```
HEADER HYDROLASE
                                      10-NOV-16 5TVV
TITLE
      COMPUTATIONALLY DESIGNED FENTANYL BINDER - FEN49* APO
COMPND MOL_ID: 1;
COMPND 2 MOLECULE: ENDO-1,4-BETA-XYLANASE A;
COMPND 3 CHAIN: A, B, C;
COMPND 4 FRAGMENT: UNP RESIDUES 30-213;
COMPND 5 SYNONYM: XYLANASE A,1,4-BETA-D-XYLAN
XYLANOHYDROLASE A:
COMPND 6 EC: 3.2.1.8;
COMPND 7 ENGINEERED: YES;
COMPND 8 MUTATION: YES SOURCE MOL_ID: 1;
SOURCE 2 ORGANIŚM_SCIENTIFIC: BACILLUS SUBTILIS (STRAIN 168);
SOURCE 3 ORGANISM_TAXID: 224308;
SOURCE 4 STRAIN: 168;
SOURCE 5 GENE: XYNA, BSU18840;
SOURCE 6 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE 7 EXPRESSION_SYSTEM_TAXID: 562
KEYWDS FENTANYL BINDER, COMPUTATIONAL DESIGN, HYDROLASE
EXPDTA X-RAY DIFFRACTION
AUTHOR
M.J.BICK, P.J.GREISEN, K.J.MOREY, A.S.ANTUNES, D.LA, B.SANKARAN, L.REYM
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REVDAT 3 01-JAN-20 5TVV
                            1
                                 REMARK
REVDAT 2 04-DEC-19 5TVV
                            1
                                 REMARK
REVDAT 1 04-OCT-17 5TVV 0
JRNL
        AUTH
M.J.BICK, P.J. GREISEN, K.J. MOREY, M.S. ANTUNES, D.LA, B. SANKARAN,
JRNL
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JRNL
         TITL COMPUTATIONAL DESIGN OF ENVIRONMENTAL SENSORS
FOR THE POTENT
JRNL
         TITL 2 OPIOID FENTANYL.
JRNL
         REF
               ELIFE
                                 V. 6
                                         2017
                        ESSN 2050-084X
JRNL
         REFN
JRNL
         PMID 28925919
         DOI
              10.7554/ELIFE.28909
JRNL
REMARK 2
REMARK 2 RESOLUTION. 1.79 ANGSTROMS.
REMARK 3
REMARK 3 REFINEMENT.
REMARK 3 PROGRAM : PHENIX DEV_2313
REMARK 3 AUTHORS
                        : PAUL ADAMS, PAVEL AFONINE, VINCENT
CHEN, IAN
REMARK 3
                   : DAVIS,KRESHNA GOPAL,RALF GROSSE-KUNSTLEVE,
REMARK 3
                  : LI-WEI HUNG, ROBERT IMMORMINO, TOM IOERGER,
                   : AIRLIE MCCOY, ERIK MCKEE, NIGEL MORIARTY,
REMARK 3
```

```
: REETAL PAI, RANDY READ, JANE RICHARDSON,
REMARK 3
REMARK 3
                 : DAVID RICHARDSON.TOD ROMO.JIM SACCHETTINI.
                 : NICHOLAS SAUTER, JACOB SMITH, LAURENT
REMARK 3
REMARK 3
                 : STORONI, TOM TERWILLIGER, PETER ZWART
REMARK
         3
            REFINEMENT TARGET: NULL
REMARK
REMARK
REMARK 3 DATA USED IN REFINEMENT.
REMARK
         3
           RESOLUTION RANGE HIGH (ANGSTROMS): 1.79
           RESOLUTION RANGE LOW (ANGSTROMS): 43.86
REMARK 3
           MIN(FOBS/SIGMA FOBS)
REMARK 3
                                       : 1.350
           COMPLETENESS FOR RANGE
REMARK 3
                                        (\%):98.3
REMARK
           NUMBER OF REFLECTIONS
                                         : 52283
REMARK 3
REMARK 3 FIT TO DATA USED IN REFINEMENT.
REMARK 3 R VALUE (WORKING + TEST SET): 0.205
                         (WORKING SET) : 0.204
REMARK 3
           R VALUE
REMARK 3 FREER VALUE
                                  : 0.225
REMARK 3
           FREE R VALUE TEST SET SIZE (%): 5.090
REMARK 3 FREE R VALUE TEST SET COUNT
REMARK 3
REMARK 3 FIT TO DATA USED IN REFINEMENT (IN BINS).
REMARK 3 BIN RESOLUTION RANGE COMPL. NWORK NFREE RWORK
RFREE
REMARK 3
            1 43.8741 - 4.7684 1.00
                                   2876 143 0.2343 0.2647
REMARK 3
            2 4.7684 - 3.7855
                             1.00
                                   2722 160 0.1716 0.1795
            3 3.7855 - 3.3072 1.00
REMARK 3
                                   2679 161 0.1704 0.1635
            4 3.3072 - 3.0049
                                   2685 133 0.1743 0.2166
REMARK
         3
                             1.00
            5 3.0049 - 2.7896 1.00
6 2.7896 - 2.6251 1.00
7 2.6251 - 2.4937 1.00
                                   2633 157 0.1841 0.2116
REMARK 3
                                  2634 163 0.1973 0.2312
REMARK 3
REMARK 3
                                  2667 118 0.2018 0.2619
            8 2.4937 - 2.3851 1.00
                                   2649 129 0.2064 0.2513
REMARK 3
           9 2.3851 - 2.2933 0.99 2619 130 0.1972 0.2495
10 2.2933 - 2.2142 0.99 2648 142 0.2006 0.2711
REMARK 3
REMARK 3
           11 2.2142 - 2.1449 0.99 2600 135 0.2133 0.2280 12 2.1449 - 2.0836 0.99 2590 145 0.2171 0.2291
REMARK 3
REMARK
         3
           REMARK 3
REMARK 3
           2595 134 0.2195 0.2342
REMARK 3
                                   2540 143 0.2452 0.2803
REMARK 3
REMARK 3
                                   2514 142 0.2626 0.2678
                                   2484 133 0.2905 0.2585
REMARK 3
            18 1.8552 - 1.8202
                             0.95
REMARK 3
            19 1.8202 - 1.7877 0.87
                                   2271 127 0.3248 0.2983
REMARK 3
REMARK 3 BULK SOLVENT MODELLING.
REMARK 3
           METHOD USED
                            : NULL
REMARK 3
           SOLVENT RADIUS
                           : 1.11
REMARK 3
           SHRINKAGE RADIUS: 0.90
REMARK 3 K SOL
                       : NULL
REMARK 3
           B SOL
                        : NULL
REMARK
         3
```

REMARK 3 ERROR ESTIMATES.

```
REMARK 3 COORDINATE ERROR (MAXIMUM-LIKELIHOOD BASED) : 0.200
REMARK 3 PHASE ERROR (DEGREES, MAXIMUM-LIKELIHOOD BASED):
21.790
REMARK 3
REMARK 3 B VALUES.
REMARK 3 FROM WILSON PLOT (A**2): 18.53
REMARK 3 MEAN B VALUE (OVERALL, A**2): 28.51
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 B11 (A**2): NULL
           B22 (A**2): NULL
REMARK 3
REMARK 3 B33 (A**2): NULL
           B12 (A**2): NULL
REMARK 3
REMARK 3
           B13 (A**2) : NULL
REMARK 3
           B23 (A**2) : NULL
REMARK 3
REMARK 3 TWINNING INFORMATION.
REMARK 3 FRACTION: NULL
REMARK 3 OPERATOR: NULL
REMARK 3
REMARK 3 DEVIATIONS FROM IDEAL VALUES.
REMARK 3
                  RMSD COUNT
REMARK 3 BOND : 0.005
REMARK 3 ANGLE : 0.714
                              4507
                              6218
REMARK 3 CHIRALITY: 0.052
                               654
REMARK 3 PLANARITY: 0.004
                                794
REMARK 3 DIHEDRAL: 8.702
                               2440
REMARK 3
REMARK 3 TLS DETAILS
REMARK 3 NUMBER OF TLS GROUPS: 20
REMARK 3 TLS GROUP: 1
REMARK 3 SELECTION: CHAIN 'A' AND (RESID 1 THROUGH 34)
REMARK 3
           ORIGIN FOR THE GROUP (A): -7.4266 -14.2785 -19.2916
REMARK 3
           T TENSOR
REMARK 3
           T11: 0.1465 T22: 0.2537
REMARK 3
           T33: 0.1747 T12: 0.1046
          T13: -0.0107 T23: -0.0033
REMARK 3
REMARK 3
REMARK 3
           L TENSOR
          L11: 1.9175 L22: 3.6960
REMARK 3
            L33: 3.6803 L12: -1.2216
REMARK 3
           L13: 0.8093 L23: -0.0721
REMARK 3
           S TENSOR
REMARK 3
           S11: -0.2795 S12: -0.4562 S13: 0.0191
REMARK 3
            S21: 0.2063 S22: 0.1995 S23: 0.2222
S31: -0.0183 S32: -0.4444 S33: 0.0242
REMARK 3
REMARK 3 TLS GROUP: 2
REMARK 3
           SELECTION: CHAIN 'A' AND (RESID 35 THROUGH 85)
REMARK 3
           ORIGIN FOR THE GROUP (A): 3.7368 -18.5591 -18.7112
REMARK 3
           T TENSOR
REMARK 3
           T11: 0.1209 T22: 0.1778
REMARK 3
           T33: 0.1018 T12: 0.0550
REMARK 3 T13: -0.0150 T23: -0.0167
REMARK 3
           L TENSOR
```

```
REMARK 3 L11: 2.0361 L22: 1.7099
REMARK 3
REMARK 3
              L33: 1.8231 L12: -1.1001
              L13: 0.0867 L23: 0.1097
REMARK 3
REMARK 3
             S TENSOR
             S11: -0.2072 S12: -0.3608 S13: 0.0899
              $21: 0.1669 $22: 0.1350 $23: 0.0397
REMARK 3
              S31: -0.1683 S32: -0.1803 S33: 0.0225
REMARK 3
REMARK 3 TLS GROUP: 3
REMARK 3 SELECTION: CHAIN 'A' AND (RESID 86 THROUGH 102)
REMARK 3
             ORIGIN FOR THE GROUP (A): 11.2092 -25.6495 -8.0892
REMARK 3
             T TENSOR
REMARK 3
             T11: 0.2308 T22: 0.2543
REMARK 3
              T33: 0.1686 T12: 0.0577
REMARK 3
              T13: -0.0027 T23: 0.0453
REMARK 3
             L TENSOR
REMARK 3
REMARK 3
             L11: 1.3594 L22: 4.8708
              L33: 2.7132 L12: -2.2527
REMARK 3
REMARK 3
             L13: -0.4914 L23: -0.8920
             S TENSOR
REMARK 3 S11: -0.3291 S12: -0.4173 S13: -0.1837 REMARK 3 S21: 0.4689 S22: 0.3497 S23: 0.3786
REMARK 3 S31: -0.0319 S
REMARK 3 TLS GROUP: 4
             S31: -0.0319 S32: -0.2347 S33: 0.0325
REMARK 3 SELECTION: CHAIN 'A' AND (RESID 103 THROUGH 112)
REMARK 3
             ORIGIN FOR THE GROUP (A): 9.9113 -28.5600 -12.5559
REMARK 3
             T TENSOR
REMARK 3
             T11: 0.1161 T22: 0.1865
REMARK 3
              T33: 0.1048 T12: 0.0516
REMARK 3
              T13: 0.0252 T23: 0.0412
REMARK 3
             L TENSOR
REMARK 3
            L11: 4.6460 L22: 7.3079
REMARK 3
REMARK 3
              L33: 3.2883 L12: 2.7736
L13: 1.7977 L23: 2.2869
REMARK 3
             S TENSOR
REMARK 3
            S11: -0.0003 S12: -0.7291 S13: -0.2368
REMARK 3
REMARK 3
              S21: 0.3632 S22: -0.1622 S23: -0.1008
S31: 0.1180 S32: -0.5140 S33: 0.1138
REMARK 3 TLS GROUP: 5
REMARK 3
             SELECTION: CHAIN 'A' AND (RESID 113 THROUGH 141)
REMARK 3
             ORIGIN FOR THE GROUP (A): 3.3591 -25.4410 -17.0045
REMARK 3
             T TENSOR
REMARK 3
             T11: 0.0913 T22: 0.2020
REMARK 3
              T33: 0.1301 T12: 0.0564
REMARK 3
              T13: 0.0268 T23: 0.0163
REMARK 3
             L TENSOR
REMARK 3
              L11: 1.8271 L22: 2.1442
REMARK 3
              L33: 1.1852 L12: -1.3140
REMARK 3
             L13: 0.0513 L23: -0.2498
REMARK 3
             S TENSOR
REMARK 3 S11: -0.0946 S12: -0.4100 S13: -0.1455
```

```
REMARK 3 S21: 0.1554 S22: 0.0800 S23: 0.1498
REMARK 3 S31: -0.0416 S32: -0.1855 S33: 0.0234 REMARK 3 TLS GROUP: 6
REMARK 3 SELECTION: CHAIN 'A' AND (RESID 142 THROUGH 156)
REMARK 3
             ORIGIN FOR THE GROUP (A): 16.7345 -21.5387 -18.8739
REMARK 3
             T TENSOR
REMARK 3
              T11: 0.0824 T22: 0.1298
REMARK 3
              T33: 0.1331 T12: -0.0083
REMARK 3
              T13: -0.0092 T23: -0.0045
REMARK 3
             L TENSOR
REMARK 3
            L11: 3.5324 L22: 3.0896
REMARK 3
             L33: 2.5064 L12: -1.9262
REMARK 3 L13: 1.0637 L23: -0.3943
REMARK 3
REMARK 3
             S TENSOR
             S11: -0.1630 S12: -0.0716 S13: 0.1040
REMARK 3
REMARK 3
              S21: -0.2080 S22: 0.0749 S23: -0.2821
              S31: -0.2703 S32: 0.0550 S33: 0.1135
REMARK 3 TLS GROUP: 7
REMARK 3 SELECTION: CHAIN 'A' AND (RESID 157 THROUGH 185)
REMARK 3
             ORIGIN FOR THE GROUP (A): 2.0072 -18.4595 -18.8159
REMARK 3
REMARK 3
             T TENSOR
            T11: 0.1197 T22: 0.1842
REMARK 3
             T33: 0.0974 T12: 0.0497
             T13: -0.0153 T23: -0.0094
REMARK 3
REMARK 3 L TENSOR
REMARK 3 L11: 2.0450 L22: 2.1579
REMARK 3 L33: 1.1541 L12: -1.0209
             L13: -0.1235 L23: 0.4893
REMARK 3
REMARK 3
             S TENSOR
REMARK 3 S11: -0.1653 S12: -0.2779 S13: 0.1061
REMARK 3
              S21: 0.1804 S22: 0.1385 S23: 0.0186
REMARK 3 S31: -0.0938 S
REMARK 3 TLS GROUP: 8
              S31: -0.0938 S32: -0.2112 S33: 0.0104
REMARK 3
             SELECTION: CHAIN 'B' AND (RESID 1 THROUGH 20)
REMARK 3
             ORIGIN FOR THE GROUP (A): -28.3573 -21.0667 -44.7718
REMARK 3
REMARK 3
             T TENSOR
             T11: 0.1757 T22: 0.1567
REMARK 3
REMARK 3
              T33: 0.1371 T12: -0.0267
              T13: 0.0045 T23: -0.0257
REMARK 3
REMARK 3
             L TENSOR
             L11: 2.4388 L22: 2.8741
REMARK 3
REMARK 3
              L33: 3.1348 L12: -1.2527
             L13: 0.8404 L23: -0.6631
REMARK 3
             S TENSOR
REMARK 3
              S11: -0.0671 S12: -0.0381 S13: -0.1501
REMARK 3
              S21: 0.2110 S22: -0.1046 S23: -0.0460
REMARK 3
              S31: 0.2016 S32: -0.1554 S33: 0.1147
REMARK 3 TLS GROUP: 9
REMARK 3 SELECTION: CHAIN 'B' AND (RESID 21 THROUGH 85)
REMARK 3 ORIGIN FOR THE GROUP (A): -22.7424 -14.6707 -39.9691
REMARK 3 TIENSOR
```

```
REMARK 3
              T11: 0.1345 T22: 0.1040
REMARK 3 T33: 0.0974 T12: -0.0229
REMARK 3 T13: 0.0052 T23: 0.0070
REMARK 3
REMARK 3
             L TENSOR
            L11: 1.4922 L22: 1.0571
REMARK 3
             L33: 1.2749 L12: 0.0664
REMARK 3
             L13: -0.2456 L23: 0.2571
REMARK 3
             S TENSOR
REMARK 3
             S11: -0.0274 S12: -0.1098 S13: -0.1216
REMARK 3
              S21: 0.1463 S22: -0.0064 S23: 0.0272
REMARK 3
              S31: 0.1860 S32: -0.0433 S33: 0.0417
REMARK 3 TLS GROUP: 10
REMARK 3 SELECTION: CHAIN 'B' AND (RESID 86 THROUGH 102)
REMARK 3
             ORIGIN FOR THE GROUP (A): -11.2103 -9.4673 -30.2715
REMARK 3
             T TENSOR
REMARK 3
             T11: 0.2137 T22: 0.1496
REMARK 3
              T33: 0.1008 T12: 0.0210
REMARK 3
REMARK 3
              T13: -0.0075 T23: -0.0208
             L TENSOR
REMARK 3 L11: 5.3646 L22: 1.4615
REMARK 3 L33: 1.0748 L12: -1.3169
REMARK 3
REMARK 3
             L13: 1.3109 L23: -0.6266
             S TENSOR
REMARK 3
             S11: -0.1303 S12: -0.1255 S13: -0.0950
REMARK 3
              S21: 0.2780 S22: 0.0451 S23: -0.1774
REMARK 3 S31: 0.0785 S3 REMARK 3 TLS GROUP: 11
             S31: 0.0785 S32: -0.0718 S33: 0.1062
REMARK 3 SELECTION: CHAIN 'B' AND (RESID 103 THROUGH 112)
REMARK 3
             ORIGIN FOR THE GROUP (A): -9.8123 -11.6432 -33.9187
REMARK 3
             T TENSOR
REMARK 3
            T11: 0.1681 T22: 0.1389
REMARK 3
REMARK 3
              T33: 0.1378 T12: -0.0021
              T13: -0.0291 T23: 0.0183
REMARK 3
REMARK 3
             L TENSOR
            L11: 5.2588 L22: 3.6616
REMARK 3
REMARK 3
             L33: 3.9269 L12: -1.8113
L13: -0.0706 L23: 0.9700
REMARK 3
REMARK 3
             S TENSOR
              S11: -0.0729 S12: -0.0776 S13: -0.3229
              S21: 0.3090 S22: 0.0589 S23: -0.0340 S31: 0.4581 S32: -0.0363 S33: -0.0025
REMARK 3
REMARK 3
REMARK 3 TLS GROUP: 12
REMARK 3
             SELECTION: CHAIN 'B' AND (RESID 113 THROUGH 124)
REMARK 3
             ORIGIN FOR THE GROUP (A): -10.2557 -26.9480 -45.5203
REMARK 3
             T TENSOR
REMARK 3
              T11: 0.4748 T22: 0.2572
REMARK 3
              T33: 0.5760 T12: 0.0773
REMARK 3
             T13: -0.1449 T23: -0.0732
REMARK 3
             L TENSOR
REMARK 3 L11: 0.5934 L22: 0.4705
```

```
REMARK 3 L33: 0.5927 L12: 0.1640
REMARK 3 L13: -0.5883 L23: -0.2007 REMARK 3 S TENSOR
REMARK 3 S11: 0.0539 S12: -0.0286 S13: -0.8568 REMARK 3 S21: 0.5617 S22: 0.3556 S23: -1.0878
REMARK 3 S31: 0.8305 S32: 0.4172 S33: -0.1149
REMARK 3 TLS GROUP: 13
REMARK 3 SELECTION: CHAIN 'B' AND (RESID 125 THROUGH 166)
REMARK 3
               ORIGIN FOR THE GROUP (A): -14.1521 -7.4796 -39.6016
REMARK 3 T TENSOR
REMARK 3
              T11: 0.0967 T22: 0.1080
REMARK 3
                T33: 0.1099 T12: 0.0175
REMARK 3
                T13: -0.0145 T23: 0.0061
REMARK 3
REMARK 3
               L TENSOR
              L11: 1.9685 L22: 1.8381
REMARK 3 L33: 1.6347 L12: 0.6634
REMARK 3 L13: 0.0649 L23: 0.6162
REMARK 3 S TENSOR
REMARK 3 S11: -0.0437 S12: -0.0497 S13: 0.0127
REMARK 3
REMARK 3
                S21: 0.0781 S22: 0.0725 S23: -0.1727
                S31: 0.1355 S32: 0.0987 S33: -0.0426
REMARK 3 TLS GROUP: 14
REMARK 3 SELECTION: CHAIN 'B' AND (RESID 167 THROUGH 185)
REMARK 3
               ORIGIN FOR THE GROUP (A): -26.1437 -16.0144 -37.9159
REMARK 3
               T TENSOR
REMARK 3
               T11: 0.1763 T22: 0.1494
REMARK 3
                T33: 0.1147 T12: -0.0192
REMARK 3
               T13: 0.0043 T23: -0.0033
REMARK 3
               L TENSOR
REMARK 3 L11: 2.2596 L22: 1.9171
REMARK 3 L33: 2.0756 L12: 1.0177
REMARK 3
REMARK 3
               L13: -0.2419 L23: 0.1930
               S TENSOR
REMARK 3 S11: 0.0309 S12: -0.2818 S13: -0.1438
REMARK 3
                S21: 0.2967 S22: -0.0375 S23: 0.0263
REMARK 3 S31: 0.3876 S3
REMARK 3 TLS GROUP: 15
REMARK 3 SELECTION: CH
REMARK 3 ORIGIN FOR THI
               S31: 0.3876 S32: -0.0012 S33: 0.0492
               SELECTION: CHAIN 'C' AND (RESID 2 THROUGH 20)
               ORIGIN FOR THE GROUP (A): -20.1145 -4.3943 0.0423
REMARK 3
REMARK 3
               T TENSOR
              T11: 0.3151 T22: 0.2981
REMARK 3
REMARK 3
                T33: 0.3679 T12: -0.0918
                T13: -0.1710 T23: 0.0889
REMARK 3
REMARK 3
               L TENSOR
               L11: 3.5236 L22: 4.5697
REMARK 3
                L33: 5.5632 L12: -0.5525
REMARK 3
               L13: 1.2117 L23: -0.1707
REMARK 3 S TENSOR

REMARK 3 S11: 0.2701 S12: -0.0212 S13: -0.5456

REMARK 3 S21: 0.0799 S22: 0.2827 S23: 1.0646

S31: 0.7478 S32: -0.6348 S33: -0.4695
```

```
REMARK 3 TLS GROUP: 16
REMARK 3
REMARK 3
            SELECTION: CHAIN 'C' AND (RESID 21 THROUGH 34)
            ORIGIN FOR THE GROUP (A): -16.8581 -6.8161 -6.2287
REMARK 3
            T TENSOR
REMARK 3
             T11: 0.4388 T22: 0.4301
REMARK 3
             T33: 0.3814 T12: 0.3165
REMARK 3
             T13: -0.3867 T23: -0.0513
REMARK 3
            L TENSOR
REMARK 3
            L11: 2.2869 L22: 3.6176
REMARK 3
             L33: 4.0125 L12: -1.5084
REMARK 3
             L13: 1.5107 L23: -1.8920
REMARK 3
            S TENSOR
REMARK 3
             S11: 0.7160 S12: 0.0451 S13: -0.9207
REMARK 3
             S21: -0.8597 S22: -0.0774 S23: 0.4664
REMARK 3
             S31: 0.8666 S32: 0.3094 S33: -0.0420
REMARK 3 TLS GROUP: 17
REMARK 3
            SELECTION: CHAIN 'C' AND (RESID 35 THROUGH 85)
REMARK 3
            ORIGIN FOR THE GROUP (A): -16.6302 6.2585 -4.2298
REMARK 3
            T TENSOR
REMARK 3
            T11: 0.3200 T22: 0.2405
REMARK 3
             T33: 0.1862 T12: 0.0609
REMARK 3
             T13: 0.0157 T23: 0.0475
REMARK 3
REMARK 3
            L TENSOR
            L11: 3.7079 L22: 3.9865
REMARK 3
             L33: 5.8413 L12: -1.5152
             L13: 1.9325 L23: -2.3472
REMARK 3
REMARK 3
            S TENSOR
REMARK 3
             S11: 0.3593 S12: 0.2912 S13: 0.0305
             S21: 0.4082 S22: -0.0794 S23: -0.0809
REMARK 3
REMARK 3
             S31: -0.4654 S32: 0.0005 S33: -0.0537
REMARK 3 TLS GROUP: 18
REMARK 3 SELECTION: CHAIN 'C' AND (RESID 86 THROUGH 112)
REMARK 3
            ORIGIN FOR THE GROUP (A): -19.4903 15.4867 -14.2949
REMARK 3
            T TENSOR
REMARK 3
            T11: 0.2696 T22: 0.2849
REMARK 3
             T33: 0.1954 T12: 0.0083
REMARK 3
             T13: -0.0205 T23: 0.0907
REMARK 3
            L TENSOR
REMARK 3
            L11: 3.2203 L22: 4.2902
REMARK 3
             L33: 3.8381 L12: -2.5010
REMARK 3
             L13: 2.4302 L23: -0.9386
REMARK 3
            S TENSOR
REMARK 3
             S11: -0.1841 S12: 0.2041 S13: 0.0396
             S21: 0.5110 S22: -0.1390 S23: -0.1358
REMARK 3
REMARK 3
             S31: -0.2556 S32: 0.5570 S33: 0.1875
REMARK 3 TLS GROUP: 19
REMARK 3
            SELECTION: CHAIN 'C' AND (RESID 113 THROUGH 124)
REMARK 3
            ORIGIN FOR THE GROUP (A): -33.1080 8.4485 1.2824
REMARK 3
            T TENSOR
REMARK 3
            T11: 0.7064 T22: 0.5772
REMARK 3
             T33: 0.7716 T12: 0.0858
```

```
REMARK 3 T13: 0.3868 T23: 0.2309
REMARK 3
REMARK 3
           L TENSOR
            L11: 0.5603 L22: 4.5862
REMARK 3
            L33: 2.8544 L12: -1.2356
REMARK 3
            L13: -0.3163 L23: -1.5391
REMARK 3
           S TENSOR
REMARK 3
            S11: -0.2752 S12: -0.5478 S13: -0.5842
REMARK 3
            S21: 0.3640 S22: 0.7865 S23: 1.2804
REMARK 3
            S31: -0.1500 S32: -1.3605 S33: -0.4396
REMARK 3 TLS GROUP: 20
REMARK 3
           SELECTION: CHAIN 'C' AND (RESID 125 THROUGH 185 )
REMARK 3
           ORIGIN FOR THE GROUP (A): -15.2944 9.7380 -6.2454
REMARK 3
           T TENSOR
REMARK 3
            T11: 0.3936 T22: 0.2809
REMARK 3
            T33: 0.1925 T12: 0.0227
            T13: -0.0247 T23: -0.0020
REMARK 3
REMARK 3
           L TENSOR
REMARK 3
           L11: 3.2440 L22: 2.6931
REMARK 3
            L33: 4.9663 L12: -0.1727
REMARK 3
            L13: 1.8322 L23: -2.2225
REMARK 3
           S TENSOR
REMARK 3
REMARK 3
            S11: 0.0340 S12: 0.2617 S13: 0.0712
            S21: 0.5482 S22: -0.0413 S23: -0.1878
REMARK 3
            S31: -0.6528 S32: 0.4477 S33: -0.0297
REMARK 3
REMARK 3 NCS DETAILS
REMARK 3 NUMBER OF NCS GROUPS : NULL
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS: ITERATIVE ROUNDS OF MODEL
BUILDING IN
REMARK 3 COOT AND REFINEMENT IN PHENIX. REFINEMENT PARAMETERS
INCLUDED
REMARK 3 REAL AND RECIPROCAL SPACE, INDIVIDUAL ADPS,
OCCUPANICES.
REMARK 3 OPTIMIZATION OF X-RAY TO STEREOCHEMICAL AND X-RAY TO
ADP
REMARK 3 WEIGHTS. HYDROGENS WERE ADDED AUTOMATICALLY AND
AUTOMATIC
REMARK 3 CORRECTION OF N/Q/H ERRORS WAS USED. UPDATED
SOLVENT MODEL WAS
REMARK 3 USED IN THE PENULTIMATE ROUND OF REFINEMENT. MANUAL
MODELING OF
REMARK 3 SOLVENT WAS CONDUCTED BEFORE THE FINAL ROUND OF
REFINEMENT.
REMARK 4
REMARK 4 5TVV COMPLIES WITH FORMAT V. 3.30, 13-JUL-11
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 17-NOV-16.
REMARK 100 THE DEPOSITION ID IS D 1000224895.
REMARK 200
```

REMARK 200 EXPERIMENTAL DETAILS

```
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION
REMARK 200 DATE OF DATA COLLECTION : 09-JUL-15
REMARK 200 TEMPERATURE
                              (KELVIN): 80
REMARK 200 PH
                            : 7.5
REMARK 200 NUMBER OF CRYSTALS USED : 1
REMARK 200
REMARK 200 SYNCHROTRON (Y/N): Y REMARK 200 RADIATION SOURCE : AL
                                : ALS
REMARK 200 BEAMLINE
REMARK 200 X-RAY GENERATOR MODEL : NULL
REMARK 200 MONOCHROMATIC OR LAUE (M/L): M
REMARK 200 WAVELENGTH OR RANGE (A): 0.976246
REMARK 200 MONOCHROMATOR : DOUBLE-CRYSTAL SI(111)
REMARK 200 OPTICS
                             : NULL
REMARK 200
REMARK 200 DETECTOR TYPE : CCD
REMARK 200 DETECTOR MANUFACTURER : ADSC QUANTUM 315R
REMARK 200 INTENSITY-INTEGRATION SOFTWARE: HKL-2000
REMARK 200 DATA SCALING SOFTWARE : HKL-2000, HKL
REMARK 200
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 52362
REMARK 200 RESOLUTION RANGE HIGH (A): 1.790
                                     (A): 43.861
REMARK 200 RESOLUTION RANGE LOW
REMARK 200 REJECTION CRITERIA (SIGMA(I)): NULL
REMARK 200
REMARK 200 OVERALL.
REMARK 200 COMPLETENESS FOR RANGE (%): 98.5
REMARK 200 DATA REDUNDANCY : 7.800
REMARK 200 R MERGE (I): 0.11000 REMARK 200 R SYM (I): NULL
                           (I) : NULL
REMARK 200 <I/SIGMA(I)> FOR THE DATA SET : 13.5280
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A): 1.79
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A): 1.85
REMARK 200 COMPLETENESS FOR SHELL (%): 92.8
REMARK 200 DATA REDUNDANCY IN SHELL : 5.90
REMARK 200 R MERGE FOR SHELL (I): 0.77800
                                 (I) : NULL
REMARK 200 R SYM FOR SHELL
REMARK 200 <I/SIGMA(I)> FOR SHELL : 1.538
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR
REPLACEMENT
REMARK 200 SOFTWARE USED: PHASER 2.5.6
REMARK 200 STARTING MODEL: 2QZ3
```

REMARK 200

```
REMARK 200 REMARK: ROD-LIKE CRYSTALS WITH LONGEST DIMENSION OF
APPROXIMATELY
REMARK 200 200 MICRONS.
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS (%): 46.13
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 2.28
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: 0.8M SODIUM PHOSPHATE.
0.8M POTASSIUM
REMARK 280 PHOSPHATE, 0.1M HEPES PH 7.5, VAPOR DIFFUSION, SITTING
DROP.
REMARK 280 TEMPERATURE 293.15K
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 21 21 21
REMARK 290
                  SYMOP SYMMETRY
REMARK 290
                  NNNMMM OPERATOR
REMARK 290
REMARK 290
                1555 X,Y,Z
                  2555 -X+1/2,-Y,Z+1/2
REMARK 290
REMARK 290 2555 -X+1/2,-1,2+1/2
REMARK 290 3555 -X,Y+1/2,-Z+1/2
REMARK 290 4555 X+1/2,-Y+1/2,-Z
REMARK 290
REMARK 290
                  WHERE NNN -> OPERATOR NUMBER
REMARK 290
                      MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE
ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE
CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290 SMTRY1 1 1.000000 0.000000 0.000000
                                                                   0.00000
REMARK 290 SMTRY1 1 1.000000 0.000000 0.000000 REMARK 290 SMTRY3 1 0.000000 0.000000 1.000000 REMARK 290 SMTRY1 2 -1.000000 0.000000 0.000000 REMARK 290 SMTRY2 2 0.000000 -1.000000 0.000000 REMARK 290 SMTRY3 2 0.000000 0.000000 1.000000 REMARK 290 SMTRY1 3 -1.000000 0.000000 0.000000 REMARK 290 SMTRY2 3 0.000000 1.000000 0.000000 REMARK 290 SMTRY3 3 0.000000 1.000000 0.000000 REMARK 290 SMTRY3 3 0.000000 0.000000 0.000000 REMARK 290 SMTRY3 4 1.000000 0.000000 0.000000
                                                                   0.00000
                                                                   0.00000
                                                                   27.38000
                                                                   0.00000
                                                                   68.77900
                                                                   0.00000
                                                                   36.62950
                                                                   68.77900
REMARK 290 SMTRY1 4 1.000000 0.000000 0.000000 REMARK 290 SMTRY2 4 0.000000 -1.000000 0.000000
                                                                   27.38000
                                                                   36.62950
REMARK 290 SMTRY3 4 0.000000 0.000000 -1.000000
                                                                   0.00000
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1, 2, 3
REMARK 300 SEE REMARK 350 FOR THE AUTHOR PROVIDED AND/OR
```

PROGRAM

REMARK 300 GENERATED ASSEMBLY INFORMATION FOR THE STRUCTURE

REMARK 300 THIS ENTRY. THE REMARK MAY ALSO PROVIDE INFORMATION ON

REMARK 300 BURIED SURFACE AREA.

REMARK 350

REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN

REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE

REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS

REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND

REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.

REMARK 350

REMARK 350 BIOMOLECULE: 1

REMARK 350 AUTHOR DETERMINED BIOLOGICAL UNIT: MONOMERIC

REMARK 350 APPLY THE FOLLOWING TO CHAINS: A

REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000 0.000000 REMARK 350 BIOMT2 1 0.000000 1.000000 0.000000 0.000000 REMARK 350 BIOMT3 1 0.000000 0.000000 1.000000 0.000000

REMARK 350

REMARK 350 BIOMOLECULE: 2

REMARK 350 AUTHOR DETERMINED BIOLOGICAL UNIT: MONOMERIC

REMARK 350 APPLY THE FOLLOWING TO CHAINS: B

REMARK 350

REMARK 350 BIOMOLECULE: 3

REMARK 350 AUTHOR DETERMINED BIOLOGICAL UNIT: MONOMERIC

REMARK 350 APPLY THE FOLLOWING TO CHAINS: C

REMARK 465

REMARK 465 MISSING RESIDUES

REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE

REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN

REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)

REMARK 465

REMARK 465 M RES C SSSEQI

REMARK 465 GLY A -2

REMARK 465 PRO A -1

```
REMARK 465
            HIS A
                   0
REMARK 465
            GLY B
                   -2
                    -1
REMARK 465
            PRO B
REMARK 465
            HIS B
                   0
REMARK 465
            GLY C
                   -2
REMARK 465
            PRO C
                    -1
REMARK 465
            HIS C
                   0
            MET C
                    1
REMARK 465
REMARK 470
REMARK 470 MISSING ATOM
REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL
NUMBER;
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
NUMBER:
REMARK 470 I=INSERTION CODE):
REMARK 470 M RES CSSEQI ATOMS
REMARK 470
            MET A 1
                      CG SD CE
                       CD NE CZ NH1 NH2
            ARG A 122
REMARK 470
REMARK 470
            MET B 1
                      CG SD CE
CG OD1 OD2
REMARK 470
            ASP B 121
            ILE C 15
                     CG1 CG2 CD1
REMARK 470
            VAL C 16
                      CG1 CG2
REMARK 470
            ASN C 17
                      CG OD1 ND2
REMARK 470
            SER C 31
REMARK 470
                      OG
            ASN C 32
                      CG OD1 ND2
REMARK 470
            ASN C 61
REMARK 470
                      CG OD1 ND2
            LYS C 95
                      CE NZ
REMARK 470
            LYS C 99
                      CG CD CE NZ
REMARK 470
            ARG C 112
REMARK 470
                       NE CZ NH1 NH2
            TYR C 113
                       CG CD1 CD2 CE1 CE2 CZ OH
REMARK 470
                       CG OD1 ND2
            ASN C 114
REMARK 470
            SER C 117
REMARK 470
                       OG
           ASP C 121
REMARK 470
                       CG OD1 OD2
           ARG C 122
REMARK 470
                       CG CD NE CZ NH1 NH2
            THR C 123 OG1 CG2
REMARK 470
            TYR C 174
                       CD1 CD2 CE1 CE2 CZ OH
REMARK 470
            GLN C 175
                       CD OE1 NE2
REMARK 470
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
REMARK 500
REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
REMARK 500
REMARK 500 ATM1 RES C SSEQI ATM2 RES C SSEQI
                                                   DISTANCE
REMARK 500
          0
               HOH B
                     346
                           0
                              HOH B 421
                                              2.02
                              HOH B 416
REMARK 500
          0
               HOH B
                     342
                           0
                                              2.17
                     334
REMARK 500
               HOH C
                              HOH C
                                    353
                                              2.18
           0
                           0
               HOH A 389
                          0
REMARK 500 O
                              HOH B 449
                                              2.19
REMARK 500
```

REMARK 500 REMARK: NULL

REMARK 500

REMARK 500 GEOMETRY AND STEREOCHEMISTRY

REMARK 500 SUBTOPIC: CLOSE CONTACTS

REMARK 500

REMARK 500 THE FOLLOWING ATOMS THAT ARE RELATED BY

CRYSTALLOGRAPHIC

REMARK 500 SYMMETRY ARE IN CLOSE CONTACT. AN ATOM LOCATED WITHIN 0.15

REMARK 500 ANGSTROMS OF A SYMMETRY RELATED ATOM IS ASSUMED TO BE ON A

REMARK 500 SPECIAL POSITION AND IS, THEREFORE, LISTED IN REMARK 375

REMARK 500 INSTEAD OF REMARK 500. ATOMS WITH NON-BLANK ALTERNATE

REMARK 500 LOCATION INDICATORS ARE NOT INCLUDED IN THE CALCULATIONS.

REMARK 500

REMARK 500 DISTANCE CUTOFF:

REMARK 500 2.2 ANGSTROMS FOR CONTACTS NOT INVOLVING HYDROGEN ATOMS

REMARK 500 1.6 ANGSTROMS FOR CONTACTS INVOLVING HYDROGEN ATOMS

REMARK 500

REMARK 500 ATM1 RES C SSEQI ATM2 RES C SSEQI SSYMOP

DISTANCE

REMARK 500 O HOH A 399 O HOH C 353 4545 2.04

REMARK 500

REMARK 500 REMARK: NULL

REMARK 500

REMARK 500 GEOMETRY AND STEREOCHEMISTRY

REMARK 500 SUBTOPIC: TORSION ANGLES

REMARK 500

REMARK 500 TORSION ANGLES OUTSIDE THE EXPECTED RAMACHANDRAN REGIONS:

REMARK 500 (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER;

REMARK 500 SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).

REMARK 500

REMARK 500 STANDARD TABLE:

REMARK 500 FORMAT:(10X,I3,1X,A3,1X,A1,I4,A1,4X,F7.2,3X,F7.2)

REMARK 500

REMARK 500 EXPECTED VALUES: GJ KLEYWEGT AND TA JONES (1996). PHI/PSI-

REMARK 500 CHOLOGY: RAMACHANDRAN REVISITED. STRUCTURE 4, 1395 - 1400

REMARK 500

REMARK 500 M RES CSSEQI PSI PHI

REMARK 500 ASP A 4 29.42 -152.55

REMARK 500 ALA A 165 -155.26 -106.09

REMARK 500 ASP B 4 20.75 -141.31

REMARK 500 SER B 74 60.39 62.17

REMARK 500 ALA B 165 -150.14 -106.68

```
REMARK 500 ASP C 4
                       26.28 -144.37
REMARK 500 SER C 117
                       -157.56 -143.80
REMARK 500 ASP C 119
                       49.08 -100.55
REMARK 500 ALA C 165
                      -151.78 -94.65
                       61.74
REMARK 500 GLN C 175
                               28.58
REMARK 500 GLN C 175
                        62.27 28.58
REMARK 500
REMARK 500 REMARK: NULL
REMARK 620
REMARK 620 METAL COORDINATION
REMARK 620 (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
IDENTIFIER;
REMARK 620 SSEQ=SEQUENCE NUMBER; I=INSERTION CODE):
REMARK 620
REMARK 620 COORDINATION ANGLES FOR: M RES CSSEQI METAL
REMARK 620
                         K A 201 K
REMARK 620 N RES CSSEQI ATOM
REMARK 620 1 ASN A 20 O
REMARK 620 2 ASN A 20 OD1 68.1
REMARK 620 3 GLY A 21 O 75.0 64.5
REMARK 620 4 TYR B 94 OH 154.1 88.7 84.8
REMARK 620 5 ASP B 106 OD1 99.0 102.2 166.6 97.1
REMARK 620 6 HOH B 390 O 84.1 143.4 86.1 111.0 105.5
REMARK 620 N
                      1
                         2
                            3
REMARK 620
REMARK 620 COORDINATION ANGLES FOR: M RES CSSEQI METAL
REMARK 620
                         K B 201 K
REMARK 620 N RES CSSEQI ATOM
REMARK 620 1 ASN B 20 O
REMARK 620 2 ASN B 20 OD1 64.0
REMARK 620 3 GLY B 21 O 73.0 64.8
REMARK 620 4 TYR C 94 OH 80.3 61.5 9.8
REMARK 620 5 ASP C 106 OD1 77.5 58.4 9.8 3.5
REMARK 620 6 HOH C 356 O 90.0 141.1 80.7 87.1 89.3
REMARK 620 N
                      1
                         2 3
                                   5
                                4
REMARK 620
REMARK 620 COORDINATION ANGLES FOR: M RES CSSEQI METAL
REMARK 620
                         K C 201 K
REMARK 620 N RES CSSEQI ATOM
REMARK 620 1 ASN C 20 O
REMARK 620 2 ASN C 20 OD1 64.4
REMARK 620 3 GLY C 21 O 71.4 64.3
REMARK 620 4 TYR A 94 OH 91.2 141.9 80.7
REMARK 620 5 ASP A 106 OD1 90.5 139.7 78.4 2.3
REMARK 620 6 HOH A 360 O 91.3 145.8 85.8 5.3 7.6
                      1
                         2 3 4
REMARK 620 N
                                   5
REMARK 800
REMARK 800 SITE
REMARK 800 SITE IDENTIFIER: AC1
```

```
REMARK 800 EVIDENCE CODE: SOFTWARE
REMARK 800 SITE DESCRIPTION: binding site for residue K A 201
REMARK 800
REMARK 800 SITE IDENTIFIER: AC2
REMARK 800 EVIDENCE CODE: SOFTWARE
REMARK 800 SITE DESCRIPTION: binding site for residue K B 201
REMARK 800
REMARK 800 SITE IDENTIFIER: AC3
REMARK 800 EVIDENCE CODE: SOFTWARE
REMARK 800 SITE DESCRIPTION: binding site for residue K C 201
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 5TVY RELATED DB: PDB
DBREF 5TVV A
              2 185 UNP P18429 XYNA BACSU
                                              30
                                                  213
DBREF 5TVV B
              2 185 UNP
                         P18429 XYNA BACSU
                                                  213
                                              30
DBREF 5TVV C
              2 185 UNP P18429 XYNA BACSU
                                              30
                                                  213
SEQADV 5TVV GLY A -2 UNP P18429
                                     EXPRESSION TAG
SEQADV 5TVV PRO A -1 UNP P18429
                                     EXPRESSION TAG
SEQADV 5TVV HIS A 0 UNP P18429
                                    EXPRESSION TAG
SEQADV 5TVV MET A 1 UNP P18429
                                     EXPRESSION TAG
SEQADV 5TVV LEU A 7 UNP P18429 GLN
                                     35 ENGINEERED MUTATION
SEQADV 5TVV PHE A 9 UNP P18429 TRP 37 ENGINEERED MUTATION
SEQADV 5TVV SER A 35 UNP P18429 ASN 63 ENGINEERED MUTATION
SEQADV 5TVV TRP A 63 UNP P18429 ASN 91 ENGINEERED MUTATION
SEQADV 5TVV ALA A 65 UNP P18429 TYR 93 ENGINEERED MUTATION
SEQADV 5TVV ALA A 67 UNP P18429 THR 95 ENGINEERED MUTATION
SEQADV 5TVV VAL A 69 UNP P18429 TYR 97 ENGINEERED MUTATION
SEQADV 5TVV ALA A 78 UNP P18429 GLU 106 ENGINEERED MUTATION
SEQADV 5TVV ALA A 88 UNP P18429 TYR 116 ENGINEERED MUTATION
SEQADV 5TVV TRP A 90 UNP P18429 PRO 118 ENGINEERED MUTATION
SEQADV 5TVV ALA A 172 UNP P18429 GLU 200 ENGINEERED MUTATION
SEQADV 5TVV GLY B -2 UNP P18429
                                     EXPRESSION TAG
SEQADV 5TVV PRO B -1 UNP P18429
                                     EXPRESSION TAG
SEQADV 5TVV HIS B 0 UNP P18429
                                    EXPRESSION TAG
SEQADV 5TVV MET B 1 UNP P18429
                                     EXPRESSION TAG
SEQADV 5TVV LEU B 7 UNP P18429 GLN
                                     35 ENGINEERED MUTATION
SEQADV 5TVV PHE B
                  9 UNP P18429 TRP 37 ENGINEERED MUTATION
SEQADV 5TVV SER B 35 UNP P18429 ASN 63 ENGINEERED MUTATION
SEQADV 5TVV TRP B 63 UNP P18429 ASN 91 ENGINEERED MUTATION
```

SEQADV 5TVV ALA B 65 UNP P18429 **TYR** 93 ENGINEERED MUTATION SEQADV 5TVV ALA B 67 UNP P18429 95 ENGINEERED MUTATION THR 97 ENGINEERED MUTATION SEQADV 5TVV VAL B 69 UNP P18429 **TYR** SEQADV 5TVV ALA B 78 UNP P18429 GLU **106 ENGINEERED MUTATION** SEQADV 5TVV ALA B 88 UNP P18429 TYR 116 ENGINEERED MUTATION SEQADV 5TVV TRP B 90 UNP P18429 PRO 118 ENGINEERED MUTATION SEQADV 5TVV ALA B 172 UNP P18429 GLU 200 ENGINEERED MUTATION SEQADV 5TVV GLY C -2 UNP P18429 **EXPRESSION TAG** SEQADV 5TVV PRO C -1 UNP P18429 **EXPRESSION TAG SEQADV 5TVV HIS C** 0 UNP P18429 **EXPRESSION TAG** SEQADV 5TVV MET C 1 UNP P18429 **EXPRESSION TAG SEQADV 5TVV LEU C** 7 UNP P18429 GLN 35 ENGINEERED MUTATION SEQADV 5TVV PHE C 9 UNP P18429 TRP 37 ENGINEERED MUTATION SEQADV 5TVV SER C 35 UNP P18429 ASN **63 ENGINEERED MUTATION** SEQADV 5TVV TRP C 63 UNP P18429 **ASN** 91 ENGINEERED MUTATION SEQADV 5TVV ALA C 65 UNP P18429 93 ENGINEERED MUTATION **TYR** 95 ENGINEERED MUTATION SEQADV 5TVV ALA C 67 UNP P18429 THR SEQADV 5TVV VAL C 69 UNP P18429 97 ENGINEERED MUTATION **TYR** SEQADV 5TVV ALA C 78 UNP P18429 GLU **106 ENGINEERED MUTATION** SEQADV 5TVV ALA C 88 UNP P18429 116 ENGINEERED MUTATION **TYR** SEQADV 5TVV TRP C 90 UNP P18429 PRO 118 ENGINEERED MUTATION SEQADV 5TVV ALA C 172 UNP P18429 GLU 200 ENGINEERED MUTATION SEQRES 1 A 188 GLY PRO HIS MET SER THR ASP TYR TRP LEU ASN PHE THR SEQRES 2 A 188 ASP GLY GLY GLY ILE VAL ASN ALA VAL ASN GLY SER GLY SEQRES 3 A 188 GLY ASN TYR SER VAL ASN TRP SER ASN THR GLY SER PHE SEQRES 4 A 188 VAL VAL GLY LYS GLY TRP THR THR GLY SER PRO PHE ARG SEQRES 5 A 188 THR ILE ASN TYR ASN ALA GLY VAL TRP ALA PRO ASN GLY SEQRES 6 A 188 TRP GLY ALA LEU ALA LEU VAL GLY TRP THR ARG SER **PRO**

```
SEQRES 7 A 188 LEUILE ALA TYR TYR VAL VAL ASP SER TRP GLY THR
ALA
SEQRES 8 A 188 ARG TRP THR GLY THR TYR LYS GLY THR VAL LYS SER
ASP
SEQRES 9 A 188 GLY GLY THR TYR ASPILE TYR THR THR THR ARG TYR
ASN
SEQRES 10 A 188 ALA PRO SER ILE ASP GLY ASP ARG THR THR PHE THR
GLN
SEQRES 11 A 188 TYR TRP SER VAL ARG GLN SER LYS ARG PRO THR GLY
SER
SEQRES 12 A 188 ASN ALA THR ILE THR PHE SER ASN HIS VAL ASN ALA
TRP
SEQRES 13 A 188 LYS SER HIS GLY MET ASN LEU GLY SER ASN TRP ALA
TYR
SEQRES 14 A 188 GLN VAL MET ALA THR ALA GLY TYR GLN SER SER GLY
SER
SEQRES 15 A 188 SER ASN VAL THR VAL TRP
SEQRES 1B 188 GLY PRO HIS MET SER THR ASP TYR TRP LEU ASN PHE
THR
SEQRES 2 B 188 ASP GLY GLY GLY ILE VAL ASN ALA VAL ASN GLY SER
GLY
SEQRES 3 B 188 GLY ASN TYR SER VAL ASN TRP SER ASN THR GLY SER
PHE
SEQRES 4 B 188 VAL VAL GLY LYS GLY TRP THR THR GLY SER PRO PHE
ARG
SEQRES 5 B 188 THR ILE ASN TYR ASN ALA GLY VAL TRP ALA PRO ASN
GLY
SEQRES 6 B 188 TRP GLY ALA LEU ALA LEU VAL GLY TRP THR ARG SER
PRO
SEQRES 7 B 188 LEU ILE ALA TYR TYR VAL VAL ASP SER TRP GLY THR
ALA
SEQRES 8 B 188 ARG TRP THR GLY THR TYR LYS GLY THR VAL LYS SER
ASP
SEQRES 9 B 188 GLY GLY THR TYR ASPILE TYR THR THR THR ARG TYR
ASN
SEQRES 10 B 188 ALA PRO SER ILE ASP GLY ASP ARG THR THR PHE THR
GLN
SEQRES 11 B 188 TYR TRP SER VAL ARG GLN SER LYS ARG PRO THR GLY
SER
SEQRES 12 B 188 ASN ALA THR ILE THR PHE SER ASN HIS VAL ASN ALA
TRP
SEQRES 13 B 188 LYS SER HIS GLY MET ASN LEU GLY SER ASN TRP ALA
TYR
SEQRES 14 B 188 GLN VAL MET ALA THR ALA GLY TYR GLN SER SER GLY
SER
SEQRES 15 B 188 SER ASN VAL THR VAL TRP
SEQRES 1 C 188 GLY PRO HIS MET SER THR ASP TYR TRP LEU ASN PHE
THR
SEQRES 2 C 188 ASP GLY GLY GLY ILE VAL ASN ALA VAL ASN GLY SER
GLY
SEQRES 3 C 188 GLY ASN TYR SER VAL ASN TRP SER ASN THR GLY SER
PHE
SEQRES 4 C 188 VAL VAL GLY LYS GLY TRP THR THR GLY SER PRO PHE
```

```
ARG
SEQRES 5 C 188 THR ILE ASN TYR ASN ALA GLY VAL TRP ALA PRO ASN
GLY
SEQRES 6 C 188 TRP GLY ALA LEU ALA LEU VAL GLY TRP THR ARG SER
PRO
SEQRES 7 C 188 LEU ILE ALA TYR TYR VAL VAL ASP SER TRP GLY THR
ALA
SEQRES 8 C 188 ARG TRP THR GLY THR TYR LYS GLY THR VAL LYS SER
ASP
SEQRES 9 C 188 GLY GLY THR TYR ASPILE TYR THR THR THR ARG TYR
ASN
SEQRES 10 C 188 ALA PRO SER ILE ASP GLY ASP ARG THR THR PHE THR
GLN
SEQRES 11 C 188 TYR TRP SER VAL ARG GLN SER LYS ARG PRO THR GLY
SER
SEQRES 12 C 188 ASN ALA THR ILE THR PHE SER ASN HIS VAL ASN ALA
TRP
SEQRES 13 C 188 LYS SER HIS GLY MET ASN LEU GLY SER ASN TRP ALA
TYR
SEQRES 14 C 188 GLN VAL MET ALA THR ALA GLY TYR GLN SER SER GLY
SER
SEQRES 15 C 188 SER ASN VAL THR VAL TRP
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HET
      K B 201
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HET
      K C 201
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HETNAM
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FORMUL 4
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FORMUL 7 HOH
                *367(H2 O)
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       3 AA3 PHE C 146 SER C 155 1
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       4 AA116 ILE A 77 TRP A 85 1 N VAL A 82 O SER A 130
SHEET
       5 AA116 THR A 50 ARG A 73 -1 N LEU A 66 O SER A 84
SHEET
       6 AA116 ASN A 163 TRP A 185 -1 O SER A 177 N ASN A 61
SHEET
SHEET
       7 AA116 SER A 35 TRP A 42 -1 N VAL A 38 O THR A 171
       8 AA116 TYR A 5 THR A 10-1 N LEU A 7 O GLY A 39
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       11 AA116 GLY B 120 ARG B 132 -1 O GLY B 120 N SER B 117
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       6 AA211 GLY B 92 SER B 100 -1 O GLY B 92 N TRP A 6
SHEET
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         6 AA310 THR A 50 ARG A 73 -1 N TYR A 53 O ALA A 142
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SHEET
         9 AA310 GLY A 103 SER A 117 -1 N ASP A 106 O VAL A 131
SHEET
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SHEET
         3 AA4 5 ASN B 163 TRP B 185 -1 O GLN B 167 N TRP B 42
SHEET
SHEET
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         5 AA4 5 ILE B 15 ASN B 20 -1 N ASN B 17 O ASN B 29
SHEET
SHEET
         1 AA5 5 ILE B 15 ASN B 20 0
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SHEET
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SHEET
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         8 AA6 8 THR C 93 SER C 100 -1 N VAL C 98 O TYR C 105
SHEET
SHEET
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SHEET
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O ASN A 20 K K A 201 1555 1555 2.78
OD1 ASN A 20 K K A 201 1555 1555 2.84
O GLY A 21 K K A 201 1555 1555 2.76
O ASN B 20 K K B 201 1555 1555 2.81
OD1 ASN B 20 K K B 201 1555 1555 2.81
OD1 ASN B 20 K K B 201 1555 1555 2.83
OH TYR B 94 K K A 201 1555 1555 2.67
OD1 ASP B 106 K K A 201 1555 1555 2.71
O ASN C 20 K K C 201 1555 1555 2.74
OD1 ASN C 20 K K C 201 1555 1555 2.74
OD1 ASN C 20 K K C 201 1555 1555 2.71
K K A 201 O HOH B 390 1555 1555 2.67
OH TYR A 94 K K C 201 1555 4545 2.72
OD1 ASP A 106 K K C 201 1555 4545 2.64
OH TYR C 94 K K B 201 1555 3454 2.80
SHEET
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CISPEP 2 SER B 74 PRO B 75 0
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CISPEP 3 SER C 74
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SITE
            2 AC1 7 ASP B 106 GLN B 133 HOH B 390
SITE
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SITE
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SITE
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SITE
SITE 2 AC3 7 HOH A 360 ASN C 20 GLY C 21
CRYST1 54.760 73.259 137.558 90.00 90.00 90.00 P 21 21 21 12
1 N MET A 1 10.518 -8.748 -29.729 1.00 63.76
ATOM
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ANISOU 1 N MET A 1 6872 7840 9513 -263 722 536
ATOM 2 CA MET A 1 9.467 -7.797 -30.197 1.00 61.68
ANISOU 2 CA MET A 1 6899 7382 9153 -335 665 566
ATOM 3 C MET A 1 8.390 -7.628 -29.131 1.00 55.67
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                                                                                                           C
                                                                                                            C
ANISOU 3 C MET A 1 6263 6561 8329 -257 389 416
ATOM 4 O MET A 1 8.363 -8.370 -28.149 1.00 56.71
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ANISOU 4 O MET A 1 6298 6802 8448 -138 273 307
ATOM 5 CB MET A 1 8.842 -8.292 -31.503 1.00 62.19
ANISOU 5 CB MET A 1 7216 7430 8983 -236 857 656
ATOM 6 H MET A 1 11.286 -8.312 -29.620 1.00 76.51
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ATOM 7 HA MET A 1 9.877 -6.935 -30.369 1.00 74.01
ATOM 8 N SER A 2 7.504 -6.652 -29.317 1.00 46.95
ANISOU 8 N SER A 2 5380 5287 7174 -306 290 415
ATOM 9 CA SER A 2 6.381 -6.514 -28.407 1.00 35.79
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ANISOU 9 CA SER A 2 4088 3836 5673 -197 64 279

ATOM 10 C SER A 2 5.413 -7.680 -28.608 1.00 26.20

ANISOU 10 C SER A 2 2987 2719 4248 -14 105 254

ATOM 11 O SER A 2 5.504 -8.446 -29.574 1.00 22.86

ANISOU 11 O SER A 2 2611 2345 3729 27 283 335

ATOM 12 CB SER A 2 4278 3611 5654 -265 -52 281

ATOM 13 OG SER A 2 4.900 -5.154 -29.789 1.00 35.73
                                                                                                           C
                                                                                                            C
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ANISOU 13 OG SER A 2 4516 3555 5503 -221
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ATOM 15 HA SER A 2 6.708 -6.550 -27.495 1.00 42.94
                                                                                                          Н
                                                                                                        Н
              16 HB2 SER A 2 5.096 -5.007 -27.847 1.00 42.77
17 HB3 SER A 2 6.348 -4.472 -28.662 1.00 42.77
18 HG SER A 2 4.525 -4.407 -29.876 1.00 42.87
ATOM 16 HB2 SER A 2
                                                                                                           Н
            17 HB3 SER A 2
ATOM
                                                                                                            Н
            19 N THR A 3 4.489 -7.823 -27.663 1.00 42.87 N
ATOM
ATOM
ANISOU 19 N THR A 3 2556 2269 3700 96 -61 140
ATOM 20 CA THR A 3 3.617 -8.986 -27.630 1.00 19.97
ANISOU 20 CA THR A 3 2306 2054 3227 240 -40 114
ATOM 21 C THR A 3 2.665 -8.991 -28.821 1.00 18.92
                                                                                                           Ν
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                                                                                                            C
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ANISOU 21 C THR A 3		С
ATOM 22 O THR A 3	2.345 -7.948 -29.397 1.00 18.10	0
ANISOU 22 O THR A 3	2402 1619 2854 212 -10 207	0
ATOM 23 CB THR A 3	2.815 -9.019 -26.327 1.00 19.45	С
ANISOU 23 CB THR A 3	2233 2038 3121 338 -209 -2	Č
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ATOM 24 OG1 THR A 3	2.113 -7.783 -26.157 1.00 20.18	0
ANISOU 24 OG1 THR A 3		0
ATOM 25 CG2 THR A 3	3.726 -9.243 -25.138 1.00 20.20	С
ANISOU 25 CG2 THR A 3	2155 2215 3305 352 -282 -67	С
ATOM 26 H THR A 3	4.349 -7.259 -27.029 1.00 26.92	Н
ATOM 27 HA THR A 3	4.158 -9.790 -27.672 1.00 23.96	H
_		
ATOM 28 HB THR A 3	2.176 -9.748 -26.362 1.00 23.35	H.
ATOM 29 HG1 THR A 3	1.586 -7.662 -26.800 1.00 24.22	Н
ATOM 30 HG21 THR A 3	3.205 -9.262 -24.320 1.00 24.24	Н
ATOM 31 HG22 THR A 3	4.193 -10.088 -25.234 1.00 24.24	Н
ATOM 32 HG23 THR A 3	4.378 -8.527 -25.081 1.00 24.24	Н
ATOM 33 N ASP A 4	2.216 -10.199 -29.197 1.00 17.87	Ν΄
ANISOU 33 N ASP A 4	2293 1792 2704 349 82 183	N
ATOM 34 CA ASP A 4	1.262 -10.339 -30.293 1.00 18.15	С
ANISOU 34 CA ASP A 4	2524 1770 2603 385 98 218	C
ATOM 35 C ASP A 4	0.396 -11.589 -30.144 1.00 17.36	С
ANISOU 35 C ASP A 4	2451 1744 2402 472 64 177	C
ATOM 36 O ASP A 4	-0.059 -12.149 -31.148 1.00 16.74	Ŏ
ANISOU 36 O ASP A 4	2515 1635 2212 501 98 206	0
ATOM 37 CB ASP A 4	1.999 -10.371 -31.634 1.00 19.80	С
ANISOU 37 CB ASP A 4	2827 1930 2766 348 274 325	C
ATOM 38 CG ASP A 4	2.829 -11.629 -31.821 1.00 19.73	C
ANISOU 38 CG ASP A 4	2748 2017 2733 398 419 346	С
ATOM 39 OD1 ASP A 4	2.972 -12.434 -30.878 1.00 19.20	ŏ
ANISOU 39 OD1 ASP A 4		Ö
ATOM 40 OD2 ASP A 4	3.340 -11.819 -32.935 1.00 22.88	0
ANISOU 40 OD2 ASP A 4	3239 2398 3058 408 580 425	0
ATOM 41 H ASP A 4	2.450 -10.942 -28.833 1.00 21.44	Н
ATOM 42 HA ASP A 4	0.673 -9.569 -30.295 1.00 21.78	Н
ATOM 43 HB2 ASP A 4	1.348 -10.332 -32.353 1.00 23.76	Н
ATOM 44 HB3 ASP A 4	2.595 -9.608 -31.685 1.00 23.76	H
ATOM 45 N TYR A 5	0.140 -12.029 -28.914 1.00 15.74	N
ANISOU 45 N TYR A 5	2128 1625 2228 509 -9 114	N
ATOM 46 CA TYR A 5	-0.614 -13.254 -28.699 1.00 15.44	C
ANISOU 46 CA TYR A 5	2108 1645 2115 559 -28 97	С
ATOM 47 C TYR A 5	-1.455 -13.128 -27.440 1.00 15.74	С
ANISOU 47 C TYR A 5	2059 1756 2167 593 -132 39	C
ATOM 48 O TYR A 5	-0.980 -12.628 -26.417 1.00 15.89	ŏ
ANISOU 48 O TYR A 5	1982 1813 2243 609 -167 0	0
ATOM 49 CB TYR A 5	0.315 -14.464 -28.580 1.00 15.85	С
ANISOU 49 CB TYR A 5	2120 1740 2162 588 69 118	С
ATOM 50 CG TYR A 5	-0.404 -15.777 -28.768 1.00 16.04	C
ANISOU 50 CG TYR A 5	2233 1762 2100 617 60 121	Č
ATOM 51 CD1 TYR A 5	-0.570 -16.323 -30.035 1.00 17.46	Č
ANISOU 51 CD1 TYR A 5		Č
ATOM 52 CD2 TYR A 5	-0.932 -16.460 -27.682 1.00 15.88	С
ANISOU 52 CD2 TYR A 5	2155 1800 2080 633 8 103	С
ATOM 53 CE1 TYR A 5	-1.232 -17.531 -30.212 1.00 17.95	C

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ANISOU 53 CE1 TYR A 5
                          2735 1898 2189
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        54 CE2 TYR A 5
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ANISOU 54 CE2 TYR A 5
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ATOM
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ANISOU 55 CZ TYR A 5
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ATOM
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        65 HH TYR A 5
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ATOM
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ANISOU 66 N TRP A 6
                         2050 1738 2070 607 -182
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        67 CA TRP A 6
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ANISOU 67 CA TRP A 6
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                         -4.069 -15.038 -26.161 1.00 15.42
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                         1946 1879 2034 625 -207
ANISOU 68 C TRP A 6
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ATOM
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                                          579 -220
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        70 CB TRPA 6
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                               1855 1951
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        72 CD1 TRP A 6
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ANISOU 73 CD2 TRP A 6
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ANISOU 74 NE1 TRP A 6
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        78 CZ3 TRP A 6
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ANISOU 78 CZ3 TRP A 6
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        79 CH2 TRP A 6
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ANISOU 79 CH2 TRP A 6
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        86 HE3 TRP A
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        88 HZ3 TRP A 6
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ATOM 89 HH2 TRP A 6 -6.636 -12.082 -20.686 1.00 22.23 Н **ATOM** 90 N LEUA 7 -3.777 -15.533 -24.959 1.00 14.52 Ν ANISOU 90 N LEUA 7 1764 1840 1913 657 -176 37 Ν C **ATOM** 91 CA LEU A 7 -4.166 -16.863 -24.515 1.00 14.46 ANISOU 91 CA LEUA 7 C 1760 1862 1873 632 -138 **ATOM** 92 C LEUA 7 -5.326 -16.741 -23.537 1.00 15.50 Č ANISOU 92 C LEUA 7 1793 2108 1988 647 -145 94 Ŏ 93 O LEUA 7 -5.233 -16.005 -22.546 1.00 15.67 ATOM 0 ANISOU 93 O LEUA 7 1755 2210 1989 731 -151 55 C 94 CB LEU A 7 -2.990 -17.577 -23.851 1.00 13.66 **ATOM** ANISOU 94 CB LEU A 7 1675 1761 1753 678 -88 108 CCCC ATOM 95 CG LEU A 7 -3.285 -18.915 -23.173 1.00 13.59 ANISOU 95 CG LEU A 7 1702 1763 1698 668 -50 96 CD1 LEU A 7 -3.750 -19.940 -24.196 1.00 14.45 **ATOM** ANISOU 96 CD1 LEU A 7 1917 1765 1807 581 214 -49 C 97 CD2 LEU A 7 -2.043 -19.394 -22.439 1.00 14.15 ATOM ANISOU 97 CD2 LEU A 7 1792 1841 1744 **758** -29 180 98 H LEUA 7 **ATOM** -3.336 -15.096 -24.364 1.00 17.43 Н **ATOM** 99 HA LEU A 7 -4.458 -17.388 -25.277 1.00 17.36 Н **ATOM** 100 HB2 LEU A 7 -2.316 -17.742 -24.528 1.00 16.39 Н 101 HB3 LEU A 7 -2.623 -16.988 -23.173 1.00 16.39 Н **ATOM** 102 HG LEU A 7 Н **ATOM** -3.994 -18.793 -22.523 1.00 16.31 103 HD11 LEU A 7 **ATOM** -3.931 -20.778 -23.743 1.00 17.34 Н **ATOM** 104 HD12 LEU A 7 -4.557 -19.614 -24.624 1.00 17.34 Н **ATOM** 105 HD13 LEU A 7 -3.051 -20.064 -24.857 1.00 17.34 Н **ATOM** 106 HD21 LEU A -2.238 -20.243 -22.012 1.00 16.98 Н -1.321 -19.503 -23.077 1.00 16.98 107 HD22 LEU A 7 Н **ATOM** Н **ATOM** 108 HD23 LEU A -1.798 -18.736 -21.770 1.00 16.98 **ATOM** 109 N ASNA 8 -6.412 -17.468 -23.807 1.00 15.66 N ANISOU 109 N ASNA 8 1794 2139 2019 567 -145 110 CA ASN A 8 -7.590 -17.432 -22.934 1.00 16.67 C ATOM C ANISOU 110 CA ASN A 8 1792 2400 2144 570 -118 166 111 C ASN A 8 -8.241 -18.819 -22.960 1.00 18.33 **ATOM** 259 ANISOU 111 C ASN A 8 2001 2590 2374 439 -82 ATOM 112 O ASNA 8 0 -9.161 -19.070 -23.741 1.00 20.24 0 ANISOU 112 O ASN A 8 267 2204 2809 2679 340 -141 CCCC 113 CB ASN A 8 -8.558 -16.349 -23.383 1.00 17.36 **ATOM** ANISOU 113 CB ASN A 8 1787 2540 2267 603 -189 108 114 CG ASN A 8 ATOM -9.744 -16.199 -22.452 1.00 18.03 ANISOU 114 CG ASN A 8 1703 2797 2350 641 -140 128 0 115 OD1 ASN A 8 -9.795 -16.801 -21.387 1.00 17.38 ATOM ANISOU 115 OD1 ASN A 8 0 1584 2798 2222 645 -37 191 -10.699 -15.370 -22.847 1.00 19.47 N ATOM 116 ND2 ASN A 8 ANISOU 116 ND2 ASN A 8 1785 3040 2573 689 -207 **79** N **ATOM** 117 H ASNA 8 -6.493 -17.989 -24.487 1.00 18.80 Н 118 HA ASN A 8 -7.313 -17.239 -22.024 1.00 20.01 Η **ATOM** -8.090 -15.499 -23.411 1.00 20.83 **ATOM** 119 HB2 ASN A 8 Н -8.895 -16.572 -24.265 1.00 20.83 Н **ATOM** 120 HB3 ASN A 8 121 HD21 ASN A 8 **ATOM** -11.394 -15.249 -22.356 1.00 23.37 Н 122 HD22 ASN A 8 -10.623 -14.952 -23.595 1.00 23.37 Н **ATOM** 123 N PHE A 9 Ν ATOM -7.761 -19.710 -22.094 1.00 17.69 ANISOU 123 N PHE A 9 1974 2505 2243 438 -3 Ν 124 CA PHE A 9 -8.212 -21.096 -22.072 1.00 18.09 C ATOM

ANISOU 124 CA PHE A 9 2071 2490 2314 303 31 430 C **ATOM** 125 C PHE A 9 -8.803 -21.440 -20.716 1.00 19.00 ANISOU 125 C PHE A 9 2103 2731 2384 298 148 529 Ö ATOM 126 O PHE A 9 -8.217 -21.120 -19.676 1.00 17.40 ANISOU 126 O PHE A 9 1921 2605 2083 433 206 5 ANISOU 126 O PHE A 9 1921 2605 2083 433 206 526 ATOM 127 CB PHE A 9 -7.069 -22.060 -22.382 1.00 17.95 ANISOU 127 CB PHE A 9 2249 2311 2261 310 23 446 ATOM 128 CG PHE A 9 -7.376 -23.490 -22.013 1.00 18.91 0 000000000 ANISOU 128 CG PHE A 9 2461 2345 2379 199 561 63 ATOM 129 CD1 PHE A 9 -8.064 -24.309 -22.890 1.00 20.12 ANISOU 129 CD1 PHE A 9 2669 2370 2607 35 -4 587 ATOM 130 CD2 PHE A 9 -6.990 -24.005 -20.790 1.00 20.13 ANISOU 130 CD2 PHE A 9 2668 2530 2452 257 150 644 131 CE1 PHE A 9 -8.350 -25.625 -22.559 1.00 21.33 CCCC **ATOM** ANISOU 131 CE1 PHE A 9 2927 2407 2772 -91 20 -7.279 -25.318 -20.450 1.00 22.01 ATOM 132 CE2 PHE A 9 ANISOU 132 CE2 PHE A 9 3020 2660 2683 148 190 769 133 CZ PHE A 9 -7.957 -26.127 -21.340 1.00 22.81 **ATOM** C ANISOU 133 CZ PHE A 9 3173 2615 2879 -37 126 798 ATOM 134 H PHEA 9 -7.164 -19.531 -21.502 1.00 21.23 Н ATOM 135 HA PHE A 9 -8.902 -21.217 -22.743 1.00 21.71 ATOM 136 HB2 PHE A 9 -6.884 -22.031 -23.334 1.00 21.54 Н Н ATOM 137 HB3 PHE A 9 -6.283 -21.785 -21.885 1.00 21.54 ATOM 138 HD1 PHE A 9 -8.329 -23.976 -23.717 1.00 24.15 Н Н ATOM 139 HD2 PHE A 9 -6.530 -23.465 -20.188 1.00 24.16 ATOM 140 HE1 PHE A 9 -8.810 -26.166 -23.158 1.00 25.60 Н Н ATOM 141 HE2 PHE A 9 -7.010 -25.656 -19.626 1.00 26.41 Н 142 HZ PHE A 9 -8.151 -27.008 -21.115 1.00 27.37 **ATOM** ATOM 143 N ATHR A 10 -9.964 -22.090 -20.730 0.43 21.24 ANISOU 143 N ATHR A 10 2294 3037 2738 141 181 618 Ν ATOM 144 N BTHR A 10 -9.964 -22.092 -20.732 0.57 21.26 ANISOU 144 N BTHR A 10 2296 3040 2740 141 181 6 Ν 618 145 CA ATHR A 10 -10.566 -22.631 -19.522 0.43 23.27 **ATOM** ANISOU 145 CA ATHR A 10 2485 3401 2955 100 328 ATOM 146 CA BTHR A 10 -10.583 -22.621 -19.527 0.57 23.25 ANISOU 146 CA BTHR A 10 2480 3400 2954 99 328 -11.219 -23.960 -19.862 0.43 26.32 147 C ATHR A 10 **ATOM** ANISOU 147 C ATHR A 10 2898 3665 3438 -137 331 872 ATOM 148 C BTHR A 10 -11.224 -23.959 -19.863 0.57 26.31 ANISOU 148 C BTHR A 10 2896 3665 3437 -138 331 872 0 -11.618 -24.196 -21.004 0.43 26.52 149 O ATHR A 10 ATOM 0 ANISOU 149 O ATHR A 10 2913 3584 3579 -267 204 830 ATOM 150 O BTHR A 10 -11.619 -24.201 -21.006 0.57 26.55 0 ANISOU 150 O BTHR A 10 2917 3588 3583 -268 204 831 CCCC **ATOM 151 CB ATHR A 10** -11.609 -21.678 -18.913 0.43 23.53 ANISOU 151 CB ATHR A 10 2280 3671 2989 165 409 745 ATOM 152 CB BTHR A 10 -11.652 -21.675 -18.953 0.57 23.54 ANISOU 152 CB BTHR A 10 2274 3672 2997 159 406 744 0 153 OG1ATHR A 10 -11.999 -22.153 -17.617 0.43 25.15 ATOM ANISOU 153 OG1ATHR A 10 2451 3996 3109 166 591 883 0 ATOM 154 OG1BTHR A 10 -12.843 -21.763 -19.742 0.57 24.56 ANISOU 154 OG1BTHR A 10 2222 3829 3282 0 353 755 0 0 ATOM 155 CG2ATHR A 10 -12.843 -21.574 -19.802 0.43 24.44 C

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ATOM
        156 CG2BTHR A 10
                            -11.157 -20.228 -18.935 0.57 21.91
                                                                  C
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                                                    345 593
                          -10.427 -22.231 -21.440 0.43 25.48
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ATOM
       158 H BTHR A 10
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-9.904 -22.766 -18.850 0.57 27.90
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       160 HA BTHR A 10
ATOM
ATOM
       161 HB ATHR A 10
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                                                                Н
      162 HB BTHR A 10
                            -11.854 -21.937 -18.041 0.57 28.24
ATOM
      163 HG1ATHR A 10
ATOM
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ATOM
       164 HG1BTHR A 10
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                            -12.594 -21.236 -20.676 0.43 29.32
ATOM
       165 HG21ATHR A 10
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      166 HG21BTHR A 10
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      167 HG22ATHR A 10
ATOM
      168 HG22BTHR A 10
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ATOM
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      169 HG23ATHR A 10
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ANISOU 172 CA ASP A 11 4693 5251 5202 -450 477 1162
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ANISOU 175 CB ASP A 11 5327 5557 5502 -454 584 1312
ATOM 176 CG ASP A 11 -11.641 -26.785 -16.648 1.00 45.64
ANISOU 176 CG ASP A 11 5575 6088 5678 -333 783 1410
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ATOM 177 OD1 ASP A 11 -12.425 -25.858 -16.352 1.00 46.33
ANISOU 177 OD1 ASP A 11 5415 6410 5779 -287 863 1385
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ANISOU 178 OD2 ASP A 11 5998 6231 5746 -260 857 1509
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      179 H AASP A 11
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ATOM
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       185 CA GLY A 12
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ANISOU 185 CA GLY A 12
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                                                               C
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ANISOU 186 C GLY A 12
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ANISOU 187 O GLY A 12
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                                                               Н
                                                               Н
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      189 HA2 GLY A 12
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       190 HA3 GLY A 12
ATOM
                          -15.914 -25.277 -18.663 1.00 64.94
ATOM 191 N GLY A 13 -15.139 -24.450 -15.817 1.00 47.45
                                                               Ν
ANISOU 191 N GLY A 13  4866 7091 6070 -343 1105 1439
ATOM 192 CA GLY A 13 -15.641 -24.383 -14.455 1.00 45.95
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ANISOU 198 N GLY A 14
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       203 HA2 GLY A 14
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ANISOU 211 CG2 ILE A 15
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      212 CD1 ILE A 15
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      218 HG21 ILE A 15
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      219 HG22 ILE A 15
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      221 HD11 ILE A 15
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ANISOU 224 N VAL A 16
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      225 CA VAL A 16
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ANISOU 225 CA VAL A 16
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ATOM 226 C VAL A 16
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                                                             C
ANISOU 226 C VAL A 16
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      227 O VAL A 16
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ANISOU 227 O VAL A 16
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ATOM
ANISOU 229 CG1 VAL A 16
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       230 CG2 VAL A 16
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ANISOU 230 CG2 VAL A 16
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       231 H VAL A 16
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       232 HA VAL A 16
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       233 HB VAL A 16
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ATOM
ATOM
      234 HG11 VAL A 16
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      235 HG12 VAL A 16
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      236 HG13 VAL A 16
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      238 HG22 VAL A 16
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      239 HG23 VAL A 16
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ANISOU 244 CB ASN A 17
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ATOM
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ANISOU 245 CG ASN A 17
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ATOM
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      253 HD22 ASN A 17
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ATOM
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      258 CB ALA A 18
                          -9.479 -13.743 -19.345 1.00 19.75
                                                             Č
ANISOU 258 CB ALA A 18
                          1868 3287 2347 1097
                                                 -70 -35
                                                            Н
      259 H ALA A 18
                         -11.850 -13.624 -18.570 1.00 26.81
ATOM
                                                            Н
ATOM
       260 HA ALA A 18
                          -9.582 -12.386 -17.805 1.00 24.44
      261 HB1 ALA A 18
                                                            Н
ATOM
                         -8.627 -13.419 -19.675 1.00 23.69
      262 HB2 ALA A 18
                         -9.341 -14.508 -18.766 1.00 23.69
ATOM
       263 HB3 ALA A 18 -10.050 -13.990 -20.090 1.00 23.69
ATOM
                                                             Н
ATOM
       264 N VAL A 19 -9.539 -10.384 -19.224 1.00 18.24
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ATOM 265 CA VAL A 19 ANISOU 265 CA VAL A 19 ATOM 266 C VAL A 19 ANISOU 267 O VAL A 19 ANISOU 268 CB VAL A 19 ANISOU 268 CB VAL A 19 ANISOU 269 CG1 VAL A 19 ANISOU 270 CG2 VAL A 19 ANISOU 270 CG2 VAL A 19 ANISOU 270 CG2 VAL A 19 ATOM 271 H VAL A 19 ATOM 273 HB VAL A 19 ATOM 274 HG11 VAL A 19 ATOM 274 HG11 VAL A 19 ATOM 275 HG21 VAL A 19 ATOM 276 HG72 VAL A 19 ATOM 277 HG21 VAL A 19 ATOM 276 HG72 VAL A 19 ATOM 277 HG21 VAL A 19 ATOM 276 HG72 VAL A 19 ATOM 276 HG72 VAL A 19 ATOM 279 HG23 VAL A 19 ATOM 280 N ASNA 20 ANISOU 286 CG ASNA 20 ANISOU 286 CG ASNA 20 ANISOU 286 OD1 ASNA 20 ANISOU 286 OD1 ASNA 20 ANISOU 287 ND2 ASNA 20 ANISOU 286 OD1 ASNA 20 ANISOU 287 ND2 ASNA 20 ATOM 287 ND2 ASNA 20 ATOM 288 H ASNA 20 ATOM 288 H ASNA 20 ATOM 298 H ASNA 20 ATOM 294 N GLYA 21 ANISOU 296 C GLYA 21 ANISOU 297 O GL	ANISOU 264 N VAL A 19	1869 2949 2113 1248 -268 -287	N
ATOM 266 C VAL A 19	ATOM 265 CA VAL A 19	-9.674 -9.122 -19.943 1.00 18.23	C
ANISOU 266 C VAL A 19	ANISOU 265 CA VAL A 19	1941 2837 2147 1268 -374 -361	C
ATOM 267 O VAL A 19	ATOM 266 C VAL A 19	-8.457 -8.944 -20.837 1.00 17.12	C
ANISOU 267 O VAL A 19 ATOM 268 CB VAL A 19 ANISOU 268 CB VAL A 19 ANISOU 269 CG1 VAL A 19 ATOM 269 CG1 VAL A 19 ATOM 270 CG2 VAL A 19 ATOM 270 CG2 VAL A 19 ATOM 271 H VAL A 19 ATOM 272 HA VAL A 19 ATOM 273 HB VAL A 19 ATOM 274 HG11 VAL A 19 ATOM 275 HG12 VAL A 19 ATOM 276 HG13 VAL A 19 ATOM 276 HG13 VAL A 19 ATOM 277 HG21 VAL A 19 ATOM 278 HG22 VAL A 19 ATOM 279 HG23 VAL A 19 ATOM 279 HG23 VAL A 19 ATOM 279 HG23 VAL A 19 ATOM 280 N ASN A 20 ANISOU 281 CA ASN A 20 ANISOU 282 C ASN A 20 ANISOU 282 C ASN A 20 ATOM 282 C ASN A 20 ANISOU 282 C ASN A 20 ANISOU 284 CB ASN A 20 ANISOU 285 CG ASN A 20 ANISOU 286 OD1 ASN A 20 ANISOU 286 OD1 ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 286 CD1 ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 286 CD1 ASN A 20 ANISOU 287 CG ASN A 20 ANISOU 286 CD1 ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 286 CG ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 287 CG ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 287 CG ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 287 CG ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 287 AD ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 287 AD ASN A 20 ANISOU 287 AD ASN A 20 ANISOU 288 CG ASN A 20 ANISOU 287 AD ASN A 20 ANISOU 288 CG ASN A 20 ANISOU 287 AD ASN A 20 ANISOU 288 CG ASN A 20 ANISOU 288 CG ASN A 20 ANISOU 287 AD ASN A 20 ANISOU 288 CG ASN A 20 ANISOU 288 CG ASN A 20 ANISOU 298 N GLY A 21 ANISOU 294 N GLY A 21 ANISOU 295 CA GLY A 21 ANISOU 296 C GLY A 21 ANISOU 297 O GLY A 21 AN	ANISOU 266 C VAL A 19	1904 2523 2079 1171 -447 -362	С
ATOM 268 CB VAL A 19 ANISOU 268 CB VAL A 19 ATOM 269 CG1 VAL A 19 ATOM 269 CG1 VAL A 19 ANISOU 269 CG1 VAL A 19 ANISOU 269 CG1 VAL A 19 ATOM 270 CG2 VAL A 19 ATOM 271 H VAL A 19 ATOM 271 H VAL A 19 ATOM 272 HA VAL A 19 ATOM 273 HB VAL A 19 ATOM 274 HG11 VAL A 19 ATOM 274 HG11 VAL A 19 ATOM 275 HG12 VAL A 19 ATOM 276 HG13 VAL A 19 ATOM 276 HG13 VAL A 19 ATOM 277 HG21 VAL A 19 ATOM 277 HG21 VAL A 19 ATOM 278 HG22 VAL A 19 ATOM 279 HG23 VAL A 19 ATOM 279 HG23 VAL A 19 ATOM 280 N ASN A 20 ANISOU 280 C ASN A 20 ANISOU 281 CA ASN A 20 ANISOU 282 C ASN A 20 ANISOU 282 C ASN A 20 ANISOU 283 C ASN A 20 ANISOU 284 CB ASN A 20 ATOM 283 O ASN A 20 ATOM 283 O ASN A 20 ATOM 284 CB ASN A 20 ATOM 285 CG ASN A 20 ATOM 286 OD1 ASN A 20 ATOM 286 OD1 ASN A 20 ATOM 286 OD1 ASN A 20 ATOM 287 ND2 ASN A 20 ATOM 290 HB2 ASN A 20 ATOM 291 HB3 ASN A 20 ATOM 292 HD21 ASN A 20 ATOM 294 N GLY A 21 ATOM 295 CA GLY A 21 ANISOU 295 CA GLY A 21 ANISOU 296 C GLY A 21 ANISOU 297 O GLY A 21 CATOM 297 O GLY A	ATOM 267 O VAL A 19	-7.330 -8.797 -20.352 1.00 16.02	0
ATOM 268 CB VAL A 19 ANISOU 268 CB VAL A 19 ATOM 269 CG1 VAL A 19 ATOM 269 CG1 VAL A 19 ANISOU 269 CG1 VAL A 19 ANISOU 269 CG1 VAL A 19 ATOM 270 CG2 VAL A 19 ATOM 271 H VAL A 19 ATOM 271 H VAL A 19 ATOM 272 HA VAL A 19 ATOM 273 HB VAL A 19 ATOM 274 HG11 VAL A 19 ATOM 274 HG11 VAL A 19 ATOM 275 HG12 VAL A 19 ATOM 276 HG13 VAL A 19 ATOM 276 HG13 VAL A 19 ATOM 277 HG21 VAL A 19 ATOM 277 HG21 VAL A 19 ATOM 278 HG22 VAL A 19 ATOM 279 HG23 VAL A 19 ATOM 279 HG23 VAL A 19 ATOM 280 N ASN A 20 ANISOU 280 C ASN A 20 ANISOU 281 CA ASN A 20 ANISOU 282 C ASN A 20 ANISOU 282 C ASN A 20 ANISOU 283 C ASN A 20 ANISOU 284 CB ASN A 20 ATOM 283 O ASN A 20 ATOM 283 O ASN A 20 ATOM 284 CB ASN A 20 ATOM 285 CG ASN A 20 ATOM 286 OD1 ASN A 20 ATOM 286 OD1 ASN A 20 ATOM 286 OD1 ASN A 20 ATOM 287 ND2 ASN A 20 ATOM 290 HB2 ASN A 20 ATOM 291 HB3 ASN A 20 ATOM 292 HD21 ASN A 20 ATOM 294 N GLY A 21 ATOM 295 CA GLY A 21 ANISOU 295 CA GLY A 21 ANISOU 296 C GLY A 21 ANISOU 297 O GLY A 21 CATOM 297 O GLY A	ANISOU 267 O VAL A 19	1831 2326 1930 1162 -473 -392	0
ANISOU 268 CB VAL A 19 ATOM 269 CG1 VAL A 19 ANISOU 269 CG1 VAL A 19 ANISOU 270 CG2 VAL A 19 ATOM 270 CG2 VAL A 19 ATOM 271 H VAL A 19 ATOM 273 HB VAL A 19 ATOM 273 HB VAL A 19 ATOM 274 HG11 VAL A 19 ATOM 275 HG12 VAL A 19 ATOM 276 HG13 VAL A 19 ATOM 277 HG21 VAL A 19 ATOM 278 HG22 VAL A 19 ATOM 279 HG23 VAL A 19 ATOM 279 HG23 VAL A 19 ATOM 280 N ASN A 20 ANISOU 280 C ASN A 20 ANISOU 281 CA ASN A 20 ANISOU 282 C ASN A 20 ANISOU 282 C ASN A 20 ANISOU 284 CB ASN A 20 ANISOU 285 CG ASN A 20 ANISOU 286 OD1 ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 287 CG ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 288 C G GLY A 21 ANISOU 294 N GLY A 21 ANISOU 294 N GLY A 21 ANISOU 295 CA GLY A 21 ANISOU 296 C GLY A 21 ANISOU 296 C GLY A 21 ANISOU 297 O GL			_
ATOM 269 CG1 VAL A 19 ANISOU 269 CG1 VAL A 19 ANISOU 270 CG2 VAL A 19 ANISOU 270 CG2 VAL A 19 ANISOU 270 CG2 VAL A 19 ATOM 271 H VAL A 19 ATOM 272 HA VAL A 19 ATOM 273 HB VAL A 19 ATOM 273 HB VAL A 19 ATOM 275 HG12 VAL A 19 ATOM 276 HG13 VAL A 19 ATOM 276 HG13 VAL A 19 ATOM 277 HG21 VAL A 19 ATOM 277 HG21 VAL A 19 ATOM 278 HG22 VAL A 19 ATOM 278 HG22 VAL A 19 ATOM 279 HG23 VAL A 19 ATOM 288 I CA ASN A 20 ANISOU 280 N ASN A 20 ANISOU 281 CA ASN A 20 ATOM 282 C ASN A 20 ATOM 282 C ASN A 20 ATOM 284 CB ASN A 20 ATOM 283 O ASN A 20 ANISOU 285 CG ASN A 20 ANISOU 285 CG ASN A 20 ANISOU 286 OD I ASN A 20 ATOM 286 OD I ASN A 20 ATOM 287 ND2 ASN A 20 ATOM 288 H ASN A 20 ATOM 288 H ASN A 20 ATOM 288 H ASN A 20 ATOM 298 HA ASN A 20 ATOM 299 HB2 ASN A 20 ATOM 299 HB2 ASN A 20 ATOM 291 HB3 ASN A 20 ATOM 294 N GLY A 21 ANISOU 295 CA GLY A 21 ANISOU 295 CA GLY A 21 ANISOU 296 C GLY A 21 ANISOU 297 O GLY A 21 ANI			_
ANISOU 269 CG1 VAL A 19			
ATOM 270 CG2 VAL A 19 ANISOU 270 CG2 VAL A 19 ATOM 271 H VAL A 19 ATOM 272 HA VAL A 19 ATOM 273 HB VAL A 19 ATOM 274 HG11 VAL A 19 ATOM 275 HG12 VAL A 19 ATOM 275 HG12 VAL A 19 ATOM 276 HG13 VAL A 19 ATOM 277 HG21 VAL A 19 ATOM 278 HG22 VAL A 19 ATOM 279 HG23 VAL A 19 ATOM 280 N ASN A 20 ANISOU 280 N ASN A 20 ANISOU 281 CA ASN A 20 ANISOU 282 C ASN A 20 ANISOU 282 C ASN A 20 ANISOU 282 C ASN A 20 ANISOU 283 O ASN A 20 ANISOU 284 CB ASN A 20 ANISOU 285 CG ASN A 20 ANISOU 286 OD1 ASN A 20 ANISOU 286 OD1 ASN A 20 ANISOU 286 OD1 ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 286 OD1 ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 288 OD1 ASN A 20 ANISOU 287 ND2 ASN A 20 ATOM 289 HA ASN A 20 ATOM 291 HB3 ASN A 20 ATOM 292 HD21 ASN A 20 ATOM 292 HD21 ASN A 20 ATOM 294 N GLY A 21 ANISOU 294 N GLY A 21 ANISOU 295 CA GLY A 21 ANISOU 295 CA GLY A 21 ANISOU 296 C GLY A 21 ANISOU 297 O GLY A 21 A			
ANISOU 270 CG2 VAL A 19 ATOM 271 H VAL A 19 ATOM 272 HA VAL A 19 ATOM 273 HB VAL A 19 ATOM 274 HG11 VAL A 19 ATOM 275 HG12 VAL A 19 ATOM 276 HG13 VAL A 19 ATOM 277 HG21 VAL A 19 ATOM 277 HG22 VAL A 19 ATOM 278 HG22 VAL A 19 ATOM 278 HG22 VAL A 19 ATOM 279 HG23 VAL A 19 ATOM 280 N ASN A 20 ANISOU 280 N ASN A 20 ANISOU 281 CA ASN A 20 ATOM 282 C ASN A 20 ANISOU 281 CA ASN A 20 ANISOU 282 C ASN A 20 ANISOU 283 O ASN A 20 ANISOU 284 CB ASN A 20 ANISOU 285 CG ASN A 20 ANISOU 286 OD1 ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 288 H ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 288 H ASN A 20 ANISOU 287 ND2 ASN A 20 ATOM 288 H ASN A 20 ANISOU 287 ND2 ASN A 20 ANISOU 287 ND2 ASN A 20 ATOM 290 HB2 ASN A 20 ATOM 291 HB3 ASN A 20 ATOM 292 HD21 ASN A 20 ATOM 293 HD22 ASN A 20 ATOM 294 N GLY A 21 ANISOU 295 CA GLY A 21 ANISOU 295 CA GLY A 21 ANISOU 296 C GLY A 21 ANISOU 297 O GLY A 21			_
ATOM 271 H VAL A 19			
ATOM 272 HA VAL A 19			_
ATOM 273 HB VAL A 19	_		
ATOM 274 HG11 VAL A 19			
ATOM 275 HG12 VAL A 19			
ATOM 276 HG13 VAL A 19			
ATOM 277 HG21 VAL A 19			
ATOM 278 HG22 VAL A 19			
ATOM 279 HG23 VAL A 19			
ATOM 280 N ASN A 20			
ANISOU 280 N ASN A 20 ATOM 281 CA ASN A 20 ANISOU 281 CA ASN A 20 ATOM 282 C ASN A 20 ANISOU 282 C ASN A 20 ANISOU 283 O ASN A 20 ANISOU 283 O ASN A 20 ANISOU 284 CB ASN A 20 ATOM 285 CG ASN A 20 ATOM 286 OD1 ASN A 20 ANISOU 286 OD1 ASN A 20 ANISOU 286 OD1 ASN A 20 ANISOU 287 ND2 ASN A 20 ATOM 288 H ASN A 20 ATOM 288 H ASN A 20 ATOM 289 HB2 ASN A 20 ATOM 289 HB2 ASN A 20 ATOM 280 HB2 ASN A 20 ATOM 280 HB2 ASN A 20 ATOM 281 CA ASN A 20 ANISOU 282 C ASN A 20 ANISOU 284 CB ASN A 20 ANISOU 285 CG ASN A 20 ANISOU 286 OD1 ASN A 20 ANISOU 286 OD1 ASN A 20 ANISOU 286 OD1 ASN A 20 ANISOU 287 ND2 ASN A 20 ATOM 280 HB2 ASN A 20 ATOM 280 HB2 ASN A 20 ATOM 293 HD22 ASN A 20 ATOM 294 N GLY A 21 ATOM 295 CA GLY A 21 ANISOU 295 CA GLY A 21 ANISOU 296 C GLY A 21 ANISOU 297 O GLY A 21			
ATOM 281 CA ASN A 20			
ANISOU 281 CA ASN A 20 ATOM 282 C ASN A 20 ANISOU 282 C ASN A 20 ANISOU 283 O ASN A 20 ANISOU 283 O ASN A 20 ANISOU 284 CB ASN A 20 ANISOU 284 CB ASN A 20 ANISOU 285 CG ASN A 20 ANISOU 285 CG ASN A 20 ANISOU 286 OD1 ASN A 20 ANISOU 286 OD1 ASN A 20 ANISOU 287 ND2 ASN A 20 ATOM 288 H ASN A 20 ANISOU 287 ND2 ASN A 20 ATOM 289 HA ASN A 20 ATOM 289 HA ASN A 20 ATOM 290 HB2 ASN A 20 ATOM 291 HB3 ASN A 20 ATOM 292 HD21 ASN A 20 ATOM 294 N GLY A 21 ANISOU 295 CA GLY A 21 ANISOU 296 C GLY A 21 ANISOU 297 O GLY A 21			
ATOM 282 C ASN A 20 ANISOU 282 C ASN A 20 ATOM 283 O ASN A 20 ANISOU 283 O ASN A 20 ANISOU 284 CB ASN A 20 ANISOU 284 CB ASN A 20 ANISOU 285 CG ASN A 20 ANISOU 285 CG ASN A 20 ANISOU 286 OD1 ASN A 20 ANISOU 287 ND2 ASN A 20 ATOM 288 H ASN A 20 ATOM 289 HA ASN A 20 ATOM 289 HA ASN A 20 ATOM 290 HB2 ASN A 20 ATOM 291 HB3 ASN A 20 ATOM 292 HD21 ASN A 20 ATOM 294 N GLY A 21 ANISOU 295 CA GLY A 21 ANISOU 296 C GLY A 21 ANISOU 297 O GLY A 21			
ANISOU 282 C ASN A 20			_
ATOM 283 O ASN A 20			_
ANISOU 283 O ASN A 20			_
ATOM 284 CB ASN A 20			_
ANISOU 284 CB ASN A 20			_
ATOM 285 CG ASN A 20			С
ANISOU 285 CG ASN A 20	ANISOU 284 CB ASN A 20	1966 2178 2183 994 -563 -262	C
ATOM 286 OD1 ASN A 20	ATOM 285 CG ASN A 20	-7.002 -8.802 -25.564 1.00 15.15	С
ANISOU 286 OD1 ASN A 20	ANISOU 285 CG ASN A 20	1909 1815 2031 945 -604 -236	C
ATOM 287 ND2 ASN A 20	ATOM 286 OD1 ASN A 20	-6.144 -7.936 -25.396 1.00 14.89	0
ANISOU 287 ND2 ASN A 20	ANISOU 286 OD1 ASN A 20	1951 1679 2026 946 -637 -264	0
ANISOU 287 ND2 ASN A 20	ATOM 287 ND2 ASN A 20	-7.094 -9.505 -26.679 1.00 15.36	N
ATOM 288 H ASN A 20 -9.449 -9.132 -22.502 1.00 19.98 H ATOM 289 HA ASN A 20 -6.811 -8.993 -22.856 1.00 21.01 H ATOM 290 HB2 ASN A 20 -8.126 -10.087 -24.453 1.00 19.98 H ATOM 291 HB3 ASN A 20 -8.875 -8.722 -24.769 1.00 19.98 H ATOM 292 HD21 ASN A 20 -6.537 -9.370 -27.320 1.00 18.43 H ATOM 293 HD22 ASN A 20 -7.711 -10.098 -26.764 1.00 18.43 H ATOM 294 N GLY A 21 -6.481 -6.584 -22.416 1.00 18.63 N ANISOU 294 N GLY A 21 2377 2298 2401 1110 -687 -452 N ATOM 295 CA GLY A 21 -6.246 -5.162 -22.277 1.00 20.36 C ANISOU 295 CA GLY A 21 2718 2388 2630 1164 -811 -537 C ATOM 296 C GLY A 21 3056 2412 2965 1084 -876 -496 C ANISOU 297 O GLY A 21 -5.188 -5.271 -24.441 1.00 19.14 O ANISOU 297 O GLY A 21 2660 1992 2620 1008 -818 -404	ANISOU 287 ND2 ASN A 20		N
ATOM 289 HA ASN A 20	ATOM 288 H ASN A 20		Н
ATOM 290 HB2 ASN A 20 -8.126 -10.087 -24.453 1.00 19.98 H ATOM 291 HB3 ASN A 20 -8.875 -8.722 -24.769 1.00 19.98 H ATOM 292 HD21 ASN A 20 -6.537 -9.370 -27.320 1.00 18.43 H ATOM 293 HD22 ASN A 20 -7.711 -10.098 -26.764 1.00 18.43 H ATOM 294 N GLY A 21 -6.481 -6.584 -22.416 1.00 18.63 N ANISOU 294 N GLY A 21 2377 2298 2401 1110 -687 -452 N ATOM 295 CA GLY A 21 -6.246 -5.162 -22.277 1.00 20.36 C ANISOU 295 CA GLY A 21 2718 2388 2630 1164 -811 -537 C ATOM 296 C GLY A 21 -5.434 -4.606 -23.433 1.00 22.19 C ANISOU 296 C GLY A 21 3056 2412 2965 1084 -876 -496 C ATOM 297 O GLY A 21 -5.188 -5.271 -24.441 1.00 19.14 O ANISOU 297 O GLY A 21 2660 1992 2620 1008 -818 -404		-6.811 -8.993 -22.856 1.00 21.01	Н
ATOM 291 HB3 ASN A 20			
ATOM 292 HD21 ASN A 20			
ATOM 293 HD22 ASN A 20 -7.711 -10.098 -26.764 1.00 18.43 H ATOM 294 N GLY A 21 -6.481 -6.584 -22.416 1.00 18.63 N ANISOU 294 N GLY A 21 2377 2298 2401 1110 -687 -452 N ATOM 295 CA GLY A 21 -6.246 -5.162 -22.277 1.00 20.36 C ANISOU 295 CA GLY A 21 2718 2388 2630 1164 -811 -537 C ATOM 296 C GLY A 21 -5.434 -4.606 -23.433 1.00 22.19 C ANISOU 296 C GLY A 21 3056 2412 2965 1084 -876 -496 C ATOM 297 O GLY A 21 -5.188 -5.271 -24.441 1.00 19.14 O ANISOU 297 O GLY A 21 2660 1992 2620 1008 -818 -404 O			
ATOM 294 N GLY A 21 -6.481 -6.584 -22.416 1.00 18.63 N ANISOU 294 N GLY A 21 2377 2298 2401 1110 -687 -452 N -6.246 -5.162 -22.277 1.00 20.36 C ANISOU 295 CA GLY A 21 2718 2388 2630 1164 -811 -537 C ATOM 296 C GLY A 21 3056 2412 2965 1084 -876 -496 C ATOM 297 O GLY A 21 3056 2412 2965 1084 -876 -496 C ANISOU 297 O GLY A 21 2660 1992 2620 1008 -818 -404 O			
ANISOU 294 N GLY A 21 2377 2298 2401 1110 -687 -452 N ATOM 295 CA GLY A 21 -6.246 -5.162 -22.277 1.00 20.36 C ANISOU 295 CA GLY A 21 2718 2388 2630 1164 -811 -537 C ATOM 296 C GLY A 21 -5.434 -4.606 -23.433 1.00 22.19 C ANISOU 296 C GLY A 21 3056 2412 2965 1084 -876 -496 C ATOM 297 O GLY A 21 -5.188 -5.271 -24.441 1.00 19.14 O ANISOU 297 O GLY A 21 2660 1992 2620 1008 -818 -404 O			
ATOM 295 CA GLY A 21 -6.246 -5.162 -22.277 1.00 20.36 C ANISOU 295 CA GLY A 21 2718 2388 2630 1164 -811 -537 C ATOM 296 C GLY A 21 -5.434 -4.606 -23.433 1.00 22.19 C ANISOU 296 C GLY A 21 3056 2412 2965 1084 -876 -496 C ATOM 297 O GLY A 21 -5.188 -5.271 -24.441 1.00 19.14 O ANISOU 297 O GLY A 21 2660 1992 2620 1008 -818 -404 O			
ANISOU 295 CA GLY A 21			
ATOM 296 C GLY A 21 -5.434 -4.606 -23.433 1.00 22.19 C ANISOU 296 C GLY A 21 3056 2412 2965 1084 -876 -496 C ATOM 297 O GLY A 21 -5.188 -5.271 -24.441 1.00 19.14 O ANISOU 297 O GLY A 21 2660 1992 2620 1008 -818 -404 O			
ANISOU 296 C GLY A 21 3056 2412 2965 1084 -876 -496 C ATOM 297 O GLY A 21 -5.188 -5.271 -24.441 1.00 19.14 O ANISOU 297 O GLY A 21 2660 1992 2620 1008 -818 -404 O			
ATOM 297 O GLY A 21 -5.188 -5.271 -24.441 1.00 19.14 O ANISOU 297 O GLY A 21 2660 1992 2620 1008 -818 -404 O			
ANISOU 297 O GLY A 21 2660 1992 2620 1008 -818 -404 O			_
			_
AIUWI 290 N GLIA 21 -3.903 -7.071-22.000 1.00 22.33 H			_
	AIUWI 290 N GLTA 21	-3.803 -7.071 -22.000 1.00 22.33	п

ATOM 299 HA2 GLY A 21	-7.096 -4.694 -22.244 1.00 24.43	Н
ATOM 300 HA3 GLY A 21	-5.766 -4.991 -21.452 1.00 24.43	H
ATOM 301 N ASER A 22	-5.010 -3.356 -23.269 0.52 23.49	Ν
ANISOU 301 N ASER A 22	3344 2416 3167 1101 -1000 -559	. N
ATOM 302 N BSER A 22	-5.006 -3.358 -23.271 0.28 23.58	N
ANISOU 302 N BSER A 22	3354 2426 3178 1101 -1000 -559	Ν
ATOM 303 N CSER A 22	-5.003 -3.359 -23.265 0.20 23.60	N
ANISOU 303 N CSER A 22	3357 2430 3181 1101 -1000 -559	N
ATOM 304 CA ASER A 22	-4.229 -2.688 -24.301 0.52 23.36	c''
ANISOU 304 CA ASER A 22	3455 2162 3259 1002 -1052 -501	C
ATOM 305 CA BSER A 22	-4.245 -2.692 -24.319 0.28 23.37	С
ANISOU 305 CA BSER A 22	3456 2163 3258 1002 -1051 -499	C
ATOM 306 CA CSER A 22	-4.231 -2.681 -24.297 0.20 23.39	С
ANISOU 306 CA CSER A 22	3459 2165 3262 1002 -1053 -501	С
ATOM 307 C ASER A 22	-2.814 -3.250 -24.357 0.52 22.91	С
ANISOU 307 C ASER A 22	3331 2051 3323 856 -1001 -447	C
ATOM 308 C BSER A 22	-2.812 -3.212 -24.361 0.28 22.97	С
ANISOU 308 C BSER A 22	3343 2053 3333 856 -1004 -448	C
ATOM 309 C CSER A 22	-2.808 -3.225 -24.355 0.20 24.96	C
ANISOU 309 C CSER A 22	3593 2307 3585 856 -1004 -448	С
ATOM 310 O ASER A 22	-2.190 -3.517 -23.327 0.52 24.39	0
ANISOU 310 O ASER A 22	3424 2307 3535 853 -1025 -508	o
		_
ATOM 311 O BSER A 22	-2.174 -3.412 -23.324 0.28 24.40	0
ANISOU 311 O BSER A 22	3436 2293 3541 853 -1036 -513	0
ATOM 312 O CSER A 22	-2.170 -3.454 -23.324 0.20 24.32	0
ANISOU 312 O CSER A 22	3421 2288 3530 852 -1032 -511	0
ATOM 313 CB ASER A 22	-4.181 -1.182 -24.037 0.52 24.88	C
ANISOU 313 CB ASER A 22	3803 2186 3464 1026 -1199 -573	C
ATOM 314 CB BSER A 22	-4.244 -1.177 -24.097 0.28 24.87	c
ANISOU 314 CB BSER A 22	3804 2186 3458 1029 -1196 -570	C
ATOM 315 CB CSER A 22	-4.207 -1.175 -24.028 0.20 24.88	С
ANISOU 315 CB CSER A 22	3804 2189 3462 1030 -1200 -575	С
ATOM 316 OG ASER A 22	-5.483 -0.629 -24.055 0.52 26.61	0
ANISOU 316 OG ASER A 22	4071 2478 3563 1156 -1231 -617	0
ATOM 317 OG BSER A 22	-3.546 -0.833 -22.914 0.28 26.81	0
ANISOU 317 OG BSER A 22	4042 2402 3744 1041 -1295 -672	_
ATOM 318 OG CSER A 22	-3.444 -0.488 -25.003 0.20 27.03	0
ANISOU 318 OG CSER A 22	4213 2216 3840 890 -1225 -493	0
ATOM 319 H ASER A 22	-5.162 -2.875 -22.572 0.52 28.19	Н
ATOM 320 H BSER A 22	-5.142 -2.879 -22.570 0.28 28.29	Н
ATOM 321 H CSER A 22	-5.144 -2.885 -22.561 0.20 28.32	Н
ATOM 322 HA ASER A 22	-4.648 -2.833 -25.163 0.52 28.03	Н
ATOM 323 HA BSER A 22	-4.658 -2.872 -25.177 0.28 28.04	H
	-4.649 -2.829 -25.160 0.20 28.07	H
ATOM 325 HB2ASER A 22	-3.782 -1.026 -23.167 0.52 29.85	Н
ATOM 326 HB2BSER A 22	-3.813 -0.749 -24.852 0.28 29.84	Н
ATOM 327 HB2CSER A 22	-5.117 -0.838 -24.046 0.20 29.86	Н
ATOM 328 HB3ASER A 22	-3.648 -0.758 -24.728 0.52 29.85	Н
ATOM 329 HB3BSER A 22	-5.161 -0.870 -24.022 0.28 29.84	Н
ATOM 330 HB3CSER A 22	-3.815 -1.018 -23.154 0.20 29.86	H
ATOM 331 HG ASER A 22	-5.840 -0.758 -24.804 0.52 31.94	Η̈́
ATOM 332 HG BSER A 22	-3.910 -1.196 -22.250 0.28 32.18	H
ATOM 333 HG CSER A 22	-3.443 0.336 -24.838 0.20 32.43	Н

ATOM 334 N GLY A 23 -2.310 -3.429 -25.572 1.00 23.03 ANISOU 334 N GLY A 23 3380 1990 3382 710 -902 -322 ATOM 335 CA GLY A 23 -0.937 -3.881 -25.739 1.00 21.39 ANISOU 335 CA GLY A 23 3072 1780 3275 535 -803 -252 -0.683 -5.210 -25.056 1.00 19.28 ATOM 336 C GLY A 23 ANISOU 336 C GLY A 23 C 2629 1716 2980 564 -726 -266 **ATOM** 337 O GLY A 23 -1.414 -6.189 -25.247 1.00 17.67 0 ANISOU 337 O GLY A 23 2394 1640 2680 633 -651 -240 0 ATOM 338 H GLY A 23 -2.744 -3.311 -26.305 1.00 27.64 Н ATOM 339 HA2 GLY A 23 -0.740 -3.978 -26.684 1.00 25.67 ATOM 340 HA3 GLY A 23 -0.331 -3.222 -25.365 1.00 25.67 Н ATOM 341 N GLY A 24 0.371 -5.254 -24.249 1.00 19.61 ANISOU 341 N GLY A 24 2561 1779 3112 508 -760 -306 342 CA GLY A 24 0.723 -6.450 -23.513 1.00 18.93 ATOM ANISOU 342 CA GLY A 24 2331 1866 2995 552 -710 -319 ATOM 343 C GLY A 24 0.052 -6.577 -22.165 1.00 19.75 ANISOU 343 C GLY A 24 2431 2076 2999 715 -805 -429 ATOM 344 O GLY A 24 0.434 -7.445 -21.371 1.00 19.44 C 0 ANISOU 344 O GLY A 24 2300 2160 2926 760 -789 -444 0 ATOM 345 H GLY A 24 0.903 -4.592 -24.112 1.00 23.54 Н ATOM 346 HA2 GLY A 24 ATOM 347 HA3 GLY A 24 0.484 -7.227 -24.042 1.00 22.71 1.683 -6.464 -23.373 1.00 22.71 Н Н ATOM 348 N ASN A 25 -0.937 -5.738 -21.877 1.00 20.20 Ν ANISOU 348 N ASN A 25 2595 2090 2991 825 -897 -502 Ν ATOM 349 CA ASN A 25 -1.596 -5.741 -20.579 1.00 19.87 ANISOU 349 CA ASN A 25 2560 2157 2833 1005 -967 -608 ATOM 350 C ASN A 25 -2.820 -6.650 -20.588 1.00 18.16 ANISOU 350 C ASN A 25 2309 2118 2474 1046 -815 -547 C ATOM 351 O ASN A 25 -3.539 -6.750 -21.588 1.00 15.96 0 2042 1826 2195 1019 -757 -483 ANISOU 351 O ASN A 25 0 ATOM 352 CB ASN A 25 -2.014 -4.325 -20.180 1.00 22.90 3610 3139 3373 1301 -1058 -809 O ANISOU 354 OD1 ASN A 25 ATOM 355 ND2 ASN A 25 -2.089 -4.483 -17.770 1.00 24.53 N 3307 2827 3187 1275 -1194 -888 N ANISOU 355 ND2 ASN A 25 ATOM 356 H ASN A 25 -1.248 -5.151 -22.424 1.00 24.24 H H ATOM 357 HA ASN A 25 -0.978 -6.074 -19.910 1.00 23.84 ATOM 358 HB2 ASN A 25 -1.219 -3.780 -20.067 1.00 27.47 -2.485 -4.476 -17.007 1.00 29.44 -1.239 -4.609 -17.812 4.00 29. Н ATOM 359 HB3 ASN A 25 -2.578 -3.952 -20.875 1.00 27.47 ATOM 360 HD21 ASN A 25 Н ATOM 361 HD22 ASN A 25 ATOM 362 N TYR A 26 -3.044 -7.329 -19.468 1.00 17.47 2183 2182 2273 1104 -762 -563 ANISOU 362 N TYR A 26 N ATOM 363 CA TYR A 26 -4.258 -8.109 -19.298 1.00 17.37 ANISOU 363 CA TYR A 26 2129 2317 2154 1137 -635 -505 ATOM 364 C TYR A 26 -4.569 -8.187 -17.815 1.00 17.95 ANISOU 364 C TYR A 26 2219 2513 2087 1258 -629 -562 C ATOM 365 O TYR A 26 -3.736 -7.864 -16.969 1.00 19.45 ANISOU 365 O TYR A 26 2460 2680 2250 1309 -723 -643 0 0 366 CB TYR A 26 -4.129 -9.516 -19.903 1.00 16.14 ATOM

ANISOU 366 CB TYR A 26 1896 2206 2029 1049 -521 -387 C 367 CG TYR A 26 -3.230 -10.468 -19.130 1.00 16.74 ATOM 1944 2336 2078 1047 -491 -364 ANISOU 367 CG TYR A 26 ATOM 368 CD1 TYR A 26 -3.753 -11.333 -18.179 1.00 17.09 ANISOU 368 CD1 TYR A 26 1975 2509 2009 1110 -416 -331 -1.862 -10.503 -19.360 1.00 16.46 **ATOM** 369 CD2 TYR A 26 ANISOU 369 CD2 TYR A 26 1892 2227 2136 997 -541 -370 ATOM 370 CE1 TYR A 26 -2.940 -12.205 -17.483 1.00 17.09 ANISOU 370 CE1 TYR A 26 1979 2547 1969 1129 -403 -305 C ATOM 371 CE2 TYR A 26 -1.038 -11.379 -18.674 1.00 16.57 ANISOU 371 CE2 TYR A 26 1879 2293 2124 1009 -527 -351 -1.582 -12.224 -17.735 1.00 16.34 **ATOM 372 CZ TYR A 26** ANISOU 372 CZ TYR A 26 C 1871 2373 1963 1078 -465 -320 373 OH TYR A 26 -0.762 -13.075 -17.049 1.00 17.13 **ATOM** ANISOU 373 OH TYR A 26 1974 2511 2025 1110 -467 -300 0 ATOM 374 H TYR A 26 -2.510 -7.352 -18.795 1.00 20.96 Н ATOM 375 HA TYR A 26 -4.993 -7.656 -19.739 1.00 20.84 Н -5.012 -9.916 -19.944 1.00 19.36 376 HB2 TYR A 26 **ATOM** Н **ATOM 377 HB3 TYR A 26** -3.767 -9.435 -20.799 1.00 19.36 Н ATOM 378 HD1 TYR A 26 -4.667 -11.326 -18.009 1.00 20.51 Н ATOM 379 HD2 TYR A 26 -1.493 -9.936 -19.998 1.00 19.75 ATOM 380 HE1 TYR A 26 -3.305 -12.778 -16.848 1.00 20.51 Н Н ATOM 381 HE2 TYR A 26 -0.123 -11.388 -18.838 1.00 19.88 Н ATOM 382 HH TYR A 26 0.032 -12.978 -17.306 1.00 20.56 Н ATOM 383 N SER A 27 -5.788 -8.626 -17.513 1.00 17.29 N ANISOU 383 N SER A 27 2091 2566 1915 1316 -527 -520 Ν **ATOM 384 CA SER A 27** -6.208 -8.845 -16.140 1.00 18.67 C ANISOU 384 CA SER A 27 2278 2885 1930 1455 -485 -544 C C 385 C SER A 27 **ATOM** -7.158 -10.033 -16.094 1.00 19.37 ANISOU 385 C SER A 27 2256 3119 1983 1449 -326 -422 C ATOM 386 O SER A 27 -7.728 -10.439 -17.110 1.00 17.65 0 ANISOU 386 O SER A 27 0 1953 2890 1864 1355 -277 -352 387 CB SER A 27 -6.873 -7.593 -15.554 1.00 20.02 ATOM ANISOU 387 CB SER A 27 2524 3078 2007 1602 -557 -654 C ATOM 388 OG SER A 27 -7.945 -7.147 -16.366 1.00 21.58 0 ANISOU 388 OG SER A 27 2671 3274 2254 1592 -531 -636 0 -6.395 -8.806 -18.095 1.00 20.75 ATOM 389 H SER A 27 Н **ATOM 390 HA SER A 27** -5.432 -9.057 -15.599 1.00 22.40 Н -7.215 -7.804 -14.671 1.00 24.03 **ATOM 391 HB2 SER A 27** Н -6.212 -6.887 -15.491 1.00 24.03 ATOM 392 HB3 SER A 27 н 393 HG SER A 27 **ATOM** -8.295 -6.462 -16.028 1.00 25.90 Н ATOM 394 N VAL A 28 -7.309 -10.594 -14.895 1.00 20.93 Ν ANISOU 394 N VAL A 28 Ν 2461 3455 2036 1561 -254 -396 395 CA VAL A 28 -8.117 -11.795 -14.687 1.00 21.29 ATOM ANISOU 395 CA VAL A 28 2399 3646 2045 1563 -87 -261 ATOM 396 C VAL A 28 -8.779 -11.703 -13.320 1.00 23.30 ANISOU 396 C VAL A 28 2672 4073 2110 1742 397 O VAL A 28 -8.106 -11.460 -12.315 1.00 23.03 **ATOM** ANISOU 397 O VAL A 28 2767 4048 1935 1867 -64 -314 ATOM 398 CB VAL A 28 -7.287 -13.095 -14.761 1.00 21.98 ANISOU 398 CB VAL A 28 2491 3709 2153 1495 -45 -167 ATOM 399 CG1 VAL A 28 -8.204 -14.284 -15.036 1.00 22.79 ANISOU 399 CG1 VAL A 28 2457 3917 2283 1444 120 -16

ATOM 400 CG2 VAL A 28 -6.177 -13.001 -15.793 1.00 21.25	С
ANISOU 400 CG2 VAL A 28 2433 3435 2204 1360 -157 -201	C
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	Η.
ATOM 402 HA VAL A 28 -8.813 -11.836 -15.363 1.00 25.55	Н
ATOM 403 HB VAL A 28 -6.870 -13.243 -13.897 1.00 26.38	Н
ATOM 404 HG11 VAL A 28 -7.669 -15.092 -15.080 1.00 27.34	Н
ATOM 405 HG12 VAL A 28 -8.853 -14.354 -14.319 1.00 27.34	Н
ATOM 406 HG13 VAL A 28 -8.659 -14.142 -15.882 1.00 27.34	Ĥ
ATOM 407 HG21 VAL A 28 -5.684 -13.837 -15.804 1.00 25.49	H
ATOM 408 HG22 VAL A 28 -6.570 -12.837 -16.665 1.00 25.49	Н
ATOM 409 HG23 VAL A 28 -5.585 -12.271 -15.554 1.00 25.49	Н
ATOM 410 N ASN A 29 -10.094 -11.904 -13.293 1.00 25.09	N
ANISOU 410 N ASN A 29 2764 4436 2334 1756 133 -181	N
ATOM 411 CA ASN A 29 -10.872 -12.122 -12.079 1.00 28.41	C
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ATOM 412 C ASN A 29 -11.451 -13.525 -12.174 1.00 28.70	C
ANISOU 412 C ASN A 29 3051 5184 2670 1780 480 64	С
ATOM 413 O ASN A 29 -12.217 -13.813 -13.099 1.00 29.62	0
ANISOU 413 O ASN A 29 2995 5317 2944 1646 523 115	0
ATOM 414 CB ASN A 29 -12.003 -11.095 -11.958 1.00 30.39	C
ANISOU 414 CB ASN A 29 3350 5373 2826 1993 285 -180	C
ATOM 415 CG ASN A 29 -11.810 -10.117 -10.809 1.00 31.94	Č
ANISOU 415 CG ASN A 29 3708 5597 2830 2211 210 -284	C
ATOM 416 OD1 ASN A 29 -10.690 -9.787 -10.429 1.00 32.18	0
ANISOU 416 OD1 ASN A 29 3910 5527 2790 2264 66 -369	0
ATOM 417 ND2 ASN A 29 -12.919 -9.631 -10.262 1.00 33.34	Ν
ANISOU 417 ND2 ASN A 29 3824 5913 2931 2345 296 -285	Ν
ATOM 418 H ASN A 29 -10.579 -11.918 -14.003 1.00 30.11	н ``
ATOM 419 HA ASN A 29 -10.300 -12.064 -11.297 1.00 34.10	'Н
ATOM 420 HB2 ASN A 29 -12.051 -10.582 -12.780 1.00 36.47	Н
ATOM 421 HB3 ASN A 29 -12.839 -11.564 -11.812 1.00 36.47	Н
ATOM 422 HD21 ASN A 29 -12.868 -9.074 -9.609 1.00 40.01	Н
ATOM 423 HD22 ASN A 29 -13.688 -9.873 -10.562 1.00 40.01	Н
ATOM 424 N TRP A 30 -11.076 -14.405 -11.251 1.00 28.14	N
ANISOU 424 N TRP A 30 3060 5170 2462 1822 590 165	Ň
ATOM 425 CA TRP A 30 -11.513 -15.791 -11.338 1.00 27.64	Ċ
ANISOU 425 CA TRP A 30 2895 5173 2434 1676 785 358	C
ATOM 426 C TRP A 30 -12.004 -16.276 -9.983 1.00 31.09	С
ANISOU 426 C TRP A 30 3379 5741 2693 1753 966 481	C
ATOM 427 O TRP A 30 -11.631 -15.751 -8.930 1.00 31.64	0
ANISOU 427 O TRP A 30 3607 5830 2585 1946 921 415	0
ATOM 428 CB TRP A 30 -10.400 -16.701 -11.893 1.00 25.44	Č
ANISOU 428 CB TRP A 30 2709 4755 2201 1570 738 404	Č
ATOM 429 CG TRP A 30 -9.289 -17.069 -10.953 1.00 25.21	C
ANISOU 429 CG TRP A 30 2908 4675 1996 1680 700 408	С
ATOM 430 CD1 TRP A 30 -9.216 -18.186 -10.163 1.00 26.67	С
ANISOU 430 CD1 TRP A 30 3202 4882 2048 1660 834 572	C
ATOM 431 CD2 TRP A 30 -8.069 -16.350 -10.741 1.00 24.24	C
ANISOU 431 CD2 TRP A 30 2931 4457 1823 1817 495 244	C
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ATOM 432 NE1 TRP A 30 -8.032 -18.195 -9.464 1.00 26.48	
ANISOU 432 NE1 TRP A 30 3390 4793 1879 1806 714 512	N
ATOM 433 CE2 TRP A 30 -7.312 -17.078 -9.799 1.00 25.15	С
ANISOU 433 CE2 TRP A 30 3228 4558 1769 1896 500 306	C

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ATOM 434 CE3 TRP A 30 -7.547 -15.154 -11.248 1.00 23.25
ANISOU 434 CE3 TRP A 30 2803 4243 1787 1865
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      435 CZ2 TRP A 30
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ATOM
                                                              C
ANISOU 435 CZ2 TRP A 30
                           3347 4455 1673 2031 300 174
      436 CZ3 TRP A 30
                           -6.308 -14.730 -10.805 1.00 22.78
ATOM
                                                              C
ANISOU 436 CZ3 TRP A 30
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                                                  111
      437 CH2 TRP A 30
                           -5.578 -15.478 -9.873 1.00 23.72
ATOM
                                                             C
ANISOU 437 CH2 TRP A 30
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      438 H TRP A 30
                         -10.576 -14.227 -10.575 1.00 33.77
                                                             Н
ATOM
ATOM
       439 HA TRP A 30
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                                                            Н
                                                             Н
ATOM
       440 HB2 TRP A 30
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                                                             Н
ATOM
                         -9.995 -16.254 -12.652 1.00 30.52
                                                             Н
      442 HD1 TRP A 30
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ATOM
ATOM 443 HE1 TRP A 30 -7.785 -18.801 -8.905 1.00 31.78
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      444 HE3 TRP A 30 -8.024 -14.655 -11.870 1.00 27.90 445 HZ2 TRP A 30 -5.575 -17.141 -8.734 1.00 29.92
                                                             Н
ATOM
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ATOM
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ATOM 446 HZ3 TRP A 30
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      447 HH2 TRP A 30
ATOM
                                                             Н
ATOM
      448 N SER A 31
                         -12.869 -17.287 -10.029 1.00 34.31
                                                             Ν
ANISOU 448 N SER A 31
                          3648 6225 3162 1585 1163 664
                                                             Ν
ATOM 449 CA SER A 31
                          -13.516 -17.778 -8.822 1.00 38.78
ANISOU 449 CA SER A 31
                          4233 6908 3592 1618 1362
                                                               C
ATOM 450 C SER A 31
ANISOU 450 C SER A 31
                         -14.100 -19.159 -9.077 1.00 40.89
                                                            C
                                                              C
                          4394 7176 3965 1352 1541 1020
      451 O SER A 31
                          -14.731 -19.382 -10.114 1.00 40.20
ATOM
                                                             0
ANISOU 451 O SER A 31
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ATOM 452 CB SER A 31
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ANISOU 452 CB SER A 31
                         4381 7345 3848 1749 1419 734
                                                             C
ATOM
      453 OG SER A 31
                          -15.380 -17.366 -7.313 1.00 44.85
                                                             0
ANISOU 453 OG SER A 31
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                          4846 7963 4230 1755 1649 882
ATOM 454 H SER A 31 -13.097 -17.702 -10.747 1.00 41.17
                                                             Н
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ATOM 455 HA SER A 31
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                         -14.211 -15.987 -8.066 1.00 49.19
ATOM 456 HB2 SER A 31
                                                             Н
                                                             Н
ATOM 457 HB3 SER A 31
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ATOM 458 HG SER A 31
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ATOM 459 N AASN A 32
ANISOU 459 N AASN A 32
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ATOM 460 N BASN A 32
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                          4872 7471 4146 1330 1667 1169
ANISOU 460 N BASN A 32
                                                              Ν
      461 CA AASN A 32
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                                                              C
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ANISOU 461 CA AASN A 32
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ATOM 462 CA BASN A 32
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                                                                C
ANISOU 462 CA BASN A 32
                           5046 7700 4489 1059 1843 1392
                                                             C
ATOM
      463 C AASN A 32
                          -14.324 -22.042 -9.517 0.50 44.15
                                                               C
ANISOU 463 C AASN A 32
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ATOM 464 C BASN A 32
                          -14.338 -22.074 -9.548 0.50 44.15
                                                             C
                          4829 7400 4547 810 1756 1443
                                                               C
ANISOU 464 C BASN A 32
      465 O AASN A 32
                          -15.290 -22.559 -10.082 0.50 45.59
ATOM
                                                              0
ANISOU 465 O AASN A 32
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ATOM 466 O BASN A 32 -15.249 -22.668 -10.129 0.50 45.54
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ANISOU 466 O BASN A 32  4805 7581 4915 556 1830 1554 ATOM 467 CB AASN A 32 -15.876 -21.401 -7.631 0.50 48.57
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ANISOU 467 CB AASN A 32 5267 8275 4913 1012 2045 1478
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ATOM 468 CB BASN A 32 -16.060 -21.218 -7.922 0.50 48.22
ANISOU 468 CB BASN A 32 5147 8248 4925 995 2025 1451
ATOM 469 CG AASN A 32
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ANISOU 469 CG AASN A 32
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ATOM 470 CG BASN A 32
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ATOM 471 OD1AASN A 32
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ANISOU 471 OD1AASN A 32
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ATOM 472 OD1BASN A 32
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ANISOU 472 OD1BASN A 32
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ATOM 473 ND2AASN A 32
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ANISOU 473 ND2AASN A 32
ATOM 474 ND2BASN A 32
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ANISOU 474 ND2BASN A 32
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                                                             Н
ATOM
ATOM 476 H BASN A 32
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                                                              Н
                                                               Н
ATOM 477 HA AASN A 32
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                            -13.918 -21.965 -7.520 0.50 54.33
-14.195 -21.960 -7.508 0.50 54.43
ATOM 478 HA BASN A 32
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-16.175 -20.810 -7.050 0.50 57.86
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ATOM 480 HB2BASN A 32
ATOM 481 HB3AASN A 32 -16.235 -22.301 -7.670 0.50 58.28
ATOM 482 HB3BASN A 32
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ATOM 483 HD21AASN A 32
                                                               Н
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ATOM 484 HD21BASN A 32
ATOM 485 HD22AASN A 32 -17.559 -19.887 -6.535 0.50 63.08
ATOM 486 HD22BASN A 32 -18.180 -21.876 -9.088 0.50 61.89
ATOM 487 N THR A 33 -13.111 -22.002 -10.059 1.00 41.85
ANISOU 487 N THR A 33
                          4707 6969 4224 878 1586 1359
      488 CA THR A 33
ATOM
                          -12.851 -22.445 -11.419 1.00 40.58
ANISOU 488 CA THR A 33 4504 6642 4271 673 1452 1354
ATOM 489 C THR A 33 -12.540 -23.939 -11.476 1.00 41.49
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ANISOU 489 C THR A 33
                          4797 6551 4416 463 1476 1534
      490 O THR A 33
ATOM
                         -12.577 -24.657 -10.475 1.00 43.11
ANISOU 490 O THR A 33 5142 6763 4477 465 1627 1694 ATOM 491 CB THR A 33 -11.694 -21.649 -12.027 1.00 37.75
ANISOU 491 CB THR A 33 4259 6159 3923 814 1199 1128 ATOM 492 OG1 THR A 33 -10.487 -21.922 -11.300 1.00 36.84
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ANISOU 492 OG1 THR A 33 4413 5957 3628 962 1146 1120
ATOM 493 CG2 THR A 33 -11.990 -20.163 -11.978 1.00 37.74
ANISOU 493 CG2 THR A 33 4124 6318 3896 1015 1155 953
ATOM 494 H THR A 33 -12.416 -21.711 -9.645 1.00 50.21 H
ATOM 495 HA THR A 33
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ATOM 496 HB THR A 33
                          -11.577 -21.908 -12.954 1.00 45.29
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ATOM 497 HG1 THR A 33 -10.307 -22.741 -11.338 1.00 44.21
ATOM 498 HG21 THR A 33 -11.253 -19.665 -12.365 1.00 45.28
ATOM 499 HG22 THR A 33
                          -12.798 -19.970 -12.479 1.00 45.28
ATOM
      500 HG23 THR A 33 -12.115 -19.880 -11.059 1.00 45.28
ATOM 501 N GLY A 34 -12.262 -24.413 -12.689 1.00 40.59
ANISOU 501 N GLY A 34
                         4701 6225 4495 283 1304 1488
ATOM 502 CA GLY A 34 -11.570 -25.669 -12.896 1.00 40.84
ANISOU 502 CA GLY A 34 4978 6002 4537 160 1244 1583 C ATOM 503 C GLY A 34 -10.124 -25.357 -13.209 1.00 38.18 C
ANISOU 503 C GLY A 34 4831 5538 4139 344 1048 1415
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ATOM 504 O GLY A 34 -9.453 -24.723 -12.395 1.00 37.74 ANISOU 504 O GLY A 34 4855 5575 3908 585 1041 1344 0 505 H GLY A 34 -12.472 -24.011 -13.420 1.00 48.71 Н **ATOM** 506 HA2 GLY A 34 **ATOM** -11.616 -26.215 -12.096 1.00 49.01 Н **ATOM** 507 HA3 GLY A 34 -11.964 -26.152 -13.639 1.00 49.01 Н ATOM 508 N SER A 35 -9.642 -25.763 -14.384 1.00 32.39 Ν ANISOU 508 N SER A 35 2854 5348 4105 413 913 **ATOM 509 CA SER A 35** -8.328 -25.377 -14.884 1.00 30.00 C ANISOU 509 CA SER A 35 C 2672 4985 3741 442 815 510 C SER A 35 ATOM -8.462 -24.212 -15.855 1.00 27.13 C ANISOU 510 C SER A 35 2297 4632 3379 489 693 ATOM 511 O SER A 35 -9.429 -24.134 -16.617 1.00 27.52 ANISOU 511 O SER A 35 2233 4689 3534 441 664 384 C 512 CB SER A 35 -7.640 -26.540 -15.600 1.00 30.44 ATOM C ANISOU 512 CB SER A 35 2741 4914 3912 305 811 616 ATOM 513 OG SER A 35 -7.413 -27.616 -14.715 1.00 33.30 0 0 ANISOU 513 OG SER A 35 3140 5244 4270 272 914 746 514 H SER A 35 -10.072 -26.277 -14.922 1.00 38.87 Н **ATOM ATOM** 515 HA SER A 35 -7.769 -25.097 -14.143 1.00 36.00 н -8.208 -26.843 -16.325 1.00 36.53 ATOM 516 HB2 SER A 35 Н 517 HB3 SER A 35 -6.789 -26.235 -15.951 1.00 36.53 Н ATOM 518 HG SER A 35 -7.035 -28.247 -15.121 1.00 39.96 **ATOM** Н ATOM 519 N PHE A 36 -7.481 -23.314 -15.835 1.00 23.34 Ν 1939 4146 2785 585 ANISOU 519 N PHE A 36 615 357 N ATOM 520 CA PHE A 36 -7.489 -22.192 -16.760 1.00 20.87 ANISOU 520 CA PHE A 36 1642 3816 2470 635 495 2 520 CA PHE A 36 233 ATOM 521 C PHE A 36 -6.079 -21.643 -16.893 1.00 19.01 ANISOU 521 C PHE A 36 1543 3525 2156 685 C 418 522 O PHE A 36 -5.261 -21.764 -15.979 1.00 18.38 **ATOM** 0000000 ANISOU 522 O PHE A 36 1546 3456 1983 729 208 450 -8.448 -21.088 -16.302 1.00 21.23 ATOM 523 CB PHE A 36 ANISOU 523 CB PHE A 36 1670 3945 2452 751 484 17 ATOM 524 CG PHE A 36 -7.920 -20.252 -15.168 1.00 21.07 ANISOU 524 CG PHE A 36 1765 3967 2272 886 480 17 ATOM 525 CD1 PHE A 36 -8.217 -20.576 -13.854 1.00 23.11 173 480 143 ANISOU 525 CD1 PHE A 36 2020 4311 2450 936 578 218 526 CD2 PHE A 36 -7.141 -19.133 -15.419 1.00 20.30 ATOM ANISOU 526 CD2 PHE A 36 1783 3818 2111 964 371 36 ATOM 527 CE1 PHE A 36 -7.731 -19.806 -12.809 1.00 24.31 ANISOU 527 CE1 PHE A 36 2277 4509 2450 1069 554 177 ATOM 528 CE2 PHE A 36 -6.654 -18.362 -14.389 1.00 20.94 C ANISOU 528 CE2 PHE A 36 1967 3930 2060 1080 349 -11 -6.950 -18.697 -13.076 1.00 23.23 ATOM 529 CZ PHE A 36 ANISOU 529 CZ PHE A 36 C 2249 4319 2260 1137 434 55 **ATOM** 530 H PHE A 36 -6.806 -23.334 -15.301 1.00 28.01 Н 531 HA PHE A 36 -7.778 -22.500 -17.633 1.00 25.04 Н ATOM -8.622 -20.495 -17.050 1.00 25.48 -9.277 -21.496 -16.007 1.00 25.48 H H H **ATOM** 532 HB2 PHE A 36 533 HB3 PHE A 36 ATOM -8.739 -21.323 -13.671 1.00 27.73 **ATOM** 534 HD1 PHE A 36 535 HD2 PHE A 36 -6.937 -18.905 -16.298 1.00 24.36 ATOM Н 536 HE1 PHE A 36 -7.933 -20.033 -11.930 1.00 29.17 537 HE2 PHE A 36 -6.130 -17.616 -14.573 1.00 25.13 ATOM ATOM Н 538 HZ PHE A 36 -6.625 -18.177 -12.378 1.00 27.88 ATOM Н

ATOM 539 N AVAL A 37 -5.797 -21.055 -18.054 0.73 17.61 Ν ANISOU 539 N AVAL A 37 1418 3251 2023 658 298 N 540 N BVAL A 37 -5.807 -21.046 -18.051 0.27 17.83 Ν ATOM ANISOU 540 N BVAL A 37 1444 3279 2049 659 298 Ν ATOM 541 CA AVAL A 37 -4.533 -20.374 -18.317 0.73 17.26 ANISOU 541 CA AVAL A 37 1521 3107 1929 675 205 28 CCCCCC 542 CA BVAL A 37 -4.527 -20.404 -18.318 0.27 17.28 ATOM ANISOU 542 CA BVAL A 37 1523 3109 1933 673 207 ATOM 543 C AVAL A 37 -4.848 -19.156 -19.183 0.73 16.75 ANISOU 543 C AVAL A 37 1486 3004 1875 729 105 -66 -4.788 -19.222 -19.245 0.27 16.68 ATOM 544 C BVAL A 37 ANISOU 544 C BVAL A 37 1480 2988 1872 719 104 -64 ATOM 545 O AVAL A 37 -5.549 -19.279 -20.194 0.73 17.27 0 1489 3056 2016 687 ANISOU 545 O AVAL A 37 **72** 0 546 O BVAL A 37 -5.380 -19.383 -20.318 0.27 17.07 ATOM 1476 3012 1999 668 ANISOU 546 O BVAL A 37 66 -73 -3.503 -21.284 -19.024 0.73 16.23 ATOM 547 CB AVAL A 37 ANISOU 547 CB AVAL A 37 1447 2861 1860 550 181 64 ATOM 548 CB BVAL A 37 -3.513 -21.395 -18.928 0.27 16.27 ANISOU 548 CB BVAL A 37 1446 2871 1863 547 192 0000000 ATOM 549 CG1AVAL A 37 -2.130 -20.611 -19.042 0.73 15.60 1499 2703 1727 572 109 ANISOU 549 CG1AVAL A 37 ATOM 550 CG1BVAL A 37 -3.255 -22.564 -17.986 0.27 17.35 1565 3042 1986 516 ANISOU 550 CG1BVAL A 37 295 177 551 CG2AVAL A 37 -3.394 -22.672 -18.381 0.73 17.37 **ATOM** 1553 3024 2025 486 ANISOU 551 CG2AVAL A 37 283 172 ATOM 552 CG2BVAL A 37 -3.997 -21.924 -20.266 0.27 16.25 ANISOU 552 CG2BVAL A 37 1392 2809 1975 447 C 154 -6.338 -21.037 -18.723 0.73 21.14 **ATOM** 553 H AVAL A 37 Н 554 H BVAL A 37 Н **ATOM** -6.360 -21.000 -18.709 0.27 21.39 -4.150 -20.067 -17.481 0.73 20.71 Н ATOM 555 HA AVAL A 37 -4.159 -20.064 -17.487 0.27 20.74 556 HA BVAL A 37 Н **ATOM** -3.780 -21.409 -19.945 0.73 19.48 ATOM 557 HB AVAL A 37 Н **ATOM** 558 HB BVAL A 37 -2.670 -20.936 -19.074 0.27 19.52 -1.497 -21.195 -19.488 0.73 18.72 559 HG11AVAL A 37 ATOM 560 HG11BVAL A 37 -2.616 -23.166 -18.398 0.27 20.82 Н **ATOM** -2.197 -19.769 -19.520 0.73 18.72 561 HG12AVAL A 37 **ATOM ATOM** 562 HG12BVAL A 37 -2.899 -22.224 -17.151 0.27 20.82 Н 563 HG13AVAL A 37 H **ATOM** -1.845 -20.451 -18.128 0.73 18.72 Н **ATOM** 564 HG13BVAL A 37 -4.091 -23.029 -17.825 0.27 20.82 **ATOM** 565 HG21AVAL A 37 -4.008 -22.721 -17.632 0.73 20.85 Н -4.858 -21.527 -20.469 0.27 19.50 Н **ATOM** 566 HG21BVAL A 37 567 HG22AVAL A 37 -3.623 -23.345 -19.042 0.73 20.85 Н **ATOM** Н **ATOM** 568 HG22BVAL A 37 -3.352 -21.687 -20.951 0.27 19.50 **ATOM** 569 HG23AVAL A 37 -2.484 -22.807 -18.074 0.73 20.85 Н 570 HG23BVAL A 37 -4.082 -22.889 -20.211 0.27 19.50 Н **ATOM** ATOM 571 N AVAL A 38 -4.337 -17.987 -18.794 0.73 16.90 Ν 1602 3000 1821 826 ANISOU 571 N AVAL A 38 52 -138 N 572 N BVAL A 38 -4.373 -18.024 -18.837 0.27 16.89 Ν **ATOM** ANISOU 572 N BVAL A 38 1596 2999 1823 822 52 -136 Ν ATOM 573 CA AVAL A 38 -4.649 -16.724 -19.463 0.73 16.41 C ANISOU 573 CA AVAL A 38 1583 2889 1763 898 -35 -219 C 574 CA BVAL A 38 -4.606 -16.824 -19.630 0.27 16.29 ATOM

ANISOU 574 CA BVAL A 38 15	567 2863 1760 880 -38 -213	С
	394 -15.861 -19.493 0.73 16.04	C
	78 2723 1693 908 -110 -274	С
	381 -15.927 -19.548 0.27 16.01	C
ANISOU 576 C BVAL A 38 16	72 2717 1694 900 -109 -270	C
ATOM 577 O AVAL A 38 -2.0	635 -15.826 -18.518 0.73 16.01	0
	21 2729 1632 931 -100 -289	Ō
	639 -15.941 -18.561 0.27 16.03	_
		0
	18 2733 1639 921 -95 -281	0
ATOM 579 CB AVAL A 38 -5	.794 -15.972 -18.744 0.73 17.66	C
ANISOU 579 CB AVAL A 38 16	692 3153 1866 1031 -12 -259	С
	.863 -16.049 -19.169 0.27 17.50	C
	660 3115 1873 1010 -25 -255	C
		Č
	5.013 -14.591 -19.358 0.73 17.61	
	766 3066 1859 1104 -106 -338	С
ATOM 582 CG1BVAL A 38 -7	7.053 -16.984 -18.991 0.27 18.08	С
ANISOU 582 CG1BVAL A 38 1	585 3300 1984 965 60 -188	C
	7.087 -16.779 -18.786 0.73 18.14	Č
	605 3314 1972 989 61 -198	C
	5.596 -15.301 -17.881 0.27 17.71	C
ANISOU 584 CG2BVAL A 38 1	762 3169 1796 1109 -18 -301	C
ATOM 585 H AVAL A 38 -3.7	795 -17.899 -18.132 0.73 20.28	Н
ATOM 586 H BVAL A 38 -3.9	953 -17.881 -18.100 0.27 20.27	Н
	.924 -16.901 -20.376 0.73 19.69	H
	.733 -17.077 -20.558 0.27 19.55	H
	.551 -15.848 -17.813 0.73 21.20	Н
ATOM 590 HB BVAL A 38 -6	.095 -15.397 -19.848 0.27 21.00	Н
ATOM 591 HG11AVAL A 38 -	6.735 -14.147 -18.886 0.73 21.13	Н
ATOM 592 HG11BVAL A 38 -	7.821 -16.466 -18.703 0.27 21.69	Н
	5.195 -14.076 -19.274 0.73 21.13	H
	7.244 -17.415 -19.839 0.27 21.69	H
	6.244 -14.696 -20.294 0.73 21.13	Н
	6.833 -17.651 -18.323 0.27 21.69	Н
ATOM 597 HG21AVAL A 38 -	7.783 -16.282 -18.328 0.73 21.76	Н
ATOM 598 HG21BVAL A 38 -	6.401 -14.827 -17.619 0.27 21.25	Н
	7.337 -16.925 -19.711 0.73 21.76	Н
	5.348 -15.937 -17.192 0.27 21.25	H
	6.942 -17.630 -18.344 0.73 21.76	Н
	4.873 -14.671 -18.026 0.27 21.25	_ Н
ATOM 603 N GLY A 39 -3.1	85 -15.132 -20.587 1.00 15.87	N
ANISOU 603 N GLY A 39 172	2 2591 1718 895 -186 -303	N
	094 -14.175 -20.596 1.00 16.51	С
	25 2551 1799 902 -250 -353	C
		_
		C
ANISOU 605 C GLY A 39 191		С
ATOM 606 O GLY A 39 -2.2	53 -14.137 -22.996 1.00 14.16	0
ANISOU 606 O GLY A 39 165	5 2134 1589 821 -305 -300	0
		H
	322 -13.425 -20.026 1.00 19.82	''Н
	296 -14.597 -20.241 1.00 19.82	Н
		N
ANISOU 610 N LYS A 40 199	5 2202 1778 869 -360 -384	N
ATOM 611 CA LYS A 40 -0.3	865 -12.032 -23.179 1.00 15.43	С
		_

ANISOU 611 CA LYS A 40 2038 2027 1798 823 -398 -356 C ATOM 612 C LYS A 40 1.051 -12.552 -23.396 1.00 14.76 C ANISOU 612 C LYS A 40 1977 1881 1751 C 698 -384 -316 ATOM 613 O LYS A 40 1.783 -12.845 -22.444 1.00 13.79 ANISOU 613 O LYS A 40 1841 1781 1618 670 -377 -343 ATOM 614 CB LYS A 40 -0.334 -10.498 -23.100 1.00 15.84 ANISOU 614 CB LYS A 40 2188 1960 1872 904 -458 -416 ATOM 615 CG LYS A 40 -1.691 -9.793 -23.166 1.00 17.79 ANISOU 615 CG LYS A 40 C 2430 2242 2088 1048 -482 -451 C ATOM 616 CD LYS A 40 -2.182 -9.663 -24.593 1.00 18.71 ANISOU 616 CD LYS A 40 2565 2322 2221 1059 -497 -388 C C ATOM 617 CE LYS A 40 -3.520 -8.969 -24.673 1.00 19.58 C ANISOU 617 CE LYS A 40 2662 2481 2296 1184 -520 -418 618 NZ LYS A 40 -3.458 -7.542 -24.266 1.00 20.58 Ν **ATOM** ANISOU 618 NZ LYS A 40 2892 2495 2433 1248 -558 -471 N 619 H LYS A 40 -0.652 -12.229 -21.252 1.00 18.87 Н ATOM **ATOM** 620 HA LYS A 40 -0.906 -12.288 -23.942 1.00 18.52 Н 0.083 -10.245 -22.262 1.00 19.01 **ATOM** 621 HB2 LYS A 40 Н **ATOM** 622 HB3 LYS A 40 Н **ATOM** 623 HG2 LYS A 40 Н -1.607 -8.902 -22.792 1.00 21.35 -1.541 -9.144 -25.104 1.00 22.45 624 HG3 LYS A 40 Н ATOM 625 HD2 LYS A 40 Н **ATOM** -2.277 -10.548 -24.978 1.00 22.45 -3.841 -9.006 -25.587 1.00 23.50 -4.146 -9.421 -24.085 1.00 23.50 -3.175 -7.478 -23.424 1.00 24.70 Н ATOM 626 HD3 LYS A 40 **ATOM** 627 HE2 LYS A 40 Н **ATOM** 628 HE3 LYS A 40 Н 629 HZ1 LYS A 40 **ATOM** -2.896 -7.099 -24.795 1.00 24.70 630 HZ2 LYS A 40 Н **ATOM** 631 HZ3 LYS A 40 -4.266 -7.173 -24.327 1.00 24.70 **ATOM** Н **ATOM** 632 N GLY A 41 1.432 -12.655 -24.665 1.00 14.84 ANISOU 632 N GLY A 41 2019 1824 1796 638 -380 -253 C ATOM 633 CA GLY A 41 2.775 -13.059 -25.008 1.00 14.55 C ANISOU 633 CA GLY A 41 2001 1731 1798 530 -359 -211 **ATOM** 634 C GLY A 41 3.050 -13.017 -26.494 1.00 13.93 C ANISOU 634 C GLY A 41 1966 1587 1739 494 -347 -138 ATOM 635 O GLY A 41 2.623 -12.091 -27.195 1.00 13.72 0 ANISOU 635 O GLY A 41 0 2003 1493 1718 549 -371 -122 636 H GLY A 41 0.926 -12.495 -25.342 1.00 17.81 Н **ATOM ATOM** 637 HA2 GLY A 41 3.408 -12.473 -24.564 1.00 17.47 Н **ATOM** 638 HA3 GLY A 41 2.926 -13.964 -24.695 1.00 17.47 Н ATOM 639 N TRP A 42 3.763 -14.025 -26.983 1.00 13.23 N ANISOU 639 N TRP A 42 1853 1523 1652 417 -308 -89 ATOM 640 CA TRP A 42 4.221 -14.058 -28.364 1.00 13.61 C C ANISOU 640 CA TRP A 42 1947 1523 1703 388 -285 -18 641 C TRP A 42 ATOM 3.719 -15.306 -29.080 1.00 13.15 ANISOU 641 C TRP A 42 1849 1552 1597 385 -271 ATOM 642 O TRP A 42 3.656 -16.401 -28.499 1.00 11.48 0 00000 ANISOU 642 O TRP A 42 1571 1411 1381 352 -256 643 CB TRP A 42 5.753 -13.993 -28.420 1.00 14.07 ATOM ANISOU 643 CB TRP A 42 2017 1515 1814 301 -251 1 ATOM 644 CG TRP A 42 6.301 -12.699 -27.907 1.00 14.90 ANISOU 644 CG TRP A 42 2161 1508 1990 288 -275 -18 ATOM 645 CD1 TRP A 42 6.663 -11.609 -28.645 1.00 15.10 C ANISOU 645 CD1 TRP A 42 2260 1411 2069 279 -266

ATOM 646 CD2 TRP A 42 6.546 -12.355 -26.541 1.00 14.70 ANISOU 646 CD2 TRP A 42 2110 1478 1997 284 -316 -88 ATOM 647 NE1 TRP A 42 7.115 -10.608 -27.827 1.00 17.09 Ν Ν ANISOU 647 NE1 TRP A 42 2528 1563 2403 256 -304 -5 C ATOM 648 CE2 TRP A 42 7.054 -11.038 -26.527 1.00 16.45 ANISOU 648 CE2 TRP A 42 C 2388 1559 2304 264 -342 -100 649 CE3 TRP A 42 6.380 -13.027 -25.328 1.00 15.28 ATOM C ANISOU 649 CE3 TRP A 42 2123 1650 2031 301 -332 -153 ATOM 650 CZ2 TRP A 42 7.403 -10.384 -25.347 1.00 17.09 C 2464 1597 2434 262 -401 -196 ANISOU 650 CZ2 TRP A 42 ATOM 651 CZ3 TRP A 42 6.732 -12.376 -24.156 1.00 16.02 2217 1719 2150 314 -383 -238 C **ANISOU 651 CZ3 TRP A 42** 7.237 -11.069 -24.175 1.00 17.04 ATOM 652 CH2 TRP A 42 2400 1708 2367 294 -425 -270 ANISOU 652 CH2 TRP A 42 653 H TRP A 42 3.998 -14.714 -26.525 1.00 15.88 Н ATOM ATOM 654 HA TRP A 42 3.871 -13.284 -28.831 1.00 16.33 Н ATOM 654 HA TRP A 42
ATOM 655 HB2 TRP A 42
ATOM 656 HB3 TRP A 42
ATOM 657 HD1 TRP A 42
ATOM 658 HE1 TRP A 42
ATOM 659 HE3 TRP A 42
ATOM 660 HZ2 TRP A 42
ATOM 661 HZ3 TRP A 42
ATOM 662 HH2 TRP A 42
ATOM 663 N THR A 43
ANISOU 663 N THR A 43
ATOM 664 CA THR A 43
ATOM 664 CA THR A 43
ATOM 665 HB2 TRP A 42
3.871 -13.284 -28.831 1.00 16.33
6.119 -14.709 -27.877 1.00 16.88
6.040 -14.096 -29.341 1.00 16.88
6.047 -11.553 -29.572 1.00 18.13
7.394 -9.837 -28.086 1.00 20.51
6.647 -13.895 -25.308 1.00 18.33
7.740 -9.517 -25.356 1.00 20.51
6.627 -12.813 -23.342 1.00 19.22
7.461 -10.656 -23.372 1.00 20.45
ATOM 663 N THR A 43
ANISOU 664 CA THR A 43 Н Н Н Н Н Н Ν 38 2.898 -16.230 -31.176 1.00 12.97 C **ATOM 664 CA THR A 43** ANISOU 664 CA THR A 43 1844 1589 1493 431 -285 C 3.968 -17.294 -31.353 1.00 12.64 **ATOM** 665 C THR A 43 ANISOU 665 C THR A 43 1790 1556 1457 357 -238 ATOM 666 O THR A 43 3.675 -18.496 -31.279 1.00 12.76 0 ANISOU 666 O THR A 43 1752 1627 1469 333 -240 29 ATOM 667 CB THR A 43 2.440 -15.699 -32.535 1.00 14.31 ANISOU 667 CB THR A 43 2083 1748 1604 509 -312 68 ATOM 668 OG1 THR A 43 1.437 -14.696 -32.331 1.00 13.31 ,00000 1970 1614 1475 593 -360 46 ANISOU 668 OG1 THR A 43 1.870 -16.833 -33.393 1.00 15.49 ATOM 669 CG2 THR A 43 ANISOU 669 CG2 THR A 43 2202 1980 1704 525 -341 ATOM 670 H THR A 43 3.434 -14.376 -30.773 1.00 16.51 Н ATOM 671 HA THR A 43
ATOM 672 HB THR A 43
ATOM 673 HG1 THR A 43
ATOM 674 HG21 THR A 43
ATOM 675 HG22 THR A 43
ATOM 676 HG23 THR A 43 Н Н Н Н **ATOM** 677 N THR A 44 5.214 -16.875 -31.579 1.00 13.02 ANISOU 677 N THR A 44 1880 1543 1525 320 -193 111 ATOM 678 CA THR A 44

ANISOU 678 CA THR A 44

ANISOU 678 CA THR A 44

ATOM 679 C THR A 44

ANISOU 679 C THR A 44

ATOM 680 O THR A 44

ATOM 680 O THR A 44

ATOM 680 O THR A 44

ANISOU 679 C THR A 44

ANISOU 679 C THR A 44

ANISOU 680 O THR A 44 ANISOU 680 O THR A 44 1729 1336 1521 180 -110 159

ATOM 681 CB THR A 44 7.026 -17.619 -33.095 1.00 16.15 ANISOU 681 CB THR A 44 2319 1930 1886 281 -99 20 -99 203 682 OG1 THR A 44 6.069 -17.784 -34.155 1.00 17.26 ATOM ANISOU 682 OG1 THR A 44 2502 2109 1947 358 -135 195 ATOM 683 CG2 THR A 44 8.145 -18.656 -33.265 1.00 15.77 ANISOU 683 CG2 THR A 44 2244 1910 1838 239 -45 219 684 H THR A 44 5.437 -16.047 -31.643 1.00 15.63 **ATOM** ATOM 685 HA THR A 44
ATOM 686 HB THR A 44
ATOM 687 HG1 THR A 44
ATOM 688 HG21 THR A 44
ATOM 689 HG22 THR A 44
ATOM 690 HG23 THR A 44 Н Н ATOM 691 N GLY A 45 7.390 -18.522 -29.687 1.00 12.12 Ν ANISOU 691 N GLY A 45 1652 1461 1492 178 -124 96 ATOM 692 CA GLY A 45 8.380 -18.460 -28.637 1.00 11.61 C ANISOU 692 CA GLY A 45 1549 1390 1471 C 136 -116 85 693 C GLY A 45 9.795 -18.542 -29.174 1.00 12.39 **ATOM** ANISOU 693 C GLY A 45 1642 1467 1598 93 -69 131 ATOM 694 O GLY A 45 10.061 -18.995 -30.293 1.00 13.10 0 ANISOU 694 O GLY A 45 1755 1564 1657 100 -30 1 ATOM 695 H GLY A 45 6.878 -19.213 -29.658 1.00 14.55 -30 173 696 HA2 GLY A 45 8.283 -17.626 -28.151 1.00 13.93 697 HA3 GLY A 45 8.242 -19.195 -28.019 1.00 13.93 ATOM 696 HA2 GLY A 45 **ATOM** Н ATOM 698 N SER A 46 10.722 -18.100 -28.330 1.00 13.28 ANISOU 698 N SER A 46 1717 1563 1767 53 -77 116 Ν Ν **ATOM 699 CA SER A 46** 12.144 -18.126 -28.609 1.00 15.24 C ANISOU 699 CA SER A 46 1926 1801 2063 5 -36 152 700 C SER A 46 12.880 -18.522 -27.337 1.00 14.44 C **ATOM** ANISOU 700 C SER A 46 1755 1743 1989 -12 -66 104 ATOM 701 O SER A 46 12.536 -18.033 -26.247 1.00 13.72 0 ANISOU 701 O SER A 46 1657 1649 1905 -1 -124 44 ATOM 702 CB SER A 46 12.663 -16.764 -29.089 1.00 16.59 ANISOU 702 CB SER A 46 2114 1882 2306 -40 -20 189 ATOM 703 OG SER A 46 14.077 -16.726 -29.076 1.00 17.16 C 0 ANISOU 703 OG SER A 46 2117 1952 2450 -101 15 213 0 704 H SER A 46 10.538 -17.767 -27.559 1.00 15.94 **ATOM** 705 HA SER A 46
706 HB2 SER A 46
707 HB3 SER A 46
708 HG SER A 46
709 N BBO A 47 Н **ATOM** Н **ATOM** Н **ATOM** Н **ATOM** 709 N PRO A 47 13.901 -19.378 -27.438 1.00 14.59 Ν ATOM 1724 1808 2013 -22 -32 127 ANISOU 709 N PRO A 47 N C **ATOM** ANISOU 710 CA PRO A 47 84 ATOM 711 C PRO A 47 15.722 -18.559 -25.934 1.00 17.17 C 1920 2142 2460 ANISOU 711 C PRO A 47 -88 -99 ANISOU 711 C PRO A 47 1920 2142 2460 -68 -99 57
ATOM 712 O PRO A 47 16.474 -18.699 -24.963 1.00 18.12
ANISOU 712 O PRO A 47 1973 2308 2603 -88 -147 7
ATOM 713 CB PRO A 47 15.487 -20.943 -26.709 1.00 15.64
ANISOU 713 CB PRO A 47 1753 2043 2145 -4 -17 123
ATOM 714 CG PRO A 47 15.601 -20.814 -28.199 1.00 15.69
ANISOU 714 CG PRO A 47 1790 2020 2152 -18 53 185 0 C C

ATOM 715 CD PRO A 47 14.343 -20.112 -28.642 1.00 15.43 ANISOU 715 CD PRO A 47 1837 1933 2093 -13 38 180 ATOM 716 HA PRO A 47 14.195 -19.865 -25.501 1.00 18.20 C 186 14.195 -19.865 -25.501 1.00 18.20 Н 716 HA PRO A 47
717 HB2 PRO A 47
718 HB3 PRO A 47
719 HG2 PRO A 47
720 HG3 PRO A 47
721 HD2 PRO A 47
722 HD3 PRO A 47
733 -19.865 -25.501 1.00 18.20
16.364 -20.969 -26.296 1.00 18.77
14.967 -21.726 -26.469 1.00 18.83
15.659 -21.696 -28.599 1.00 18.83
14.539 -19.492 -29.361 1.00 18.52
13.671 -20.760 -28.906 1.00 18.52 Н **ATOM ATOM** ATOM **ATOM** Н **ATOM** 722 HD3 PRO A 47 13.671 -20.760 -28.906 1.00 18.52 **ATOM** ATOM 723 N PHE A 48 15.735 -17.468 -26.699 1.00 17.61 Ν ANISOU 723 N PHE A 48 2001 2112 2579 -138 -76 Ν **ATOM 724 CA PHE A 48** 16.632 -16.348 -26.452 1.00 19.26 C ANISOU 724 CA PHE A 48 2153 2254 2910 -217 -102 725 C PHE A 48 15.889 -15.103 -26.012 1.00 18.95 **ATOM** ANISOU 725 C PHE A 48 2174 2118 2909 -225 -166 ATOM 726 O PHE A 48 16.511 -14.048 -25.849 1.00 19.51 0 2213 2100 3099 -298 -195 -13 ANISOU 726 O PHE A 48 17.445 -16.046 -27.713 1.00 22.45 CCCC 727 CB PHE A 48 **ATOM** ANISOU 727 CB PHE A 48 2530 2619 3381 -278 -6 166 ATOM 728 CG PHE A 48 17.996 -17.269 -28.358 1.00 24.37 ANISOU 728 CG PHE A 48 2737 2957 3565 -244 69 222 ATOM 729 CD1 PHE A 48 19.010 -17.982 -27.752 1.00 25.74 69 222 ANISOU 729 CD1 PHE A 48 2807 3214 3760 -243 54 191 ATOM 730 CD2 PHE A 48 17.481 -17.725 -29.559 1.00 25.76 ANISOU 730 CD2 PHE A 48 2987 3143 3656 -197 144 29 296 731 CE1 PHE A 48 19.512 -19.126 -28.337 1.00 26.42 ATOM ANISOU 731 CE1 PHE A 48 2866 3381 3790 -195 121 237 ATOM 732 CE2 PHE A 48 17.980 -18.872 -30.145 1.00 26.51 3059 3321 3694 -152 206 331 ANISOU 732 CE2 PHE A 48 ATOM 733 CZ PHE A 48 18.994 -19.569 -29.530 1.00 26.37 ANISOU 733 CZ PHE A 48 2941 3376 3704 -151 197 303 C 734 H PHE A 48 15.221 -17.354 -27.379 1.00 21.14 Н ATOM H H 734 H PHE A 48 15.221 -17.354 -27.379 1.00 21.14 H 735 HA PHE A 48 17.252 -16.591 -25.747 1.00 23.11 H 736 HB2 PHE A 48 16.874 -15.600 -28.357 1.00 26.94 H 737 HB3 PHE A 48 18.190 -15.471 -27.477 1.00 26.94 H 738 HD1 PHE A 48 19.360 -17.687 -26.942 1.00 30.89 H 739 HD2 PHE A 48 16.793 -17.257 -29.973 1.00 30.91 H 740 HE1 PHE A 48 20.199 -19.598 -27.923 1.00 31.70 H 741 HE2 PHE A 48 17.633 -19.170 -30.955 1.00 31.82 H 742 HZ PHE A 48 19.335 -20.337 -29.927 1.00 31.65 H 743 N ARG A 49 21.08 1980 2673 -153 -188 -9 N ATOM **ATOM** ATOM 737 HB3 PHE A 48 ATOM 738 HD1 PHE A 48 **ATOM ATOM ATOM ATOM ATOM** ANISOU 743 N ARG A 49 2108 1980 2673 -153 -188 -9 Ν 13.806 -14.012 -25.481 1.00 16.69 ATOM 744 CA ARG A 49 C ANISOU 744 CA ARG A 49 2031 1751 2559 -139 -244 -60 CC 745 C ARG A 49 13.929 -13.704 -23.998 1.00 15.92 ATOM ANISOU 745 C ARG A 49 ATOM 746 O ARG A 49 1903 1673 2471 -118 -344 -183 746 O ARG A 49 13.866 -14.600 -23.151 1.00 15.25 U 746 O ARG A 49 1788 1701 2305 -65 -367 -221 747 CB ARG A 49 12.341 -14.209 -25.853 1.00 15.84 0 **ANISOU 746 O ARG A 49** C ATOM ANISOU 747 CB ARG A 49 2005 1662 2353 -58 -231 -39 ATOM 748 CG ARG A 49 11.432 -13.100 -25.345 1.00 16.84 ANISOU 748 CG ARG A 49 2193 1718 2488 -13 -293 -104 ATOM 749 CD ARG A 49 10.033 -13.165 -25.946 1.00 17.82

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ANISOU 749 CD ARG A 49
                            2382 1857 2532 64 -275
                                                                C
                                                          -72
ATOM
        750 NE ARG A 49
                             10.002 -12.754 -27.357 1.00 20.07
                                                                 Ν
ANISOU 750 NE ARG A 49
                             2721 2070 2835
                                                49 -222
                                                          24
                                                                N
      751 CZ ARG A 49 9.642 -13.530 -28.380 1.00 20.30
U 751 CZ ARG A 49 2764 2156 2794 74 -171 93
                                                                 C
ATOM
ANISOU 751 CZ ARG A 49
                            2764 2156 2794
                                               74 -171
                                                          93
       752 NH1 ARG A 49
                                                                Ν
ATOM
                           9.255 -14.781 -28.189 1.00 19.40
ANISOU 752 NH1 ARG A 49
                            2611 2153 2608
                                                99 -165
                                                           76
                                                                Ν
ATOM 753 NH2 ARG A 49
                             9.658 -13.038 -29.613 1.00 21.88
                                                                Ν
                            3022 2294 2995
                                                                 Ν
ANISOU 753 NH2 ARG A 49
                                                78 -127
                                                          178
ATOM
       754 H ARG A 49
                            14.119 -15.913 -25.889 1.00 21.35
                                                                Н
ATOM
       755 HA ARG A 49
                            14.145 -13.251 -25.978 1.00 20.03
                                                                Н
                            12.263 -14.238 -26.820 1.00 19.01
ATOM
       756 HB2 ARG A 49
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       757 HB3 ARG A 49
ATOM
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       758 HG2 ARG A 49
ATOM
                           759 HG3 ARG A 49
                                                                  Н
ATOM
       760 HD2 ARG A 49
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ATOM
       761 HD3 ARG A 49
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ATOM
                                                                 Н
                            9.240 -15.110 -27.395 1.00 23.28
ATOM
       763 HH11 ARG A 49
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ATOM
       764 HH12 ARG A 49
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ATOM
       765 HH21 ARG A 49
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                                                                  Н
       766 HH22 ARG A 49
                              9.423 -13.533 -30.277 1.00 26.25
ATOM
                                                                  Н
       767 N THR A 50
ATOM
                            14.103 -12.425 -23.686 1.00 16.88
                                                                Ν
ANISOU 767 N THR A 50
                            2042 1681 2690 -154 -404 -246
                                                                Ν
       768 CA THR A 50
                            13.969 -11.933 -22.323 1.00 18.36
ATOM
ANISOU 768 CA THR A 50
                            2231 1876 2871 -109 -513 -384
ATOM 769 C THR A 50
                            12.544 -11.423 -22.168 1.00 17.89
ANISOU 769 C THR A 50
                            2269 1790 2741
                                             -16 -530 -413
      770 O THR A 50
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ANISOU 770 O THR A 50
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ATOM 771 CB THR A 50
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                                                                 C
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ANISOU 771 CB THR A 50
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ATOM
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ANISOU 772 OG1 THR A 50
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ATOM 773 CG2 THR A 50
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ANISOU 773 CG2 THR A 50
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       774 H THR A 50
                                                                Н
ATOM
ATOM
       775 HA THR A 50
                          14.105 -12.664 -21.700 1.00 22.04
                                                                Н
                          14.895 -10.119 -22.659 1.00 25.61
ATOM
       776 HB THR A 50
                                                                Н
      777 HG1 THR A 50 16.880 -10.801 -21.945 1.00 27.33 778 HG21 THR A 50 15.439 -9.588 -20.438 1.00 27.02
ATOM
                                                                Н
ATOM
                                                                 Н
       779 HG22 THR A 50
                                                                 Н
ATOM
                             13.895 -9.901 -20.540 1.00 27.02
ATOM
       780 HG23 THR A 50
                             14.883 -10.987 -19.960 1.00 27.02
                                                                  Н
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ATOM
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ANISOU 781 N ILE A 51
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       782 CA ILE A 51
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                                                                C
ATOM
                                                                C
ANISOU 782 CA ILE A 51
                          2181 1757 2374
                                              185 -556 -485
       783 C ILE A 51
                          10.397 -10.670 -19.950 1.00 17.95
ATOM
ANISOU 783 C ILE A 51
                          2378 1881 2560 237 -661 -630
ATOM 784 O ILE A 51 10.961 -10.897 -18.874 1.00 17.97 ANISOU 784 O ILE A 51 2341 1958 2529 261 -722 -717 ATOM 785 CB ILE A 51 9.529 -12.921 -20.707 1.00 17.20 ANISOU 785 CB ILE A 51 2236 1987 2312 263 -507 -448
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	9.407 -13.863 -21.905 1.00 17.12	С
ANISOU 786 CG1 ILE A 51	2212 1998 2297 217 -419 -324	С
ATOM 787 CG2 ILE A 51	8.137 -12.494 -20.294 1.00 17.71	C
ANISOU 787 CG2 ILE A 51	2346 2078 2304 372 -517 -489	С
ATOM 788 CD1 ILE A 51	10.491 -14.909 -21.971 1.00 16.61	C
ANISOU 788 CD1 ILE A 51		Č
	12.032 -12.776 -20.873 1.00 19.60	Η
ATOM 790 HA ILE A 51	10.027 -11.289 -21.862 1.00 19.93	¨Η
ATOM 791 HB ILE A 51		H
ATOM 792 HG12 ILE A 51	8.555 -14.323 -21.855 1.00 20.55	Ή
ATOM 792 HG13 ILE A 51	9.450 -13.340 -22.720 1.00 20.55	H
	7.617 -13.283 -20.075 1.00 21.25	H
	8.202 -11.914 -19.519 1.00 21.25	H
	7.722 -12.017 -21.030 1.00 21.25	H
ATOM 797 HD11 ILE A 51		H
ATOM 798 HD12 ILE A 51	11.352 -14.466 -22.034 1.00 19.93	H
ATOM 799 HD13 ILE A 51	10.456 -15.451 -21.168 1.00 19.93	. Н
ATOM 800 N ASN A 52	9.793 -9.521 -20.220 1.00 17.71	N
ANISOU 800 N ASN A 52	2424 1727 2579 263 -688 -661	N
ATOM 801 CA ASN A 52	9.587 -8.490 -19.221 1.00 19.72	C
ANISOU 801 CA ASN A 52	2726 1926 2841 336 -790 -811	C
ATOM 802 C ASN A 52	8.130 -8.514 -18.806 1.00 19.85	С
ANISOU 802 C ASN A 52	2786 2029 2726 486 -775 -833	С
ATOM 803 O ASN A 52	7.244 -8.723 -19.639 1.00 20.14	0
ANISOU 803 O ASN A 52	2842 2077 2734 509 -705 -737	0
ATOM 804 CB ASN A 52	9.945 -7.104 -19.761 1.00 21.36	C
ANISOU 804 CB ASN A 52		C
ATOM 805 CG ASN A 52	11.342 -7.043 -20.324 1.00 22.67	C
ANISOU 805 CG ASN A 52		Č
	12.300 -6.784 -19.600 1.00 24.84	ŏ
ANISOU 806 OD1 ASN A 52		Ö
		N
ATOM 807 ND2 ASN A 52	11.468 -7.275 -21.625 1.00 21.33	IN .
	2020 4772 2402 22 722 624	
ANISOU 807 ND2 ASN A 52	2928 1773 3402 32 -723 -634	N
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52	9.487 -9.312 -20.997 1.00 21.25	N H
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67	H H
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63	N H H H
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52 ATOM 811 HB3 ASN A 52	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63 9.884 -6.458 -19.040 1.00 25.63	N H H H
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52 ATOM 811 HB3 ASN A 52 ATOM 812 HD21 ASN A 52	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63 9.884 -6.458 -19.040 1.00 25.63 12.245 -7.251 -21.992 1.00 25.59	N H H H H
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52 ATOM 811 HB3 ASN A 52 ATOM 812 HD21 ASN A 52 ATOM 813 HD22 ASN A 52	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63 9.884 -6.458 -19.040 1.00 25.63 12.245 -7.251 -21.992 1.00 25.59 10.773 -7.450 -22.100 1.00 25.59	N H H H H
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52 ATOM 811 HB3 ASN A 52 ATOM 812 HD21 ASN A 52	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63 9.884 -6.458 -19.040 1.00 25.63 12.245 -7.251 -21.992 1.00 25.59	N H H H H
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52 ATOM 811 HB3 ASN A 52 ATOM 812 HD21 ASN A 52 ATOM 813 HD22 ASN A 52	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63 9.884 -6.458 -19.040 1.00 25.63 12.245 -7.251 -21.992 1.00 25.59 10.773 -7.450 -22.100 1.00 25.59	N H H H H
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52 ATOM 811 HB3 ASN A 52 ATOM 812 HD21 ASN A 52 ATOM 813 HD22 ASN A 52 ATOM 814 N TYR A 53	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63 9.884 -6.458 -19.040 1.00 25.63 12.245 -7.251 -21.992 1.00 25.59 10.773 -7.450 -22.100 1.00 25.59 7.880 -8.306 -17.518 1.00 19.63	N H H H H H N
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52 ATOM 811 HB3 ASN A 52 ATOM 812 HD21 ASN A 52 ATOM 813 HD22 ASN A 52 ATOM 814 N TYR A 53 ANISOU 814 N TYR A 53 ATOM 815 CA TYR A 53	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63 9.884 -6.458 -19.040 1.00 25.63 12.245 -7.251 -21.992 1.00 25.59 10.773 -7.450 -22.100 1.00 25.59 7.880 -8.306 -17.518 1.00 19.63 2769 2075 2613 596 -843 -963 6.509 -8.185 -17.063 1.00 19.23	N H H H H N N
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52 ATOM 811 HB3 ASN A 52 ATOM 812 HD21 ASN A 52 ATOM 813 HD22 ASN A 52 ATOM 814 N TYR A 53 ANISOU 814 N TYR A 53 ATOM 815 CA TYR A 53	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63 9.884 -6.458 -19.040 1.00 25.63 12.245 -7.251 -21.992 1.00 25.59 10.773 -7.450 -22.100 1.00 25.59 7.880 -8.306 -17.518 1.00 19.63 2769 2075 2613 596 -843 -963	N H H H H H H N N C C
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52 ATOM 811 HB3 ASN A 52 ATOM 812 HD21 ASN A 52 ATOM 813 HD22 ASN A 52 ATOM 814 N TYR A 53 ANISOU 814 N TYR A 53 ANISOU 815 CA TYR A 53 ANISOU 816 C TYR A 53	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63 9.884 -6.458 -19.040 1.00 25.63 12.245 -7.251 -21.992 1.00 25.59 10.773 -7.450 -22.100 1.00 25.59 7.880 -8.306 -17.518 1.00 19.63 2769 2075 2613 596 -843 -963 6.509 -8.185 -17.063 1.00 19.23 2754 2108 2444 749 -825 -993 6.471 -7.340 -15.801 1.00 20.36	N H H H H H N N C
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52 ATOM 811 HB3 ASN A 52 ATOM 812 HD21 ASN A 52 ATOM 813 HD22 ASN A 52 ATOM 814 N TYR A 53 ANISOU 814 N TYR A 53 ANISOU 815 CA TYR A 53 ANISOU 816 C TYR A 53 ANISOU 816 C TYR A 53	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63 9.884 -6.458 -19.040 1.00 25.63 12.245 -7.251 -21.992 1.00 25.59 10.773 -7.450 -22.100 1.00 25.59 7.880 -8.306 -17.518 1.00 19.63 2769 2075 2613 596 -843 -963 6.509 -8.185 -17.063 1.00 19.23 2754 2108 2444 749 -825 -993 6.471 -7.340 -15.801 1.00 20.36 2924 2264 2547 847 -912 -1128	N HHHHHH N NC C C
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52 ATOM 811 HB3 ASN A 52 ATOM 812 HD21 ASN A 52 ATOM 813 HD22 ASN A 52 ATOM 814 N TYR A 53 ANISOU 814 N TYR A 53 ANISOU 815 CA TYR A 53 ANISOU 816 C TYR A 53 ANISOU 816 C TYR A 53 ANISOU 816 C TYR A 53 ANISOU 817 O TYR A 53	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63 9.884 -6.458 -19.040 1.00 25.63 12.245 -7.251 -21.992 1.00 25.59 10.773 -7.450 -22.100 1.00 25.59 7.880 -8.306 -17.518 1.00 19.63 2769 2075 2613 596 -843 -963 6.509 -8.185 -17.063 1.00 19.23 2754 2108 2444 749 -825 -993 6.471 -7.340 -15.801 1.00 20.36 2924 2264 2547 847 -912 -1128 7.480 -7.157 -15.114 1.00 21.79	N HHHHHH N NC C C C
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52 ATOM 811 HB3 ASN A 52 ATOM 812 HD21 ASN A 52 ATOM 813 HD22 ASN A 52 ATOM 814 N TYR A 53 ANISOU 814 N TYR A 53 ANISOU 815 CA TYR A 53 ANISOU 816 C TYR A 53 ANISOU 816 C TYR A 53 ANISOU 817 O TYR A 53	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63 9.884 -6.458 -19.040 1.00 25.63 12.245 -7.251 -21.992 1.00 25.59 10.773 -7.450 -22.100 1.00 25.59 7.880 -8.306 -17.518 1.00 19.63 2769 2075 2613 596 -843 -963 6.509 -8.185 -17.063 1.00 19.23 2754 2108 2444 749 -825 -993 6.471 -7.340 -15.801 1.00 20.36 2924 2264 2547 847 -912 -1128 7.480 -7.157 -15.114 1.00 21.79 3081 2438 2762 808 -981 -1198	N HHHHH N NC C C O
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52 ATOM 811 HB3 ASN A 52 ATOM 812 HD21 ASN A 52 ATOM 813 HD22 ASN A 52 ATOM 814 N TYR A 53 ANISOU 814 N TYR A 53 ANISOU 815 CA TYR A 53 ANISOU 816 C TYR A 53 ANISOU 816 C TYR A 53 ANISOU 817 O TYR A 53	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63 9.884 -6.458 -19.040 1.00 25.63 12.245 -7.251 -21.992 1.00 25.59 10.773 -7.450 -22.100 1.00 25.59 7.880 -8.306 -17.518 1.00 19.63 2769 2075 2613 596 -843 -963 6.509 -8.185 -17.063 1.00 19.23 2754 2108 2444 749 -825 -993 6.471 -7.340 -15.801 1.00 20.36 2924 2264 2547 847 -912 -1128 7.480 -7.157 -15.114 1.00 21.79 3081 2438 2762 808 -981 -1198 5.868 -9.564 -16.830 1.00 17.08	N HHHHH N NC C C O C
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52 ATOM 811 HB3 ASN A 52 ATOM 812 HD21 ASN A 52 ATOM 813 HD22 ASN A 52 ATOM 814 N TYR A 53 ANISOU 814 N TYR A 53 ANISOU 815 CA TYR A 53 ANISOU 816 C TYR A 53 ANISOU 816 C TYR A 53 ANISOU 817 O TYR A 53 ANISOU 817 O TYR A 53 ANISOU 818 CB TYR A 53 ANISOU 818 CB TYR A 53	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63 9.884 -6.458 -19.040 1.00 25.63 12.245 -7.251 -21.992 1.00 25.59 10.773 -7.450 -22.100 1.00 25.59 7.880 -8.306 -17.518 1.00 19.63 2769 2075 2613 596 -843 -963 6.509 -8.185 -17.063 1.00 19.23 2754 2108 2444 749 -825 -993 6.471 -7.340 -15.801 1.00 20.36 2924 2264 2547 847 -912 -1128 7.480 -7.157 -15.114 1.00 21.79 3081 2438 2762 808 -981 -1198 5.868 -9.564 -16.830 1.00 17.08 2415 2038 2036 794 -730 -901	N HHHHH N NC C C O O C C
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52 ATOM 811 HB3 ASN A 52 ATOM 812 HD21 ASN A 52 ATOM 813 HD22 ASN A 52 ATOM 814 N TYR A 53 ANISOU 814 N TYR A 53 ANISOU 815 CA TYR A 53 ANISOU 816 C TYR A 53 ANISOU 816 C TYR A 53 ANISOU 817 O TYR A 53 ANISOU 817 O TYR A 53 ANISOU 817 O TYR A 53 ANISOU 818 CB TYR A 53 ANISOU 818 CB TYR A 53 ANISOU 818 CB TYR A 53 ANISOU 819 CG TYR A 53	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63 9.884 -6.458 -19.040 1.00 25.63 12.245 -7.251 -21.992 1.00 25.59 10.773 -7.450 -22.100 1.00 25.59 7.880 -8.306 -17.518 1.00 19.63 2769 2075 2613 596 -843 -963 6.509 -8.185 -17.063 1.00 19.23 2754 2108 2444 749 -825 -993 6.471 -7.340 -15.801 1.00 20.36 2924 2264 2547 847 -912 -1128 7.480 -7.157 -15.114 1.00 21.79 3081 2438 2762 808 -981 -1198 5.868 -9.564 -16.830 1.00 17.08 2415 2038 2036 794 -730 -901 6.332 -10.301 -15.594 1.00 17.20	N THHHH ZZCC COCCC
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52 ATOM 811 HB3 ASN A 52 ATOM 812 HD21 ASN A 52 ATOM 813 HD22 ASN A 52 ATOM 814 N TYR A 53 ANISOU 814 N TYR A 53 ANISOU 815 CA TYR A 53 ANISOU 816 C TYR A 53 ANISOU 816 C TYR A 53 ANISOU 817 O TYR A 53 ANISOU 817 O TYR A 53 ANISOU 818 CB TYR A 53 ANISOU 818 CB TYR A 53 ANISOU 819 CG TYR A 53	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63 9.884 -6.458 -19.040 1.00 25.59 10.773 -7.450 -22.100 1.00 25.59 7.880 -8.306 -17.518 1.00 19.63 2769 2075 2613 596 -843 -963 6.509 -8.185 -17.063 1.00 19.23 2754 2108 2444 749 -825 -993 6.471 -7.340 -15.801 1.00 20.36 2924 2264 2547 847 -912 -1128 7.480 -7.157 -15.114 1.00 21.79 3081 2438 2762 808 -981 -1198 5.868 -9.564 -16.830 1.00 17.08 2415 2038 2036 794 -730 -901 6.332 -10.301 -15.594 1.00 17.20 2390 2203 1944 843 -746 -948	SHITTE ZCCCOOCCC
ANISOU 807 ND2 ASN A 52 ATOM 808 H ASN A 52 ATOM 809 HA ASN A 52 ATOM 810 HB2 ASN A 52 ATOM 811 HB3 ASN A 52 ATOM 812 HD21 ASN A 52 ATOM 813 HD22 ASN A 52 ATOM 814 N TYR A 53 ANISOU 814 N TYR A 53 ANISOU 815 CA TYR A 53 ANISOU 816 C TYR A 53 ANISOU 816 C TYR A 53 ANISOU 817 O TYR A 53 ANISOU 817 O TYR A 53 ANISOU 818 CB TYR A 53 ANISOU 818 CB TYR A 53 ANISOU 819 CG TYR A 53	9.487 -9.312 -20.997 1.00 21.25 10.137 -8.673 -18.443 1.00 23.67 9.325 -6.871 -20.469 1.00 25.63 9.884 -6.458 -19.040 1.00 25.63 12.245 -7.251 -21.992 1.00 25.59 10.773 -7.450 -22.100 1.00 25.59 7.880 -8.306 -17.518 1.00 19.63 2769 2075 2613 596 -843 -963 6.509 -8.185 -17.063 1.00 19.23 2754 2108 2444 749 -825 -993 6.471 -7.340 -15.801 1.00 20.36 2924 2264 2547 847 -912 -1128 7.480 -7.157 -15.114 1.00 21.79 3081 2438 2762 808 -981 -1198 5.868 -9.564 -16.830 1.00 17.08 2415 2038 2036 794 -730 -901 6.332 -10.301 -15.594 1.00 17.20 2390 2203 1944 843 -746 -948 7.434 -11.143 -15.629 1.00 17.14	N THHHH ZZCC COCCC

ATOM 821 CD2 TYR A 53	5.645 -10.176 -14.396 1.00 18.18 C
ANISOU 821 CD2 TYR A 53	2527 2447 1934 998 -760 -1025 C
ATOM 822 CE1 TYR A 53	7.853 -11.823 -14.492 1.00 16.91 C
ANISOU 822 CE1 TYR A 53	2268 2337 1819 812 -758 -935 C
ATOM 823 CE2 TYR A 53	6.051 -10.849 -13.264 1.00 18.76 C
ANISOU 823 CE2 TYR A 53	2561 2660 1906 1049 -758 -1028 C
ATOM 824 CZ TYR A 53	7.151 -11.667 -13.314 1.00 17.95 C
ANISOU 824 CZ TYR A 53	2421 2583 1817 966 -766 -1000 C
ATOM 825 OH TYR A 53	7.530 -12.324 -12.171 1.00 19.60 O
ANISOU 825 OH TYR A 53	2597 2925 1924 1035 -760 -992 O
ATOM 826 H TYR A 53	8.475 -8.233 -16.901 1.00 23.55 H
ATOM 827 HA TYR A 53	5.991 -7.727 -17.744 1.00 23.08 H
ATOM 828 HB2 TYR A 53	4.908 -9.447 -16.755 1.00 20.49 H
ATOM 829 HB3 TYR A 53	6.067 -10.127 -17.594 1.00 20.49 H
ATOM 830 HD1 TYR A 53	7.908 -11.244 -16.423 1.00 20.57 H
ATOM 831 HD2 TYR A 53	4.901 -9.620 -14.353 1.00 21.81 H
ATOM 832 HE1 TYR A 53	8.597 -12.380 -14.526 1.00 20.29 H
ATOM 833 HE2 TYR A 53	5.582 -10.747 -12.467 1.00 22.51 H
ATOM 834 HH TYR A 53	8.210 -12.794 -12.322 1.00 23.51 H
ATOM 835 N ASN A 54	5.292 -6.800 -15.527 1.00 20.29 N
ANISOU 835 N ASN A 54	2948 2289 2471 967 -900 -1141 N
ATOM 836 CA ASN A 54	5.015 -6.133 -14.262 1.00 22.52 C
ANISOU 836 CA ASN A 54	3243 2630 2682 1082 -960 -1238 C
ATOM 837 C ASN A 54	3.627 -6.577 -13.839 1.00 22.18 C
ANISOU 837 C ASN A 54	3179 2758 2490 1221 -888 -1198 C
ATOM 838 O ASN A 54	2.638 -6.258 -14.512 1.00 21.35 O
ANISOU 838 O ASN A 54	3095 2628 2391 1255 -850 -1155 O
ATOM 839 CB ASN A 54	5.096 -4.615 -14.396 1.00 23.60 C
ANISOU 839 CB ASN A 54	
ATOM 840 CG ASN A 54	4.972 -3.906 -13.065 1.00 25.48 C
ANISOU 840 CG ASN A 54	3706 2872 3103 1189 -1117 -1428 C
ATOM 841 OD1 ASN A 54	4.163 -4.284 -12.217 1.00 25.54 O
ANISOU 841 OD1 ASN A 54	
	5.799 -2.889 -12.864 1.00 27.17 N
ANISOU 842 ND2 ASN A 54	3954 2937 3433 1134 -1212 -1521 N
ATOM 843 H ASN A 54	4.623 -6.808 -16.067 1.00 24.34 H
ATOM 844 HA ASN A 54	5.653 -6.422 -13.591 1.00 27.02 H
	5.953 -4.377 -14.784 1.00 28.32 H
	4.376 -4.309 -14.968 1.00 28.32 H
ATOM 847 HD21 ASN A 54	5.770 -2.451 -12.124 1.00 32.61 H
	6.364 -2.667 -13.473 1.00 32.61 H
	3.562 -7.340 -12.752 1.00 20.94 N
ANISOU 849 N ALA A 55	2974 2778 2204 1298 -863 -1199 N
	2.290 -7.753 -12.169 1.00 21.14 C
ANISOU 850 CA ALA A 55	2966 2977 2090 1426 -788 -1153 C
ATOM 851 C ALA A 55	1.877 -6.665 -11.191 1.00 23.07 C
ANISOU 851 C ALA A 55	3250 3229 2285 1552 -859 -1252 C
ATOM 852 O ALA A 55	2.321 -6.632 -10.042 1.00 24.23 O
ANISOU 852 O ALA A 55	
ATOM 853 CB ALA A 55	2.412 -9.108 -11.485 1.00 20.61 C
	2833 3086 1911 1446 -713 -1083 C
ATOM 854 H ALA A 55	4.250 -7.635 -12.328 1.00 25.13 H
ATOM 855 HA ALA A 55	1.617 -7.816 -12.865 1.00 25.37 H

ATOM 856 HB1 ALA A 55 1.551 -9.350 -11.110 1.00 24.73 H ATOM 857 HB2 ALA A 55 2.686 -9.768 -12.140 1.00 24.73 H ATOM 858 HB3 ALA A 55 3.075 -9.047 -10.779 1.00 24.73 H ATOM 859 N GLY A 56 1.035 -5.747 -11.670 1.00 23.57 ANISOU 859 N GLY A 56 3355 3220 2381 1591 -871 -1269 ANISOU 859 N GLY A 56 3355 3220 2381 1591 -871 -1269 N ATOM 860 CA GLY A 56 0.529 -4.691 -10.814 1.00 25.48 ANISOU 860 CA GLY A 56 3641 3469 2572 1721 -936 -1364 ATOM 861 C GLY A 56 -0.380 -5.212 -9.723 1.00 26.64 C ANISOU 861 C GLY A 56 3739 3835 2548 1865 -876 -1339 C ATOM 862 O GLY A 56 -0.489 -4.601 -8.659 1.00 28.40 O ANISOU 862 O GLY A 56 3989 4103 2698 1987 -935 -1427 O ATOM 863 H GLY A 56 0.748 -5.718 -12.480 1.00 28.29 H ATOM 864 HA2 GLY A 56 1.274 -4.229 -10.397 1.00 30.58 ATOM 865 HA3 GLY A 56 0.032 -4.052 -11.348 1.00 30.58 ATOM 866 N VAL A 57 -1.054 -6.334 -9.972 1.00 25.05 N 3465 3769 2285 1853 -756 -1218 N ANISOU 866 N VAL A 57 ANISOU 860 N VAL A 57 3465 3769 2265 1855 -756 -1218 ATOM 867 CA VAL A 57 -1.858 -7.012 -8.964 1.00 25.74 C ANISOU 867 CA VAL A 57 3494 4066 2221 1964 -674 -1162 ATOM 868 C VAL A 57 -1.585 -8.503 -9.067 1.00 24.89 ANISOU 868 C VAL A 57 3316 4054 2089 1885 -573 -1040 ANISOU 868 C VAL A 57 3316 4054 2089 1885 -573 -1040 C ATOM 869 O VAL A 57 -1.630 -9.076 -10.161 1.00 22.84 O ANISOU 869 O VAL A 57 3025 3749 1904 1772 -518 -967 O -3.364 -6.736 -9.123 1.00 26.92 C ANISOU 870 CB VAL A 57 3614 4293 2321 2045 -610 -1125 C ATOM 871 CG1 VAL A 57 -4.163 -7.494 -8.059 1.00 28.04 C ANISOU 871 CG2 VAL A 57 3688 4652 2315 2147 -511 -1052 C ATOM 872 CG2 VAL A 57 3815 4315 2463 2134 -711 -1246 C ATOM 873 H VAL A 57 -1.060 -6.738 -10.737 1.00 30.06 ATOM 873 H VAL A 57 -1.060 -6.728 -10.737 1.00 30.06 H ATOM 874 HA VAL A 57 -1.585 -6.713 -8.082 1.00 30.89 H ATOM 874 HA VAL A 57
ATOM 875 HB VAL A 57
ATOM 876 HG11 VAL A 57
ATOM 877 HG12 VAL A 57
ATOM 878 HG13 VAL A 57
ATOM 879 HG21 VAL A 57
ATOM 879 HG21 VAL A 57
ATOM 880 HG22 VAL A 57
ATOM 881 HG23 VAL A 57 ATOM 882 N TRP A 58 -1.308 -9.130 -7.926 1.00 25.05 3314 4202 2002 1952 -549 -1017 N ANISOU 882 N TRP A 58 ATOM 883 CA TRP A 58 -1.133 -10.580 -7.858 1.00 24.43 ANISOU 883 CA TRP A 58 3174 4223 1887 1895 -443 -887 ATOM 884 C TRP A 58 -1.762 -11.041 -6.550 1.00 25.78 ANISOU 884 C TRP A 58 3313 4576 1907 2027 -373 -3313 4576 1907 2027 -373 -827 C ATOM 885 O TRP A 58 -1.155 -10.905 -5.482 1.00 26.76 0 ANISOU 885 O TRP A 58 3466 4745 1956 2121 -428 -881 0 ATOM 886 CB TRP A 58 0.331 -10.984 -7.939 1.00 24.63 ANISOU 886 CB TRP A 58
ANISOU 886 CB TRP A 58
ANISOU 887 CG TRP A 58
ANISOU 887 CG TRP A 58
ANISOU 888 CD1 TRP A 58
ANISOU 888 CD1 TRP A 58
ANISOU 888 CD1 TRP A 58
ANISOU 889 CD2 TRP A 58

ATOM 890 NE1 TRP A 58	1.113 -14.515 -7.141 1.00 25.90	N
ANISOU 890 NE1 TRP A 58	3273 4571 1999 1743 -262 -595	N
ATOM 891 CE2 TRP A 58	0.338 -14.717 -8.253 1.00 25.13	С
ANISOU 891 CE2 TRP A 58	3140 4436 1972 1649 -194 -534	С
ATOM 892 CE3 TRP A 58	-0.869 -13.379 -9.867 1.00 24.28	С
ANISOU 892 CE3 TRP A 58	3033 4199 1994 1595 -227 -613	С
ATOM 893 CZ2 TRP A 58	-0.038 -15.900 -8.886 1.00 25.40	С
ANISOU 893 CZ2 TRP A 58	3117 4494 2041 1553 -75 -394	C
ATOM 894 CZ3 TRP A 58	-1.244 -14.554 -10.492 1.00 23.42	С
ANISOU 894 CZ3 TRP A 58	2855 4125 1919 1504 -112 -483	C
ATOM 895 CH2 TRP A 58	-0.824 -15.799 -10.004 1.00 24.07	C
ANISOU 895 CH2 TRP A 58	2910 4277 1959 1477 -37 -376	С
ATOM 896 H TRP A 58	-1.216 -8.734 -7.169 1.00 30.06	Н
ATOM 897 HA TRP A 58	-1.608 -10.999 -8.593 1.00 29.32	Н
ATOM 898 HB2 TRP A 58	0.698 -10.689 -8.788 1.00 29.56	Н
ATOM 899 HB3 TRP A 58	0.817 -10.576 -7.205 1.00 29.56	Н
ATOM 900 HD1 TRP A 58	1.669 -12.774 -6.195 1.00 32.21	Н
ATOM 901 HE1 TRP A 58	1.479 -15.133 -6.667 1.00 31.09	Н
ATOM 902 HE3 TRP A 58	-1.151 -12.557 -10.197 1.00 29.14	н
ATOM 903 HZ2 TRP A 58	0.240 -16.728 -8.565 1.00 30.48	Н
ATOM 904 HZ3 TRP A 58	-1.778 -14.518 -11.253 1.00 28.11	н
ATOM 905 HH2 TRP A 58	-1.089 -16.573 -10.445 1.00 28.88	Н
ATOM 906 N ALA A 59	-2.977 -11.575 -6.637 1.00 26.15	N
ANISOU 906 N ALA A 59	3294 4725 1916 2035 -249 -716	N
ATOM 907 CA ALA A 59	-3.772 -11.924 -5.457 1.00 28.25	C
ANISOU 907 CA ALA A 59	3526 5161 2047 2163 -166 -647	C
ATOM 908 C ALA A 59	-4.473 -13.253 -5.689 1.00 27.57	С
ANISOU 908 C ALA A 59	3349 5159 1969 2084 -3 -469	C
ATOM 909 O ALA A 59	-5.701 -13.317 -5.823 1.00 27.88	Õ
ANISOU 909 O ALA A 59	3323 5265 2007 2094 87 -409	o
ATOM 910 CB ALA A 59	-4.783 -10.822 -5.138 1.00 30.13	č
ANISOU 910 CB ALA A 59	3776 5438 2234 2287 -193 -722	C
ATOM 911 H ALA A 59	-3.372 -11.750 -7.381 1.00 31.38	н
ATOM 912 HA ALA A 59	-3.182 -12.022 -4.693 1.00 33.90	'H
ATOM 913 HB1 ALA A 59	-5.293 -11.079 -4.355 1.00 36.16	Ή
ATOM 914 HB2 ALA A 59	-4.305 -9.996 -4.966 1.00 36.16	H
ATOM 915 HB3 ALA A 59	-5.376 -10.709 -5.898 1.00 36.16	Ή
ATOM 916 N PRO A 60	-3.716 -14.344 -5.744 1.00 27.86	N
ANISOU 916 N PRO A 60	3374 5185 2025 2000 40 -382	N
ATOM 917 CA PRO A 60	-4.332 -15.671 -5.820 1.00 28.79	C
ANISOU 917 CA PRO A 60		C
	3410 5370 2160 1927 197 -206	_
ATOM 918 C PRO A 60	-4.833 -16.142 -4.465 1.00 32.56	C
ANISOU 918 C PRO A 60	3867 5994 2509 2049 287 -112	C
ATOM 919 O PRO A 60	-4.264 -15.826 -3.417 1.00 32.59	0
ANISOU 919 O PRO A 60	3929 6050 2404 2179 227 -164	0
ATOM 920 CB PRO A 60	-3.181 -16.556 -6.308 1.00 26.96	C
ANISOU 920 CB PRO A 60	3194 5058 1990 1811 190 -162	C
ATOM 921 CG PRO A 60	-1.971 -15.907 -5.707 1.00 26.52	C
ANISOU 921 CG PRO A 60	3222 4973 1880 1892 56 -287	C
ATOM 922 CD PRO A 60	-2.244 -14.419 -5.770 1.00 26.82	C
ANISOU 922 CD PRO A 60	3300 4971 1918 1964 -54 -442	C
ATOM 923 HA PRO A 60	-5.055 -15.682 -6.465 1.00 34.55	H.
ATOM 924 HB2 PRO A 60	-3.293 -17.460 -5.975 1.00 32.35	Н

ATOM 925 HB3 PRO A 60	-3.139 -16.542 -7.277 1.00 32.35 H
ATOM 926 HG2 PRO A 60	-1.867 -16.197 -4.787 1.00 31.82 H
ATOM 927 HG3 PRO A 60	-1.185 -16.134 -6.229 1.00 31.82 H
ATOM 928 HD2 PRO A 60	-1.868 -13.973 -4.996 1.00 32.18 H
ATOM 929 HD3 PRO A 60	-1.901 -14.047 -6.598 1.00 32.18 H
ATOM 930 N ASN A 61	-5.912 -16.924 -4.504 1.00 36.02 N
	4215 6498 2973 2005 434 27 N
ATOM 931 CA ASN A 61	-6.532 -17.496 -3.306 1.00 40.50 C
	4749 7203 3436 2105 551 146 C
ATOM 932 C ASN A 61	-6.809 -18.967 -3.597 1.00 40.58 C
ANISOU 932 C ASN A 61	4684 7199 3535 1969 697 327 C
ATOM 933 O ASN A 61	-7.921 -19.333 -3.987 1.00 41.49 O
ANISOU 933 O ASN A 61	4699 7336 3730 1896 804 405 O
ATOM 934 CB ASN A 61	-7.806 -16.744 -2.927 1.00 44.12 C
ANISOU 934 CB ASN A 61	5162 7763 3839 2210 588 120 C
ATOM 935 CG ASN A 61	-8.451 -17.288 -1.663 1.00 48.32 C
ANISOU 935 CG ASN A 61	
ATOM 936 OD1 ASN A 61	-7.860 -18.103 -0.953 1.00 49.20 O
ANISOU 936 OD1 ASN A 61	5799 8584 4311 2352 759 337 O
ATOM 937 ND2 ASN A 61	-9.669 -16.837 -1.375 1.00 50.33 N
ANISOU 937 ND2 ASN A 61	5851 8800 4473 2402 781 252 N
ATOM 938 H ASN A 61	-6.314 -17.144 -5.232 1.00 43.22 H
	-5.911 -17.441 -2.563 1.00 48.60 H
ATOM 940 HB2 ASN A 61	
ATOM 941 HB3 ASN A 61	
ATOM 942 HD21 ASN A 61	-10.075 -17.115 -0.670 1.00 60.40 H
ATOM 943 HD22 ASN A 61	-10.050 -16.266 <i>-</i> 1.894 1.00 60.40 H
ATOM 944 N GLY A 62	-5.795 -19.808 -3.384 1.00 39.28 N
ANISOU 944 N GLY A 62	4564 6994 3365 1937 698 389 N
ATOM 945 CA GLY A 62	-5.837 -21.204 -3.769 1.00 37.58 C
ANISOU 945 CA GLY A 62	4298 6727 3252 1797 813 546 C
ATOM 946 C GLY A 62	-4.691 -21.545 -4.707 1.00 34.61 C
	3965 6219 2965 1678 737 510 C
ATOM 947 O GLY A 62	-3.644 -20.885 -4.703 1.00 32.72 O
	3804 5949 2679 1729 606 388 O
ATOM 948 H GLY A 62	-5.056 -19.580 -3.007 1.00 47.13 H
	-5.770 -21.764 -2.979 1.00 45.09 H
	-6.675 -21.396 -4.217 1.00 45.09 H
ATOM 951 N TRP A 63	-4.899 -22.574 -5.521 1.00 34.76 N
ANISOU 951 N TRP A 63	3927 6160 3121 1518 817 612 N
ATOM 952 CA TRP A 63	-3.884 -22.940 -6.505 1.00 33.48 C
	3797 5875 3047 1404 754 584 C
ATOM 953 C TRP A 63	-3.959 -21.951 -7.664 1.00 30.30 C
ANISOU 953 C TRP A 63	3383 5417 2712 1351 660 444 C
ATOM 954 O TRP A 63	-4.792 -22.081 -8.562 1.00 30.74 O
ANISOU 954 O TRP A 63	3356 5439 2885 1250 701 459 O
ATOM 955 CB TRP A 63	
ANISOU 955 CB TRP A 63	
ATOM 956 CG TRP A 63	-2.771 -24.937 -7.548 1.00 36.69 C
ANISOU 956 CG TRP A 63	4215 6103 3622 1191 807 730 C
ATOM 957 CD1 TRP A 63	-1.935 -25.833 -6.941 1.00 37.90 C
	4425 6237 3737 1219 830 815 C
ATOM 958 CD2 TRP A 63	-2.166 -24.620 -8.811 1.00 36.22 C

ANISOU 958 CD2 TRP A 63 4165 5953 3642 1100 721 636 C ATOM 959 NE1 TRP A 63 -0.855 -26.097 -7.751 1.00 36.89 Ν ANISOU 959 NE1 TRP A 63 4340 6014 3664 1147 762 N ATOM 960 CE2 TRP A 63 -0.974 -25.366 -8.904 1.00 35.67 ANISOU 960 CE2 TRP A 63 C 4157 5817 3579 1072 698 961 CE3 TRP A 63 -2.522 -23.782 -9.874 1.00 35.78 ATOM ANISOU 961 CE3 TRP A 63 4073 5868 3654 1049 528 ATOM 962 CZ2 TRP A 63 -0.136 -25.298 -10.017 1.00 34.19 ANISOU 962 CZ2 TRP A 63 3992 5541 3457 C 626 607 990 ATOM 963 CZ3 TRP A 63 -1.688 -23.717 -10.976 1.00 33.92 C **ANISOU 963 CZ3 TRP A 63** 3862 5542 3485 972 591 ATOM 964 CH2 TRP A 63 -0.510 -24.472 -11.040 1.00 33.36 3849 5413 3413 941 ANISOU 964 CH2 TRP A 63 578 507 965 H TRP A 63 -5.603 -23.068 -5.526 1.00 41.71 **ATOM** Н ATOM 966 HA TRP A 63 -3.006 -22.864 -6.100 1.00 40.17 Н -4.337 -24.930 -6.246 1.00 42.89 ATOM 967 HB2 TRP A 63 Н -4.728 -24.394 -7.692 1.00 42.89 -2.076 -26.209 -6.103 1.00 45.47 Н ATOM 968 HB3 TRP A 63 969 HD1 TRP A 63 **ATOM** ATOM 970 HE1 TRP A 63 -0.211 -26.635 -7.564 1.00 44.27 ATOM 971 HE3 TRP A 63 -3.302 -23.278 -9.840 1.00 42.94 ATOM 972 HZ2 TRP A 63 0.647 -25.798 -10.063 1.00 41.02 ATOM 973 HZ3 TRP A 63 -1.915 -23.163 -11.688 1.00 40.71 0.030 -24.408 -11.793 1.00 40.03 Н ATOM 974 HH2 TRP A 63 **ATOM** 975 N GLY A 64 -3.097 -20.949 -7.622 1.00 26.76 N ANISOU 975 N GLY A 64 3015 4955 2199 1425 528 304 Ν 976 CA GLY A 64 -2.918 -20.040 -8.737 1.00 23.38 C ATOM C ANISOU 976 CA GLY A 64 2597 4448 1839 1377 431 **ATOM** 977 C GLY A 64 -1.445 -19.734 -8.882 1.00 22.04 ANISOU 977 C GLY A 64 2513 4212 1650 1382 316 80 C 978 O GLY A 64 -0.703 -19.687 -7.898 1.00 21.69 0 ATOM ANISOU 978 O GLY A 64 0 2523 4207 1511 1474 273 60 ATOM 979 H GLY A 64 -2.595 -20.772 -6.946 1.00 32.11 Н -3.242 -20.447 -9.556 1.00 28.06 -3.402 -19.215 -8.578 1.00 28.06 ATOM 980 HA2 GLY A 64 Н ATOM 981 HA3 GLY A 64 ATOM 982 N ALA A 65 -1.022 -19.532 -10.131 1.00 20.16 Ν ANISOU 982 N ALA A 65 2278 3873 1510 1285 265 **ATOM 983 CA ALA A 65** 0.392 -19.412 -10.448 1.00 20.74 C ANISOU 983 CA ALA A 65 2416 3874 1589 1260 173 -51 ATOM 984 C ALA A 65 0.617 -18.277 -11.435 1.00 19.76 ANISOU 984 C ALA A 65 2319 3653 1534 1234 72 -191 985 O ALA A 65 -0.151 -18.107 -12.383 1.00 20.22 ATOM 0 ANISOU 985 O ALA A 65 2331 3673 1678 1182 97 -188 C ATOM 986 CB ALA A 65 0.938 -20.725 -11.029 1.00 20.86 C 2412 3848 1665 1151 ANISOU 986 CB ALA A 65 238 60 -1.541 -19.462 -10.813 1.00 24.19 ATOM 987 H ALA A 65 Н **ATOM** 988 HA ALA A 65 0.885 -19.211 -9.637 1.00 24.88 1.880 -20.613 -11.230 1.00 25.03 0.820 -21.432 -10.375 1.00 25.03 0.449 -20.938 -11.839 1.00 25.03 ATOM 989 HB1 ALA A 65 ATOM 990 HB2 ALA A 65 Н **ATOM** 991 HB3 ALA A 65 ATOM 992 N LEU A 66 1.669 -17.492 -11.189 1.00 20.28 Ν ANISOU 992 N LEU A 66 2457 3671 1578 1268 -49 -314 ATOM 993 CA LEU A 66 2.132 -16.455 -12.110 1.00 19.34 C ANISOU 993 CA LEU A 66 2381 3422 1546 1222 -154 -438 C

ATOM 994 C LEU A 66 3.374 -17.006 -12.797 1.00 17.31 ANISOU 994 C LEU A 66 2133 3063 1382 1085 -195 -403 ATOM 995 O LEU A 66 4.423 -17.148 -12.161 1.00 17.67 0 ANISOU 995 O LEUA 66 2206 3130 1378 1108 -248 -438 0 ATOM 996 CB LEU A 66 2.437 -15.157 -11.360 1.00 21.09 ANISOU 996 CB LEU A 66 2659 3615 1738 1312 -273 -577 997 CG LEU A 66 3.064 -13.993 -12.131 1.00 20.77 ATOM ANISOU 997 CG LEU A 66 2676 3413 1804 1259 -393 -704 ATOM 998 CD1 LEU A 66 2.101 -13.449 -13.188 1.00 21.11 ANISOU 998 CD1 LEU A 66 2716 3385 1921 1241 -371 -705 C ATOM 999 CD2 LEU A 66 3.493 -12.887 -11.169 1.00 22.34 ANISOU 999 CD2 LEU A 66 2917 3582 1988 1338 -504 -827 C ATOM 1000 H LEU A 66 2.144 -17.545 -10.474 1.00 24.34 Н ATOM 1001 HA LEU A 66 1.453 -16.280 -12.780 1.00 23.21 Н 1.604 -14.829 -10.986 1.00 25.30 3.044 -15.370 -10.634 1.00 25.30 **ATOM 1002 HB2 LEU A 66** ATOM 1003 HB3 LEU A 66 Н 3.044 -15.370 -10.55-3.857 -14.312 -12.589 1.00 24.93 Н ATOM 1004 HG LEU A 66 2.528 -12.715 -13.657 1.00 25.34 1.884 -14.159 -13.813 1.00 25.34 1.294 -13.137 -12.749 1.00 25.34 3.887 -12.161 -11.678 1.00 26.80 2.714 -12.568 -10.686 1.00 26.80 ATOM 1005 HD11 LEU A 66 ATOM 1006 HD12 LEU A 66 ATOM 1007 HD13 LEU A 66 ATOM 1008 HD21 LEU A 66 ATOM 1009 HD22 LEU A 66 ATOM 1010 HD23 LEU A 66 ATOM 1011 N ALA A 67 Н 4.145 -13.246 -10.546 1.00 26.80 3.258 -17.329 -14.087 1.00 15.15 Ν **ANISOU 1011 N ALA A 67** 1832 2691 1235 955 -172 -340 4.274 -18.150 -14.726 1.00 14.82 ATOM 1012 CA ALA A 67 ANISOU 1012 CA ALA A 67 1785 2583 1265 838 -175 -278 C ATOM 1013 C ALA A 67 ANISOU 1013 C ALA A 67 4.353 -17.901 -16.219 1.00 13.57 C 1627 2293 1237 721 -196 -269 C ATOM 1014 O ALA A 67 0 3.333 -17.718 -16.896 1.00 12.33 **ANISOU 1014 O ALA A 67** 0 1449 2119 1117 710 -168 -251 4.001 -19.640 -14.495 1.00 15.53 C ATOM 1015 CB ALA A 67 ANISOU 1015 CB ALA A 67 1833 2743 1326 820 -67 -143 C Н ATOM 1016 H ALA A 67 2.612 -17.088 -14.601 1.00 18.18 ATOM 1017 HA ALA A 67 Н 5.139 -17.939 -14.340 1.00 17.79 4.695 -20.159 -14.932 1.00 18.64 4.007 -19.817 -13.541 1.00 18.64 3.135 -19.864 -14.868 1.00 18.64 ATOM 1018 HB1 ALA A 67 ATOM 1019 HB2 ALA A 67 ATOM 1020 HB3 ALA A 67 Н ATOM 1021 N LEU A 68 5.581 -17.920 -16.724 1.00 13.83 Ν **ANISOU 1021 N LEU A 68** 1676 2246 1333 643 -244 -279 **ATOM 1022 CA LEU A 68** 5.791 -18.083 -18.150 1.00 13.28 ANISOU 1022 CA LEU A 68 1604 2076 1366 534 -236 -235 ATOM 1023 C LEU A 68 5.341 -19.477 -18.552 1.00 13.32 CCOOC ANISOU 1023 C LEU A 68 1571 2113 1377 492 -153 -130 ATOM 1024 O LEU A 68 5.715 -20.467 -17.919 1.00 11.96 **ANISOU 1024 O LEU A 68** 1384 1995 1165 502 -115 -79 ATOM 1025 CB LEU A 68 7.257 -17.877 -18.509 1.00 12.65 ANISOU 1025 CB LEU A 68 1536 1924 1347 467 -288 -258 7.574 -17.844 -20.010 1.00 12.33 ATOM 1026 CG LEU A 68 ANISOU 1026 CG LEU A 68 1502 1783 1400 371 -276 -215 ATOM 1027 CD1 LEU A 68 7.173 -16.507 -20.629 1.00 12.35 ANISOU 1027 CD1 LEU A 68 1545 1694 1451 369 -315 -259 C ATOM 1028 CD2 LEU A 68 9.056 -18.121 -20.224 1.00 12.17

ANISOU 1028 CD2 LEU A 68	1464 1733 1426 309 -292 -207	C
ATOM 1029 H LEU A 68	6.303 -17.841 -16.263 1.00 16.60	Н
ATOM 1030 HA LEU A 68	5.258 -17.433 -18.635 1.00 15.94	Н
ATOM 1031 HB2 LEU A 68	7.550 -17.033 -18.132 1.00 15.18	Н
ATOM 1032 HB3 LEU A 68	7.773 -18.601 -18.120 1.00 15.18	Н
ATOM 1033 HG LEU A 68	7.070 -18.544 -20.455 1.00 14.80	Н
ATOM 1034 HD11 LEU A 68	7.386 -16.521 -21.575 1.00 14.82	Н
ATOM 1035 HD12 LEU A 68	6.219 -16.376 -20.506 1.00 14.82	H
ATOM 1036 HD13 LEU A 68	7.664 -15.796 -20.189 1.00 14.82	H
ATOM 1037 HD21 LEU A 68	9.248 -18.098 -21.175 1.00 14.60	H
ATOM 1038 HD22 LEU A 68	9.574 -17.440 -19.766 1.00 14.60	H
ATOM 1039 HD23 LEU A 68	9.269 -18.996 -19.865 1.00 14.60	H
ATOM 1040 N AVAL A 69	4.536 -19.551 -19.607 0.55 12.75	N
ANISOU 1040 N AVAL A 69	1485 2001 1357 449 -131 -103	N
ATOM 1041 N BVAL A 69	4.507 -19.549 -19.582 0.45 12.80	N.
ANISOU 1041 N BVAL A 69	1491 2010 1362 451 -130 -103	N
ATOM 1042 CA AVAL A 69	3.988 -20.804 -20.113 0.55 12.97	C
ANISOU 1042 CA AVAL A 69	1474 2041 1414 399 -68 -25	C
ATOM 1043 CA BVAL A 69	4.007 -20.810 -20.113 0.45 12.94	С
ANISOU 1043 CA BVAL A 69	1470 2036 1410 398 -68 -25	С
ATOM 1044 C AVAL A 69	4.183 -20.818 -21.620 0.55 12.34	C
ANISOU 1044 C AVAL A 69	1411 1874 1403 327 -90 -21	C
ATOM 1045 C BVAL A 69	4.237 -20.803 -21.613 0.45 12.32	C
ANISOU 1045 C BVAL A 69	1411 1871 1401 327 -91 -21	C
ATOM 1046 O AVAL A 69	3.885 -19.828 -22.294 0.55 12.79	0
ANISOU 1046 O AVAL A 69	1491 1890 1477 337 -130 -59	0
ATOM 1047 O BVAL A 69	4.037 -19.780 -22.275 0.45 12.81	Ö
ANISOU 1047 O BVAL A 69	1498 1888 1480 335 -134 -61	Ŏ
ATOM 1048 CB AVAL A 69	2.495 -20.958 -19.759 0.55 13.52	Č
ANISOU 1048 CB AVAL A 69	1486 2182 1467 437 -20 -5	C
ATOM 1049 CB BVAL A 69	2.510 -21.025 -19.790 0.45 13.48	C
ANISOU 1049 CB BVAL A 69	1481 2176 1465 432 -18 -2	C
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	1.957 -22.299 -20.249 0.55 13.34	C
ANISOU 1050 CG1AVAL A 69	1413 2154 1500 366 38 68	C
ATOM 1051 CG1BVAL A 69	2.280 -21.018 -18.280 0.45 14.10	C
ANISOU 1051 CG1BVAL A 69	1546 2358 1454 521 22 6	C
ATOM 1052 CG2AVAL A 69	2.283 -20.813 -18.256 0.55 14.07	С
ANISOU 1052 CG2AVAL A 69	1547 2354 1445 531 12 -7	C
ATOM 1053 CG2BVAL A 69	1.646 -19.971 -20.471 0.45 13.96	C
ANISOU 1053 CG2BVAL A 69	1539 2219 1547 458 -60 -56	C
ATOM 1054 H AVAL A 69	4.286 -18.865 -20.061 0.55 15.30	Н
ATOM 1055 H BVAL A 69	4.208 -18.860 -20.001 0.45 15.36	Н
ATOM 1056 HA AVAL A 69	4.476 -21.550 -19.731 0.55 15.56	Н
ATOM 1057 HA BVAL A 69	4.512 -21.544 -19.729 0.45 15.53	Н
ATOM 1058 HB AVAL A 69	1.992 -20.256 -20.200 0.55 16.22	Н
ATOM 1059 HB BVAL A 69	2.239 -21.893 -20.127 0.45 16.18	Н
ATOM 1060 HG11AVAL A 69	2.673 -22.784 -20.688 0.55 16.00	Н
ATOM 1061 HG11BVAL A 69	3.129 -20.879 -17.832 0.45 16.92	H
ATOM 1062 HG12AVAL A 69	1.631 -22.805 -19.489 0.55 16.00	H
ATOM 1063 HG12BVAL A 69	1.667 -20.300 -18.058 0.45 16.92	H
ATOM 1064 HG13AVAL A 69	1.234 -22.138 -20.875 0.55 16.00	H
ATOM 1004 HG13AVAL A 09 ATOM 1065 HG13BVAL A 69	1.902 -21.871 -18.015 0.45 16.92	H
ATOM 1066 HG21AVAL A 69	1.339 -20.914 -18.059 0.55 16.88	Н

ATOM 1067 HG21BVAL A 69 ATOM 1068 HG22AVAL A 69 ATOM 1069 HG22BVAL A 69 ATOM 1070 HG23AVAL A 69 ATOM 1071 HG23BVAL A 69 ATOM 1072 N GLY A 70 ANISOU 1072 N GLY A 70 ANISOU 1073 CA GLY A 70 ANISOU 1074 C GLY A 70 ANISOU 1074 C GLY A 70 ANISOU 1075 O GLY A 70 ATOM 1076 H GLY A 70 ATOM 1076 H GLY A 70 ATOM 1077 HA2 GLY A 70 ATOM 1079 N TRP A 71 ANISOU 1079 N TRP A 71 ANISOU 1080 CA TRP A 71 ANISOU 1080 CA TRP A 71 ANISOU 1081 C TRP A 71 ANISOU 1081 C TRP A 71 ANISOU 1082 O TRP A 71 ANISOU 1083 CB TRP A 71 ANISOU 1083 CB TRP A 71 ANISOU 1084 CG TRP A 71 ANISOU 1085 CD1 TRP A 71 ANISOU 1085 CD1 TRP A 71 ANISOU 1086 CD2 TRP A 71 ANISOU 1086 CD2 TRP A 71 ANISOU 1087 NE1 TRP A 71 ANISOU 1088 CE2 TRP A 71 ANISOU 1089 CE3 TRP A 71 ANISOU 1090 CZ2 TRP A 71 ANISOU 1091 CZ3 TRP A 71	0.716 -20.134 -20.249 0.45 16.75 2.792 -21.500 -17.798 0.55 16.88 1.912 -19.093 -20.157 0.45 16.75 2.588 -19.935 -17.978 0.55 16.88 1.772 -20.032 -21.431 0.45 16.75 4.663 -21.938 -22.151 1.00 11.03 1241 1681 1267 270 -63 27 4.858 -22.027 -23.582 1.00 10.72 1225 1575 1273 221 -80 28 4.933 -23.461 -24.047 1.00 9.43 1050 1394 1140 175 -46 70 4.866 -24.401 -23.250 1.00 8.54 913 1306 1026 173 -3 110 4.859 -22.649 -21.709 1.00 13.23 4.120 -21.592 -24.039 1.00 12.86 5.682 -21.578 -23.827 1.00 12.86 5.089 -24.914 -26.019 1.00 11.02 1276 1514 1397 109 -48 75 6.125 -24.956 -27.136 1.00 11.74 1418 1564 1480 106 -58 69 6.458 -23.939 -27.757 1.00 10.29 1263 1372 1274 121 -77 58 3.730 -25.273 -26.652 1.00 11.73 1330 1605 1523 90 -68 50 2.587 -25.426 -25.702 1.00 13.98 1543 1937 1831 85 -43 65 1.819 -24.429 -25.179 1.00 14.12 1527 2014 1825 127 -50 50 2.052 -26.654 -25.196 1.00 14.02 1499 1934 1895 40 3 104 0.849 -24.954 -24.369 1.00 14.53 1502 2113 1907 115 -4 79 0.970 -26.319 -24.357 1.00 15.08 1559 2137 2033 54 33 120 2.388 -28.001 -25.361 1.00 15.06 1642 1998 2080 -8 27 130 0.221 -27.279 -23.688 1.00 16.55 1675 2332 2281 12 97 175 1.644 -28.957 -24.688 1.00 16.63 1783 2185 2348 -53 82 182	SZOOOOTITI TITII
ATOM 1092 CH2 TRP A 71 ANISOU 1092 CH2 TRP A 71	0.571 -28.588 -23.862 1.00 16.62 1701 2260 2355 -49 121 210	C
ATOM 1093 H TRP A 71	5.170 -22.954 -25.916 1.00 11.79	н
ATOM 1094 HA TRP A 71	5.313 -25.596 -25.368 1.00 13.22	H.
ATOM 1095 HB2 TRP A 71 ATOM 1096 HB3 TRP A 71	3.492 -24.574 -27.281	H
ATOM 1090 HB3 TRF A 71 ATOM 1097 HD1 TRP A 71	1.936 -23.522 -25.348 1.00 16.95	H
ATOM 1098 HE1 TRP A 71	0.262 -24.501 -23.934 1.00 17.44	Н
ATOM 1099 HE3 TRP A 71	3.099 -28.250 -25.906 1.00 18.07	H
ATOM 1100 HZ2 TRP A 71 ATOM 1101 HZ3 TRP A 71	-0.489 -27.038 -23.137	H
ATOM THE HEATT	1.030 -23.031 -24.103 1.00 13.33	• • • • • • • • • • • • • • • • • • • •

ATOM 1102 HH2 TRP A 71	0.086 -29.250 -23.423 1.00 19.95	Н
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ATOM 1103 N THR A 72	6.605 -26.160 -27.402 1.00 11.22	N
ANISOU 1103 N THR A 72	1363 1468 1432 91 -37 82	N
ATOM 1104 CA THR A 72	7.215 -26.496 -28.672 1.00 10.69	С
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ANISOU 1104 CA THR A 72	1339 1369 1352 98 -44 66	C
ATOM 1105 C THR A 72	6.444 -27.655 -29.286 1.00 11.93	С
ANISOU 1105 C THR A 72	1499 1488 1544 80 -62 33	С
ATOM 1106 O THR A 72	5.709 -28.375 -28.603 1.00 13.30	0
ANISOU 1106 O THR A 72	1635 1647 1770 47 -53 42	0
		_
ATOM 1107 CB THR A 72	8.697 -26.879 -28.526 1.00 10.32	С
ANISOU 1107 CB THR A 72	1307 1317 1296 114 -9 94	С
ATOM 1108 OG1 THR A 72	8.842 -28.092 -27.767 1.00 11.33	0
ANISOU 1108 OG1 THR A 72	1427 1426 1453 112 14 118	0
ATOM 1109 CG2 THR A 72	9.458 -25.769 -27.851 1.00 11.37	С
		_
ANISOU 1109 CG2 THR A 72	1420 1483 1417 118 -5 113	С
ATOM 1110 H THR A 72	6.587 -26.815 -26.846 1.00 13.46	Н
ATOM 1111 HA THR A 72	7.153 -25.735 -29.271 1.00 12.82	Н
ATOM 1112 HB THR A 72	9.078 -27.011 -29.408 1.00 12.38	Н
ATOM 1113 HG1 THR A 72	8.516 -27.991 -26.999 1.00 13.60	Н
ATOM 1114 HG21 THR A 72	10.392 -26.015 -27.761 1.00 13.64	Н
ATOM 1115 HG22 THR A 72	9.396 -24.957 -28.378 1.00 13.64	Н
ATOM 1116 HG23 THR A 72	9.090 -25.603 -26.970 1.00 13.64	H
ATOM 1117 N ARG A 73	6.586 -27.795 -30.592 1.00 12.64	N
ANISOU 1117 N ARG A 73	1632 1564 1606 103 -88 -7	N
ATOM 1118 CA ARG A 73	6.277 -29.032 -31.288 1.00 13.96	С
ANISOU 1118 CA ARG A 73	1819 1682 1803 97 -114 -57	С
ATOM 1119 C ARG A 73	7.583 -29.637 -31.780 1.00 13.71	С
ANISOU 1119 C ARG A 73	1841 1629 1740 138 -83 -52	С
ATOM 1120 O ARG A 73	8.630 -28.989 -31.776 1.00 13.79	0
ANISOU 1120 O ARG A 73	1862 1675 1705 168 -44 -11	0
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ATOM 1121 CB ARG A 73	5.316 -28.799 -32.458 1.00 14.91	С
ANISOU 1121 CB ARG A 73	1949 1816 1900 113 -184 -129	C
ATOM 1122 CG ARG A 73	3.911 -28.386 -32.038 1.00 15.99	C
ANISOU 1122 CG ARG A 73	2016 1979 2082 78 -221 -146	C
ATOM 1123 CD ARG A 73	3.052 -28.099 -33.263 1.00 18.03	C
		C
ANISOU 1123 CD ARG A 73		
ATOM 1124 NE ARG A 73	1.622 -28.033 -32.951 1.00 20.51	N
ANISOU 1124 NE ARG A 73	2506 2604 2683 77 -351 -258	N
ATOM 1125 CZ ARG A 73	0.896 -26.915 -32.896 1.00 21.16	C
ANISOU 1125 CZ ARG A 73	2555 2750 2737 111 -376 -254	С
ATOM 1126 NH1 ARG A 73	1.443 -25.729 -33.121 1.00 21.09	N
ANISOU 1126 NH1 ARG A 73	2606 2767 2641 174 -360 -213	N
ATOM 1127 NH2 ARG A 73	-0.393 -26.984 -32.608 1.00 21.80	N
ANISOU 1127 NH2 ARG A 73	2537 2861 2884 80 -414 -288	N
ATOM 1128 H ARG A 73	6.868 -27.171 -31.112 1.00 15.17	Н
ATOM 1129 HA ARG A 73	5.864 -29.655 -30.671 1.00 16.75	Н
ATOM 1130 HB2 ARG A 73	5.675 -28.095 -33.020 1.00 17.89	 H
ATOM 1131 HB3 ARG A 73	5.242 -29.620 -32.968 1.00 17.89	Н
ATOM 1132 HG2 ARG A 73	3.498 -29.106 -31.536 1.00 19.19	Н
	3.957 -27.580 -31.500 1.00 19.19	Н
ATOM 1134 HD2 ARG A 73	3.316 -27.245 -33.641 1.00 21.63	Н
ATOM 1135 HD3 ARG A 73	3.185 -28.805 -33.914 1.00 21.63	H
ATOM 1136 HE ARG A 73	1.217 -28.775 -32.792 1.00 24.61	Н

ATOM 1137 HH11 ARG A 73 2.280 -25.670 -33.310 1.00 25.31 ATOM 1138 HH12 ARG A 73 0.961 -25.018 -33.080 1.00 25.31 ATOM 1139 HH21 ARG A 73 -0.760 -27.747 -32.458 1.00 26.16 Н -0.864 -26.265 -32.569 1.00 26.16 ATOM 1140 HH22 ARG A 73 ATOM 1141 N SER A 74 7.512 -30.902 -32.184 1.00 14.44 **ANISOU 1141 N SER A 74** 1962 1659 1868 140 -100 -98 8.670 -31.613 -32.714 1.00 16.41 ATOM 1142 CA SER A 74 ANISOU 1142 CA SER A 74 C 2264 1885 2085 198 -74 -107 ATOM 1143 C SER A 74 9.820 -31.650 -31.707 1.00 15.06 ANISOU 1143 C SER A 74 2074 1728 1919 210 -9 -29 ATOM 1144 O SER A 74 10.917 -31.152 -32.003 1.00 15.21 ANISOU 1144 O SER A 74 2098 1799 1884 255 27 -4 ATOM 1145 CB SER A 74 9.118 -30.964 -34.024 1.00 19.09 ANISOU 1145 CB SER A 74 2648 2282 2323 266 -78 -134 ATOM 1146 OG SER A 74 10.084 -31.761 -34.682 1.00 21.17 ANISOU 1146 OG SER A 74 2963 2531 2549 336 -55 -158 0 ATOM 1147 H SER A 74
ATOM 1148 HA SER A 74
ATOM 1149 HB2 SER A 74
ATOM 1150 HB3 SER A 74 ATOM 1151 HG SER A 74 10.758 -31.860 -34.191 1.00 25.40 ATOM 1152 N PRO A 75 9.622 -32.244 -30.511 1.00 14.40 H N **ANISOU 1152 N PRO A 75** 1966 1606 1901 175 8 14 ATOM 1153 CA PRO A 75 8.366 -32.855 -30.058 1.00 14.62 1973 1571 2009 111 -13 6 **ANISOU 1153 CA PRO A 75** ATOM 1154 C PRO A 75 7.459 -31.896 -29.300 1.00 12.72 **ANISOU 1154 C PRO A 75** ANISOU 1154 O TRO. ATOM 1155 O PRO A 75 1670 1388 1774 64 -13 37 7.848 -30.774 -28.979 1.00 11.00 0 **ANISOU 1155 O PRO A 75** 1434 1243 1501 83 -2 ATOM 1156 CB PRO A 75 8.835 -33.979 -29.113 1.00 14.95 **ANISOU 1156 CB PRO A 75** 31 65 2030 1548 2103 118 ATOM 1157 CG PRO A 75 10.333 -33.770 -28.919 1.00 15.51 **ANISOU 1157 CG PRO A 75** 2114 1670 2108 193 64 100 10.688 -32.454 -29.515 1.00 14.07 ATOM 1158 CD PRO A 75 1910 1580 1855 205 55 80 C 7.883 -33.239 -30.806 1.00 17.54 H 8.369 -33.905 -28.266 1.00 17.94 H 8.662 -34.840 -29.523 1.00 17.94 H 10.536 -33.773 -27.970 1.00 18.61 ANISOU 1158 CD PRO A 75 ATOM 1159 HA PRO A 75 ATOM 1160 HB2 PRO A 75 ATOM 1161 HB3 PRO A 75 ATOM 1162 HG2 PRO A 75 ATOM 1163 HG3 PRO A 75 10.816 -34.482 -29.367 1.00 18.61 ATOM 1164 HD2 PRO A 75 10.663 -31.757 -28.840 1.00 16.88 ATOM 1165 HD3 PRO A 75 11.554 -32.500 -29.950 1.00 16.88 ATOM 1166 N LEU A 76 6.254 -32.380 -29.018 1.00 12.34 Ν 1585 1299 1803 **ANISOU 1166 N LEU A 76** 4 -25 30 5.273 -31.645 -28.231 1.00 12.06 **ATOM 1167 CA LEU A 76** ANISOU 1167 CA LEU A 76 1480 1321 1780 -32 -16 60 ATOM 1168 C LEU A 76 5.682 -31.623 -26.760 1.00 11.39

ANISOU 1171 CG LEU A 76	1376 1380 1942 -137 -28 52	С
ATOM 1172 CD1 LEU A 76	2.434 -30.275 -28.345 1.00 12.97	C
ANISOU 1172 CD1 LEU A 76	1443 1539 1945 -96 -82 -2	c
_	1.502 -32.533 -27.757 1.00 14.63	
		C
ANISOU 1173 CD2 LEU A 76	1590 1608 2360 -223 -36 34	C
ATOM 1174 H LEU A 76	5.976 -33.152 -29.277 1.00 14.80	Н
ATOM 1175 HA LEU A 76	5.220 -30.730 -28.551 1.00 14.47	Н
ATOM 1176 HB2 LEU A 76	3.698 -32.333 -29.339 1.00 15.98	Н
ATOM 1177 HB3 LEU A 76	3.955 -33.197 -28.040 1.00 15.98	Н
ATOM 1178 HG LEU A 76	2.944 -31.465 -26.776 1.00 14.84	Н
ATOM 1179 HD11 LEU A 76	1.679 -29.867 -27.892 1.00 15.56	Н
ATOM 1180 HD12 LEU A 76	3.217 -29.710 -28.258 1.00 15.56	H
ATOM 1181 HD13 LEU A 76	2.224 -30.409 -29.282 1.00 15.56	H
		H
	0.759 -32.090 -27.319 1.00 17.55	
ATOM 1183 HD22 LEU A 76	1.281 -32.713 -28.684 1.00 17.55	H
ATOM 1184 HD23 LEU A 76	1.711 -33.362 -27.299 1.00 17.55	Н.
	5.977 -30.433 -26.247 1.00 10.98	N
ANISOU 1185 N ILE A 77	1313 1299 1558 16 53 167	N
ATOM 1186 CA ILE A 77	6.420 -30.248 -24.871 1.00 11.63	C
ANISOU 1186 CA ILE A 77	1385 1431 1602 50 97 235	С
	5.828 -28.943 -24.368 1.00 12.13	Č
	1409 1577 1623 63 85 221	Č
ATOM 1188 O ILE A 77	5.844 -27.928 -25.075 1.00 11.90	Ö
	1385 1566 1569 70 41 168	0
ATOM 1189 CB ILE A 77	7.961 -30.222 -24.757 1.00 12.49	C
ANISOU 1189 CB ILE A 77	1532 1552 1661 104 98 245	C
ATOM 1190 CG1 ILE A 77	8.576 -31.514 -25.319 1.00 13.06	С
ANISOU 1190 CG1 ILE A 77	1648 1543 1770 112 109 251	С
ATOM 1191 CG2 ILE A 77	8.401 -29.991 -23.304 1.00 13.73	C
ANISOU 1191 CG2 ILE A 77	1675 1774 1766 152 123 299	C
ATOM 1192 CD1 ILE A 77	10.025 -31.377 -25.632 1.00 13.95	C
ANISOU 1192 CD1 ILE A 77	1782 1678 1840 166 103 241	Č
	5.928 -29.698 -26.691 1.00 13.17	н
ATOM 1193 II ILL A 77	6.082 -30.973 -24.321 1.00 13.17	'H
ATOM 1195 HB ILE A 77	8.287 -29.480 -25.290 1.00 14.99	Η
ATOM 1196 HG12 ILE A 77	8.477 -32.222 -24.664 1.00 15.67	H
ATOM 1197 HG13 ILE A 77	8.114 -31.753 -26.138 1.00 15.67	Н
ATOM 1198 HG21 ILE A 77	9.370 -29.980 -23.267 1.00 16.47	Н
ATOM 1199 HG22 ILE A 77	8.048 -29.141 -23.000 1.00 16.47	Н
ATOM 1200 HG23 ILE A 77	8.056 -30.710 -22.752 1.00 16.47	Н
ATOM 1201 HD11 ILE A 77	10.353 -32.221 -25.981 1.00 16.74	Н
ATOM 1202 HD12 ILE A 77	10.140 -30.678 -26.294 1.00 16.74	Н
ATOM 1203 HD13 ILE A 77	10.502 -31.147 -24.820 1.00 16.74	H
ATOM 1204 N ALA A 78	5.307 -28.972 -23.146 1.00 11.99	Ν
ANISOU 1204 N ALA A 78	1359 1607 1592 78 129 273	N
ATOM 1205 CA ALA A 78	4.898 -27.769 -22.434 1.00 12.41	C
ANISOU 1205 CA ALA A 78	1384 1745 1587 117 121 257	C
ATOM 1206 C ALA A 78	5.962 -27.405 -21.408 1.00 11.87	C
ANISOU 1206 C ALA A 78	1342 1728 1442 183 122 273	С
ATOM 1207 O ALA A 78	6.552 -28.287 -20.774 1.00 12.04	0
ANISOU 1207 O ALA A 78	1381 1744 1448 208 157 332	0
ATOM 1208 CB ALA A 78	3.555 -27.977 -21.731 1.00 12.93	С
ANISOU 1208 CB ALA A 78	1387 1852 1673 107 172 298	C
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ATOM 1209 H ALA A 78 5.177 -29.695 -22.699 1.00 14.39 Н ATOM 1210 HA ALA A 78
ATOM 1211 HB1 ALA A 78
ATOM 1212 HB2 ALA A 78
ATOM 1213 HB3 ALA A 78
3.312 -27.161 -21.267 1.00 15.51
3.641 -28.706 -21.096 1.00 15.51 н Н Н Н ATOM 1214 N TYR A 79 6.204 -26.106 -21.237 1.00 9.88 **ANISOU 1214 N TYR A 79** 1092 1519 1144 217 76 ATOM 1215 CA TYR A 79 7.160 -25.646 -20.245 1.00 10.69 C **ANISOU 1215 CA TYR A 79** 1208 1673 1179 278 55 206 ATOM 1216 C TYR A 79 6.580 -24.487 -19.440 1. ANISOU 1216 C TYR A 79 1371 1914 1297 332 6.580 -24.487 -19.440 1.00 12.06 ATOM 1217 O TYR A 79 5.671 -23.774 -19.888 1.00 11.27 ANISOU 1217 O TYR A 79 1258 1808 1218 320 20 124 C ATOM 1218 CB TYR A 79 8.489 -25.252 -20.898 1.00 10.57 ANISOU 1218 CB TYR A 79 1210 1623 1182 262 5 165 ATOM 1219 CG TYR A 79 8.418 -24.086 -21.832 1.00 10.44 ANISOU 1219 CG TYR A 79 1199 1568 1198 228 -37 107 CCCC 8.377 -22.784 -21.347 1.00 10.46 ATOM 1220 CD1 TYR A 79 ANISOU 1220 CD1 TYR A 79 1203 1592 1181 254 -82 49 ATOM 1221 CD2 TYR A 79 8.403 -24.273 -23.207 1.00 9.86 ANISOU 1221 CD2 TYR A 79 1140 1435 1171 180 -33 109 ATOM 1222 CE1 TYR A 79 8.319 -21.716 -22.195 1.00 9.76 ANISOU 1222 CE1 TYR A 79 1130 1450 1128 226 -115 11 ATOM 1223 CE2 TYR A 79 8.338 -23.209 -24.065 1.00 9.43 C 00000 ANISOU 1223 CE2 TYR A 79 1101 1347 1133 162 -63 75 ATOM 1224 CZ TYR A 79 8.307 -21.925 -23.561 1.00 10.69 ANISOU 1224 CZ TYR A 79 1263 1513 1285 181 -100 33 ATOM 1225 OH TYR A 79 8.239 -20.840 -24.414 1.00 10.95 ANISOU 1225 OH TYR A 79 1322 1494 1343 166 -124 13 0 ANISOU 1225 OH TYR A 79
ATOM 1226 H TYR A 79
ATOM 1227 HA TYR A 79
ATOM 1227 HA TYR A 79
ATOM 1228 HB2 TYR A 79
ATOM 1229 HB3 TYR A 79
ATOM 1230 HD1 TYR A 79
ATOM 1231 HD2 TYR A 79
ATOM 1232 HE1 TYR A 79
ATOM 1232 HE1 TYR A 79
ATOM 1233 HE2 TYR A 79
ATOM 1234 HH TYR A 79
ATOM 1235 N TYR A 80
ANISOU 1235 N TYR A 80
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ATOM 1235 N TYR A 80
ANISOU 1235 N TYR A 80 ATOM 1234 FIR TTR A 73 0.200 2.1101 2012 1.101 1 6.618 -23.397 -17.232 1.00 14.52 ATOM 1236 CA TYR A 80 ANISOU 1236 CA TYR A 80 1690 2373 1454 486 3 107 7.783 -22.828 -16.428 1.00 14.20 ATOM 1237 C TYR A 80 1670 2373 1354 547 -70 ANISOU 1237 C TYR A 80 41 ATOM 1238 O TYR A 80 8.638 -23.583 -15.954 1.00 15.02 0 ANISOU 1238 O TYR A 80 1778 2505 1424 576 -68 79 ATOM 1239 CB TYR A 80 5.638 -24.097 -16.271 1.00 16.36 1903 2688 1624 542 91 ANISOU 1239 CB TYR A 80 187 ATOM 1240 CG TYR A 80 4.600 -24.950 -16.952 1.00 16.93 ANISOU 1240 CG TYR A 80 1938 2719 1777 467 166 262 ATOM 1241 CD1 TYR A 80 4.892 -26.256 -17.333 1.00 17.34 ANISOU 1241 CD1 TYR A 80 1994 2709 1886 410 210 341 ATOM 1242 CD2 TYR A 80 3.332 -24.461 -17.216 1.00 17.50

ANISOU 1242 CD2 TYR A 80	1963 2810 1874 457 184 243	С
ATOM 1243 CE1 TYR A 80	3.957 -27.040 -17.967 1.00 17.77	C
ANISOU 1243 CE1 TYR A 80	2010 2711 2032 332 263 391	C
ATOM 1244 CE2 TYR A 80	2.387 -25.246 -17.850 1.00 18.62	C
ANISOU 1244 CE2 TYR A 80	2053 2917 2104 381 238 297	C
ATOM 1245 CZ TYR A 80	2.703 -26.531 -18.218 1.00 19.30	C
ANISOU 1245 CZ TYR A 80	2145 2932 2256 313 274 367	С
ATOM 1246 OH TYR A 80	1.762 -27.312 -18.852 1.00 21.67	ŏ
ANISOU 1246 OH TYR A 80	2390 3185 2661 229 313 403	Ö
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ATOM 1247 H TYR A 80	7.828 -24.751 -17.972 1.00 16.42	Η
ATOM 1248 HA TYR A 80	6.155 -22.665 -17.669 1.00 17.42	Н
ATOM 1249 HB2 TYR A 80	6.145 -24.670 -15.675 1.00 19.63	Н
ATOM 1250 HB3 TYR A 80	5.171 -23.421 -15.756 1.00 19.63	Н
ATOM 1251 HD1 TYR A 80	5.740 -26.601 -17.167 1.00 20.81	Н
ATOM 1252 HD2 TYR A 80	3.115 -23.591 -16.971 1.00 21.00	H
ATOM 1253 HE1 TYR A 80	4.168 -27.911 -18.217 1.00 21.33	H
ATOM 1254 HE2 TYR A 80	1.539 -24.906 -18.024 1.00 22.34	H
ATOM 1255 HH TYR A 80	1.046 -26.882 -18.942 1.00 26.01	Н
ATOM 1256 N VAL A 81	7.813 -21.509 -16.258 1.00 12.15	N
ANISOU 1256 N VAL A 81	1420 2112 1085 572 -142 -62	Ν
ATOM 1257 CA VAL A 81	8.727 -20.865 -15.312 1.00 12.89	С
ANISOU 1257 CA VAL A 81	1525 2252 1121 640 -227 -149	C
ATOM 1258 C VAL A 81	7.842 -20.123 -14.317 1.00 14.15	C
ANISOU 1258 C VAL A 81		C
		_
ATOM 1259 O VAL A 81	7.287 -19.068 -14.638 1.00 13.92	0
ANISOU 1259 O VAL A 81	1687 2414 1189 743 -270 -278	0
ATOM 1260 CB VAL A 81	9.721 -19.922 -15.998 1.00 13.67	C
ANISOU 1260 CB VAL A 81	1618 2259 1316 568 -315 -235	C
ATOM 1261 CG1 VAL A 81	10.633 -19.244 -14.972 1.00 13.97	С
ANISOU 1261 CG1 VAL A 81	1655 2343 1311 630 -419 -345	Č
ATOM 1262 CG2 VAL A 81	10.537 -20.686 -17.051 1.00 13.82	Č
		Č
ANISOU 1262 CG2 VAL A 81	1613 2218 1419 475 -286 -169	
ATOM 1263 H VAL A 81	7.309 -20.957 -16.683 1.00 14.58	Η
ATOM 1264 HA VAL A 81	9.228 -21.543 -14.833 1.00 15.47	Н
ATOM 1265 HB VAL A 81	9.225 -19.226 -16.457 1.00 16.40	Н
ATOM 1266 HG11 VAL A 81	11.248 -18.656 -15.437 1.00 16.77	Н
ATOM 1267 HG12 VAL A 81	10.087 -18.732 -14.356 1.00 16.77	Н
ATOM 1268 HG13 VAL A 81	11.126 -19.926 -14.490 1.00 16.77	H
ATOM 1269 HG21 VAL A 81	11.159 -20.074 -17.473 1.00 16.58	H
ATOM 1203 HG22 VAL A 81	11.022 -21.404 -16.614 1.00 16.58	H
ATOM 1271 HG23 VAL A 81	9.931 -21.052 -17.714 1.00 16.58	Н
ATOM 1272 N VAL A 82	7.704 -20.673 -13.112 1.00 14.46	N _.
ANISOU 1272 N VAL A 82	1751 2648 1094 857 -204 -173	N
ATOM 1273 CA VAL A 82	6.778 -20.157 -12.106 1.00 16.35	C
ANISOU 1273 CA VAL A 82	2007 2988 1216 982 -187 -209	С
ATOM 1274 C VAL A 82	7.521 -19.180 -11.200 1.00 17.22	C
ANISOU 1274 C VAL A 82	2149 3137 1255 1075 -309 -357	C
ATOM 1275 O VAL A 82	8.495 -19.557 -10.538 1.00 17.39	o
ANISOU 1275 O VAL A 82	2170 3186 1253 1105 -340 -365	0
ATOM 1276 CB VAL A 82	6.166 -21.300 -11.282 1.00 18.01	C
ANISOU 1276 CB VAL A 82	2211 3314 1318 1059 -66 -75	C
ATOM 1277 CG1 VAL A 82	5.183 -20.749 -10.230 1.00 19.61	С
ANISOU 1277 CG1 VAL A 82	2414 3616 1420 1187 -32 -101	С
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ATOM 1278 CG2 VAL A 82	5.470 -22.300 -12.184 1.00 17.40	С
ANISOU 1278 CG2 VAL A 82	2093 3174 1343 947 44 58	Č
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ATOM 1279 H VAL A 82	8.146 -21.362 -12.848 1.00 17.35	Н
ATOM 1280 HA VAL A 82	6.059 -19.679 -12.547 1.00 19.62	Н
ATOM 1281 HB VAL A 82	6.876 -21.765 -10.813 1.00 21.61	Н
ATOM 1282 HG11 VAL A 82	4.813 -21.491 -9.725 1.00 23.53	Н
ATOM 1283 HG12 VAL A 82	5.662 -20.151 -9.635 1.00 23.53	Н
ATOM 1284 HG13 VAL A 82	4.473 -20.269 -10.682 1.00 23.53	Н
ATOM 1285 HG21 VAL A 82	5.094 -23.008 -11.638 1.00 20.88	Н
ATOM 1286 HG22 VAL A 82	4.764 -21.847 -12.671 1.00 20.88	H
ATOM 1287 HG23 VAL A 82	6.118 -22.668 -12.805 1.00 20.88	Н
ATOM 1288 N ASP A 83	7.050 -17.932 -11.153 1.00 18.06	N
ANISOU 1288 N ASP A 83	2276 3209 1378 1106 -364 -473	N
ATOM 1289 CA ASP A 83	7.651 -16.897 -10.316 1.00 20.07	C
ANISOU 1289 CA ASP A 83	2550 3444 1632 1169 -471 -615	C
ATOM 1290 C ASP A 83	6.918 -16.685 -9.001 1.00 21.26	C
ANISOU 1290 C ASP A 83	2709 3699 1670 1324 -442 -628	С
ATOM 1291 O ASP A 83	7.555 -16.353 -7.995 1.00 22.87	0
ANISOU 1291 O ASP A 83	2923 3934 1832 1404 -510 -707	O
		_
ATOM 1292 CB ASP A 83	7.704 -15.560 -11.068 1.00 20.70	C
ANISOU 1292 CB ASP A 83	2652 3389 1823 1106 -565 -736	С
ATOM 1293 CG ASP A 83	9.037 -15.322 -11.765 1.00 20.37	С
ANISOU 1293 CG ASP A 83	2595 3239 1905 982 -657 -786	C
ATOM 1294 OD1 ASP A 83	9.951 -16.156 -11.607 1.00 20.75	ŏ
ANISOU 1294 OD1 ASP A 83	2610 3328 1945 956 -655 -740	0
ATOM 1295 OD2 ASP A 83	9.179 -14.283 -12.453 1.00 19.99	0
ANISOU 1295 OD2 ASP A 83	2566 3061 1970 913 -727 -866	0
ATOM 1296 H ASP A 83	6.372 -17.658 -11.606 1.00 21.68	Н
ATOM 1297 HA ASP A 83	8.562 -17.156 -10.108 1.00 24.08	H.
ATOM 1298 HB2 ASP A 83	7.008 -15.550 -11.743 1.00 24.84	Н
ATOM 1299 HB3 ASP A 83	7.564 -14.837 -10.437 1.00 24.84	Н
ATOM 1300 N SER A 84	5.598 -16.854 -8.978 1.00 19.98	N
ANISOU 1300 N SER A 84	2536 3597 1459 1370 -347 -552	N
ATOM 1301 CA SER A 84	4.848 -16.732 -7.738 1.00 19.81	
		C
ANISOU 1301 CA SER A 84	2512 3687 1327 1517 -313 -539	С
ATOM 1302 C SER A 84	3.622 -17.622 -7.825 1.00 19.63	С
ANISOU 1302 C SER A 84	2450 3745 1265 1518 -167 -379	С
ATOM 1303 O SER A 84	3.286 -18.154 -8.891 1.00 18.39	0
ANISOU 1303 O SER A 84	2268 3545 1175 1408 -102 -304	Õ
ATOM 1304 CB SER A 84	4.439 -15.281 -7.457 1.00 21.11	C
ANISOU 1304 CB SER A 84	2706 3818 1498 1589 -403 -677	С
ATOM 1305 OG SER A 84	3.914 -15.157 -6.139 1.00 22.47	0
ANISOU 1305 OG SER A 84	2880 4109 1548 1746 -388 -675	0
	5.117 -17.039 -9.666 1.00 23.98	
		Н.
ATOM 1307 HA SER A 84	5.396 -17.042 -7.000 1.00 23.77	H.
ATOM 1308 HB2 SER A 84	5.219 -14.711 -7.543 1.00 25.34	Н
ATOM 1309 HB3 SER A 84	3.760 -15.014 -8.096 1.00 25.34	Н
ATOM 1310 HG SER A 84		Н
ATOM 1311 N TRP A 85	3.693 =14.360 =5.993 1 00 /6 96	
	3.693 -14.360 -5.993 1.00 26.96 2 937 -17 751 -6 694 1 00 22 59	N
	2.937 -17.751 -6.694 1.00 22.59	N
ANISOU 1311 N TRP A 85	2.937 -17.751 -6.694 1.00 22.59 2816 4232 1536 1640 -115 -329	N
ANISOU 1311 N TRP A 85 ATOM 1312 CA TRP A 85	2.937 -17.751 -6.694 1.00 22.59 2816 4232 1536 1640 -115 -329 1.761 -18.599 -6.606 1.00 23.69	N C
ANISOU 1311 N TRP A 85	2.937 -17.751 -6.694 1.00 22.59 2816 4232 1536 1640 -115 -329	N
ANISOU 1311 N TRP A 85 ATOM 1312 CA TRP A 85	2.937 -17.751 -6.694 1.00 22.59 2816 4232 1536 1640 -115 -329 1.761 -18.599 -6.606 1.00 23.69	N C

ANISOU 1313 C TRP A 85 3191 4845 1812 1791 53 -163 C ATOM 1314 O TRP A 85 1.464 -17.453 -4.507 1.00 28.80 ANISOU 1314 O TRP A 85 3595 5237 2110 1908 -44 -2 0 **ANISOU 1314 O TRP A 85** 3595 5237 2110 1908 -44 -280 0 ATOM 1315 CB TRP A 85 2.150 -20.080 -6.619 1.00 23.43 ANISOU 1315 CB TRP A 85 2859 4419 1623 1576 122 -16 ATOM 1316 CG TRP A 85 3.033 -20.462 -5.472 1.00 24.45 ANISOU 1316 CG TRP A 85 3020 4604 1663 1680 97 -11 ATOM 1317 CD1 TRP A 85 2.638 -20.951 -4.255 1.00 27.12 **ANISOU 1317 CD1 TRP A 85** 3358 5048 1896 1801 4.461 -20.367 -5.421 1.00 24.80 ATOM 1318 CD2 TRP A 85 C **ANISOU 1318 CD2 TRP A 85** 3099 4607 1717 1680 -6 -104 ATOM 1319 NE1 TRP A 85 3.738 -21.170 -3.451 1.00 28.16 Ν 3526 5209 1963 1887 Ν **ANISOU 1319 NE1 TRP A 85** ATOM 1320 CE2 TRP A 85 4.868 -20.823 -4.145 1.00 26.94 ANISOU 1320 CE2 TRP A 85 3388 4967 1881 1810 5.437 -19.946 -6.330 1.00 24.35 ATOM 1321 CE3 TRP A 85 C **ANISOU 1321 CE3 TRP A 85** 3055 4448 1749 1581 -103 -209 C ATOM 1322 CZ2 TRP A 85 6.207 -20.866 -3.761 1.00 27.55 **ANISOU 1322 CZ2 TRP A 85** 3490 5037 1940 1843 -82 -150 C ATOM 1323 CZ3 TRP A 85 6.765 -19.991 -5.945 1.00 24.71 **ANISOU 1323 CZ3 TRP A 85** 3121 4484 1786 1600 -187 -281 ATOM 1324 CH2 TRP A 85 7.139 -20.446 -4.671 1.00 26.33 **ANISOU 1324 CH2 TRP A 85** 3338 4782 1883 1732 -178 -256 ATOM 1325 H TRP A 85 3.137 -17.352 -5.958 1.00 27.11 Н 1.181 -18.427 -7.364 1.00 28.42 ATOM 1326 HA TRP A 85 1.344 -20.618 -6.568 1.00 28.12 ATOM 1327 HB2 TRP A 85 ATOM 1328 HB3 TRP A 85 2.626 -20.274 -7.441 1.00 28.12 Н ATOM 1329 HD1 TRP A 85 1.756 -21.111 -4.006 1.00 32.54 3.718 -21.479 -2.040 1.00 29.22 5.198 -19.642 -7.175 1.00 29.22 3.718 -21.479 -2.648 1.00 33.79 ATOM 1330 HE1 TRP A 85 Н ATOM 1331 HE3 TRP A 85 ATOM 1332 HZ2 TRP A 85 Н 6.457 -21.168 -2.918 1.00 33.06 ATOM 1333 HZ3 TRP A 85 7.423 -19.713 -6.542 1.00 29.66 ATOM 1334 HH2 TRP A 85 8.040 -20.466 -4.441 1.00 31.59 ATOM 1335 N GLY A 86 -0.167 -18.856 -5.183 1.00 33.21 ANISOU 1335 N GLY A 86 3618 5050 3950 2020 1365 1400 ATOM 1336 CA GLY A 86 -0.946 -18.693 -3.973 1.00 35.92 C ANISOU 1336 CA GLY A 86 4038 5399 4212 2270 1670 1603 ATOM 1337 C GLY A 86 ANISOU 1337 C GLY A 86 -0.600 -19.769 -2.972 1.00 37.18 4293 5505 4328 2291 1822 1707 ATOM 1338 O GLY A 86 0.386 -19.650 -2.238 1.00 37.23 0 ANISOU 1338 O GLY A 86 4648 5469 4030 2407 1790 1597 ATOM 1339 H GLY A 86 -0.529 -19.368 -5.771 1.00 39.85 ATOM 1340 HA2 GLY A 86 -0.764 -17.826 -3.578 1.00 43.10 Н ATOM 1341 HA3 GLY A 86 -1.892 -18.750 -4.180 1.00 43.10 ATOM 1342 N THR A 87 -1.398 -20.832 -2.943 1.00 39.67 Ν **ANISOU 1342 N THR A 87** 4312 5805 4957 2171 1961 1908 ATOM 1343 CA THR A 87 -1.127 -22.010 -2.129 1.00 41.63 ANISOU 1343 CA THR A 87 4620 5978 5217 2164 2106 2019 ATOM 1344 C THR A 87 -0.888 -23.180 -3.071 1.00 41.53 ANISOU 1344 C THR A 87 4308 5966 5507 1855 1994 1993 ATOM 1345 O THR A 87 -1.785 -23.564 -3.829 1.00 42.37 ANISOU 1345 O THR A 87 4051 6071 5976 1665 1956 2075 ATOM 1346 CB THR A 87 -2.288 -22.301 -1.172 1.00 45.50

ANISOU 1346 CB THR A 87 5061 6397 5831 2307 2389 2297 ATOM 1347 OG1 THR A 87 -2.490 -21.174 -0.306 1.00 47.29 ANISOU 1347 OG1 THR A 87 5596 6611 5760 2612 2482 5596 6611 5760 2612 2482 2330 O ATOM 1348 CG2 THR A 87 -2.004 -23.536 -0.327 1.00 46.79 C ANISOU 1348 CG2 THR A 87 5309 6455 6014 2327 2539 2409 C ATOM 1349 H THR A 87 -2.124 -20.895 -3.400 1.00 47.61 H ATOM 1350 HA THR A 87 -0.323 -21.865 -1.605 1.00 49.95 H ATOM 1351 HB THR A 87 -3.095 -22.461 -1.685 1.00 54.60 H ATOM 1351 HB 1HR A 67 -3.093 -22.401 -1.003 1.00 34.60
ATOM 1352 HG1 THR A 87 -2.672 -20.491 -0.761 1.00 56.74
ATOM 1353 HG21 THR A 87 -2.747 -23.706 0.272 1.00 56.15
ATOM 1355 HG23 THR A 87 -1.200 -23.400 0.199 1.00 56.15
ATOM 1355 HG23 THR A 87 -1.200 -23.400 0.199 1.00 56.15 Н ATOM 1356 N ALA A 88 0.320 -23.734 -3.035 1.00 41.21 N **ANISOU 1356 N ALA A 88** 4437 5912 5309 1797 1908 1871 N ATOM 1357 CA ALA A 88 0.675 -24.837 -3.916 1.00 41.88 ANISOU 1357 CA ALA A 88 4349 5938 5624 1468 1721 1811 ATOM 1358 C ALA A 88 1.895 -25.547 -3.353 1.00 42.69 C ANISOU 1358 C ALA A 88 4733 5988 5498 1475 1697 1738 C ATOM 1359 O ALA A 88 2.863 -24.899 -2.948 1.00 41.83 O ANISOU 1359 O ALA A 88 4940 5897 5055 1607 1584 1580 O ATOM 1360 CB ALA A 88 0.967 -24.347 -5.337 1.00 39.36 C ANISOU 1360 CB ALA A 88 3953 5632 5371 1247 1356 1592 C ATOM 1361 H ALA A 88
ATOM 1362 HA ALA A 88
ATOM 1363 HB1 ALA A 88
ATOM 1364 HB2 ALA A 88
ATOM 1365 HB3 ALA A 88
ATOM 1366 N ARG A 89
ANISOU 1366 N ARG A 89
ATOM 1367 CA ARG A 89
ATOM 1368 C ARG A 89
ATOM 1367 CA ARG A 89 ATOM 1367 CA ARG A 89 2.988 -27.690 -2.947 1.00 46.16 ANISOU 1367 CA ARG A 89 5290 6301 5947 1322 1756 1790 ATOM 1368 C ARG A 89 3.568 -28.283 -4.219 1.00 44.41 C ANISOU 1368 C ARG A 89 4974 6027 5874 1002 1461 1637 ATOM 1369 O ARG A 89 2.875 -28.999 -4.949 1.00 47.26 O ANISOU 1369 O ARG A 89 5069 6323 6565 782 1445 1707 ATOM 1370 CB ARG A 89 2.624 -28.813 -1.973 1.00 49.37 C ANISOU 1370 CB ARG A 89 5705 6629 6426 1419 2082 2022 ATOM 1371 CG ARG A 89 1.346 -28.643 -1.152 1.00 52.66 C ANISOU 1371 CG ARG A 89 6040 6989 6977 1591 2315 2208 ATOM 1372 CD ARG A 89 1.565 -27.938 0.190 1.00 53.65 C ANISOU 1372 CD ARG A 89 6522 7115 6748 1963 2417 2213 ATOM 1373 NE ARG A 89 2.741 -28.402 0.923 1.00 52.39 ANISOU 1373 NE ARG A 89 6684 6923 6300 2092 2366 2116 ATOM 1374 CZ ARG A 89 3.168 -27.856 2.058 1.00 53.05 ANISOU 1374 CZ ARG A 89 7103 6989 6065 2405 2370 2064 ATOM 1375 NH1 ARG A 89 2.510 -26.839 2.594 1.00 54.12 7327 7124 6112 2622 2445 2118 N **ANISOU 1375 NH1 ARG A 89** ATOM 1376 NH2 ARG A 89 4.251 -28.326 2.662 1.00 52.97 N ANISOU 1376 NH2 ARG A 89 7343 6951 5833 2506 2281 1955 ATOM 1377 H ARG A 89 1.147 -27.333 -3.542 1.00 54.07 H ATOM 1378 HA ARG A 89 3.662 -27.129 -2.532 1.00 55.39 H ATOM 1380 HB3 ARG A 89 3.355 -28.914 -1.344 1.00 59.25 H

ATOM 1381 HG2 ARG A 89	0.713 -28.116 -1.664 1.00 63.19	Н
ATOM 1382 HG3 ARG A 89	0.973 -29.519 -0.969 1.00 63.19	Н
ATOM 1383 HD2 ARG A 89	1.673 -26.988 0.029 1.00 64.38	Н
ATOM 1384 HD3 ARG A 89	0.789 -28.090 0.752 1.00 64.38	Н
ATOM 1385 HE ARG A 89	3.124 -29.123 0.654 1.00 62.87	Η
ATOM 1386 HH11 ARG A 89	1.809 -26.528 2.205 1.00 64.94	Н
ATOM 1387 HH12 ARG A 89	2.786 -26.488 3.329 1.00 64.94	Н
ATOM 1388 HH21 ARG A 89	4.680 -28.988 2.320 1.00 63.56	Ĥ
ATOM 1389 HH22 ARG A 89	4.520 -27.973 3.398 1.00 63.56	. Н
ATOM 1390 N TRP A 90	4.825 -27.984 -4.484 1.00 39.86	N
ANISOU 1390 N TRP A 90	4616 5466 5064 985 1227 1433	N
ATOM 1391 CA TRP A 90	5.489 -28.495 -5.667 1.00 36.70	C
ANISOU 1391 CA TRP A 90	4179 5008 4757 733 976 1296	С
ATOM 1392 C TRP A 90	6.059 -29.870 -5.344 1.00 39.48	C
ANISOU 1392 C TRP A 90	4612 5280 5109 686 1060 1366	С
ATOM 1393 O TRP A 90	6.743 -30.042 -4.328 1.00 39.19	0
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ANISOU 1393 O TRP A 90	4789 5265 4838 873 1162 1391	0
ATOM 1394 CB TRP A 90	6.554 -27.501 -6.118 1.00 32.04	С
ANISOU 1394 CB TRP A 90	3757 4461 3955 746 727 1076	С
ATOM 1395 CG TRP A 90	5.943 -26.122 -6.251 1.00 30.18	C
ANISOU 1395 CG TRP A 90	3484 4290 3692 835 694 1029	С
ATOM 1396 CD1 TRP A 90	6.066 -25.076 -5.379 1.00 30.56	С
ANISOU 1396 CD1 TRP A 90	3706 4396 3511 1060 747 996	С
ATOM 1397 CD2 TRP A 90	5.081 -25.668 -7.301 1.00 28.43	C
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ANISOU 1397 CD2 TRP A 90	3059 4073 3670 720 599 1011	С
ATOM 1398 NE1 TRP A 90	5.346 -23.992 -5.834 1.00 29.61	Ν
ANISOU 1398 NE1 TRP A 90	3506 4310 3435 1090 714 967	N
ATOM 1399 CE2 TRP A 90	4.732 -24.331 -7.011 1.00 28.45	C
		_
ANISOU 1399 CE2 TRP A 90	3118 4142 3550 890 623 979	С
ATOM 1400 CE3 TRP A 90	4.580 -26.256 -8.466 1.00 27.61	С
ANISOU 1400 CE3 TRP A 90	2756 3913 3820 505 475 1009	С
ATOM 1401 CZ2 TRP A 90	3.906 -23.578 -7.846 1.00 27.16	С
ANISOU 1401 CZ2 TRP A 90	2802 4005 3512 861 546 960	C
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ATOM 1402 CZ3 TRP A 90	3.758 -25.501 -9.295 1.00 26.76	C
ANISOU 1402 CZ3 TRP A 90	2498 3835 3835 477 366 977	С
ATOM 1403 CH2 TRP A 90	3.430 -24.183 -8.978 1.00 26.31	C
ANISOU 1403 CH2 TRP A 90	2484 3858 3653 658 413 960	C
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ATOM 1404 H TRP A 90	5.321 -27.482 -3.991 1.00 47.83	H.
ATOM 1405 HA TRP A 90	4.841 -28.594 -6.382 1.00 44.04	Н
ATOM 1406 HB2 TRP A 90	7.264 -27.462 -5.457 1.00 38.44	Н
ATOM 1407 HB3 TRP A 90	6.905 -27.768 -6.981 1.00 38.44	Н
		H
ATOM 1408 HD1 TRP A 90	6.565 -25.092 -4.595 1.00 36.68	
ATOM 1409 HE1 TRP A 90	5.289 -23.229 -5.441 1.00 35.53	Н
ATOM 1410 HE3 TRP A 90	4.794 -27.134 -8.683 1.00 33.13	Н
ATOM 1411 HZ2 TRP A 90	3.687 -22.698 -7.640 1.00 32.59	Н
ATOM 1412 HZ3 TRP A 90	3.417 -25.883 -10.071 1.00 32.11	Ĥ
ATOM 1413 HH2 TRP A 90	2.877 -23.702 -9.552 1.00 31.57	H
ATOM 1414 N THR A 91	5.712 -30.854 -6.173 1.00 41.83	N
ANISOU 1414 N THR A 91	4754 5473 5666 454 1018 1402	Ν
ATOM 1415 CA THR A 91	6.057 -32.249 -5.945 1.00 42.84	C.
ANISOU 1415 CA THR A 91	4946 5492 5840 391 1126 1491	C
ATOM 1416 C THR A 91	6.330 -32.910 -7.287 1.00 39.22	С
ANISOU 1416 C THR A 91	4448 4923 5530 133 897 1386	С
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ATOM 1417 O THR A 91 5.721 -32.560 -8.299 1.00 41.08 ANISOU 1417 O THR A 91 4525 5140 5945 -19 722 1316 ATOM 1418 CB THR A 91 5.343 5976 6622 408 1442 1737 ATOM 1419 OG1 THR A 91 4.798 -32.495 -3.875 1.00 48.91 5674 6273 6637 707 1695 1852 5.183 -34.497 -5.150 1.00 47.92 **ANISOU 1419 OG1 THR A 91** ATOM 1420 CG2 THR A 91 ANISOU 1420 CG2 THR A 91
ATOM 1421 H THR A 91
ATOM 1422 HA THR A 91
ATOM 1423 HB THR A 91
ATOM 1424 HG1 THR A 91
ATOM 1425 HG21 THR A 91
ATOM 1426 HG22 THR A 91
ATOM 1427 HG23 THR A 91 ANISOU 1420 CG2 THR A 91 5487 5911 6807 302 1550 1830 C Н 3862 4089 4676 111 897 1376 **ANISOU 1428 N GLY A 92** Ν ATOM 1429 CA GLY A 92 7.498 -34.689 -8.452 1.00 29.09 ANISOU 1429 CA GLY A 92 3356 3426 4272 -101 728 1304 ATOM 1430 C GLY A 92 8.980 -34.864 -8.707 1.00 25.51 ANISOU 1430 C GLY A 92 3138 2979 3574 -41 623 1199 C ATOM 1431 O GLY A 92 9.826 -34.549 -7.868 1.00 23.42 ANISOU 1431 O GLY A 92 3003 2817 3078 149 683 1195 ATOM 1432 H GLY A 92 7.755 -34.056 -6.618 1.00 39.88 0 Н 7.101 -35.565 -8.322 1.00 34.91 7.096 -34.279 -9.233 1.00 34.91 ATOM 1433 HA2 GLY A 92 Н ATOM 1434 HA3 GLY A 92 ATOM 1435 N THR A 93 9.294 -35.386 -9.895 1.00 23.87 **ANISOU 1435 N THR A 93** 2991 2651 3426 -193 454 1114 ATOM 1436 CA THR A 93 10.682 -35.622 -10.262 1.00 22.25 ANISOU 1436 CA THR A 93 2992 2436 3024 -133 379 1039 ATOM 1437 C THR A 93 11.445 -34.304 -10.299 1.00 19.80 ANISOU 1437 C THR A 93 2699 2275 2547 -18 268 925 ATOM 1438 O THR A 93 10.989 -33.320 -10.892 1.00 19.18 ANISOU 1438 O THR A 93 2531 2236 2522 -62 146 841 ATOM 1439 CB THR A 93 10.770 -36.334 -11.616 1.00 22.99 0 ANISOU 1439 CB THR A 93 3177 2356 3201 -290 228 974 ATOM 1440 OG1 THR A 93 10.182 -37.635 -11.506 1.00 26.89 **ANISOU 1440 OG1 THR A 93** 3682 2681 3853 -406 325 1074 ATOM 1441 CG2 THR A 93 12.226 -36.491 -12.055 1.00 21.83 ANISOU 1441 CG2 THR A 93 3235 2202 2856 -197 182 919 ATOM 1442 H THR A 93 8.723 -35.610 -10.498 1.00 28.64 ATOM 1443 HA THR A 93 11.095 -36.191 -9.594 1.00 26.70 ATOM 1444 HB THR A 93 10.297 -35.818 -12.287 1.00 27.58 Н Н Н ATOM 1445 HG1 THR A 93 9.376 -37.568 -11.280 1.00 32.26 ATOM 1446 HG21 THR A 93 12.266 -36.942 -12.913 1.00 26.19 ATOM 1447 HG22 THR A 93 12.642 -35.619 -12.139 1.00 26.19 ATOM 1448 HG23 THR A 93 12.715 -37.013 -11.401 1.00 26.19 ATOM 1449 N TYR A 94 12.623 -34.312 -9.678 1.00 19.14 Ν ANISOU 1449 N TYR A 94 2732 2265 2276 130 304 924 ATOM 1450 CA TYR A 94 13.408 -33.124 -9.380 1.00 18.26 ANISOU 1450 CA TYR A 94 2625 2286 2025 246 215 831 ATOM 1451 C TYR A 94 14.793 -33.279 -9.985 1.00 19.09 ANISOU 1451 C TYR A 94 2824 2373 2057 267 129 779 C C

ATOM 1452 O TYR A 94 15.478 -34.279 -9.734 1.00 18.43 0 ANISOU 1452 O TYR A 94 2836 2256 1909 326 198 84 ATOM 1453 CB TYR A 94 13.509 -32.917 -7.864 1.00 20.26 198 847 ANISOU 1453 CB TYR A 94 2911 2652 2135 433 319 8 ATOM 1454 CG TYR A 94 14.548 -31.910 -7.459 1.00 19.64 884 ANISOU 1454 CG TYR A 94 2871 2683 1908 552 777 190 14.369 -30.564 -7.726 1.00 18.44 ATOM 1455 CD1 TYR A 94 ANISOU 1455 CD1 TYR A 94 2657 2577 1771 530 77 669 ATOM 1456 CD2 TYR A 94 15.709 -32.303 -6.800 1.00 20.94 ANISOU 1456 CD2 TYR A 94 3129 2895 1931 688 169 784 ATOM 1457 CE1 TYR A 94 15.318 -29.635 -7.362 1.00 18.97 ANISOU 1457 CE1 TYR A 94 2755 2713 1740 612 -56 563 ATOM 1458 CE2 TYR A 94 16.666 -31.371 -6.424 1.00 20.98 ANISOU 1458 CE2 TYR A 94 3140 2987 1844 776 9 676 ATOM 1459 CZ TYR A 94 16.460 -30.041 -6.713 1.00 20.24 ANISOU 1459 CZ TYR A 94 C 2984 2916 1791 724 -103 563 ATOM 1460 OH TYR A 94 17.393 -29.101 -6.348 1.00 21.51 ANISOU 1460 OH TYR A 94 3146 3132 1895 784 -274 448 0 13.003 -35.035 -9.408 1.00 22.97 ATOM 1461 H TYR A 94 Н ATOM 1462 HA TYR A 94 12.983 -32.345 -9.772 1.00 21.91 Н ATOM 1463 HB2 TYR A 94 12.651 -32.608 -7.533 1.00 24.31 ATOM 1464 HB3 TYR A 94 13.737 -33.763 -7.448 1.00 24.31 Н Н Ь Н . У ATOM 1465 HD1 TYR A 94
ATOM 1466 HD2 TYR A 94
ATOM 1467 HE1 TYR A 94
ATOM 1468 HE2 TYR A 94 ATOM 1469 HIT LINES ATOM 1470 N LYS A 95 15.210 -32.283 -10.76. 20114470 N LYS A 95 2759 2352 2035 237 ATOM 1469 HH TYR A 94 18.040 -29.472 -5.962 1.00 25.81 15.210 -32.283 -10.767 1.00 18.81 Ν 1 675 Ν 16.407 -32.391 -11.584 1.00 20.52 C ANISOU 1471 CA LYS A 95 3040 2522 2234 245 -49 649 CCOO ATOM 1472 C LYS A 95 17.560 -31.511 -11.127 1.00 20.12 ANISOU 1472 C LYS A 95 2941 2573 2131 338 -115 596 18.702 -31.776 -11.510 1.00 21.52 ATOM 1473 O LYS A 95 **ANISOU 1473 O LYS A 95** 3140 2729 2309 377 -119 616 ATOM 1474 CB LYS A 95 16.073 -32.036 -13.042 1.00 22.21 ANISOU 1474 CB LYS A 95 3281 2630 2528 145 -122 590 ATOM 1475 CG LYS A 95 15.196 -33.053 -13.734 1.00 24.70 ANISOU 1475 CG LYS A 95 3671 2807 2908 44 -118 623 C ATOM 1476 CD LYS A 95 15.924 -34.368 -13.880 1.00 26.74 ANISOU 1476 CD LYS A 95 4076 2968 3115 76 -42 698 C ATOM 1477 CE LYS A 95 15.263 -35.267 -14.881 1.00 28.34 C ANISOU 1477 CE LYS A 95 4410 2984 3376 -28 -85 696 ATOM 1478 NZ LYS A 95 15.958 -36.570 -14.900 1.00 29.77 Ν ANISOU 1478 NZ LYS A 95 4764 3059 3490 20 **12 776** Ν ATOM 1479 H LYS A 95 14.808 -31.526 -10.840 1.00 22.57 Н ATOM 1480 HA LYS A 95 16.713 -33.311 -11.566 1.00 24.62 Н Н ATOM 1481 HB2 LYS A 95 15.608 -31.185 -13.057 1.00 26.65 ATOM 1482 HB3 LYS A 95 16.900 -31.968 -13.544 1.00 26.65 ATOM 1483 HG2 LYS A 95 14.396 -33.203 -13.206 1.00 29.64 H ATOM 1484 HG3 LYS A 95 14.963 -32.731 -14.618 1.00 29.64 H ATOM 1485 HD2 LYS A 95 16.831 -34.198 -14.178 1.00 32.08 H ATOM 1486 HD3 LYS A 95 15.933 -34.824 -13.024 1.00 32.08 H

ATOM 1487 HE2 LYS A 95
ATOM 1488 HE3 LYS A 95
ATOM 1489 HZ1 LYS A 95
ATOM 1490 HZ2 LYS A 95
ATOM 1491 HZ3 LYS A 95
ATOM 1492 N GLY A 96
ANISOU 1493 CA GLY A 96 Н Ν C ANISOU 1493 CA GLY A 96 2451 2357 1702 437 -276 459 ATOM 1494 C GLY A 96 17.782 -28.177 -9.854 1.00 16.80 ANISOU 1494 C GLY A 96 2369 2338 1674 411 -349 359 ATOM 1495 O GLY A 96 16.575 -27.985 -9.739 1.00 16.49 O ANISOU 1495 O GLY A 96 2337 2306 1624 396 -302 366 O ATOM 1496 H GLY A 96 16.528 -30.305 -10.018 1.00 21.85 H ATOM 1497 HA2 GLY A 96 18.693 -29.826 -9.072 1.00 20.56 ATOM 1498 HA3 GLY A 96 19.063 -29.826 -9.072 1.00 20.56 HATOM 1499 N THR A 97 18.670 -27.195 -9.941 1.00 17.58 N ANISOU 1499 N THR A 97 2418 2440 1821 405 -456 276 N ATOM 1500 CA THR A 97 18.298 -25.805 -9.745 1.00 17.73 C ANISOU 1500 CA THR A 97 2430 2466 1842 394 -532 171 C ATOM 1501 C THR A 97 18.295 24.004 40.005 4.005 24.004 ATOM 1500 CA THR A 97
ANISOU 1500 CA THR A 97
ANISOU 1501 C THR A 97
ANISOU 1501 C THR A 97
ANISOU 1501 C THR A 97
ANISOU 1502 O THR A 97
ANISOU 1502 O THR A 97
ANISOU 1503 CB THR A 97
ANISOU 1503 CB THR A 97
ANISOU 1503 CB THR A 97
ANISOU 1504 OG1 THR A 97
ANISOU 1505 CG2 THR A 97
ATOM 1505 CG2 THR A 97
ATOM 1505 CG2 THR A 97
ATOM 1506 H THR A 97
ATOM 1507 HA THR A 97
ATOM 1508 HB THR A 97
ATOM 1509 HG1 THR A 97
ATOM 1511 HG22 THR A 97
ATOM 1511 HG22 THR A 97
ATOM 1513 N VAL A 98
ANISOU 1500 CA THR A 97
ANISOU 1500 C THR ATOM 1513 N VAL A 98 18.364 -23.775 -11.072 1.00 15.70 ANISOU 1513 N VAL A 98 2136 2084 1744 277 -586 47 ATOM 1514 CA VAL A 98 18.955 -22.773 -11.957 1.00 16.07 C ANISOU 1514 CA VAL A 98 2152 2029 1924 210 -598 0 C CCCO ANISOU 1514 CA VAL A 98 2152 2029 1924 210 -598 0 C ATOM 1515 C VAL A 98 18.812 -21.404 -11.308 1.00 16.52 C ANISOU 1515 C VAL A 98 2236 2078 1963 218 -694 -117 C ATOM 1516 O VAL A 98 17.778 -21.087 -10.709 1.00 15.42 O ANISOU 1516 O VAL A 98 2172 1991 1697 281 -696 -148 O ATOM 1517 CB VAL A 98 18.313 -22.778 -13.361 1.00 15.44 C ANISOU 1517 CB VAL A 98 2125 1864 1876 177 -494 42 C ATOM 1518 CG1 VAL A 98 16.810 -22.642 -13.275 1.00 16.24 C ANISOU 1518 CG1 VAL A 98 2278 2009 1883 202 -484 30 C ATOM 1519 CG2 VAL A 98 18.914 -21.664 -14.234 1.00 17.26 C ANISOU 1519 CG2 VAL A 98 2355 1973 2231 140 -467 10 C ATOM 1520 H VAL A 98 17.626 -23.521 -10.710 1.00 18.84 H ATOM 1521 HA VAL A 98 19.901 -22.960 -12.059 1.00 19.28

ATOM 1522 HB VAL A 98	18.509 -23.626 -13.789 1.00 18.52	Н
ATOM 1523 HG11 VAL A 98	16.441 -22.649 -14.172 1.00 19.49	Н
ATOM 1524 HG12 VAL A 98	16.455 -23.387 -12.765 1.00 19.49	Н
ATOM 1525 HG13 VAL A 98	16.594 -21.805 -12.834 1.00 19.49	н
ATOM 1526 HG21 VAL A 98	18.495 -21.689 -15.108 1.00 20.71	Н
ATOM 1527 HG22 VAL A 98	18.747 -20.807 -13.811 1.00 20.71	H
ATOM 1528 HG23 VAL A 98	19.869 -21.811 -14.320 1.00 20.71	H
	19.860 -20.600 -11.409 1.00 18.59	Ν
	2436 2262 2367 160 -765 -176	N
ATOM 1530 CA LYS A 99	19.822 -19.224 -10.941 1.00 21.18	Ċ
ANISOU 1530 CA LYS A 99	2812 2533 2704 147 -864 -300	C
		_
	19.550 -18.308 -12.126 1.00 20.30	C
	2733 2292 2687 94 -754 -299	C
	20.201 -18.423 -13.168 1.00 19.75	0
	2600 2134 2770 40 -656 -229	0
	21.131 -18.840 -10.253 1.00 25.43	C
ANISOU 1533 CB LYS A 99	3255 3037 3371 98 -1043 -379	С
ATOM 1534 CG LYS A 99	21.367 -19.548 -8.927 1.00 29.43	C
ANISOU 1534 CG LYS A 99	3777 3668 3736 194 -1193 -407	С
ATOM 1535 CD LYS A 99	22.592 -18.999 -8.220 1.00 34.02	С
ANISOU 1535 CD LYS A 99	4270 4207 4448 150 -1436 -518	С
ATOM 1536 CE LYS A 99	22.927 -19.786 -6.965 1.00 37.19	С
ANISOU 1536 CE LYS A 99	4704 4735 4693 280 -1603 -543	C
	24.203 -19.301 -6.343 1.00 41.78	N
ANISOU 1537 NZ LYS A 99	5171 5273 5430 230 -1864 -650	N
	20.615 -20.832 -11.750 1.00 22.31	н'`
ATOM 1539 HA LYS A 99	19.099 -19.121 -10.303 1.00 25.42	Ή.
ATOM 1540 HB2 LYS A 99	21.870 -19.061 -10.842 1.00 30.52	¨H
ATOM 1540 HB2 LT3 A 99 ATOM 1541 HB3 LYS A 99	21.124 -17.885 -10.080 1.00 30.52	H
	20.598 -19.416 -8.351 1.00 35.31	
		H
ATOM 1543 HG3 LYS A 99	21.507 -20.494 -9.089 1.00 35.31	Н
ATOM 1544 HD2 LYS A 99	23.353 -19.047 -8.819 1.00 40.82	Н
ATOM 1545 HD3 LYS A 99	22.425 -18.078 -7.964 1.00 40.82	Н
ATOM 1546 HE2 LYS A 99	22.212 -19.678 -6.318 1.00 44.63	Н
ATOM 1547 HE3 LYS A 99	23.035 -20.722 -7.193 1.00 44.63	Н
ATOM 1548 HZ1 LYS A 99	24.382 -19.773 -5.610 1.00 50.14	Н
ATOM 1549 HZ2 LYS A 99	24.876 -19.393 -6.918 1.00 50.14	Н
ATOM 1550 HZ3 LYS A 99	24.126 -18.442 -6.122 1.00 50.14	Н
ATOM 1551 N SER A 100	18.587 -17.405 -11.966 1.00 19.61	N
ANISOU 1551 N SER A 100	2765 2190 2495 140 -750 -363	N
ATOM 1552 CA SER A 100	18.228 -16.502 -13.044 1.00 18.83	С
ANISOU 1552 CA SER A 100	2729 1973 2452 126 -643 -361	С
	17.467 -15.319 -12.468 1.00 18.56	C
ANISOU 1553 C SER A 100	2829 1916 2309 186 -683 -459	Č
ATOM 1554 O SER A 100	16.608 -15.491 -11.602 1.00 18.20	ŏ
ANISOU 1554 O SER A 100	2845 1982 2090 283 -715 -473	ŏ
ATOM 1555 CB SER A 100	17.379 -17.225 -14.096 1.00 17.49	Č
ANISOU 1555 CB SER A 100	2586 1837 2223 170 -520 -262	Č
ATOM 1556 OG SER A 100	17.300 -16.467 -15.287 1.00 17.51	
		0
ANISOU 1556 OG SER A 100	2662 1709 2283 178 -417 -248	0
ATOM 1557 H SER A 100	18.130 -17.298 -11.246 1.00 23.53	Η
ATOM 1558 HA SER A 100	19.034 -16.172 -13.471 1.00 22.59	H.
ATOM 1559 HB2 SER A 100	17.785 -18.083 -14.295 1.00 20.99	Н

ATOM 1560 HB3 SER A 100 16.484 -17.354 -13.745 1.00 20.99 Н ATOM 1561 HG SER A 100 16.950 -15.720 -15.130 1.00 21.02 Н ATOM 1562 N ASP A 101 17.803 -14.123 -12.949 1.00 20.27 N **ANISOU 1562 N ASP A 101** Ν 3100 1972 2629 141 -655 -512 ATOM 1563 CA ASP A 101 17.053 -12.902 -12.650 1.00 20.88 **ANISOU 1563 CA ASP A 101** 3341 1991 2601 213 -657 -594 ATOM 1564 C ASP A 101 ANISOU 1564 C ASP A 101 16.902 -12.694 -11.147 1.00 21.97 3565 2189 2594 275 -811 -695 C ATOM 1565 O ASP A 101 15.820 -12.403 -10.636 1.00 21.83 0 **ANISOU 1565 O ASP A 101** 0 3676 2237 2382 414 -783 -705 C ATOM 1566 CB ASP A 101 15.695 -12.934 -13.346 1.00 19.99 **ANISOU 1566 CB ASP A 101** 3297 1946 2354 332 -530 -523 ATOM 1567 CG ASP A 101 15.822 -13.243 -14.810 1.00 19.27 **ANISOU 1567 CG ASP A 101** 3172 1793 2356 309 -409 -434 ATOM 1568 OD1 ASP A 101 16.192 -12.320 -15.563 1.00 19.44 0 **ANISOU 1568 OD1 ASP A 101** 3268 1651 2468 294 -324 -443 0 15.578 -14.405 -15.203 1.00 18.55 ATOM 1569 OD2 ASP A 101 **ANISOU 1569 OD2 ASP A 101** 3005 1799 2244 316 -394 -353 0 ATOM 1570 H ASP A 101 18.479 -13.990 -13.464 1.00 24.32 Н ATOM 1571 HA ASP A 101 17.545 -12.144 -13.002 1.00 25.06 Н ATOM 1572 HB2 ASP A 101 15.144 -13.621 -12.938 1.00 23.99 Н ATOM 1573 HB3 ASP A 101 15.270 -12.067 -13.255 1.00 23.99 Н ATOM 1574 N GLY A 102 18.020 -12.821 -10.440 1.00 23.48 Ν **ANISOU 1574 N GLY A 102** 3692 2349 2880 190 -976 -767 Ν ATOM 1575 CA GLY A 102 18.043 -12.599 -9.012 1.00 27.10 **ANISOU 1575 CA GLY A 102** 4274 2837 3185 268 -1160 -882 ATOM 1576 C GLY A 102 17.375 -13.664 -8.173 1.00 28.25 C **ANISOU 1576 C GLY A 102** 4446 3175 3112 416 -1153 -820 C ATOM 1577 O GLY A 102 17.262 -13.484 -6.955 1.00 30.19 0 **ANISOU 1577 O GLY A 102** 4849 3444 3176 537 -1277 -903 0 ATOM 1578 H GLY A 102 18.783 -13.038 -10.772 1.00 28.17 Н ATOM 1579 HA2 GLY A 102 18.966 -12.529 -8.722 1.00 32.51 Н 17.606 -11.754 -8.821 1.00 32.51 ATOM 1580 HA3 GLY A 102 ATOM 1581 N GLY A 103 16.936 -14.776 -8.775 1.00 24.82 Ν **ANISOU 1581 N GLY A 103** 3385 2896 3152 1090 -1136 -1018 Ν ATOM 1582 CA GLY A 103 16.275 -15.830 -8.038 1.00 25.09 C 3387 3175 2972 1177 -1058 -1037 **ANISOU 1582 CA GLY A 103** ATOM 1583 C GLY A 103 ANISOU 1583 C GLY A 103 16.895 -17.187 -8.322 1.00 23.12 C 3085 2940 2759 1083 -995 -801 C ATOM 1584 O GLY A 103 17.703 -17.350 -9.241 1.00 23.70 0 **ANISOU 1584 O GLY A 103** 3128 2815 3063 983 -946 -684 0 ATOM 1585 H GLY A 103 17.016 -14.935 -9.616 1.00 29.79 Н ATOM 1586 HA2 GLY A 103 16.339 -15.652 -7.087 1.00 30.11 Н ATOM 1587 HA3 GLY A 103 15.337 -15.860 -8.285 1.00 30.11 Н ATOM 1588 N THR A 104 16.499 -18.165 -7.506 1.00 20.87 Ν **ANISOU 1588 N THR A 104** 2785 2893 2252 1059 -961 -718 Ν C ATOM 1589 CA THR A 104 16.890 -19.559 -7.678 1.00 19.47 2551 2714 2133 970 -916 -464 **ANISOU 1589 CA THR A 104** C ATOM 1590 C THR A 104 ANISOU 1590 C THR A 104 15.625 -20.381 -7.886 1.00 18.54 C 2432 2764 1849 978 -737 -399 C ATOM 1591 O THR A 104 14.640 -20.193 -7.162 1.00 20.49 ANISOU 1591 O THR A 104 2713 3238 1835 994 -674 -524 0 ATOM 1592 CB THR A 104 17.676 -20.080 -6.463 1.00 22.07

ANISOU 1592 CB THR A 104	2902 3106 2378 870 -1089 -358	С
ATOM 1593 OG1 THR A 104	18.868 -19.304 -6.299 1.00 23.53	0
ANISOU 1593 OG1 THR A 104	3051 3124 2763 854 -1257 -437	0
ATOM 1594 CG2 THR A 104	18.060 -21.536 -6.637 1.00 22.27	С
ANISOU 1594 CG2 THR A 104	2861 3070 2530 787 -1087 -100	С
ATOM 1595 H THR A 104	15.988 -18.038 -6.826 1.00 25.04	Н
ATOM 1596 HA THR A 104	17.448 -19.646 -8.467 1.00 23.37	Н
ATOM 1597 HB THR A 104	17.127 -20.001 -5.666 1.00 26.48	Н
ATOM 1598 HG1 THR A 104	19.303 -19.582 -5.636 1.00 28.23	Н
ATOM 1599 HG21 THR A 104	18.553 -21.843 -5.860 1.00 26.72	Н
ATOM 1600 HG22 THR A 104	17.262 -22.079 -6.739 1.00 26.72	Н
ATOM 1601 HG23 THR A 104	18.615 -21.640 -7.425 1.00 26.72	Н
ATOM 1602 N TYR A 105	15.653 -21.279 -8.872 1.00 16.45	N
ANISOU 1602 N TYR A 105	2112 2386 1751 940 -624 -238	N
ATOM 1603 CA TYR A 105	14.496 -22.072 -9.269 1.00 14.95	C
ANISOU 1603 CA TYR A 105	1907 2309 1465 932 -459 -176	С
ATOM 1604 C TYR A 105	14.793 -23.561 -9.152 1.00 14.74	C
ANISOU 1604 C TYR A 105	1854 2272 1475 835 -452 61	С
ATOM 1605 O TYR A 105	15.884 -24.017 -9.506 1.00 13.15	0
ANISOU 1605 O TYR A 105		
		0
ATOM 1606 CB TYR A 105	14.081 -21.791 -10.717 1.00 13.71	С
ANISOU 1606 CB TYR A 105	1757 1986 1465 911 -336 -212	C
ATOM 1607 CG TYR A 105	13.633 -20.372 -10.990 1.00 12.97	Č
ANISOU 1607 CG TYR A 105	1722 1840 1367 946 -388 -390	C
ATOM 1608 CD1 TYR A 105	14.555 -19.346 -11.068 1.00 12.88	C
ANISOU 1608 CD1 TYR A 105	1761 1676 1457 926 -489 -450	Č
ATOM 1609 CD2 TYR A 105	12.297 -20.069 -11.207 1.00 13.28	C
ANISOU 1609 CD2 TYR A 105	1740 1957 1350 976 -371 -477	С
ATOM 1610 CE1 TYR A 105	14.173 -18.059 -11.330 1.00 13.71	C
ANISOU 1610 CE1 TYR A 105	1923 1705 1581 943 -580 -567	C
ATOM 1611 CE2 TYR A 105	11.891 -18.761 -11.468 1.00 14.45	C
ANISOU 1611 CE2 TYR A 105	1917 2015 1559 998 -483 -602	С
ATOM 1612 CZ TYR A 105	12.841 -17.764 -11.528 1.00 14.81	C
ANISOU 1612 CZ TYR A 105	2040 1909 1679 985 -590 -634	С
ATOM 1613 OH TYR A 105	12.483 -16.463 -11.784 1.00 17.05	0
ANISOU 1613 OH TYR A 105	2359 2084 2037 1015 -729 -736	O
		_
ATOM 1614 H TYR A 105	16.355 -21.450 -9.339 1.00 19.74	Н
ATOM 1615 HA TYR A 105	13.747 -21.862 -8.689 1.00 17.94	Н
ATOM 1616 HB2 TYR A 105	14.838 -21.975 -11.296 1.00 16.45	Н
ATOM 1617 HB3 TYR A 105	13.345 -22.379 -10.947 1.00 16.45	Н
ATOM 1618 HD1 TYR A 105	15.456 -19.534 -10.933 1.00 15.46	Н
ATOM 1619 HD2 TYR A 105	11.661 -20.746 -11.162 1.00 15.94	Н
ATOM 1620 HE1 TYR A 105	14.810 -17.382 -11.368 1.00 16.45	Н
ATOM 1621 HE2 TYR A 105	10.993 -18.564 -11.604 1.00 17.34	Н
ATOM 1622 HH TYR A 105	11.651 -16.409 -11.886 1.00 20.47	Н
ATOM 1623 N ASP A 106	13.804 -24.317 -8.680 1.00 15.15	N
ANISOU 1623 N ASP A 106	1928 2516 1312 770 -364 133	N
ATOM 1624 CA ASP A 106	13.852 -25.773 -8.706 1.00 14.81	С
ANISOU 1624 CA ASP A 106	1882 2427 1316 667 -358 368	Č
		_
ATOM 1625 C ASP A 106	13.335 -26.287 -10.042 1.00 13.51	C
ANISOU 1625 C ASP A 106	1649 2153 1333 679 -191 374	С
ATOM 1626 O ASP A 106	12.329 -25.798 -10.557 1.00 13.09	Ŏ
ANISOU 1626 O ASP A 106	1573 2186 1214 720 -71 239	0

ATOM 1627 CB ASP A 106 13.020 -26.357 -7.567 1.00 16.19 **ANISOU 1627 CB ASP A 106** 2153 2856 1144 526 -326 460 ATOM 1628 CG ASP A 106 13.595 -26.026 -6.207 1.00 19.52 **ANISOU 1628 CG ASP A 106** 2713 3381 1321 455 -519 486 ATOM 1629 OD1 ASP A 106 14.834 -26.097 -6.061 1.00 19.01 0 2659 3107 1457 473 -761 579 0 **ANISOU 1629 OD1 ASP A 106** ATOM 1630 OD2 ASP A 106 12.815 -25.682 -5.293 1.00 22.49 **ANISOU 1630 OD2 ASP A 106** 3176 3992 1377 342 -410 367 0 ATOM 1631 H ASP A 106 13.082 -24.002 -8.334 1.00 18.18 ATOM 1632 HA ASP A 106 14.769 -26.067 -8.598 1.00 17.77 Н ATOM 1633 HB2 ASP A 106 12.121 -25.994 -7.612 1.00 19.43 ATOM 1634 HB3 ASP A 106 12.994 -27.323 -7.657 1.00 19.43 Н ATOM 1635 N ILE A 107 14.021 -27.291 -10.591 1.00 13.85 **ANISOU 1635 N ILE A 107** 1651 1989 1624 644 -210 509 C ATOM 1636 CA ILE A 107 13.686 -27.864 -11.895 1.00 13.25 **ANISOU 1636 CA ILE A 107** 1534 1788 1713 627 -54 494 C ATOM 1637 C ILE A 107 ANISOU 1637 C ILE A 107 12.938 -29.176 -11.678 1.00 14.29 C O 1673 1966 1793 526 -16 654 ATOM 1638 O ILE A 107 13.432 -30.068 -10.978 1.00 15.78 o c 1879 2078 2039 466 -149 834 **ANISOU 1638 O ILE A 107** ATOM 1639 CB ILE A 107 14.953 -28.096 -12.744 1.00 13.61 ANISOU 1639 CB ILE A 107 1532 1574 2065 577 -49 407 ATOM 1640 CG1 ILE A 107 15.699 -26.781 -12.983 1.00 13.73 1555 1546 2116 604 -72 251 **ANISOU 1640 CG1 ILE A 107** ATOM 1641 CG2 ILE A 107 14.605 -28.764 -14.092 1.00 12.65 **ANISOU 1641 CG2 ILE A 107** 1412 1360 2033 506 123 361 ATOM 1642 CD1 ILE A 107 17.125 -26.970 -13.549 1.00 14.53 C **ANISOU 1642 CD1 ILE A 107** 1584 1489 2450 551 C -29 180 14.700 -27.665 -10.218 1.00 16.62 ATOM 1643 H ILE A 107 Н ATOM 1644 HA ILE A 107 13.104 -27.254 -12.375 1.00 15.90 Н 15.540 -28.692 -12.253 1.00 16.33 ATOM 1645 HB ILE A 107 Н 15.196 -26.247 -13.617 1.00 16.48 ATOM 1646 HG12 ILE A 107 15.775 -26.306 -12.140 1.00 16.48 ATOM 1647 HG13 ILE A 107 ATOM 1648 HG21 ILE A 107 15.421 -28.895 -14.599 1.00 15.18 14.181 -29.619 -13.919 1.00 15.18 13.999 -28.186 -14.582 1.00 15.18 17.533 -26.099 -13.674 1.00 17.44 ATOM 1649 HG22 ILE A 107 ATOM 1650 HG23 ILE A 107 ATOM 1651 HD11 ILE A 107 ATOM 1652 HD12 ILE A 107 17.647 -27.493 -12.921 1.00 17.44 Н ATOM 1653 HD13 ILE A 107 17.068 -27.433 -14.399 1.00 17.44 Н ATOM 1654 N TYR A 108 11.757 -29.304 -12.289 1.00 14.30 Ν 1663 2059 1709 495 **ANISOU 1654 N TYR A 108** 126 598 ATOM 1655 CA TYR A 108 10.967 -30.529 -12.208 1.00 15.03 **ANISOU 1655 CA TYR A 108** 1749 2185 1775 370 185 730 ATOM 1656 C TYR A 108 10.540 -30.963 -13.603 1.00 16.05 1850 2188 2060 358 **ANISOU 1656 C TYR A 108** 293 658 Ŏ ATOM 1657 O TYR A 108 10.505 -30.164 -14.546 1.00 13.84 0 **ANISOU 1657 O TYR A 108** 1586 1867 1804 426 328 505 ATOM 1658 CB TYR A 108 9.696 -30.357 -11.355 1.00 13.68 **ANISOU 1658 CB TYR A 108** 1566 2317 1314 287 268 708 ATOM 1659 CG TYR A 108 9.901 -29.837 -9.954 1.00 14.72 ANISOU 1659 CG TYR A 108 1769 2637 1188 252 207 728 ATOM 1660 CD1 TYR A 108 10.259 -30.693 -8.924 1.00 16.78 ANISOU 1660 CD1 TYR A 108 2157 2901 1317 91 103 969

ATOM 1661 CD2 TYR A 108 9.703 -28.493 -9.652 1.00 14.77 **ANISOU 1661 CD2 TYR A 108** 1743 2800 1068 361 227 504 ATOM 1662 CE1 TYR A 108 10.431 -30.229 -7.640 1.00 18.79 2533 3302 1302 15 **ANISOU 1662 CE1 TYR A 108** 31 953 ATOM 1663 CE2 TYR A 108 9.877 -28.018 -8.366 1.00 16.39 **ANISOU 1663 CE2 TYR A 108** 2032 3188 1007 309 186 481 ATOM 1664 CZ TYR A 108 10.237 -28.893 -7.361 1.00 18.55 ANISOU 1664 CZ TYR A 108 2459 3467 1120 118 94 709 ATOM 1665 OH TYR A 108 10.413 -28.432 -6.070 1.00 20.93 0 2903 3888 1161 23 35 656 11.391 -28.687 -12.762 1.00 17.15 11.505 -31.235 -11.818 1.00 18.03 9.106 -29.736 -11.810 1.00 16.41 9.260 -31.220 -11.282 1.00 16.41 **ANISOU 1665 OH TYR A 108** ATOM 1666 H TYR A 108 ATOM 1667 HA TYR A 108 ATOM 1668 HB2 TYR A 108 ATOM 1669 HB3 TYR A 108 ATOM 1670 HD1 TYR A 108 ATOM 1671 HD2 TYR A 108 9.458 -27.903 -10.328 1.00 17.72 Н ATOM 1672 HE1 TYR A 108 ATOM 1672 HE1 TYR A 108 10.676 -30.816 -6.962 1.00 22.54 ATOM 1673 HE2 TYR A 108 9.746 -27.117 -8.178 1.00 19.67 10.676 -30.816 -6.962 1.00 22.54 Н ATOM 1674 HH TYR A 108 10.264 -27.606 -6.037 1.00 25.11 ATOM 1675 N ATHR A 109 10.228 -32.258 -13.731 0.75 17.72 **ANISOU 1675 N ATHR A 109** 2053 2316 2362 245 320 780 ATOM 1676 N BTHR A 109 10.191 -32.240 -13.719 0.25 17.77 **ANISOU 1676 N BTHR A 109** 2060 2331 2361 244 322 779 **ATOM 1677 CA ATHR A 109** 9.612 -32.805 -14.934 0.75 18.29 C 2113 2300 2537 196 413 707 **ANISOU 1677 CA ATHR A 109** ATOM 1678 CA BTHR A 109 9.587 -32.767 -14.932 0.25 18.22 **ANISOU 1678 CA BTHR A 109** 2104 2298 2521 197 414 703 ATOM 1679 C ATHR A 109 8.401 -33.638 -14.543 0.75 19.10 **ANISOU 1679 C ATHR A 109** 2176 2528 2553 51 458 799 ATOM 1680 C BTHR A 109 8.402 -33.640 -14.555 0.25 19.03 C **ANISOU 1680 C BTHR A 109** 2167 2518 2545 51 458 ATOM 1681 O ATHR A 109 8.417 -34.334 -13.520 0.75 20.52 **ANISOU 1681 O ATHR A 109** 2382 2736 2677 -60 0 421 987 0 ATOM 1682 O BTHR A 109 8.443 -34.366 -13.556 0.25 20.72 **ANISOU 1682 O BTHR A 109** 2409 2751 2714 -59 419 988 CCC ATOM 1683 CB ATHR A 109 10.586 -33.679 -15.769 0.75 18.60 2162 2035 2869 183 431 ANISOU 1683 CB ATHR A 109 696 ATOM 1684 CB BTHR A 109 10.589 -33.573 -15.772 0.25 18.47 2148 2030 2840 191 432 687 Č ANISOU 1684 CB BTHR A 109 ATOM 1685 OG1ATHR A 109 10.993 -34.838 -15.024 0.75 20.35 2366 2131 3236 126 326 861 **ANISOU 1685 OG1ATHR A 109** ATOM 1686 OG1BTHR A 109 9.988 -33.923 -17.025 0.25 18.56 **ANISOU 1686 OG1BTHR A 109** 2191 1977 2885 127 528 570 ATOM 1687 CG2ATHR A 109 11.806 -32.878 -16.199 0.75 18.19 **ANISOU 1687 CG2ATHR A 109** 2114 1871 2928 278 446 568 C ATOM 1688 CG2BTHR A 109 11.028 -34.842 -15.038 0.25 20.47 Č **ANISOU 1688 CG2BTHR A 109** 2380 2140 3259 128 325 858 10.368 -32.847 -13.120 0.75 21.26 H 10.296 -32.827 -13.100 0.25 21.33 H 9.308 -32.075 -15.495 0.75 21.95 H ATOM 1689 H ATHR A 109 ATOM 1690 H BTHR A 109 ATOM 1691 HA ATHR A 109 9.308 -32.075 -15.495 0.75 21.95 ATOM 1692 HA BTHR A 109 9.262 -32.031 -15.472 0.25 21.86 ATOM 1693 HB ATHR A 109 10.128 -33.972 -16.573 0.75 22.32 ATOM 1694 HB BTHR A 109 11.376 -33.030 -15.936 0.25 22.16 Н

ATOM	1605	HC1	ATHR A 109	11.383 -34.603 -14.318 0.75 24.42	Н
		_		9.300 -34.387 -16.895 0.25 22.27	Η̈́
ATOM		_	BTHR A 109		= =
ATOM			1ATHR A 109	12.403 -33.438 -16.719 0.75 21.83	H
ATOM	1698 F	HG2	1BTHR A 109	11.660 -35.337 -15.583 0.25 24.57	Н
ATOM	1699 H	1G2 2	2ATHR A 109	11.531 -32.121 -16.741 0.75 21.83	Н
ATOM	1700 H	HG2	2BTHR A 109	11.452 -34.609 -14.198 0.25 24.57	Н
ATOM		_	3ATHR A 109	12.279 -32.551 -15.418 0.75 21.83	Ĥ
ATOM	_	_	3BTHR A 109		H
ATOM					Ν
_			THR A 110	7.343 -33.551 -15.355 1.00 18.28	
ANISOL			_	2020 2491 2432 26 517 673	N
ATOM	1704	CA	THR A 110	6.133 -34.336 -15.153 1.00 18.91	C
ANISOL	J 1704	CA	THR A 110	2016 2684 2485 -132 579 716	С
ATOM	1705	C 1	THR A 110	5.578 -34.735 -16.514 1.00 16.01	C
ANISOL	J 1705	C	THR A 110	1641 2195 2249 -163 574 604	С
ATOM			ΓHR A 110	6.100 -34.344 -17.562 1.00 13.63	Ŏ
ANISOL			THR A 110	1435 1747 1997 -81 537 496	Ö
		_	_		
ATOM	_	_	THR A 110	5.078 -33.556 -14.361 1.00 21.91	C
	_	_	THR A 110	2260 3383 2681 -140 646 615	C
ATOM			THR A 110	4.794 -32.328 -15.038 1.00 20.58	0
ANISOL	J 1708	OG	1 THR A 110	2041 3252 2528 37 580 397	0
ATOM	1709	CG ₂	THR A 110	5.568 -33.249 -12.943 1.00 23.49	С
_			2 THR A 110	2531 3703 2690 -163 646 690	C
ATOM			THR A 110	7.303 -33.032 -16.040 1.00 21.93	н
ATOM	_		THR A 110	6.351 -35.143 -14.662 1.00 22.69	Ή
ATOM			THR A 110	4.267 -34.085 -14.297 1.00 26.29	H.
ATOM			THR A 110	4.502 -32.486 -15.810 1.00 24.70	Н
ATOM	1714 H	HG2	1 THR A 110	4.888 -32.757 -12.457 1.00 28.19	Н
ATOM	1715 H	1G2 2	2 THR A 110	5.756 -34.076 -12.471 1.00 28.19	Н
ATOM	1716 H	HG2 :	3 THR A 110	6.377 -32.716 -12.981 1.00 28.19	Н
ATOM	1717	N 1	THR A 111	4.502 -35.519 -16.493 1.00 17.17	N
_			THR A 111	1691 2407 2428 -318 617 623	N
			THR A 111	3.762 -35.882 -17.694 1.00 17.14	Ċ
_	_	_	THR A 111		C
	_	_		1664 2320 2529 -371 575 501	
			THR A 111	2.280 -35.626 -17.460 1.00 18.10	C
ANISOL	_	_	THR A 111	1563 2680 2635 -430 585 392	С
ATOM	_	_	ΓHR A 111	1.769 -35.869 -16.364 1.00 20.05	0
ANISOL	J 1720	0	THR A 111	1680 3117 2822 -550 710 456	0
ATOM	1721	CB	THR A 111	3.979 -37.357 -18.061 1.00 17.91	С
ANISOL	J 1721	CB	THR A 111	1830 2182 2793 -526 597 599	С
			THR A 111	5.372 -37.593 -18.275 1.00 18.63	Ŏ
			1 THR A 111	2060 2035 2982 -450 595 637	Ö
			? THR A 111		
				3.198 -37.748 -19.319 1.00 17.07	C
			2 THR A 111	1723 1993 2770 -604 540 449	C
ATOM			THR A 111	4.176 -35.860 -15.775 1.00 20.61	Н
ATOM	1725	HA	THR A 111	4.057 -35.332 -18.437 1.00 20.57	Н
ATOM	1726	HB	THR A 111	3.671 -37.915 -17.329 1.00 21.49	Н
ATOM	1727	HG1	THR A 111	5.499 -38.399 -18.476 1.00 22.35	Н
ATOM		_	1 THR A 111	3.353 -38.682 -19.528 1.00 20.48	Н
ATOM			2 THR A 111	2.249 -37.610 -19.176 1.00 20.48	H
	_	_	3 THR A 111	3.486 -37.205 -20.069 1.00 20.48	H
ATOM			ARG A 112	1.593 -35.137 -18.489 1.00 18.87	N _.
ANISOL			ARG A 112	1616 2762 2790 -366 446 215	N
ATOM	1732	CA	ARG A 112	0.138 -35.040 -18.491 1.00 22.18	С

ANISOU 1732 CA ARG A 112 1765 3349 3311 -417 405 65 ATOM 1733 C ARG A 112 -0.426 -36.045 -19.482 1.00 23.41 **ANISOU 1733 C ARG A 112** 1934 3359 3603 -571 319 43 ATOM 1734 O ARG A 112 0.081 -36.182 -20.599 1.00 21.85 **ANISOU 1734 O ARG A 112** 1970 2946 3386 -554 195 30 -0.343 -33.632 -18.867 1.00 24.06 1913 3652 3577 -204 209 -138 ATOM 1735 CB ARG A 112 **ANISOU 1735 CB ARG A 112** 209 -138 ATOM 1736 CG ARG A 112 0.154 -32.553 -17.936 1.00 25.22 **ANISOU 1736 CG ARG A 112** 2041 3928 3615 -43 276 -165 ATOM 1737 CD ARG A 112 -0.766 -32.209 -16.751 1.00 29.63 **ANISOU 1737 CD ARG A 112** 2261 4784 4212 -56 437 -321 -1.950 -33.064 -16.613 1.00 34.03 ATOM 1738 NE ARG A 112 Ν **ANISOU 1738 NE ARG A 112** 2595 5430 4902 -246 532 -370 ATOM 1739 CZ ARG A 112 -3.214 -32.644 -16.694 1.00 37.86 **ANISOU 1739 CZ ARG A 112** 2843 5969 5573 -192 448 -582 ATOM 1740 NH1 ARG A 112 -3.506 -31.364 -16.918 1.00 38.73 2894 6041 5779 45 250 -774 **ANISOU 1740 NH1 ARG A 112** ATOM 1741 NH2 ARG A 112 -4.205 -33.515 -16.545 1.00 41.25 **ANISOU 1741 NH2 ARG A 112** 3106 6459 6106 -381 550 -596 ATOM 1742 H ARG A 112 1.957 -34.850 -19.214 1.00 22.64 ATOM 1743 HA ARG A 112 -0.201 -35.255 -17.608 1.00 26.61 Н ATOM 1744 HB2 ARG A 112 -0.029 -33.422 -19.760 1.00 28.87 -1.313 -33.617 -18.847 1.00 28.87 ATOM 1745 HB3 ARG A 112 ATOM 1746 HG2 ARG A 112 Н 1.006 -32.835 -17.569 1.00 30.27 0.278 -31.740 -18.451 1.00 30.27 -0.253 -32.286 -15.931 1.00 35.55 ATOM 1747 HG3 ARG A 112 ATOM 1748 HD2 ARG A 112 ATOM 1749 HD3 ARG A 112 -1.076 -31.296 -16.856 1.00 35.55 Н ATOM 1750 HE ARG A 112 -1.819 -33.901 -16.469 1.00 40.83 ATOM 1751 HH11 ARG A 112 -2.874 -30.789 -17.014 1.00 46.47 -4.327 -31.112 -16.967 1.00 46.47 Н ATOM 1752 HH12 ARG A 112 ATOM 1753 HH21 ARG A 112 -4.030 -34.345 -16.401 1.00 49.50 Н ATOM 1754 HH22 ARG A 112 -5.022 -33.251 -16.598 1.00 49.50 ATOM 1755 N TYR A 113 -1.486 -36.733 -19.072 1.00 22.58 **ANISOU 1755 N TYR A 113** 1777 2759 4044 -14 340 830 ATOM 1756 CA TYR A 113 -2.086 -37.802 -19.858 1.00 24.34 **ANISOU 1756 CA TYR A 113** 1939 2813 4498 -101 258 811 -3.491 -37.405 -20.286 1.00 25.50 ATOM 1757 C TYR A 113 C ANISOU 1757 C TYR A 113 ATOM 1758 O TYR A 113 1955 2963 4772 -138 207 754 -4.298 -36.975 -19.456 1.00 26.42 **ANISOU 1758 O TYR A 113** 1971 3183 4885 -131 304 833 ATOM 1759 CB TYR A 113 -2.142 -39.099 -19.052 1.00 26.24 CCCCC **ANISOU 1759 CB TYR A 113** 2111 2976 4883 -160 352 985 ATOM 1760 CG TYR A 113 -0.796 -39.569 -18.572 1.00 25.60 **ANISOU 1760 CG TYR A 113** 2148 2894 4684 -115 402 1054 ATOM 1761 CD1 TYR A 113 -0.303 -39.181 -17.334 1.00 25.48 2154 3028 4500 -46 526 1167 **ANISOU 1761 CD1 TYR A 113** -0.016 -40.407 -19.354 1.00 25.51 ATOM 1762 CD2 TYR A 113 **ANISOU 1762 CD2 TYR A 113** 2230 2735 4726 -129 317 1002 0.930 -39.615 -16.892 1.00 25.79 ATOM 1763 CE1 TYR A 113 ANISOU 1763 CE1 TYR A 113 2292 3071 4435 1 557 1227 ATOM 1764 CE2 TYR A 113 1.214 -40.838 -18.925 1.00 25.71 ANISOU 1764 CE2 TYR A 113 2354 2764 4652 -81 362 1068 C ATOM 1765 CZ TYR A 113 1.686 -40.443 -17.694 1.00 26.48

ANISOU 1765 CZ TYR A 113	2458 3011 4591 -19 478 1182	С
ATOM 1766 OH TYR A 113	2.923 -40.888 -17.273 1.00 28.28	0
ANISOU 1766 OH TYR A 113	2776 3245 4725 35 507 1244	0
ATOM 1767 H TYR A 113	-1.885 -36.595 -18.323 1.00 27.10	Н
ATOM 1768 HA TYR A 113	-1.554 -37.957 -20.654 1.00 29.21	Н
ATOM 1769 HB2 TYR A 113	-2.703 -38.961 -18.273 1.00 31.49	Н
ATOM 1770 HB3 TYR A 113	-2.518 -39.798 -19.609 1.00 31.49	Н
ATOM 1771 HD1 TYR A 113	-0.813 -38.621 -16.793 1.00 30.58	Н
ATOM 1772 HD2 TYR A 113	-0.329 -40.676 -20.188 1.00 30.61	Н
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ATOM 1773 HE1 TYR A 113	1.251 -39.347 -16.061 1.00 30.94	Н
ATOM 1774 HE2 TYR A 113	1.725 -41.399 -19.462 1.00 30.85	Н
_		
ATOM 1775 HH TYR A 113	3.266 -41.381 -17.860 1.00 33.94	Н
ATOM 1776 N ASN A 114	-3.779 -37.557 -21.576 1.00 26.32	N
ANISOU 1776 N ASN A 114	2077 2955 4969 -161 49 608	N
ATOM 1777 CA ASN A 114	-5.131 -37.348 -22.093 1.00 29.17	C
ANISOU 1777 CA ASN A 114	2303 3298 5484 -200 -32 543	С
ATOM 1778 C ASN A 114	-5.663 -35.978 -21.694 1.00 26.29	C
ANISOU 1778 C ASN A 114	1895 3106 4988 -135 27 533	C
ATOM 1779 O ASN A 114	-6.820 -35.832 -21.295 1.00 27.35	0
ANISOU 1779 O ASN A 114	1926 3282 5184 -156 65 569	0
ATOM 1780 CB ASN A 114	-6.076 -38.445 -21.603 1.00 33.58	С
ANISOU 1780 CB ASN A 114	2720 3762 6278 -298 7 653	C
ATOM 1781 CG ASN A 114	-5.616 -39.825 -22.002 1.00 36.00	С
ANISOU 1781 CG ASN A 114	3052 3876 6751 -366 -57 661	C
ATOM 1782 OD1 ASN A 114	-5.193 -40.046 -23.136 1.00 36.66	0
ANISOU 1782 OD1 ASN A 114	3220 3853 6855 -360 -212 516	0
ATOM 1783 ND2 ASN A 114	-5.690 -40.765 -21.068 1.00 37.61	Ν
ANISOU 1783 ND2 ASN A 114	3228 4036 7025 -401 59 819	N
ATOM 1784 H ASN A 114	-3.206 -37.782 -22.177 1.00 31.59	Н
ATOM 1785 HA ASN A 114		Н
ATOM 1786 HB2 ASN A 114	-6.124 -38.413 -20.635 1.00 40.30	Н
ATOM 1787 HB3 ASN A 114	-6.955 -38.300 -21.985 1.00 40.30	Н
ATOM 1788 HD21 ASN A 114	-5.440 -41.568 -21.245 1.00 45.13	H
ATOM 1789 HD22 ASN A 114	-5.988 -40.570 -20.285 1.00 45.13	Н
ATOM 1790 N ALA A 115	-4.806 -34.963 -21.812 1.00 22.28	N
ANISOU 1790 N ALA A 115	1533 2689 4245 -43 32 466	N
ATOM 1791 CA ALA A 115	-5.141 -33.619 -21.367 1.00 21.08	C
ANISOU 1791 CA ALA A 115	1367 2691 3951 30 92 453	C
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ATOM 1792 C ALA A 115	-5.147 -32.655 -22.546 1.00 20.55	
ANISOU 1792 C ALA A 115	1387 2625 3795 95 -32 289	С
ATOM 1793 O ALA A 115	-4.661 -32.994 -23.634 1.00 19.64	0
ANISOU 1793 O ALA A 115	1370 2408 3683 100 -147 193	0
ATOM 1794 CB ALA A 115	-4.150 -33.145 -20.301 1.00 19.74	C
ANISOU 1794 CB ALA A 115	1286 2630 3586 88 215 527	C
ATOM 1795 H ALA A 115	-4.018 -35.032 -22.150 1.00 26.74	Н
ATOM 1796 HA ALA A 115	-6.029 -33.624 -20.975 1.00 25.30	Н
ATOM 1797 HB1 ALA A 115	-4.393 -32.249 -20.020 1.00 23.69	Н
ATOM 1798 HB2 ALA A 115	-4.187 -33.751 -19.544 1.00 23.69	Н
ATOM 1799 HB3 ALA A 115	-3.257 -33.143 -20.680 1.00 23.69	Н
ATOM 1800 N PRO A 116	-5.699 -31.456 -22.379 1.00 21.81	N
ANISOU 1800 N PRO A 116	1520 2896 3870 158 -7 256	N
ATOM 1801 CA PRO A 116	-5.682 -30.485 -23.476 1.00 22.02	С
		Č
ANISOU 1801 CA PRO A 116	1638 2924 3805 232 -112 116	C

ATOM 1802 C PRO A 116 -4.278 -29.978 -23.760 1.00 20.99 **ANISOU 1802 C PRO A 116** 1691 2788 3495 290 -105 76 ATOM 1803 O PRO A 116 0 -3.474 -29.768 -22.849 1.00 21.49 **ANISOU 1803 O PRO A 116** 1799 2909 3460 299 -5 141 ATOM 1804 CB PRO A 116 -6.591 -29.357 -22.968 1.00 22.91 **ANISOU 1804 CB PRO A 116** 1668 3160 3876 288 -57 119 ATOM 1805 CG PRO A 116 -7.393 -29.959 -21.882 1.00 23.85 Č **ANISOU 1805 CG PRO A 116** 1650 3321 4091 226 45 239 ATOM 1806 CD PRO A 116 -6.524 -30.993 -21.252 1.00 23.47 **ANISOU 1806 CD PRO A 116** 1622 3226 4068 170 C 114 342 ATOM 1807 HA PRO A 116 -6.060 -30.871 -24.282 1.00 26.42 ATOM 1808 HB2 PRO A 116 -6.047 -28.628 -22.629 1.00 27.49 Н ATOM 1809 HB3 PRO A 116 -7.164 -29.051 -23.688 1.00 27.49 -7.630 -29.275 -21.237 1.00 28.62 ATOM 1810 HG2 PRO A 116 ATOM 1811 HG3 PRO A 116 -8.191 -30.366 -22.255 1.00 28.62 ATOM 1812 HD2 PRO A 116 -5.968 -30.597 -20.564 1.00 28.16 Н ATOM 1813 HD3 PRO A 116 -7.062 -31.722 -20.902 1.00 28.16 ATOM 1814 N SER A 117 -3.995 -29.779 -25.044 1.00 18.95 Ν **ANISOU 1814 N SER A 117** 1538 2463 3200 336 -214 -32 ATOM 1815 CA SER A 117 -2.749 -29.173 -25.488 1.00 16.77 **ANISOU 1815 CA SER A 117** 1424 2177 2770 400 -202 -68 ATOM 1816 C SER A 117 -3.039 -28.353 -26.733 1.00 16.48 ANISOU 1816 C SER A 117 ATOM 1817 O SER A 117 1462 2124 2674 488 -293 -176 C -4.176 -28.302 -27.216 1.00 17.17 0 **ANISOU 1817 O SER A 117** 1478 2213 2834 500 -378 -230 0 ATOM 1818 CB SER A 117 -1.687 -30.228 -25.773 1.00 15.64 Č **ANISOU 1818 CB SER A 117** 1361 1942 2639 372 -213 -48 ATOM 1819 OG SER A 117 -1.991 -30.937 -26.960 1.00 16.06 **ANISOU 1819 OG SER A 117** 1446 1893 2763 380 -337 -127 -4.522 -29.993 -25.690 1.00 22.74 ATOM 1820 H SER A 117 Н ATOM 1821 HA SER A 117 -2.415 -28.578 -24.798 1.00 20.12 Н ATOM 1822 HB2 SER A 117 -0.827 -29.791 -25.878 1.00 18.77 ATOM 1823 HB3 SER A 117 -1.654 -30.852 -25.032 1.00 18.77 Н Н ATOM 1824 HG SER A 117 -2.735 -31.320 -26.884 1.00 19.27 ATOM 1825 N ILE A 118 -1.993 -27.724 -27.274 1.00 16.77 **ANISOU 1825 N ILE A 118** 1641 2145 2585 556 -275 -201 N ATOM 1826 CA ILE A 118 -2.128 -27.043 -28.552 1.00 17.98 **ANISOU 1826 CA ILE A 118** 1890 2272 2669 657 -350 -286 ATOM 1827 C ILE A 118 -2.438 -28.012 -29.687 1.00 19.61 C **ANISOU 1827 C ILE A 118** 2131 2393 2929 675 -481 -357 ATOM 1828 O ILE A 118 0 -2.812 -27.568 -30.774 1.00 19.79 O **ANISOU 1828 O ILE A 118** 2221 2402 2897 772 -568 -437 ATOM 1829 CB ILE A 118 -0.854 -26.220 -28.872 1.00 17.60 **ANISOU 1829 CB ILE A 118** 1981 2214 2493 723 -280 -273 ATOM 1830 CG1 ILE A 118 0.395 -27.119 -28.870 1.00 17.92 2082 2195 2531 691 -244 -229 **ANISOU 1830 CG1 ILE A 118** ATOM 1831 CG2 ILE A 118 -0.713 -25.062 -27.884 1.00 17.47 **ANISOU 1831 CG2 ILE A 118** 1939 2270 2428 709 -182 -232 ATOM 1832 CD1 ILE A 118 1.645 -26.422 -29.383 1.00 18.39 ANISOU 1832 CD1 ILE A 118 2267 2235 2485 719 -169 -199 C ATOM 1833 H ILE A 118 -1.209 -27.680 -26.923 1.00 20.12 Н ATOM 1834 HA ILE A 118 -2.869 -26.420 -28.491 1.00 21.57 Н ATOM 1835 HB ILE A 118 -0.953 -25.847 -29.761 1.00 21.12

ATOM 1836 HG12 ILE A 118	0.570 -27.412 -27.962 1.00 21.50	Н
ATOM 1837 HG13 ILE A 118	0.229 -27.888 -29.438 1.00 21.50	Н
ATOM 1838 HG21 ILE A 118	0.088 -24.559 -28.100 1.00 20.96	Н
ATOM 1839 HG22 ILE A 118	-1.492 -24.489 -27.957 1.00 20.96	Н
ATOM 1840 HG23 ILE A 118	-0.647 -25.420 -26.985 1.00 20.96	Н
ATOM 1841 HD11 ILE A 118	2.388 -27.045 -29.353 1.00 22.07	H
ATOM 1842 HD12 ILE A 118	1.492 -26.132 -30.295 1.00 22.07	Н
ATOM 1843 HD13 ILE A 118	1.833 -25.656 -28.818 1.00 22.07	Н
ATOM 1844 N ASP A 119	-2.303 -29.328 -29.459 1.00 20.03	N
ANISOU 1844 N ASP A 119	2143 2382 3084 595 -504 -335	N
ATOM 1845 CA ASP A 119	-2.551 -30.339 -30.487 1.00 21.38	С
ANISOU 1845 CA ASP A 119	2352 2453 3319 610 -642 -417	С
ATOM 1846 C ASP A 119	-3.918 -31.012 -30.383 1.00 22.82	C
ANISOU 1846 C ASP A 119	2377 2609 3683 536 -749 -453	С
ATOM 1847 O ASP A 119	-4.276 -31.781 -31.284 1.00 24.98	0
ANISOU 1847 O ASP A 119	2673 2794 4026 551 -895 -548	O
ATOM 1848 CB ASP A 119	-1.470 -31.427 -30.433 1.00 21.77	C
ANISOU 1848 CB ASP A 119	2469 2420 3382 577 -611 -380	C
ATOM 1849 CG ASP A 119	-0.245 -31.093 -31.282 1.00 21.77	C
ANISOU 1849 CG ASP A 119	2649 2399 3225 688 -580 -396	C
ATOM 1850 OD1 ASP A 119	-0.187 -29.988 -31.865 1.00 22.47	0
ANISOU 1850 OD1 ASP A 119	2811 2533 3192 783 -567 -423	0
ATOM 1851 OD2 ASP A 119		
	0.665 -31.941 -31.358 1.00 21.63	0
ANISOU 1851 OD2 ASP A 119	2694 2315 3208 682 -557 -372	0
ATOM 1852 H ASP A 119	-2.065 -29.660 -28.702 1.00 24.03	Н
ATOM 1853 HA ASP A 119	-2.498 -29.914 -31.357 1.00 25.66	H
ATOM 1854 HB2 ASP A 119	-1.177 -31.535 -29.515 1.00 26.12	Н
ATOM 1855 HB3 ASP A 119	-1.844 -32.259 -30.762 1.00 26.12	Н
ATOM 1856 N GLY A 120	-4.679 -30.774 -29.328 1.00 22.86	N
ANISOU 1856 N GLY A 120	2223 2685 3776 462 -682 -383	N
ATOM 1857 CA GLY A 120	-5.982 -31.398 -29.210 1.00 24.63	C
ANISOU 1857 CA GLY A 120	2273 2884 4202 387 -768 -400	C
ATOM 1858 C GLY A 120	-6.452 -31.463 -27.772 1.00 25.60	C
ANISOU 1858 C GLY A 120	2228 3074 4423 292 -633 -269	С
ATOM 1859 O GLY A 120	-5.747 -31.077 -26.839 1.00 22.77	0
ANISOU 1859 O GLY A 120	1901 2784 3965 290 -486 -176	0
ATOM 1860 H GLY A 120	-4.465 -30.261 -28.672 1.00 27.43	H
ATOM 1861 HA2 GLY A 120	-6.631 -30.892 -29.724 1.00 29.56	Н
ATOM 1862 HA3 GLY A 120	-5.943 -32.300 -29.563 1.00 29.56	Н
ATOM 1863 N AASP A 121	-7.678 -31.978 -27.618 0.63 28.46	N
ANISOU 1863 N AASP A 121	2407 3415 4991 221 -690 -264	N
ATOM 1864 N BASP A 121	-7.669 -31.991 -27.618 0.37 28.54	N
ANISOU 1864 N BASP A 121	2419 3425 5002 220 -690 -264	N
ATOM 1865 CA AASP A 121	-8.331 -32.030 -26.313 0.63 29.83	С
ANISOU 1865 CA AASP A 121	2413 3660 5260 146 -551 -129	
		C
ATOM 1866 CA BASP A 121	-8.327 -32.023 -26.317 0.37 29.86	C
ANISOU 1866 CA BASP A 121	2417 3664 5263 147 -551 -130	С
ATOM 1867 C AASP A 121	-7.790 -33.147 -25.430 0.63 30.01	C
ANISOU 1867 C AASP A 121	2395 3625 5380 51 -452 -2	C
ATOM 1868 C BASP A 121	-7.822 -33.157 -25.433 0.37 30.03	C
ANISOU 1868 C BASP A 121	2394 3628 5389 50 -453 -2	С
ATOM 1869 O AASP A 121	-7.808 -33.021 -24.200 0.63 30.14	0
ANISOU 1869 O AASP A 121	2355 3727 5369 29 -287 131	0

ATOM 1870 O BASP A 121 -7.893 -33.053 -24.203 0.37 30.30 0 2367 3745 5399 **ANISOU 1870 O BASP A 121** 24 -290 132 ATOM 1871 CB AASP A 121 -9.840 -32.221 -26.484 0.63 33.03 CCCCC **ANISOU 1871 CB AASP A 121** 2687 4056 5806 97 -608 -147 ATOM 1872 CB BASP A 121 -9.839 -32.154 -26.509 0.37 32.94 **ANISOU 1872 CB BASP A 121** 2680 4049 5785 103 -610 -151 -10.485 -31.112 -27.285 0.63 33.58 ATOM 1873 CG AASP A 121 ANISOU 1873 CG AASP A 121 2793 4191 5774 193 -694 -254 ATOM 1874 CG BASP A 121 -10.595 -32.151 -25.198 0.37 34.36 ANISOU 1874 CG BASP A 121 2722 4314 6020 46 -446 -10.012 -29.959 -27.197 0.63 32.96 ATOM 1875 OD1AASP A 121 **ANISOU 1875 OD1AASP A 121** 2804 4207 5512 287 -634 -260 ATOM 1876 OD1BASP A 121 -10.376 -31.227 -24.386 0.37 33.83 **ANISOU 1876 OD1BASP A 121** 2674 4376 5803 53 104 -314 ATOM 1877 OD2AASP A 121 -11.469 -31.395 -28.003 0.63 35.79 0 **ANISOU 1877 OD2AASP A 121** 3016 4421 6163 177 -820 -329 0 ATOM 1878 OD2BASP A 121 -11.406 -33.077 -24.981 0.37 36.59 0 **ANISOU 1878 OD2BASP A 121** 2885 4527 6492 -46 -451 0 ATOM 1879 H AASP A 121 -8.151 -32.304 -28.258 0.63 34.15 Н ATOM 1880 H BASP A 121 -8.132 -32.337 -28.254 0.37 34.25 Н **ATOM 1881 HA AASP A 121** -8.186 -31.188 -25.853 0.63 35.79 Н ATOM 1882 HA BASP A 121 -8.155 -31.187 -25.857 0.37 35.83 Н ATOM 1883 HB2AASP A 121 ATOM 1884 HB2BASP A 121 -10.001 -33.058 -26.946 0.63 39.63 Н -10.156 -31.406 -27.040 0.37 39.52 Н **ATOM 1885 HB3AASP A 121** -10.257 -32.240 -25.608 0.63 39.63 Н **ATOM 1886 HB3BASP A 121** -10.029 -32.989 -26.964 0.37 39.52 ATOM 1887 N ARG A 122 -7.321 -34.241 -26.026 1.00 28.67 Ν **ANISOU 1887 N ARG A 122** 2286 3313 5293 7 -542 -41 -6.855 -35.410 -25.281 1.00 26.50 ATOM 1888 CA ARG A 122 **ANISOU 1888 CA ARG A 122** 1984 2961 5124 -82 -457 ATOM 1889 C ARG A 122 -5.496 -35.821 -25.837 1.00 23.95 **ANISOU 1889 C ARG A 122** 1861 2562 4678 -42 -490 ATOM 1890 O ARG A 122 0 -5.413 -36.636 -26.760 1.00 24.35 **ANISOU 1890 O ARG A 122** 1962 2473 4815 -54 -627 -60 ATOM 1891 CB ARG A 122 -7.864 -36.545 -25.368 1.00 28.84 2125 3130 5704 -193 -528 **ANISOU 1891 CB ARG A 122** 95 -7.447 -37.786 -24.598 1.00 30.24 ATOM 1892 CG ARG A 122 **ANISOU 1892 CG ARG A 122** 2276 3211 6005 -281 -433 234 ATOM 1893 H ARG A 122 -7.249 -34.331 -26.878 1.00 34.40 Н ATOM 1894 HA ARG A 122 -6.744 -35.173 -24.347 1.00 31.80 Н ATOM 1895 HB2 ARG A 122 -8.711 -36.240 -25.006 1.00 34.61 ATOM 1896 HB3 ARG A 122 -7.975 -36.795 -26.299 1.00 34.61 Н ATOM 1897 N THR A 123 -4.435 -35.270 -25.258 1.00 21.78 Ν **ANISOU 1897 N THR A 123** 1692 2375 4208 10 -368 ATOM 1898 CA THR A 123 -3.080 -35.540 -25.707 1.00 20.68 C **ANISOU 1898 CA THR A 123** 1728 2182 3946 58 -376 C C ATOM 1899 C THR A 123 -2.214 -35.870 -24.502 1.00 19.59 **ANISOU 1899 C THR A 123** 1599 2085 3761 34 -226 212 ATOM 1900 O THR A 123 0 -2.564 -35.571 -23.356 1.00 19.99 **ANISOU 1900 O THR A 123** 1554 2235 3806 11 -110 321 0 ATOM 1901 CB THR A 123 -2.498 -34.341 -26.471 1.00 20.32 ANISOU 1901 CB THR A 123 1823 2203 3694 171 -403 -31 ATOM 1902 OG1 THR A 123 -2.453 -33.203 -25.609 1.00 19.70

ANISOU 1902 OG1 THR A 123 1720 2267 3500 198 -290 27 0 ATOM 1903 CG2 THR A 123 -3.371 -34.007 -27.684 1.00 21.43 1967 2312 3862 218 -557 -172 **ANISOU 1903 CG2 THR A 123** ATOM 1904 H THR A 123 -4.477 -34.728 -24.591 1.00 26.13 H ATOM 1905 HA THR A 123 -3.084 -36.307 -26.300 1.00 24.81 Н ATOM 1906 HB THR A 123 -1.603 -34.553 -26.780 1.00 24.38 ATOM 1907 HG1 THR A 123 -3.228 -33.012 -25.344 1.00 23.65 ATOM 1908 HG21 THR A 123 ATOM 1909 HG22 THR A 123 -2.998 -33.249 -28.162 1.00 25.71 -3.411 -34.768 -28.283 1.00 25.71 ATOM 1910 HG23 THR A 123 -4.270 -33.785 -27.394 1.00 25.71 ATOM 1911 N THR A 124 -1.074 -36.495 -24.769 1.00 18.36 ANISOU 1911 N THR A 124 1561 1856 3559 53 -229 214 ATOM 1912 CA THR A 124 -0.112 -36.832 -23.732 1.00 17.08 ANISOU 1912 CA THR A 124 1422 1729 3337 48 -107 342 ATOM 1913 C THR A 124 1.204 -36.142 -24.054 1.00 15.94 ANISOU 1913 C THR A 124 1421 1632 3002 134 -91 300 ATOM 1914 O THR A 124 1.667 -36.188 -25.197 1.00 16.84 ANISOU 1914 O THR A 124 1641 1676 3081 185 -171 202 CO ATOM 1915 CB THR A 124 0.061 -38.351 -23.630 1.00 18.24 1557 1734 3641 -14 -114 407 **ANISOU 1915 CB THR A 124** ATOM 1916 OG1 THR A 124 -1.194 -38.945 -23.274 1.00 19.62 O ANISOU 1916 OG1 THR A 124 1575 1857 4022 -105 -116 462 ATOM 1917 CG2 THR A 124 1.091 -38.712 -22.576 1.00 18.07 C ANISOU 1917 CG2 THR A 124 1566 1754 3545 -2 7 543 C ATOM 1917 CG2 THR A 124
ANISOU 1917 CG2 THR A 124
ATOM 1918 H THR A 124
ATOM 1919 HA THR A 124
ATOM 1920 HB THR A 124
ATOM 1921 HG1 THR A 124
ATOM 1922 HG21 THR A 124
ATOM 1923 HG22 THR A 124
ATOM 1924 HG23 THR A 124
ATOM 1925 N PHE A 125
ANISOU 1917 CG2 THR A 124
1.091 -38.712 -22.576 1.00 18.07
1566 1754 3545 -2 7 543
C
-0.832 -36.739 -25.557 1.00 22.03
H
0.357 -38.703 -24.485 1.00 21.89
H
1.188 -39.676 -22.524 1.00 21.68
H
1.948 -38.320 -22.802 1.00 21.68
H
1.948 -38.320 -22.802 1.00 21.68
H
1.794 -35.485 -23.060 1.00 14.89
N
1.794 -35.485 -23.060 1.00 14.89
N **ANISOU 1925 N PHE A 125** 1290 1619 2751 158 10 373 2.966 -34.670 -23.327 1.00 14.84 ATOM 1926 CA PHE A 125 1390 1659 2591 229 23 333 **ANISOU 1926 CA PHE A 125** ATOM 1927 C PHE A 125 3.777 -34.483 -22.058 1.00 14.39 ANISOU 1927 C PHE A 125 1322 1696 2447 239 117 430 CO ATOM 1928 O PHE A 125 3.247 -34.502 -20.943 1.00 14.90 0 **ANISOU 1928 O PHE A 125** 1307 1837 2519 215 181 512 2.585 -33.298 -23.916 1.00 14.00 ATOM 1929 CB PHE A 125 **ANISOU 1929 CB PHE A 125** 1306 1612 2401 278 -9 236 ATOM 1930 CG PHE A 125 1.582 -32.530 -23.094 1.00 14.96 **ANISOU 1930 CG PHE A 125** 1330 1839 2516 263 31 256 ATOM 1931 CD1 PHE A 125 0.221 -32.708 -23.292 1.00 15.61 ANISOU 1931 CD1 PHE A 125 1317 1905 2707 228 -11 237 ATOM 1932 CD2 PHE A 125 1.999 -31.622 -22.135 1.00 14.87 **ANISOU 1932 CD2 PHE A 125** 1318 1939 2392 292 103 288 ATOM 1933 CE1 PHE A 125 -0.706 -32.001 -22.537 1.00 16.51 ANISOU 1933 CE1 PHE A 125
ATOM 1934 CE2 PHE A 125
ANISOU 1934 CE2 PHE A 125
ANISOU 1935 CZ PHE A 125

ATOM 1936 H PHE A 125	1.539 -35.495 -22.239 1.00 17.87	Н
	3.525 -35.127 -23.975 1.00 17.81	
ATOM 1937 HA PHE A 125		H.
ATOM 1938 HB2 PHE A 125	3.386 -32.756 -23.986 1.00 16.80	Н
ATOM 1939 HB3 PHE A 125	2.202 -33.433 -24.797 1.00 16.80	Н
ATOM 1940 HD1 PHE A 125	-0.075 -33.314 -23.933 1.00 18.73	Н
ATOM 1941 HD2 PHE A 125	2.909 -31.491 -21.992 1.00 17.84	Н
ATOM 1942 HE1 PHE A 125	-1.616 -32.132 -22.675 1.00 19.82	Н
ATOM 1943 HE2 PHE A 125	1.375 -30.311 -20.736 1.00 18.59	н
ATOM 1944 HZ PHE A 125	-0.892 -30.632 -21.076 1.00 19.77	H
ATOM 1945 N THR A 126	5.075 -34.294 -22.260 1.00 12.84	N
ANISOU 1945 N THR A 126	1209 1500 2170 284 124 420	Ň
ATOM 1946 CA THR A 126	5.999 -33.966 -21.189 1.00 12.61	C
ANISOU 1946 CA THR A 126	1179 1562 2051 306 184 484	C
ATOM 1947 C THR A 126	5.892 -32.487 -20.816 1.00 11.44	C
ANISOU 1947 C THR A 126	1022 1521 1805 335 195 432	C
ATOM 1948 O THR A 126	5.599 -31.625 -21.654 1.00 11.20	0
ANISOU 1948 O THR A 126	1020 1477 1758 354 161 345	0
ATOM 1949 CB THR A 126	7.423 -34.318 -21.627 1.00 12.87	C
ANISOU 1949 CB THR A 126	1285 1545 2062 342 179 488	C
ATOM 1950 OG1 THR A 126	7.504 -35.730 -21.849 1.00 15.12	Ŏ
ANISOU 1950 OG1 THR A 126	1582 1727 2437 324 172 538	Ö
ATOM 1951 CG2 THR A 126	8.464 -33.902 -20.583 1.00 13.87	C
ANISOU 1951 CG2 THR A 126	1402 1766 2104 369 217 537	., С
ATOM 1952 H THR A 126	5.452 -34.352 -23.030 1.00 15.41	Η
ATOM 1953 HA THR A 126	5.781 -34.494 -20.405 1.00 15.13	Н
ATOM 1954 HB THR A 126	7.624 -33.854 -22.455 1.00 15.45	Н
ATOM 1955 HG1 THR A 126	8.281 -35.939 -22.090 1.00 18.15	Н
ATOM 1956 HG21 THR A 126	9.353 -34.138 -20.890 1.00 16.65	Н
ATOM 1957 HG22 THR A 126	8.425 -32.943 -20.440 1.00 16.65	Н
ATOM 1958 HG23 THR A 126	8.290 -34.354 -19.743 1.00 16.65	Н
ATOM 1959 N GLN A 127	6.144 -32.206 -19.539 1.00 11.76	N
ANISOU 1959 N GLN A 127	1031 1663 1773 349 239 486	Ň
ATOM 1960 CA GLN A 127	6.183 -30.851 -19.002 1.00 12.41	Ċ
ANISOU 1960 CA GLN A 127	1114 1843 1760 384 242 433	
		C
ATOM 1961 C GLN A 127	7.530 -30.597 -18.336 1.00 12.28	C
ANISOU 1961 C GLN A 127	1121 1871 1671 416 239 444	С
ATOM 1962 O GLN A 127	7.985 -31.410 -17.521 1.00 14.64	0
ANISOU 1962 O GLN A 127	1409 2201 1954 424 261 528	0
ATOM 1963 CB GLN A 127	5.072 -30.628 -17.976 1.00 13.88	C
ANISOU 1963 CB GLN A 127	1236 2127 1912 392 288 469	С
ATOM 1964 CG GLN A 127	3.668 -30.887 -18.470 1.00 15.62	C
ANISOU 1964 CG GLN A 127	1398 2313 2223 357 292 469	C
ATOM 1965 CD GLN A 127	2.654 -30.842 -17.337 1.00 17.65	C
ANISOU 1965 CD GLN A 127	1576 2671 2459 371 365 539	C
ATOM 1966 OE1 GLN A 127	2.688 -31.677 -16.426 1.00 19.16	ŏ
ANISOU 1966 OE1 GLN A 127	1736 2895 2650 370 427 654	ŏ
ATOM 1967 NE2 GLN A 127	1.752 -29.865 -17.378 1.00 18.77	N
ANISOU 1967 NE2 GLN A 127	1688 2866 2577 395 367 479	N
ATOM 1968 H GLN A 127	6.301 -32.808 -18.945 1.00 14.11	Η
ATOM 1969 HA GLN A 127	6.070 -30.213 -19.724 1.00 14.90	H
ATOM 1970 HB2 GLN A 127	5.229 -31.218 -17.222 1.00 16.66	Н
ATOM 1971 HB3 GLN A 127	5.111 -29.705 -17.678 1.00 16.66	Н
ATOM 1972 HG2 GLN A 127	3.428 -30.207 -19.119 1.00 18.74	Н

ATOM 1973 HG3 GLN A 127 3.630 -31.767 -18.876 1.00 18.74 Н 1.762 -29.298 -18.025 1.00 22.52 1.159 -29.800 -16.759 1.00 22.52 ATOM 1974 HE21 GLN A 127 Н ATOM 1975 HE22 GLN A 127 ATOM 1976 N TYR A 128 **ANISOU 1976 N TYR A 128** 1008 1731 1497 436 208 363 ATOM 1977 CA TYR A 128 9.375 -29.003 -18.010 1.00 11.43 **ANISOU 1977 CA TYR A 128** 1049 1809 1486 461 185 ATOM 1978 C TYR A 128 9.031 -27.833 -17.098 1.00 11.46 **ANISOU 1978 C TYR A 128** 1043 1904 1408 492 169 290 ATOM 1979 O TYR A 128 0 8.339 -26.901 -17.520 1.00 10.05 **ANISOU 1979 O TYR A 128** 875 1716 1230 494 166 221 ATOM 1980 CB TYR A 128 10.424 -28.540 -19.026 1.00 11.40 **ANISOU 1980 CB TYR A 128** 1072 1723 1535 458 165 ATOM 1981 CG TYR A 128 10.965 -29.581 -19.988 1.00 11.24 **ANISOU 1981 CG TYR A 128** 1076 1612 1581 452 182 358 10.757 -30.936 -19.786 1.00 12.10 ATOM 1982 CD1 TYR A 128 **ANISOU 1982 CD1 TYR A 128** 1182 1707 1710 443 198 ATOM 1983 CD2 TYR A 128 11.686 -29.190 -21.109 1.00 11.26 **ANISOU 1983 CD2 TYR A 128** 1111 1539 1628 465 189 ATOM 1984 CE1 TYR A 128 11.259 -31.881 -20.679 1.00 12.26 **ANISOU 1984 CE1 TYR A 128** 1237 1634 1788 449 207 464 ATOM 1985 CE2 TYR A 128 12.192 -30.123 -22.001 1.00 10.79 **ANISOU 1985 CE2 TYR A 128** 1087 1402 1612 482 209 369 ATOM 1986 CZ TYR A 128 11.969 -31.467 -21.781 1.00 10.63 **ANISOU 1986 CZ TYR A 128** 1069 1365 1606 475 211 427 ATOM 1987 OH TYR A 128 0 12.466 -32.400 -22.664 1.00 11.28 **ANISOU 1987 OH TYR A 128** 0 1196 1361 1729 502 225 453 ATOM 1988 H TYR A 128 7.863 -28.921 -19.263 1.00 13.38 ATOM 1989 HA TYR A 128 9.751 -29.719 -17.474 1.00 13.72 Н ATOM 1990 HB2 TYR A 128 10.032 -27.833 -19.562 1.00 13.67 ATOM 1991 HB3 TYR A 128 11.181 -28.185 -18.535 1.00 13.67 Н 10.276 -31.219 -19.043 1.00 14.52 ATOM 1992 HD1 TYR A 128 ATOM 1993 HD2 TYR A 128 11.837 -28.286 -21.262 1.00 13.51 ATOM 1994 HE1 TYR A 128 11.111 -32.788 -20.532 1.00 14.71 ATOM 1995 HE2 TYR A 128 12.672 -29.845 -22.747 1.00 12.95 ATOM 1996 HH TYR A 128 12.876 -32.015 -23.288 1.00 13.53 ATOM 1997 N TRP A 129 9.531 -27.866 -15.862 1.00 12.11 Ν **ANISOU 1997 N TRP A 129** 1115 2076 1412 529 152 309 ATOM 1998 CA TRP A 129 9.220 -26.845 -14.873 1.00 13.37 **ANISOU 1998 CA TRP A 129** 1279 2329 1473 578 127 242 ATOM 1999 C TRP A 129 10.486 -26.217 -14.305 1.00 13.63 ANISOU 1999 C TRP A 129 ATOM 2000 O TRP A 129 1316 2384 1480 603 46 178 0 11.454 -26.918 -13.989 1.00 13.73 **ANISOU 2000 O TRP A 129** 1314 2405 1495 609 22 228 ATOM 2001 CB TRP A 129 8.415 -27.419 -13.689 1.00 16.00 **ANISOU 2001 CB TRP A 129** 1599 2774 1705 630 179 318 ATOM 2002 CG TRP A 129 7.108 -28.054 -14.036 1.00 16.43 **ANISOU 2002 CG TRP A 129** 1623 2815 1805 603 258 390 ATOM 2003 CD1 TRP A 129 6.913 -29.326 -14.501 1.00 16.92 ANISOU 2003 CD1 TRP A 129
ATOM 2004 CD2 TRP A 129
ANISOU 2004 CD2 TRP A 129
ANISOU 2004 CD2 TRP A 129
ATOM 2005 NE1 TRP A 129
5.806 -27.474 -13.898 1.00 17.67
1759 3018 1937 624 300 368
ATOM 2005 NE1 TRP A 129
5.571 -29.564 -14.677 1.00 18.02

ANISOU 2005 NE1 TRP A 129	1755 2949 2141 534 356 527	N
ATOM 2006 CE2 TRP A 129	4.870 -28.441 -14.319 1.00 17.76	С
ANISOU 2006 CE2 TRP A 129	1719 2990 2039 578 362 458	С
ATOM 2007 CE3 TRP A 129	5.339 -26.225 -13.475 1.00 18.07	С
ANISOU 2007 CE3 TRP A 129	1826 3132 1907 681 288 276	С
ATOM 2008 CZ2 TRP A 129	3.503 -28.201 -14.323 1.00 18.58	С
ANISOU 2008 CZ2 TRP A 129		C
ATOM 2009 CZ3 TRP A 129		Č
ANISOU 2009 CZ3 TRP A 129		C
	3.079 -26.970 -13.909 1.00 19.14	Č
ANISOU 2010 CH2 TRP A 129		C
ATOM 2011 H TRP A 129	10.059 -28.480 -15.572 1.00 14.54	H
ATOM 2012 HA TRP A 129	8.693 -26.145 -15.290 1.00 16.05	Ĥ
	8.957 -28.093 -13.250 1.00 19.20	H
ATOM 2014 HB3 TRP A 129		H
ATOM 2015 HD1 TRP A 129		H
ATOM 2016 HE1 TRP A 129		H
ATOM 2017 HE3 TRP A 129		H
	2.899 -28.849 -14.605 1.00 22.30	H
ATOM 2010 HZ2 TRP A 129 ATOM 2019 HZ3 TRP A 129		H
ATOM 2019 H23 TRP A 129 ATOM 2020 HH2 TRP A 129	2.169 -26.781 -13.903 1.00 22.97	
		H
ATOM 2021 N SER A 130	10.456 -24.892 -14.170 1.00 12.07	N
	1132 2188 1265 619 -2 64	N
ATOM 2022 CA SER A 130	11.286 -24.151 -13.223 1.00 13.02	C
ANISOU 2022 CA SER A 130	1256 2357 1334 661 -97 -22	C
ATOM 2023 C SER A 130	10.339 -23.464 -12.249 1.00 13.69	С
ANISOU 2023 C SER A 130	1376 2540 1286 739 -101 -84	C
	9.445 -22.721 -12.675 1.00 14.11	0
ANISOU 2024 O SER A 130		0
	12.166 -23.104 -13.918 1.00 12.96	C
ANISOU 2025 CB SER A 130		C
	13.224 -23.682 -14.645 1.00 12.38	0
ANISOU 2026 OG SER A 130	1121 2094 1487 563 -154 -55	0
ATOM 2027 H SER A 130	9.942 -24.383 -14.634 1.00 14.48	Η
ATOM 2028 HA SER A 130	11.854 -24.763 -12.731 1.00 15.63	H.
ATOM 2029 HB2 SER A 130	11.614 -22.592 -14.529 1.00 15.56	Н
ATOM 2030 HB3 SER A 130	12.538 -22.516 -13.243 1.00 15.56	Н
ATOM 2031 HG SER A 130	13.717 -24.127 -14.130 1.00 14.85	H
ATOM 2032 N VAL A 131	10.528 -23.706 -10.954 1.00 14.79	N
ANISOU 2032 N VAL A 131	1533 2798 1290 822 -137 -81	N
ATOM 2033 CA VAL A 131	9.689 -23.122 -9.911 1.00 16.08	C
ANISOU 2033 CA VAL A 131	1741 3072 1297 926 -134 -134	C
ATOM 2034 C VAL A 131	10.590 -22.353 -8.951 1.00 17.37	С
ANISOU 2034 C VAL A 131	1936 3281 1384 995 -275 -265	С
ATOM 2035 O VAL A 131	11.498 -22.936 -8.346 1.00 17.66	0
ANISOU 2035 O VAL A 131	1965 3367 1379 1026 -338 -239	0
ATOM 2036 CB VAL A 131	8.884 -24.192 -9.157 1.00 16.90	С
ANISOU 2036 CB VAL A 131	1848 3293 1279 993 -29 6	С
ATOM 2037 CG1 VAL A 131	7.959 -23.540 -8.151 1.00 17.51	С
ANISOU 2037 CG1 VAL A 131	1972 3489 1192 1115 -3 -40	C
ATOM 2038 CG2 VAL A 131	8.083 -25.066 -10.128 1.00 15.88	С
ANISOU 2038 CG2 VAL A 131	1672 3099 1263 910 88 129	С
ATOM 2039 H VAL A 131	11.149 -24.216 -10.648 1.00 17.75	Н

ATOM 2040 HA VAL A 131	9.065 -22.497 -10.312 1.00 19.29 H
ATOM 2041 HB VAL A 131	9.498 -24.766 -8.673 1.00 20.28 H
ATOM 2042 HG11 VAL A 131	7.461 -24.231 -7.687 1.00 21.01 H
ATOM 2043 HG12 VAL A 131	8.490 -23.032 -7.518 1.00 21.01 H
ATOM 2044 HG13 VAL A 131	7.349 -22.950 -8.620 1.00 21.01 H
ATOM 2045 HG21 VAL A 131	7.588 -25.729 -9.620 1.00 19.06 H
ATOM 2046 HG22 VAL A 131	7.469 -24.504 -10.626 1.00 19.06 H
ATOM 2047 HG23 VAL A 131	8.697 -25.506 -10.736 1.00 19.06 H
ATOM 2048 N ARG A 132	10.324 -21.055 -8.790 1.00 18.20 N
ANISOU 2048 N ARG A 132	2077 3367 1472 1027 -334 -410 N
ATOM 2049 CA ARG A 132	11.157 -20.227 -7.927 1.00 18.85 C
ANISOU 2049 CA ARG A 132	
ATOM 2050 C ARG A 132	11.127 -20.772 -6.503 1.00 20.30 C
ANISOU 2050 C ARG A 132	2425 3826 1463 1234 -518 -541 C
ATOM 2051 O ARG A 132	10.084 -21.208 -6.013 1.00 21.06 O
ANISOU 2051 O ARG A 132	2555 4030 1417 1319 -402 -454 O
ATOM 2052 CB ARG A 132	
ANISOU 2052 CB ARG A 132	
ATOM 2053 CG ARG A 132	11.777 -17.757 -7.700 1.00 20.43 C
ANISOU 2053 CG ARG A 132	2432 3535 1795 1099 -720 -894 C
ATOM 2054 CD ARG A 132	11.255 -16.345 -7.837 1.00 21.60 C
ANISOU 2054 CD ARG A 132	2627 3601 1978 1115 -754 -1041 C
ATOM 2055 NE ARG A 132	
ANISOU 2055 NE ARG A 132	
ATOM 2056 CZ ARG A 132	12.693 -14.752 -6.593 1.00 25.34 C
ANISOU 2056 CZ ARG A 132	3130 3986 2512 1164 -1064 -1342 C
ATOM 2057 NH1 ARG A 132	12.158 -15.109 <i>-</i> 5.431 1.00 25.76 N
ATOM ZUJI NITI ANG A IJZ	12.136 - 13.109 - 3.431 1.00 23.70 N
	3247 4176 2363 1297 -1026 -1307 N
	3247 4176 2363 1297 -1026 -1307 N
ANISOU 2057 NH1 ARG A 132	3247 4176 2363 1297 -1026 -1307 N
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132 ATOM 2063 HG2 ARG A 132	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132 ATOM 2063 HG2 ARG A 132 ATOM 2064 HG3 ARG A 132	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H 12.488 -17.884 -8.347 1.00 24.52
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132 ATOM 2063 HG2 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2065 HD2 ARG A 132	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H 12.488 -17.884 -8.347 1.00 24.52 H 10.834 -16.249 -8.705 1.00 25.92
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2063 HG2 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2065 HD2 ARG A 132 ATOM 2066 HD3 ARG A 132	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H 12.488 -17.884 -8.347 1.00 24.52 H 10.834 -16.249 -8.705 1.00 25.92 H 10.604 -16.182 -7.136 1.00 25.92
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132 ATOM 2063 HG2 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2065 HD2 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2067 HE ARG A 132	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H 12.488 -17.884 -8.347 1.00 24.52 H 10.834 -16.249 -8.705 1.00 25.92 H 10.604 -16.182 -7.136 1.00 25.92 H 12.683 -15.071 -8.455 1.00 27.43 H
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132 ATOM 2063 HG2 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2065 HD2 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2067 HE ARG A 132 ATOM 2067 HE ARG A 132	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H 12.488 -17.884 -8.347 1.00 24.52 H 10.834 -16.249 -8.705 1.00 25.92 H 10.604 -16.182 -7.136 1.00 25.92 H 12.683 -15.071 -8.455 1.00 27.43 H 11.543 -15.709 -5.407 1.00 30.91 H
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132 ATOM 2063 HG2 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2065 HD2 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2068 HH11 ARG A 132 ATOM 2068 HH11 ARG A 132	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H 12.488 -17.884 -8.347 1.00 24.52 H 10.834 -16.249 -8.705 1.00 25.92 H 10.604 -16.182 -7.136 1.00 25.92 H 11.543 -15.709 -5.407 1.00 30.91 H 12.424 -14.736 -4.703 1.00 30.91 H
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132 ATOM 2063 HG2 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2065 HD2 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2067 HE ARG A 132 ATOM 2068 HH11 ARG A 132 ATOM 2069 HH12 ARG A 132 ATOM 2069 HH12 ARG A 132	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H 12.488 -17.884 -8.347 1.00 24.52 H 10.834 -16.249 -8.705 1.00 25.92 H 10.604 -16.182 -7.136 1.00 25.92 H 11.543 -15.071 -8.455 1.00 27.43 H 11.543 -15.709 -5.407 1.00 30.91 H 12.424 -14.736 -4.703 1.00 30.91 H 13.992 -13.586 -7.364 1.00 32.71 H
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132 ATOM 2063 HG2 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2065 HD2 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2067 HE ARG A 132 ATOM 2068 HH11 ARG A 132 ATOM 2069 HH12 ARG A 132 ATOM 2070 HH21 ARG A 132 ATOM 2071 HH22 ARG A 132	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H 12.488 -17.884 -8.347 1.00 24.52 H 10.834 -16.249 -8.705 1.00 25.92 H 10.604 -16.182 -7.136 1.00 25.92 H 12.683 -15.071 -8.455 1.00 27.43 H 11.543 -15.709 -5.407 1.00 30.91 H 12.424 -14.736 -4.703 1.00 30.91 H 13.992 -13.586 -7.364 1.00 32.71 H 13.991 -13.456 -5.883 1.00 32.71
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132 ATOM 2063 HG2 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2067 HE ARG A 132 ATOM 2068 HH11 ARG A 132 ATOM 2069 HH12 ARG A 132 ATOM 2070 HH21 ARG A 132 ATOM 2071 HH22 ARG A 132 ATOM 2071 HH22 ARG A 133	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H 12.488 -17.884 -8.347 1.00 24.52 H 10.834 -16.249 -8.705 1.00 25.92 H 10.604 -16.182 -7.136 1.00 25.92 H 11.543 -15.709 -5.407 1.00 30.91 H 13.992 -13.586 -7.364 1.00 32.71 H 13.901 -13.456 -5.883 1.00 32.71 H 13.901 -13.456 -5.883 1.00 21.38 N
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132 ATOM 2063 HG2 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2067 HE ARG A 132 ATOM 2068 HH11 ARG A 132 ATOM 2069 HH12 ARG A 132 ATOM 2070 HH21 ARG A 132 ATOM 2071 HH22 ARG A 132 ATOM 2072 N GLN A 133 ANISOU 2072 N GLN A 133	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H 12.488 -17.884 -8.347 1.00 24.52 H 10.834 -16.249 -8.705 1.00 25.92 H 10.604 -16.182 -7.136 1.00 25.92 H 12.683 -15.071 -8.455 1.00 27.43 H 11.543 -15.709 -5.407 1.00 30.91 H 13.992 -13.586 -7.364 1.00 32.71 H 13.901 -13.456 -5.883 1.00 32.71 H 13.901 -13.456 -5.883 1.00 32.71 H 12.287 -20.761 -5.841 1.00 21.38 N 2559 3988 1575 1270 -666 -613 N
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132 ATOM 2063 HG2 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2065 HD2 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2067 HE ARG A 132 ATOM 2068 HH11 ARG A 132 ATOM 2069 HH12 ARG A 132 ATOM 2070 HH21 ARG A 132 ATOM 2071 HH22 ARG A 132 ATOM 2072 N GLN A 133 ANISOU 2072 N GLN A 133 ANISOU 2073 CA GLN A 133	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H 10.834 -16.249 -8.705 1.00 25.92 H 10.604 -16.182 -7.136 1.00 25.92 H 11.543 -15.071 -8.455 1.00 27.43 H 11.543 -15.709 -5.407 1.00 30.91 H 12.424 -14.736 -4.703 1.00 30.91 H 13.992 -13.586 -7.364 1.00 32.71 H 13.901 -13.456 -5.883 1.00 32.71 H 12.287 -20.761 -5.841 1.00 21.38 N 2559 3988 1575 1270 -666 -613 N 12.369 -21.322 -4.495 1.00 23.06 C
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132 ATOM 2063 HG2 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2065 HD2 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2067 HE ARG A 132 ATOM 2068 HH11 ARG A 132 ATOM 2069 HH12 ARG A 132 ATOM 2070 HH21 ARG A 132 ATOM 2071 HH22 ARG A 132 ATOM 2072 N GLN A 133 ANISOU 2072 N GLN A 133 ANISOU 2073 CA GLN A 133	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H 10.834 -16.249 -8.705 1.00 24.52 H 10.604 -16.182 -7.136 1.00 25.92 H 10.604 -16.182 -7.136 1.00 25.92 H 11.543 -15.709 -5.407 1.00 30.91 H 12.424 -14.736 -4.703 1.00 30.91 H 13.992 -13.586 -7.364 1.00 32.71 H 13.901 -13.456 -5.883 1.00 32.71 H 12.287 -20.761 -5.841 1.00 21.38 N 2559 3988 1575 1270 -666 -613 N 12.369 -21.322 -4.495 1.00 23.06 C 2821 4306 1633 1385 -654 -572 C
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132 ATOM 2063 HG2 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2065 HD2 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2067 HE ARG A 132 ATOM 2068 HH11 ARG A 132 ATOM 2069 HH12 ARG A 132 ATOM 2070 HH21 ARG A 132 ATOM 2071 HH22 ARG A 132 ATOM 2072 N GLN A 133 ANISOU 2072 N GLN A 133 ANISOU 2073 CA GLN A 133 ANISOU 2073 CA GLN A 133 ANISOU 2074 C GLN A 133	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H 12.488 -17.884 -8.347 1.00 24.52 H 10.834 -16.249 -8.705 1.00 25.92 H 10.604 -16.182 -7.136 1.00 25.92 H 12.683 -15.071 -8.455 1.00 27.43 H 11.543 -15.709 -5.407 1.00 30.91 H 13.992 -13.586 -7.364 1.00 32.71 H 13.991 -13.456 -5.883 1.00 32.71 H 12.287 -20.761 -5.841 1.00 21.38 N 2559 3988 1575 1270 -666 -613 N 12.369 -21.322 -4.495 1.00 23.06 C 2821 4306 1633 1385 -654 -572 C
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132 ATOM 2063 HG2 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2065 HD2 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2067 HE ARG A 132 ATOM 2068 HH11 ARG A 132 ATOM 2069 HH12 ARG A 132 ATOM 2070 HH21 ARG A 132 ATOM 2071 HH22 ARG A 132 ATOM 2072 N GLN A 133 ANISOU 2072 N GLN A 133 ANISOU 2073 CA GLN A 133 ANISOU 2074 C GLN A 133 ANISOU 2074 C GLN A 133	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H 10.834 -16.249 -8.705 1.00 25.92 H 10.604 -16.182 -7.136 1.00 25.92 H 11.543 -15.071 -8.455 1.00 27.43 H 11.543 -15.709 -5.407 1.00 30.91 H 13.992 -13.586 -7.364 1.00 32.71 H 13.901 -13.456 -5.883 1.00 32.71 H 13.901 -13.456 -5.883 1.00 32.71 H 12.287 -20.761 -5.841 1.00 21.38 N 2559 3988 1575 1270 -666 -613 N 12.369 -21.322 -4.495 1.00 23.06 C 2821 4306 1633 1385 -654 -572 C 11.605 -20.469 -3.489 1.00 25.11 C 3160 4613 1767 1509 -651 -666 C
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132 ATOM 2063 HG2 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2065 HD2 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2067 HE ARG A 132 ATOM 2069 HH11 ARG A 132 ATOM 2069 HH12 ARG A 132 ATOM 2070 HH21 ARG A 132 ATOM 2071 HH22 ARG A 132 ATOM 2072 N GLN A 133 ANISOU 2072 N GLN A 133 ANISOU 2073 CA GLN A 133 ANISOU 2074 C GLN A 133 ANISOU 2074 C GLN A 133 ANISOU 2075 O GLN A 133	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H 12.488 -17.884 -8.347 1.00 24.52 H 10.834 -16.249 -8.705 1.00 25.92 H 10.604 -16.182 -7.136 1.00 25.92 H 11.543 -15.709 -5.407 1.00 30.91 H 11.543 -15.709 -5.407 1.00 30.91 H 13.992 -13.586 -7.364 1.00 32.71 H 13.901 -13.456 -5.883 1.00 32.71 H 12.287 -20.761 -5.841 1.00 21.38 N 2559 3988 1575 1270 -666 -613 N 12.369 -21.322 -4.495 1.00 23.06 C 2821 4306 1633 1385 -654 -572 C 11.605 -20.469 -3.489 1.00 25.11 C 3160 4613 1767 1509 -651 -666 C
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132 ATOM 2063 HG2 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2065 HD2 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2067 HE ARG A 132 ATOM 2068 HH11 ARG A 132 ATOM 2069 HH12 ARG A 132 ATOM 2070 HH21 ARG A 132 ATOM 2071 HH22 ARG A 132 ATOM 2072 N GLN A 133 ANISOU 2072 N GLN A 133 ANISOU 2073 CA GLN A 133 ANISOU 2074 C GLN A 133 ANISOU 2074 C GLN A 133 ANISOU 2075 O GLN A 133 ANISOU 2075 O GLN A 133 ANISOU 2075 O GLN A 133	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H 12.488 -17.884 -8.347 1.00 24.52 H 10.834 -16.249 -8.705 1.00 25.92 H 10.604 -16.182 -7.136 1.00 25.92 H 11.543 -15.709 -5.407 1.00 30.91 H 11.543 -15.709 -5.407 1.00 30.91 H 12.424 -14.736 -4.703 1.00 30.91 H 13.992 -13.586 -7.364 1.00 32.71 H 13.901 -13.456 -5.883 1.00 32.71 H 12.287 -20.761 -5.841 1.00 21.38 N 2559 3988 1575 1270 -666 -613 N 12.369 -21.322 -4.495 1.00 23.06 C 2821 4306 1633 1385 -654 -572 C 11.605 -20.469 -3.489 1.00 25.11 C 3160 4613 1767 1509 -651 -666 C 11.102 -20.988 -2.487 1.00 25.56 O 3258 4774 1678 1625 -574 -587 O
ANISOU 2057 NH1 ARG A 132 ATOM 2058 NH2 ARG A 132 ANISOU 2058 NH2 ARG A 132 ATOM 2059 H ARG A 132 ATOM 2060 HA ARG A 132 ATOM 2061 HB2 ARG A 132 ATOM 2062 HB3 ARG A 132 ATOM 2063 HG2 ARG A 132 ATOM 2064 HG3 ARG A 132 ATOM 2065 HD2 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2066 HD3 ARG A 132 ATOM 2067 HE ARG A 132 ATOM 2068 HH11 ARG A 132 ATOM 2069 HH12 ARG A 132 ATOM 2070 HH21 ARG A 132 ATOM 2071 HH22 ARG A 132 ATOM 2072 N GLN A 133 ANISOU 2072 N GLN A 133 ANISOU 2073 CA GLN A 133 ANISOU 2074 C GLN A 133 ANISOU 2074 C GLN A 133 ANISOU 2075 O GLN A 133 ANISOU 2075 O GLN A 133 ANISOU 2075 O GLN A 133	3247 4176 2363 1297 -1026 -1307 N 13.636 -13.819 -6.616 1.00 27.26 N 3339 4088 2929 1104 -1207 -1474 N 9.674 -20.636 -9.167 1.00 21.84 H 12.073 -20.252 -8.244 1.00 22.62 H 10.296 -18.587 -8.827 1.00 23.14 H 10.000 -18.656 -7.269 1.00 23.14 H 12.117 -17.870 -6.798 1.00 24.52 H 12.488 -17.884 -8.347 1.00 24.52 H 10.834 -16.249 -8.705 1.00 25.92 H 10.604 -16.182 -7.136 1.00 25.92 H 11.543 -15.709 -5.407 1.00 30.91 H 11.543 -15.709 -5.407 1.00 30.91 H 13.992 -13.586 -7.364 1.00 32.71 H 13.901 -13.456 -5.883 1.00 32.71 H 12.287 -20.761 -5.841 1.00 21.38 N 2559 3988 1575 1270 -666 -613 N 12.369 -21.322 -4.495 1.00 23.06 C 2821 4306 1633 1385 -654 -572 C 11.605 -20.469 -3.489 1.00 25.11 C 3160 4613 1767 1509 -651 -666 C

ATOM 2077 CG GLN A 133	14.596 -22.505 -4.908 1.00 22.65 C
ANISOU 2077 CG GLN A 133	2658 4194 1753 1273 -784 -499 C
ATOM 2078 CD GLN A 133	15.974 -22.827 -4.351 1.00 24.31 C
ANISOU 2078 CD GLN A 133	2839 4400 1997 1277 -906 -525 C
ATOM 2079 OE1 GLN A 133	16.623 -21.987 -3.714 1.00 26.17 O
ANISOU 2079 OE1 GLN A 133	3087 4613 2242 1304 -1051 -680 O
ATOM 2080 NE2 GLN A 133	16.417 -24.061 -4.565 1.00 23.29 N
ANISOU 2080 NE2 GLN A 133	2670 4288 1891 1254 -850 -373 N
ATOM 2081 H GLN A 133	13.026 -20.442 -6.144 1.00 25.65 H
ATOM 2082 HA GLN A 133	11.967 -22.205 -4.499 1.00 27.67 H
ATOM 2083 HB2 GLN A 133	14.280 -20.622 -4.174 1.00 28.66 H
ATOM 2084 HB3 GLN A 133	13.865 -21.760 -3.148 1.00 28.66 H
ATOM 2085 HG2 GLN A 133	14.085 -23.329 -4.935 1.00 27.18 H
ATOM 2086 HG3 GLN A 133	14.711 -22.158 -5.806 1.00 27.18 H
ATOM 2000 HG3 GEN A 133	15.931 -24.623 -4.998 1.00 27.95 H
ATOM 2087 HE21 GEN A 133	17.190 -24.297 -4.272 1.00 27.95 H
ATOM 2000 HE22 GEN A 133 ATOM 2089 N SER A 134	11.511 -19.170 -3.732 1.00 27.93 N
ANISOU 2089 N SER A 134	3264 4616 1919 1491 -730 -824 N
ATOM 2090 CA SER A 134	
ATOM 2091 C SER A 134	9.892 -17.397 -3.869 1.00 26.54 C
ANISOU 2091 C SER A 134	3423 4651 2012 1543 -680 -952 C
ATOM 2092 O SER A 134	10.331 -17.100 -4.984 1.00 23.58 O
ANISOU 2092 O SER A 134	3004 4168 1788 1421 -721 -996 O
ATOM 2093 CB SER A 134	11.524 -17.444 -1.965 1.00 31.45 C
ANISOU 2093 CB SER A 134	4095 5333 2522 1674 -896 -1075 C
ATOM 2094 OG SER A 134	12.394 -16.583 -2.676 1.00 32.97 O
ANISOU 2094 OG SER A 134	4248 5380 2900 1561 -1035 -1213 O
ATOM 2095 H SER A 134	11.926 -18.769 -4.370 1.00 30.95 H
ATOM 2096 HA SER A 134	10.060 -18.817 -2.409 1.00 33.79 H
ATOM 2097 HB2 SER A 134	10.931 -16.910 -1.415 1.00 37.74 H
ATOM 2098 HB3 SER A 134	12.053 -18.035 -1.406 1.00 37.74 H
ATOM 2099 HG SER A 134	12.849 -16.126 -2.138 1.00 39.57 H
ATOM 2100 N LYS A 135	8.707 -16.998 -3.420 1.00 27.22 N
ANISOU 2100 N LYS A 135	3550 4782 2011 1631 -595 -932 N
ATOM 2101 CA LYS A 135	7.832 -16.197 -4.260 1.00 26.79 C
ANISOU 2101 CA LYS A 135	3490 4651 2039 1582 -541 -958 C
ATOM 2102 C LYS A 135	8.505 -14.880 -4.618 1.00 27.01 C
ANISOU 2102 C LYS A 135	3534 4533 2194 1531 -687 -1142 C
	9.034 -14.174 -3.753 1.00 28.08 O
ANISOU 2103 O LYS A 135	3713 4651 2304 1597 -814 -1268 O
ATOM 2104 CB LYS A 135	6.506 -15.941 -3.551 1.00 28.01 C
ANISOU 2104 CB LYS A 135	3682 4882 2080 1694 -445 -905 C
ATOM 2105 CG LYS A 135	5.641 -17.175 -3.435 1.00 27.95 C
ANISOU 2105 CG LYS A 135	3636 4982 2003 1714 -279 -704 C
ATOM 2106 CD LYS A 135	4.319 -16.833 -2.782 1.00 29.45 C
ANISOU 2106 CD LYS A 135	3849 5234 2104 1817 -190 -654 C
ATOM 2107 CE LYS A 135	3.530 -18.083 -2.449 1.00 30.65 C
ANISOU 2107 CE LYS A 135	3959 5489 2198 1847 -34 -450 C
ATOM 2108 NZ LYS A 135	2.264 -17.751 -1.743 1.00 32.19 N
ANISOU 2108 NZ LYS A 135	4173 5750 2309 1956 52 -399 N
ATOM 2109 H LYS A 135	8.390 -17.176 -2.641 1.00 32.66 H
ATOM 2110 HA LYS A 135	7.650 -16.679 -5.082 1.00 32.15 H

ATOM 2111 HB2 LYS A 135	6.687 -15.618 -2.655 1.00 33.62	Н
ATOM 2112 HB3 LYS A 135	6.008 -15.274 -4.049 1.00 33.62	Н
ATOM 2113 HG2 LYS A 135	5.464 -17.531 -4.319 1.00 33.54	Н
ATOM 2114 HG3 LYS A 135	6.092 -17.836 -2.887 1.00 33.54	Н
ATOM 2115 HD2 LYS A 135	4.484 -16.348 -1.959 1.00 35.33	Η̈́
ATOM 2116 HD3 LYS A 135		Н
ATOM 2117 HE2 LYS A 135	3.307 -18.550 -3.270 1.00 36.78	Н
ATOM 2118 HE3 LYS A 135	4.061 -18.653 -1.871 1.00 36.78	Н
_		H
ATOM 2120 HZ2 LYS A 135	2.443 -17.324 -0.983 1.00 38.63	Н
ATOM 2121 HZ3 LYS A 135	1.757 -17.230 -2.256 1.00 38.63	Н
ATOM 2122 N ARG A 136	8.480 -14.561 -5.892 1.00 24.97 N	J
ANISOU 2122 N ARG A 136	3239 4164 2083 1415 -666 -1154	N
ATOM 2123 CA ARG A 136		С
ANISOU 2123 CA ARG A 136	3244 4003 2247 1348 -784 -1305	С
ATOM 2124 C ARG A 136	8.273 -12.131 -6.021 1.00 26.19	•
ANISOU 2124 C ARG A 136		
	3456 4117 2380 1416 -787 -1376	C
ATOM 2125 O ARG A 136)
ANISOU 2125 O ARG A 136	3482 4178 2340 1445 -662 -1291	0
ATOM 2126 CB ARG A 136	9.271 -13.437 -7.901 1.00 23.60	С
ANISOU 2126 CB ARG A 136	3017 3716 2236 1218 -735 -1277	C
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ATOM 2127 CG ARG A 136	10.162 -12.370 -8.487 1.00 23.32	С
ANISOU 2127 CG ARG A 136	2962 3490 2409 1128 -851 -1408	C
ATOM 2128 CD ARG A 136	10.413 -12.634 -9.959 1.00 20.50	C
ANISOU 2128 CD ARG A 136	2535 3012 2243 991 -764 -1305	C
ATOM 2129 NE ARG A 136	11.407 -11.711 -10.478 1.00 21.03	N.
ANISOU 2129 NE ARG A 136	2562 2887 2539 894 -857 -1388	N
ATOM 2130 CZ ARG A 136	11.935 -11.790 -11.693 1.00 20.62	C
ANISOU 2130 CZ ARG A 136	2441 2707 2687 772 -792 -1289	C
ATOM 2131 NH1 ARG A 136	11.568 -12.762 -12.512 1.00 19.30	Ň
ANISOU 2131 NH1 ARG A 136	2247 2582 2502 737 -653 -1121	N
ATOM 2132 NH2 ARG A 136	12.842 -10.900 -12.077 1.00 21.92	Ν
ANISOU 2132 NH2 ARG A 136	2561 2695 3073 691 -868 -1357	Ν
ATOM 2133 H ARG A 136	8.099 -15.032 -6.502 1.00 29.96 H	
ATOM 2134 HA ARG A 136		H.
ATOM 2135 HB2 ARG A 136	9.655 -14.299 -8.126 1.00 28.33	Н
ATOM 2136 HB3 ARG A 136		
	8.397 -13.351 -8.312 1.00 28.33	Н
ATOM 2137 HG2 ARG A 136		
ATOM 2137 HG2 ARG A 136	9.730 -11.506 -8.399 1.00 27.99	Н
ATOM 2138 HG3 ARG A 136	9.730 -11.506 -8.399 1.00 27.99 11.015 -12.372 -8.025 1.00 27.99	H H
ATOM 2138 HG3 ARG A 136 ATOM 2139 HD2 ARG A 136	9.730 -11.506 -8.399 1.00 27.99 11.015 -12.372 -8.025 1.00 27.99 10.744 -13.539 -10.074 1.00 24.60	H H H
ATOM 2138 HG3 ARG A 136	9.730 -11.506 -8.399 1.00 27.99 11.015 -12.372 -8.025 1.00 27.99	H H
ATOM 2138 HG3 ARG A 136 ATOM 2139 HD2 ARG A 136 ATOM 2140 HD3 ARG A 136	9.730 -11.506 -8.399 1.00 27.99 11.015 -12.372 -8.025 1.00 27.99 10.744 -13.539 -10.074 1.00 24.60 9.589 -12.509 -10.456 1.00 24.60	H H H
ATOM 2138 HG3 ARG A 136 ATOM 2139 HD2 ARG A 136 ATOM 2140 HD3 ARG A 136 ATOM 2141 HE ARG A 136	9.730 -11.506 -8.399 1.00 27.99 11.015 -12.372 -8.025 1.00 27.99 10.744 -13.539 -10.074 1.00 24.60 9.589 -12.509 -10.456 1.00 24.60 11.684 -11.084 -9.959 1.00 25.23	H H H H
ATOM 2138 HG3 ARG A 136 ATOM 2139 HD2 ARG A 136 ATOM 2140 HD3 ARG A 136 ATOM 2141 HE ARG A 136 ATOM 2142 HH11 ARG A 136	9.730 -11.506 -8.399 1.00 27.99 11.015 -12.372 -8.025 1.00 27.99 10.744 -13.539 -10.074 1.00 24.60 9.589 -12.509 -10.456 1.00 24.60 11.684 -11.084 -9.959 1.00 25.23 10.981 -13.339 -12.260 1.00 23.16	H H H H H
ATOM 2138 HG3 ARG A 136 ATOM 2139 HD2 ARG A 136 ATOM 2140 HD3 ARG A 136 ATOM 2141 HE ARG A 136 ATOM 2142 HH11 ARG A 136 ATOM 2143 HH12 ARG A 136	9.730 -11.506 -8.399 1.00 27.99 11.015 -12.372 -8.025 1.00 27.99 10.744 -13.539 -10.074 1.00 24.60 9.589 -12.509 -10.456 1.00 24.60 11.684 -11.084 -9.959 1.00 25.23 10.981 -13.339 -12.260 1.00 23.16 11.911 -12.814 -13.299 1.00 23.16	H
ATOM 2138 HG3 ARG A 136 ATOM 2139 HD2 ARG A 136 ATOM 2140 HD3 ARG A 136 ATOM 2141 HE ARG A 136 ATOM 2142 HH11 ARG A 136 ATOM 2143 HH12 ARG A 136 ATOM 2144 HH21 ARG A 136	9.730 -11.506 -8.399 1.00 27.99 11.015 -12.372 -8.025 1.00 27.99 10.744 -13.539 -10.074 1.00 24.60 9.589 -12.509 -10.456 1.00 24.60 11.684 -11.084 -9.959 1.00 25.23 10.981 -13.339 -12.260 1.00 23.16 11.911 -12.814 -13.299 1.00 23.16 13.080 -10.270 -11.542 1.00 26.31	H
ATOM 2138 HG3 ARG A 136 ATOM 2139 HD2 ARG A 136 ATOM 2140 HD3 ARG A 136 ATOM 2141 HE ARG A 136 ATOM 2142 HH11 ARG A 136 ATOM 2143 HH12 ARG A 136	9.730 -11.506 -8.399 1.00 27.99 11.015 -12.372 -8.025 1.00 27.99 10.744 -13.539 -10.074 1.00 24.60 9.589 -12.509 -10.456 1.00 24.60 11.684 -11.084 -9.959 1.00 25.23 10.981 -13.339 -12.260 1.00 23.16 11.911 -12.814 -13.299 1.00 23.16	H
ATOM 2138 HG3 ARG A 136 ATOM 2139 HD2 ARG A 136 ATOM 2140 HD3 ARG A 136 ATOM 2141 HE ARG A 136 ATOM 2142 HH11 ARG A 136 ATOM 2143 HH12 ARG A 136 ATOM 2144 HH21 ARG A 136 ATOM 2145 HH22 ARG A 136	9.730 -11.506 -8.399 1.00 27.99 11.015 -12.372 -8.025 1.00 27.99 10.744 -13.539 -10.074 1.00 24.60 9.589 -12.509 -10.456 1.00 24.60 11.684 -11.084 -9.959 1.00 25.23 10.981 -13.339 -12.260 1.00 23.16 11.911 -12.814 -13.299 1.00 23.16 13.080 -10.270 -11.542 1.00 26.31 13.187 -10.950 -12.863 1.00 26.31	H
ATOM 2138 HG3 ARG A 136 ATOM 2139 HD2 ARG A 136 ATOM 2140 HD3 ARG A 136 ATOM 2141 HE ARG A 136 ATOM 2142 HH11 ARG A 136 ATOM 2143 HH12 ARG A 136 ATOM 2144 HH21 ARG A 136 ATOM 2145 HH22 ARG A 136 ATOM 2146 N PRO A 137	9.730 -11.506 -8.399 1.00 27.99 11.015 -12.372 -8.025 1.00 27.99 10.744 -13.539 -10.074 1.00 24.60 9.589 -12.509 -10.456 1.00 24.60 11.684 -11.084 -9.959 1.00 25.23 10.981 -13.339 -12.260 1.00 23.16 11.911 -12.814 -13.299 1.00 23.16 13.080 -10.270 -11.542 1.00 26.31 13.187 -10.950 -12.863 1.00 26.31 8.876 -11.061 -5.495 1.00 26.36	H
ATOM 2138 HG3 ARG A 136 ATOM 2139 HD2 ARG A 136 ATOM 2140 HD3 ARG A 136 ATOM 2141 HE ARG A 136 ATOM 2142 HH11 ARG A 136 ATOM 2143 HH12 ARG A 136 ATOM 2144 HH21 ARG A 136 ATOM 2145 HH22 ARG A 136 ATOM 2146 N PRO A 137 ANISOU 2146 N PRO A 137	9.730 -11.506 -8.399 1.00 27.99 11.015 -12.372 -8.025 1.00 27.99 10.744 -13.539 -10.074 1.00 24.60 9.589 -12.509 -10.456 1.00 24.60 11.684 -11.084 -9.959 1.00 25.23 10.981 -13.339 -12.260 1.00 23.16 11.911 -12.814 -13.299 1.00 23.16 13.080 -10.270 -11.542 1.00 26.31 13.187 -10.950 -12.863 1.00 26.31 8.876 -11.061 -5.495 1.00 26.36	HHHHHHH Z
ATOM 2138 HG3 ARG A 136 ATOM 2139 HD2 ARG A 136 ATOM 2140 HD3 ARG A 136 ATOM 2141 HE ARG A 136 ATOM 2142 HH11 ARG A 136 ATOM 2143 HH12 ARG A 136 ATOM 2144 HH21 ARG A 136 ATOM 2145 HH22 ARG A 136 ATOM 2146 N PRO A 137 ANISOU 2146 N PRO A 137 ATOM 2147 CA PRO A 137	9.730 -11.506 -8.399 1.00 27.99 11.015 -12.372 -8.025 1.00 27.99 10.744 -13.539 -10.074 1.00 24.60 9.589 -12.509 -10.456 1.00 24.60 11.684 -11.084 -9.959 1.00 25.23 10.981 -13.339 -12.260 1.00 23.16 11.911 -12.814 -13.299 1.00 23.16 13.080 -10.270 -11.542 1.00 26.31 13.187 -10.950 -12.863 1.00 26.31 8.876 -11.061 -5.495 1.00 26.36 3509 4051 2454 1437 -931 -1528 8.119 -9.817 -5.319 1.00 27.40	HITITIE Z
ATOM 2138 HG3 ARG A 136 ATOM 2139 HD2 ARG A 136 ATOM 2140 HD3 ARG A 136 ATOM 2141 HE ARG A 136 ATOM 2142 HH11 ARG A 136 ATOM 2143 HH12 ARG A 136 ATOM 2144 HH21 ARG A 136 ATOM 2145 HH22 ARG A 136 ATOM 2146 N PRO A 137 ANISOU 2146 N PRO A 137 ATOM 2147 CA PRO A 137	9.730 -11.506 -8.399 1.00 27.99 11.015 -12.372 -8.025 1.00 27.99 10.744 -13.539 -10.074 1.00 24.60 9.589 -12.509 -10.456 1.00 24.60 11.684 -11.084 -9.959 1.00 25.23 10.981 -13.339 -12.260 1.00 23.16 11.911 -12.814 -13.299 1.00 23.16 13.080 -10.270 -11.542 1.00 26.31 13.187 -10.950 -12.863 1.00 26.31 8.876 -11.061 -5.495 1.00 26.36 3509 4051 2454 1437 -931 -1528 8.119 -9.817 -5.319 1.00 27.40 3698 4125 2588 1488 -937 -1599	HETELETE & C
ATOM 2138 HG3 ARG A 136 ATOM 2139 HD2 ARG A 136 ATOM 2140 HD3 ARG A 136 ATOM 2141 HE ARG A 136 ATOM 2142 HH11 ARG A 136 ATOM 2143 HH12 ARG A 136 ATOM 2144 HH21 ARG A 136 ATOM 2145 HH22 ARG A 136 ATOM 2146 N PRO A 137 ANISOU 2146 N PRO A 137 ATOM 2147 CA PRO A 137	9.730 -11.506 -8.399 1.00 27.99 11.015 -12.372 -8.025 1.00 27.99 10.744 -13.539 -10.074 1.00 24.60 9.589 -12.509 -10.456 1.00 24.60 11.684 -11.084 -9.959 1.00 25.23 10.981 -13.339 -12.260 1.00 23.16 11.911 -12.814 -13.299 1.00 23.16 13.080 -10.270 -11.542 1.00 26.31 13.187 -10.950 -12.863 1.00 26.31 8.876 -11.061 -5.495 1.00 26.36 3509 4051 2454 1437 -931 -1528 8.119 -9.817 -5.319 1.00 27.40	HETELETE & C
ATOM 2138 HG3 ARG A 136 ATOM 2139 HD2 ARG A 136 ATOM 2140 HD3 ARG A 136 ATOM 2141 HE ARG A 136 ATOM 2142 HH11 ARG A 136 ATOM 2143 HH12 ARG A 136 ATOM 2144 HH21 ARG A 136 ATOM 2145 HH22 ARG A 136 ATOM 2146 N PRO A 137 ANISOU 2146 N PRO A 137 ATOM 2147 CA PRO A 137 ANISOU 2147 CA PRO A 137 ANISOU 2148 C PRO A 137	9.730 -11.506 -8.399 1.00 27.99 11.015 -12.372 -8.025 1.00 27.99 10.744 -13.539 -10.074 1.00 24.60 9.589 -12.509 -10.456 1.00 24.60 11.684 -11.084 -9.959 1.00 25.23 10.981 -13.339 -12.260 1.00 23.16 11.911 -12.814 -13.299 1.00 23.16 13.080 -10.270 -11.542 1.00 26.31 13.187 -10.950 -12.863 1.00 26.31 8.876 -11.061 -5.495 1.00 26.36 8.509 4051 2454 1437 -931 -1528 8.119 -9.817 -5.319 1.00 27.40 3698 4125 2588 1488 -937 -1599 7.500 -9.373 -6.635 1.00 25.87	HITHH I C
ATOM 2138 HG3 ARG A 136 ATOM 2139 HD2 ARG A 136 ATOM 2140 HD3 ARG A 136 ATOM 2141 HE ARG A 136 ATOM 2142 HH11 ARG A 136 ATOM 2143 HH12 ARG A 136 ATOM 2144 HH21 ARG A 136 ATOM 2145 HH22 ARG A 136 ATOM 2146 N PRO A 137 ANISOU 2146 N PRO A 137 ATOM 2147 CA PRO A 137	9.730 -11.506 -8.399 1.00 27.99 11.015 -12.372 -8.025 1.00 27.99 10.744 -13.539 -10.074 1.00 24.60 9.589 -12.509 -10.456 1.00 24.60 11.684 -11.084 -9.959 1.00 25.23 10.981 -13.339 -12.260 1.00 23.16 11.911 -12.814 -13.299 1.00 23.16 13.080 -10.270 -11.542 1.00 26.31 13.187 -10.950 -12.863 1.00 26.31 8.876 -11.061 -5.495 1.00 26.36 3509 4051 2454 1437 -931 -1528 8.119 -9.817 -5.319 1.00 27.40 3698 4125 2588 1488 -937 -1599	HETELETE Z C C

ANISOU 2149 O PRO A 137 3263 3561 2502 1279 -831 -1531 ATOM 2150 CB PRO A 137 9.176 -8.819 -4.831 1.00 29.17 C 3939 4233 2913 1484 -1124 -1772 C **ANISOU 2150 CB PRO A 137** ATOM 2151 CG PRO A 137 10.256 -9.665 -4.219 1.00 30.26 C 4045 4434 3017 1491 -1213 -1783 C **ANISOU 2151 CG PRO A 137** 10.268 -10.932 -5.029 1.00 27.52 C ATOM 2152 CD PRO A 137 **ANISOU 2152 CD PRO A 137** 3637 4145 2673 1414 -1099 -1638 7.429 -9.924 -4.646 1.00 32.88 H ATOM 2153 HA PRO A 137 9.520 -8.313 -5.583 1.00 35.01 H 8.786 -8.228 -4.168 1.00 35.01 H 11.108 -9.207 -4.287 1.00 36.31 H 10.040 -9.852 -3.292 1.00 36.31 H 10.870 -10.844 -5.785 1.00 33.02 H 10.508 -11.688 -4.470 1.00 33.02 H 10.508 -8.752 -6.538 1.00 26.24 N 2575 2888 2508 1458 772 4534 ATOM 2154 HB2 PRO A 137 ATOM 2155 HB3 PRO A 137 ATOM 2156 HG2 PRO A 137 ATOM 2157 HG3 PRO A 137 ATOM 2158 HD2 PRO A 137 ATOM 2159 HD3 PRO A 137 ATOM 2160 N THR A 138 3575 3888 2508 1458 -772 -1534 N **ANISOU 2160 N THR A 138** ATOM 2161 CA THR A 138 5.608 -8.230 -7.690 1.00 25.14 C 3426 3655 2471 1391 -681 -1487 **ANISOU 2161 CA THR A 138** ATOM 2162 C THR A 138 5.346 -6.738 -7.506 1.00 26.68 C ANISOU 2162 C THR A 138 3680 3743 2712 1426 -740 -1597 3680 3743 2712 1426 -740 -1597 ATOM 2163 O THR A 138 5.463 -6.190 -6.407 1.00 28.46 O ANISOU 2163 O THR A 138 3960 3996 2858 1521 -833 -1699 3960 3996 2858 1521 -833 -1699 ATOM 2164 CB THR A 138 4.277 -8.963 -7.892 1.00 24.16 C 3283 3652 2246 1423 -524 -1337 C **ANISOU 2164 CB THR A 138** ANISOU 2164 CB THR A 138 3263 3652 2246 1423 -524 -1337 O ANISOU 2165 OG1 THR A 138 3605 4053 2359 1557 -509 -1337 O ATOM 2166 CG2 THR A 138 4.520 -10.419 -8.239 1.00 23.55 C ANISOU 2166 CG2 THR A 138 3142 3655 2151 1373 -458 -1221 C ATOM 2167 H THR A 138 5.923 -8.617 -5.793 1.00 31.49 H ATOM 2168 HA THR A 138 6.147 -8.349 -8.488 1.00 30.17 H ATOM 2169 HB THR A 138
ATOM 2170 HG1 THR A 138
ATOM 2171 HG21 THR A 138
ATOM 2172 HG22 THR A 138
ATOM 2173 HG23 THR A 138
ATOM 2174 N GLY A 139

0.147 -0.349 -0.488 1.00 30.17
3.794 -8.552 -8.626 1.00 28.99
3.905 -9.211 -6.052 1.00 31.64
3.673 -10.875 -8.365 1.00 28.26
5.009 -10.853 -7.523 1.00 28.26
4 973 -6.085 -8.605 1.00 25.20 ATOM 2174 N GLY A 139 4.973 -6.085 -8.605 1.00 25.83 N **ANISOU 2174 N GLY A 139** 3569 3514 2730 1357 -683 -1572 N ATOM 2175 CA GLY A 139 ANISOU 2175 CA GLY A 139 4.668 -4.668 -8.618 1.00 27.08 C 3784 3558 2949 1380 -718 -1658 ATOM 2176 C GLY A 139 ANISOU 2176 C GLY A 139 5.738 -3.814 -9.262 1.00 27.85 C 3871 3448 3261 1279 -802 -1740 C ATOM 2177 O GLY A 139 ANISOU 2177 O GLY A 139 5.489 -2.633 -9.538 1.00 28.47 O 3991 3402 3422 1277 -810 -1790 ATOM 2178 H GLY A 139 4.888 -6.458 -9.375 1.00 30.99 H 3.838 -4.526 -9.100 1.00 32.50 H ATOM 2179 HA2 GLY A 139 3.838 -4.526 -9.100 1.00 32.50 ATOM 2180 HA3 GLY A 139 4.545 -4.361 -7.707 1.00 32.50 ATOM 2181 N SER A 140 6.925 -4.364 -9.481 1.00 27.55 ANISOU 2181 N SER A 140 3776 3366 3326 1195 -864 -1752 N ATOM 2182 CA SER A 140 7.989 -3.690 -10.203 1.00 28.93 C ANISOU 2182 CA SER A 140 3915 3336 3740 1081 -926 -1800 C ATOM 2183 C SER A 140 8.282 -4.448 -11.488 1.00 26.80 C ANISOU 2183 C SER A 140 3581 3022 3579 980 -825 -1676 C ATOM 2184 O SER A 140 7.839 -5.582 -11.683 1.00 26.14 O

ANISOU 2184 O SER A 140	3478 3071 3383 997 -739 -1578 O
ATOM 2185 CB SER A 140	9.251 -3.584 -9.339 1.00 30.77 C
ANISOU 2185 CB SER A 140	4117 3533 4039 1065 -1101 -1926 C
ATOM 2186 OG SER A 140	
ANISOU 2186 OG SER A 140	4449 3812 4221 1164 -1203 -2050 O
ATOM 2187 H SER A 140	7.141 -5.152 -9.213 1.00 33.06 H
ATOM 2188 HA SER A 140	7.702 -2.793 -10.436 1.00 34.71 H
ATOM 2189 HB2 SER A 140	9.492 -4.469 -9.024 1.00 36.92 H
ATOM 2190 HB3 SER A 140	9.970 -3.216 -9.876 1.00 36.92 H
ATOM 2191 HG SER A 140	9.732 -2.694 -7.760 1.00 39.42 H
ATOM 2192 N ASN A 141	9.022 -3.801 -12.384 1.00 27.15 N
	5.5 <u>—</u> 5.55. 1—155. 1155 — 11.
ANISOU 2192 N ASN A 141	3591 2871 3852 879 -828 -1672 N
ATOM 2193 CA ASN A 141	9.400 -4.457 -13.626 1.00 25.18 C
ANISOU 2193 CA ASN A 141	3283 2562 3720 793 -729 -1548 C
ATOM 2194 C ASN A 141	10.271 -5.669 -13.317 1.00 25.55 C
ANISOU 2194 C ASN A 141	3261 2687 3761 763 -782 -1551 C
ATOM 2195 O ASN A 141	11.247 -5.574 -12.567 1.00 26.49 O
ANISOU 2195 O ASN A 141	3341 2781 3945 738 -921 -1651 O
ATOM 2196 CB ASN A 141	10.133 -3.483 -14.553 1.00 26.13 C
ANISOU 2196 CB ASN A 141	3375 2453 4100 696 -716 -1526 C
ATOM 2197 CG ASN A 141	9.229 -2.379 -15.080 1.00 26.02 C
ANISOU 2197 CG ASN A 141	
ATOM 2198 OD1 ASN A 141	8.017 -2.416 -14.901 1.00 25.58 O
ANISOU 2198 OD1 ASN A 141	3444 2420 3853 818 -579 -1478 O
ATOM 2199 ND2 ASN A 141	9.820 -1.395 -15.747 1.00 27.63 N
ANISOU 2199 ND2 ASN A 141	3630 2364 4506 660 -623 -1478 N
ATOM 2200 H ASN A 141	9.313 -2.996 -12.297 1.00 32.58 H
ATOM 2201 HA ASN A 141	8.601 -4.765 -14.081 1.00 30.21 H
ATOM 2202 HB2 ASN A 141	10.861 -3.068 -14.064 1.00 31.35 H
ATOM 2203 HB3 ASN A 141	10.483 -3.974 -15.314 1.00 31.35 H
ATOM 2204 HD21 ASN A 141	9.350 -0.748 -16.064 1.00 33.16 H
ATOM 2205 HD22 ASN A 141	10.672 -1.404 -15.862 1.00 33.16 H
ATOM 2206 N ALA A 142	9.898 -6.815 -13.882 1.00 24.58 N
ANISOU 2206 N ALA A 142	3938 2440 2961 1344 -1743 -1007 N
ATOM 2207 CA ALA A 142	10.592 -8.069 -13.655 1.00 23.45 C
ANISOU 2207 CA ALA A 142	3676 2384 2849 1269 -1595 -971 C
ATOM 2208 C ALA A 142	11.005 -8.664 -14.991 1.00 23.09 C
ANISOU 2208 C ALA A 142	3647 2251 2874 1057 -1544 -848 C
ATOM 2209 O ALA A 142	10.376 -8.415 -16.020 1.00 23.75 O
ANISOU 2209 O ALA A 142	3825 2269 2930 1031 -1539 -784 O
ATOM 2210 CB ALA A 142	9.704 -9.067 -12.896 1.00 22.10 C
ANISOU 2210 CB ALA A 142	3401 2499 2496 1383 -1364 -999 C
ATOM 2211 H ALA A 142	9.227 -6.887 -14.414 1.00 29.50 H
ATOM 2212 HA ALA A 142	11.391 -7.907 -13.130 1.00 28.14 H
ATOM 2213 HB1 ALA A 142	10.199 -9.891 -12.763 1.00 26.52 H
ATOM 2214 HB2 ALA A 142	9.462 -8.685 -12.038 1.00 26.52 H
ATOM 2215 HB3 ALA A 142	8.906 -9.241 -13.418 1.00 26.52 H
ATOM 2216 N THR A 143	12.070 -9.457 -14.972 1.00 22.88 N
ANISOU 2216 N THR A 143	3527 2247 2920 875 -1471 -813 N
ATOM 2217 CA THR A 143	
ANISOU 2217 CA THR A 143	3261 1984 2757 638 -1318 -645 C
ATOM 2218 C THR A 143	12.676 -11.607 -15.957 1.00 19.31 C
ANISOU 2218 C THR A 143	2873 2007 2456 600 -1148 -584 C

ATOM 2219 O THR A 143 13.054 -12.058 -14.869 1.00 19.83	0
ANISOU 2219 O THR A 143 2850 2192 2492 667 -1172 -664	0
ATOM 2220 CB THR A 143 13.894 -9.537 -16.631 1.00 23.62	C
ANISOU 2220 CB THR A 143 3606 2057 3313 414 -1356 -595	С
ATOM 2221 OG1 THR A 143 14.846 -9.682 -15.574 1.00 25.45	Ö
ANISOU 2221 OG1 THR A 143 3743 2298 3628 399 -1442 -710	O
ATOM 2222 CG2 THR A 143 13.763 -8.066 -16.986 1.00 25.92	C
ANISOU 2222 CG2 THR A 143	Č
ATOM 2223 H THR A 143 12.535 -9.634 -14.270 1.00 27.46	н
ATOM 2224 HA THR A 143 11.902 -9.963 -16.895 1.00 25.27	¨H
ATOM 2225 HB THR A 143 14.204 -10.017 -17.415 1.00 28.35	¨H
ATOM 2226 HG1 THR A 143 14.939 -10.494 -15.381 1.00 20.53	¨H
ATOM 2220 HG1 THR A 143 14.939 -10.494 -13.381 1.00 30.34 ATOM 2227 HG21 THR A 143 13.124 -7.955 -17.708 1.00 31.11	H
ATOM 2228 HG22 THR A 143 13.456 -7.564 -16.215 1.00 31.11	H
ATOM 2229 HG23 THR A 143 14.622 -7.715 -17.269 1.00 31.11	Н
ATOM 2230 N ILE A 144 12.348 -12.374 -16.991 1.00 17.26	N
ANISOU 2230 N ILE A 144 2584 1815 2160 508 -993 -448	N
ATOM 2231 CA ILE A 144 12.663 -13.797 -17.056 1.00 15.13	С
ANISOU 2231 CA ILE A 144 2174 1705 1871 425 -838 -374	C
ATOM 2232 C ILE A 144 13.593 -13.960 -18.248 1.00 15.48	С
ANISOU 2232 C ILE A 144 2234 1632 2015 220 -736 -263	С
ATOM 2233 O ILE A 144 13.172 -13.796 -19.401 1.00 14.74	Ö
ANISOU 2233 O ILE A 144 2227 1488 1886 186 -690 -182	Ö
ATOM 2234 CB ILE A 144 11.409 -14.676 -17.186 1.00 14.02	C
	C
ANISOU 2234 CB ILE A 144 1971 1750 1608 517 -762 -330	
ATOM 2235 CG1 ILE A 144 10.576 -14.565 -15.907 1.00 14.11	C
ANISOU 2235 CG1 ILE A 144 1930 1904 1526 710 -787 -403	С
ATOM 2236 CG2 ILE A 144 11.805 -16.148 -17.453 1.00 14.50	C
ANISOU 2236 CG2 ILE A 144 1908 1910 1690 405 -619 -248	С
ATOM 2237 CD1 ILE A 144 9.256 -15.321 -15.937 1.00 13.87	C
ANISOU 2237 CD1 ILE A 144 1808 2029 1434 751 -661 -333	C
ATOM 2238 H ILE A 144 11.932 -12.085 -17.686 1.00 20.71	Н
ATOM 2239 HA ILE A 144 13.141 -14.061 -16.254 1.00 18.16	Н
ATOM 2240 HB ILE A 144 10.880 -14.355 -17.933 1.00 16.83	Н
ATOM 2241 HG12 ILE A 144 11.097 -14.915 -15.167 1.00 16.93	Н
ATOM 2242 HG13 ILE A 144 10.374 -13.630 -15.750 1.00 16.93	Н
ATOM 2243 HG21 ILE A 144 11.000 -16.682 -17.532 1.00 17.39	H
ATOM 2244 HG22 ILE A 144 12.314 -16.193 -18.278 1.00 17.39	H
ATOM 2245 HG23 ILE A 144 12.345 -16.469 -16.714 1.00 17.39	H
ATOM 2246 HD11 ILE A 144 8.800 -15.194 -15.090 1.00 16.64	H'
ATOM 2247 HD12 ILE A 144 8.711 -14.976 -16.662 1.00 16.64	H
ATOM 2248 HD13 ILE A 144 9.436 -16.264 -16.078 1.00 16.64	H
ATOM 2249 N THR A 145 14.869 -14.212 -17.964 1.00 15.36	N
ANISOU 2249 N THR A 145 2136 1585 2117 105 -707 -259	N
ATOM 2250 CA THR A 145 15.886 -14.449 -18.984 1.00 15.46	С
ANISOU 2250 CA THR A 145 2125 1526 2223 -72 -580 -144	С
ATOM 2251 C THR A 145 15.757 -15.920 -19.352 1.00 14.43	С
ANISOU 2251 C THR A 145 1912 1560 2009 -77 -435 -99	С
ATOM 2252 O THR A 145 16.412 -16.792 -18.778 1.00 13.97	0
ANISOU 2252 O THR A 145 1731 1588 1990 -96 -390 -116	Ŏ
ATOM 2253 CB THR A 145 17.275 -14.098 -18.466 1.00 16.96	C
ANISOU 2253 CB THR A 145 2227 1620 2599 -183 -623 -165	Č
ATOM 2254 OG1 THR A 145 2227 1020 2399 -103 -023 -103 ATOM 2254 OG1 THR A 145 17.298 -12.727 -18.025 1.00 19.43	Ö
A 10m 2207 001 11m A 170 11.230 12.121 10.025 1.00 13.45	9

ANISOU 2254 OG1 THR A 145 2622 1747 3013 -169 -806 -236 0 C ATOM 2255 CG2 THR A 145 18.326 -14.286 -19.555 1.00 17.74 2276 1667 2800 -356 -464 -20 **ANISOU 2255 CG2 THR A 145** ATOM 2256 H THR A 145 15.178 -14.252 -17.163 1.00 18.44 Н ATOM 2257 HA THR A 145 15.698 -13.911 -19.769 1.00 18.55 ATOM 2258 HB THR A 145 17.498 -14.679 -17.721 1.00 20.36 ATOM 2259 HG1 THR A 145 16.738 -12.614 -17.409 1.00 23.32 ATOM 2260 HG21 THR A 145 19.204 -14.059 -19.211 1.00 21.29 ATOM 2261 HG22 THR A 145 18.332 -15.210 -19.852 1.00 21.29 ATOM 2262 HG23 THR A 145 18.125 -13.713 -20.311 1.00 21.29 ATOM 2263 N PHE A 146 14.852 -16.200 -20.293 1.00 13.97 **ANISOU 2263 N PHE A 146** 1930 1538 1842 -43 -386 -53 14.421 -17.577 -20.524 1.00 12.62 ATOM 2264 CA PHE A 146 **ANISOU 2264 CA PHE A 146** 1691 1501 1603 -20 -306 -45 ATOM 2265 C PHE A 146 ANISOU 2265 C PHE A 146 15.578 -18.474 -20.952 1.00 12.88 1651 1554 1690 -115 -178 -4 0 ATOM 2266 O PHE A 146 15.546 -19.684 -20.695 1.00 13.09 **ANISOU 2266 O PHE A 146** 1589 1670 1714 -97 -136 -20 ATOM 2267 CB PHE A 146 13.301 -17.588 -21.563 1.00 12.78 1812 1531 1514 30 -317 -23 **ANISOU 2267 CB PHE A 146** C ATOM 2268 CG PHE A 146 12.723 -18.951 -21.836 1.00 11.95 **ANISOU 2268 CG PHE A 146** 1639 1528 1372 50 -282 -34 CCC ATOM 2269 CD1 PHE A 146 12.318 -19.771 -20.798 1.00 11.34 **ANISOU 2269 CD1 PHE A 146** 1428 1546 1333 89 -296 -58 ATOM 2270 CD2 PHE A 146 12.566 -19.400 -23.140 1.00 12.30 ANISOU 2270 CD2 PHE A 146 1761 1566 1348 40 -245 -18 CC ATOM 2271 CE1 PHE A 146 11.784 -21.015 -21.053 1.00 10.58 1263 1504 1253 86 -280 -53 **ANISOU 2271 CE1 PHE A 146** 2000 ATOM 2272 CE2 PHE A 146 12.024 -20.642 -23.394 1.00 12.28 **ANISOU 2272 CE2 PHE A 146** 1701 1621 1343 56 -254 -53 ATOM 2273 CZ PHE A 146 11.638 -21.450 -22.349 1.00 11.23 **ANISOU 2273 CZ PHE A 146** 1421 1550 1295 64 -275 -66 ATOM 2274 H PHE A 146 14.477 -15.618 -20.803 1.00 16.77 14.061 -17.934 -19.697 1.00 15.15 12.581 -17.019 -21.250 1.00 15.34 ATOM 2275 HA PHE A 146 ATOM 2276 HB2 PHE A 146 13.650 -17.243 -22.400 1.00 15.34 ATOM 2277 HB3 PHE A 146 13.650 -17.243 -22.400 1.00 15.34 ATOM 2278 HD1 PHE A 146 12.416 -19.484 -19.919 1.00 13.60 ATOM 2279 HD2 PHE A 146 12.828 -18.858 -23.848 1.00 14.76 ATOM 2280 HE1 PHE A 146 11.519 -21.560 -20.348 1.00 12.70 Н ATOM 2281 HE2 PHE A 146 11.928 -20.938 -24.271 1.00 14.74 Н ATOM 2282 HZ PHE A 146 11.275 -22.289 -22.519 1.00 13.47 ATOM 2283 N SER A 147 ANISOU 2283 N SER A 147 16.599 -17.908 -21.607 1.00 14.33 Ν 1859 1652 1932 -210 -109 Ν ATOM 2284 CA SER A 147 17.737 -18.706 -22.060 1.00 14.64 **ANISOU 2284 CA SER A 147** 1813 1730 2017 -277 30 ATOM 2285 C SER A 147 18.428 -19.417 -20.906 1.00 13.49 C **ANISOU 2285 C SER A 147** 1511 1645 1969 -281 15 ATOM 2286 O SER A 147 0 18.949 -20.524 -21.083 1.00 12.43 **ANISOU 2286 O SER A 147** 1302 1580 1842 -279 105 ATOM 2287 CB SER A 147
ANISOU 2287 CB SER A 147
ATOM 2288 OG SER A 147
ANISOU 2288 OG SER A 147
ANISOU 2288 OG SER A 147
2102 1913 2366 -381 116 216
19.235 -16.797 -21.949 1.00 17.97
2203 1951 2672 -447 13 205

ATOM 2289 H SER A 147 16.654 -17.071 -21.7	798 1.00 17.19 H
ATOM 2290 HA SER A 147 17.422 -19.380 -22	
ATOM 2291 HB2 SER A 147 19.489 -18.367 -23	
ATOM 2292 HB3 SER A 147 18.309 -17.413 -23	
ATOM 2293 HG SER A 147 19.787 -16.320 -22	
ATOM 2294 N ASN A 148 18.474 -18.792 -19.	
ANISOU 2294 N ASN A 148 1517 1663 2081	
ATOM 2295 CA ASN A 148 19.068 -19.457 -18	
	-236 -144 -60 C
ATOM 2296 C ASN A 148 18.315 -20.738 -18.3	
ANISOU 2296 C ASN A 148 1025 1523 1723	-145 -118 -68 C
ATOM 2297 O ASN A 148 18.922 -21.739 -17.	835 1.00 11.43 O
ANISOU 2297 O ASN A 148 948 1608 1788	-135 -75 -63 O
ATOM 2298 CB ASN A 148 19.072 -18.519 -17	
	-190 -312 -145 C
ATOM 2299 CG ASN A 148 20.072 -17.393 -17	
	-305 -369 -144 C
ATOM 2300 OD1 ASN A 148 21.100 -17.535 -18	
ANISOU 2300 OD1 ASN A 148 1658 1904 283	
ATOM 2301 ND2 ASN A 148 19.781 -16.267 -16	
ANISOU 2301 ND2 ASN A 148 1616 1646 2562	
ATOM 2302 H ASN A 148 18.173 -18.001 -19.	575 1.00 16.62 H
ATOM 2303 HA ASN A 148 19.987 -19.691 -18	.777 1.00 15.40 H
ATOM 2304 HB2 ASN A 148 18.190 -18.126 -17	7.273 1.00 16.27 H
ATOM 2305 HB3 ASN A 148 19.298 -19.027 -16	6.575 1.00 16.27 H
ATOM 2306 HD21 ASN A 148 20.318 -15.597 -1	
ATOM 2307 HD22 ASN A 148 19.057 -16.209 -1	
ATOM 2308 N HIS A 149 16.988 -20.707 -18.3	
ANISOU 2308 N HIS A 149 10.386 -20.767 -18.3	-79 -153 -70 N
ATOM 2309 CA HIS A 149 16.190 -21.899 -18.	
ANISOU 2309 CA HIS A 149 881 1465 1415	-17 -132 -50 C
ATOM 2310 C HIS A 149 16.375 -22.953 -19.1	
ANISOU 2310 C HIS A 149 981 1541 1528	
ATOM 2311 O HIS A 149 16.575 -24.138 -18.8	
ANISOU 2311 O HIS A 149 774 1443 1446	-52 -8 -11 O
ATOM 2312 CB HIS A 149 14.720 -21.513 -17.9	911 1.00 10.44
ANISOU 2312 CB HIS A 149 997 1568 1403	60 -196 -52 C
ATOM 2313 CG HIS A 149 14.456 -20.608 -16.	749 1.00 12.05 C
	159 -287 -94 C
ATOM 2314 ND1 HIS A 149 14.242 -21.083 -15	
ANISOU 2314 ND1 HIS A 149 1204 2031 1619	263 -299 -81 N
ATOM 2315 CD2 HIS A 149 14.423 -19.256 -16	
ANISOU 2315 CD2 HIS A 149 1453 1912 1706	
ANISOU 2316 CE1 HIS A 149 1410 2225 1720	
ATOM 2317 NE2 HIS A 149 14.178 -18.944 -15.	
ANISOU 2317 NE2 HIS A 149 1434 2011 1660	324 -456 -207 N
ATOM 2318 H HIS A 149 16.529 -20.016 -18.5	
ATOM 2319 HA HIS A 149 16.478 -22.281 -17.	
ATOM 2320 HB2 HIS A 149 14.441 -21.053 -18	.718 1.00 12.53 H
ATOM 2321 HB3 HIS A 149 14.193 -22.318 -17.	.789 1.00 12.53 H
ATOM 2322 HD1 HIS A 149 14.219 -21.914 -15	.251 1.00 15.33 H
ATOM 2323 HD2 HIS A 149 14.542 -18.652 -17.	
	

ATOM 2324 HE1 HIS A 149	13.897 -20.129 -13.736 1.00 16.91	Н
ATOM 2325 N VAL A 150	16.293 -22.543 -20.391 1.00 10.55	N
ANISOU 2325 N VAL A 150	1071 1472 1467 -101 -9 -25	N
ATOM 2326 CA VAL A 150	16.509 -23.478 -21.492 1.00 10.47	С
ANISOU 2326 CA VAL A 150	1090 1451 1437 -110 65 -31	C
ATOM 2327 C VAL A 150	17.855 -24.168 -21.339 1.00 10.82	C
ANISOU 2327 C VAL A 150	1042 1512 1559 -130 154 -27	C
ATOM 2328 O VAL A 150	17.976 -25.387 -21.511 1.00 10.99	0
ANISOU 2328 O VAL A 150	1030 1538 1606 -100 180 -50	0
ATOM 2329 CB VAL A 150	16.402 -22.744 -22.842 1.00 10.00	С
ANISOU 2329 CB VAL A 150	1169 1354 1276 -117 98 -17	С
ATOM 2330 CG1 VAL A 150	16.725 -23.691 -24.002 1.00 10.68	С
ANISOU 2330 CG1 VAL A 150	1303 1452 1302 -85 174 -44	C
ATOM 2331 CG2 VAL A 150	15.013 -22.138 -23.013 1.00 9.85	С
ANISOU 2331 CG2 VAL A 150	1238 1322 1183 -76 -9 -28	С
ATOM 2332 H VAL A 150	16.116 -21.737 -20.635 1.00 12.67	Н
ATOM 2333 HA VAL A 150	15.819 -24.160 -21.467 1.00 12.57	Н
ATOM 2334 HB VAL A 150	17.048 -22.020 -22.858 1.00 12.00	Н
ATOM 2335 HG11 VAL A 150	16.650 -23.203 -24.837 1.00 12.81	Н
ATOM 2336 HG12 VAL A 150	17.628 -24.026 -23.894 1.00 12.81	Н
ATOM 2337 HG13 VAL A 150	16.094 -24.428 -23.992 1.00 12.81	Н
ATOM 2338 HG21 VAL A 150	14.971 -21.682 -23.868 1.00 11.82	Н
ATOM 2339 HG22 VAL A 150	14.353 -22.848 -22.983 1.00 11.82	Н
ATOM 2340 HG23 VAL A 150	14.853 -21.508 -22.293 1.00 11.82	Н
ATOM 2341 N ASN A 151	18.894 -23.398 -21.017 1.00 12.53	N
ANISOU 2341 N ASN A 151	1206 1723 1832 -180 187 -1	N
ATOM 2342 CA ASN A 151	20.229 -23.979 -20.925 1.00 13.26	С
ANISOU 2342 CA ASN A 151	1185 1843 2010 -195 271 6	С
ATOM 2343 C ASN A 151	20.349 -24.910 -19.725 1.00 12.55	С
ANISOU 2343 C ASN A 151	988 1793 1986 -146 218 -16	С
ATOM 2344 O ASN A 151	20.969 -25.972 -19.827 1.00 11.79	0
ANISOU 2344 O ASN A 151	831 1716 1935 -112 274 -24	0
ATOM 2345 CB ASN A 151	21.284 -22.876 -20.865 1.00 16.85	C
ANISOU 2345 CB ASN A 151	1578 2273 2551 -278 300 48	C
ATOM 2346 CG ASN A 151	21.487 -22.204 -22.208 1.00 21.37	С
ANISOU 2346 CG ASN A 151	2233 2817 3071 -323 412 121	С
ATOM 2347 OD1 ASN A 151	21.320 -22.832 -23.246 1.00 23.07	0
ANISOU 2347 OD1 ASN A 151	2521 3068 3177 -268 503 124	0
ATOM 2348 ND2 ASN A 151	21.853 -20.927 -22.193 1.00 23.90	N
ANISOU 2348 ND2 ASN A 151	2548 3066 3468 -413 397 182	N
ATOM 2349 H ASN A 151	18.853 -22.556 -20.850 1.00 15.04	Н
ATOM 2350 HA ASN A 151	20.396 -24.504 -21.723 1.00 15.91	Н
ATOM 2351 HB2 ASN A 151	21.002 -22.200 -20.229 1.00 20.22	Н
ATOM 2352 HB3 ASN A 151	22.131 -23.261 -20.590 1.00 20.22	Н
ATOM 2353 HD21 ASN A 151	21.979 -20.508 -22.933 1.00 28.68	Н
ATOM 2354 HD22 ASN A 151	21.964 -20.521 -21.444 1.00 28.68	Н
ATOM 2355 N ALA A 152	19.767 -24.532 -18.584 1.00 13.34	N
ANISOU 2355 N ALA A 152	1073 1914 2083 -119 113 -20	N
ATOM 2356 CA ALA A 152	19.783 -25.416 -17.421 1.00 13.66	С
ANISOU 2356 CA ALA A 152	1026 2010 2153 -50 73 -9	C
ATOM 2357 C ALA A 152	19.049 -26.714 -17.725 1.00 13.25	С
ANISOU 2357 C ALA A 152		С
ATOM 2358 O ALA A 152	19.560 -27.809 -17.462 1.00 13.65	0

ANISOU 2358 O ALA A 152	981 1991 2213 16 122 37	0
ATOM 2359 CB ALA A 152	19.161 -24.716 -16.214 1.00 13.55	C
ANISOU 2359 CB ALA A 152	1013 2049 2087 9 -31 -13	C
ATOM 2360 H ALA A 152	19.362 -23.783 -18.461 1.00 16.01	Н
ATOM 2361 HA ALA A 152	20.703 -25.634 -17.202 1.00 16.39	Н
ATOM 2362 HB1 ALA A 152	19.182 -25.319 -15.454 1.00 16.26	H
ATOM 2363 HB2 ALA A 152	19.672 -23.916 -16.016 1.00 16.26	H
ATOM 2364 HB3 ALA A 152	18.244 -24.480 -16.424 1.00 16.26	H
ATOM 2365 N TRP A 153	17.844 -26.609 -18.288 1.00 11.05	N
ANISOU 2365 N TRP A 153	790 1637 1772 -28 76 22	N
ATOM 2366 CA TRP A 153	17.109 -27.806 -18.686 1.00 10.57	С
ANISOU 2366 CA TRP A 153	734 1529 1755 -18 68 35	С
ATOM 2367 C TRP A 153	17.938 -28.658 -19.641 1.00 10.76	C
ANISOU 2367 C TRP A 153	781 1492 1816 -15 124 -19	C
ATOM 2368 O TRP A 153	18.012 -29.887 -19.494 1.00 10.30	0
ANISOU 2368 O TRP A 153	683 1382 1847 13 114 -10	0
ATOM 2369 CB TRP A 153	15.777 -27.404 -19.332 1.00 9.62	C
ANISOU 2369 CB TRP A 153	687 1386 1581 -34 14 22	C
ATOM 2370 CG TRP A 153	14.823 -26.642 -18.427 1.00 9.75	C
ANISOU 2370 CG TRP A 153	674 1476 1555 -5 -35 72	C
ATOM 2371 CD1 TRP A 153	14.879 -26.538 -17.065 1.00 10.68	C
ANISOU 2371 CD1 TRP A 153	711 1680 1667 51 -37 131	C
ATOM 2372 CD2 TRP A 153	13.667 -25.898 -18.836 1.00 9.93	C
ANISOU 2372 CD2 TRP A 153	749 1507 1515 3 -90 59	C
ATOM 2373 NE1 TRP A 153	13.830 -25.775 -16.606 1.00 11.46	N
ANISOU 2373 NE1 TRP A 153	810 1849 1696 102 -79 152	N
ATOM 2374 CE2 TRP A 153	13.076 -25.366 -17.672 1.00 10.74	Ċ
ANISOU 2374 CE2 TRP A 153	793 1707 1582 68 -113 109	C
ATOM 2375 CE3 TRP A 153	13.082 -25.619 -20.074 1.00 10.50	C
ANISOU 2375 CE3 TRP A 153	919 1527 1543 -16 -129 5	C
ATOM 2376 CZ2 TRP A 153	11.928 -24.571 -17.712 1.00 11.35	C
ANISOU 2376 CZ2 TRP A 153	891 1825 1598 113 -165 106	Č
ATOM 2377 CZ3 TRP A 153	11.936 -24.825 -20.109 1.00 11.42	Č
ANISOU 2377 CZ3 TRP A 153	1058 1676 1605 18 -195 8	C
ATOM 2378 CH2 TRP A 153	11.372 -24.323 -18.934 1.00 11.05	ČC
ANISOU 2378 CH2 TRP A 153	936 1721 1542 81 -209 58	C
ATOM 2379 H TRP A 153	17.437 -25.869 -18.447 1.00 13.26	H
ATOM 2380 HA TRP A 153	16.915 -28.337 -17.898 1.00 12.69	н
ATOM 2381 HB2 TRP A 153		¨H
ATOM 2382 HB3 TRP A 153	15.322 -28.208 -19.625 1.00 11.54	H
ATOM 2383 HD1 TRP A 153	15.526 -26.934 -16.526 1.00 12.82	H
ATOM 2384 HE1 TRP A 153	13.676 -25.580 -15.782 1.00 13.76	H
ATOM 2385 HE3 TRP A 153	13.451 -25.953 -20.859 1.00 12.60	H
ATOM 2386 HZ2 TRP A 153	11.550 -24.232 -16.933 1.00 13.63	H
ATOM 2387 HZ3 TRP A 153	11.534 -24.638 -20.927 1.00 13.70	H
ATOM 2388 HH2 TRP A 153	10.608 -23.796 -18.986 1.00 13.26	H
ATOM 2389 N LYS A 154	18.582 -28.018 -20.621 1.00 12.15	N
ANISOU 2389 N LYS A 154	1020 1673 1925 -31 187 -66	N
ATOM 2390 CA LYS A 154	19.435 -28.746 -21.554 1.00 14.89	C
ANISOU 2390 CA LYS A 154	1386 2000 2271 10 263 -120	C
ATOM 2391 C LYS A 154	20.530 -29.513 -20.819 1.00 12.50	C
ANISOU 2391 C LYS A 154	964 1713 2073 46 299 -106	C
ATOM 2392 O LYS A 154	20.851 -30.657 -21.175 1.00 11.72	0

ANISOU 2392 O LYS A 154	866 1567 2019 112 311 -152	0
ATOM 2393 CB LYS A 154	20.054 -27.767 -22.553 1.00 19.57	C
ANISOU 2393 CB LYS A 154	2037 2633 2765 -6 362 -122	C
ATOM 2394 CG LYS A 154	20.322 -28.334 -23.911 1.00 24.72	C
ANISOU 2394 CG LYS A 154	2780 3287 3327 72 432 -186	Č
ATOM 2395 CD LYS A 154	20.992 -27.297 -24.822 1.00 28.71	Č
ANISOU 2395 CD LYS A 154	3325 3858 3725 61 566 -133	C
ATOM 2396 CE LYS A 154	20.002 -26.249 -25.331 1.00 31.32	C
ANISOU 2396 CE LYS A 154	3786 4169 3944 26 517 -102	C
	20.680 -25.142 -26.087 1.00 34.67	N
ANISOU 2397 NZ LYS A 154	4242 4640 4291 -2 654 0	N
	18.541 -27.170 -20.763 1.00 14.58	H.
ATOM 2399 HA LYS A 154	18.897 -29.384 -22.048 1.00 17.87	H.
ATOM 2400 HB2 LYS A 154	19.449 -27.016 -22.664 1.00 23.48	H
ATOM 2401 HB3 LYS A 154	20.899 -27.453 -22.195 1.00 23.48	H
ATOM 2402 HG2 LYS A 154	20.916 -29.097 -23.829 1.00 29.67	Н
ATOM 2403 HG3 LYS A 154	19.484 -28.603 -24.318 1.00 29.67	Н
ATOM 2404 HD2 LYS A 154	21.687 -26.838 -24.324 1.00 34.45	Н
ATOM 2405 HD3 LYS A 154	21.374 -27.748 -25.590 1.00 34.45	Н
ATOM 2406 HE2 LYS A 154	19.367 -26.676 -25.926 1.00 37.58	Н
ATOM 2407 HE3 LYS A 154	19.538 -25.857 -24.574 1.00 37.58	Н
ATOM 2408 HZ1 LYS A 154	20.077 -24.551 -26.368 1.00 41.61	Н
ATOM 2409 HZ2 LYS A 154	21.266 -24.728 -25.560 1.00 41.61	Н
ATOM 2410 HZ3 LYS A 154	21.110 -25.474 -26.792 1.00 41.61	Н
ATOM 2411 N SER A 155	21.110 -28.907 -19.782 1.00 12.56	N
ANISOU 2411 N SER A 155	873 1780 2121 21 295 -57	N
ATOM 2412 CA SER A 155	22.196 -29.561 -19.061 1.00 13.54	C
ANISOU 2412 CA SER A 155	890 1932 2323 69 306 -44	C
ATOM 2413 C SER A 155	21.731 -30.834 -18.369 1.00 13.32	Č
ANISOU 2413 C SER A 155	854 1853 2352 127 243 -12	C
ATOM 2414 O SER A 155	22.565 -31.681 -18.031 1.00 13.91	o
ANISOU 2414 O SER A 155	889 1925 2471 187 246 -9	o
ATOM 2415 CB SER A 155	22.813 -28.606 -18.028 1.00 14.85	C
ANISOU 2415 CB SER A 155	1023 2168 2452 38 246 -16	C
ATOM 2416 OG SER A 155	21.992 -28.466 -16.882 1.00 14.04	o
ANISOU 2416 OG SER A 155	941 2086 2307 57 154 13	o
ATOM 2417 H SER A 155	20.896 -28.130 -19.482 1.00 15.08	Н
ATOM 2417 H SER A 155	22.890 -29.803 -19.693 1.00 16.25	
		H
ATOM 2419 HB2 SER A 155	23.675 -28.956 -17.754 1.00 17.82	Н
	22.927 -27.734 -18.438 1.00 17.82	Н
ATOM 2421 HG SER A 155	21.241 -28.160 -17.101 1.00 16.85	H
	20.425 -30.985 -18.143	N
	727 1656 2208 108 187 30	N
ATOM 2423 CA HIS A 156	19.870 -32.212 -17.590 1.00 13.05	C
ANISOU 2423 CA HIS A 156	831 1706 2422 140 138 99	C
	19.226 -33.089 -18.658 1.00 13.69	C
	986 1650 2567 131 105 39	C
	18.467 -34.007 -18.323 1.00 14.10	0
	1019 1603 2734 121 43 106	0
ATOM 2426 CB HIS A 156	18.858 -31.881 -16.490 1.00 13.70	С
ANISOU 2426 CB HIS A 156	933 1842 2430 121 90 198	C
ATOM 2427 CG HIS A 156	19.446 -31.109 -15.351 1.00 14.15	С
ANISOU 2427 CG HIS A 156	994 2014 2367 155 79 200	С

ATOM 2428 ND1 HIS A 156 20.221 -31.701 -14.379 1.00 15.18 N **ANISOU 2428 ND1 HIS A 156** 1094 2171 2504 218 68 235 Ν ATOM 2429 CD2 HIS A 156 19.408 -29.791 -15.051 1.00 13.70 C **ANISOU 2429 CD2 HIS A 156** 957 2034 2216 146 58 153 ATOM 2430 CE1 HIS A 156 C 20.615 -30.786 -13.512 1.00 15.06 C **ANISOU 2430 CE1 HIS A 156** 1075 2245 2403 248 33 198 Ν ATOM 2431 NE2 HIS A 156 20.134 -29.617 -13.897 1.00 14.57 **ANISOU 2431 NE2 HIS A 156** 1040 2203 2292 204 24 146 Ν ATOM 2432 H HIS A 156 19.835 -30.381 -18.306 1.00 14.50 Н ATOM 2433 HA HIS A 156 20.588 -32.722 -17.184 1.00 15.66 Н ATOM 2434 HB2 HIS A 156 18.143 -31.348 -16.872 1.00 16.44 18.499 -32.708 -16.135 1.00 16.44 ATOM 2435 HB3 HIS A 156 Н ATOM 2436 HD1 HIS A 156 20.409 -32.540 -14.335 1.00 18.22 18.960 -29.129 -15.526 1.00 16.44 ATOM 2437 HD2 HIS A 156 ATOM 2438 HE1 HIS A 156 21.143 -30.937 -12.762 1.00 18.08 Н ATOM 2439 N GLY A 157 19.528 -32.840 -19.933 1.00 14.69 N **ANISOU 2439 N GLY A 157** Ν 1563 1734 2286 476 -445 -120 18.959 -33.620 -21.016 1.00 13.80 ATOM 2440 CA GLY A 157 **ANISOU 2440 CA GLY A 157** 1477 1566 2199 395 -341 -72 ATOM 2441 C GLY A 157 17.520 -33.302 -21.343 1.00 12.33 **ANISOU 2441 C GLY A 157** 1348 1400 1936 319 -271 -14 0 ATOM 2442 O GLY A 157 16.893 -34.047 -22.106 1.00 11.87 **ANISOU 2442 O GLY A 157 ATOM 2443 H GLY A 157** 0 1317 1300 1892 262 -202 20.064 -32.219 -20.193 1.00 17.63 Н ATOM 2444 HA2 GLY A 157 19.486 -33.477 -21.818 1.00 16.56 Н ATOM 2445 HA3 GLY A 157 19.012 -34.561 -20.787 1.00 16.56 ATOM 2446 N MET A 158 16.973 -32.226 -20.780 1.00 11.71 Ν **ANISOU 2446 N MET A 158** 323 -295 -15 1280 1384 1784 Ν **ATOM 2447 CA MET A 158** 15.592 -31.808 -21.022 1.00 11.39 **ANISOU 2447 CA MET A 158** 1281 1372 1676 263 -238 15.584 -30.861 -22.220 1.00 10.73 ATOM 2448 C MET A 158 **ANISOU 2448 C MET A 158** 1156 1284 1637 181 -196 -25 ATOM 2449 O MET A 158 0 15.629 -29.631 -22.089 1.00 11.16 **ANISOU 2449 O MET A 158** 1188 1368 1684 177 -218 -66 ATOM 2450 CB MET A 158 15.019 -31.142 -19.776 1.00 11.56 ANISOU 2450 CB MET A 158 1339 1464 1591 326 -282 ATOM 2451 CG MET A 158 14.976 -32.023 -18.535 1.00 13.64 **ANISOU 2451 CG MET A 158** 1663 1741 1779 425 -311 134 ATOM 2452 SD MET A 158 14.901 -31.073 -16.987 1.00 14.46 **ANISOU 2452 SD MET A 158** 1803 1945 1748 544 -396 ATOM 2453 CE MET A 158 13.466 -30.040 -17.307 1.00 14.03 C **ANISOU 2453 CE MET A 158** 1753 1934 1645 469 -327 126 ATOM 2454 H MET A 158 17.394 -31.708 -20.238 1.00 14.05 Н 15.052 -32.588 -21.227 1.00 13.67 ATOM 2455 HA MET A 158 Н ATOM 2456 HB2 MET A 158 15.560 -30.365 -19.565 1.00 13.88 Н ATOM 2457 HB3 MET A 158 14.110 -30.862 -19.967 1.00 13.88 Н ATOM 2458 HG2 MET A 158 14.189 -32.588 -18.577 1.00 16.37 Н ATOM 2459 HG3 MET A 158 15.776 -32.571 -18.511 1.00 16.37 Н ATOM 2460 HE1 MET A 158 13.311 -29.469 -16.539 1.00 16.84 ATOM 2461 HE2 MET A 158 13.636 -29.499 -18.094 1.00 16.84 ATOM 2462 HE3 MET A 158 12.695 -30.610 -17.457 1.00 16.84 Н ATOM 2463 N ASN A 159 15.553 -31.452 -23.412 1.00 10.34 Ν **ANISOU 2463 N ASN A 159** 1102 1193 1633 122 -134 -29 Ν

ATOM 2464 CA ASN A 159	15.627 -30.683 -24.644 1.00 12.33	С
ANISOU 2464 CA ASN A 159	1331 1441 1912 61 -82 -70	C
ATOM 2465 C ASN A 159	14.230 -30.312 -25.113 1.00 11.63	C
ANISOU 2465 C ASN A 159	1284 1384 1751 16 -50 -35	C
ATOM 2466 O ASN A 159	13.301 -31.117 -25.032 1.00 11.47	O
ANISOU 2466 O ASN A 159		o Č
ATOM 2467 CB ASN A 159	16.349 -31.472 -25.735 1.00 13.54	C
ANISOU 2467 CB ASN A 159	1465 1548 2132 39 -33 -103	C
ATOM 2468 CG ASN A 159		_
	17.803 -31.713 -25.406 1.00 15.98	C
ANISOU 2468 CG ASN A 159	1711 1828 2533 84 -61 -151	C
ATOM 2469 OD1 ASN A 159	18.658 -30.883 -25.704 1.00 17.60	0
ANISOU 2469 OD1 ASN A 159		Q.
ATOM 2470 ND2 ASN A 159	18.092 -32.848 -24.790 1.00 16.61	N
ANISOU 2470 ND2 ASN A 159	1799 1879 2631 136 -99 -135	. N
ATOM 2471 H ASN A 159	15.489 -32.301 -23.531 1.00 12.41	H
ATOM 2472 HA ASN A 159	16.121 -29.865 -24.482 1.00 14.79	Н
ATOM 2473 HB2 ASN A 159	15.917 -32.334 -25.841 1.00 16.25	Н
ATOM 2474 HB3 ASN A 159	16.307 -30.974 -26.566 1.00 16.25	Н
ATOM 2475 HD21 ASN A 159	18.907 -33.029 -24.583 1.00 19.93	Н
ATOM 2476 HD22 ASN A 159	17.465 -33.405 -24.598 1.00 19.93	Н
ATOM 2477 N LEU A 160	14.087 -29.080 -25.583 1.00 10.99	N
ANISOU 2477 N LEU A 160	1198 1323 1657 -6 -34 -52	N
ATOM 2478 CA LEU A 160	12.836 -28.605 -26.153 1.00 12.30	С
ANISOU 2478 CA LEU A 160	1396 1519 1756 -36 -12 -27	C
ATOM 2479 C LEU A 160	12.780 -28.893 -27.654 1.00 12.85	Č
ANISOU 2479 C LEU A 160	1483 1576 1822 -71 42 -44	C
ATOM 2480 O LEU A 160	13.794 -29.162 -28.301 1.00 13.12	Õ
ANISOU 2480 O LEU A 160	1502 1579 1904 -75 78 -74	o
ATOM 2481 CB LEU A 160	12.677 -27.112 -25.895 1.00 12.39	C
ANISOU 2481 CB LEU A 160		_
		C
ATOM 2482 CG LEU A 160	12.462 -26.767 -24.417 1.00 13.29	C
ANISOU 2482 CG LEU A 160	1515 1696 1839 21 -85 -29	C
ATOM 2483 CD1 LEU A 160	12.667 -25.285 -24.178 1.00 14.25	C
ANISOU 2483 CD1 LEU A 160	1623 1814 1979 33 -106 -64	C
ATOM 2484 CD2 LEU A 160	11.068 -27.188 -23.984 1.00 14.50	C
ANISOU 2484 CD2 LEU A 160	1697 1895 1916 27 -84 20	C
ATOM 2485 H LEU A 160	14.712 -28.489 -25.582 1.00 13.19	Н
ATOM 2486 HA LEU A 160	12.096 -29.067 -25.728 1.00 14.75	Н
ATOM 2487 HB2 LEU A 160	13.479 -26.655 -26.194 1.00 14.87	Н
ATOM 2488 HB3 LEU A 160	11.909 -26.788 -26.391 1.00 14.87	Н
ATOM 2489 HG LEU A 160	13.107 -27.253 -23.879 1.00 15.95	Н
ATOM 2490 HD11 LEU A 160	12.526 -25.095 -23.238 1.00 17.11	Н
ATOM 2491 HD12 LEU A 160	13.573 -25.047 -24.432 1.00 17.11	Н
ATOM 2492 HD13 LEU A 160	12.031 -24.788 -24.716 1.00 17.11	Н
ATOM 2493 HD21 LEU A 160	10.947 -26.964 -23.048 1.00 17.40	Ĥ
ATOM 2494 HD22 LEU A 160	10.415 -26.717 -24.525 1.00 17.40	Ĥ
ATOM 2495 HD23 LEU A 160	10.974 -28.146 -24.111 1.00 17.40	H
ATOM 2496 N GLY A 161	11.567 -28.848 -28.198 1.00 13.20	Ν
ANISOU 2496 N GLY A 161	1558 1653 1806 -87 43 -30	N
ATOM 2497 CA GLY A 161	11.364 -29.140 -29.605 1.00 12.92	"C
ANISOU 2497 CA GLY A 161	1549 1621 1740 -102 75 -56	C
ATOM 2498 C GLY A 161	11.866 -28.026 -30.511 1.00 13.85	C
		C
ANISOU 2498 C GLY A 161	1688 1741 1831 -94 123 -54	C

ATOM 2499 O GLY A 161	12.287 -26.953 -30.076 1.00 13.36	0
ANISOU 2499 O GLY A 161	1613 1667 1794 -88 132 -35	0
ATOM 2500 H GLY A 161	10.847 -28.652 -27.770 1.00 15.85	H
ATOM 2501 HA2 GLY A 161	11.833 -29.958 -29.836 1.00 15.51	
ATOM 2502 HA3 GLY A 161	10.418 -29.270 -29.775 1.00 15.51	H
ATOM 2502 HAS GET A 101 ATOM 2503 N SER A 162	11.824 -28.300 -31.816 1.00 15.38	N
ANISOU 2503 N SER A 162	1921 1947 1976 -89 159 -75	N
ATOM 2504 CA SER A 162	12.370 -27.381 -32.810 1.00 17.59	C
ANISOU 2504 CA SER A 162	2237 2227 2221 -72 232 -56	C
ATOM 2505 C SER A 162	11.337 -26.421 -33.393 1.00 17.55	С
ANISOU 2505 C SER A 162	2287 2262 2118 -46 219 -22	C
ATOM 2506 O SER A 162	11.729 -25.450 -34.047 1.00 19.25	0
ANISOU 2506 O SER A 162	2541 2466 2307 -28 285 19	0
ATOM 2507 CB SER A 162	13.016 -28.172 -33.946 1.00 19.35	С
ANISOU 2507 CB SER A 162	2484 2449 2421 -59 291 -95	С
ATOM 2508 OG SER A 162	12.085 -29.047 -34.549 1.00 20.29	0
ANISOU 2508 OG SER A 162	2636 2604 2470 -46 241 -142	Ö
ATOM 2509 H SER A 162	11.482 -29.015 -32.150 1.00 18.46	Н
ATOM 2510 HA SER A 162	13.063 -26.847 -32.391 1.00 21.11	
ATOM 2511 HB2 SER A 162	13.344 -27.551 -34.616 1.00 23.23	Ή
ATOM 2512 HB3 SER A 162	13.752 -28.693 -33.589 1.00 23.23	Н
ATOM 2513 HG SER A 162	12.454 -29.474 -35.171 1.00 24.35	H
ATOM 2514 N ASN A 163	10.043 -26.660 -33.178 1.00 16.81	N
ANISOU 2514 N ASN A 163	2195 2211 1981 -41 142 -33	N
ATOM 2515 CA ASN A 163	8.970 -25.857 -33.771 1.00 17.77	С
ANISOU 2515 CA ASN A 163	2362 2380 2010 -3 112 -12	С
ATOM 2516 C ASN A 163	8.261 -25.103 -32.648 1.00 15.86	C
ANISOU 2516 C ASN A 163	2085 2141 1798 -6 66 16	С
ATOM 2517 O ASN A 163	7.427 -25.670 -31.940 1.00 15.31	0
ANISOU 2517 O ASN A 163	1971 2096 1749 -22 10 -5	0
ATOM 2518 CB ASN A 163	7.998 -26.741 -34.550 1.00 20.36	С
ANISOU 2518 CB ASN A 163	2704 2761 2272 14 51 -71	С
ATOM 2519 CG ASN A 163	6.851 -25.955 -35.158 1.00 24.49	C
ANISOU 2519 CG ASN A 163	3266 3341 2698 69 -1 -61	C
ATOM 2520 OD1 ASN A 163	6.802 -24.732 -35.056 1.00 25.97	O
ANISOU 2520 OD1 ASN A 163	3482 3523 2864 98 19 2	o
ATOM 2521 ND2 ASN A 163	5.923 -26.659 -35.809 1.00 26.67	N
ANISOU 2521 ND2 ASN A 163	3539 3669 2926 89 -75 -130	N
ATOM 2522 H ASN A 163	9.753 -27.299 -32.681 1.00 20.17	H
ATOM 2523 HA ASN A 163	9.353 -25.208 -34.382 1.00 21.33	H.
ATOM 2524 HB2 ASN A 163		H
ATOM 2525 HB3 ASN A 163	7.622 -27.404 -33.950 1.00 24.43	H
ATOM 2526 HD21 ASN A 163	5.254 -26.258 -36.170 1.00 32.00	Н
ATOM 2527 HD22 ASN A 163	5.995 -27.514 -35.867 1.00 32.00	Н
ATOM 2528 N TRP A 164	8.579 -23.821 -32.496 1.00 14.81	N
ANISOU 2528 N TRP A 164	1972 1980 1676 11 97 63	N
ATOM 2529 CA TRP A 164	8.134 -23.065 -31.334 1.00 14.08	С
ANISOU 2529 CA TRP A 164	1846 1882 1622 14 59 76	С
ATOM 2530 C TRP A 164	6.718 -22.530 -31.526 1.00 14.45	C
ANISOU 2530 C TRP A 164	1909 1980 1601 57 4 85	C
ATOM 2531 O TRP A 164	6.408 -21.914 -32.556 1.00 14.43	0
ANISOU 2531 O TRP A 164	1966 1989 1529 102 11 111	ŏ
ATOM 2532 CB TRP A 164	9.113 -21.924 -31.048 1.00 14.13	C
ALOM LOOL OD THE A TOT	SILIO ELIGET CHUTC HUCHTHU	•

ANISOU 2532 CB TRP A 164 1856 1818 1695 11 107 102 ATOM 2533 CG TRP A 164 C 10.410 -22.443 -30.506 1.00 15.08 **ANISOU 2533 CG TRP A 164** 1927 1895 1907 -28 135 74 C ATOM 2534 CD1 TRP A 164 11.399 -23.077 -31.207 1.00 16.58 **ANISOU 2534 CD1 TRP A 164** 2115 2063 2121 -49 196 ATOM 2535 CD2 TRP A 164 10.841 -22.413 -29.144 1.00 14.71 C **ANISOU 2535 CD2 TRP A 164** 1824 1831 1935 -38 95 Ν ATOM 2536 NE1 TRP A 164 12.420 -23.434 -30.367 1.00 17.05 **ANISOU 2536 NE1 TRP A 164** 2112 2088 2279 Ν -73 193 ATOM 2537 CE2 TRP A 164 12.104 -23.043 -29.093 1.00 16.33 C 1989 2001 2213 **ANISOU 2537 CE2 TRP A 164** -63 124 ATOM 2538 CE3 TRP A 164 10.287 -21.911 -27.962 1.00 14.60 C **ANISOU 2538 CE3 TRP A 164** 1790 1833 1923 -15 34 ATOM 2539 CZ2 TRP A 164 12.820 -23.185 -27.908 1.00 16.03 C 1895 1946 2250 -62 **ANISOU 2539 CZ2 TRP A 164** 80 -24 ATOM 2540 CZ3 TRP A 164 11.003 -22.045 -26.786 1.00 15.38 C **ANISOU 2540 CZ3 TRP A 164** 1843 1919 2081 -12 -3 -12 ATOM 2541 CH2 TRP A 164 12.256 -22.681 -26.768 1.00 15.74 C **ANISOU 2541 CH2 TRP A 164** 1851 1932 2198 -33 14 -38 C ATOM 2542 H TRP A 164 9.052 -23.367 -33.053 1.00 17.77 Н ATOM 2543 HA TRP A 164 8.127 -23.652 -30.562 1.00 16.90 Н 9.297 -21.445 -31.871 1.00 16.96 ATOM 2544 HB2 TRP A 164 ATOM 2545 HB3 TRP A 164 8.726 -21.326 -30.390 1.00 16.96 Н ATOM 2546 HD1 TRP A 164 11.378 -23.247 -32.121 1.00 19.89 Н ATOM 2547 HE1 TRP A 164 13.139 -23.843 -30.600 1.00 20.46 Н ATOM 2548 HE3 TRP A 164 9.454 -21.496 -27.966 1.00 17.52 Н ATOM 2549 HZ2 TRP A 164 13.655 -23.593 -27.894 1.00 19.24 ATOM 2550 HZ3 TRP A 164 10.643 -21.721 -25.992 1.00 18.45 ATOM 2551 HH2 TRP A 164 12.716 -22.756 -25.963 1.00 18.89 ATOM 2552 N ALA A 165 5.868 -22.754 -30.519 1.00 12.58 1619 1778 1384 53 -46 67 **ANISOU 2552 N ALA A 165** ATOM 2553 CA ALA A 165 4.501 -22.241 -30.467 1.00 13.05 **ANISOU 2553 CA ALA A 165** 1666 1888 1403 95 -97 67 C ATOM 2554 C ALA A 165 ANISOU 2554 C ALA A 165 4.452 -21.096 -29.450 1.00 12.51 1589 1799 1366 121 **-99** 83 0 ATOM 2555 O ALA A 165 5.487 -20.458 -29.194 1.00 13.17 **ANISOU 2555 O ALA A 165** 1693 1819 1492 114 -65 95 ATOM 2556 CB ALA A 165 3.554 -23.401 -30.168 1.00 13.86 **ANISOU 2556 CB ALA A 165** 1704 2042 1519 68 -134 30 Н ATOM 2557 H ALA A 165 6.074 -23.221 -29.827 1.00 15.10 ATOM 2558 HA ALA A 165 4.266 -21.880 -31.336 1.00 15.65 ATOM 2559 HB1 ALA A 165 2.645 -23.064 -30.132 1.00 16.63 Н 3.634 -24.063 -30.871 1.00 16.63 ATOM 2560 HB2 ALA A 165 Н ATOM 2561 HB3 ALA A 165 3.795 -23.793 -29.314 1.00 16.63 Н ATOM 2562 N TYR A 166 Ν 3.280 -20.833 -28.884 1.00 10.88 **ANISOU 2562 N TYR A 166** 1343 1642 1147 153 -139 **72** Ν ATOM 2563 CA TYR A 166 3.123 -19.601 -28.128 1.00 11.58 **ANISOU 2563 CA TYR A 166 77** C 1435 1712 1252 198 -146 C ATOM 2564 C TYR A 166 ANISOU 2564 C TYR A 166 3.972 -19.608 -26.861 1.00 11.03 1348 1614 1230 178 -130 59 ATOM 2565 O TYR A 166 4.401 -20.651 -26.356 1.00 10.79 0 ANISOU 2565 O TYR A 166 1292 1595 1212 140 -118 0 52 ATOM 2566 CB TYR A 166 1.645 -19.339 -27.794 1.00 12.55

ANISOU 2566 CB TYR A 166 1513 1903 1352 246 -186 00000000000 ATOM 2567 CG TYR A 166 0.981 -20.242 -26.779 1.00 13.08 **ANISOU 2567 CG TYR A 166** 1504 2031 1433 224 -181 ATOM 2568 CD1 TYR A 166 1.363 -20.230 -25.437 1.00 12.67 **ANISOU 2568 CD1 TYR A 166** 1440 1978 1395 226 -157 40 ATOM 2569 CD2 TYR A 166 -0.092 -21.056 -27.144 1.00 14.13 **ANISOU 2569 CD2 TYR A 166** 1576 2222 1569 209 -198 29 ATOM 2570 CE1 TYR A 166 0.734 -21.027 -24.509 1.00 13.25 **ANISOU 2570 CE1 TYR A 166** 216 -131 43 1458 2107 1469 ATOM 2571 CE2 TYR A 166 -0.729 -21.856 -26.215 1.00 13.95 **ANISOU 2571 CE2 TYR A 166** 1479 2242 1578 183 -170 27 ATOM 2572 CZ TYR A 166 -0.316 -21.834 -24.900 1.00 14.22 **ANISOU 2572 CZ TYR A 166** 1518 2275 1611 189 -127 45 ATOM 2573 OH TYR A 166 -0.926 -22.621 -23.943 1.00 16.46 0 **ANISOU 2573 OH TYR A 166** 1742 2600 1913 173 -78 63 0 ATOM 2574 H TYR A 166 2.582 -21.333 -28.922 1.00 13.05 Н ATOM 2575 HA TYR A 166 3.430 -18.864 -28.678 1.00 13.89 Н ATOM 2576 HB2 TYR A 166 1.571 -18.433 -27.457 1.00 15.06 ATOM 2577 HB3 TYR A 166 1.135 -19.415 -28.615 1.00 15.06 ATOM 2578 HD1 TYR A 166 2.068 -19.686 -25.168 1.00 15.20 ATOM 2579 HD2 TYR A 166 -0.375 -21.070 -28.030 1.00 16.95 Н ATOM 2580 HE1 TYR A 166 1.010 -21.016 -23.620 1.00 15.90 ATOM 2581 HE2 TYR A 166 -1.435 -22.404 -26.475 1.00 16.73 Н ATOM 2582 HH TYR A 166 -1.547 -23.067 -24.291 1.00 19.75 Н ATOM 2583 N GLN A 167 4.206 -18.400 -26.355 1.00 9.96 Ν **ANISOU 2583 N GLN A 167** 1227 1435 1122 215 -138 47 Ν ATOM 2584 CA GLN A 167 5.055 -18.167 -25.196 1.00 10.99 **ANISOU 2584 CA GLN A 167** 1343 1535 1297 215 -145 ATOM 2585 C GLN A 167 4.439 -16.980 -24.469 1.00 12.34 C **ANISOU 2585 C GLN A 167** 1514 1705 1469 282 -175 -24 ATOM 2586 O GLN A 167 0 4.531 -15.845 -24.955 1.00 13.19 **ANISOU 2586 O GLN A 167** 1653 1743 1617 304 -176 -20 ATOM 2587 CB GLN A 167 6.486 -17.884 -25.643 1.00 12.60 1565 1647 1576 175 -118 **ANISOU 2587 CB GLN A 167** ATOM 2588 CG GLN A 167 7.493 -17.643 -24.545 1.00 12.74 **ANISOU 2588 CG GLN A 167** 1555 1628 1658 175 -144 -54 ATOM 2589 CD GLN A 167 8.886 -17.442 -25.113 1.00 13.94 **ANISOU 2589 CD GLN A 167** 1700 1687 1910 125 -109 -59 0 ATOM 2590 OE1 GLN A 167 9.131 -16.513 -25.894 1.00 14.43 **ANISOU 2590 OE1 GLN A 167** 1785 1669 2029 114 -69 -35 ATOM 2591 NE2 GLN A 167 9.800 -18.321 -24.746 1.00 13.89 N **ANISOU 2591 NE2 GLN A 167** 1659 1687 1931 97 -114 -85 Ν ATOM 2592 H GLN A 167 3.870 -17.677 -26.679 1.00 11.95 Н ATOM 2593 HA GLN A 167 5.048 -18.941 -24.612 1.00 13.18 Н ATOM 2594 HB2 GLN A 167 6.799 -18.644 -26.159 1.00 15.12 Н ATOM 2595 HB3 GLN A 167 6.479 -17.094 -26.205 1.00 15.12 Н ATOM 2596 HG2 GLN A 167 7.246 -16.845 -24.052 1.00 15.29 ATOM 2597 HG3 GLN A 167 7.513 -18.412 -23.953 1.00 15.29 ATOM 2598 HE21 GLN A 167 9.590 -18.963 -24.214 1.00 16.67 ATOM 2599 HE22 GLN A 167 10.605 -18.251 -25.040 1.00 16.67 Н **ATOM 2600 N AVAL A 168** 3.784 -17.226 -23.335 0.16 12.27 Ν ANISOU 2600 N AVAL A 168 1474 1770 1417 320 -191 -51 Ν ATOM 2601 N BVAL A 168 3.834 -17.245 -23.314 0.84 12.20 N

ANISOU 2601 N BVAL A 168 1466 1761 1410 318 -191 -52 Ν **ATOM 2602 CA AVAL A 168** 2.957 -16.210 -22.691 0.16 12.80 **ANISOU 2602 CA AVAL A 168** 1537 1857 1469 396 -215 -86 2.948 -16.297 -22.643 0.84 12.68 **ATOM 2603 CA BVAL A 168** C ANISOU 2603 CA BVAL A 168 1520 1849 1451 395 -213 C 3.288 -16.128 -21.208 0.16 13.48 **ATOM 2604 C AVAL A 168** ANISOU 2604 C AVAL A 168 1615 1973 1533 440 -235 -147 ATOM 2605 C BVAL A 168 3.357 -16.137 -21.184 0.84 13.49 ANISOU 2605 C BVAL A 168 1616 1972 1536 439 -236 -149 C **ATOM 2606 O AVAL A 168** 3.543 -17.147 -20.556 0.16 13.43 0 0 **ANISOU 2606 O AVAL A 168** 1598 2020 1486 427 -223 -137 3.712 -17.113 -20.516 0.84 13.61 ATOM 2607 O BVAL A 168 0 **ANISOU 2607 O BVAL A 168** 1623 2034 1514 426 -227 -143 CCCCCCC **ATOM 2608 CB AVAL A 168** 1.453 -16.497 -22.890 0.16 12.97 **ANISOU 2608 CB AVAL A 168** 1523 1965 1441 424 -205 -60 **ATOM 2609 CB BVAL A 168** 1.479 -16.769 -22.743 0.84 12.89 1506 1968 1424 417 -199 -58 ANISOU 2609 CB BVAL A 168 1.086 -16.412 -24.366 0.16 12.95 **ATOM 2610 CG1AVAL A 168** ANISOU 2610 CG1AVAL A 168 1536 1940 1446 408 -210 -18 **ATOM 2611 CG1BVAL A 168** 0.545 -15.978 -21.814 0.84 13.75 **ANISOU 2611 CG1BVAL A 168** 1593 2126 1505 504 -209 -100 CCC **ATOM 2612 CG2AVAL A 168** 1.084 -17.860 -22.321 0.16 12.88 **ANISOU 2612 CG2AVAL A 168** 1468 2035 1390 394 -171 1.004 -16.696 -24.208 0.84 12.84 ATOM 2613 CG2BVAL A 168 1509 1945 1424 401 -206 **ANISOU 2613 CG2BVAL A 168** ATOM 2614 H AVAL A 168 3.803 -17.977 -22.918 0.16 14.72 **ATOM 2615 H BVAL A 168** 3.925 -17.987 -22.888 0.84 14.65 Н **ATOM 2616 HA AVAL A 168** 3.152 -15.347 -23.089 0.16 15.36 Н **ATOM 2617 HA BVAL A 168** 3.019 -15.432 -23.075 0.84 15.22 Н **ATOM 2618 HB AVAL A 168 ATOM 2619 HB BVAL A 168** 1.438 -17.699 -22.472 0.84 15.47 **ATOM 2620 HG11AVAL A 168** 0.139 -16.595 -24.467 0.16 15.55 ATOM 2621 HG11BVAL A 168 1.066 -15.318 -21.330 0.84 16.50 Н Н **ATOM 2622 HG12AVAL A 168** 1.287 -15.520 -24.691 0.16 15.55 ATOM 2623 HG12BVAL A 168 Н -0.133 -15.536 -22.349 0.84 16.50 1.604 -17.068 -24.858 0.16 15.55 Н **ATOM 2624 HG13AVAL A 168** ATOM 2625 HG13BVAL A 168 0.127 -16.592 -21.190 0.84 16.50 Н **ATOM 2626 HG21AVAL A 168** 1.879 -18.271 -21.947 0.16 15.45 Н 1.731 -16.367 -24.759 0.84 15.41 **ATOM 2627 HG21BVAL A 168** Н **ATOM 2628 HG22AVAL A 168** 0.415 -17.742 -21.628 0.16 15.45 Н **ATOM 2629 HG22BVAL A 168** 0.742 -17.583 -24.499 0.84 15.41 Н **ATOM 2630 HG23AVAL A 168** 0.729 -18.414 -23.034 0.16 15.45 Н ATOM 2631 HG23BVAL A 168 0.247 -16.092 -24.264 0.84 15.41 Н ATOM 2632 N MET A 169 3.273 -14.905 -20.680 1.00 14.19 N **ANISOU 2632 N MET A 169** 1717 2027 1648 503 -271 -212 Ν ATOM 2633 CA MET A 169 3.418 -14.655 -19.246 1.00 14.96 C **ANISOU 2633 CA MET A 169** 1814 2167 1705 573 -304 -291 ATOM 2634 C MET A 169 2.018 -14.730 -18.656 1.00 15.19 C **ANISOU 2634 C MET A 169** 1824 2304 1646 643 -275 -282 ATOM 2635 O MET A 169 1.222 -13.786 -18.773 1.00 15.04 0 **ANISOU 2635 O MET A 169** 1799 2276 1639 697 -283 -307 0 4.066 -13.304 -18.969 1.00 15.82 ATOM 2636 CB MET A 169 **ANISOU 2636 CB MET A 169** 1938 2176 1897 608 -361 -386

ATOM 2637 CG MET A 169	4.442 -13.125 -17.505 1.00 16.14	С
ANISOU 2637 CG MET A 169	1982 2260 1889 685 -417 -492	Č
ATOM 2638 SD MET A 169	5.705 -14.324 -16.995 1.00 15.56	S
ANISOU 2638 SD MET A 169	1904 2217 1792 649 -441 -494	S
ATOM 2639 CE MET A 169	5.393 -14.423 -15.229 1.00 17.11	C
ANISOU 2639 CE MET A 169	2126 2542 1835 785 -482 -572	C
ATOM 2640 H AMET A 169	3.179 -14.187 -21.143 0.16 17.03	H
ATOM 2641 H BMET A 169	3.133 -14.197 -21.147 0.84 17.03	Н
ATOM 2642 HA MET A 169	3.972 -15.347 -18.852 1.00 17.96	Н
ATOM 2643 HB2 MET A 169	4.874 -13.226 -19.499 1.00 18.99	Н
ATOM 2644 HB3 MET A 169	3.443 -12.600 -19.207 1.00 18.99	Ĥ
ATOM 2645 HG2 MET A 169	4.798 -12.233 -17.372 1.00 19.36	H
ATOM 2646 HG3 MET A 169	3.655 -13.259 -16.953 1.00 19.36	Н
ATOM 2647 HE1 MET A 169	6.020 -15.048 -14.833 1.00 20.54	Н
ATOM 2648 HE2 MET A 169	5.511 -13.543 -14.839 1.00 20.54	Н
ATOM 2649 HE3 MET A 169	4.484 -14.730 -15.086 1.00 20.54	H
ATOM 2650 N ALA A 170	1.723 -15.849 -18.010 1.00 12.97	N _.
ANISOU 2650 N ALA A 170	1528 2118 1283 644 -233 -242	N
ATOM 2651 CA ALA A 170	0.355 -16.268 -17.775 1.00 12.43	C
ANISOU 2651 CA ALA A 170	1418 2146 1157 673 -171 -199	С
ATOM 2652 C ALA A 170	-0.038 -16.156 -16.312 1.00 14.05	C
ANISOU 2652 C ALA A 170	1632 2445 1263 775 -147 -237	С
ATOM 2653 O ALA A 170	0.796 -16.167 -15.400 1.00 14.67	0
ANISOU 2653 O ALA A 170	1755 2533 1287 820 -180 -282	0
ATOM 2654 CB ALA A 170	0.151 -17.718 -18.234 1.00 12.82	С
ANISOU 2654 CB ALA A 170	1439 2226 1208 590 -114 -109	C
		_
ATOM 2655 H ALA A 170	2.310 -16.391 -17.694 1.00 15.57	Η
ATOM 2656 HA ALA A 170	-0.241 -15.703 -18.290 1.00 14.91	Н
ATOM 2657 HB1 ALA A 170	-0.769 -17.975 -18.067 1.00 15.39	Н
ATOM 2658 HB2 ALA A 170	0.345 -17.779 -19.183 1.00 15.39	Н
ATOM 2659 HB3 ALA A 170	0.752 -18.294 -17.736 1.00 15.39	H
	-1.347 -16.058 -16.124 1.00 14.45	
ATOM 2660 N THR A 171		N
ANISOU 2660 N THR A 171	1635 2570 1286 818 -90 -221	N
ATOM 2661 CA THR A 171	-2.015 -16.372 -14.875 1.00 15.63	С
ANISOU 2661 CA THR A 171	1776 2832 1328 900 -16 -213	C
ATOM 2662 C THR A 171	-2.723 -17.708 -15.067 1.00 15.49	C
ANISOU 2662 C THR A 171	1702 2865 1319 830 85 -102	Č
ATOM 2663 O THR A 171	-3.523 -17.861 -15.995 1.00 16.56	0
ANISOU 2663 O THR A 171	1765 2990 1536 772 103 -74	0
ATOM 2664 CB THR A 171	-3.006 -15.267 -14.506 1.00 17.45	C
ANISOU 2664 CB THR A 171	1979 3107 1543 1002 -9 -281	С
ATOM 2665 OG1 THR A 171	-2.298 -14.029 -14.322 1.00 17.00	Ö
ANISOU 2665 OG1 THR A 171	1977 2981 1501 1063 -107 -393	0
ATOM 2666 CG2 THR A 171	-3.746 -15.624 -13.235 1.00 19.42	C
ANISOU 2666 CG2 THR A 171	2219 3485 1674 1092 92 -265	С
ATOM 2667 H THR A 171	-1.891 -15.799 -16.737 1.00 17.34	Н
ATOM 2668 HA THR A 171	-1.362 -16.460 -14.164 1.00 18.75	Н
	-3.655 -15.163 -15.219 1.00 20.94	H
ATOM 2670 HG1 THR A 171	-1.900 -13.818 -15.031 1.00 20.40	H.
ATOM 2671 HG21 THR A 171	-4.372 -14.919 -13.007 1.00 23.30	Н
ATOM 2672 HG22 THR A 171	-4.235 -16.452 -13.358 1.00 23.30	Н
ATOM 2673 HG23 THR A 171	-3.116 -15.734 -12.505 1.00 23.30	H
ATOM 2674 N ALA A 172	-2.414 -18.680 -14.217 1.00 16.85	Ν
AION ZUIT IN ALA A IIZ	-2.714 -10.000 -14.21 <i>1</i> 1.00 10.00	1.4

ANISOU 2674 N ALA A 172 1905 3082 1413 838 147 -42 N ATOM 2675 CA ALA A 172 -2.995 -20.011 -14.339 1.00 18.45 2057 3308 1644 764 **ANISOU 2675 CA ALA A 172** 252 ATOM 2676 C ALA A 172 -3.499 -20.464 -12.982 1.00 21.91 **ANISOU 2676 C ALA A 172** 2510 3847 1967 846 372 126 C ATOM 2677 O ALA A 172 -3.005 -20.026 -11.941 1.00 22.67 0 **ANISOU 2677 O ALA A 172** 2688 3992 1935 958 352 86 ATOM 2678 CB ALA A 172 C -1.990 -21.029 -14.885 1.00 18.92 **ANISOU 2678 CB ALA A 172** 2149 3291 1748 669 224 120 ATOM 2679 H ALA A 172 -1.868 -18.595 -13.558 1.00 20.21 Н ATOM 2680 HA ALA A 172 -3.750 -19.975 -14.947 1.00 22.14 ATOM 2681 HB1 ALA A 172 -2.422 -21.895 -14.947 1.00 22.70 Н -1.695 -20.742 -15.763 1.00 22.70 ATOM 2682 HB2 ALA A 172 ATOM 2683 HB3 ALA A 172 -1.233 -21.079 -14.281 1.00 22.70 ATOM 2684 N GLY A 173 -4.496 -21.341 -13.001 1.00 23.11 Ν **ANISOU 2684 N GLY A 173** 2583 4029 2169 795 499 217 Ν ATOM 2685 CA GLY A 173 -5.102 -21.761 -11.752 1.00 24.95 **ANISOU 2685 CA GLY A 173** 2829 4342 2310 864 635 289 ATOM 2686 C GLY A 173 ANISOU 2686 C GLY A 173 -5.873 -23.054 -11.880 1.00 26.13 2902 4465 2562 761 C 767 409 ATOM 2687 O GLY A 173 -6.119 -23.565 -12.974 1.00 24.06 0 **ANISOU 2687 O GLY A 173** 2546 4159 2435 653 769 423 ATOM 2688 H GLY A 173 ATOM 2689 HA2 GLY A 173 -4.830 -21.700 -13.708 1.00 27.73 -4.410 -21.882 -11.083 1.00 29.94 Н ATOM 2690 HA3 GLY A 173 -5.710 -21.071 -11.442 1.00 29.94 ATOM 2691 N TYR A 174 -6.257 -23.576 -10.717 1.00 29.89 Ν **ANISOU 2691 N TYR A 174** 3419 4959 2980 797 873 487 ATOM 2692 CA TYR A 174 -6.976 -24.842 -10.636 1.00 31.90 ANISOU 2692 CA TYR A 174 3614 5169 3337 703 1012 ATOM 2693 C TYR A 174 ANISOU 2693 C TYR A 174 -7.857 -24.785 -9.395 1.00 33.28 C 3799 5398 3448 771 1133 644 ATOM 2694 O TYR A 174 -7.340 -24.696 -8.278 1.00 34.46 0 **ANISOU 2694 O TYR A 174** 4067 5582 3444 878 1133 668 0 ATOM 2695 CB TYR A 174 -6.008 -26.020 -10.578 1.00 33.49 **ANISOU 2695 CB TYR A 174** 3895 5297 3534 660 1016 ATOM 2696 CG TYR A 174 -6.682 -27.378 -10.531 1.00 35.94 **ANISOU 2696 CG TYR A 174** 4151 5535 3972 556 1153 809 ATOM 2697 CD1 TYR A 174 ANISOU 2697 CD1 TYR A 174 -7.253 -27.929 -11.666 1.00 36.43 C 4081 5531 4228 417 1169 ATOM 2698 CD2 TYR A 174 -6.737 -28.111 -9.350 1.00 38.79 **ANISOU 2698 CD2 TYR A 174** C 4588 5886 4263 601 1258 916 ATOM 2699 CE1 TYR A 174 -7.864 -29.170 -11.631 1.00 38.20 C **ANISOU 2699 CE1 TYR A 174** 4251 5674 4590 315 1283 885 ATOM 2700 CE2 TYR A 174 -7.350 -29.350 -9.305 1.00 40.67 **ANISOU 2700 CE2 TYR A 174** 4778 6045 4631 504 1385 1018 ATOM 2701 CZ TYR A 174 -7.910 -29.875 -10.452 1.00 40.81 **ANISOU 2701 CZ TYR A 174** C 4661 5989 4855 357 1395 996 ATOM 2702 OH TYR A 174 -8.522 -31.108 -10.420 1.00 42.87 0 4867 6160 5263 256 1510 1080 0 **ANISOU 2702 OH TYR A 174** ATOM 2703 H TYR A 174 -6.111 -23.210 -9.953 1.00 35.87 ATOM 2704 HA TYR A 174 -7.544 -24.946 -11.415 1.00 38.27 ATOM 2705 HB2 TYR A 174 -5.444 -25.998 -11.367 1.00 40.19 Н Н ATOM 2706 HB3 TYR A 174 -5.461 -25.935 -9.781 1.00 40.19

ATOM 2707 HD1 TYR A 174	-7.224 -27.457 -12.466 1.00 43.71	Н
	-6.360 -27.760 -8.576 1.00 46.54	H'
ATOM 2708 HD2 TYR A 174		
ATOM 2709 HE1 TYR A 174	-8.245 -29.524 -12.402 1.00 45.84	H
ATOM 2710 HE2 TYR A 174	-7.380 -29.828 -8.508 1.00 48.81	Н
ATOM 2711 HH TYR A 174	-8.818 -31.301 -11.182 1.00 51.45	Н
ATOM 2712 N GLN A 175	-9.173 -24.799 -9.594 1.00 32.75	N
ANISOU 2712 N GLN A 175	3602 5342 3498 716 1228 641	N
ATOM 2713 CA GLN A 175	-10.146 -24.786 -8.501 1.00 33.81	Ċ
ANISOU 2713 CA GLN A 175	3725 5530 3593 767 1365 681	C
		_
ATOM 2714 C GLN A 175	-9.770 -23.744 -7.452 1.00 33.99	C
ANISOU 2714 C GLN A 175	3862 5637 3417 931 1317 629	С
ATOM 2715 O GLN A 175	-9.538 -24.050 -6.284 1.00 34.42	0
ANISOU 2715 O GLN A 175	4018 5719 3341 1012 1377 697	0
ATOM 2716 CB GLN A 175	-10.270 -26.177 -7.869 1.00 35.92	C
ANISOU 2716 CB GLN A 175	4019 5744 3885 715 1506 826	C
ATOM 2717 CG GLN A 175	-10.318 -27.301 -8.888 1.00 37.05	C
ANISOU 2717 CG GLN A 175		C
ATOM 2718 CD GLN A 175	-10.630 -28.661 -8.286 1.00 40.91	C
ANISOU 2718 CD GLN A 175	4576 6202 4766 497 1671 1007	С
ATOM 2719 OE1 GLN A 175	-11.250 -29.504 -8.938 1.00 42.22	0
ANISOU 2719 OE1 GLN A 175	4626 6291 5126 362 1727 1027	0
ATOM 2720 NE2 GLN A 175	-10.194 -28.890 -7.048 1.00 42.67	N
ANISOU 2720 NE2 GLN A 175	4936 6449 4826 604 1728 1096	
ATOM 2721 H GLN A 175	-9.537 -24.816 -10.374 1.00 39.29	'н '`
ATOM 2722 HA GLN A 175	-11.015 -24.546 -8.859 1.00 40.58	Н
ATOM 2723 HB2 GLN A 175	-9.504 -26.329 -7.293 1.00 43.10	H
ATOM 2724 HB3 GLN A 175	-11.087 -26.212 -7.347 1.00 43.10	Н
ATOM 2725 HG2 GLN A 175	-11.005 -27.100 -9.542 1.00 44.46	Н
ATOM 2726 HG3 GLN A 175	-9.455 -27.361 -9.327 1.00 44.46	Н
ATOM 2727 HE21 GLN A 175	-9.757 -28.281 -6.627 1.00 51.20	Н
ATOM 2728 HE22 GLN A 175	-10.349 -29.647 -6.671 1.00 51.20	Н
ATOM 2729 N SER A 176	-9.722 -22.489 -7.891 1.00 33.83	N
ANISOU 2729 N SER A 176	3822 5653 3378 985 1200 502	N
ATOM 2730 CA SER A 176	-9.245 -21.415 -7.037 1.00 34.38	
		C
ANISOU 2730 CA SER A 176	3996 5785 3281 1133 1120 423	C
ATOM 2731 C SER A 176	-9.942 -20.114 -7.412 1.00 32.79	C
ANISOU 2731 C SER A 176	3720 5621 3117 1175 1067 298	С
ATOM 2732 O SER A 176	-10.754 -20.060 -8.340 1.00 32.83	0
ANISOU 2732 O SER A 176	3595 5609 3271 1097 1085 276	0
ATOM 2733 CB SER A 176	-7.723 -21.276 -7.143 1.00 33.33	С
ANISOU 2733 CB SER A 176	3976 5621 3065 1169 968 385	С
ATOM 2734 OG SER A 176	-7.323 -20.937 -8.463 1.00 31.68	O
ANISOU 2734 OG SER A 176	3717 5364 2955 1099 859 318	o
	-9.961 -22.237 -8.677 1.00 40.59	Н
ATOM 2736 HA SER A 176	-9.465 -21.620 -6.115 1.00 41.26	H.
ATOM 2737 HB2 SER A 176	-7.429 -20.579 -6.537 1.00 39.99	Н
ATOM 2738 HB3 SER A 176	-7.313 -22.121 -6.898 1.00 39.99	Н
ATOM 2739 HG SER A 176	-6.487 -20.866 -8.501 1.00 38.02	Н
ATOM 2740 N ASER A 177	-9.619 -19.063 -6.663 0.58 31.52	N
ANISOU 2740 N ASER A 177	3641 5507 2827 1306 991 210	N
ATOM 2741 N BSER A 177	-9.623 -19.062 -6.661 0.42 31.55	N
ANISOU 2741 N BSER A 177	3645 5512 2831 1306 991 210	N
ATOM 2742 CA ASER A 177	-10.122 -17.722 -6.914 0.58 30.89	C
ATOW ZI4Z CA ASER A III	-10.122 -11.122 -0.314 0.30 30.09	C

ANISOU 2742 CA ASER A 177 3516 5451 2771 1365 921 C C ATOM 2743 CA BSER A 177 -10.122 -17.722 -6.922 0.42 30.88 C ANISOU 2743 CA BSER A 177 3514 5448 2770 1365 921 ATOM 2744 C ASER A 177 -8.953 -16.755 -6.802 0.58 29.62 **ANISOU 2744 C ASER A 177** 3459 5271 2523 1449 747 C ATOM 2745 C BSER A 177 -8.959 -16.750 -6.792 0.42 29.61 ANISOU 2745 C BSER A 177 3459 5271 2522 1450 747 C **ATOM 2746 O ASER A 177** -7.908 -17.080 -6.231 0.58 29.60 0 0 **ANISOU 2746 O ASER A 177** 3560 5264 2422 1485 697 ATOM 2747 O BSER A 177 -7.926 -17.067 -6.194 0.42 29.63 0 **ANISOU 2747 O BSER A 177** 3565 5270 2423 1489 699 ATOM 2748 CB ASER A 177 -11.234 -17.341 -5.927 0.58 32.76 ANISOU 2748 CB ASER A 177 C 3725 5763 2958 1446 1037 **ATOM 2749 CB BSER A 177** -11.251 -17.337 -5.957 0.42 32.73 C ANISOU 2749 CB BSER A 177 3718 5758 2959 1444 1037 **ATOM 2750 OG ASER A 177** -12.227 -18.352 -5.861 0.58 33.63 0 ANISOU 2750 OG ASER A 177 0 3743 5883 3152 1365 1214 184 **ATOM 2751 OG BSER A 177** -10.769 -17.200 -4.631 0.42 33.97 0 **ANISOU 2751 OG BSER A 177** 3999 5969 2939 1563 1039 0 ATOM 2752 H ASER A 177 -9.094 -19.107 -5.983 0.58 37.82 Н ATOM 2753 H BSER A 177 **-9.104 -19.105 -5.977 0.42 37.86** Н **ATOM 2754 HA ASER A 177** -10.478 -17.673 -7.815 0.58 37.07 Н ATOM 2755 HA BSER A 177 Н -10.463 -17.674 -7.829 0.42 37.05 **ATOM 2756 HB2ASER A 177** -10.846 -17.223 -5.045 0.58 39.31 Н -11.634 -16.493 -6.241 0.42 39.27 **ATOM 2757 HB2BSER A 177** Н **ATOM 2758 HB3ASER A 177** -11.645 -16.513 -6.220 0.58 39.31 **ATOM 2759 HB3BSER A 177** -11.929 -18.031 -5.974 0.42 39.27 Н **ATOM 2760 HG ASER A 177** Н -12.827 -18.129 -5.318 0.58 40.35 **ATOM 2761 HG BSER A 177** -11.399 -16.989 -4.116 0.42 40.76 Н ATOM 2762 N GLY A 178 -9.128 -15.567 -7.361 1.00 28.59 **ANISOU 2762 N GLY A 178** 3296 5120 2446 1478 650 -146 Ν -8.111 -14.544 -7.244 1.00 27.16 ATOM 2763 CA GLY A 178 C **ANISOU 2763 CA GLY A 178** 3201 4905 2215 1550 489 -267 ATOM 2764 C GLY A 178 ANISOU 2764 C GLY A 178 -8.286 -13.445 -8.272 1.00 25.79 C 2978 4668 2153 1540 C 390 -368 ATOM 2765 O GLY A 178 -9.288 -13.377 -8.980 1.00 24.78 0 **ANISOU 2765 O GLY A 178** 2750 4540 2127 1499 439 -353 0 ATOM 2766 H GLY A 178 -9.822 -15.336 -7.814 1.00 34.31 Н ATOM 2767 HA2 GLY A 178 -8.151 -14.148 -6.359 1.00 32.60 Н ATOM 2768 HA3 GLY A 178 -7.235 -14.943 -7.364 1.00 32.60 Н **ATOM 2769 N ASER A 179** -7.276 -12.580 -8.321 0.68 26.25 Ν 3107 4664 2203 1579 246 -474 **ANISOU 2769 N ASER A 179** Ν ATOM 2770 N BSER A 179 -7.279 -12.574 -8.318 0.32 26.26 Ν **ANISOU 2770 N BSER A 179** 3108 4665 2203 1580 246 -474 Ν -7.229 -11.488 -9.279 0.68 25.48 **ATOM 2771 CA ASER A 179 ANISOU 2771 CA ASER A 179** 2988 4478 2217 1571 143 -566 C C **ATOM 2772 CA BSER A 179** -7.250 -11.468 -9.261 0.32 25.56 C **ANISOU 2772 CA BSER A 179** 2997 4488 2225 1573 144 -568 C ATOM 2773 C ASER A 179 -5.779 -11.234 -9.650 0.68 24.27 **ANISOU 2773 C ASER A 179** 2903 4230 2088 1546 15 -625 C ATOM 2774 C BSER A 179 -5.807 -11.226 -9.674 0.32 24.20 C **ANISOU 2774 C BSER A 179** C 2893 4221 2082 1545 16 -625 ATOM 2775 O ASER A 179 -4.889 -11.333 -8.799 0.68 25.00 0

ANISOU 2775 O ASER A 179 3067 4335 2099 1586 -33 -657 0 ATOM 2776 O BSER A 179 -4.881 -11.401 -8.876 0.32 24.96 **ANISOU 2776 O BSER A 179** 3058 4328 2098 1578 -30 -650 0 **ATOM 2777 CB ASER A 179** -7.859 -10.208 -8.713 0.68 27.89 C ANISOU 2777 CB ASER A 179 3296 4790 2512 1671 112 -670 -7.852 -10.190 -8.659 0.32 27.89 **ATOM 2778 CB BSER A 179 ANISOU 2778 CB BSER A 179** 3298 4792 2508 1676 112 -673 **ATOM 2779 OG ASER A 179** 0 -9.255 -10.357 -8.579 0.68 29.03 ANISOU 2779 OG ASER A 179 3357 5006 2666 1687 230 -625 0 -6.842 -9.334 -8.154 0.32 28.15 ATOM 2780 OG BSER A 179 0 3414 4771 2513 1733 -15 -786 **ANISOU 2780 OG BSER A 179** ATOM 2781 H ASER A 179 -6.594 -12.608 -7.798 0.68 31.50 ATOM 2782 H BSER A 179 -6.591 -12.607 -7.803 0.32 31.51 ATOM 2783 HA ASER A 179 -7.713 -11.740 -10.082 0.68 30.58 Н ATOM 2784 HA BSER A 179 -7.760 -11.704 -10.051 0.32 30.67 **ATOM 2785 HB2ASER A 179** -7.475 -10.026 -7.840 0.68 33.47 Н ATOM 2786 HB2BSER A 179 -8.346 -9.720 -9.349 0.32 33.47 ATOM 2787 HB3ASER A 179 -7.675 -9.471 -9.316 0.68 33.47 ATOM 2788 HB3BSER A 179 -8.448 -10.435 -7.934 0.32 33.47 Н **ATOM 2789 HG ASER A 179** -9.591 -9.653 -8.269 0.68 34.83 **ATOM 2790 HG BSER A 179** -6.405 -9.727 -7.554 0.32 33.79 Н ATOM 2791 N ASER A 180 -5.552 -10.899 -10.920 0.68 22.03 Ν 2595 3849 1928 1483 -41 -639 Ν **ANISOU 2791 N ASER A 180** -5.624 -10.816 -10.928 0.32 22.16 ATOM 2792 N BSER A 180 Ν 2608 3864 1947 1487 -42 -644 **ANISOU 2792 N BSER A 180** -4.230 -10.543 -11.402 0.68 19.58 **ATOM 2793 CA ASER A 180** 2338 3426 1676 1450 -152 -699 **ANISOU 2793 CA ASER A 180 ATOM 2794 CA BSER A 180** -4.299 -10.562 -11.467 0.32 19.86 C ANISOU 2794 CA BSER A 180 2369 3462 1716 1447 -147 -694 -4.347 -9.437 -12.439 0.68 19.43 ATOM 2795 C ASER A 180 **ANISOU 2795 C ASER A 180** 2304 3282 1795 1436 -218 -748 C ATOM 2796 C BSER A 180 -4.373 -9.409 -12.457 0.32 19.49 C **ANISOU 2796 C BSER A 180** 2312 3288 1806 1436 -219 -749 ATOM 2797 O ASER A 180 -5.363 -9.306 -13.127 0.68 19.28 **ANISOU 2797 O ASER A 180** 2226 3268 1830 1428 -180 -705 0 ATOM 2798 O BSER A 180 -5.392 -9.210 -13.123 0.32 19.34 2235 3272 1842 1433 -184 -711 **ANISOU 2798 O BSER A 180** 0 **ATOM 2799 CB ASER A 180** -3.505 -11.747 -12.020 0.68 18.30 C 2174 3257 1521 1363 -127 -616 ANISOU 2799 CB ASER A 180 **ATOM 2800 CB BSER A 180** -3.733 -11.807 -12.160 0.32 18.25 C ANISOU 2800 CB BSER A 180 2153 3258 1523 1357 -111 -601 **ATOM 2801 OG ASER A 180** -3.930 -11.978 -13.356 0.68 17.35 **ANISOU 2801 OG ASER A 180** 1991 3094 1506 1289 -104 -552 0 **ATOM 2802 OG BSER A 180** -2.365 -11.639 -12.480 0.32 17.74 2139 3094 1506 1325 -204 -655 0 **ANISOU 2802 OG BSER A 180** ATOM 2803 H ASER A 180 -6.161 -10.873 -11.527 0.68 26.44 Н -6.262 -10.678 -11.489 0.32 26.59 ATOM 2804 H BSER A 180 Н **ATOM 2805 HA ASER A 180** -3.697 -10.213 -10.663 0.68 23.50 Н **ATOM 2806 HA BSER A 180** -3.699 -10.311 -10.747 0.32 23.83 ATOM 2807 HB2ASER A 180 -2.551 -11.573 -12.020 0.68 21.96 Н ATOM 2808 HB2BSER A 180 -3.826 -12.567 -11.565 0.32 21.90 H
ATOM 2809 HB3ASER A 180 -3.696 -12.536 -11.488 0.68 21.96 H
ATOM 2810 HB3BSER A 180 -4.230 -11.965 -12.978 0.32 21.90 H

ATOM 2811 HG ASER A 180	-3.524 -12.639 -13.677 0.68 20.82	Н
ATOM 2812 HG BSER A 180	-2.071 -12.329 -12.859 0.32 21.29	Н
ATOM 2813 N ASN A 181	-3.284 -8.647 -12.543 1.00 20.01	N
ANISOU 2813 N ASN A 181	2430 3234 1938 1429 -321 -834	N
ATOM 2814 CA ASN A 181	-3.132 -7.655 -13.603 1.00 20.96	C
ANISOU 2814 CA ASN A 181	2554 3202 2209 1399 -379 -856	С
ATOM 2815 C ASN A 181	-1.658 -7.640 -13.973 1.00 20.95	C
ANISOU 2815 C ASN A 181	2590 3080 2289 1334 -447 -885	C
ATOM 2816 O ASN A 181	-0.800 -7.414 -13.112 1.00 20.66	0
ANISOU 2816 O ASN A 181	2586 3031 2234 1350 -509 -976	0
ATOM 2817 CB ASN A 181	-3.613 -6.274 -13.165 1.00 21.73	C
ANISOU 2817 CB ASN A 181	2665 3250 2342 1472 -422 -948	C
ATOM 2818 CG ASN A 181	-3.652 -5.282 -14.305 1.00 22.05	С
ANISOU 2818 CG ASN A 181	2712 3132 2535 1448 -460 -940	C
ATOM 2819 OD1 ASN A 181	-2.665 -5.088 -15.014 1.00 22.43	o
ANISOU 2819 OD1 ASN A 181	2788 3047 2687 1383 -500 -931	0
ATOM 2820 ND2 ASN A 181	-4.804 -4.657 -14.500 1.00 22.53	N
ANISOU 2820 ND2 ASN A 181	2747 3203 2611 1502 -441 -932	N
ATOM 2821 H ASN A 181	-2.619 -8.675 -11.999 1.00 24.01	H _.
ATOM 2822 HA ASN A 181	-3.643 -7.928 -14.381 1.00 25.16	Н
ATOM 2823 HB2 ASN A 181	-4.511 -6.351 -12.804 1.00 26.08	Н
ATOM 2824 HB3 ASN A 181	-3.011 -5.929 -12.487 1.00 26.08	H
ATOM 2825 HD21 ASN A 181	-4.880 -4.082 -15.135 1.00 27.04	Н
ATOM 2826 HD22 ASN A 181	-5.477 -4.825 -13.991 1.00 27.04	Н
ATOM 2827 N VAL A 182	-1.364 -7.930 -15.235 1.00 20.19	N
		N
ANISOU 2827 N VAL A 182	2483 2903 2284 1262 -438 -806	
ATOM 2828 CA VAL A 182	0.004 -8.131 -15.691 1.00 19.56	С
ANISOU 2828 CA VAL A 182	2429 2717 2286 1158 -476 -794	С
ATOM 2829 C VAL A 182	0.178 -7.433 -17.027 1.00 18.90	С
ANISOU 2829 C VAL A 182	2359 2478 2346 1097 -484 -736	C
ATOM 2830 O VAL A 182	-0.681 -7.534 -17.910 1.00 18.51	0
ANISOU 2830 O VAL A 182	2295 2445 2292 1090 -446 -642	0
ATOM 2831 CB VAL A 182	0.346 -9.632 -15.827 1.00 20.33	C
ANISOU 2831 CB VAL A 182	2514 2901 2309 1070 -429 -693	С
ATOM 2832 CG1 VAL A 182	1.821 -9.813 -16.122 1.00 20.78	C
ANISOU 2832 CG1 VAL A 182	2588 2859 2449 980 -472 -703	С
ATOM 2833 CG2 VAL A 182	-0.045 -10.393 -14.583 1.00 19.91	C
ANISOU 2833 CG2 VAL A 182	2457 3008 2101 1141 -395 -709	C
ATOM 2834 H VAL A 182	-1.952 -8.018 -15.857 1.00 24.23	Н
ATOM 2835 HA VAL A 182	0.618 -7.733 -15.054 1.00 23.47	H
ATOM 2836 HB VAL A 182	-0.155 -10.002 -16.572 1.00 24.39	Η
ATOM 2837 HG11 VAL A 182	2.013 -10.761 -16.204 1.00 24.94	Н
ATOM 2838 HG12 VAL A 182	2.035 -9.359 -16.952 1.00 24.94	Н
ATOM 2839 HG13 VAL A 182	2.337 -9.432 -15.394 1.00 24.94	Н
ATOM 2840 HG21 VAL A 182	0.182 -11.328 -14.701 1.00 23.90	¨H
ATOM 2841 HG22 VAL A 182	0.439 -10.027 -13.826 1.00 23.90	Н
ATOM 2842 HG23 VAL A 182	-1.000 -10.298 -14.443 1.00 23.90	Н
ATOM 2843 N THR A 183	1.294 -6.726 -17.173 1.00 18.65	N
ANISOU 2843 N THR A 183	2350 2292 2443 1057 -532 -794	N
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ATOM 2844 CA THR A 183	1.702 -6.151 -18.445 1.00 18.92	C
ANISOU 2844 CA THR A 183	2407 2165 2617 987 -517 -719	C
ATOM 2845 C THR A 183	2.963 -6.859 -18.908 1.00 18.55	C
ANISOU 2845 C THR A 183	2356 2074 2619 865 -502 -672	C
,	AND ANT AND OUR OIL OIL	•

ATOM 2846 O THR A 183	3.893 -7.055 -18.117 1.00 18.71	0
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ANISOU 2846 O THR A 183	2358 2094 2658 849 -545 -764	0
ATOM 2847 CB THR A 183	1.944 -4.645 -18.323 1.00 20.07	C
ANISOU 2847 CB THR A 183	2576 2139 2912 1035 -563 -814	С
ATOM 2848 OG1 THR A 183	0.792 -4.026 -17.746 1.00 20.50	0
ANISOU 2848 OG1 THR A 183	2629 2256 2903 1136 -575 -860	0
ATOM 2849 CG2 THR A 183	2.211 -4.036 -19.703 1.00 21.28	С
ANISOU 2849 CG2 THR A 183		_
		C
ATOM 2850 H THR A 183	1.843 -6.562 -16.532 1.00 22.38	Н
ATOM 2851 HA THR A 183	1.007 -6.298 -19.105 1.00 22.71	Н
		H
ATOM 2852 HB THR A 183	2.716 -4.484 -17.758 1.00 24.09	
ATOM 2853 HG1 THR A 183	0.916 -3.199 -17.675 1.00 24.60	Н
ATOM 2854 HG21 THR A 183	2.363 -3.081 -19.620 1.00 25.54	Н
ATOM 2855 HG22 THR A 183	2.995 -4.447 -20.100 1.00 25.54	H
ATOM 2856 HG23 THR A 183	1.449 -4.184 -20.284 1.00 25.54	Н
ATOM 2857 N VAL A 184	2.985 -7.251 -20.180 1.00 18.07	N
ANISOU 2857 N VAL A 184	2310 1984 2572 793 -444 -538	N
ATOM 2858 CA VAL A 184	4.034 -8.090 -20.742 1.00 17.80	С
ANISOU 2858 CA VAL A 184	2269 1931 2563 683 -411 -478	С
ATOM 2859 C VAL A 184	4.658 -7.351 -21.914 1.00 19.00	С
ANISOU 2859 C VAL A 184	2453 1912 2854 626 -368 -409	С
ATOM 2860 O VAL A 184	3.946 -6.749 -22.728 1.00 19.00	0
ANISOU 2860 O VAL A 184	2496 1865 2858 663 -342 -333	0
ATOM 2861 CB VAL A 184	3.472 -9.454 -21.206 1.00 17.23	C
ANISOU 2861 CB VAL A 184	2187 2001 2358 653 -369 -378	С
ATOM 2862 CG1 VAL A 184	4.600 -10.416 -21.584 1.00 16.79	C
ANISOU 2862 CG1 VAL A 184	2120 1937 2321 553 -342 -340	C
ATOM 2863 CG2 VAL A 184	2.567 -10.057 -20.142 1.00 17.71	С
ANISOU 2863 CG2 VAL A 184	2219 2221 2289 719 -384 -418	С
ATOM 2864 H VAL A 184	2.380 -7.036 -20.753 1.00 21.69	Н
ATOM 2865 HA VAL A 184	4.719 -8.247 -20.074 1.00 21.36	Н
ATOM 2866 HB VAL A 184	2.934 -9.310 -22.000 1.00 20.67	Н
ATOM 2867 HG11 VAL A 184	4.213 -11.258 -21.869 1.00 20.14	Н
ATOM 2868 HG12 VAL A 184	5.117 -10.027 -22.307 1.00 20.14	H
ATOM 2869 HG13 VAL A 184	5.167 -10.557 -20.810 1.00 20.14	Н
ATOM 2870 HG21 VAL A 184	2.231 -10.910 -20.461 1.00 21.25	Н
ATOM 2871 HG22 VAL A 184	3.079 -10.186 -19.328 1.00 21.25	Н
ATOM 2872 HG23 VAL A 184	1.828 -9.451 -19.976 1.00 21.25	Н
ATOM 2873 N TRP A 185	5.981 -7.411 -22.014 1.00 18.56	N
ANISOU 2873 N TRP A 185	2376 1765 2911 542 -354 -429	N
ATOM 2874 CA TRP A 185	6.665 -6.804 -23.151 1.00 20.04	C
ANISOU 2874 CA TRP A 185	2590 1789 3234 477 -283 -345	С
ATOM 2875 C TRP A 185	8.048 -7.401 -23.348 1.00 20.72	C
ANISOU 2875 C TRP A 185	2631 1836 3404 373 -248 -346	С
		_
ATOM 2876 O TRP A 185	8.508 -8.213 -22.545 1.00 20.50	0
ANISOU 2876 O TRP A 185	2553 1899 3338 358 -297 -423	0
ATOM 2877 CB TRP A 185	6.756 -5.286 -22.970 1.00 21.08	C
ANISOU 2877 CB TRP A 185	2736 1743 3531 510 -300 -403	C
ATOM 2878 CG TRP A 185	7.676 -4.817 -21.877 1.00 22.44	C
ANISOU 2878 CG TRP A 185	2843 1837 3845 492 -370 -572	С
ATOM 2879 CD1 TRP A 185	8.971 -4.417 -22.016 1.00 23.38	C
ANISOU 2879 CD1 TRP A 185	2915 1801 4169 403 -347 -611	C
		_
ATOM 2880 CD2 TRP A 185	7.357 -4.665 -20.485 1.00 23.43	С

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ANISOU 2880 CD2 TRP A 185
                            2940 2038 3923 574 -478 -736
                                                              C
ATOM 2881 NE1 TRP A 185
                           9.483 -4.026 -20.800 1.00 24.61
                                                             Ν
ANISOU 2881 NE1 TRP A 185
                            3007 1954 4391 414 -446 -787
                                                              N
                            8.513 -4.173 -19.844 1.00 24.55
ATOM 2882 CE2 TRP A 185
ANISOU 2882 CE2 TRP A 185
                                                              C
                            3019 2083 4225 526 -530 -868
ATOM 2883 CE3 TRP A 185
                           6.211 -4.905 -19.720 1.00 22.93
                                                              C
ANISOU 2883 CE3 TRP A 185
                            2894 2131 3686 681 -526 -776
ATOM 2884 CZ2 TRP A 185
                            8.559 -3.926 -18.473 1.00 25.98
                                                            C
ANISOU 2884 CZ2 TRP A 185
                            3164 2347 4359
                                            581 -635 -1023
                                                              C
ATOM 2885 CZ3 TRP A 185
                            6.257 -4.659 -18.365 1.00 24.11
                                                            C
ANISOU 2885 CZ3 TRP A 185
                            3018 2328 3814 754 -621 -947
                                                              C
ATOM 2886 CH2 TRP A 185
                            7.423 -4.172 -17.752 1.00 25.80
                                                             C
                                                              C
ANISOU 2886 CH2 TRP A 185
                            3179 2473 4153 696 -676 -1057
ATOM 2887 OXT TRP A 185
                            8.719 -7.099 -24.335 1.00 21.58
                                                             0
ANISOU 2887 OXT TRP A 185
                            2755 1825 3618 308 -163 -264
                                                              0
ATOM 2888 H TRP A 185
                           6.501 -7.792 -21.445 1.00 22.27
                                                           Н
ATOM 2889 HA TRP A 185
                            6.149 -6.977 -23.954 1.00 24.05
                                                            Н
ATOM 2890 HB2 TRP A 185
                           7.070 -4.897 -23.802 1.00 25.30
                                                            Н
ATOM 2891 HB3 TRP A 185
                           5.869 -4.948 -22.769 1.00 25.30
                                                             Н
ATOM 2892 HD1 TRP A 185
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            TRP A 185
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ATOM 2929 HG22 THR B 3 -27.929 -8.566 -47.471 1.00 19.90
ATOM 2930 HG23 THR B 3 -29.320 -7.847 -47.266 1.00 19.90 ATOM 2931 N ASP B 4 -28.557 -10.194 -51.529 1.00 15.98
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ATOM 2936 CG ASP B 4 -26.711 -10.198 -53.916 1.00 20.93
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ATOM 2946 O TYR B 5 -28.142 -14.190 -48.804 1.00 14.28
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ATOM 2948 CG TYR B 5 -25.057 -15.347 -51.050 1.00 14.98 C ANISOU 2948 CG TYR B 5 1696 2098 1898 -35 -68 116 C ATOM 2949 CD1 TYR B 5 -24.778 -15.875 -52.305 1.00 16.02 ANISOU 2949 CD1 TYR B 5 1796 2317 1974 42 36 151 ATOM 2950 CD2 TYR B 5 C -24.640 -16.058 -49.934 1.00 14.40 ANISOU 2950 CD2 TYR B 5 1639 1970 1863 -71 -94 95 ATOM 2951 CE1 TYR B 5 -24.096 -17.076 -52.438 1.00 17.69 ANISOU 2951 CE1 TYR B 5 1994 2550 2177 90 111 153 ATOM 2952 CE2 TYR B 5 -23.960 -17.255 -50.059 1.00 15.02 C ANISOU 2952 CE2 TYR B 5 1698 2065 1943 -33 -24 112 C -23.696 -17.761 -51.313 1.00 16.82 ATOM 2953 CZ TYR B 5 ANISOU 2953 CZ TYR B 5 1896 2370 2123 51 78 135 ATOM 2954 OH TYR B 5 -23.017 -18.950 -51.446 1.00 18.22 0 ANISOU 2954 OH TYR B 5 2073 2555 2296 119 145 139 0 ATOM 2955 H TYR B 5 -28.138 -12.460 -50.561 1.00 17.14 Н ATOM 2956 HA TYR B 5 -27.497 -14.758 -51.823 1.00 16.77 Н ATOM 2957 HB2 TYR B 5 -25.476 -13.430 -51.583 1.00 17.25 Н ATOM 2958 HB3 TYR B -25.612 -13.683 -50.021 1.00 17.25 5 ATOM 2959 HD1 TYR B 5 -25.050 -15.415 -53.066 1.00 19.23 Н ATOM 2960 HD2 TYR B 5 -24.820 -15.722 -49.086 1.00 17.28 Н ATOM 2961 HE1 TYR B 5 -23.914 -17.419 -53.283 1.00 21.23 Н **ATOM 2962 HE2 TYR B 5** -23.687 -17.719 -49.300 1.00 18.02 Н ATOM 2963 HH TYR B 5 -22.833 -19.262 -50.688 1.00 21.87 Н ATOM 2964 N TRPB 6 -28.188 -16.151 -49.944 1.00 14.40 Ν ANISOU 2964 N TRP B 6 1754 2053 1663 -63 -83 -223 Ν ATOM 2965 CA TRPB 6 -28.712 -16.978 -48.863 1.00 15.59 C 1941 2184 1799 -110 -68 -293 C ANISOU 2965 CA TRP B 6 ATOM 2966 C TRPB 6 C -27.700 -18.084 -48.608 1.00 15.39 ANISOU 2966 C TRP B 6 1932 2106 1810 -125 -34 -245 ATOM 2967 O TRPB 6 0 -27.475 -18.939 -49.473 1.00 14.47 ANISOU 2967 O TRP B 6 1812 2003 1683 -99 21 -255 ATOM 2968 CB TRPB 6 -30.081 -17.556 -49.220 1.00 15.36 C ANISOU 2968 CB TRP B 6 1896 2222 1716 -126 -29 -403 C ATOM 2969 CG TRPB 6 -30.571 -18.628 -48.282 1.00 15.38 ANISOU 2969 CG TRP B 6 1922 2203 1718 -195 13 -442 ATOM 2970 CD1 TRP B 6 -30.973 -19.884 -48.619 1.00 16.03 ANISOU 2970 CD1 TRP B 6 2008 2274 1807 -248 55 -490 ATOM 2971 CD2 TRP B 6 -30.717 -18.531 -46.855 1.00 16.22 ANISOU 2971 CD2 TRP B 6 2064 2287 1811 -218 16 -426 Ν ATOM 2972 NE1 TRP B 6 -31.356 -20.578 -47.495 1.00 17.28 ANISOU 2972 NE1 TRP B 6 2192 2400 1975 -319 Ν 93 -483 ATOM 2973 CE2 TRP B 6 -31.206 -19.772 -46.400 1.00 17.38 C ANISOU 2973 CE2 TRP B 6 2224 2420 1960 -291 80 -441 -30.472 -17.521 -45.921 1.00 16.82 ATOM 2974 CE3 TRP B 6 ANISOU 2974 CE3 TRP B 6 2178 2346 1866 -177 -38 -402 ATOM 2975 CZ2 TRP B 6 -31.468 -20.025 -45.051 1.00 18.45 ANISOU 2975 CZ2 TRP B 6 2401 2547 2062 -318 116 -411 C ATOM 2976 CZ3 TRP B 6 -30.728 -17.776 -44.584 1.00 18.02 ANISOU 2976 CZ3 TRP B 6 -17 -400 2385 2493 1969 -186 ATOM 2977 CH2 TRP B 6 -31.222 -19.016 -44.164 1.00 18.40 C ANISOU 2977 CH2 TRP B 6 2436 2550 2006 -252 72 -394 C ATOM 2978 H TRPB 6 -28.067 -16.591 -50.673 1.00 17.28 Н Н ATOM 2979 HA TRPB 6 -28.801 -16.445 -48.058 1.00 18.71

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ATOM 3054 HG23 THR B 10 -25.077 -29.623 -42.913 1.00 27.46
ATOM 3055 N ASP B 11 -21.742 -28.896 -41.807 1.00 21.08
ANISOU 3055 N ASP B 11 3413 1948 2648 163 -32 245
ATOM 3056 CA ASP B 11 -20.913 -30.060 -42.110 1.00 23.23
ANISOU 3056 CA ASP B 11 3753 2107 2965 298 -30 274
ATOM 3057 C ASP B 11 -21.647 -31.375 -41.871 1.00 24.96
                                                                               C
ANISOU 3057 C ASP B 11 4168 2138 3178 247
                                                               16 273
ATOM 3058 O ASP B 11 -21.050 -32.443 -42.047 1.00 26.18
                                                                              0
ATOM 3061 OD1 ASP B 11 -20.948 -30.481 -39.375 1.00 24.69
ANISOU 3061 OD1 ASP B 11 4149 2208 3025 269 -121 461
ATOM 3062 OD2 ASP B 11 -18.818 -30.084 -39.065 1.00 25.41 O
ANISOU 3062 OD2 ASP B 11 4096 2387 3170 490 -291 551
ATOM 3063 H ASP B 11 -21.557 -28.492 -41.071 1.00 25.29 H
ATOM 3064 HA ASP B 11 -20.675 -30.029 -43.049 1.00 27.87
ATOM 3065 HB2 ASP B 11 -19.027 -30.743 -41.611 1.00 29.00
ATOM 3066 HB3 ASP B 11 -19.171 -29.170 -41.442 1.00 29.00
ATOM 3067 N GLY B 12 -22.923 -31.328 -41.488 1.00 25.27
                                                                             Н
                                                                              Ν
ANISOU 3067 N GLY B 12 4258 2159 3184 75 62 258
ATOM 3068 CA GLY B 12 -23.712 -32.521 -41.286 1.00 26.45
                                                                               C
ANISOU 3068 CA GLY B 12 4569 2125 3354 -18 106 277
ATOM 3069 C GLY B 12 -23.890 -32.935 -39.840 1.00 27.29
ANISOU 3069 C GLY B 12 4798 2169 3401 -60 113 422
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ATOM 3070 O GLY B 12 -24.656 -33.868 -39.573 1.00 29.18
ANISOU 3070 O GLY B 12 5164 2258 3666 -172 162 470 O
ATOM 3071 H GLY B 12 -23.354 -30.599 -41.338 1.00 30.32
ATOM 3072 HA2 GLY B 12 -24.593 -32.383 -41.667 1.00 31.74
ATOM 3073 HA3 GLY B 12 -23.294 -33.258 -41.758 1.00 31.74
ATOM 3074 N GLY B 13 -23.211 -32.274 -38.904 1.00 25.91
                                                                              Ν
ANISOU 3074 N GLY B 13 4595 2101 3147 24 57 499 ATOM 3075 CA GLY B 13 -23.345 -32.620 -37.498 1.00 26.72
                                                                            C
ANISOU 3075 CA GLY B 13 4833 2166 3154 14 60 640
                                                                              C
ATOM 3076 C GLY B 13 -24.644 -32.088 -36.921 1.00 27.11
ANISOU 3076 C GLY B 13 4865 2314 3122 -141 151 656
                                                                              0
ATOM 3077 O GLY B 13 -25.017 -30.934 -37.158 1.00 24.47
ANISOU 3077 O GLY B 13 4396 2143 2760 -175 154 568
ATOM 3078 H GLY B 13 -22.669 -31.625 -39.059 1.00 31.09
ATOM 3079 HA2 GLY B 13 -23.331 -33.584 -37.396 1.00 32.07
ATOM 3080 HA3 GLY B 13 -22.605 -32.243 -36.997 1.00 32.07
ATOM 3081 N GLY B 14 -25.342 -32.937 -36.173 1.00 31.03
                                                                              Ν
ANISOU 3081 N GLY B 14 5497 2711 3584 -229 234 779
ATOM 3082 CA GLY B 14 -26.527 -32.518 -35.449 1.00 32.00
ANISOU 3082 CA GLY B 14 5599 2948 3610 -350 345 833
ATOM 3083 C GLY B 14 -27.618 -32.006 -36.372 1.00 29.52
ANISOU 3083 C GLY B 14 5121 2722 3374 -494 413 711 C ATOM 3084 O GLY B 14 -27.803 -32.483 -37.498 1.00 30.71 O
ANISOU 3084 O GLY B 14 5232 2772 3664 -563 403 622 O
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ATOM 3085 H GLY B 14 -25.145 -33.768 -36.070 1.00 37.24
                                                                         H
ATOM 3086 HA2 GLY B 14 -26.878 -33.268 -34.943 1.00 38.40
ATOM 3087 HA3 GLY B 14 -26.292 -31.811 -34.828 1.00 38.40
                             -28.343 -30.997 -35.887 1.00 25.58
ATOM 3088 N ILE B 15
ANISOU 3088 N ILE B 15
                             4534 2417 2770 -518 470 697
ATOM 3089 CA ILE B 15
                               -29.510 -30.439 -36.561 1.00 24.01
ANISOU 3089 CA ILE B 15 4171 2332 2621 -640 542
                                                                  603
ATOM 3090 C ILE B 15 -29.281 -28.950 -36.788 1.00 21.93
ANISOU 3090 C ILE B 15 3798 2242 2294 -538
                                                          474 476
ATOM 3091 O ILE B 15
                              -28.949 -28.226 -35.844 1.00 21.95
ANISOU 3091 O ILE B 15
                              3848 2340 2153 -430 444 502
ATOM 3092 CB ILE B 15
                                                                         CCCC
                               -30.788 -30.640 -35.725 1.00 25.80
ANISOU 3092 CB ILE B 15 4381 2637 2785 -759 702 725
ATOM 3093 CG1 ILE B 15 -31.014 -32.120 -35.363 1.00 29.38
ANISOU 3093 CG1 ILE B 15 4957 2896 3308 -881 772 892
ATOM 3094 CG2 ILE B 15 -31.991 -30.018 -36.451 1.00 25.22
ANISOU 3094 CG2 ILE B 15 4104 2703 2774 -868 763 624
ATOM 3095 CD1 ILE B 15
                                -31.595 -32.964 -36.478 1.00 30.74
ANISOU 3095 CD1 ILE B 15 5074 2914 3692 -1062 765 839 C
ATOM 3096 H ILE B 15 -28.168 -30.607 -35.141 1.00 30.70 H
                               -30.669 -30.154 -34.894 1.00 30.96 H
ATOM 3097 HA ILE B 15 -29.630 -30.871 -37.422 1.00 28.82
ATOM 3098 HB ILE B 15
ATOM 3099 HG12 ILE B 15 -30.162 -32.510 -35.113 1.00 35.25
ATOM 3100 HG13 ILE B 15 -31.626 -32.164 -34.612 1.00 35.25
ATOM 3101 HG21 ILE B 15 -32.787 -30.151 -35.914 1.00 30.26
ATOM 3102 HG22 ILE B 15 -31.829 -29.069 -36.574 1.00 30.26
                                -32.097 -30.450 -37.313 1.00 30.26
-31.701 -33.874 -36.162 1.00 36.89
-32.456 -32.599 -36.734 1.00 36.89
ATOM 3103 HG23 ILE B 15
                                                                           Н
ATOM 3104 HD11 ILE B 15
ATOM 3105 HD12 ILE B 15
                                -30.989 -32.945 -37.236 1.00 36.89
ATOM 3106 HD13 ILE B 15
ATOM 3107 N VAL B 16
                               -29.498 -28.481 -38.021 1.00 20.61
                                                                        Ν
ANISOU 3107 N VAL B 16 3498 2109 2225 -572 443 340
ATOM 3108 CA VAL B 16 -29.472 -27.049 -38.336 1.00 19.62
ANISOU 3108 CA VAL B 16 3265 2133 2058 -501 388
ATOM 3109 C VAL B 16
                                                                         C
                               -30.699 -26.762 -39.191 1.00 20.43
ANISOU 3109 C VAL B 16
                              3222 2317 2221 -604 450 145
ATOM 3110 O VAL B 16
                                                                         Ö
                               -30.690 -26.994 -40.406 1.00 19.68
ANISOU 3110 O VAL B 16
                              3070 2173 2234 -644 413 62
ATOM 3111 CB VAL B 16 -28.187 -26.615 -39.047 1.00 18.05
ANISOU 3111 CB VAL B 16 3048 1898 1912 -399 260 168
ATOM 3112 CG1 VAL B 16 -28.252 -25.124 -39.421 1.00 16.59
ANISOU 3112 CG1 VAL B 16 2757 1842 1704 -352 204 73
                                 -26.987 -26.876 -38.167 1.00 18.72
ATOM 3113 CG2 VAL B 16
ANISOU 3113 CG2 VAL B 16 3246 1920 1948 -294
                                                            180 255
ATOM 3114 H VAL B 16 -29.666 -28.980 -38.701 1.00 24.74
                                                                         Н
ATOM 3115 HA VAL B 16 -29.549 -26.540 -37.514 1.00 23.55
                                                                        Н
ATOM 3116 HB VAL B 16 -28.084 -27.129 -39.863 1.00 21.66
                                                                         Н
ATOM 3116 HB VAL B 16 -28.084 -27.129 -39.863 1.00 21.66 H
ATOM 3117 HG11 VAL B 16 -27.429 -24.875 -39.869 1.00 19.91 H
ATOM 3118 HG12 VAL B 16 -29.008 -24.980 -40.012 1.00 19.91 H
ATOM 3119 HG13 VAL B 16 -28.361 -24.600 -38.612 1.00 19.91 H
ATOM 3120 HG21 VAL B 16 -26.185 -26.595 -38.635 1.00 22.47 H
ATOM 3121 HG22 VAL B 16 -27.083 -26.371 -37.344 1.00 22.47 H
ATOM 3122 HG23 VAL B 16 -26.940 -27.824 -37.970 1.00 22.47 H
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ATOM 3123 N ASN B 17 -31.754 -26.243 -38.563 1.00 22.49
ANISOU 3123 N ASN B 17 3423 2718 2402 -628 539
                                                       164
ATOM 3124 CA ASN B 17
                          -33.009 -25.913 -39.240 1.00 24.88
ANISOU 3124 CA ASN B 17 3563 3131 2759 -714 596
ATOM 3125 C ASN B 17
                          -32.998 -24.427 -39.571 1.00 21.88
ANISOU 3125 C ASN B 17
                          3112 2878 2325 -598 532 -17
                                                             0
ATOM 3126 O ASN B 17
                          -33.201 -23.583 -38.697 1.00 20.40
ANISOU 3126 O ASN B 17
                         2943 2798 2010 -501 555 -10
ATOM 3127 CB ASN B 17
                           -34.207 -26.270 -38.367 1.00 32.14
ANISOU 3127 CB ASN B 17 4431 4145 3635 -800 750
                                                       201
ATOM 3128 CG ASN B 17
                           -35.516 -25.827 -38.982 1.00 37.98
ANISOU 3128 CG ASN B 17 4967 5032 4432 -871 802 135
ATOM 3129 OD1 ASN B 17 -35.697 -25.908 -40.198 1.00 39.72
                           5102 5216 4773 -935
ANISOU 3129 OD1 ASN B 17
ATOM 3130 ND2 ASN B 17
                           -36.427 -25.328 -38.154 1.00 41.10
ANISOU 3130 ND2 ASN B 17 5282 5607 4726 -836 926 188
                                                              Ν
ATOM 3131 H ASN B 17 -31.767 -26.068 -37.721 1.00 26.98
                                                            Н
ATOM 3132 HA ASN B 17
                           -33.072 -26.414 -40.068 1.00 29.86
                                                            Н
ATOM 3133 HB2 ASN B 17 -34.239 -27.232 -38.249 1.00 38.57 ATOM 3134 HB3 ASN B 17 -34.114 -25.832 -37.506 1.00 38.57
                                                              Н
ATOM 3135 HD21 ASN B 17 -37.187 -25.063 -38.458 1.00 49.32 ATOM 3136 HD22 ASN B 17 -36.257 -25.269 -37.313 1.00 49.32
ATOM 3137 N ALA B 18 -32.760 -24.110 -40.837 1.00 20.61
ANISOU 3137 N ALA B 18
                         2887 2696 2250 -595 449 -117
ATOM 3138 CA ALA B 18 -32.645 -22.733 -41.295 1.00 20.20
ANISOU 3138 CA ALA B 18 2780 2728 2166 -493 376 -206
ATOM 3139 C ALA B 18 -33.821 -22.394 -42.200 1.00 20.53
ANISOU 3139 C ALA B 18 2672 2874 2253 -537 398 -286
ATOM 3140 O ALA B 18
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                          -34.208 -23.198 -43.057 1.00 20.53
ANISOU 3140 O ALA B 18 2617 2836 2346 -639 401 -313
ATOM 3141 CB ALA B 18 -31.331 -22.512 -42.049 1.00 18.02
ANISOU 3141 CB ALA B 18 2545 2361 1941 -436 265 -230
                          -32.660 -24.689 -41.465 1.00 24.74 H
ATOM 3142 H ALA B 18
ATOM 3143 HA ALA B 18
ATOM 3144 HB1 ALA B 18
                                                            Н
                         -32.663 -22.136 -40.530 1.00 24.24
                          -31.285 -21.588 -42.340 1.00 21.62
ATOM 3145 HB2 ALA B 18 -30.589 -22.710 -41.456 1.00 21.62
ATOM 3146 HB3 ALA B 18 -31.306 -23.103 -42.819 1.00 21.62
ATOM 3147 N VAL B 19 -34.366 -21.191 -42.028 1.00 18.43
                                                             Ν
ANISOU 3147 N VAL B 19
                         2351 2732 1921 -446 394 -334
                                                             N
ATOM 3148 CA VAL B 19
                         -35.515 -20.727 -42.799 1.00 18.06
ANISOU 3148 CA VAL B 19 2151 2806 1903 -455 404 -407
ATOM 3149 C VAL B 19 -35.092 -19.490 -43.583 1.00 16.65
ANISOU 3149 C VAL B 19 1978 2633 1715 -342 296 -480
                                                             C
                                                             Ŏ
ATOM 3150 O VAL B 19 -34.642 -18.500 -42.993 1.00 16.07
ANISOU 3150 O VAL B 19 1981 2553 1572 -230 251 -483
ATOM 3151 CB VAL B 19 -36.720 -20.426 -41.893 1.00 20.37
ANISOU 3151 CB VAL B 19 2356 3258 2125 -427 517 -383
ATOM 3152 CG1 VAL B 19 -37.906 -19.915 -42.707 1.00 21.04
ANISOU 3152 CG1 VAL B 19 2258 3485 2251 -419 514 -457
ATOM 3153 CG2 VAL B 19 -37.107 -21.676 -41.099 1.00 21.31
ANISOU 3153 CG2 VAL B 19 2467 3370 2260 -556 641 -271
ATOM 3154 H VAL B 19 -34.081 -20.614 -41.457 1.00 22.12
                                                             Н
ATOM 3155 HA VAL B 19 -35.775 -21.414 -43.432 1.00 21.67
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ATOM 3156 HB VAL B 19 -36.472 -19.734 -41.260 1.00 24.44
                                                              Н
ATOM 3157 HG11 VAL B 19
                          -38.647 -19.735 -42.107 1.00 25.25
                                                              Н
                           -37.647 -19.100 -43.166 1.00 25.25
ATOM 3158 HG12 VAL B 19
                                                               Н
ATOM 3159 HG13 VAL B 19
                           -38.160 -20.592 -43.353 1.00 25.25
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ATOM 3160 HG21 VAL B 19
                           -37.868 -21.467 -40.534 1.00 25.57
                                                               Н
ATOM 3161 HG22 VAL B 19
                           -37.340 -22.384 -41.719 1.00 25.57
                                                               Н
ATOM 3162 HG23 VAL B 19
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ATOM 3163 N ASN B 20
                          -35.219 -19.558 -44.908 1.00 15.88
ANISOU 3163 N ASN B 20
                           1815 2535 1684 -371 244 -535
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ATOM 3164 CA ASN B 20
                           -34.982 -18.414 -45.789 1.00 14.94
ANISOU 3164 CA ASN B 20
                          1689 2432 1556 -271
                                                  155 -583
ATOM 3165 C ASN B 20
                          -36.238 -17.553 -45.753 1.00 15.61
ANISOU 3165 C ASN B 20
                          1668 2660 1602 -199
                                                 166 -635
ATOM 3166 O ASN B 20
                          -37.228 -17.849 -46.418 1.00 15.70
ANISOU 3166 O ASN B 20
                         1552 2763 1649 -242 174 -680
                           -34.656 -18.882 -47.204 1.00 16.28
ATOM 3167 CB ASN B 20
ANISOU 3167 CB ASN B 20
                          1844 2564 1777 -305
                                                 107 -613
                                                              Č
ATOM 3168 CG ASN B 20
                           -34.533 -17.740 -48.193 1.00 16.17
ANISOU 3168 CG ASN B 20
                           1818 2583 1741 -203
                                                   33 -638
                                                              0
ATOM 3169 OD1 ASN B 20
                           -34.821 -16.587 -47.885 1.00 16.28
ANISOU 3169 OD1 ASN B 20
                           1828 2638 1721 -116
                                                              0
                                                   5 -643
ATOM 3170 ND2 ASN B 20
                           -34.103 -18.071 -49.406 1.00 17.47
                                                             Ν
ANISOU 3170 ND2 ASN B 20
                           1995 2727 1918 -201 1 -651
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ATOM 3171 H ASN B 20
                          -35.447 -20.272 -45.330 1.00 19.06
                                                             Н
ATOM 3172 HA ASN B 20
                           -34.236 -17.891 -45.454 1.00 17.93
                                                             Н
ATOM 3173 HB2 ASN B 20
                           -33.811 -19.359 -47.191 1.00 19.53
ATOM 3174 HB3 ASN B 20
                           -35.363 -19.470 -47.512 1.00 19.53
ATOM 3175 HD21 ASN B 20
                           -34.013 -17.466 -50.011 1.00 20.97
ATOM 3176 HD22 ASN B 20
                           -33.915 -18.891 -49.587 1.00 20.97
ATOM 3177 N GLY B 21
                          -36.210 -16.484 -44.960 1.00 16.15
ANISOU 3177 N GLY B 21
                           1658 2341 2139 -752 199 -283
ATOM 3178 CA GLY B 21
                           -37.388 -15.682 -44.710 1.00 16.71
ANISOU 3178 CA GLY B 21
                           1621 2501 2229 -740 204 -301
ATOM 3179 C GLY B 21
ANISOU 3179 C GLY B 21
                          -37.606 -14.611 -45.765 1.00 16.88
                          1572 2599 2242 -668 126 -312
                                                             C
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ATOM 3180 O GLY B 21
                          -36.911 -14.529 -46.780 1.00 16.58
ANISOU 3180 O GLY B 21
                          1567 2556 2178 -638
                                                             0
                                                  68 -308
ATOM 3181 H GLY B 21
                          -35.506 -16.205 -44.552 1.00 19.38
ATOM 3182 HA2 GLY B 21
                          -38.170 -16.255 -44.690 1.00 20.06
ATOM 3183 HA3 GLY B 21
                           -37.304 -15.248 -43.846 1.00 20.06
ATOM 3184 N SER B 22
                          -38.593 -13.766 -45.503 1.00 19.97
                                                             Ν
ANISOU 3184 N SER B 22
                           1866 3065 2657 -635 127 -321
                                                             Ν
ATOM 3185 CA SER B 22
                           -38.921 -12.689 -46.428 1.00 21.52
                                                              C
                                                             C
ANISOU 3185 CA SER B 22
                           1991 3333 2852 -555
                                                  52 -320
                                                             C
ATOM 3186 C SER B 22
ANISOU 3186 C SER B 22
                          -37.809 -11.646 -46.460 1.00 20.76
                                                             000
                          1970 3188 2730 -459
                                                  26 -266
ATOM 3187 O SER B 22
                          -37.299 -11.231 -45.415 1.00 19.25
ANISOU 3187 O SER B 22
                         1831 2943 2539 -431
                                                  72 -241
ATOM 3188 CB SER B 22 -40.241 -12.042 -46.026 1.00 24.38
ANISOU 3188 CB SER B 22 2228 3779 3257 -533 67 -343
ATOM 3189 OG SER B 22 -40.552 -10.981 -46.902 1.00 27.03
ANISOU 3189 OG SER B 22 2498 4176 3595 -443 -9 -331
                                                             0
ATOM 3190 H SER B 22 -39.087 -13.793 -44.799 1.00 23.96
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ATOM 3191 HA SER B 22 -39.021 -13.055 -47.321 1.00 25.82 Н ATOM 3192 HB2 SER B 22 -40.946 -12.706 -46.069 1.00 29.26 Н ATOM 3193 HB3 SER B 22 -40.163 -11.696 -45.123 1.00 29.26 ATOM 3194 HG SER B 22 -41.280 -10.627 -46.677 1.00 32.43 Н ATOM 3195 N GLY B 23 -37.441 -11.222 -47.667 1.00 20.20 Ν ANISOU 3195 N GLY B 23 1903 3140 2633 -415 -46 -250 Ν ATOM 3196 CA GLY B 23 -36.446 -10.174 -47.835 1.00 19.73 C ANISOU 3196 CA GLY B 23 1904 3036 2555 -331 -71 -197 C ATOM 3197 C GLY B 23 -35.092 -10.578 -47.282 1.00 17.99 C **ANISOU 3197 C GLY B 23** 1798 2725 2314 -347 -35 -177 0 ATOM 3198 O GLY B 23 -34.478 -11.561 -47.723 1.00 17.48 **ANISOU 3198 O GLY B 23** 1785 2633 2225 -396 -37 -189 0 ATOM 3199 H GLY B 23 -37.756 -11.528 -48.406 1.00 24.24 ATOM 3200 HA2 GLY B 23 -36.345 -9.971 -48.778 1.00 23.67 Н ATOM 3201 HA3 GLY B 23 -36.739 -9.372 -47.376 1.00 23.67 ATOM 3202 N GLY B 24 -34.609 -9.802 -46.312 1.00 17.47 Ν ANISOU 3202 N GLY B 24 1768 2611 2258 -302 -3 -152 ATOM 3203 CA GLY B 24 -33.355 -10.059 -45.639 1.00 16.02 ANISOU 3203 CA GLY B 24 1679 2352 2054 -309 26 -134 ATOM 3204 C GLY B 24 -33.476 -10.836 -44.344 1.00 14.88 ANISOU 3204 C GLY B 24 1561 2182 1911 -359 89 -145 0 ATOM 3205 O GLY B 24 -32.493 -10.922 -43.598 1.00 14.23 **ANISOU 3205 O GLY B 24** 1551 2046 1809 -353 109 -125 0 ATOM 3206 H GLY B 24 -35.011 -9.098 -46.023 1.00 20.96 Н ATOM 3207 HA2 GLY B 24 -32.775 -10.559 -46.234 1.00 19.22 Н ATOM 3208 HA3 GLY B 24 -32.925 -9.213 -45.441 1.00 19.22 Н ATOM 3209 N ASN B 25 -34.635 -11.426 -44.063 1.00 15.22 Ν ANISOU 3209 N ASN B 25 1545 2264 1972 -411 120 -174 -34.880 -12.116 -42.804 1.00 14.68 **ATOM 3210 CA ASN B 25** ANISOU 3210 CA ASN B 25 1500 2177 1901 -463 190 -176 -34.586 -13.605 -42.929 1.00 14.78 ATOM 3211 C ASN B 25 **ANISOU 3211 C ASN B 25** 1565 2145 1906 -539 207 -175 ATOM 3212 O ASN B 25 -34.800 -14.216 -43.982 1.00 14.79 ANISOU 3212 O ASN B 25 1544 2156 1919 -574 176 -200 -36.330 -11.919 -42.357 1.00 16.91 ATOM 3213 CB ASN B 25 ANISOU 3213 CB ASN B 25 1684 2527 2212 -483 229 -209 ATOM 3214 CG ASN B 25 -36.668 -12.716 -41.104 1.00 18.44 ANISOU 3214 CG ASN B 25 1903 2709 2396 -551 312 -207 ATOM 3215 OD1 ASN B 25 -37.347 -13.744 -41.165 1.00 19.86 **ANISOU 3215 OD1 ASN B 25** 2057 2898 2593 -633 343 -224 ATOM 3216 ND2 ASN B 25 -36.186 -12.246 -39.961 1.00 17.55 **ANISOU 3216 ND2 ASN B 25** 1841 2575 2251 -520 349 -188 Ν ATOM 3217 H ASN B 25 -35.307 -11.440 -44.598 1.00 18.26 Н ATOM 3218 HA ASN B 25 Н -34.299 -11.749 -42.120 1.00 17.62 Н ATOM 3219 HB2 ASN B 25 -36.477 -10.980 -42.164 1.00 20.29 ATOM 3220 HB3 ASN B 25 -36.923 -12.210 -43.067 1.00 20.29 ATOM 3221 HD21 ASN B 25 -36.348 -12.659 -39.224 1.00 21.06 Н ATOM 3222 HD22 ASN B 25 -35.712 -11.528 -39.956 1.00 21.06 -34.090 -14.182 -41.835 1.00 14.88 ATOM 3223 N TYR B 26 Ν 1651 2106 1898 -562 255 -147 ANISOU 3223 N TYR B 26 ATOM 3224 CA TYR B 26 -33.873 -15.615 -41.738 1.00 14.99 ANISOU 3224 CA TYR B 26 1722 2060 1914 -631 284 -136 C ATOM 3225 C TYR B 26 -33.923 -16.017 -40.275 1.00 15.42

ANISOU 3225 C TYR B 26 1826 2090 1945 -659 353 -99 ATOM 3226 O TYR B 26 -33.826 -15.176 -39.376 1.00 16.64 ANISOU 3226 O TYR B 26 1984 2272 2068 -617 369 -86 0 ATOM 3227 CB TYR B 26 -32.534 -16.030 -42.358 1.00 14.37 ANISOU 3227 CB TYR B 26 1719 1916 1824 -603 243 -118 ATOM 3228 CG TYR B 26 -31.303 -15.607 -41.581 1.00 14.05 ANISOU 3228 CG TYR B 26 1750 1841 1749 -542 236 -74 C ATOM 3229 CD1 TYR B 26 -30.732 -16.445 -40.630 1.00 14.41 ANISOU 3229 CD1 TYR B 26 1873 1827 1774 -556 269 -31 ATOM 3230 CD2 TYR B 26 -30.706 -14.372 -41.800 1.00 14.23 ANISOU 3230 CD2 TYR B 26 1760 1889 1759 -471 195 -73 ATOM 3231 CE1 TYR B 26 -29.601 -16.066 -39.924 1.00 14.10 ANISOU 3231 CE1 TYR B 26 1888 1770 1698 -499 253 6 ATOM 3232 CE2 TYR B 26 -29.574 -13.985 -41.094 1.00 13.99 ANISOU 3232 CE2 TYR B 26 1784 1832 1698 -425 186 -43 C ATOM 3233 CZ TYR B 26 -29.026 -14.840 -40.160 1.00 14.60 ANISOU 3233 CZ TYR B 26 1930 1866 1752 -438 211 -6 ATOM 3234 OH TYR B 26 -27.899 -14.469 -39.452 1.00 14.80 0 ANISOU 3234 OH TYR B 26 2001 1880 1743 -391 192 20 O ATOM 3235 H TYR B 26 -33.868 -13.752 -41.124 1.00 17.86 H ATOM 3236 HA TYR B 26 -34.583 -16.080 -42.207 1.00 17.99 ATOM 3237 HB2 TYR B 26 -32.515 -16.997 -42.431 1.00 17.24 ATOM 3238 HB3 TYR B 26 -32.470 -15.637 -43.243 1.00 17.24 ATOM 3239 HD1 TYR B 26 -31.112 -17.278 -40.468 1.00 17.29 ATOM 3240 HD2 TYR B 26 -31.070 -13.795 -42.432 1.00 17.08 ATOM 3241 HE1 TYR B 26 -29.232 -16.641 -39.293 1.00 16.91 ATOM 3244 N SER B 27 -34.080 -17.318 -40.042 1.00 16.01 N ANISOU 3244 N SER B 27 1942 2110 2030 -733 396 -84 N ATOM 3245 CA SER B 27 -34.020 -17.853 -38 693 1 00 45 60 ANISOU 3245 CA SER B 27 ANISOU 3245 CA SER B 27 -34.020 -17.853 -38 693 1 00 45 60 ANISOU 3245 CA SER B 27 -34.020 -17.853 -38 60 ANISOU 3245 CA SER B 27 -34.020 -17.853 -38 60 ANISOU 3245 CA SER B 27 -34.020 -17.853 -38 60 ANISOU 3245 CA SER B 27 -34.020 -17.853 -38 60 ANISOU 3245 CA SER B 27 -34.020 -17.853 -38 60 ANISOU 3245 CA SER B 27 -34.020 -17.853 -38 60 ANISOU 3245 CA SER B 27 -34.020 -17.853 -38 60 ANISOU 3245 CA SER B 27 -34.020 -17.853 -38 60 ANISOU 3245 CA SER B 27 -34.020 -17.853 -38 60 ANISOU 3245 CA Н Н ANISOU 3245 CA SER B 27 1916 1987 1906 -762 462 -32 C ATOM 3246 C SER B 27 -33.280 -19.182 -38.728 1.00 16.14 ANISOU 3246 C SER B 27 2119 1990 2022 -791 469 9 ATOM 3247 O SER B 27 -33.176 -19.835 -39.772 1.00 15.27 0 ANISOU 3247 O SER B 27 2008 1837 1955 -816 443 -21 O ATOM 3248 CB SER B 27 -35.424 -18.017 -38.085 1.00 17.60 C ANISOU 3248 CB SER B 27 2146 2331 2211 -838 538 -49 ATOM 3249 OG SER B 27 -36.234 -18.879 -38.854 1.00 19.83 ANISOU 3249 OG SER B 27 2382 2602 2551 -923 552 -87 O ATOM 3250 H SER B 27 -34.223 -17.908 -40.651 1.00 19.21 H ATOM 3251 HA SER B 27 -33.518 -17.243 -38.131 1.00 18.35 ATOM 3252 HB2 SER B 27 -35.336 -18.386 -37.192 1.00 21.13 ATOM 3253 HB3 SER B 27 -35.848 -17.146 -38.041 1.00 21.13 ATOM 3254 HG SER B 27 -36.993 -18.951 -38.501 1.00 23.80 ATOM 3255 N VAL B 28 -32.751 -19.567 -37.570 1.00 16.52 Ν ANISOU 3255 N VAL B 28 2252 1998 2025 -783 503 78 ATOM 3256 CA VAL B 28 -32.013 -20.812 -37.417 1.00 16.87 ANISOU 3256 CA VAL B 28 2396 1935 2078 -796 513 134 C C ATOM 3257 C VAL B 28 -32.346 -21.389 -36.050 1.00 17.47 ANISOU 3257 C VAL B 28 2533 1992 2112 -840 588 206 ATOM 3258 O VAL B 28 -32.339 -20.667 -35.047 1.00 17.00 0 ANISOU 3258 O VAL B 28 2478 1998 1984 -811 603 232

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ATOM 3259 CB VAL B 28 -30.487 -20.630 -37.531 1.00 16.72
ANISOU 3259 CB VAL B 28 2435 1881 2036 -701 446 163 ATOM 3260 CG1 VAL B 28 -29.827 -21.983 -37.849 1.00 17.56
ANISOU 3260 CG1 VAL B 28 2621 1868 2182 -708 447 195
ATOM 3261 CG2 VAL B 28
                                -30.110 -19.563 -38.561 1.00 18.29
ANISOU 3261 CG2 VAL B 28 2569 2133 2245 -643 378 102
ATOM 3262 H VAL B 28
                               -32.808 -19.111 -36.843 1.00 19.82
                                                                         Н
ATOM 3263 HA VAL B 28
                              -32.299 -21.443 -38.096 1.00 20.24
                                                                        Н
ATOM 3264 HB VAL B 28
                                -30.148 -20.336 -36.671 1.00 20.06
                                                                         Н
                                                                        Н
ATOM 3265 HG11 VAL B 28 -28.868 -21.857 -37.918 1.00 21.07
ATOM 3266 HG12 VAL B 28
                                -30.029 -22.607 -37.134 1.00 21.07
ATOM 3267 HG13 VAL B 28
                               -30.180 -22.316 -38.689 1.00 21.07
                                                                          Н
ATOM 3268 HG21 VAL B 28 -29.144 -19.486 -38.596 1.00 21.94
ATOM 3269 HG22 VAL B 28 -30.453 -19.829 -39.429 1.00 21.94
ATOM 3270 HG23 VAL B 28 -30.501 -18.716 -38.295 1.00 21.94
ATOM 3271 N ASN B 29 -32.634 -22.681 -36.015 1.00 19.08
ANISOU 3271 N ASN B 29
                              2789 2106 2356 -914 639 238
                                                                         Ν
ATOM 3272 CA ASN B 29 -32.722 -23.458 -34.784 1.00 21.74
ANISOU 3272 CA ASN B 29 3202 2403 2656 -932 694 326
ATOM 3273 C ASN B 29
                               -31.761 -24.622 -34.952 1.00 22.28
ANISOU 3273 C ASN B 29
                              3368 2341 2758 -903 672 383
ATOM 3274 O ASN B 29
                                                                         0
                               -31.901 -25.401 -35.901 1.00 21.62
ANISOU 3274 O ASN B 29 3275 2185 2756 -935 665 340
ATOM 3275 CB ASN B 29 -34.143 -23.970 -34.539 1.00 25.57
                                                                         C
ANISOU 3275 CB ASN B 29 3630 2909 3176 -1015 759 307
ATOM 3276 CG ASN B 29
                                -35.149 -22.851 -34.330 1.00 28.31
ANISOU 3276 CG ASN B 29
                               3872 3386 3499 -1034 784 249
ATOM 3277 OD1 ASN B 29
                                -34.940 -21.951 -33.519 1.00 29.60
ANISOU 3277 OD1 ASN B 29
                                4040 3620 3586 -994 792 268
                                 -36.262 -22.915 -35.057 1.00 29.66
ATOM 3278 ND2 ASN B 29
ANISOU 3278 ND2 ASN B 29 3945 3590 3735 -1092 795 174 N
                               -32.790 -23.150 -36.720 1.00 22.90 H
ATOM 3279 H ASN B 29
ATOM 3280 HA ASN B 29 -32.442 -22.920 -34.028 1.00 26.09
ATOM 3281 HB2 ASN B 29 -34.428 -24.489 -35.308 1.00 30.68
ATOM 3282 HB3 ASN B 29 -34.145 -24.527 -33.745 1.00 30.68
ATOM 3283 HD21 ASN B 29 -36.864 -22.306 -34.976 1.00 35.59
ATOM 3284 HD22 ASN B 29 -36.379 -23.565 -35.608 1.00 35.59
                               -36.379 -23.565 -35.608 1.00 35.59
ATOM 3285 N TRP B 30 -30.781 -24.737 -34.055 1.00 22.17
                              3442 2300 2680 -837 657 474
ANISOU 3285 N TRP B 30
                                                                         Ν
ATOM 3286 CA TRP B 30
                              -29.729 -25.727 -34.224 1.00 22.50
ANISOU 3286 CA TRP B 30 3571 2222 2756 -786
                                                           625
                                                                 528
ATOM 3287 C TRP B 30 -29.474 -26.467 -32.917 1.00 23.08
ANISOU 3287 C TRP B 30 3726 2262 2780 -761 647 647
                               -29.474 -26.467 -32.917 1.00 23.08
                                                                         Č
                                                                         ŏ
ATOM 3288 O TRP B 30 -29.791 -25.979 -31.827 1.00 23.64
ANISOU 3288 O TRP B 30 3799 2418 2764 -764 672 688
ATOM 3289 CB TRP B 30 -28.438 -25.072 -34.755 1.00 21.68
ANISOU 3292 CD2 TRP B 30

ANISOU 3292 CD2 TRP B 30

-28.438 -25.072 -34.755 1.00 21.68

3474 2125 2637 -691 546 511

C 3474 2125 2637 -691 546 511

-27.686 -24.164 -33.809 1.00 21.75

3492 2224 2546 -608 500 554

C -26.604 -24.502 -33.041 1.00 22.15

C ANISOU 3291 CD1 TRP B 30

ANISOU 3292 CD2 TRP B 30

-27.929 -22.766 -33.560 1.00 20.52

C 3262 2202 2234 502 460 502
ANISOU 3292 CD2 TRP B 30 3263 2202 2331 -593 480 502
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ATOM 3293 NE1 TRP B 30 -26.169 -23.410 -32.329 1.00 22.27 ANISOU 3293 NE1 TRP B 30 3612 2376 2471 -477 421 642 ATOM 3294 CE2 TRP B 30 -26.961 -22.334 -32.630 1.00 20.55 ANISOU 3294 CE2 TRP B 30 3306 2251 2250 -515 434 554 ATOM 3295 CE3 TRP B 30 -28.868 -21.842 -34.033 1.00 18.93 **ANISOU 3295 CE3 TRP B 30** 2965 2082 2145 -634 495 415 -26.914 -21.020 -32.154 1.00 19.33 ATOM 3296 CZ2 TRP B 30 **ANISOU 3296 CZ2 TRP B 30** 3103 2214 2028 -487 410 514 ATOM 3297 CZ3 TRP B 30 -28.812 -20.534 -33.564 1.00 18.84 **ANISOU 3297 CZ3 TRP B 30** 2907 2178 2071 -595 472 383 ATOM 3298 CH2 TRP B 30 -27.843 -20.141 -32.632 1.00 18.63 ANISOU 3298 CH2 TRP B 30 2928 2188 1964 -527 433 429 C -30.706 -24.255 -33.346 1.00 26.60 Н ATOM 3299 H TRP B 30 **ATOM 3300 HA TRPB 30** -30.020 -26.380 -34.880 1.00 27.00 Н ATOM 3301 HB2 TRP B 30 -27.828 -25.779 -35.018 1.00 26.01 ATOM 3301 HB2 IRP B 30 -27.828 -23.779 -35.018 1.00 26.01 H
ATOM 3302 HB3 TRP B 30 -28.668 -24.543 -35.536 1.00 26.01 H
ATOM 3303 HD1 TRP B 30 -26.219 -25.347 -33.006 1.00 26.58 H
ATOM 3304 HE1 TRP B 30 -25.507 -23.404 -31.780 1.00 26.72 H
ATOM 3305 HE3 TRP B 30 -29.514 -22.097 -34.651 1.00 22.71 H
ATOM 3306 HZ2 TRP B 30 -26.270 -20.754 -31.538 1.00 23.20 H ATOM 3307 HZ3 TRP B 30 -29.433 -19.912 -33.868 1.00 22.60 ATOM 3308 HH2 TRP B 30 -27.831 -19.260 -32.333 1.00 22.36 -29.433 -19.912 -33.868 1.00 22.60 ATOM 3309 N SER B 31 -28.908 -27.671 -33.042 1.00 22.58 ANISOU 3309 N SER B 31 3731 2075 2775 -735 637 698 ANISOU 3309 N SER B 31 3731 2075 2775 -735 637 698 ATOM 3310 CA SER B 31 -28.716 -28.529 -31.880 1.00 24.21 ANISOU 3310 CA SER B 31 4014 2238 2948 -716 656 818 818 ATOM 3311 C SER B 31 -27.577 -29.516 -32.119 1.00 26.18 ANISOU 3311 C SER B 31 4337 2360 3252 -639 612 873 ATOM 3312 O SER B 31 -27.534 -30.179 -33.160 1.00 25.22 0 ANISOU 3312 O SER B 31 4209 2141 3232 -655 611 816 ATOM 3313 CB SER B 31 -30.007 -29.288 -31.564 1.00 25.08 ANISOU 3313 CB SER B 31 4110 2325 3094 -820 735 828 ATOM 3314 OG SER B 31 -29.783 -30.246 -30.548 1.00 28.39 ANISOU 3314 OG SER B 31 4611 2684 3492 -805 754 952 ATOM 3315 H SER B 31 -28.631 -28.008 -33.783 1.00 27.10 Н ATOM 3316 HA SER B 31 ATOM 3316 HA SER B 31 -28.489 -27.982 -31.112 1.00 29.06 ATOM 3317 HB2 SER B 31 -30.679 -28.657 -31.263 1.00 30.10 Н ATOM 3318 HB3 SER B 31 -30.311 -29.742 -32.366 1.00 30.10 Н ATOM 3319 HG SER B 31 -29.201 -30.798 -30.796 1.00 34.07 Н ATOM 3320 N ASN B 32 -26.675 -29.626 -31.141 1.00 28.71 Ν ANISOU 3320 N ASN B 32 4719 2688 3503 -555 575 980 ATOM 3321 CA ASN B 32 -25.597 -30.619 -31.169 1.00 31.02 ANISOU 3321 CA ASN B 32 5077 2864 3844 -471 531 1049 ATOM 3322 C ASN B 32 -24.894 -30.625 -32.524 1.00 29.79 ANISOU 3322 C ASN B 32 4900 2641 3776 -427 491 960 0 ATOM 3323 O ASN B 32 -24.600 -31.674 -33.098 1.00 30.75 **ANISOU 3323 O ASN B 32** 5051 2635 3997 -412 492 955 ATOM 3324 CB ASN B 32 -26.136 -32.001 -30.822 1.00 34.46 ANISOU 3324 CB ASN B 32 5564 3187 4342 -524 582 1117 ATOM 3325 CG ASN B 32 -26.741 -32.054 -29.439 1.00 36.91 ANISOU 3325 CG ASN B 32 5901 3562 4559 -562 623 121 ATOM 3326 OD1 ASN B 32 -26.434 -31.224 -28.582 1.00 36.94 623 1217 ANISOU 3326 OD1 ASN B 32 5903 3686 4446 -520 597 1258 O

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ATOM 3327 ND2 ASN B 32 -27.606 -33.033 -29.210 1.00 39.01
  ANISOU 3327 ND2 ASN B 32 6192 3754 4875 -646 689 1254 N
 ANISOU 3327 ND2 ASN B 32 6192 3754 4875 -646 689 1254 N
ATOM 3328 H ASN B 32 -26.666 -29.129 -30.439 1.00 34.46 H
ATOM 3329 HA ASN B 32 -24.939 -30.382 -30.497 1.00 37.22 H
ATOM 3330 HB2 ASN B 32 -26.824 -32.243 -31.461 1.00 41.35 H
ATOM 3331 HB3 ASN B 32 -25.409 -32.643 -30.857 1.00 41.35 H
ATOM 3332 HD21 ASN B 32 -27.978 -33.106 -28.438 1.00 46.81 H
ATOM 3333 HD22 ASN B 32 -27.794 -33.595 -29.833 1.00 46.81 H
ATOM 3334 N THR B 33 -24.615 -29.433 -33.035 1.00 27.70 N
ANISOU 3334 N THR B 33 -24.615 -29.433 -33.035 1.00 27.70 N
ANISOU 3335 CA THR B 33 -24.104 -29.310 -34.386 1.00 26.63 C
  ANISOU 3335 CA THR B 33 4420 2282 3415 -379 432 791
 ATOM 3336 C THR B 33 -22.640 -29.740 -34.448 1.00 28.91
ANISOU 3336 C THR B 33 4749 2506 3729 -251 369 836
 ATOM 3337 O THR B 33 -21.999 -30.039 -33.434 1.00 29.34 O ANISOU 3337 O THR B 33 4848 2565 3737 -178 335 941 O ATOM 3338 CB THR B 33 -24.242 -27.872 -34.885 1.00 24.69 C ANISOU 3338 CB THR B 33 4108 2153 3121 -396 413 708 C ATOM 3339 OG1 THR B 33 -23.368 -27.013 -34.140 1.00 24.54
ATOM 3350 C GLY B 34 -20.387 -28.285 -36.201 1.00 29.07
ANISOU 3350 C GLY B 34 4642 2623 3778 -74 230 682
 ATOM 3351 O GLY B 34 -20.712 -27.413 -35.390 1.00 30.16 O ANISOU 3351 O GLY B 34 4761 2875 3823 -95 218 709 O ATOM 3352 H GLY B 34 -22.603 -29.915 -36.387 1.00 34.83 H ATOM 3353 HA2 GLY B 34 -20.213 -30.035 -35.139 1.00 35.59 H ATOM 3355 N SER B 35 -19.779 -28.003 -37.347 1.00 26.20 N
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ATOM 3362 HA SER B 35 -19.643 -26.025 -37.066 1.00 29.30 Н ATOM 3363 HB2 SER B 35 -18.248 -27.100 -39.280 1.00 30.64 Н -18.250 -25.554 -38.911 1.00 30.64 ATOM 3364 HB3 SER B 35 Н ATOM 3365 HG SER B 35 -16.479 -26.564 -38.096 1.00 33.70 Н ATOM 3366 N PHE B 36 -21.238 -25.036 -38.671 1.00 20.81 Ν ANISOU 3366 N PHE B 36 3324 1882 2698 -182 190 378 Ν **ATOM 3367 CA PHE B 36** -22.305 -24.567 -39.546 1.00 19.49 ANISOU 3367 CA PHE B 36 C 3103 1757 2544 -268 218 294 ATOM 3368 C PHE B 36 -22.253 -23.047 -39.626 1.00 18.24 C ANISOU 3368 C PHE B 36 2869 1732 2331 -257 179 258 0 ATOM 3369 O PHE B 36 -21.717 -22.378 -38.737 1.00 18.24 **ANISOU 3369 O PHE B 36** 0 2866 1791 2275 -211 147 300 ATOM 3370 CB PHE B 36 -23.684 -25.025 -39.055 1.00 20.02 ANISOU 3370 CB PHE B 36 3199 1796 2610 -366 280 316 ATOM 3371 CG PHE B 36 -24.196 -24.255 -37.865 1.00 19.80 ANISOU 3371 CG PHE B 36 3167 1855 2503 -383 287 367 ATOM 3372 CD1 PHE B 36 -23.884 -24.654 -36.576 1.00 21.45 **ANISOU 3372 CD1 PHE B 36** 3446 2041 2664 -353 294 469 ATOM 3373 CD2 PHE B 36 -25.007 -23.149 -38.040 1.00 19.20 3017 1884 2397 -426 ANISOU 3373 CD2 PHE B 36 290 313 ATOM 3374 CE1 PHE B 36 -24.361 -23.953 -35.488 1.00 21.16 ANISOU 3374 CE1 PHE B 36 3406 2091 2542 -372 305 506 ATOM 3375 CE2 PHE B 36 -25.483 -22.443 -36.960 1.00 19.07 2993 1944 2309 -439 ANISOU 3375 CE2 PHE B 36 303 347 ATOM 3376 CZ PHE B 36 -25.161 -22.841 -35.680 1.00 20.41 C ANISOU 3376 CZ PHE B 36 3234 2097 2424 -416 314 439 ATOM 3377 H PHE B 36 -20.947 -24.443 -38.120 1.00 24.97 Н **ATOM 3378 HA PHE B 36** -22.167 -24.923 -40.438 1.00 23.38 Н ATOM 3379 HB2 PHE B 36 -24.324 -24.916 -39.776 1.00 24.02 ATOM 3380 HB3 PHE B 36 -23.630 -25.959 -38.802 1.00 24.02 ATOM 3381 HD1 PHE B 36 -23.344 -25.398 -36.443 1.00 25.74 ATOM 3382 HD2 PHE B 36 -25.225 -22.872 -38.901 1.00 23.05 ATOM 3383 HE1 PHE B 36 -24.141 -24.226 -34.626 1.00 25.39 ATOM 3384 HE2 PHE B 36 -26.023 -21.697 -37.094 1.00 22.88 ATOM 3385 HZ PHE B 36 -25.485 -22.367 -34.948 1.00 24.49 Н -22.813 -22.518 -40.713 0.40 17.98 Ν **ATOM 3386 N AVAL B 37** ANISOU 3386 N AVAL B 37 2776 1742 2315 -300 177 Ν 182 **ATOM 3387 N BVAL B 37** -22.831 -22.510 -40.698 0.60 17.96 Ν 2773 1740 2312 -301 183 ANISOU 3387 N BVAL B 37 178 Ν ATOM 3388 CA AVAL B 37 -22.950 -21.077 -40.923 0.40 17.27 ANISOU 3388 CA AVAL B 37 2615 1761 2184 -297 154 143 **ATOM 3389 CA BVAL B 37** -22.966 -21.064 -40.864 0.60 17.27 C ANISOU 3389 CA BVAL B 37 2617 1763 2183 -297 154 ATOM 3390 C AVAL B 37 -24.203 -20.841 -41.758 0.40 16.84 ANISOU 3390 C AVAL B 37 2514 1739 2145 -371 177 82 ATOM 3391 C BVAL B 37 -24.160 -20.794 -41.771 0.60 16.82 C C ANISOU 3391 C BVAL B 37 2511 1739 2142 -368 174 82 **ATOM 3392 O AVAL B 37** 0 -24.401 -21.495 -42.788 0.40 17.01 ANISOU 3392 O AVAL B 37 32 2533 1723 2208 -401 187 0 ATOM 3393 O BVAL B 37 -24.278 -21.382 -42.852 0.60 16.83 0 ANISOU 3393 O BVAL B 37 2506 1706 2182 -393 181 30 ATOM 3394 CB AVAL B 37 -21.717 -20.464 -41.622 0.40 16.93 ANISOU 3394 CB AVAL B 37 2537 1751 2145 -231 108 113

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ATOM 3395 CB BVAL B 37
                            -21.673 -20.425 -41.420 0.60 16.93
ANISOU 3395 CB BVAL B 37
                            2540 1753 2138 -227
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                                                         123
ATOM 3396 CG1AVAL B 37
                            -21.807 -18.939 -41.630 0.40 16.61
                             2438 1808 2066 -228 83
ANISOU 3396 CG1AVAL B 37
                                                         93
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ATOM 3397 CG1BVAL B 37
                            -21.267 -21.064 -42.741 0.60 16.92
ANISOU 3397 CG1BVAL B 37
                             2534 1708 2188 -221
                                                    110
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ATOM 3398 CG2AVAL B 37
                            -20.423 -20.915 -40.958 0.40 17.22
ANISOU 3398 CG2AVAL B 37
                             2609 1752 2181 -155 82 163
ATOM 3399 CG2BVAL B 37
                            -21.827 -18.910 -41.566 0.60 16.69
ANISOU 3399 CG2BVAL B 37
                            2449 1820 2074 -229
                                                         95
                                                    83
                                                               Н
ATOM 3400 H AVAL B 37
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ATOM 3401 H BVAL B 37
                           -23.157 -22.967 -41.350 0.60 21.55
ATOM 3402 HA AVAL B 37
                            -23.066 -20.637 -40.067 0.40 20.72
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ATOM 3403 HA BVAL B 37
                            -23.149 -20.663 -40.000 0.60 20.73
                                                               Н
ATOM 3404 HB AVAL B 37
                            -21.698 -20.765 -42.544 0.40 20.32
ATOM 3405 HB BVAL B 37
                                                               Н
                            -20.956 -20.585 -40.788 0.60 20.31
ATOM 3406 HG11AVAL B 37
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                            -22.628 -18.670 -41.190 0.40 19.93
ATOM 3407 HG11BVAL B 37
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ATOM 3408 HG12AVAL B 37
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ATOM 3409 HG12BVAL B 37
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                            -21.254 -20.381 -43.430 0.60 20.30
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ATOM 3411 HG13BVAL B 37
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ATOM 3412 HG21AVAL B 37
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ATOM 3413 HG21BVAL B 37
                             -21.001 -18.541 -41.916 0.60 20.03
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ATOM 3414 HG22AVAL B 37
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ATOM 3415 HG22BVAL B 37
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ATOM 3416 HG23AVAL B 37
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                                                                Н
ATOM 3417 HG23BVAL B 37
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                             -22.018 -18.527 -40.695 0.60 20.03
ATOM 3418 N VAL B 38
                          -25.042 -19.901 -41.323 1.00 15.64
                                                              N
ANISOU 3418 N VAL B 38
                           2321 1661 1959 -398 182
ATOM 3419 CA VAL B 38
                                                              C
                           -26.307 -19.595 -41.990 1.00 14.44
ANISOU 3419 CA VAL B 38
                           2112 1553 1820 -460
                                                   197
                                                              C
ATOM 3420 C VAL B 38
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ANISOU 3420 C VAL B 38
                           1948 1540 1684 -435 172
                                                       16
ATOM 3421 O VAL B 38
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                          -26.297 -17.442 -40.942 1.00 13.73
ANISOU 3421 O VAL B 38
                          1971 1581 1664 -406
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ATOM 3422 CB VAL B 38
                           -27.491 -20.295 -41.286 1.00 15.71
ANISOU 3422 CB VAL B 38
                           2286 1692 1990 -535 253
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ATOM 3423 CG1 VAL B 38
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ANISOU 3423 CG1 VAL B 38
                           2258 1810 2055 -595
                                                  263 -10
                                                               C
                           -27.325 -21.810 -41.334 1.00 15.92
ATOM 3424 CG2 VAL B 38
                                                               C
ANISOU 3424 CG2 VAL B 38
                           2381 1609 2060 -566 285
                                                         62
                                                              Н
ATOM 3425 H AVAL B 38
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                           -24.924 -19.443 -40.605 0.60 18.76
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ATOM 3426 H BVAL B 38
ATOM
      3427 HA VAL B 38
                           -26.272 -19.894 -42.912 1.00 17.32
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ATOM 3428 HB VAL B 38
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ATOM 3429 HG11 VAL B 38
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ATOM 3430 HG12 VAL B 38
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ATOM 3431 HG13 VAL B 38
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ATOM 3432 HG21 VAL B 38
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ATOM 3433 HG22 VAL B 38
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                          -26.500 -22.051 -40.885 1.00 19.10
ATOM 3434 HG23 VAL B 38
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ATOM 3435 N GLY B 39 -26.989 -17.523 -43.082 1.00 13.38
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ANISOU 3435 N GLY B 39 1861 1559 1666 -445 151 -32 ATOM 3436 CA GLY B 39 -27.339 -16.116 -43.060 1.00 14.13 ANISOU 3436 CA GLY B 39 1901 1726 1742 -420 132 -39 ATOM 3437 C GLY B 39 -27.655 -15.547 -44.427 1.00 13.46 ANISOU 3437 C GLY B 39 1763 1687 1665 -418 100 -77 0 ATOM 3438 O GLY B 39 -27.529 -16.209 -45.463 1.00 12.61 0 **ANISOU 3438 O GLY B 39** 1658 1567 1567 -436 90 -107 ATOM 3439 H GLY B 39 -27.110 -17.921 -43.835 1.00 16.06 ATOM 3440 HA2 GLY B 39 -28.116 -15.989 -42.493 1.00 16.96 ATOM 3441 HA3 GLY B 39 -26.602 -15.609 -42.684 1.00 16.96 ATOM 3442 N LYS B 40 -28.067 -14.279 -44.397 1.00 13.96 ANISOU 3442 N LYS B 40 1780 1804 1720 -391 85 -77 ATOM 3443 CA LYS B 40 -28.340 -13.493 -45.591 1.00 14.08 C ANISOU 3443 CA LYS B 40 1746 1868 1734 -373 49 -94 ATOM 3444 C LYS B 40 ANISOU 3444 C LYS B 40 C -27.250 -12.442 -45.750 1.00 13.17 1646 1749 1608 -317 26 -71 ATOM 3445 O LYS B 40 -26.771 -11.867 -44.763 1.00 11.16 0 **ANISOU 3445 O LYS B 40** 1410 1479 1352 -292 **35** -**53** ATOM 3446 CB LYS B 40 -29.713 -12.808 -45.517 1.00 15.70 ANISOU 3446 CB LYS B 40 1883 2132 1952 -379 50 -106 ATOM 3447 CG LYS B 40 -30.923 -13.753 -45.588 1.00 16.73 ANISOU 3447 CG LYS B 40 1975 2284 2099 -445 70 -138 ATOM 3448 CD LYS B 40 -31.468 -13.876 -46.981 1.00 17.21 ANISOU 3448 CD LYS B 40 1987 2395 2156 -463 30 -172 C -32.704 -14.768 -47.074 1.00 17.29 ATOM 3449 CE LYS B 40 ANISOU 3449 CE LYS B 40 1947 2435 2189 -538 47 -216 Ν ATOM 3450 NZ LYS B 40 -33.971 -14.141 -46.605 1.00 16.45 ANISOU 3450 NZ LYS B 40 1756 2392 2103 -538 57 -223 Ν ATOM 3451 H LYS B 40 -28.199 -13.841 -43.668 1.00 16.75 Н **ATOM 3452 HA LYS B 40** -28.326 -14.072 -46.369 1.00 16.89 ATOM 3453 HB2 LYS B 40 -29.771 -12.323 -44.679 1.00 18.84 ATOM 3454 HB3 LYS B 40 -29.786 -12.185 -46.257 1.00 18.84 ATOM 3455 HG2 LYS B 40 -30.654 -14.636 -45.291 1.00 20.08 ATOM 3456 HG3 LYS B 40 -31.628 -13.410 -45.018 1.00 20.08 ATOM 3457 HD2 LYS B 40 -31.713 -12.994 -47.301 1.00 20.65 Н ATOM 3458 HD3 LYS B 40 -30.783 -14.256 -47.553 1.00 20.65 Н ATOM 3459 HE2 LYS B 40 -32.831 -15.025 -48.000 1.00 20.75 ATOM 3460 HE3 LYS B 40 -32.554 -15.561 -46.535 1.00 20.75 Н ATOM 3461 HZ1 LYS B 40 -33.895 -13.906 -45.750 1.00 19.74 Н ATOM 3462 HZ2 LYS B 40 -34.148 -13.416 -47.090 1.00 19.74 ATOM 3463 HZ3 LYS B 40 -34.645 -14.716 -46.688 1.00 19.74 Н -26.859 -12.202 -46.990 1.00 13.45 Ν ATOM 3464 N GLY B 41 ANISOU 3464 N GLY B 41 1674 1804 1633 -304 -2 -76 ATOM 3465 CA GLY B 41 -25.873 -11.188 -47.284 1.00 13.66 C 1710 1827 1652 -262 -18 -53 ANISOU 3465 CA GLY B 41 Č ATOM 3466 C GLY B 41 -25.714 -10.954 -48.769 1.00 13.73 1707 1871 1639 -257 -42 -53 ANISOU 3466 C GLY B 41 ATOM 3467 O GLY B 41 -26.702 -10.863 -49.505 1.00 13.81 0 **ANISOU 3467 O GLY B 41** 1682 1929 1637 -267 -62 -61 ATOM 3468 H GLY B 41 -27.155 -12.617 -47.683 1.00 16.14 ATOM 3469 HA2 GLY B 41 -26.134 -10.352 -46.867 1.00 16.39 ATOM 3470 HA3 GLY B 41 -25.014 -11.458 -46.922 1.00 16.39 Ν ATOM 3471 N TRP B 42 -24.469 -10.882 -49.216 1.00 12.78

ANISOU 3471 N TRP B 42 1613 1735 1507 -243 -41 -46 ATOM 3472 CA TRP B 42 -24.162 -10.518 -50.584 1.00 13.82 ANISOU 3472 CA TRP B 42 1741 1905 1607 -238 -55 -38 C ATOM 3473 C TRP B 42 ANISOU 3473 C TRP B 42 -23.295 -11.578 -51.253 1.00 13.68 1747 1881 1570 -253 -41 -71 ATOM 3474 O TRP B 42 -22.427 -12.186 -50.616 1.00 13.35 0 **ANISOU 3474 O TRP B 42** 1728 1794 1551 -248 -22 -82 C ATOM 3475 CB TRP B 42 -23.491 -9.143 -50.597 1.00 13.94 ANISOU 3475 CB TRP B 42 1757 1910 1628 -207 -56 ATOM 3476 CG TRP B 42 -24.444 -8.063 -50.126 1.00 14.89 ANISOU 3476 CG TRP B 42 1854 2031 1772 -185 -68 ATOM 3477 CD1 TRP B 42 -25.261 -7.302 -50.902 1.00 16.03 **ANISOU 3477 CD1 TRP B 42** 1974 2211 1904 -165 60 -93 ATOM 3478 CD2 TRP B 42 -24.693 -7.660 -48.768 1.00 14.47 **ANISOU 3478 CD2 TRP B 42** 1797 1944 1756 -174 -56 27 -25.996 -6.441 -50.120 1.00 15.71 ATOM 3479 NE1 TRP B 42 **ANISOU 3479 NE1 TRP B 42** 1913 2153 1903 -138 **72** -94 ATOM 3480 CE2 TRP B 42 -25.667 -6.644 -48.806 1.00 14.88 ANISOU 3480 CE2 TRP B 42 1821 2007 1826 -147 -68 47 C ATOM 3481 CE3 TRP B 42 -24.191 -8.063 -47.525 1.00 14.77 **ANISOU 3481 CE3 TRP B 42** 1855 1948 1809 -182 -37 8 CC ATOM 3482 CZ2 TRP B 42 -26.144 -6.021 -47.652 1.00 14.48 **ANISOU 3482 CZ2 TRP B 42** 1759 1932 1811 -129 -54 38 C ATOM 3483 CZ3 TRP B 42 -24.667 -7.437 -46.384 1.00 13.76 **ANISOU 3483 CZ3 TRP B 42** 3 1719 1805 1703 -170 -27 C ATOM 3484 CH2 TRP B 42 -25.631 -6.433 -46.458 1.00 13.65 1676 1800 1711 -145 -32 12 C ANISOU 3484 CH2 TRP B 42 -23.774 -11.044 -48.735 1.00 15.33 -24 990 -10.451 -51.085 1.00 16.59 ATOM 3485 H TRP B 42 Н -24.990 -10.451 -51.085 1.00 16.59 Н ATOM 3486 HA TRP B 42 ATOM 3487 HB2 TRP B 42 -22.725 -9.154 -50.002 1.00 16.73 ATOM 3488 HB3 TRP B 42 -23.213 -8.930 -51.501 1.00 16.73 ATOM 3489 HD1 TRP B 42 -25.310 -7.351 -51.830 1.00 19.23 ATOM 3490 HE1 TRP B 42 -26.569 -5.869 -50.410 1.00 18.85 ATOM 3491 HE3 TRP B 42 ATOM 3492 HZ2 TRP B 42 -23.548 -8.733 -47.467 1.00 17.73 -26.785 -5.349 -47.696 1.00 17.38 Н ATOM 3493 HZ3 TRP B 42 -24.339 -7.693 -45.553 1.00 16.51 Н ATOM 3494 HH2 TRP B 42 -25.929 -6.031 -45.674 1.00 16.38 ATOM 3495 N THR B 43 -23.554 -11.791 -52.550 1.00 14.28 Ν ANISOU 3495 N THR B 43 1816 2008 1602 -267 -53 -90 Ν ATOM 3496 CA THR B 43 -22.840 -12.804 -53.326 1.00 15.54 ANISOU 3496 CA THR B 43 1996 2169 1739 -283 -35 -136 ATOM 3497 C THR B 43 ANISOU 3497 C THR B 43 -21.359 -12.487 -53.428 1.00 16.11 C 2083 2224 1814 -258 -10 -121 0 ATOM 3498 O THR B 43 -20.509 -13.377 -53.288 1.00 16.62 ANISOU 3498 O THR B 43 2164 2254 1898 -253 14 -155 ATOM 3499 CB THR B 43 -23.447 -12.896 -54.727 1.00 17.03 ANISOU 3499 CB THR B 43 2173 2434 1864 -304 -56 -160 ATOM 3500 OG1 THR B 43 -24.811 -13.301 -54.626 1.00 18.12 ANISOU 3500 OG1 THR B 43 2285 2594 2006 -333 -82 -185 ATOM 3501 CG2 THR B 43 -22.683 -13.889 -55.607 1.00 18.70 ANISOU 3501 CG2 THR B 43 2407 2652 2045 -320 -31 -221 ATOM 3502 H THR B 43 -24.143 -11.357 -53.002 1.00 17.14 Н ATOM 3503 HA THR B 43 -22.938 -13.667 -52.894 1.00 18.64 Н

ATOM 3504 HB THR B 43 -23.405 -12.024 -55.149 1.00 20.43 Н ATOM 3505 HG1 THR B 43 -25.244 -12.742 -54.173 1.00 21.75 ATOM 3506 HG21 THR B 43 -23.087 -13.929 -56.488 1.00 22.44 ATOM 3507 HG22 THR B 43 -21.759 -13.609 -55.696 1.00 22.44

ATOM 3508 HG23 THR B 43 -22.709 -14.772 -55.208 1.00 22.44

ATOM 3509 N THR B 44 -21.033 -11.233 -53.718 1.00 16.14

ANISOU 3509 N THR B 44 2078 2252 1802 -242 -14 -72 N ATOM 3510 CA THR B 44 -19.658 -10.772 -53.811 1.00 16.17 C ANISOU 3510 CA THR B 44 2085 2246 1814 -229 14 -56 ATOM 3511 C THR B 44 -19.445 -9.726 -52.731 1.00 15.09 ANISOU 3511 C THR B 44 1940 2070 1722 -213 ATOM 3512 O THR B 44 -20.098 -8.674 -52.741 1.00 15.29 ANISOU 3512 O THR B 44 1961 2100 1747 -208 -7 27 O
ATOM 3513 CB THR B 44 -19.360 -10.199 -55.194 1.00 18.58 C
ANISOU 3513 CB THR B 44 2392 2609 2057 -236 25 -36 C
ATOM 3514 OG1 THR B 44 -19.672 -11.182 -56.181 1.00 20.02 ANISOU 3514 OGT TIRE 377
ATOM 3515 CG2 THR B 44 -17.886 -9.807 -55.309 1.00 19.44
ANISOU 3515 CG2 THR B 44 2496 2711 2179 -233 65 -26 C
ATOM 3516 H THR B 44 -21.611 -10.614 -53.868 1.00 19.37 H
ATOM 2517 HA THR B 44 -19.054 -11.514 -53.647 1.00 19.41 H ANISOU 3514 OG1 THR B 44 2582 2837 2187 -254 26 -87 ATOM 3516 H THR B 44 -21.611 -10.614 -53.868 1.00 19.37 H
ATOM 3517 HA THR B 44 -19.054 -11.514 -53.647 1.00 19.41 H
ATOM 3518 HB THR B 44 -19.902 -9.408 -55.341 1.00 22.29 H
ATOM 3519 HG1 THR B 44 -20.485 -11.389 -56.133 1.00 24.03 H
ATOM 3520 HG21 THR B 44 -17.708 -9.444 -56.190 1.00 23.33 H
ATOM 3521 HG22 THR B 44 -17.669 -9.137 -54.642 1.00 23.33 H
ATOM 3522 HG23 THR B 44 -17.325 -10.585 -55.168 1.00 23.33 H
ATOM 3523 N GLY B 45 -18.538 -10.024 -51.806 1.00 14.04 N
ANISOU 3523 N GLY B 45 1805 1898 1629 -203 20 -29 N ATOM 3523 N GLY B 45 -18.538 -10.024 -51.806 1.00 14.04 N ANISOU 3523 N GLY B 45 1805 1898 1629 -203 20 -29 N ATOM 3524 CA GLY B 45 -18.240 -9.105 -50.733 1.00 13.51 C ANISOU 3524 CA GLY B 45 1731 1802 1601 -194 14 -5 C ATOM 3525 C GLY B 45 17504 -7.876 -51.219 1.00 12.28 C ANISOU 3525 C GLY B 45 1566 1652 1449 -201 29 26 C ATOM 3526 O GLY B 45 1566 1652 1449 -201 29 26 C ANISOU 3526 O GLY B 45 1579 1699 1442 -211 53 28 O ATOM 3527 H GLY B 45 1579 1699 1442 -211 53 28 O ATOM 3528 HA2 GLY B 45 -18.084 -10.755 -51.784 1.00 16.84 H ATOM 3529 HA3 GLY B 45 -19.066 -8.823 -50.311 1.00 16.21 H ATOM 3530 N SER B 46 17.638 -6.802 -50.438 1.00 11.69 N ANISOU 3530 N SER B 46 1488 1546 1407 -200 21 46 N ATOM 3531 CA SER B 46 -16.926 -5.562 -50.668 1.00 12.09 C ANISOU 3531 CA SER B 46 -16.926 -5.562 -50.668 1.00 12.09 C
ATOM 3532 C SER B 46 -16.227 -5 135 -49 395 4 00 44 47 ATOM 3532 C SER B 46 -16.227 -5.135 -49.385 1.00 11.47 ANISOU 3532 C SER B 46 1440 1471 1448 -220 35 49 ATOM 3533 O SER B 46 -16.795 -5.277 -48.293 1.00 10.21 ANISOU 3533 O SER B 46 1285 1295 1298 -207 14 31 ATOM 3534 CB SER B 46 -17.869 -4.439 -51.127 1.00 11.59 0 ATOM 3535 HB2 SER B 46 -18.135 -4.603 -52.045 1.00 13.91 H

ATOM 3539 HB3 SER B 46 -18.648 -4.423 -50.550 1.00 13.91 H

ATOM 3540 HG SER B 46 -17.725 -2.568 -51.303 1.00 14.82 Н ATOM 3541 N PRO B 47 -15.007 -4.596 -49.476 1.00 13.08 Ν **ANISOU 3541 N PRO B 47** 1622 1672 1677 -243 Ν 56 45 ATOM 3542 CA PRO B 47 -14.367 -4.022 -48.285 1.00 13.77 C ANISOU 3542 CA PRO B 47 1690 1736 1807 -256 46 15 C -14.969 -2.693 -47.849 1.00 14.43 ATOM 3543 C PRO B 47 1792 1767 1923 -266 ANISOU 3543 C PRO B 47 47 28 ATOM 3544 O PROB 47 -14.567 -2.163 -46.805 1.00 16.04 0 ANISOU 3544 O PRO B 47 1984 1951 2159 -280 -9 37 ATOM 3545 CB PRO B 47 -12.911 -3.852 -48.729 1.00 14.33 C ANISOU 3545 CB PRO B 47 1721 1826 1898 -285 **73** ATOM 3546 CG PRO B 47 -13.004 -3.646 -50.192 1.00 14.65 ANISOU 3546 CG PROB 47 1776 1878 1912 -299 110 48 ATOM 3547 CD PRO B 47 -14.145 -4.491 -50.666 1.00 13.44 ANISOU 3547 CD PRO B 47 1654 1743 1708 -266 93 62 Н ATOM 3548 HA PRO B 47 -14.406 -4.650 -47.547 1.00 16.53 -12.521 -3.077 -48.294 1.00 17.20 -12.407 -4.655 -48.524 1.00 17.20 ATOM 3549 HB2 PRO B 47 ATOM 3550 HB3 PRO B 47 -12.407 -4.000 -40.024 ...00 -13.176 -2.709 -50.376 1.00 17.58 ATOM 3551 HG2 PRO B 47 ATOM 3552 HG3 PRO B 47 -12.176 -3.928 -50.612 1.00 17.58 -14.618 -4.048 -51.388 1.00 16.12 ATOM 3553 HD2 PRO B 47 ATOM 3554 HD3 PRO B 47 -13.829 -5.368 -50.933 1.00 16.12 ATOM 3555 N PHE B 48 -15.929 -2.158 -48.601 1.00 13.18 Ν **ANISOU 3555 N PHE B 48** 1661 1588 1757 -256 55 74 ATOM 3556 CA PHE B 48 -16.646 -0.942 -48.231 1.00 12.27 C ANISOU 3556 CA PHE B 48 1566 1415 1681 -251 57 88 C ATOM 3557 C PHE B 48 -18.115 -1.203 -47.926 1.00 13.22 ANISOU 3557 C PHE B 48 1698 1538 1785 -209 92 34 ATOM 3558 O PHE B 48 -18.900 -0.255 -47.817 1.00 13.43 0 ANISOU 3558 O PHE B 48 1739 1520 1843 -190 36 110 C ATOM 3559 CB PHE B 48 -16.483 0.090 -49.339 1.00 12.45 ANISOU 3559 CB PHE B 48 1607 1402 1720 -267 87 149 ATOM 3560 CG PHE B 48 -15.058 0.484 -49.550 1.00 13.26 ANISOU 3560 CG PHE B 48 1691 1496 1849 -320 119 142 ATOM 3561 CD1 PHE B 48 -14.385 1.221 -48.585 1.00 14.30 **ANISOU 3561 CD1 PHE B 48** 1808 1584 2040 -354 125 -14.370 0.073 -50.672 1.00 13.87 ATOM 3562 CD2 PHE B 48 **ANISOU 3562 CD2 PHE B 48** 1760 1619 1891 -340 146 171 ATOM 3563 CE1 PHE B 48 -13.062 1.568 -48.757 1.00 15.21 ANISOU 3563 CE1 PHE B 48 1895 1700 2186 -410 155 81 ATOM 3564 CE2 PHE B 48 -13.045 0.424 -50.855 1.00 15.01 C 1876 1765 2064 -392 184 160 **ANISOU 3564 CE2 PHE B 48** ATOM 3565 CZ PHE B 48 -12.388 1.169 -49.885 1.00 15.41 C ANISOU 3565 CZ PHE B 48 1904 1769 2180 -429 187 115 C ATOM 3566 H PHE B 48 -16.189 -2.492 -49.349 1.00 15.81 Н ATOM 3567 HA PHE B 48 -16.241 -0.577 -47.428 1.00 14.72 Н ATOM 3567 HA PHE B 48 -16.241 -0.577 -47.428 1.00 14.72
ATOM 3568 HB2 PHE B 48 -16.818 -0.282 -50.170 1.00 14.94
ATOM 3569 HB3 PHE B 48 -16.984 0.887 -49.106 1.00 14.94
ATOM 3570 HD1 PHE B 48 -14.835 1.493 -47.819 1.00 17.16 Н ATOM 3571 HD2 PHE B 48 -14.807 -0.427 -51.322 1.00 16.64 ATOM 3572 HE1 PHE B 48 -12.625 2.072 -48.108 1.00 18.26 Н ATOM 3573 HE2 PHE B 48 -12.591 0.151 -51.619 1.00 18.02 H ATOM 3574 HZ PHF R 48 -11.027 1.007 50.005 4.00 40 40 ATOM 3574 HZ PHE B 48 -11.497 1.407 -50.005 1.00 18.49 Н

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ATOM 3575 N ARG B 49 -18.480 -2.464 -47.727 1.00 13.35
ANISOU 3575 N ARG B 49 1708 1603 1761 -196 16 72
ATOM 3576 CA ARG B 49 -19.843 -2.840 -47.376 1.00 14.39
                                                          C
ANISOU 3576 CA ARG B 49 1841 1746 1879 -168 0 68
                                                            C
ATOM 3577 C ARG B 49 -20.269 -2.214 -46.055 1.00 13.75
ANISOU 3577 C ARG B 49
                         1761 1633 1829 -159
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ATOM 3578 O ARG B 49
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ANISOU 3578 O ARG B 49 1587 1453 1664 -176 1 -6
ATOM 3579 CB ARG B 49 -19.933 -4.367 -47.275 1.00 14.99
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ANISOU 3579 CB ARG B 49 1914 1868 1915 -169 -11
ATOM 3580 CG ARG B 49
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ANISOU 3580 CG ARG B 49 2103 2081 2094 -155 -21 42
ATOM 3581 CD ARG B 49
                           -22.176 -4.868 -48.271 1.00 17.51
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ANISOU 3581 CD ARG B 49
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ATOM 3582 NE ARG B 49
ANISOU 3582 NE ARG B 49 2185 2225 2123 -161 -31 78
ATOM 3583 CZ ARG B 49
                          -21.952 -5.668 -50.597 1.00 19.06
ANISOU 3583 CZ ARG B 49 2420 2497 2326 -160 -41 105
ATOM 3584 NH1 ARG B 49 -22.894 -4.832 -51.001 1.00 20.55
ANISOU 3584 NH1 ARG B 49 2090 2092 2010 100 19.97 ATOM 3585 NH2 ARG B 49 -21.358 -6.461 -51.478 1.00 19.97 N
ANISOU 3584 NH1 ARG B 49 2598 2692 2516 -136 -57 141
ATOM 3595 HH11 ARG B 49 -23.279 -4.313 -50.434 1.00 24.66
ATOM 3596 HH12 ARG B 49 -23.122 -4.810 -51.829 1.00 24.66
ATOM 3597 HH21 ARG B 49
                          -20.746 -7.007 -51.221 1.00 23.97
ATOM 3598 HH22 ARG B 49 -21.593 -6.436 -52.305 1.00 23.97
                                                         N
ATOM 3599 N THR B 50 -21.506 -1.723 -46.018 1.00 14.94
ANISOU 3599 N THR B 50
                         1910 1772 1996 -130
                                                           Ν
                                                 0 44
ATOM 3600 CA THR B 50
                         -22.168 -1.298 -44.785 1.00 15.66
ANISOU 3600 CA THR B 50 1997 1845 2108 -115
ATOM 3601 C THR B 50 -23.295 -2.287 -44.518 1.00 15.01 ANISOU 3601 C THR B 50 1898 1811 1993 -103 2 -6
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ATOM 3602 O THR B 50 -24.250 -2.371 -45.300 1.00 15.21
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ANISOU 3602 O THR B 50 1905 1857 2018 -83
                                                -6
ATOM 3603 CB THR B 50 -22.709 0.126 -44.903 1.00 17.88
ANISOU 3603 CB THR B 50 2281 2066 2446 -86 20 14
                                                          C
ATOM 3604 OG1 THR B 50 -21.649 1.010 -45.275 1.00 19.61
ANISOU 3604 OG1 THR B 50 2519 2231 2700 -109
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ATOM 3610 HG21 THR B 50 -23.649 1.489 -43.662 1.00 21.43
ATOM 3611 HG22 THR B 50 -24.036 -0.004 -43.321 1.00 21.43
ATOM 3612 HG23 THR B 50 -22.630 0.567 -42.883 1.00 21.43
ATOM 3613 N ILE B 51 -23.174 -3.049 -43.436 1.00 12.41
                                                                                            Ν
 ANISOU 3613 N ILE B 51 1574 1504 1635 -119
                                                                            7 -42
                                                                                             Ν
ATOM 3614 CA ILE B 51 -24.139 -4.087 -43.099 1.00 12.00
ANISOU 3614 CA ILE B 51 1511 1493 1554 -122 11 -48
ATOM 3615 C ILE B 51 -25.038 -3.565 -41.990 1.00 14.17
ANISOU 3615 C ILE B 51 1775 1770 1840 -108
ATOM 3616 O ILE B 51
                                        -24.558 -3.205 -40.908 1.00 14.63
ANISOU 3616 O ILE B 51 1851 1818 1890 -114 46 -120
ATOM 3617 CB ILE B 51
                                                                                                C
                                       -23.449 -5.391 -42.669 1.00 11.03
ANISOU 3617 CB ILE B 51 1409 1392 1390 -147 6 -51 ATOM 3618 CG1 ILE B 51 -22.509 -5.912 -43.774 1.00 11.46
                                                                                               CCC
ANISOU 3618 CG1 ILE B 51 1470 1446 1439 -156 -10 -27 ATOM 3619 CG2 ILE B 51 -24.504 -6.450 -42.292 1.00 10.74
ANISOU 3619 CG2 ILE B 51 1367 1384 1330 -160
                                                                              21 -53
ATOM 3620 CD1 ILE B 51 -21.060 -5.434 -43.614 1.00 10.45
ANISOU 3620 CD1 ILE B 51 1350 1300 1321 -160 -18 -34 C ATOM 3621 H ILE B 51 -22.529 -2.981 -42.871 1.00 14.89 H
ATOM 3622 HA ILE B 51 -24.691 -4.276 -43.874 1.00 14.39 H
ATOM 3623 HB ILE B 51 -22.915 -5.204 -41.882 1.00 13.24 H
ATOM 3623 HB ILE B 51 -22.915 -5.204 -41.882 1.00 13.24 H
ATOM 3624 HG12 ILE B 51 -22.506 -6.882 -43.752 1.00 13.75 H
ATOM 3625 HG13 ILE B 51 -22.832 -5.602 -44.634 1.00 13.75 H
ATOM 3626 HG21 ILE B 51 -24.050 -7.265 -42.024 1.00 12.89 H
ATOM 3627 HG22 ILE B 51 -25.040 -6.113 -41.558 1.00 12.89 H
ATOM 3628 HG23 ILE B 51 -25.067 -6.622 -43.062 1.00 12.89 H
ATOM 3629 HD11 ILE B 51 -20.527 -5.797 -44.339 1.00 12.54 H
ATOM 3630 HD12 ILE B 51 -21.043 -4.465 -43.644 1.00 12.54 H
ATOM 3631 HD13 ILE B 51 -20.717 -5.746 -42.762 1.00 12.54 H
ATOM 3632 N ASN B 52 -26.339 -3.546 -42.255 1.00 13.82 N
ANISOU 3632 N ASN B 52 1697 1746 1810 -90 44 -80 N
ANISOU 3632 N ASN B 52 1697 1746 1810 -90
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ATOM 3633 CA ASN B 52 -27.353 -3.255 -41.255 1.00 13.85
                                                                                                CCC
ANISOU 3633 CA ASN B 52 1677 1763 1820 -77 76 -118
ATOM 3634 C ASN B 52 -28.085 -4.538 -40.888 1.00 12.90
ANISOU 3634 C ASN B 52 1544 1694 1663 -108
                                                                              93 -120
                                         -28.359 -5.380 -41.751 1.00 13.19
                                                                                                Ö
ATOM 3635 O ASN B 52
ANISOU 3635 O ASN B 52 1567 1752 1693 -125 76 -93
ATOM 3636 CB ASN B 52 -28.354 -2.225 -41.774 1.00 16.18
ANISOU 3636 CB ASN B 52 1930 2045 2171 -28 78 -114 ATOM 3637 CG ASN B 52 -27.681 -0.988 -42.303 1.00 18.42
ANISOU 3637 CG ASN B 52 2234 2264 2499 0 65 -97
ATOM 3638 OD1 ASN B 52 -27.245 -0.136 -41.534 1.00 19.40
                                                                                                0
ATOM 3649 HB2 ASN B 52 -26.667 -3.703 -43.034 1.00 16.59 H ATOM 3642 HB2 ASN B 52 -28.870 -2.619 -42.495 1.00 19.41 H ATOM 3644 HD21 ASN B 52 -28.943 -1.962 -41.049 1.00 19.41 H ATOM 3645 HD22 ASN B 52 -27.212 -0.191 -43.974 1.00 23.30 H ATOM 3646 N TYR B 53 -28.416 -4.683 -39.611 1.00 11.54 N
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ANISOU 3646 N TYR B 53 1378 1543 1465 -120 130 -153 Ν ATOM 3647 CA TYR B 53 -29.117 -5.882 -39.195 1.00 12.73 ANISOU 3647 CA TYR B 53 1521 1734 1582 -158 156 -148 ATOM 3648 C TYR B 53 ANISOU 3648 C TYR B 53 -29.854 -5.624 -37.892 1.00 13.38 1593 1847 1645 -160 209 -189 C ATOM 3649 O TYR B 53 -29.550 -4.682 -37.145 1.00 13.52 0 **ANISOU 3649 O TYR B 53** 1624 1853 1660 -138 222 -227 ATOM 3650 CB TYR B 53 -28.157 -7.071 -39.042 1.00 12.71 ANISOU 3650 CB TYR B 53 1572 1724 1533 -193 142 -119 ATOM 3651 CG TYR B 53 -27.308 -7.035 -37.780 1.00 12.93 ANISOU 3651 CG TYR B 53 1649 1753 1512 -197 150 -130 ATOM 3652 CD1 TYR B 53 C -26.052 -6.440 -37.785 1.00 13.96 C **ANISOU 3652 CD1 TYR B 53** 1804 1858 1642 -180 115 -136 CC ATOM 3653 CD2 TYR B 53 -27.755 -7.615 -36.599 1.00 13.73 **ANISOU 3653 CD2 TYR B 53** 1769 1886 1562 -222 190 -133 -25.270 -6.404 -36.646 1.00 14.23 ATOM 3654 CE1 TYR B 53 C **ANISOU 3654 CE1 TYR B 53** 1875 1907 1626 -184 112 -151 ATOM 3655 CE2 TYR B 53 -26.987 -7.586 -35.448 1.00 13.20 **ANISOU 3655 CE2 TYR B 53** 1748 1832 1433 -223 189 -140 -25.744 -6.981 -35.474 1.00 13.59 ATOM 3656 CZ TYR B 53 **ANISOU 3656 CZ TYR B 53 ATOM 3657 OH TYR B 53** C 1816 1864 1484 -202 145 -152 -24.964 -6.951 -34.338 1.00 13.57 0 1852 1888 1416 -204 134 -165 **ANISOU 3657 OH TYR B 53** 0 ATOM 3658 H TYR B 53 -28.251 -4.117 -38.984 1.00 13.85 Н ATOM 3659 HA TYR B 53 -29.774 -6.113 -39.870 1.00 15.28 Н ATOM 3660 HB2 TYR B 53 -28.677 -7.889 -39.024 1.00 15.25 Н ATOM 3661 HB3 TYR B 53 -27.555 -7.083 -39.803 1.00 15.25 Н ATOM 3662 HD1 TYR B 53 ATOM 3663 HD2 TYR B 53 -25.735 -6.049 -38.568 1.00 16.75 Н -28.592 -8.019 -36.577 1.00 16.48 Н ATOM 3664 HE1 TYR B 53 -24.434 -5.998 -36.664 1.00 17.08 ATOM 3665 HE2 TYR B 53 -27.302 -7.975 -34.665 1.00 15.83 Н ATOM 3666 HH TYR B 53 -24.239 -6.559 -34.498 1.00 16.29 Н ATOM 3667 N ASN B 54 -30.820 -6.496 -37.629 1.00 13.94 Ν ANISOU 3667 N ASN B 54 1638 1958 1701 -194 245 -186 N -31.547 -6.502 -36.366 1.00 14.91 ATOM 3668 CA ASN B 54 C ANISOU 3668 CA ASN B 54 1751 2121 1791 -210 309 -219 ATOM 3669 C ASN B 54 -31.785 -7.954 -35.977 1.00 14.57 ANISOU 3669 C ASN B 54 ATOM 3670 O ASN B 54 C 1733 2101 1703 -273 338 -185 0 -32.435 -8.698 -36.722 1.00 14.24 **ANISOU 3670 O ASN B 54** 1655 2066 1691 -303 338 -168 ATOM 3671 CB ASN B 54 -32.869 -5.734 -36.492 1.00 16.78 ANISOU 3671 CB ASN B 54 1905 2388 2083 -179 340 -259 C ATOM 3672 CG ASN B 54 -33.624 -5.643 -35.180 1.00 18.91 C ANISOU 3672 CG ASN B 54 2159 2706 2318 -192 417 -304 0 ATOM 3673 OD1 ASN B 54 -33.669 -6.598 -34.407 1.00 19.32 **ANISOU 3673 OD1 ASN B 54** 2244 2788 2308 -247 456 -287 0 ATOM 3674 ND2 ASN B 54 -34.217 -4.482 -34.918 1.00 19.66 Ν 2207 2808 2455 -141 444 -360 **ANISOU 3674 ND2 ASN B 54** Ν ATOM 3675 H ASN B 54 -31.077 -7.107 -38.177 1.00 16.73 Н ATOM 3676 HA ASN B 54 -31.008 -6.081 -35.677 1.00 17.89 Н ATOM 3677 HB2 ASN B 54 -32.682 -4.831 -36.793 1.00 20.14 Н ATOM 3678 HB3 ASN B 54 -33.437 -6.186 -37.135 1.00 20.14 ATOM 3679 HD21 ASN B 54 -34.658 -4.380 -34.187 1.00 23.59

ATOM 3680 HD22 ASN B 54 -34.160 -3.834 -35.480 1.00 23.59 ATOM 3681 N ALA B 55 -31.237 -8.369 -34.835 1.00 13.36 **ANISOU 3681 N ALA B 55** 1643 1955 1478 -294 361 -174 ATOM 3682 CA ALA B 55 -31.376 -9.743 -34.358 1.00 14.05 ANISOU 3682 CA ALA B 55 1769 2051 1520 -351 393 -128 ATOM 3683 C ALA B 55 -32.522 -9.769 -33.356 1.00 15.70 C ANISOU 3683 C ALA B 55 1951 2317 1698 -382 476 -152 ATOM 3684 O ALA B 55 -32.334 -9.479 -32.172 1.00 16.50 0 **ANISOU 3684 O ALA B 55** 2089 2451 1730 -380 509 -165 0 ATOM 3685 CB ALA B 55 -30.079 -10.252 -33.737 1.00 14.71 ANISOU 3685 CB ALA B 55 1939 2111 1537 -349 364 -86 ATOM 3686 H ALA B 55 -30.774 -7.866 -34.313 1.00 16.03 H ATOM 3687 HA ALA B 55 -31.606 -10.320 -35.103 1.00 16.86 ATOM 3688 HB1 ALA B 55 -30.212 -11.164 -33.434 1.00 17.65 ATOM 3689 HB2 ALA B 55 -29.377 -10.224 -34.406 1.00 17.65 ATOM 3690 HB3 ALA B 55 -29.845 -9.685 -32.986 1.00 17.65 ATOM 3691 N GLY B 56 -33.715 -10.118 -33.841 1.00 15.90 ANISOU 3691 N GLY B 56 1905 2363 1772 -415 511 -161 Ν ATOM 3692 CA GLY B 56 -34.873 -10.178 -32.970 1.00 16.51 C ANISOU 3692 CA GLY B 56 1941 2502 1830 -451 599 -187 ATOM 3693 C GLY B 56 -34.787 -11.299 -31.956 1.00 17.84 ANISOU 3693 C GLY B 56 2182 2678 1919 -516 655 -135 ATOM 3694 O GLY B 56 -35.346 -11.189 -30.861 1.00 18.84 ANISOU 3694 O GLY B 56 2308 2861 1990 -538 731 -151 0 0 ATOM 3695 H GLY B 56 -33.873 -10.321 -34.661 1.00 19.08 ATOM 3696 HA2 GLY B 56 -34.959 -9.339 -32.492 1.00 19.81 ATOM 3697 HA3 GLY B 56 -35.671 -10.310 -33.505 1.00 19.81 ATOM 3698 N VAL B 57 -34.099 -12.386 -32.305 1.00 17.43 Ν ANISOU 3698 N VAL B 57 2195 2567 1859 -544 622 -69 Ν ATOM 3699 CA VAL B 57 -33.828 -13.490 -31.395 1.00 17.77 С ANISOU 3699 CA VAL B 57 2326 2598 1830 -594 662 0 C ATOM 3700 C VAL B 57 ANISOU 3700 C VAL B 57 -32.349 -13.818 -31.493 1.00 16.12 2203 2331 1591 -555 587 51 ATOM 3701 O VAL B 57 -31.836 -14.081 -32.588 1.00 15.76 ANISOU 3701 O VAL B 57 2153 2228 1605 -538 526 58 0 ANISOU 3701 O VAL B 57 2153 2228 1605 -538 526 58 ATOM 3702 CB VAL B 57 -34.676 -14.737 -31.719 1.00 19.05 ANISOU 3702 CB VAL B 57 2473 2734 2031 -680 714 33 ATOM 3703 CG1 VAL B 57 -34.302 -15.899 -30.798 1.00 20.00 ANISOU 3703 CG1 VAL B 57 2699 2820 2079 -726 756 122 2699 2820 2019 -120 .00 -36.170 -14.423 -31.584 1.00 20.51 C ATOM 3704 CG2 VAL B 57 ANISOU 3704 CG2 VAL B 57 2555 2990 2248 -723 793 -22 ATOM 3705 H VAL B 57 -33.771 -12.507 -33.090 1.00 20.91 H Н ATOM 3706 HA VAL B 57 -34.022 -13.215 -30.485 1.00 21.33 ATOM 3706 HA VAL B 57 -34.022 -13.215 -30.485 1.00 21.33 H ATOM 3707 HB VAL B 57 -34.506 -15.009 -32.634 1.00 22.86 H ATOM 3708 HG11 VAL B 57 -34.850 -16.668 -31.023 1.00 24.00 H ATOM 3709 HG12 VAL B 57 -33.364 -16.112 -30.925 1.00 24.00 H ATOM 3710 HG13 VAL B 57 -34.462 -15.637 -29.878 1.00 24.00 H ATOM 3711 HG21 VAL B 57 -36.680 -15.221 -31.792 1.00 24.61 H ATOM 3712 HG22 VAL B 57 -36.352 -14.142 -30.673 1.00 24.61 H ATOM 3713 HG23 VAL B 57 -36.400 -13.712 -32.202 1.00 24.61 H ATOM 3714 N TRP B 58 -31.669 -13.815 -30.352 1.00 15.50 N ANISOU 3714 N TRP B 58 -30.272 -14.240 -30.294 1.00 15.50 C

ANISOU 3715 CA TRP B 58 2276 2231 1382 -501 519 139 C ATOM 3716 C TRP B 58 -30.121 -15.057 -29.014 1.00 16.41 C Č **ANISOU 3716 C TRP B 58** 2479 2363 1392 -527 559 216 Ŏ ATOM 3717 O TRP B 58 -30.071 -14.506 -27.909 1.00 16.35 2494 2429 1289 -517 579 203 0 **ANISOU 3717 O TRP B 58** ATOM 3718 CB TRP B 58 -29.307 -13.056 -30.350 1.00 15.27 C ANISOU 3718 CB TRP B 58 2236 2222 1344 -433 449 88 ATOM 3719 CG TRP B 58 -27.904 -13.517 -30.240 1.00 16.27 ANISOU 3719 CG TRP B 58 2427 2317 1436 -396 378 ATOM 3720 CD1 TRP B 58 C -26.997 -13.189 -29.270 1.00 17.01 **ANISOU 3720 CD1 TRP B 58** 2566 2455 1441 -363 342 -27.250 -14.447 -31.107 1.00 16.80 C ATOM 3721 CD2 TRP B 58 **ANISOU 3721 CD2 TRP B 58** 2518 2308 1558 -386 335 190 ATOM 3722 NE1 TRP B 58 -25.814 -13.856 -29.490 1.00 17.86 ANISOU 3722 NE1 TRP B 58 2716 2521 1549 -328 205 276 -25.942 -14.629 -30.615 1.00 16.97 C ATOM 3723 CE2 TRP B 58 **ANISOU 3723 CE2 TRP B 58** 2592 2330 1527 -339 274 230 CC ATOM 3724 CE3 TRP B 58 -27.643 -15.136 -32.262 1.00 17.13 ANISOU 3724 CE3 TRP B 58 2536 2285 1687 -411 342 196 CC ATOM 3725 CZ2 TRP B 58 -25.026 -15.478 -31.231 1.00 17.88 **ANISOU 3725 CZ2 TRP B 58** 2734 2377 1680 -310 226 278 Č ATOM 3726 CZ3 TRP B 58 -26.728 -15.979 -32.876 1.00 17.43 Č **ANISOU 3726 CZ3 TRP B 58** 2609 2254 1758 -388 296 238 Č -25.438 -16.147 -32.354 1.00 17.02 ATOM 3727 CH2 TRP B 58 Č 2608 2199 1660 -334 **ANISOU 3727 CH2 TRP B 58** 242 279 ATOM 3728 H TRP B 58 -31.994 -13.571 -29.594 1.00 18.60 Н ATOM 3729 HA TRP B 58 -30.083 -14.820 -31.048 1.00 18.60 Н ATOM 3730 HB2 TRP B 58 -29.413 -12.594 -31.196 1.00 18.33 Н ATOM 3731 HB3 TRP B 58 -29.491 -12.455 -29.611 1.00 18.33 ATOM 3732 HD1 TRP B 58 -27.159 -12.607 -28.563 1.00 20.41 ATOM 3733 HE1 TRP B 58 -25.106 -13.791 -29.005 1.00 21.43 Н ATOM 3734 HE3 TRP B 58 -28.502 -15.038 -32.604 1.00 20.55 ATOM 3735 HZ2 TRP B 58 -24.166 -15.584 -30.895 1.00 21.45 Н ATOM 3736 HZ3 TRP B 58 -26.976 -16.445 -33.641 1.00 20.91 -24.841 -16.709 -32.792 1.00 20.42 ATOM 3737 HH2 TRP B 58 -30.086 -16.380 -29.164 1.00 16.95 ATOM 3738 N ALA B 59 Ν **ANISOU 3738 N ALA B 59** 2601 2363 1475 -561 573 297 -30.127 -17.304 -28.029 1.00 17.50 ATOM 3739 CA ALA B 59 ANISOU 3739 CA ALA B 59 2759 2435 1453 -594 C 624 390 ATOM 3740 C ALA B 59 -29.176 -18.469 -28.275 1.00 18.85 C ANISOU 3740 C ALA B 59 3010 2510 1641 -572 576 482 Ŏ ATOM 3741 O ALA B 59 -29.599 -19.627 -28.396 1.00 19.84 0 **ANISOU 3741 O ALA B 59** 3177 2562 1801 -625 624 545 ATOM 3742 CB ALA B 59 -31.556 -17.798 -27.795 1.00 18.55 C C ANISOU 3742 CB ALA B 59 2870 2580 1599 -686 735 397 ATOM 3743 H ALA B 59 -30.038 -16.775 -29.927 1.00 20.34 Н ATOM 3744 HA ALA B 59 -29.835 -16.838 -27.230 1.00 20.99 Н ATOM 3745 HB1 ALA B 59 -31.559 -18.408 -27.040 1.00 22.26 Н ATOM 3746 HB2 ALA B 59 -32.127 -17.037 -27.609 1.00 22.26 ATOM 3747 HB3 ALA B 59 -31.866 -18.257 -28.592 1.00 22.26 Н ATOM 3748 N PRO B 60 -27.872 -18.199 -28.329 1.00 19.31 Ν ANISOU 3748 N PRO B 60 3092 2566 1681 -493 484 489 Ν ATOM 3749 CA PRO B 60 -26.894 -19.279 -28.491 1.00 21.32 C

ANISOU 3749 CA PRO B 60 3417 2734 1951 -455 436 C 576 ATOM 3750 C PRO B 60 -26.630 -20.026 -27.192 1.00 25.52 ANISOU 3750 C PRO B 60 4050 3275 2370 -450 453 690 0 ATOM 3751 O PROB 60 -26.689 -19.466 -26.096 1.00 24.34 **ANISOU 3751 O PRO B 60** 0 3919 3226 2103 -448 465 694 ATOM 3752 CB PRO B 60 -25.635 -18.534 -28.942 1.00 19.84 C ANISOU 3752 CB PRO B 60 3196 2564 1777 -372 334 ATOM 3753 CG PRO B 60 Č -25.744 -17.212 -28.242 1.00 18.70 Č ANISOU 3753 CG PRO B 60 3015 2534 1558 -365 330 ATOM 3754 CD PRO B 60 C -27.220 -16.875 -28.279 1.00 19.15 C ANISOU 3754 CD PROB 60 3026 2618 1634 -436 420 413 ATOM 3755 HA PRO B 60 Н -27.174 -19.900 -29.181 1.00 25.59 ATOM 3756 HB2 PRO B 60 -24.843 -19.015 -28.654 1.00 23.80 ATOM 3757 HB3 PRO B 60 -25.643 -18.420 -29.905 1.00 23.80 Н ATOM 3758 HG2 PRO B 60 -25.434 -17.298 -27.327 1.00 22.45 Н 3759 HG3 PRO B 60 -25.227 -16.544 -28.720 1.00 22.45 Н ATOM -27.478 -16.401 -27.473 1.00 22.99 ATOM 3760 HD2 PRO B 60 Н ATOM 3761 HD3 PRO B 60 -27.430 -16.364 -29.076 1.00 22.99 Н ATOM 3762 N AASN B 61 -26.324 -21.317 -27.333 0.67 29.16 Ν ANISOU 3762 N AASN B 61 4583 3630 2867 -446 455 N ATOM 3763 N BASN B 61 -26.316 -21.313 -27.338 0.33 29.26 Ν ANISOU 3763 N BASN B 61 4595 3642 2879 -446 455 Ν **785 ATOM 3764 CA AASN B 61** -25.957 -22.175 -26.203 0.67 31.67 C ANISOU 3764 CA AASN B 61 4974 3944 3114 -413 451 901 Č **ATOM 3765 CA BASN B 61** -25.961 -22.185 -26.216 0.33 31.66 C ANISOU 3765 CA BASN B 61 4972 3941 3114 -414 451 901 C ATOM 3766 C AASN B 61 -24.650 -22.874 -26.565 0.67 32.56 ANISOU 3766 C AASN B 61 5134 3975 3263 -329 367 964 Č ATOM 3767 C BASN B 61 -24.647 -22.876 -26.571 0.33 32.51 C ANISOU 3767 C BASN B 61 5127 3967 3257 -329 367 964 ATOM 3768 O AASN B 61 -24.652 -23.925 -27.214 0.67 33.55 0 ANISOU 3768 O AASN B 61 0 5281 3975 3490 -334 381 1000 ATOM 3769 O BASN B 61 -24.644 -23.924 -27.224 0.33 33.43 ANISOU 3769 O BASN B 61 5266 3960 3476 -334 381 1000 **ATOM 3770 CB AASN B 61** CCCCCC -27.065 -23.171 -25.882 0.67 33.95 ANISOU 3770 CB AASN B 61 5275 4184 3441 -485 543 953 ATOM 3771 CB BASN B 61 -27.072 -23.190 -25.925 0.33 34.02 ANISOU 3771 CB BASN B 61 5283 4189 3454 -486 544 952 ATOM 3772 CG AASN B 61 -26.669 -24.154 -24.790 0.67 35.88 ANISOU 3772 CG AASN B 61 5592 4415 3626 -450 537 1085 CC -28.273 -22.555 -25.251 0.33 34.84 ATOM 3773 CG BASN B 61 ANISOU 3773 CG BASN B 61 5342 4394 3502 -551 624 906 0 ATOM 3774 OD1AASN B 61 -25.677 -23.957 -24.087 0.67 36.13 0 ANISOU 3774 OD1AASN B 61 5656 4505 3567 -373 467 1132 **ATOM 3775 OD1BASN B 61** -28.149 -21.545 -24.559 0.33 35.42 0 ANISOU 3775 OD1BASN B 61 5400 4583 3476 -528 611 0 867 **ATOM 3776 ND2AASN B 61** -27.446 -25.223 -24.646 0.67 37.34 Ν ANISOU 3776 ND2AASN B 61 5798 4526 3862 -510 607 1145 Ν -29.444 -23.153 -25.442 0.33 35.96 **ATOM 3777 ND2BASN B 61** Ν ANISOU 3777 ND2BASN B 61 5457 4493 3712 -632 708 Ν **ATOM 3778 H AASN B 61** -26.322 -21.727 -28.089 0.67 35.00 Н ATOM 3779 H BASN B 61 -26.302 -21.716 -28.098 0.33 35.11 Н ATOM 3780 HA AASN B 61 -25.803 -21.626 -25.419 0.67 38.00 Н

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ATOM 3781 HA BASN B 61
                           -25.820 -21.646 -25.422 0.33 37.99
                                                              Н
ATOM 3782 HB2AASN B 61
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ATOM 3783 HB2BASN B 61
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ATOM 3784 HB3AASN B 61
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ATOM 3785 HB3BASN B 61
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ATOM 3786 HD21AASN B 61
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                                                              Н
ATOM 3787 HD21BASN B 61
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ATOM 3788 HD22AASN B 61
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ATOM 3789 HD22BASN B 61
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ATOM 3790 N GLY B 62
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ANISOU 3790 N GLY B 62
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                          -22.222 -22.811 -26.462 1.00 25.93
ATOM 3791 CA GLY B 62
ANISOU 3791 CA GLY B 62
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ATOM 3792 C GLY B 62
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ANISOU 3792 C GLY B 62
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ATOM 3793 O GLY B 62
                          -21.755 -20.733 -27.547 1.00 19.51
                                                            0
ANISOU 3793 O GLY B 62
                          3352 2446 1616 -139 119 805
ATOM 3794 H GLY B 62
                         -23.518 -21.586 -25.640 1.00 35.59
ATOM 3795 HA2 GLY B 62
                          -21.673 -22.840 -25.663 1.00 31.11
ATOM 3796 HA3 GLY B 62
                           -22.307 -23.711 -26.814 1.00 31.11
                                                             Н
ATOM 3797 N TRP B 63
                         -20.687 -22.558 -28.331 1.00 24.75
                                                            Ν
ANISOU 3797 N TRP B 63
                          4078 2927 2397 -56
                                                           N
                                                78 914
ATOM 3798 CA TRP B 63
                          -19.945 -21.793 -29.332 1.00 25.83
                                                             C
ANISOU 3798 CA TRP B 63
                           4123 3086 2606 -18
                                                 19 811
                                                            C
ATOM 3799 C TRP B 63
                         -20.880 -21.500 -30.495 1.00 24.76
ANISOU 3799 C TRP B 63
                          3933 2912 2564 -92
                                                 78 720
ATOM 3800 O TRP B 63
                          -20.959 -22.244 -31.473 1.00 25.80
                                                            0
ANISOU 3800 O TRP B 63
                          4066 2941 2795 -99
                                                 99 711
ATOM 3801 CB TRP B 63
                          -18.693 -22.527 -29.798 1.00 29.13
                                                             C
ANISOU 3801 CB TRP B 63
                          4545 3436 3088 75
                                                 -46
ATOM 3802 CG TRP B 63
                          -17.620 -21.556 -30.248 1.00 30.72
ANISOU 3802 CG TRP B 63
                                           128 -125 765
                          4655 3714 3305
ATOM 3803 CD1 TRP B 63
                           -16.445 -21.278 -29.605 1.00 31.92
ANISOU 3803 CD1 TRP B 63
                          4787 3942 3398 206 -212 786
ATOM 3804 CD2 TRP B 63
                           -17.647 -20.712 -31.412 1.00 30.13
                           4493 3650 3305
ANISOU 3804 CD2 TRP B 63
                                            100 -120
                                                       650
ATOM 3805 NE1 TRP B 63
                           -15.736 -20.324 -30.305 1.00 31.66
ANISOU 3805 NE1 TRP B 63
                           4657 3962 3408 220 -256 686
                                                              C
ATOM 3806 CE2 TRP B 63
                           -16.451 -19.962 -31.415 1.00 29.99
ANISOU 3806 CE2 TRP B 63
                           4409 3708 3276 157 -199
                                                       608
                                                              C
ATOM 3807 CE3 TRP B 63
                           -18.559 -20.526 -32.457 1.00 29.11
ANISOU 3807 CE3 TRP B 63
                           4334 3477 3247 32 -60 582
ATOM 3808 CZ2 TRP B 63
                           -16.147 -19.046 -32.418 1.00 28.97
                                                             C
ANISOU 3808 CZ2 TRP B 63
                           4197 3604 3208 144 -209
                                                       508
                                                             C
                           -18.250 -19.614 -33.454 1.00 27.79
ATOM 3809 CZ3 TRP B 63
ANISOU 3809 CZ3 TRP B 63
                          4085 3341 3131 28 -78 488
                                                             C
ATOM 3810 CH2 TRP B 63
                           -17.058 -18.888 -33.426 1.00 27.91
                           4046 3423 3136
ANISOU 3810 CH2 TRP B 63
                                            82 -147 455
                                                             C
ATOM 3811 H TRP B 63
                                                            Н
                         -20.529 -23.404 -28.339 1.00 29.69
ATOM 3812 HA TRP B 63
                          -19.671 -20.947 -28.945 1.00 31.00
                                                            Н
ATOM 3813 HB2 TRP B 63 -18.338 -23.054 -29.065 1.00 34.96
ATOM 3814 HB3 TRP B 63 -18.917 -23.101 -30.547 1.00 34.96
ATOM 3815 HD1 TRP B 63 -16.165 -21.673 -28.811 1.00 38.30
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ATOM 3816 HE1 TRP B 63 -14.969 -20.007 -30.080 1.00 37.99 ATOM 3817 HE3 TRP B 63 -19.355 -21.006 -32.483 1.00 34.93 Н ATOM 3818 HZ2 TRP B 63 -15.353 -18.563 -32.405 1.00 34.77 -18.850 -19.480 -34.153 1.00 33.34 Н ATOM 3819 HZ3 TRP B 63 -16.879 -18.282 -34.108 1.00 33.49 ATOM 3820 HH2 TRP B 63 ATOM 3821 N GLY B 64 -21.612 -20.401 -30.369 1.00 21.66 ANISOU 3821 N GLY B 64 3490 2603 2135 -144 104 648 ATOM 3822 CA GLY B 64 -22.404 -19.870 -31.453 1.00 18.48 C ANISOU 3822 CA GLY B 64 3020 2190 1810 -198 140 ATOM 3823 C GLY B 64 -22.178 -18.375 -31.508 1.00 18.33 ANISOU 3823 C GLY B 64 2929 2267 1769 -187 105 470 ATOM 3824 O GLY B 64 0 -22.104 -17.730 -30.456 1.00 18.53 ANISOU 3824 O GLY B 64 0 2963 2377 1703 -180 94 ATOM 3825 H GLY B 64 -21.662 -19.939 -29.646 1.00 25.99 ATOM 3826 HA2 GLY B 64 -22.133 -20.268 -32.295 1.00 22.17 ATOM 3827 HA3 GLY B 64 -23.346 -20.048 -31.301 1.00 22.17 -22.052 -17.814 -32.707 1.00 16.88 ATOM 3828 N ALA B 65 Ν 2678 2071 1663 -185 ANISOU 3828 N ALA B 65 Ν 88 395 ATOM 3829 CA ALA B 65 -21.687 -16.414 -32.869 1.00 16.53 C 2571 2097 1613 -170 ANISOU 3829 CA ALA B 65 52 C ATOM 3830 C ALA B 65 -22.622 -15.716 -33.842 1.00 15.60 ANISOU 3830 C ALA B 65 2395 1978 1556 -212 87 250 0 ATOM 3831 O ALA B 65 -23.042 -16.294 -34.851 1.00 14.63 0 **ANISOU 3831 O ALA B 65** 2261 1799 1500 -234 107 245 ATOM 3832 CB ALA B 65 -20.252 -16.270 -33.377 1.00 15.82 ANISOU 3832 CB ALA B 65 2454 2003 1554 -108 -19 308 Н ATOM 3833 H ALA B 65 -22.175 -18.230 -33.450 1.00 20.25 ATOM 3834 HA ALA B 65 Н -21.752 -15.966 -32.011 1.00 19.84 ATOM 3835 HB1 ALA B 65 -20.044 -15.327 -33.472 1.00 18.98 ATOM 3836 HB2 ALA B 65 -19.648 -16.678 -32.736 1.00 18.98 ATOM 3837 HB3 ALA B 65 -20.175 -16.715 -34.235 1.00 18.98 Н -22.925 -14.461 -33.525 1.00 14.18 Ν ATOM 3838 N LEU B 66 ANISOU 3838 N LEU B 66 2177 1861 1352 -220 195 90 **ATOM 3839 CA LEU B 66** -23.635 -13.548 -34.412 1.00 14.37 2138 1890 1431 -240 ANISOU 3839 CA LEU B 66 107 131 C ATOM 3840 C LEU B 66 -22.577 -12.635 -35.017 1.00 14.25 ANISOU 3840 C LEU B 66 2087 1882 1447 -203 92 53 ATOM 3841 O LEUB 66 -21.986 -11.813 -34.307 1.00 13.46 0 1982 1823 1308 -185 ANISOU 3841 O LEU B 66 27 ATOM 3842 CB LEU B 66 -24.684 -12.755 -33.634 1.00 14.24 ANISOU 3842 CB LEU B 66 2106 1927 1379 -266 96 153 ATOM 3843 CG LEU B 66 -25.480 -11.672 -34.367 1.00 13.49 ANISOU 3843 CG LEU B 66 1944 1842 1339 -273 170 33 ATOM 3844 CD1 LEU B 66 C -26.318 -12.283 -35.480 1.00 14.40 ANISOU 3844 CD1 LEU B 66 2030 1923 1517 -302 191 ATOM 3845 CD2 LEU B 66 -26.352 -10.905 -33.396 1.00 15.73 C ANISOU 3845 CD2 LEU B 66 2214 2180 1583 -286 217 -5 ATOM 3846 H LEU B 66 -22.721 -14.104 -32.770 1.00 17.02 Н **ATOM 3847 HA LEU B 66** -24.073 -14.043 -35.122 1.00 17.24 Н ATOM 3848 HB2 LEU B 66 -25.330 -13.386 -33.281 1.00 17.09 Н ATOM 3849 HB3 LEU B 66 -24.234 -12.318 -32.894 1.00 17.09 ATOM 3850 HG LEU B 66 -24.860 -11.045 -34.771 1.00 16.18 ATOM 3851 HD11 LEU B 66 -26.811 -11.577 -35.927 1.00 17.28

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ATOM 3852 HD12 LEU B 66 -25.729 -12.726 -36.111 1.00 17.28
                                                                                                          Н
ATOM 3853 HD13 LEU B 66 -26.935 -12.925 -35.095 1.00 17.28
ATOM 3854 HD21 LEU B 66 -26.846 -10.227 -33.883 1.00 18.88
ATOM 3855 HD22 LEU B 66 -26.969 -11.522 -32.971 1.00 18.88
ATOM 3856 HD23 LEU B 66 -25.788 -10.488 -32.727 1.00 18.88
                                                                                                         Н
                                            -22.327 -12.785 -36.317 1.00 13.46 N
ATOM 3857 N ALA B 67
ANISOU 3857 N ALA B 67
                                            1960 1742 1412 -197
ATOM 3858 CA ALA B 67 -21.119 -12.221 -36.898 1.00 12.44
                                                                                                     C
ANISOU 3858 CA ALA B 67 1805 1613 1309 -165
                                                                                     -8
ATOM 3859 C ALA B 67
                                            -21.275 -12.019 -38.394 1.00 12.54
                                                                                                       C
ANISOU 3859 C ALA B 67
                                             1782 1600 1384 -172
ATOM 3860 O ALA B 67 -21.908 -12.825 -39.088 1.00 12.59
                                                                                                        0
ANISOU 3860 O ALA B 67 1793 1577 1414 -191 17 50 O ATOM 3861 CB ALA B 67 -19.914 -13.136 -36.650 1.00 13.22 C
ANISOU 3861 CB ALA B 67 1930 1697 1395 -129 -44 100 C
ATOM 3862 H ALA B 67 -22.834 -13.201 -36.873 1.00 16.15 H
ATOM 3863 HA ALA B 67 -20.938 -11.359 -36.491 1.00 14.93
ATOM 3864 HB1 ALA B 67 -19.126 -12.734 -37.048 1.00 15.86
ATOM 3865 HB2 ALA B 67 -19.787 -13.237 -35.693 1.00 15.86
ATOM 3866 HB3 ALA B 67 -20.085 -14.000 -37.055 1.00 15.86
                                                                                                   N
N
ATOM 3867 N LEU B 68 -20.653 -10.951 -38.884 1.00 11.11
                                           1565 1430 1225 -161 -26
ANISOU 3867 N LEU B 68
                                                                                           10
ATOM 3868 CA LEU B 68 -20.350 -10.861 -40.304 1.00 10.81
                                                                                                     С
ANISOU 3868 CA LEU B 68 1501 1374 1232 -159 -31
ATOM 3869 C LEU B 68 -19.313 -11.923 -40.638 1.00 12.05
ANISOU 3869 C LEU B 68 1671 1511 1398 -136 -48 19
ATOM 3870 O LEU B 68 -18.281 -12.014 -39.969 1.00 12.91
ANISOU 3870 O LEU B 68 1782 1631 1492 -110 -75 26
                                                                                                       0
                                          1782 1631 1492 -110 -75
ANISOU 3870 O LEU B 68
ATOM 3871 CB LEU B 68 -19.825 -9.467 -40.650 1.00 11.27 C
ANISOU 3871 CB LEU B 68 1527 1443 1312 -155 -43 -26
ATOM 3872 CG LEU B 68 -19.511 -9.195 -42.116 1.00 12.95
ANISOU 3872 CG LEU B 68 1715 1645 1560 -157 -43 -27
ATOM 3873 CD1 LEU B 68 -20.781 -9.049 -42.904 1.00 13.98
ANISOU 3873 CD1 LEU B 68 1837 1774 1699 -170 -24 -23 ATOM 3874 CD2 LEU B 68 -18.658 -7.933 -42.230 1.00 13.61
ATOM 3874 CD2 LEU B 68 -18.658 -7.933 -42.230 1.00 13.61 C ANISOU 3874 CD2 LEU B 68 1776 1732 1665 -157 -52 -44 C ATOM 3875 H LEU B 68 -20.399 -10.273 -38.420 1.00 13.33 H ATOM 3876 HA LEU B 68 -21.152 -11.032 -40.823 1.00 12.97 H ATOM 3877 HB2 LEU B 68 -20.490 -8.816 -40.375 1.00 13.52 H ATOM 3878 HB3 LEU B 68 -19.007 -9.319 -40.150 1.00 13.52 H ATOM 3879 HG LEU B 68 -19.007 -9.939 -42.481 1.00 15.54 H ATOM 3880 HD11 LEU B 68 -20.558 -8.878 -43.833 1.00 16.77 H ATOM 3881 HD12 LEU B 68 -21.292 -9.871 -42.833 1.00 16.77 H ATOM 3882 HD13 LEU B 68 -21.292 -8.308 -42.544 1.00 16.77 H ATOM 3883 HD21 LEU B 68 -18.463 -7.768 -43.165 1.00 16.34 H ATOM 3884 HD22 LEU B 68 -19.151 -7.185 -41.857 1.00 16.34 H ATOM 3885 HD23 LEU B 68 -17.833 -8.064 -41.737 1.00 16.34 H ATOM 3886 N VAL B 69 -19.607 -12.756 -41.638 1.00 11.57 N ANISOU 3886 N VAL B 69 1614 1421 1359 -144 -32 21 N
ANISOU 3886 N VAL B 69 1614 1421 1359 -144 -32 21
ATOM 3887 CA VAL B 69 -18.718 -13.826 -42.078 1.00 11.37 ANISOU 3887 CA VAL B 69 1601 1367 1353 -119 -39 29
                                                                                                     C
ATOM 3888 C VAL B 69 -18.557 -13.732 -43.587 1.00 10.91
ANISOU 3888 C VAL B 69 1517 1309 1320 -126 -30 1
                                                                                                       C
```

ATOM 3889 O VAL B 69 -19.552 -13.670 -44.316 1.00 12.49 0 **ANISOU 3889 O VAL B 69** 1712 1512 1520 -157 -13 -12 C ATOM 3890 CB VAL B 69 -19.260 -15.214 -41.684 1.00 12.53 ANISOU 3890 CB VAL B 69 1796 1466 1499 -125 -21 ATOM 3891 CG1 VAL B 69 -18.341 -16.340 -42.189 1.00 14.23 C **ANISOU 3891 CG1 VAL B 69** 2026 1636 1746 -90 -24 58 ATOM 3892 CG2 VAL B 69 -19.423 -15.295 -40.170 1.00 12.04 **ANISOU 3892 CG2 VAL B 69** 1765 1412 1396 -119 -26 93 C ATOM 3893 H VAL B 69 -20.339 -12.718 -42.087 1.00 13.88 Н ATOM 3894 HA VAL B 69 -17.846 -13.710 -41.669 1.00 13.65 Н ATOM 3895 HB VAL B 69 -20.134 -15.337 -42.087 1.00 15.04 ATOM 3896 HG11 VAL B 69 -18.714 -17.195 -41.923 1.00 17.08 Н ATOM 3897 HG12 VAL B 69 ATOM 3898 HG13 VAL B 69 -18.283 -16.290 -43.156 1.00 17.08 -17.461 -16.226 -41.798 1.00 17.08 Н ATOM 3899 HG21 VAL B 69 -19.765 -16.172 -39.936 1.00 14.44 ATOM 3900 HG22 VAL B 69 -18.559 -15.153 -39.752 1.00 14.44 Н ATOM 3901 HG23 VAL B 69 ATOM 3902 N GLY B 70 -20.046 -14.609 -39.883 1.00 14.44 -17.315 -13.757 -44.057 1.00 9.84 Ν ANISOU 3902 N GLY B 70 1360 1178 1201 -98 -40 -10 ATOM 3903 CA GLY B 70 -17.076 -13.739 -45.486 1.00 9.14 ANISOU 3903 CA GLY B 70 1251 1097 1125 -105 -24 -37 C ATOM 3904 C GLY B 70 -15.737 -14.359 -45.815 1.00 11.06 ANISOU 3904 C GLY B 70 ATOM 3905 O GLY B 70 1479 1333 1391 -67 -24 -51 0 -14.974 -14.765 -44.931 1.00 11.65 **ANISOU 3905 O GLY B 70** 1554 1398 1476 -28 -45 -35 ATOM 3906 H GLY B 70 -16.604 -13.784 -43.573 1.00 11.81 ATOM 3907 HA2 GLY B 70 -17.772 -14.239 -45.942 1.00 10.97 ATOM 3908 HA3 GLY B 70 -17.085 -12.825 -45.809 1.00 10.97 ATOM 3909 N TRPB 71 -15.462 -14.421 -47.118 1.00 11.43 **ANISOU 3909 N TRP B 71** 1509 1393 1442 -74 -1 -80 ATOM 3910 CA TRP B 71 -14.265 -15.058 -47.638 1.00 13.04 C **ANISOU 3910 CA TRP B 71** 1691 1594 1671 -37 11 -106 C ATOM 3911 C TRP B 71 -13.654 -14.216 -48.743 1.00 13.31 **ANISOU 3911 C TRP B 71** 1683 1678 1694 -54 33 -127 ATOM 3912 O TRP B 71 -14.360 -13.547 -49.499 1.00 13.10 0 **ANISOU 3912 O TRP B 71** 1663 1677 1639 -93 45 -124 ATOM 3913 CB TRP B 71 -14.550 -16.436 -48.245 1.00 14.66 C ANISOU 3913 CB TRP B 71 1930 1751 1890 -28 **35** -136 ATOM 3914 CG TRP B 71 C -14.994 -17.490 -47.305 1.00 16.25 **ANISOU 3914 CG TRP B 71** 2178 1886 2111 -12 26 -113 ATOM 3915 CD1 TRP B 71 -16.271 -17.732 -46.892 1.00 16.42 **ANISOU 3915 CD1 TRP B 71** 2239 1881 2120 -51 **27** -96 C ATOM 3916 CD2 TRP B 71 -14.178 -18.493 -46.700 1.00 16.81 **ANISOU 3916 CD2 TRP B 71** C 2261 1905 2220 49 19 -101 ATOM 3917 NE1 TRP B 71 -16.296 -18.815 -46.061 1.00 15.87 **ANISOU 3917 NE1 TRP B 71** 2213 1743 2075 -27 27 -70 ATOM 3918 CE2 TRP B 71 -15.022 -19.299 -45.918 1.00 16.35 **ANISOU 3918 CE2 TRP B 71** 2262 1784 2167 40 18 -67 -12.811 -18.779 -46.731 1.00 16.81 ATOM 3919 CE3 TRP B 71 **ANISOU 3919 CE3 TRP B 71** 2224 1909 2253 114 C 13 -111 ATOM 3920 CZ2 TRP B 71 -14.547 -20.369 -45.172 1.00 17.84 C ANISOU 3920 CZ2 TRP B 71 2485 1905 2390 95 10 C ATOM 3921 CZ3 TRP B 71 -12.340 -19.845 -45.993 1.00 18.06

ANISOU 3921 CZ3 TRP B 71 2407 2004 2449 177 0 -84	С
ATOM 3922 CH2 TRP B 71 -13.207 -20.626 -45.221 1.00 18.34	С
ANISOU 3922 CH2 TRP B 71 2514 1970 2486 169 -3 -41	С
ATOM 3923 H TRP B 71 -15.968 -14.092 -47.730 1.00 13.72	Н
ATOM 3924 HA TRP B 71 -13.613 -15.159 -46.926 1.00 15.65	Н
ATOM 3925 HB2 TRP B 71 -15.245 -16.335 -48.914 1.00 17.60	н
ATOM 3926 HB3 TRP B 71 -13.738 -16.753 -48.670 1.00 17.60	H
ATOM 3927 HD1 TRP B 71 -17.016 -17.238 -47.147 1.00 19.71	H
ATOM 3928 HE1 TRP B 71 -16.997 -19.133 -45.678 1.00 19.04	H
ATOM 3929 HE3 TRP B 71 -12.229 -18.262 -47.241 1.00 20.17	H
ATOM 3930 HZ2 TRP B 71 -15.120 -20.891 -44.659 1.00 21.41	Ĥ
ATOM 3931 HZ3 TRP B 71 -11.432 -20.044 -46.006 1.00 21.67	H
ATOM 3932 HH2 TRP B 71 -12.862 -21.339 -44.733 1.00 22.01	H
ATOM 3933 N THR B 72 -12.332 -14.296 -48.849 1.00 14.10	N
ANISOU 3933 N THR B 72 1741 1796 1821 -22 41 -144	N N
ATOM 3934 CA THR B 72 -11.623 -13.989 -50.079 1.00 14.23	С
ANISOU 3934 CA THR B 72 1721 1855 1832 -33 80 -173	C
ATOM 3935 C THR B 72 -10.844 -15.217 -50.526 1.00 15.89	Č
ANISOU 3935 C THR B 72 1919 2050 2071 15 105 -217	Č
ATOM 3936 O THR B 72 -10.610 -16.151 -49.754 1.00 15.63	Ö
ANISOU 3936 O THR B 72 1896 1970 2073 64 85 -215	o
ATOM 3937 CB THR B 72 -10.643 -12.815 -49.920 1.00 13.34	C
ANISOU 3937 CB THR B 72 1550 1786 1731 -46 81 -163	C
ATOM 3938 OG1 THR B 72 -9.566 -13.200 -49.061 1.00 14.04	O
ANISOU 3938 OG1 THR B 72 1596 1877 1863 1 57 -172	o
ATOM 3939 CG2 THR B 72 -11.332 -11.586 -49.375 1.00 13.11	C
ANISOU 3939 CG2 THR B 72 1536 1758 1688 -87 58 -126	C
ATOM 3940 H THR B 72 -11.813 -14.532 -48.205 1.00 16.92	н
ATOM 3940 II THIR B 72 -11.813 -14.332 -48.203 1.00 10.92 ATOM 3941 HA THR B 72 -12.264 -13.763 -50.772 1.00 17.08	'н
ATOM 3942 HB THR B 72 -10.282 -12.590 -50.792 1.00 16.00	H
ATOM 3943 HG1 THR B 72 -9.864 -13.414 -48.305 1.00 16.85	H
ATOM 3944 HG21 THR B 72 -10.694 -10.861 -49.285 1.00 15.74	
ATOM 3945 HG22 THR B 72 -12.041 -11.309 -49.977 1.00 15.74	H
ATOM 3946 HG23 THR B 72 -11.715 -11.779 -48.505 1.00 15.74	H
ATOM 3947 N ARG B 73 -10.471 -15.208 -51.801 1.00 16.34	Ν
ANISOU 3947 N ARG B 73 1957 2143 2108 1 153 -256	N.
ATOM 3948 CA ARG B 73 -9.443 -16.074 -52.358 1.00 18.19	``c
ANISOU 3948 CA ARG B 73 2157 2380 2373 46 190 -309	č
ATOM 3949 C ARG B 73 -8.251 -15.220 -52.772 1.00 17.36	c
ANISOU 3949 C ARG B 73 1977 2344 2273 38 220 -317	Č
ATOM 3950 O ARG B 73 -8.358 -13.997 -52.917 1.00 16.21	ŏ
ANISOU 3950 O ARG B 73 1822 2239 2100 -15 222 -284	ŏ
ATOM 3951 CB ARG B 73 -9.970 -16.858 -53.567 1.00 18.67	C
ANISOU 3951 CB ARG B 73 2257 2435 2400 32 232 -364	C
ATOM 3952 CG ARG B 73 -11.085 -17.833 -53.253 1.00 19.23	C
ANISOU 3952 CG ARG B 73 2396 2434 2478 32 211 -370	C
ATOM 3953 CD ARG B 73 -11.427 -18.677 -54.491 1.00 20.43	Č
ANISOU 3953 CD ARG B 73 2576 2584 2603 16 255 -446	Č
ATOM 3954 NE ARG B 73 -12.325 -19.783 -54.168 1.00 22.27	N
ANISOU 3954 NE ARG B 73	N
ATOM 3955 CZ ARG B 73 -13.645 -19.783 -54.356 1.00 23.31	Č
ANISOU 3955 CZ ARG B 73	C
ATOM 3956 NH1 ARG B 73 -14.268 -18.738 -54.885 1.00 24.54	N
A 1 O 11 3330 11 A 10 O D 13 - 14.200 - 10.730 - 34.003 1.00 24.34	IA

	3188 3095 3041 -95 214 -441	N
	-14.348 -20.846 -54.019 1.00 24.18	N
ANISOU 3957 NH2 ARG B 73		N
	0.818 -14.683 -52.387 1.00 19.61	Н
ATOM 3959 HA ARG B 73	-9.151 -16.707 -51.683 1.00 21.82	Н
ATOM 3960 HB2 ARG B 73	-10.307 -16.226 -54.221 1.00 22.40	Н
ATOM 3961 HB3 ARG B 73	-9.236 -17.364 -53.950 1.00 22.40	Н
ATOM 3962 HG2 ARG B 73	-10.803 -18.430 -52.543 1.00 23.08	Н
ATOM 3963 HG3 ARG B 73	-11.879 -17.342 -52.988 1.00 23.08	Н
ATOM 3964 HD2 ARG B 73	-11.864 -18.115 -55.150 1.00 24.52	Н
	-10.610 -19.049 -54.859 1.00 24.52	Н
ATOM 3966 HE ARG B 73 -	11.975 -20.491 -53.828 1.00 26.73	Н
ATOM 3967 HH11 ARG B 73	-13.820 -18.039 -55.109 1.00 29.45	Н
	-15.120 -18.759 -55.000 1.00 29.45	H
	-13.956 -21.531 -53.678 1.00 29.02	H
		H
	7.104 -15.869 -52.930 1.00 19.18	Ν
ANISOU 3971 N SER B 74 2		N
ATOM 3972 CA SER B 74 -		C
	2251 2839 2742 81 288 -380	Č
	5.439 -14.118 -52.435 1.00 19.35	C
	042 2704 2605 59 247 -337	C
	5.327 -12.945 -52.822 1.00 18.92	Ö
		o
		_
	6.106 -14.636 -54.804 1.00 22.53	C
	2506 3136 2917 17 352 -393	C
	-6.323 -15.680 -55.736	0
ANISOU 3976 OG SER B 74		O H
ATOM 3977 H SER B 74 -7		
	5.178 -15.869 -53.456 1.00 24.74	H.
	-6.882 -14.054 -54.793	Н
	-5.318 -14.135 -55.067 1.00 27.03	Н
	5.657 -16.192 -55.753 1.00 30.65	H
	5.136 -14.461 -51.175 1.00 18.66	N.
	935 2591 2563 111 185 -323	N
	-5.150 -15.812 -50.606 1.00 18.11	C
	1889 2464 2529 194 155 -330	С
	5.511 -16.212 -50.037 1.00 17.26	C
	880 2285 2393 187 118 -291	С
	7.395 -15.367 -49.887 1.00 16.98	0
	884 2253 2315 125 105 -258	0
	-4.100 -15.734 -49.486 1.00 19.83	C
	2030 2710 2796 246 101 -320	С
	-3.634 -14.294 -49.433 1.00 19.22	C
	1891 2701 2709 175 103 -315	С
	-4.620 -13.484 -50.206 1.00 18.62	C
	1878 2618 2578 90 141 -298	C
ATOM 3989 HA PRO B 75	-4.870 -16.464 -51.268 1.00 21.74	Н
	-4.507 -15.990 -48.643 1.00 23.80	Н
ATOM 3991 HB3 PRO B 75	-3.358 -16.323 -49.696 1.00 23.80	Н
ATOM 3992 HG2 PRO B 75	-3.606 -13.999 -48.510 1.00 23.06	Н
ATOM 3993 HG3 PRO B 75	-2.754 -14.227 -49.835 1.00 23.06	Н
ATOM 3994 HD2 PRO B 75	-5.331 -13.169 -49.627 1.00 22.34	Н

ATOM 3995 HD3 PRO B 75 -4.176 -12.752 -50.663 1.00 22.34 Н ATOM 3996 N LEUB 76 -6.670 -17.495 -49.722 1.00 16.65 **ANISOU 3996 N LEU B 76** 1841 2140 2344 249 107 -295 **ATOM 3997 CA LEUB 76** C -7.899 -17.983 -49.106 1.00 16.13 Č ANISOU 3997 CA LEU B 76 1865 2004 2260 240 78 -257 -7.933 -17.564 -47.637 1.00 15.96 ATOM 3998 C LEUB 76 **ANISOU 3998 C LEU B 76** 1844 1986 2233 251 12 -197 ATOM 3999 O LEUB 76 0 -7.152 -18.062 -46.821 1.00 16.73 **ANISOU 3999 O LEU B 76** 1914 2077 2365 321 0 -26 -179 C ATOM 4000 CB LEU B 76 -7.983 -19.497 -49.242 1.00 16.67 1977 1988 2370 298 ANISOU 4000 CB LEU B 76 ATOM 4001 CG LEU B 76 -9.224 -20.170 -48.669 1.00 16.57 ANISOU 4001 CG LEU B 76 2057 1892 2348 282 78 -243 ATOM 4002 CD1 LEU B 76 -10.465 -19.768 -49.448 1.00 15.12 **ANISOU 4002 CD1 LEU B 76** 1915 1718 2111 194 103 -261 -9.046 -21.692 -48.649 1.00 18.01 ATOM 4003 CD2 LEU B 76 2278 1975 2591 350 93 -2 -6.079 -18.105 -49.857 1.00 19.98 C **ANISOU 4003 CD2 LEU B 76** 93 -259 ATOM 4004 H LEU B 76 Н **ATOM 4005 HA LEUB 76** -8.664 -17.591 -49.555 1.00 19.36 Н ATOM 4006 HB2 LEU B 76 -7.947 -19.718 -50.186 1.00 20.01 Н ATOM 4007 HB3 LEU B 76 -7.214 -19.884 -48.794 1.00 20.01 Н ATOM 4008 HG LEU B 76 -9.343 -19.875 -47.752 1.00 19.89 Н ATOM 4009 HD11 LEU B 76 -11.237 -20.210 -49.061 1.00 18.14 Н ATOM 4010 HD12 LEU B 76 -10.574 -18.805 -49.394 1.00 18.14 Н ATOM 4011 HD13 LEU B 76 -10.358 -20.038 -50.373 1.00 18.14 Н ATOM 4012 HD21 LEU B 76 -9.846 -22.099 -48.282 1.00 21.62 Н -8.903 -22.004 -49.557 1.00 21.62 ATOM 4013 HD22 LEU B 76 Н ATOM 4014 HD23 LEU B 76 Н -8.278 -21.913 -48.098 1.00 21.62 ATOM 4015 N ILE B 77 -8.834 -16.646 -47.299 1.00 15.13 N **ANISOU 4015 N ILE B 77** 1769 1896 2083 186 -4 -167 ATOM 4016 CA ILE B 77 -8.964 -16.127 -45.940 1.00 14.83 C **ANISOU 4016 CA ILE B 77** 1737 1871 2027 185 -60 -122 ATOM 4017 C ILE B 77 -10.439 -16.073 -45.580 1.00 14.50 **ANISOU 4017 C ILE B 77** 1772 1792 1946 140 -61 -91 ATOM 4018 O ILE B 77 -11.256 -15.582 -46.364 1.00 14.60 0 **ANISOU 4018 O ILE B 77** 1803 1808 1936 84 -31 -104 CCCCCC ATOM 4019 CB ILE B 77 -8.346 -14.723 -45.788 1.00 15.45 ANISOU 4019 CB ILE B 77 1750 2022 2097 147 -73 -131 ATOM 4020 CG1 ILE B 77 -6.852 -14.764 -46.112 1.00 17.24 **ANISOU 4020 CG1 ILE B 77** 1886 2297 2369 185 -68 -166 ATOM 4021 CG2 ILE B 77 -8.571 -14.197 -44.359 1.00 16.24 **ANISOU 4021 CG2 ILE B 77** 1863 2137 2171 142 -130 -98 C -6.203 -13.389 -46.234 1.00 18.59 ATOM 4022 CD1 ILE B 77 C 1987 2535 2542 129 -63 -186 **ANISOU 4022 CD1 ILE B 77** -9.394 -16.300 -47.852 1.00 18.15 ATOM 4023 H ILE B 77 Н **ATOM 4024 HA ILE B 77** -8.518 -16.727 -45.321 1.00 17.80 Н ATOM 4025 HB ILE B 77 -8.782 -14.123 -46.413 1.00 18.54 Н -6.393 -15.246 -45.406 1.00 20.69 Н ATOM 4026 HG12 ILE B 77 Н ATOM 4027 HG13 ILE B 77 -6.728 -15.225 -46.956 1.00 20.69 ATOM 4028 HG21 ILE B 77 -8.176 -13.314 -44.282 1.00 19.49 ATOM 4029 HG22 ILE B 77 -9.524 -14.150 -44.186 1.00 19.49 ATOM 4031 HD11 ILE B 77 -8.150 -14.804 -43.730 1.00 19.49 -5.262 -13.501 -46.439 1.00 22.31 Н Н Ĥ

ATOM 4032 HD12 ILE B 77 -6.641 -12.896 -46.946 1.00 22.31 Н ATOM 4033 HD13 ILE B 77 -6.305 -12.917 -45.393 1.00 22.31 Н ATOM 4034 N ALA B 78 -10.772 -16.539 -44.382 1.00 12.83 Ν **ANISOU 4034 N ALA B 78** 1601 1552 1723 165 -97 -47 Ν **ATOM 4035 CA ALAB 78** C -12.084 -16.326 -43.793 1.00 11.78 ANISOU 4035 CA ALA B 78 1527 1400 1550 120 -99 -17 ATOM 4036 C ALA B 78 ANISOU 4036 C ALA B 78 C -11.986 -15.151 -42.836 1.00 11.63 1485 1437 1498 99 -135 -5 ATOM 4037 O ALA B 78 -11.026 -15.051 -42.067 1.00 11.88 0 **ANISOU 4037 O ALA B 78** 1482 1504 1529 138 -177 ATOM 4038 CB ALA B 78 -12.565 -17.569 -43.043 1.00 12.20 ANISOU 4038 CB ALA B 78 1645 1386 1604 150 -105 26 Н ATOM 4039 H ALA B 78 -10.240 -16.992 -43.880 1.00 15.40 **ATOM 4040 HA ALAB 78** -12.726 -16.112 -44.488 1.00 14.14 Н ATOM 4041 HB1 ALA B 78 -13.440 -17.391 -42.665 1.00 14.64 ATOM 4042 HB2 ALA B 78 -12.617 -18.312 -43.664 1.00 14.64 Н ATOM 4043 HB3 ALA B 78 -11.934 -17.774 -42.335 1.00 14.64 ATOM 4044 N TYR B 79 N -12.971 -14.264 -42.875 1.00 11.66 ANISOU 4044 N TYR B 79 1505 1452 1475 42 -121 **ATOM 4045 CA TYR B 79** -12.980 -13.131 -41.961 1.00 12.10 ANISOU 4045 CA TYR B 79 1546 1550 1503 20 -147 C ATOM 4046 C TYR B 79 -14.300 -13.076 -41.207 1.00 11.87 ANISOU 4046 C TYR B 79 ATOM 4047 O TYR B 79 1569 1505 1435 -7 -140 -15.340 -13.537 -41.693 1.00 11.61 0 **ANISOU 4047 O TYR B 79** 1570 1438 1404 -28 -109 21 -12.713 -11.801 -42.687 1.00 12.02 **ATOM 4048 CB TYR B 79** C ANISOU 4048 CB TYR B 79 1489 1568 1508 -20 -132 -42 ATOM 4049 CG TYR B 79 -13.741 -11.401 -43.713 1.00 11.52 ANISOU 4049 CG TYR B 79 1446 1486 1446 -60 -93 -45 ATOM 4050 CD1 TYR B 79 -14.924 -10.789 -43.335 1.00 11.06 **ANISOU 4050 CD1 TYR B 79** 1415 1420 1367 -89 -88 -37 C ATOM 4051 CD2 TYR B 79 -13.510 -11.601 -45.064 1.00 12.31 **ANISOU 4051 CD2 TYR B 79** 1530 1583 1562 -65 -63 ATOM 4052 CE1 TYR B 79 -15.859 -10.409 -44.272 1.00 11.58 **ANISOU 4052 CE1 TYR B 79** 1490 1477 1434 -116 -61 -36 ATOM 4053 CE2 TYR B 79 -14.436 -11.228 -46.013 1.00 10.84 **ANISOU 4053 CE2 TYR B 79** 1361 1393 1366 -97 -36 C **ATOM 4054 CZ TYR B 79** -15.610 -10.628 -45.612 1.00 10.61 ANISOU 4054 CZ TYR B 79 1355 1356 1320 -120 -40 -43 ATOM 4055 OH TYR B 79 0 -16.545 -10.260 -46.547 1.00 10.96 ANISOU 4055 OH TYR B 79 1407 1402 1353 -144 -23 -37 0 ATOM 4056 H TYR B 79 -13.640 -14.294 -43.415 1.00 14.00 Н **ATOM 4057 HA TYR B 79** -12.274 -13.255 -41.308 1.00 14.52 Н ATOM 4058 HB2 TYR B 79 -12.673 -11.094 -42.024 1.00 14.42 ATOM 4059 HB3 TYR B 79 -11.859 -11.866 -43.142 1.00 14.42 ATOM 4060 HD1 TYR B 79 -15.094 -10.640 -42.433 1.00 13.27 Н -12.718 -12.006 -45.336 1.00 14.77 ATOM 4061 HD2 TYR B 79 -16.654 -10.007 -44.003 1.00 13.90 ATOM 4062 HE1 TYR B 79 ATOM 4063 HE2 TYR B 79 -14.270 -11.377 -46.915 1.00 13.01 ATOM 4064 HH TYR B 79 -16.270 -10.448 -47.318 1.00 13.15 Н ATOM 4065 N TYR B 80 -14.232 -12.495 -40.011 1.00 12.28 Ν ANISOU 4065 N TYR B 80 1622 1592 1450 -8 -169 ATOM 4066 CA TYR B 80 -15.334 -12.465 -39.057 1.00 12.09 C

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ANISOU 4066 CA TYR B 80 1645 1567 1381 -28 -161
                                                              C
ATOM 4067 C TYR B 80
                          -15.353 -11.125 -38.325 1.00 12.97
                                                              C
ANISOU 4067 C TYR B 80
                           1738 1724 1467 -53 -174
ATOM 4068 O TYR B 80
                                                              0
                          -14.315 -10.675 -37.829 1.00 14.02
ANISOU 4068 O TYR B 80
                          1837 1897 1591
                                            -41 -213 -18
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ATOM 4069 CB TYR B 80
                           -15.195 -13.588 -38.019 1.00 13.64
                                                              C
ANISOU 4069 CB TYR B 80 1885 1758 1539
                                            9 -182
                                                       87
ATOM 4070 CG TYR B 80
                           -14.901 -14.966 -38.587 1.00 13.85
ANISOU 4070 CG TYR B 80
                          1933 1728 1602
                                             46 -175
ATOM 4071 CD1 TYR B 80
                           -13.615 -15.322 -38.974 1.00 15.00
                                                               C
ANISOU 4071 CD1 TYR B 80
                            2040 1877 1784 97 -203
                                                               C
ATOM 4072 CD2 TYR B 80
                           -15.905 -15.911 -38.711 1.00 14.64
ANISOU 4072 CD2 TYR B 80
                           2087 1769 1706
                                             29 -136
ATOM 4073 CE1 TYR B 80
                           -13.345 -16.581 -39.490 1.00 15.85
ANISOU 4073 CE1 TYR B 80
                           2167 1923 1931 137 -191
                                                        132
                           -15.646 -17.167 -39.222 1.00 16.35
ATOM 4074 CE2 TYR B 80
ANISOU 4074 CE2 TYR B 80
                           2327 1920 1963
                                             60 -125
                           -14.362 -17.498 -39.604 1.00 16.49
ATOM 4075 CZ TYR B 80
ANISOU 4075 CZ TYR B 80
                           2311 1936 2018 118 -152 159
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ATOM 4076 OH TYR B 80
                           -14.098 -18.748 -40.112 1.00 17.58
                                                               0
ANISOU 4076 OH TYR B 80
                           2475 2001 2204 156 -136 171
ATOM 4077 H TYR B 80
                          -13.527 -12.097 -39.720 1.00 14.73
                                                              Н
ATOM 4078 HA TYR B 80
                           -16.175 -12.576 -39.526 1.00 14.51
                                                             Н
ATOM 4079 HB2 TYR B 80
                          -14.471 -13.361 -37.416 1.00 16.37
ATOM 4080 HB3 TYR B 80
                           -16.025 -13.649 -37.521 1.00 16.37
ATOM 4081 HD1 TYR B 80
                           -12.926 -14.702 -38.896 1.00 18.01
ATOM 4082 HD2 TYR B 80
                           -16.772 -15.693 -38.454 1.00 17.57
ATOM 4083 HE1 TYR B 80
                           -12.480 -16.806 -39.748 1.00 19.02
ATOM 4084 HE2 TYR B 80
                           -16.332 -17.790 -39.302 1.00 19.62
                           -14.801 -19.207 -40.127 1.00 21.10
ATOM 4085 HH TYR B 80
ATOM 4086 N VAL B 81
                          -16.526 -10.499 -38.233 1.00 11.64
                                                              Ν
ANISOU 4086 N VAL B 81
                          1586 1549 1288 -87 -143 -10
                                                             Ν
ATOM 4087 CA VAL B 81
                           -16.766 -9.408 -37.289 1.00 10.09
ANISOU 4087 CA VAL B 81 1387 1386 1061 -107 -147 -44 ATOM 4088 C VAL B 81 -17.837 -9.906 -36.329 1.00 10.41
ANISOU 4088 C VAL B 81
                         1475 1435 1046 -113 -125 -21
ATOM 4089 O VAL B 81
                                                              o
o
                          -19.019 -9.978 -36.679 1.00 11.02
ANISOU 4089 O VAL B 81
                          1563 1489 1136 -132 -83 -15
ATOM 4090 CB VAL B 81
                           -17.188 -8.101 -37.974 1.00 11.67
ANISOU 4090 CB VAL B 81 1561 1567 1304 -135 -122 -83
ATOM 4091 CG1 VAL B 81
                           -17.430 -7.019 -36.947 1.00 13.76
ANISOU 4091 CG1 VAL B 81
                           1828 1855 1544 -152 -122 -129
ATOM 4092 CG2 VAL B 81
                           -16.115 -7.660 -38.967 1.00 12.15
                                                               Č
                            1581 1620 1417 -138 -134 -96
ANISOU 4092 CG2 VAL B 81
ATOM 4093 H VAL B 81
                          -17.211 -10.693 -38.715 1.00 13.97
                                                              Н
ATOM 4094 HA VAL B 81
                           -15.956 -9.238 -36.782 1.00 12.11
                                                              Н
ATOM 4095 HB VAL B 81
                           -18.013 -8.248 -38.462 1.00 14.00
                                                              Н
ATOM 4096 HG11 VAL B 81
                          -17.695 -6.205 -37.403 1.00 16.51
                                                              Н
ATOM 4097 HG12 VAL B 81
                            -18.135 -7.306 -36.346 1.00 16.51
ATOM 4098 HG13 VAL B 81
                          -16.612 -6.868 -36.448 1.00 16.51
                                                               Н
ATOM 4099 HG21 VAL B 81 -16.398 -6.834 -39.390 1.00 14.58
ATOM 4100 HG22 VAL B 81 -15.282 -7.519 -38.490 1.00 14.58
ATOM 4101 HG23 VAL B 81 -16.001 -8.352 -39.637 1.00 14.58
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ATOM 4102 N VAL B 82 -17.422 -10.269 -35.124 1.00 10.70
ANISOU 4102 N VAL B 82
                          1536 1512 1018 -96 -153
ATOM 4103 CA VAL B 82
                          -18.283 -10.940 -34.158 1.00 10.43
                                                              C
ANISOU 4103 CA VAL B 82 1554 1490 920 -102 -129
                                                       32
ATOM 4104 C VAL B 82
                          -18.867 -9.902 -33.211 1.00 10.50
ANISOU 4104 C VAL B 82
                          1566 1545 880 -127 -112 -17
ATOM 4105 O VAL B 82
                                                             0
                          -18.132 -9.278 -32.436 1.00 10.94
ANISOU 4105 O VAL B 82
                          1612 1651 892 -122 -150 -54
ATOM 4106 CB VAL B 82
                          -17.506 -12.008 -33.375 1.00 11.55
                                                              C
ANISOU 4106 CB VAL B 82
                           1731 1651 1008 -64 -170
ATOM 4107 CG1 VAL B 82
                           -18.431 -12.735 -32.416 1.00 12.98
                           1974 1838 1118 -76 -135 143
ANISOU 4107 CG1 VAL B 82
ATOM 4108 CG2 VAL B 82
                           -16.798 -12.986 -34.333 1.00 11.89
                           1765 1640 1112 -29 -187 128
ANISOU 4108 CG2 VAL B 82
ATOM 4109 H VAL B 82
                          -16.624 -10.133 -34.833 1.00 12.84
                                                             Н
ATOM 4110 HA VAL B 82
                          -19.014 -11.375 -34.625 1.00 12.52
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ATOM 4111 HB VAL B 82
                          -16.822 -11.567 -32.847 1.00 13.87
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ATOM 4112 HG11 VAL B 82
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                                                              Н
ATOM 4113 HG12 VAL B 82
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ATOM 4114 HG13 VAL B 82
                           -19.139 -13.161 -32.924 1.00 15.57
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ATOM 4115 HG21 VAL B 82
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                                                               Н
ATOM 4116 HG22 VAL B 82
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                                                               Н
                           -16.179 -12.489 -34.891 1.00 14.27
ATOM 4117 HG23 VAL B 82
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ATOM 4118 N ASP B 83
                          -20.193 -9.741 -33.243 1.00 10.93
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ANISOU 4118 N ASP B 83
                           1628 1587 938 -153 -54 -25
ATOM 4119 CA ASP B 83
                           -20.887 -8.826 -32.345 1.00 12.05
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ANISOU 4119 CA ASP B 83
                           1772 1769 1037 -173 -24 -77
                                                             C
                                                             C
ATOM 4120 C ASP B 83
                          -21.414 -9.499 -31.080 1.00 12.34
ANISOU 4120 C ASP B 83
                           1859 1854 976 -182
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                                                           C
                          -21.480 -8.852 -30.026 1.00 13.43
ATOM 4121 O ASP B 83
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ANISOU 4121 O ASP B 83
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ATOM 4122 CB ASP B 83
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                           1807 1804 1171 -189
ANISOU 4122 CB ASP B 83
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ATOM 4123 CG ASP B 83
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ANISOU 4123 CG ASP B 83
                           1818 1828 1290 -183
                                                  9 -165
ATOM 4124 OD1 ASP B 83
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                           2004 2032 1476 -178 -35 -189
ANISOU 4124 OD1 ASP B 83
ATOM 4125 OD2 ASP B 83
                           -22.420 -6.286 -34.544 1.00 12.90
ANISOU 4125 OD2 ASP B 83
                           1779 1784 1339 -184
                                                  39 -182
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ATOM 4126 H ASP B 83
                          -20.715 -10.157 -33.785 1.00 13.12
                                                             Н
ATOM 4127 HA ASP B 83
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ATOM 4128 HB2 ASP B 83
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ATOM 4129 HB3 ASP B 83
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                                                              Н
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ATOM 4130 N SER B 84
                                                             Ν
ANISOU 4130 N SER B 84
                          1959 1894 1030 -185
                                                  22
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ATOM 4131 CA SER B 84
                          -22.204 -11.484 -29.942 1.00 14.62
                                                              C
ANISOU 4131 CA SER B 84
                          2240 2158 1157 -197
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                                                       80
                                                             C
ATOM 4132 C SER B 84
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ANISOU 4132 C SER B 84
                         2362 2187 1234 -185
ATOM 4133 O SER B 84
                                                             0
                          -21.632 -13.466 -31.189 1.00 13.96
ANISOU 4133 O SER B 84 2186 1962 1156 -172 26 193
ATOM 4134 CB SER B 84 -23.677 -11.232 -29.629 1.00 14.98
                                                             C
ANISOU 4134 CB SER B 84 2280 2221 1191 -238 133
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ATOM 4135 OG SER B 84 -24.007 -11.773 -28.350 1.00 16.39 0 ANISOU 4135 OG SER B 84 2516 2453 1259 -255 166 98 ATOM 4136 H SER B 84 -21.779 -11.255 -31.855 1.00 15.42 Н ATOM 4137 HA SER B 84 Н -21.681 -11.170 -29.188 1.00 17.54 ATOM 4138 HB2 SER B 84 -23.842 -10.277 -29.622 1.00 17.98 -24.223 -11.661 -30.306 1.00 17.98 ATOM 4139 HB3 SER B 84 ATOM 4140 HG SER B 84 -24.818 -11.633 -28.180 1.00 19.67 ATOM 4141 N TRP B 85 -22.095 -13.695 -28.997 1.00 16.46 Ν ANISOU 4141 N TRP B 85 Ν 2581 2375 1297 -189 58 **ATOM 4142 CA TRP B 85** -21.780 -15.114 -28.962 1.00 16.48 C ANISOU 4142 CA TRP B 85 2642 2324 1295 -171 **50** ATOM 4143 C TRPB 85 -22.406 -15.702 -27.705 1.00 17.66 C **ANISOU 4143 C TRP B 85** 2863 2511 1336 -197 98 411 ATOM 4144 O TRP B 85 0 -22.911 -14.977 -26.842 1.00 18.99 **ANISOU 4144 O TRP B 85** 3031 2760 1424 -222 129 371 ATOM 4145 CB TRP B 85 -20.263 -15.336 -28.995 1.00 16.58 ANISOU 4145 CB TRP B 85 2654 2340 1306 -104 -42 368 C ATOM 4146 CG TRP B 85 -19.550 -14.708 -27.835 1.00 18.10 ANISOU 4146 CG TRP B 85 2853 2634 1389 -80 -96 353 ATOM 4147 CD1 TRP B 85 -19.252 -15.300 -26.644 1.00 19.83 **ANISOU 4147 CD1 TRP B 85** 3136 2905 1493 -56 -120 429 C ATOM 4148 CD2 TRP B 85 -19.051 -13.367 -27.749 1.00 18.10 **ANISOU 4148 CD2 TRP B 85** 2796 2700 1382 -80 -135 253 -18.595 -14.419 -25.824 1.00 20.16 N ATOM 4149 NE1 TRP B 85 Ν **ANISOU 4149 NE1 TRP B 85** 3159 3052 1448 -42 -176 376 C ATOM 4150 CE2 TRP B 85 -18.457 -13.225 -26.476 1.00 19.33 **ANISOU 4150 CE2 TRP B 85** 2979 2952 1413 -59 -184 263 C ATOM 4151 CE3 TRP B 85 -19.042 -12.277 -28.624 1.00 17.13 **ANISOU 4151 CE3 TRP B 85** 2604 2560 1345 -97 -132 159 ATOM 4152 CZ2 TRP B 85 -17.865 -12.033 -26.054 1.00 19.38 **ANISOU 4152 CZ2 TRP B 85** 2942 3038 1384 -63 -230 168 ATOM 4153 CZ3 TRP B 85 -18.450 -11.097 -28.204 1.00 17.60 C **ANISOU 4153 CZ3 TRP B 85** 2627 2686 1377 -99 -172 **75** C ATOM 4154 CH2 TRP B 85 -17.874 -10.984 -26.932 1.00 18.76 2798 2927 1404 -85 -220 73 **ANISOU 4154 CH2 TRP B 85** C ATOM 4155 H TRP B 85 -22.380 -13.380 -28.249 1.00 19.75 Н ATOM 4156 HA TRP B 85 -22.171 -15.551 -29.734 1.00 19.77 Н ATOM 4157 HB2 TRP B 85 -20.084 -16.290 -28.974 1.00 19.90 Н ATOM 4158 HB3 TRP B 85 -19.906 -14.950 -29.810 1.00 19.90 ATOM 4159 HD1 TRP B 85 -19.462 -16.178 -26.421 1.00 23.79 ATOM 4160 HE1 TRP B 85 -18.317 -14.589 -25.028 1.00 24.19 ATOM 4161 HE3 TRP B 85 -19.423 -12.343 -29.470 1.00 20.56 Н ATOM 4162 HZ2 TRP B 85 -17.479 -11.956 -25.211 1.00 23.26 Н ATOM 4163 HZ3 TRP B 85 -18.440 -10.364 -28.776 1.00 21.13 Н ATOM 4164 HH2 TRP B 85 -17.485 -10.178 -26.680 1.00 22.52 Н ATOM 4165 N GLY B 86 -22.378 -17.028 -27.615 1.00 21.40 Ν ANISOU 4165 N GLY B 86 2744 2653 2735 -228 492 946 Ν ATOM 4166 CA GLY B 86 -22.877 -17.694 -26.429 1.00 23.54 2902 3002 3041 -231 ANISOU 4166 CA GLY B 86 554 1294 ATOM 4167 C GLY B 86 -21.773 -17.873 -25.416 1.00 24.64 ANISOU 4167 C GLY B 86 3089 3204 3067 -152 544 1423 C ATOM 4168 O GLY B 86 -21.509 -16.984 -24.601 1.00 24.56 0 ANISOU 4168 O GLY B 86 3156 3440 2735 -35 589 1421

ATOM 4169 H GLY B 86 -22.078 -17.557 -28.223 1.00 25.68 Н ATOM 4170 HA2 GLY B 86 -23.587 -17.166 -26.029 1.00 28.25 Н ATOM 4171 HA3 GLY B 86 -23.231 -18.566 -26.665 1.00 28.25 ATOM 4172 N THR B 87 -21.114 -19.023 -25.465 1.00 26.31 Ν ANISOU 4172 N THR B 87 3249 3191 3558 -208 467 1519 Ν ATOM 4173 CA THR B 87 -19.937 -19.296 -24.653 1.00 29.55 ANISOU 4173 CA THR B 87 3702 3623 3905 -142 434 1627 ATOM 4174 C THR B 87 -18.781 -19.543 -25.608 1.00 30.08 ANISOU 4174 C THR B 87 3848 3448 4132 -160 322 1361 C ATOM 4175 O THR B 87 -18.760 -20.560 -26.311 1.00 31.66 **ANISOU 4175 O THR B 87** 3968 3379 4683 -241 244 1329 ATOM 4176 CB THR B 87 -20.172 -20.494 -23.737 1.00 32.65 ANISOU 4176 CB THR B 87 3929 3978 4499 -179 448 2040 ATOM 4177 OG1 THR B 87 -21.282 -20.212 -22.876 1.00 34.38 **ANISOU 4177 OG1 THR B 87** 4055 4478 4531 -140 556 2243 -18.930 -20.797 -22.901 1.00 33.49 ATOM 4178 CG2 THR B 87 **ANISOU 4178 CG2 THR B 87** 4072 4116 4536 -105 406 2164 ATOM 4179 H THR B 87 -21.336 -19.679 -25.975 1.00 31.58 Н ATOM 4180 HA THR B 87 -19.730 -18.522 -24.106 1.00 35.47 Н ATOM 4181 HB THR B 87 -20.374 -21.274 -24.276 1.00 39.18 Н ATOM 4182 HG1 THR B 87 -21.972 -20.070 -23.334 1.00 41.26 ATOM 4183 HG21 THR B 87 -19.096 -21.560 -22.326 1.00 40.18 ATOM 4184 HG22 THR B 87 -18.180 -20.998 -23.483 1.00 40.18 ATOM 4185 HG23 THR B 87 -18.706 -20.030 -22.351 1.00 40.18 ATOM 4186 N ALA B 88 -17.831 -18.616 -25.636 1.00 28.98 3848 3408 3754 -76 304 1165 **ANISOU 4186 N ALA B 88** ATOM 4187 CA ALA B 88 -16.714 -18.707 -26.560 1.00 29.53 ANISOU 4187 CA ALA B 88 3981 3305 3934 -77 215 921 ATOM 4188 C ALA B 88 -15.578 -17.852 -26.031 1.00 29.39 C 4078 3421 3669 ANISOU 4188 C ALA B 88 21 195 854 ATOM 4189 O ALA B 88 -15.814 -16.772 -25.482 1.00 30.35 0 ANISOU 4189 O ALA B 88 4259 3756 3516 86 236 834 ATOM 4190 CB ALA B 88 -17.108 -18.251 -27.971 1.00 28.21 ANISOU 4190 CB ALA B 88 3833 3087 3799 -113 205 639 ATOM 4191 H ALA B 88 -17.813 -17.923 -25.128 1.00 34.77 Н ATOM 4192 HA ALA B 88 -16.409 -19.627 -26.609 1.00 35.44 ATOM 4193 HB1 ALA B 88 -16.336 -18.327 -28.554 1.00 33.85 ATOM 4194 HB2 ALA B 88 -17.826 -18.816 -28.296 1.00 33.85 ATOM 4195 HB3 ALA B 88 -17.403 -17.328 -27.932 1.00 33.85 Н ATOM 4196 N ARG B 89 -14.352 -18.343 -26.205 1.00 28.37 Ν **ANISOU 4196 N ARG B 89** 3965 3154 3660 36 119 803 Ν ATOM 4197 CA ARG B 89 -13.146 -17.618 -25.834 1.00 27.70 ANISOU 4197 CA ARG B 89 3971 3154 3400 117 76 726 ATOM 4198 C ARG B 89 -12.192 -17.616 -27.015 1.00 26.94 **ANISOU 4198 C ARG B 89** 3893 2919 3425 111 18 498 ATOM 4199 O ARG B 89 -11.983 -18.656 -27.649 1.00 28.71 0 **ANISOU 4199 O ARG B 89** 4053 2956 3900 77 -18 ATOM 4200 CB ARG B 89 -12.477 -18.251 -24.615 1.00 29.15 ANISOU 4200 CB ARG B 89 44 958 4133 3362 3579 163 ATOM 4201 CG ARG B 89 -13.388 -18.313 -23.425 1.00 30.79 ANISOU 4201 CG ARG B 89 4294 3768 3638 191 111 1220 ATOM 4202 CD ARG B 89 -12.660 -18.751 -22.180 1.00 30.95 ANISOU 4202 CD ARG B 89 4292 3886 3581 263 78 1452

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ATOM 4203 NE ARG B 89 -13.518 -18.580 -21.009 1.00 33.04
                                                            Ν
ANISOU 4203 NE ARG B 89 4506 4439 3606 327
                                                155 1688
                                                            N
ATOM 4204 CZ ARG B 89
                          -13.333 -17.683 -20.045 1.00 33.53
ANISOU 4204 CZ ARG B 89
                         4625 4799 3317 460 151 1665
ATOM 4205 NH1 ARG B 89
                          -12.295 -16.857 -20.069 1.00 31.72
ANISOU 4205 NH1 ARG B 89
                          4503 4583 2967 526
                                                 58 1426
ATOM 4206 NH2 ARG B 89
                          -14.193 -17.623 -19.037 1.00 36.55
ANISOU 4206 NH2 ARG B 89
                          4926 5430 3530 505 219 1781
                                                            Ν
                         -14.193 -19.116 -26.547 1.00 34.04
ATOM 4207 H ARG B 89
                                                           Н
ATOM 4208 HA ARG B 89
                          -13.372 -16.700 -25.618 1.00 33.24
                                                          Н
ATOM 4209 HB2 ARG B 89
                          -12.210 -19.157 -24.835 1.00 34.97
ATOM 4210 HB3 ARG B 89
                          -11.700 -17.725 -24.371 1.00 34.97
                                                           Н
ATOM 4211 HG2 ARG B 89
                          -13.761 -17.432 -23.263 1.00 36.95
ATOM 4212 HG3 ARG B 89
                          -14.098 -18.949 -23.600 1.00 36.95
                                                           Н
ATOM 4213 HD2 ARG B 89
                          -12.424 -19.689 -22.255 1.00 37.14
ATOM 4214 HD3 ARG B 89
                                                            Н
                          -11.865 -18.208 -22.061 1.00 37.14
ATOM 4215 HE ARG B 89
                          -14.199 -19.101 -20.939 1.00 39.64
                                                           Н
ATOM 4216 HH11 ARG B 89
                         -11.734 -16.889 -20.720 1.00 38.07
                                                           Н
ATOM 4217 HH12 ARG B 89
                         -12.186 -16.284 -19.436 1.00 38.07
ATOM 4218 HH21 ARG B 89
                          -14.866 -18.158 -19.013 1.00 43.86
                                                            Н
ATOM 4219 HH22 ARG B 89 -14.076 -17.051 -18.406 1.00 43.86
                                                            Н
ATOM 4220 N TRP B 90
                        -11.630 -16.451 -27.320 1.00 24.08
ANISOU 4220 N TRP B 90
                         3598 2652 2899 153 4 345
ATOM 4221 CA TRP B 90
                         -10.718 -16.310 -28.444 1.00 23.43
ANISOU 4221 CA TRP B 90
                          3510 2500 2893 160 -33
                                                   163
ATOM 4222 C TRPB 90
                         -9.274 -16.374 -27.970 1.00 23.55
ANISOU 4222 C TRP B 90 3542 2486 2920 214 -102 191
                                                          C
ATOM 4223 O TRP B 90 -8.874 -15.649 -27.048 1.00 24.36
                                                          0
ANISOU 4223 O TRP B 90
                       3695 2687 2872 258 -134 246
                         -10.989 -15.010 -29.199 1.00 22.34
                                                          C
ATOM 4224 CB TRP B 90
ANISOU 4224 CB TRP B 90 3396 2475 2619 161
                                                -8 24
ATOM 4225 CG TRP B 90 -12.136 -15.191 -30.150 1.00 21.63
ANISOU 4225 CG TRP B 90
                          3262 2381 2574
                                          110
                                                44
                                                   -52
ATOM 4226 CD1 TRP B 90
                          -12.063 -15.512 -31.471 1.00 21.45
ANISOU 4226 CD1 TRP B 90
                         3183 2326 2641 102 41 -202
ATOM 4227 CD2 TRP B 90
                          -13.532 -15.111 -29.832 1.00 21.62
ANISOU 4227 CD2 TRP B 90
                          3256 2429 2528
                                            71
                                                    14
                                                99
ATOM 4228 NE1 TRP B 90
                          -13.327 -15.629 -32.000 1.00 21.56
                                                            N
                          3163 2355 2674
ANISOU 4228 NE1 TRP B 90
                                            56
                                                77 -244
                                                           Ν
ATOM 4229 CE2 TRP B 90
                          -14.246 -15.392 -31.012 1.00 21.20
ANISOU 4229 CE2 TRP B 90
                          3147 2347 2562
                                            28
                                                116 -103
ATOM 4230 CE3 TRP B 90
                          -14.244 -14.825 -28.664 1.00 21.81
ANISOU 4230 CE3 TRP B 90
                          3306 2548 2432 83
                                                135 158
ATOM 4231 CZ2 TRP B 90
                                                            C
                          -15.637 -15.392 -31.060 1.00 21.52
ANISOU 4231 CZ2 TRP B 90
                          3157 2418 2601 -20
                                                162 -70
ATOM 4232 CZ3 TRP B 90
                          -15.624 -14.822 -28.713 1.00 22.08
                                                            C
ANISOU 4232 CZ3 TRP B 90
                         3305 2631 2455
                                            42
                                               197 200
ATOM 4233 CH2 TRP B 90
                          -16.307 -15.100 -29.904 1.00 21.98
                                                          C
ANISOU 4233 CH2 TRP B 90 3237 2556 2558 -17 208 92
                                                           C
ATOM 4234 H TRP B 90 -11.762 -15.722 -26.885 1.00 28.90 H
ATOM 4235 HA TRP B 90 -10.863 -17.046 -29.059 1.00 28.12
                                                          Н
ATOM 4236 HB2 TRP B 90 -11.219 -14.310 -28.567 1.00 26.81
                                                          Н
ATOM 4237 HB3 TRP B 90 -10.202 -14.762 -29.709 1.00 26.81
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ATOM 4238 HD1 TRP B 90 -11.273 -15.642 -31.944 1.00 25.74 Н ATOM 4239 HE1 TRP B 90 -13.511 -15.824 -32.817 1.00 25.87 Н ATOM 4240 HE3 TRP B 90 -13.798 -14.644 -27.868 1.00 26.17 -16.093 -15.567 -31.852 1.00 25.82 ATOM 4241 HZ2 TRP B 90 Н ATOM 4242 HZ3 TRP B 90 -16.108 -14.636 -27.941 1.00 26.50 Н ATOM 4243 HH2 TRP B 90 -17.237 -15.091 -29.907 1.00 26.38 Н ATOM 4244 N THR B 91 -8.515 -17.268 -28.587 1.00 23.00 **ANISOU 4244 N THR B 91** 3420 2281 3037 220 -135 136 Ν ATOM 4245 CA THR B 91 -7.087 -17.411 -28.379 1.00 23.52 3481 2306 3149 272 -199 ANISOU 4245 CA THR B 91 142 ATOM 4246 C THR B 91 ANISOU 4246 C THR B 91 -6.416 -17.305 -29.736 1.00 21.95 3230 2099 3010 297 -198 -42 C ATOM 4247 O THR B 91 0 -6.874 -17.913 -30.707 1.00 23.91 0 **ANISOU 4247 O THR B 91** 3425 2299 3363 289 -176 -163 ATOM 4248 CB THR B 91 -6.744 -18.769 -27.729 1.00 25.70 ANISOU 4248 CB THR B 91 3715 2431 3618 279 -243 282 ATOM 4249 OG1 THR B 91 -7.153 -18.775 -26.360 1.00 26.40 3834 2593 3604 278 -241 **ANISOU 4249 OG1 THR B 91** 501 ATOM 4250 CG2 THR B 91 -5.238 -19.073 -27.798 1.00 26.37 3774 2449 3798 337 -310 C ANISOU 4250 CG2 THR B 91 ATOM 4251 H THR B 91 -8.825 -17.831 -29.159 1.00 27.60 Н ATOM 4252 HA THR B 91 -6.762 -16.696 -27.808 1.00 28.22 Н ATOM 4253 HB THR B 91 -7.214 -19.473 -28.202 1.00 30.84 Н ATOM 4254 HG1 THR B 91 -6.966 -19.514 -26.008 1.00 31.68 Н ATOM 4255 HG21 THR B 91 -5.054 -19.931 -27.383 1.00 31.65 Н ATOM 4256 HG22 THR B 91 -4.948 -19.102 -28.723 1.00 31.65 -4.739 -18.384 -27.332 1.00 31.65 ATOM 4257 HG23 THR B 91 Н ATOM 4258 N GLY B 92 -5.340 -16.540 -29.814 1.00 18.65 **ANISOU 4258 N GLY B 92** 2811 1748 2528 335 -228 -62 ATOM 4259 CA GLY B 92 -4.578 -16.488 -31.043 1.00 17.52 ANISOU 4259 CA GLY B 92 2589 1640 2429 376 -216 -191 C ATOM 4260 C GLY B 92 -3.735 -15.234 -31.100 1.00 16.02 C ANISOU 4260 C GLY B 92 C 2383 1555 2148 390 -237 -162 0 ATOM 4261 O GLY B 92 -3.634 -14.479 -30.132 1.00 15.93 **ANISOU 4261 O GLY B 92** 2430 1555 2068 375 -288 -78 0 ATOM 4262 H GLY B 92 -5.035 -16.048 -29.178 1.00 22.38 Н ATOM 4263 HA2 GLY B 92 -3.994 -17.260 -31.100 1.00 21.03 Н ATOM 4264 HA3 GLY B 92 -5.180 -16.494 -31.803 1.00 21.03 Н ATOM 4265 N THR B 93 -3.118 -15.048 -32.259 1.00 16.00 Ν **ANISOU 4265 N THR B 93** 2283 1638 2157 429 -207 -234 ATOM 4266 CA THR B 93 -2.351 -13.842 -32.508 1.00 15.50 2162 1673 2053 432 -225 -173 ANISOU 4266 CA THR B 93 C ATOM 4267 C THR B 93 -3.251 -12.633 -32.319 1.00 15.28 C **ANISOU 4267 C THR B 93** C 2181 1693 1930 373 -224 -137 ATOM 4268 O THR B 93 -4.398 -12.619 -32.777 1.00 14.75 0 0 **ANISOU 4268 O THR B 93** 2135 1671 1796 347 -164 -191 ATOM 4269 CB THR B 93 -1.761 -13.877 -33.920 1.00 16.28 ANISOU 4269 CB THR B 93 2119 1916 2152 493 -164 -226 ATOM 4270 OG1 THR B 93 -0.857 -14.981 -34.011 1.00 17.04 2165 1962 2348 568 -177 -282 **ANISOU 4270 OG1 THR B 93** 0 ATOM 4271 CG2 THR B 93 -1.010 -12.591 -34.247 1.00 16.14 ANISOU 4271 CG2 THR B 93 2002 2005 2126 484 -177 -103 C ATOM 4272 H THR B 93 -3.129 -15.605 -32.914 1.00 19.20 Н

ATOM 4273 HA THR B 93 -1.621 -13.785 -31.871 1.00 18.60 Н -2.475 -13.990 -34.567 1.00 19.54 ATOM 4274 HB THR B 93 Н Н ATOM 4275 HG1 THR B 93 -1.264 -15.699 -33.857 1.00 20.45 ATOM 4276 HG21 THR B 93 -0.647 -12.639 -35.145 1.00 19.37 ATOM 4277 HG22 THR B 93 -1.612 -11.833 -34.190 1.00 19.37 Н ATOM 4278 HG23 THR B 93 -0.282 -12.464 -33.619 1.00 19.37 ATOM 4279 N TYR B 94 -2.742 -11.648 -31.594 1.00 14.57 **ANISOU 4279 N TYR B 94** 2103 1579 1854 359 -308 -62 Ν ATOM 4280 CA TYR B 94 -3.493 -10.464 -31.213 1.00 14.91 ANISOU 4280 CA TYR B 94 2188 1634 1843 321 -344 -51 ATOM 4281 C TYR B 94 -2.769 -9.250 -31.781 1.00 15.73 ANISOU 4281 C TYR B 94 2172 1770 2036 309 -392 21 C ATOM 4282 O TYR B 94 -1.578 -9.051 -31.510 1.00 16.32 2186 1800 2214 323 -473 **ANISOU 4282 O TYR B 94** ATOM 4283 CB TYR B 94 -3.631 -10.375 -29.691 1.00 15.78 CCCC ANISOU 4283 CB TYR B 94 2408 1678 1910 334 -434 -52 ATOM 4284 CG TYR B 94 -4.114 -9.020 -29.243 1.00 15.17 ANISOU 4284 CG TYR B 94 2351 1607 1805 326 -509 -79 ATOM 4285 CD1 TYR B 94 -5.410 -8.610 -29.508 1.00 16.01 2487 1761 1833 304 -447 -118 ANISOU 4285 CD1 TYR B 94 ATOM 4286 CD2 TYR B 94 -3.267 -8.138 -28.586 1.00 15.80 2406 1632 1965 347 -658 -81 ANISOU 4286 CD2 TYR B 94 ATOM 4287 CE1 TYR B 94 -5.857 -7.362 -29.128 1.00 17.19 2644 1903 1985 311 -525 -162 C ANISOU 4287 CE1 TYR B 94 ATOM 4288 CE2 TYR B 94 -3.711 -6.886 -28.193 1.00 17.82 C ANISOU 4288 CE2 TYR B 94 2666 1866 2238 355 -755 -143 ATOM 4289 CZ TYR B 94 -5.010 -6.506 -28.471 1.00 17.46 2652 1868 2115 340 -684 -185 ANISOU 4289 CZ TYR B 94 C ATOM 4290 OH TYR B 94 -5.469 -5.267 -28.089 1.00 19.01 0 ANISOU 4290 OH TYR B 94 2844 2030 2349 361 -788 -265 0 ATOM 4291 H TYR B 94 -1.934 -11.645 -31.301 1.00 17.48 ATOM 4292 HA TYR B 94 -4.381 -10.503 -31.602 1.00 17.89 ATOM 4293 HB2 TYR B 94 -4.272 -11.039 -29.391 1.00 18.94 ATOM 4294 HB3 TYR B 94 -2.766 -10.538 -29.283 1.00 18.94 ATOM 4295 HD1 TYR B 94 -5.987 -9.184 -29.957 1.00 19.21 Н ATOM 4296 HD2 TYR B 94 -2.392 -8.393 -28.403 1.00 18.96 ATOM 4297 HE1 TYR B 94 -6.732 -7.105 -29.309 1.00 20.63 Н Н ATOM 4298 HE2 TYR B 94 -3.137 -6.304 -27.750 1.00 21.38 Н ATOM 4299 HH TYR B 94 -4.859 -4.841 -27.699 1.00 22.81 Н ATOM 4300 N LYS B 95 -3.481 -8.447 -32.573 1.00 15.11 N 2040 1763 1936 278 -348 ANISOU 4300 N LYS B 95 41 ATOM 4301 CA LYS B 95 -2.858 -7.377 -33.336 1.00 18.07 ANISOU 4301 CA LYS B 95 2259 2184 2423 C 261 -375 ATOM 4302 C LYS B 95 -3.206 -5.975 -32.853 1.00 19.19 2393 2234 2664 223 -489 C **ANISOU 4302 C LYS B 95** 193 ATOM 4303 O LYS B 95 -2.567 -5.016 -33.297 1.00 21.46 0 **ANISOU 4303 O LYS B 95** 2531 2506 3117 199 -550 0 ATOM 4304 CB LYS B 95 -3.242 -7.506 -34.819 1.00 19.91 ANISOU 4304 CB LYS B 95 2383 2603 2578 270 -243 204 ATOM 4305 CG LYS B 95 -2.740 -8.776 -35.509 1.00 23.36 ANISOU 4305 CG LYS B 95 2780 3153 2945 336 -151 147 ATOM 4306 CD LYS B 95 -1.211 -8.891 -35.417 1.00 27.20 ANISOU 4306 CD LYS B 95 3165 3627 3541 371 -194 233 C

ATOM 4307 CE LYS B 95	-0.543 -8.945 -36.775 1.00 30.30	С
ANISOU 4307 CE LYS B 95	3359 4253 3899 434 -100 321	C
ATOM 4308 NZ LYS B 95	-0.565 -10.315 -37.343 1.00 31.88	N
ANISOU 4308 NZ LYS B 95	3569 4556 3987 527 -15 152	N
ATOM 4309 H LYS B 95	-4.332 -8.506 -32.683 1.00 18.13	Н
		Ή
	-1.895 -7.476 -33.273 1.00 21.68	
ATOM 4311 HB2 LYS B 95	-4.210 -7.499 -34.889 1.00 23.89	Н
ATOM 4312 HB3 LYS B 95	-2.876 -6.748 -35.300 1.00 23.89	Н
ATOM 4313 HG2 LYS B 95	-3.131 -9.552 -35.077 1.00 28.04	Н
ATOM 4314 HG3 LYS B 95	-2.988 -8.752 -36.446 1.00 28.04	H
ATOM 4315 HD2 LYS B 95	-0.864 -8.118 -34.943 1.00 32.64	Н
ATOM 4316 HD3 LYS B 95	-0.983 -9.703 -34.938 1.00 32.64	Н
ATOM 4317 HE2 LYS B 95	-1.013 -8.356 -37.386 1.00 36.35	Н
ATOM 4318 HE3 LYS B 95	0.382 -8.668 -36.688 1.00 36.35	Н
ATOM 4319 HZ1 LYS B 95	-0.135 -10.875 -36.802 1.00 38.25	H
ATOM 4320 HZ2 LYS B 95	-1.405 -10.592 -37.438 1.00 38.25	Н
ATOM 4321 HZ3 LYS B 95	-0.168 -10.320 -38.140 1.00 38.25	Н
ATOM 4322 N GLY B 96	-4.184 -5.823 -31.961 1.00 17.88	N
ANISOU 4322 N GLY B 96	2364 2007 2423 226 -525 78	N
_	-4.630 -4.523 -31.516 1.00 17.58	C
ANISOU 4323 CA GLY B 96	2318 1884 2479 215 -640 55	С
ATOM 4324 C GLY B 96	-6.139 -4.457 -31.515 1.00 15.73	С
ANISOU 4324 C GLY B 96	2168 1698 2109 215 -567 -25	С
ATOM 4325 O GLY B 96	-6.825 -5.483 -31.442 1.00 13.88	0
ANISOU 4325 O GLY B 96	2030 1537 1709 224 -457 -81	Ŏ
ATOM 4326 H GLY B 96	-4.607 -6.477 -31.597 1.00 21.46	Н
ATOM 4327 HA2 GLY B 96	-4.308 -4.353 -30.617 1.00 21.10	Н
ATOM 4328 HA3 GLY B 96	-4.287 -3.836 -32.108 1.00 21.10	Н
ATOM 4329 N THR B 97	-6.664 -3.235 -31.615 1.00 14.87	N
ANISOU 4329 N THR B 97	2007 1538 2105 202 -637 -21	Ň
ATOM 4330 CA THR B 97	-8.096 -2.994 -31.518 1.00 14.39	C
ANISOU 4330 CA THR B 97	2015 1515 1939 211 -587 -102	С
ATOM 4331 C THR B 97	-8.568 -2.068 -32.632 1.00 14.52	C
ANISOU 4331 C THR B 97	1901 1549 2068 167 -566 11	C
ATOM 4332 O THR B 97	-7.797 -1.287 -33.195 1.00 15.79	ŏ
ANISOU 4332 O THR B 97	1910 1656 2433 136 -638 153	0
ATOM 4333 CB THR B 97	-8.469 -2.373 -30.158 1.00 15.03	C
ANISOU 4333 CB THR B 97	2181 1514 2014 279 -721 -265	С
ATOM 4334 OG1 THR B 97	-7.859 -1.082 -30.034 1.00 16.70	0
ANISOU 4334 OG1 THR B 97		Ō
_		
		C
ANISOU 4335 CG2 THR B 97		С
ATOM 4336 H THR B 97	-6.201 -2.522 -31.740 1.00 17.85	Н
ATOM 4337 HA THR B 97	-8.568 -3.838 -31.605 1.00 17.27	Н
ATOM 4338 HB THR B 97		Н
ATOM 4339 HG1 THR B 97	-7.023 -1.154 -30.085 1.00 20.03	Ĥ
ATOM 4340 HG21 THR B 97	-8.247 -2.860 -28.162 1.00 18.95	H
ATOM 4341 HG22 THR B 97	-8.427 -4.134 -29.077 1.00 18.95	Н
ATOM 4342 HG23 THR B 97	-7.043 -3.374 -29.045 1.00 18.95	Н
ATOM 4343 N VAL B 98	-9.863 -2.151 -32.930 1.00 13.47	N
ANISOU 4343 N VAL B 98	1811 1496 1811 164 -472 -28	N
ATOM 4344 CA VAL B 98	-10.522 -1.217 -33.840 1.00 14.12	Ċ
ANISOU 4344 CA VAL B 98	1779 1600 1985 133 -462 72	С

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ATOM 4345 C VAL B 98 -11.819 -0.746 -33.196 1.00 13.84
ANISOU 4345 C VAL B 98 1824 1531 1904 168 -482 -63
ATOM 4346 O VAL B 98 -12.561 -1.542 -32.607 1.00 13.36
ANISOU 4346 O VAL B 98 1891 1537 1650 196 -405 -179
ATOM 4347 CB VAL B 98 -10.779 -1.853 -35.231 1.00 14.69
ANISOU 4347 CB VAL B 98 1780 1865 1935 101 -305 185
ATOM 4348 CG1 VAL B 98 -11.607 -3.112 -35.131 1.00 14.94
ATOM 4348 CG1 VAL B 98 -11.607 -3.112 -35.131 1.00 14.94 C ANISOU 4348 CG1 VAL B 98 1940 1994 1743 112 -185 57 ATOM 4349 CG2 VAL B 98 -11.431 -0.862 -36.163 1.00 15.96 C ANISOU 4349 CG2 VAL B 98 1809 2077 2180 75 -300 320 C ATOM 4350 H VAL B 98 -10.390 -2.751 -32.611 1.00 16.16 H ATOM 4351 HA VAL B 98 -9.952 -0.443 -33.966 1.00 16.94 H ATOM 4352 HB VAL B 98 -9.924 -2.098 -35.619 1.00 17.62 H ATOM 4353 HG11 VAL B 98 -11.742 -3.473 -36.021 1.00 17.93 H ATOM 4354 HG12 VAL B 98 -11.136 -3.756 -34.580 1.00 17.93 H ATOM 4355 HG13 VAL B 98 -11.578 -1.286 -37.022 1.00 19.16 H ATOM 4357 HG22 VAL B 98 -11.578 -1.286 -37.022 1.00 19.16 H ATOM 4358 HG23 VAL B 98 -12.277 -0.581 -35.782 1.00 19.16 H ATOM 4359 N LYS B 99 -12.074 0.559 -33.276 1.00 14.97 N ANISOU 4359 N LYS B 99 1875 1565 2249 171 -593 -35 N ATOM 4360 CA LYS B 99 -13.325 1.142 -32.819 1.00 16.78 C ANISOU 4360 CA LYS B 99 2148 1770 2459 217 -615 -158 C
ANISOU 4360 CA LYS B 99 2148 1770 2459 217 -615 -158
ATOM 4361 C LYS B 99 -14.259 1.330 -34.007 1.00 16.05
ANISOU 4361 C LYS B 99 1971 1779 2347 170 -509 -28
ATOM 4362 O LYS B 99 -13.882 1.947 -35.008 1.00 16.21
                                                                                                                                        00000
ANISOU 4362 O LYS B 99 1834 1794 2530 121 -529 169
ATOM 4363 CB LYS B 99 -13.074 2.478 -32.118 1.00 22.55
ANISOU 4363 CB LYS B 99 2819 2292 3456 270 -831 -249
ATOM 4364 CG LYS B 99 -12.539 2.321 -30.701 1.00 26.55
 ANISOU 4364 CG LYS B 99 3434 2741 3914 357 -948 -461
 ATOM 4365 CD LYS B 99 -12.254 3.675 -30.052 1.00 31.96
 ANISOU 4365 CD LYS B 99 4043 3206 4893 424 -1199 -598 C
ATOM 4366 CE LYS B 99 -12.175 3.551 -28.530 1.00 35.68
 ANISOU 4366 CE LYS B 99 4638 3697 5224 560 -1308 -883 C
ATOM 4367 NZ LYS B 99 -11.354 2.380 -28.105 1.00 36.34 N
ANISOU 4367 NZ LYS B 99 4816 3889 5101 550 -1239 -858 N
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ANISOU 4382 CA SER B 100 1738 1755 1862 148 -304 -14 ATOM 4383 C SER B 100 -17.835 0.725 -34.426 1.00 14.47 ANISOU 4383 C SER B 100 1873 1849 1775 189 -247 -151 ATOM 4384 O SER B 100 -18.069 -0.135 -33.575 1.00 14.79 ANISOU 4384 O SER B 100 2034 1933 1651 219 -194 -268 0 ATOM 4385 CB SER B 100 -16.139 -0.180 -36.044 1.00 12.78 ANISOU 4385 CB SER B 100 1548 1764 1546 97 -175 84 ATOM 4386 OG SER B 100 -16.886 0.048 -37.220 1.00 13.20 0 ANISOU 4386 OG SER B 100 1498 1950 1568 70 -111 197 0 ATOM 4387 H SER B 100 -15.774 0.409 -33.190 1.00 17.77 H ATOM 4388 HA SER B 100 -16.368 1.765 -35.402 1.00 16.91 ATOM 4389 HB2 SER B 100 -15.194 -0.158 -36.263 1.00 15.34 Н ATOM 4390 HB3 SER B 100 -16.374 -1.050 -35.686 1.00 15.34 ATOM 4391 HG SER B 100 -17.707 0.030 -37.046 1.00 15.84 ATOM 4392 N ASP B 101 -18.756 1.565 -34.901 1.00 13.62 Ν ANISOU 4392 N ASP B 101 1684 1740 1750 191 -258 -108 ATOM 4393 CA ASP B 101 -20.189 1.392 -34.649 1.00 13.48 ANISOU 4393 CA ASP B 101 1714 1802 1605 220 -181 -197 ATOM 4394 C ASP B 101 -20.486 1.312 -33.155 1.00 14.63 ANISOU 4394 C ASP B 101 1972 1918 1668 315 -208 -391 C ATOM 4395 O ASP B 101 -21.235 0.452 -32.693 1.00 14.42 ANISOU 4395 O ASP B 101 2021 2007 1451 330 -101 -445 ATOM 4396 CB ASP B 101 -20.717 0.157 -35.377 1.00 13.40 ANISOU 4396 CB ASP B 101 1727 1963 1401 159 -32 -154 ATOM 4397 CG ASP B 101 -20.375 0.173 -36.850 1.00 12.90 C ANISOU 4397 CG ASP B 101 1545 1995 1361 98 -6 ATOM 4398 OD1 ASP B 101 -20.982 0.986 -37.588 1.00 14.48 0 ANISOU 4398 OD1 ASP B 101 1635 2228 1639 90 -20 111 ATOM 4399 OD2 ASP B 101 -19.492 -0.611 -37.264 1.00 12.14 O ANISOU 4399 OD2 ASP B 101 1453 1958 1201 72 28 42 O ATOM 4400 H ASP B 101 -18.573 2.254 -35.382 1.00 16.34 H ATOM 4401 HA ASP B 101 -20.660 2.164 -35.000 1.00 16.17 ATOM 4402 HB2 ASP B 101 -20.322 -0.637 -34.985 1.00 16.08 ATOM 4403 HB3 ASP B 101 -21.683 0.126 -35.292 1.00 16.08 ATOM 4404 N GLY B 102 -19.886 2.220 -32.397 1.00 14.77 Ν ANISOU 4404 N GLY B 102 1983 1793 1837 388 -362 -489 ATOM 4405 CA GLY B 102 -20.147 2.292 -30.976 1.00 17.53 ANISOU 4405 CA GLY B 102 2418 2158 2086 514 -408 -697 ATOM 4406 C GLY B 102 -19.476 1.228 -30.130 1.00 18.09 ANISOU 4406 C GLY B 102 2600 2306 1969 533 -369 -740 C ATOM 4407 O GLY B 102 -19.692 1.211 -28.911 1.00 20.88 ANISOU 4407 O GLY B 102 3015 2728 2188 653 -396 -894 O ATOM 4408 H GLY B 102 -19.324 2.804 -32.685 1.00 17.73 H 0 ATOM 4409 HA2 GLY B 102 -19.856 3.157 -30.649 1.00 21.04 ATOM 4410 HA3 GLY B 102 -21.104 2.225 -30.831 1.00 21.04 ATOM 4411 N GLY B 103 -18.652 0.362 -30.723 1.00 17.77 Ν ANISOU 4411 N GLY B 103 1861 2818 2073 656 -194 -397 ATOM 4412 CA GLY B 103 -18.007 -0.705 -29.991 1.00 16.95 ANISOU 4412 CA GLY B 103 1830 2761 1849 537 -155 -369 ATOM 4413 C GLY B 103 -16.508 -0.705 -30.229 1.00 15.70 ANISOU 4413 C GLY B 103 1774 2417 1773 467 -255 -331 C ATOM 4414 O GLY B 103 -15.994 -0.047 -31.146 1.00 14.56 O ANISOU 4414 O GLY B 103 1630 2116 1787 464 -319 -287 O

ATOM 4415 H GLY B 103 -18.453 0.379 -31.560 1.00 21.32 Н ATOM 4416 HA2 GLY B 103 -18.171 -0.595 -29.041 1.00 20.34 Н ATOM 4417 HA3 GLY B 103 -18.367 -1.560 -30.273 1.00 20.34 ATOM 4418 N THR B 104 -15.811 -1.448 -29.373 1.00 14.81 Ν ANISOU 4418 N THR B 104 1741 2338 1549 424 -259 -337 Ν ATOM 4419 CA THR B 104 -14.383 -1.687 -29.520 1.00 14.71 ANISOU 4419 CA THR B 104 1788 2200 1603 360 -352 -310 ATOM 4420 C THR B 104 -14.169 -3.179 -29.734 1.00 13.92 ANISOU 4420 C THR B 104 1716 2152 1419 C 257 -295 -176 ATOM 4421 O THR B 104 -14.703 -3.999 -28.978 1.00 15.20 ANISOU 4421 O THR B 104 1918 2430 1427 252 -209 -138 ATOM 4422 CB THR B 104 -13.605 -1.193 -28.294 1.00 17.94 ANISOU 4422 CB THR B 104 2263 2594 1962 444 -458 -469 ATOM 4423 OG1 THR B 104 -13.904 0.194 -28.075 1.00 19.58 ANISOU 4423 OG1 THR B 104 2448 2718 2274 544 -512 -631 ATOM 4424 CG2 THR B 104 -12.106 -1.348 -28.492 1.00 17.92 ANISOU 4424 CG2 THR B 104 2267 2475 2067 382 -572 -469 ATOM 4425 H THR B 104 -16.154 -1.832 -28.684 1.00 17.78 Н ATOM 4426 HA THR B 104 -14.056 -1.215 -30.302 1.00 17.66 Н ATOM 4427 HB THR B 104 -13.868 -1.708 -27.515 1.00 21.53 Н ATOM 4428 HG1 THR B 104 -14.727 0.293 -27.941 1.00 23.50 ATOM 4429 HG21 THR B 104 -11.634 -1.030 -27.706 1.00 21.50 ATOM 4430 HG22 THR B 104 -11.886 -2.281 -28.636 1.00 21.50 ATOM 4431 HG23 THR B 104 -11.819 -0.833 -29.262 1.00 21.50 ATOM 4432 N TYR B 105 -13.376 -3.520 -30.743 1.00 12.25 Ν **ANISOU 4432 N TYR B 105** 1491 1846 1317 182 -328 -102 C ATOM 4433 CA TYR B 105 -13.165 -4.900 -31.166 1.00 12.94 **ANISOU 4433 CA TYR B 105** 1605 1944 1369 98 -285 -1 C -11.690 -5.259 -31.040 1.00 12.80 ATOM 4434 C TYR B 105 **ANISOU 4434 C TYR B 105** 1629 1851 1383 105 -371 ATOM 4435 O TYR B 105 0 -10.820 -4.496 -31.473 1.00 12.71 1565 1764 1499 108 -438 -36 **ANISOU 4435 O TYR B 105** ATOM 4436 CB TYR B 105 -13.614 -5.119 -32.623 1.00 12.26 1444 1859 1355 36 -248 **ANISOU 4436 CB TYR B 105** 52 ATOM 4437 CG TYR B 105 -15.079 -4.868 -32.916 1.00 12.01 35 **ANISOU 4437 CG TYR B 105** 1328 1931 1305 39 -189 ATOM 4438 CD1 TYR B 105 -15.579 -3.578 -33.017 1.00 12.64 **ANISOU 4438 CD1 TYR B 105** 1358 2020 1425 134 -213 -6 ATOM 4439 CD2 TYR B 105 -15.959 -5.928 -33.138 1.00 11.55 1223 1948 1218 -50 -118 **ANISOU 4439 CD2 TYR B 105** ATOM 4440 CE1 TYR B 105 -16.915 -3.345 -33.302 1.00 12.60 **ANISOU 4440 CE1 TYR B 105** 1250 2135 1405 171 -176 -33 C ATOM 4441 CE2 TYR B 105 -17.291 -5.700 -33.422 1.00 12.42 7 **ANISOU 4441 CE2 TYR B 105** 1205 2182 1332 -48 -79 ATOM 4442 CZ TYR B 105 -17.764 -4.399 -33.495 1.00 13.43 **ANISOU 4442 CZ TYR B 105** 1275 2355 1473 78 -112 -34 0 ATOM 4443 OH TYR B 105 -19.089 -4.152 -33.781 1.00 13.86 1179 2556 1531 115 -89 -86 **ANISOU 4443 OH TYR B 105** 0 ATOM 4444 H TYR B 105 -12.936 -2.951 -31.214 1.00 14.70 H ATOM 4445 HA TYR B 105 -13.676 -5.495 -30.595 1.00 15.53 Н ATOM 4446 HB2 TYR B 105 -13.100 -4.525 -33.192 1.00 14.71 ATOM 4447 HB3 TYR B 105 -13.425 -6.039 -32.864 1.00 14.71 ATOM 4448 HD1 TYR B 105 -15.010 -2.856 -32.879 1.00 15.17 ATOM 4448 HD1 TYR B 105 -15.010 -2.856 -32.879 1.00 15.17

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ATOM 4449 HD2 TYR B 105
                           -15.646 -6.802 -33.082 1.00 13.86
                                                               Н
ATOM 4450 HE1 TYR B 105
                           -17.234 -2.474 -33.354 1.00 15.12
ATOM 4451 HE2 TYR B 105
                            -17.869 -6.416 -33.557 1.00 14.91
                           -19.502 -4.878 -33.877 1.00 16.63
                                                              Н
ATOM 4452 HH TYR B 105
ATOM 4453 N ASP B 106
                           -11.418 -6.421 -30.453 1.00 11.69
                                                              Ν
ANISOU 4453 N ASP B 106
                           1573 1725 1144 110 -360
                                                        55
                                                              Ν
ATOM 4454 CA ASP B 106
                           -10.077 -6.991 -30.453 1.00 12.37
                                                              C
                                                              C
ANISOU 4454 CA ASP B 106
                            1684 1755 1260 142 -445
ATOM 4455 C ASP B 106
                           -9.806 -7.676 -31.788 1.00 12.01
ANISOU 4455 C ASP B 106
                           1597 1651 1315
                                            77 -407
                                                       114
                                                              0
ATOM 4456 O ASP B 106
                           -10.670 -8.368 -32.330 1.00 12.25
ANISOU 4456 O ASP B 106
                           1642 1679 1335 10 -323 158
                                                              0
ATOM 4457 CB ASP B 106
                            -9.929 -8.000 -29.316 1.00 13.05
                            1903 1867 1186 216 -452
ANISOU 4457 CB ASP B 106
                                                        129
ATOM 4458 CG ASP B 106
                            -9.986 -7.351 -27.945 1.00 15.37
                                                              C
ANISOU 4458 CG ASP B 106
                           2249 2268 1322 327 -510
ATOM 4459 OD1 ASP B 106
                            -9.352 -6.288 -27.766 1.00 14.92
                             2120 2221 1330 372 -633
                                                               0
ANISOU 4459 OD1 ASP B 106
                                                         -91
ATOM 4460 OD2 ASP B 106
                            -10.662 -7.905 -27.049 1.00 16.51
                            2505 2487 1282 369 -425
ANISOU 4460 OD2 ASP B 106
                                                         146
                                                               0
ATOM 4461 H ASP B 106
                           -12.000 -6.903 -30.043 1.00 14.03
                                                              Н
ATOM 4462 HA ASP B 106
                            -9.423 -6.286 -30.328 1.00 14.84
                                                              Н
                            -10.650 -8.647 -29.371 1.00 15.66
ATOM 4463 HB2 ASP B 106
                                                               Н
ATOM 4464 HB3 ASP B 106
                            -9.073 -8.448 -29.400 1.00 15.66
                                                              Н
ATOM 4465 N ILE B 107
                          -8.600 -7.485 -32.320 1.00 13.20
                                                            N
ANISOU 4465 N ILE B 107
                          1678 1770 1566
                                            97 -468
                                                            Ν
                                                      85
ATOM 4466 CA ILE B 107
                           -8.230 -8.025 -33.627 1.00 13.06
                                                             C
ANISOU 4466 CA ILE B 107
                                             68 -424
                                                             C
                           1612 1735 1616
ATOM 4467 C ILE B 107
                          -7.364 -9.265 -33.423 1.00 13.82
                                                            C
                                                             C
ANISOU 4467 C ILE B 107
                          1760 1790 1703 136 -463
                                                       115
ATOM 4468 O ILE B 107
                          -6.322 -9.202 -32.759 1.00 15.13
                                                            0
                          1901 1961 1885
ANISOU 4468 O ILE B 107
                                           217 -557
                                                       83
                                                             CCC
ATOM 4469 CB ILE B 107
                           -7.493 -6.984 -34.484 1.00 14.42
ANISOU 4469 CB ILE B 107
                           1655 1915 1909 50 -417
                                                       101
ATOM 4470 CG1 ILE B 107
                           -8.359 -5.736 -34.687 1.00 14.16
ANISOU 4470 CG1 ILE B 107
                                             13 -384 119
                            1599 1879 1901
ATOM 4471 CG2 ILE B 107
                            -7.117 -7.594 -35.840 1.00 14.45
                                                              C
ANISOU 4471 CG2 ILE B 107
                            1615 1952 1923 52 -349 128
                                                              C
ATOM 4472 CD1 ILE B 107
                           -7.584 -4.545 -35.235 1.00 14.52
ANISOU 4472 CD1 ILE B 107
                            1542 1872 2102 -14 -369 143
ATOM 4473 H ILE B 107
                          -7.971 -7.041 -31.938 1.00 15.84
                                                            Н
ATOM 4474 HA ILE B 107
                           -9.033 -8.292 -34.100 1.00 15.67
                                                             Н
ATOM 4475 HB ILE B 107
                           -6.679 -6.725 -34.024 1.00 17.30
                                                             Н
ATOM 4476 HG12 ILE B 107
                                                              Н
                            -9.068 -5.945 -35.315 1.00 16.99
ATOM 4477 HG13 ILE B 107
                            -8.740 -5.477 -33.833 1.00 16.99
                                                              Н
ATOM 4478 HG21 ILE B 107
                            -6.654 -6.926 -36.368 1.00 17.34
                                                             Н
ATOM 4479 HG22 ILE B 107
                            -6.539 -8.359 -35.692 1.00 17.34
                                                              Н
ATOM 4480 HG23 ILE B 107
                            -7.927 -7.874 -36.295 1.00 17.34
                                                              Н
                            -8.190 -3.795 -35.338 1.00 17.42
                                                              Н
ATOM 4481 HD11 ILE B 107
ATOM 4482 HD12 ILE B 107
                           -6.876 -4.316 -34.612 1.00 17.42
                                                              Н
                          -7.204 -4.785 -36.095 1.00 17.42
ATOM 4483 HD13 ILE B 107
                                                              Н
ATOM 4484 N TYR B 108
                           -7.778 -10.385 -34.017 1.00 12.93
                                                             Ν
ANISOU 4484 N TYR B 108
                          1707 1629 1578 116 -408 135
                                                             Ν
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ATOM 4485 CA TYR B 108 -7.035 -11.636 -33.928 1.00 13.22 ANISOU 4485 CA TYR B 108 1812 1579 1630 201 -440 138 ATOM 4486 C TYR B 108 -6.776 -12.214 -35.314 1.00 13.20 Č ANISOU 4486 C TYR B 108 ATOM 4487 O TYR B 108 1760 1570 1685 205 -399 Ö -7.493 -11.930 -36.271 1.00 11.77 **ANISOU 4487 O TYR B 108** 1532 1447 1492 131 -342 40 ATOM 4488 CB TYR B 108 -7.786 -12.699 -33.118 1.00 14.11 **ANISOU 4488 CB TYR B 108** 2092 1576 1692 187 -408 220 COCCCCC ATOM 4489 CG TYR B 108 -8.187 -12.303 -31.725 1.00 15.27 **ANISOU 4489 CG TYR B 108** 2316 1764 1722 206 -416 299 ATOM 4490 CD1 TYR B 108 -7.252 -12.260 -30.702 1.00 16.51 **ANISOU 4490 CD1 TYR B 108** 2520 1953 1801 355 -524 320 ATOM 4491 CD2 TYR B 108 -9.518 -12.015 -31.416 1.00 15.24 **ANISOU 4491 CD2 TYR B 108** 2329 1796 1667 338 96 -319 ATOM 4492 CE1 TYR B 108 -7.619 -11.918 -29.417 1.00 17.98 CC **ANISOU 4492 CE1 TYR B 108** 2789 2215 1828 405 -536 -9.892 -11.674 -30.129 1.00 16.44 ATOM 4493 CE2 TYR B 108 2552 2019 1676 138 -304 **ANISOU 4493 CE2 TYR B 108** 401 ATOM 4494 CZ TYR B 108 -8.941 -11.626 -29.137 1.00 17.43 C **ANISOU 4494 CZ TYR B 108** 2746 2183 1693 297 -413 419 ATOM 4495 OH TYR B 108 -9.303 -11.302 -27.851 1.00 18.23 0 **ANISOU 4495 OH TYR B 108** 2932 2393 1603 371 -405 466 ATOM 4496 H TYR B 108 -8.497 -10.444 -34.485 1.00 15.52 Н ATOM 4497 HA TYR B 108 -6.180 -11.473 -33.500 1.00 15.86 Н -8.597 -12.932 -33.597 1.00 16.93 ATOM 4498 HB2 TYR B 108 Н -7.220 -13.483 -33.044 1.00 16.93 ATOM 4499 HB3 TYR B 108 -6.362 -12.456 -30.887 1.00 19.82 ATOM 4500 HD1 TYR B 108 ATOM 4501 HD2 TYR B 108 -10.161 -12.047 -32.087 1.00 18.29 -6.981 -11.889 -28.742 1.00 21.58 ATOM 4502 HE1 TYR B 108 **ATOM 4503 HE2 TYR B 108** -10.781 -11.479 -29.935 1.00 19.73 ATOM 4504 HH TYR B 108 -8.630 -11.319 -27.350 1.00 21.88 Н -5.757 -13.065 -35.404 1.00 14.67 ATOM 4505 N THR B 109 Ν **ANISOU 4505 N THR B 109** 1959 1702 1913 323 -440 39 ATOM 4506 CA THR B 109 -5.588 -13.943 -36.555 1.00 15.97 **ANISOU 4506 CA THR B 109** 2120 1834 2114 362 -405 -54 ATOM 4507 C THR B 109 -5.312 -15.353 -36.057 1.00 17.28 Č **ANISOU 4507 C THR B 109** 2431 1804 2330 461 -447 -52 ATOM 4508 O THR B 109 ANISOU 4508 O THR B 109 Ö -4.603 -15.543 -35.063 1.00 17.75 2536 1820 2386 576 -520 ATOM 4509 CB THR B 109 -4.456 -13.492 -37.490 1.00 17.11 2098 2126 2278 444 -382 -118 **ANISOU 4509 CB THR B 109** ATOM 4510 OG1 THR B 109 -3.191 -13.592 -36.823 1.00 19.84 0 **ANISOU 4510 OG1 THR B 109** 2382 2475 2680 572 -455 -117 ATOM 4511 CG2 THR B 109 -4.681 -12.075 -37.956 1.00 15.60 Č **ANISOU 4511 CG2 THR B 109** 1787 2081 2058 349 -322 -70 ATOM 4512 H THR B 109 -5.145 -13.152 -34.805 1.00 17.60 Н ATOM 4513 HA THR B 109 -6.412 -13.959 -37.065 1.00 19.17 Н ATOM 4514 HB THR B 109 -4.446 -14.066 -38.272 1.00 20.53 Н ATOM 4515 HG1 THR B 109 Н -3.050 -14.387 -36.592 1.00 23.80 ATOM 4516 HG21 THR B 109 -3.961 -11.802 -38.546 1.00 18.72 Н ATOM 4517 HG22 THR B 109 -5.522 -12.014 -38.437 1.00 18.72 ATOM 4518 HG23 THR B 109 -4.710 -11.476 -37.194 1.00 18.72 ATOM 4519 N THR B 110 -5.888 -16.331 -36.751 1.00 17.14

ANISOU 4519 N THR B 110 2488 1660 2363 427 -413 -136 ATOM 4520 CA THR B 110 -5.724 -17.742 -36.447 1.00 19.26 **ANISOU 4520 CA THR B 110** 2916 1674 2728 509 -439 -143 ATOM 4521 C THR B 110 ANISOU 4521 C THR B 110 -5.678 -18.520 -37.757 1.00 20.48 3054 1779 2949 547 -429 -352 ATOM 4522 O THR B 110 -5.966 -17.990 -38.833 1.00 18.89 **ANISOU 4522 O THR B 110** 0 2733 1763 2680 496 -397 -472 ATOM 4523 CB THR B 110 C -6.869 -18.272 -35.575 1.00 20.19 **ANISOU 4523 CB THR B 110** 3193 1592 2885 366 -393 -14 ATOM 4524 OG1 THR B 110 -8.118 -18.097 -36.265 1.00 19.05 **ANISOU 4524 OG1 THR B 110** 2990 1485 2763 166 -333 -102 ATOM 4525 CG2 THR B 110 -6.921 -17.543 -34.238 1.00 18.75 3045 1493 2588 367 -398 176 C **ANISOU 4525 CG2 THR B 110** ATOM 4526 H THR B 110 -6.398 -16.190 -37.429 1.00 20.57 Н ATOM 4527 HA THR B 110 -4.887 -17.878 -35.976 1.00 23.12 Н ATOM 4528 HB THR B 110 -6.729 -19.216 -35.401 1.00 24.22 Н ATOM 4529 HG1 THR B 110 -8.750 -18.385 -35.793 1.00 22.86 Н ATOM 4530 HG21 THR B 110 -7.649 -17.891 -33.700 1.00 22.51 ATOM 4531 HG22 THR B 110 -6.087 -17.670 -33.759 1.00 22.51 ATOM 4532 HG23 THR B 110 -7.061 -16.595 -34.383 1.00 22.51 Н ATOM 4533 N THR B 111 -5.325 -19.796 -37.654 1.00 23.30 Ν **ANISOU 4533 N THR B 111** 3545 1880 3428 659 -462 -399 -5.347 -20.715 -38.781 1.00 26.64 ATOM 4534 CA THR B 111 **ANISOU 4534 CA THR B 111** 3986 2200 3938 708 -468 -640 ATOM 4535 C THR B 111 -6.235 -21.901 -38.436 1.00 29.87 ANISOU 4535 C THR B 111 4583 2231 4536 590 -462 -643 ATOM 4536 O THR B 111 -6.137 -22.455 -37.338 1.00 30.62 0 0 **ANISOU 4536 O THR B 111** 4840 2082 4713 621 -460 -446 ATOM 4537 CB THR B 111 -3.935 -21.222 -39.122 1.00 29.58 **ANISOU 4537 CB THR B 111** 4328 2578 4332 990 -512 -746 ATOM 4538 OG1 THR B 111 -3.042 -20.115 -39.268 1.00 29.01 **ANISOU 4538 OG1 THR B 111** 4056 2837 4129 1071 -495 -706 -3.947 -22.026 -40.412 1.00 32.17 ATOM 4539 CG2 THR B 111 4654 2860 4708 1067 -515 -1046 **ANISOU 4539 CG2 THR B 111** ATOM 4540 H THR B 111 -5.061 -20.161 -36.921 1.00 27.96 Н ATOM 4541 HA THR B 111 -5.714 -20.268 -39.560 1.00 31.97 Н ATOM 4542 HB THR B 111 -3.620 -21.797 -38.407 1.00 35.49 ATOM 4543 HG1 THR B 111 -2.271 -20.391 -39.454 1.00 34.81 ATOM 4544 HG21 THR B 111 -3.052 -22.340 -40.615 1.00 38.60 ATOM 4545 HG22 THR B 111 -4.536 -22.792 -40.319 1.00 38.60 ATOM 4546 HG23 THR B 111 -4.262 -21.473 -41.144 1.00 38.60 ATOM 4547 N ARG B 112 -7.089 -22.303 -39.375 1.00 31.64 **ANISOU 4547 N ARG B 112** 4784 2405 4833 459 -460 -867 Ν ATOM 4548 CA ARG B 112 -7.897 -23.508 -39.223 1.00 35.67 C **ANISOU 4548 CA ARG B 112** 5441 2521 5592 319 -453 -928 ATOM 4549 C ARG B 112 -7.407 -24.564 -40.206 1.00 37.35 **ANISOU 4549 C ARG B 112** C 5686 2601 5904 460 -502 -1216 ATOM 4550 O ARG B 112 -7.188 -24.267 -41.384 1.00 37.43 0 **ANISOU 4550 O ARG B 112** 5565 2875 5782 548 -541 -1466 ATOM 4551 CB ARG B 112 -9.383 -23.205 -39.433 1.00 36.85 ANISOU 4551 CB ARG B 112 5499 2725 5777 20 -417 -982 ATOM 4552 CG ARG B 112 -10.299 -24.260 -38.816 1.00 41.20 C ANISOU 4552 CG ARG B 112 6178 2871 6604 -200 -353 -916

ATOM 4553 CD ARG B 112	-11.645 -23.684 -38.418 1.00 41.82	C
ANISOU 4553 CD ARG B 112	6146 3043 6702 -487 -277 -821	C
ATOM 4554 NE ARG B 112	-12.290 -24.498 -37.385 1.00 45.69	Ν
ANISOU 4554 NE ARG B 112	6776 3236 7350 -666 -144 -584	Ν
ATOM 4555 CZ ARG B 112	-13.342 -25.293 -37.571 1.00 50.13	C
ANISOU 4555 CZ ARG B 112	7318 3662 8069 -899 -109 -662	С
ATOM 4556 NH1 ARG B 112	-13.914 -25.407 -38.763 1.00 51.74	N
ANISOU 4556 NH1 ARG B 112	7361 3993 8306 -978 -202 -991	N
ATOM 4557 NH2 ARG B 112	-13.833 -25.979 -36.546 1.00 53.13	Ν
ANISOU 4557 NH2 ARG B 112	7830 3798 8560 -1042 3 -399	N
ATOM 4558 H ARG B 112	-7.218 -21.890 -40.118 1.00 37.97	Н
ATOM 4559 HA ARG B 112	-7.784 -23.855 -38.325 1.00 42.81	Н
ATOM 4560 HB2 ARG B 112	-9.592 -22.351 -39.023 1.00 44.22	Н
ATOM 4561 HB3 ARG B 112	-9.566 -23.170 -40.384 1.00 44.22	Н
ATOM 4562 HG2 ARG B 112	-10.452 -24.966 -39.463 1.00 49.44	Н
ATOM 4563 HG3 ARG B 112	-9.878 -24.621 -38.020 1.00 49.44	Н
ATOM 4564 HD2 ARG B 112	-11.519 -22.789 -38.066 1.00 50.19	Н
ATOM 4565 HD3 ARG B 112	-12.226 -23.662 -39.194 1.00 50.19	Н
ATOM 4566 HE ARG B 112	-11.961 -24.459 -36.591 1.00 54.83	H
ATOM 4567 HH11 ARG B 112	-13.603 -24.966 -39.433 1.00 62.09	Н
ATOM 4568 HH12 ARG B 112	-14.593 -25.924 -38.866 1.00 62.09	H
ATOM 4569 HH21 ARG B 112	-13.470 -25.911 -35.769 1.00 63.76	H
ATOM 4570 HH22 ARG B 112		H
ATOM 4571 N TYR B 113	-7.228 -25.791 -39.716 1.00 45.41	Ν
ANISOU 4571 N TYR B 113	6227 3839 7188 1378 -2765 -280	''N
ATOM 4572 CA TYR B 113	-6.598 -26.863 -40.476 1.00 46.84	C
ANISOU 4572 CA TYR B 113	6284 3856 7658 1511 -2757 -452	C
ATOM 4573 C TYR B 113	-7.606 -27.952 -40.821 1.00 46.92	C
ANISOU 4573 C TYR B 113	6532 3686 7609 1446 -2670 -356	C
ATOM 4574 O TYR B 113	-8.456 -28.309 -39.999 1.00 45.28	o
ANISOU 4574 O TYR B 113	6595 3444 7164 1350 -2712 -130	0
	-5.440 -27.481 -39.689 1.00 50.75	C
ANISOU 4575 CB TYR B 113	6705 4287 8291 1656 -2963 -473	C
	-4.259 -26.559 -39.483 1.00 51.92	_
ATOM 4576 CG TYR B 113		C
ANISOU 4576 CG TYR B 113	6592 4596 8538 1721 -3028 -608	C
ATOM 4577 CD1 TYR B 113	-4.157 -25.773 -38.343 1.00 51.91	C
ANISOU 4577 CD1 TYR B 113	6653 4719 8353 1671 -3136 -485	C
ATOM 4578 CD2 TYR B 113	-3.242 -26.481 -40.427 1.00 52.93	C
ANISOU 4578 CD2 TYR B 113	6417 4764 8930 1808 -2951 -863	C
ATOM 4579 CE1 TYR B 113	-3.076 -24.931 -38.150 1.00 52.68	C
ANISOU 4579 CE1 TYR B 113	6523 4962 8531 1714 -3178 -609	C
ATOM 4580 CE2 TYR B 113	-2.158 -25.642 -40.243 1.00 53.49	C
ANISOU 4580 CE2 TYR B 113	6260 4991 9074 1843 -2987 -984	C
ATOM 4581 CZ TYR B 113	-2.080 -24.871 -39.103 1.00 53.37	C
ANISOU 4581 CZ TYR B 113	6316 5084 8877 1800 -3107 -856	C
ATOM 4582 OH TYR B 113	-1.002 -24.036 -38.918 1.00 53.63	0
ANISOU 4582 OH TYR B 113	6136 5266 8976 1824 -3126 -977	0
ATOM 4583 H TYR B 113	-7.470 -26.029 -38.926 1.00 54.49	Η.
ATOM 4584 HA TYR B 113	-6.244 -26.502 -41.304 1.00 56.21	H.
ATOM 4585 HB2 TYR B 113	-5.765 -27.743 -38.814 1.00 60.90	Н
ATOM 4586 HB3 TYR B 113	-5.123 -28.263 -40.168 1.00 60.90	Н
ATOM 4587 HD1 TYR B 113	-4.827 -25.812 -37.699 1.00 62.29	Н
ATOM 4588 HD2 TYR B 113	-3.292 -27.000 -41.197 1.00 63.52	Н

ATOM 4589 HE1 TYR B 113 -3.021 -24.409 -37.382 1.00 63.21 ATOM 4590 HE2 TYR B 113 -1.485 -25.599 -40.883 1.00 64.19 Н ATOM 4591 HH TYR B 113 -0.476 -24.098 -39.570 1.00 64.36 Н ATOM 4592 N ASN B 114 -7.492 -28.482 -42.040 1.00 48.74 Ν **ANISOU 4592 N ASN B 114** 6644 3833 8041 1474 -2514 -546 N -8.320 -29.597 -42.504 1.00 50.16 ATOM 4593 CA ASN B 114 C **ANISOU 4593 CA ASN B 114** 7018 3840 8200 1412 -2413 -496 -9.788 -29.373 -42.154 1.00 45.82 ATOM 4594 C ASN B 114 **ANISOU 4594 C ASN B 114** C 6764 3336 7311 1205 -2325 -261 ATOM 4595 O ASN B 114 -10.451 -30.226 -41.559 1.00 47.68 0 **ANISOU 4595 O ASN B 114** 7237 3468 7412 1163 -2377 -82 0 ATOM 4596 CB ASN B 114 -7.824 -30.922 -41.924 1.00 55.11 C **ANISOU 4596 CB ASN B 114** 7710 4300 8930 1536 -2572 -443 ATOM 4597 CG ASN B 114 -6.332 -31.115 -42.098 1.00 58.68 **ANISOU 4597 CG ASN B 114** 7883 4744 9671 1718 -2662 -635 C ATOM 4598 OD1 ASN B 114 -5.810 -31.077 -43.213 1.00 58.94 0 0 **ANISOU 4598 OD1 ASN B 114** 7692 4799 9901 1748 -2517 -861 ATOM 4599 ND2 ASN B 114 -5.633 -31.316 -40.987 1.00 61.07 **ANISOU 4599 ND2 ASN B 114** 8193 5030 9979 1822 -2883 -546 Ν ATOM 4600 H ASN B 114 -6.930 -28.206 -42.629 1.00 58.49 Н ATOM 4601 HA ASN B 114 -8.252 -29.653 -43.470 1.00 60.19 н ATOM 4602 HB2 ASN B 114 -8.021 -30.944 -40.974 1.00 66.14 Н ATOM 4603 HB3 ASN B 114 -8.276 -31.653 -42.374 1.00 66.14 Н ATOM 4604 HD21 ASN B 114 -4.781 -31.432 -41.029 1.00 73.28 -6.031 -31.331 -40.225 1.00 73.28 ATOM 4605 HD22 ASN B 114 ATOM 4606 N ALA B 115 -10.293 -28.205 -42.525 1.00 39.58 Ν **ANISOU 4606 N ALA B 115** 5908 2809 6321 1019 -2115 -266 ATOM 4607 CA ALA B 115 -11.650 -27.792 -42.218 1.00 35.66 **ANISOU 4607 CA ALA B 115** 5654 2409 5486 806 -2002 -46 ATOM 4608 C ALA B 115 ANISOU 4608 C ALA B 115 -12.381 -27.424 -43.502 1.00 36.14 5640 2636 5455 606 -1657 -143 C -11.749 -27.148 -44.529 1.00 33.22 ATOM 4609 O ALA B 115 **ANISOU 4609 O ALA B 115** 5002 2365 5256 623 -1505 -383 -11.644 -26.593 -41.260 1.00 34.75 ATOM 4610 CB ALA B 115 5554 2472 5175 763 -2083 85 C **ANISOU 4610 CB ALA B 115** ATOM 4611 H ALA B 115 -9.852 -27.616 -42.970 1.00 47.49 Н ATOM 4612 HA ALA B 115 -12.123 -28.524 -41.793 1.00 42.79 Н ATOM 4613 HB1 ALA B 115 -12.560 -26.336 -41.070 1.00 41.69 Н ATOM 4614 HB2 ALA B 115 Н -11.195 -26.848 -40.439 1.00 41.69 ATOM 4615 HB3 ALA B 115 -11.173 -25.856 -41.679 1.00 41.69 Н ATOM 4616 N PRO B 116 -13.713 -27.410 -43.485 1.00 37.97 Ν **ANISOU 4616 N PRO B 116** 6101 2908 5417 414 -1525 Ν -14.448 -27.070 -44.707 1.00 37.32 ATOM 4617 CA PRO B 116 **ANISOU 4617 CA PRO B 116** 5949 2996 5235 218 -1198 CC ATOM 4618 C PRO B 116 -14.362 -25.583 -45.012 1.00 34.10 **ANISOU 4618 C PRO B 116** 5347 2893 4716 115 -1022 -96 ATOM 4619 O PROB 116 0 -14.443 -24.737 -44.119 1.00 34.37 **ANISOU 4619 O PRO B 116** 5437 3030 4592 92 -1101 45 ATOM 4620 CB PRO B 116 -15.883 -27.502 -44.392 1.00 38.08 6367 3036 5067 56 -1149 203 **ANISOU 4620 CB PRO B 116** ATOM 4621 CG PRO B 116 -15.990 -27.378 -42.924 1.00 39.45 С ANISOU 4621 CG PRO B 116 6744 3135 5110 113 -1395 435 ATOM 4622 CD PRO B 116 -14.624 -27.705 -42.364 1.00 40.69

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ANISOU 4622 CD PRO B 116
                             6778 3150 5532 363 -1664 330
                                                                  C
ATOM 4623 HA PRO B 116
                            -14.112 -27.579 -45.462 1.00 44.78
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ATOM 4624 HB2 PRO B 116
                             -16.510 -26.910 -44.835 1.00 45.70
                                                                 Н
ATOM 4625 HB3 PRO B 116
                                                                 Н
                             -16.018 -28.421 -44.672 1.00 45.70
                             -16.243 -26.471 -42.695 1.00 47.34
ATOM 4626 HG2 PRO B 116
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ATOM 4627 HG3 PRO B 116
                             -16.651 -28.008 -42.595 1.00 47.34
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ATOM 4628 HD2 PRO B 116
                             -14.424 -27.132 -41.607 1.00 48.83
                                                                  Н
ATOM 4629 HD3 PRO B 116
                             -14.572 -28.643 -42.124 1.00 48.83
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ATOM 4630 N SER B 117
                           -14.185 -25.276 -46.292 1.00 30.31
                                                                Ν
ANISOU 4630 N SER B 117
                            4639 2555 4325 53 -778 -306
                                                                Ν
ATOM 4631 CA SER B 117
                            -14.101 -23.911 -46.775 1.00 25.87
ANISOU 4631 CA SER B 117
                             3871 2282 3677 -48 -573 -382
ATOM 4632 C SER B 117
ANISOU 4632 C SER B 117
                           -14.824 -23.840 -48.111 1.00 23.41
                            3492 2108 3293 -222 -253 -466
                                                                C
ATOM 4633 O SER B 117
ANISOU 4633 O SER B 117
                                                                0
                           -15.369 -24.835 -48.601 1.00 23.71
                            3646 2018 3344 -267 -203 -465
                                                                0
ATOM 4634 CB SER B 117
                            -12.644 -23.459 -46.915 1.00 26.22
ANISOU 4634 CB SER B 117
                             3614 2368 3981 120 -648 -610
ATOM 4635 OG SER B 117
                            -12.014 -24.115 -48.013 1.00 27.04
ANISOU 4635 OG SER B 117
                             3529 2399 4345 196 -567 -858
                                                                 0
ATOM 4636 H SER B 117
                           -14.109 -25.863 -46.916 1.00 36.38
                                                                Н
ATOM 4637 HA SER B 117
                            -14.548 -23.318 -46.151 1.00 31.04
                                                                 Н
ATOM 4638 HB2 SER B 117
                            -12.622 -22.501 -47.065 1.00 31.47
                                                                 Н
ATOM 4639 HB3 SER B 117
                            -12.165 -23.678 -46.100 1.00 31.47
                                                                 Н
ATOM 4640 HG SER B 117
                            -11.216 -23.860 -48.080 1.00 32.45
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ATOM 4641 N ILE B 118
                          -14.826 -22.650 -48.711 1.00 21.21
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ANISOU 4641 N ILE B 118
                           3023 2098 2937 -324 -30 -540
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ATOM 4642 CA ILE B 118
                           -15.354 -22.504 -50.057 1.00 21.41
                                                                C
                                                                C
ANISOU 4642 CA ILE B 118
                            2938 2279 2918 -476 278 -647
ATOM 4643 C ILE B 118
                          -14.545 -23.289 -51.082 1.00 23.02
ANISOU 4643 C ILE B 118
                                                               C
                           2952 2378 3415 -373 313 -921
                                                               0
ATOM 4644 O ILE B 118
                          -15.023 -23.496 -52.201 1.00 21.79
ANISOU 4644 O ILE B 118
                           2745 2297 3238 -492 540 -1010
ATOM 4645 CB ILE B 118
                           -15.430 -21.007 -50.448 1.00 19.75
ANISOU 4645 CB ILE B 118
                            2549 2379 2578 -589 505 -670
ATOM 4646 CG1 ILE B 118
                            -14.070 -20.324 -50.277 1.00 20.80
ANISOU 4646 CG1 ILE B 118
                            2427 2560 2915 -433 416 -847
ATOM 4647 CG2 ILE B 118
                            -16.475 -20.311 -49.599 1.00 19.08
                                                                 Č
ANISOU 4647 CG2 ILE B 118
                            2677 2399 2173 -727
                                                    526 -385
                                                                Č
ATOM 4648 CD1 ILE B 118
                            -14.003 -18.917 -50.851 1.00 20.04
                            2117 2759 2740 -531
                                                    664 -919
                                                                C
ANISOU 4648 CD1 ILE B 118
ATOM 4649 H ILE B 118
                          -14.529 -21.922 -48.362 1.00 25.45
                                                               Н
ATOM 4650 HA ILE B 118
                           -16.259 -22.854 -50.071 1.00 25.70
                                                                Н
ATOM 4651 HB ILE B 118
                           -15.694 -20.943 -51.379 1.00 23.70
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ATOM 4652 HG12 ILE B 118
                            -13.867 -20.266 -49.331 1.00 24.96
                                                                 Н
ATOM 4653 HG13 ILE B 118
                            -13.395 -20.857 -50.725 1.00 24.96
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                            -16.514 -19.376 -49.852 1.00 22.89
ATOM 4654 HG21 ILE B 118
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ATOM 4655 HG22 ILE B 118
                            -17.335 -20.732 -49.751 1.00 22.89
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ATOM 4656 HG23 ILE B 118
                            -16.227 -20.392 -48.665 1.00 22.89
ATOM 4657 HD11 ILE B 118
                            -13.114 -18.558 -50.702 1.00 24.05
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ATOM 4658 HD12 ILE B 118
                            -14.190 -18.955 -51.802 1.00 24.05
                                                                 Н
                            -14.663 -18.363 -50.405 1.00 24.05
ATOM 4659 HD13 ILE B 118
                                                                 Н
ATOM 4660 N ASP B 119
                           -13.341 -23.755 -50.726 1.00 25.06
                                                                Ν
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ANISOU 4660 N ASP B 119 3110 2466 3947 -157 93 -1053 Ν ATOM 4661 CA ASP B 119 -12.507 -24.525 -51.644 1.00 27.21 C **ANISOU 4661 CA ASP B 119** 3203 2621 4516 -43 117 -1312 ATOM 4662 C ASP B 119 -12.598 -26.033 -51.442 1.00 28.80 **ANISOU 4662 C ASP B 119** 3591 2519 4832 42 -41 -1285 ATOM 4663 O ASP B 119 -12.057 -26.780 -52.266 1.00 31.02 0 **ANISOU 4663 O ASP B 119** 3754 2687 5344 117 4 -1490 ATOM 4664 CB ASP B 119 C -11.034 -24.105 -51.518 1.00 29.63 **ANISOU 4664 CB ASP B 119** -3 -1502 3243 2932 5082 151 C ATOM 4665 CG ASP B 119 -10.734 -22.807 -52.243 1.00 28.95 **ANISOU 4665 CG ASP B 119** 2893 3131 4975 77 223 -1638 ATOM 4666 OD1 ASP B 119 -11.668 -22.239 -52.845 1.00 27.01 0 **ANISOU 4666 OD1 ASP B 119** 0 2670 3079 4514 -120 473 -1581 ATOM 4667 OD2 ASP B 119 -9.573 -22.344 -52.198 1.00 30.31 0 **ANISOU 4667 OD2 ASP B 119** 2835 3336 5345 215 151 -1797 0 ATOM 4668 H ASP B 119 -12.986 -23.635 -49.952 1.00 30.08 Н ATOM 4669 HA ASP B 119 -12.790 -24.334 -52.552 1.00 32.66 Н ATOM 4670 HB2 ASP B 119 -10.819 -23.982 -50.580 1.00 35.55 Н ATOM 4671 HB3 ASP B 119 -10.473 -24.798 -51.900 1.00 35.55 Н ATOM 4672 N GLY B 120 -13.249 -26.503 -50.389 1.00 27.68 Ν **ANISOU 4672 N GLY B 120** 3735 2237 4544 36 -216 -1043 N ATOM 4673 CA GLY B 120 -13.377 -27.934 -50.193 1.00 29.70 C 4179 2202 4904 113 -354 -1009 **ANISOU 4673 CA GLY B 120** ATOM 4674 C GLY B 120 -13.752 -28.276 -48.772 1.00 31.06 **ANISOU 4674 C GLY B 120** 4628 2220 4954 163 -610 -747 0 ATOM 4675 O GLY B 120 -13.813 -27.423 -47.886 1.00 29.97 **ANISOU 4675 O GLY B 120** 4530 2192 4667 154 -702 -601 0 ATOM 4676 H GLY B 120 -13.619 -26.021 -49.781 1.00 33.21 ATOM 4677 HA2 GLY B 120 -14.062 -28.283 -50.786 1.00 35.64 Н Н ATOM 4678 HA3 GLY B 120 -12.536 -28.368 -50.404 1.00 35.64 ATOM 4679 N ASP B 121 -13.994 -29.571 -48.566 1.00 33.72 Ν **ANISOU 4679 N ASP B 121** N 5159 2292 5360 218 -723 -693 -14.392 -30.079 -47.260 1.00 34.94 ATOM 4680 CA ASP B 121 C C **ANISOU 4680 CA ASP B 121** 5597 2269 5410 271 -964 -443 ATOM 4681 C ASP B 121 -13.228 -30.172 -46.282 1.00 36.21 C **ANISOU 4681 C ASP B 121** 5699 2299 5760 513 -1263 -448 ATOM 4682 O ASP B 121 -13.461 -30.197 -45.070 1.00 36.90 0 0 **ANISOU 4682 O ASP B 121** 5983 2311 5726 553 -1469 -231 C ATOM 4683 CB ASP B 121 -15.035 -31.460 -47.416 1.00 36.84 C 6063 2264 5670 247 -971 -390 **ANISOU 4683 CB ASP B 121** ATOM 4684 H ASP B 121 -13.933 -30.178 -49.173 1.00 40.46 Н ATOM 4685 HA ASP B 121 -15.054 -29.481 -46.880 1.00 41.93 Н ATOM 4686 N ARG B 122 N -11.989 -30.216 -46.773 1.00 36.57 5477 2323 6097 674 -1291 -686 Ν **ANISOU 4686 N ARG B 122** -10.817 -30.473 -45.933 1.00 39.01 C ATOM 4687 CA ARG B 122 **ANISOU 4687 CA ARG B 122** 5714 2488 6622 920 -1579 -707 C ATOM 4688 C ARG B 122 -9.697 -29.554 -46.417 1.00 39.19 C **ANISOU 4688 C ARG B 122** 5390 2690 6811 995 -1529 -929 C ATOM 4689 O ARG B 122 -8.907 -29.931 -47.286 1.00 40.09 0 **ANISOU 4689 O ARG B 122** 5294 2751 7187 1090 -1463 -1163 0 ATOM 4690 CB ARG B 122 -10.423 -31.943 -46.008 1.00 42.20 C 6184 2578 7270 1081 -1699 -763 **ANISOU 4690 CB ARG B 122** C ATOM 4691 CG ARG B 122 C -9.779 -32.478 -44.752 1.00 44.37

ANISOU 4691 CG ARG B 122 6527 2726 7604 1264 -1995 -628 C
ATOM 4692 CD ARG B 122 -9.338 -33.921 -44.941 1.00 47.30 C
ANISOU 4692 CD ARG B 122 6905 2908 8159 1375 -2023 -678 C
ATOM 4693 NE ARG B 122 -8.318 -34.301 -43.969 1.00 49.94 N
ANISOU 4693 NE ARG B 122 7184 3183 8609 1564 -2269 -630 N
ATOM 4694 CZ ARG B 122 -7.008 -34.307 -44.207 1.00 51.89 C
ANISOU 4694 CZ ARG B 122 7172 3442 9103 1719 -2327 -803 C
ATOM 4695 NH1 ARG B 122 -6.532 -33.957 -45.398 1.00 51.20 N
ANISOU 4695 NH1 ARG B 122 6844 3437 9172 1709 -2149 -1041 N
ATOM 4696 NH2 ARG B 122 -6.165 -34.671 -43.248 1.00 54.21 N
ANISOU 4696 NH2 ARG B 122 7442 3683 9472 1869 -2551 -736 N
ATOM 4697 H ARG B 122 -11.798 -30.099 -47.603 1.00 43.89 H
ATOM 4698 HA ARG B 122 -11.022 -30.253 -45.010 1.00 46.82 H
ATOM 4699 HB2 ARG B 122 -11.219 -32.470 -46.179 1.00 50.63 H
ATOM 4700 HB3 ARG B 122 -9.791 -32.058 -46.735 1.00 50.63 H
ATOM 4701 HG2 ARG B 122 -8.998 -31.945 -44.538 1.00 53.24 H
ATOM 4702 HG3 ARG B 122 -10.419 -32.447 -44.024 1.00 53.24 H
ATOM 4703 HD2 ARG B 122 -10.103 -34.507 -44.824 1.00 56.76 H
ATOM 4704 HD3 ARG B 122 -8.966 -34.028 -45.830 1.00 56.76 H
ATOM 4705 HE ARG B 122 -8.582 -34.538 -43.185 1.00 59.93 H
ATOM 4706 HH11 ARG B 122 -7.072 -33.720 -46.024 1.00 61.44 H
ATOM 4707 HH12 ARG B 122 -5.684 -33.965 -45.542 1.00 61.44 H
ATOM 4707 HH12 ARG B 122 -5.004 -53.905 -43.542 1.00 01.44 H
ATOM 4708 HH21 ARG B 122 -0.400 -34.900 -42.473 1.00 03.03 H
ATOM 4709 HHZZ ARG B 122 -3.318 -34.078 -43.399 1.00 03.03 H
ANISOU 4710 N THR B 123 5119 2685 6445 948 -1556 -856 N
ATOM 4711 CA THR B 123 -8.714 -27.321 -46.316 1.00 37.93 C
ANISOU 4711 CA THR B 123
ANISOU 4712 C THR B 123 4867 3048 6612 1072 -1703 -957 C
ATOM 4713 O THR B 123 -8.628 -26.643 -43.999 1.00 37.29 O
ANISOU 4714 CB THR B 123
ATOM 4715 OG1 THR B 123 -10.438 -25.631 -46.555 1.00 33.99 O
ANISOU 4715 OG1 THR B 123
ATOM 4716 CG2 THR B 123 -10.039 -27.068 -48.441 1.00 35.58 C
ANISOU 4716 CG2 THR B 123
ATOM 4717 H THR B 123 -10.125 -28.099 -45.188 1.00 45.00 H
ATOM 4718 HA THR B 123 -7.985 -27.741 -46.799 1.00 45.52 H
ATOM 4719 HB THR B 123 -8.763 -25.700 -47.608 1.00 42.53 H
ATOM 4720 HG1 THR B 123 -11.005 -26.175 -46.256 1.00 40.79 H
ATOM 4721 HG21 THR B 123 -10.476 -26.435 -49.032 1.00 42.70 H
ATOM 4722 HG22 THR B 123 -9.354 -27.542 -48.938 1.00 42.70 H
ATOM 4723 HG23 THR B 123 -10.695 -27.707 -48.122 1.00 42.70 H
ATOM 4724 N THR B 124 -7.053 -25.832 -45.393 1.00 39.43 N
ANISOU 4724 N THR B 124 4723 3331 6927 1156 -1697 -1146 N
ATOM 4725 CA THR B 124 -6.391 -25.000 -44.397 1.00 41.73 C
ANISOU 4725 CA THR B 124 4943 3718 7193 1230 -1887 -1096 C
ATOM 4726 C THR B 124 -6.463 -23.546 -44.843 1.00 39.52 C
ANISOU 4726 C THR B 124 4492 3740 6785 1081 -1664 -1171 C
ATOM 4727 O THR B 124 -6.153 -23.235 -45.997 1.00 38.35 O
ANISOU 4727 O THR B 124 4115 3702 6755 1049 -1443 -1384 O

ATOM 4728 CB THR B 124 -4.933 -25.428 -44.209 1.00 45.94 **ANISOU 4728 CB THR B 124** 5266 4132 8056 1480 -2107 -1251 ATOM 4729 OG1 THR B 124 -4.888 -26.789 -43.758 1.00 48.85 5803 4214 8543 1623 -2311 -1166 **ANISOU 4729 OG1 THR B 124** ATOM 4730 CG2 THR B 124 -4.233 -24.539 -43.193 1.00 46.78 5288 4355 8132 1546 -2302 -1207 C **ANISOU 4730 CG2 THR B 124** ATOM 4731 H THR B 124 -6.679 -25.798 -46.167 1.00 47.32 Н ATOM 4732 HA THR B 124 -6.850 -25.085 -43.546 1.00 50.07 Н ATOM 4733 HB THR B 124 -4.464 -25.354 -45.055 1.00 55.12 Н ATOM 4734 HG1 THR B 124 -4.090 -27.030 -43.653 1.00 58.62 ATOM 4735 HG21 THR B 124 -3.311 -24.821 -43.085 1.00 56.14 ATOM 4736 HG22 THR B 124 -4.246 -23.617 -43.495 1.00 56.14 Н ATOM 4737 HG23 THR B 124 -4.683 -24.596 -42.336 1.00 56.14 ATOM 4738 N PHE B 125 -6.868 -22.657 -43.935 1.00 26.21 **ANISOU 4738 N PHE B 125** 3287 2360 4311 987 -17 -506 ATOM 4739 CA PHE B 125 -7.029 -21.256 -44.294 1.00 25.04 **ANISOU 4739 CA PHE B 125** 3073 2399 4043 880 31 -505 ATOM 4740 C PHE B 125 -6.780 -20.365 -43.084 1.00 23.85 ANISOU 4740 C PHE B 125 ATOM 4741 O PHE B 125 2893 2313 3856 910 -84 -392 -6.966 -20.774 -41.933 1.00 24.86 **ANISOU 4741 O PHE B 125** 3102 2359 3984 966 -196 -281 ATOM 4742 CB PHE B 125 -8.425 -20.983 -44.862 1.00 24.02 **ANISOU 4742 CB PHE B 125** 3048 2317 3763 723 102 -475 ATOM 4743 CG PHE B 125 -9.542 -21.511 -44.013 1.00 22.64 3022 2048 3531 693 **ANISOU 4743 CG PHE B 125** 40 -354 ATOM 4744 CD1 PHE B 125 -9.974 -22.820 -44.151 1.00 22.67 **ANISOU 4744 CD1 PHE B 125** 3130 1899 3586 701 56 -372 ATOM 4745 CD2 PHE B 125 -10.170 -20.698 -43.086 1.00 21.23 **ANISOU 4745 CD2 PHE B 125** 2882 1934 3249 647 -22 -231 -11.003 -23.308 -43.376 1.00 22.48 ATOM 4746 CE1 PHE B 125 **ANISOU 4746 CE1 PHE B 125** 3244 1791 3506 655 11 -260 ATOM 4747 CE2 PHE B 125 -11.205 -21.183 -42.306 1.00 20.95 **ANISOU 4747 CE2 PHE B 125** 2979 1826 3155 605 -61 -129 -11.617 -22.495 -42.454 1.00 21.69 ATOM 4748 CZ PHE B 125 C **ANISOU 4748 CZ PHE B 125** 3176 1770 3296 604 -43 -138 ATOM 4749 H PHE B 125 -7.054 -22.840 -43.116 1.00 31.45 Н Н ATOM 4750 HA PHE B 125 -6.377 -21.027 -44.975 1.00 30.05 -8.545 -20.024 -44.946 1.00 28.83 -8.494 -21.400 -45.735 1.00 28.83 ATOM 4751 HB2 PHE B 125 ATOM 4752 HB3 PHE B 125 Н ATOM 4753 HD1 PHE B 125 -9.562 -23.377 -44.772 1.00 27.21 ATOM 4754 HD2 PHE B 125 -9.891 -19.816 -42.984 1.00 25.47 ATOM 4755 HE1 PHE B 125 -11.282 -24.190 -43.476 1.00 26.98 Н ATOM 4756 HE2 PHE B 125 -11.618 -20.631 -41.682 1.00 25.14 Н ATOM 4757 HZ PHE B 125 -12.312 -22.826 -41.932 1.00 26.03 -6.353 -19.142 -43.365 1.00 22.02 ATOM 4758 N THR B 126 Ν **ANISOU 4758 N THR B 126** 2552 2227 3586 862 -52 -422 Ν ATOM 4759 CA THR B 126 -6.190 -18.129 -42.335 1.00 19.99 **ANISOU 4759 CA THR B 126** 2266 2048 3282 863 -144 -336 ATOM 4760 C THR B 126 -7.538 -17.510 -41.993 1.00 18.67 ANISOU 4760 C THR B 126 2213 1919 2964 750 -144 -235 C ATOM 4761 O THR B 126 -8.423 -17.382 -42.849 1.00 18.38 0 ANISOU 4761 O THR B 126 2224 1906 2853 648 -56 -250 0 ATOM 4762 CB THR B 126 -5.227 -17.042 -42.815 1.00 21.21

ANISOU 4762 CB THR B 126 2261 2333 3465 842 -100 -415 ATOM 4763 OG1 THR B 126 -3.949 -17.625 -43.084 1.00 24.20 **ANISOU 4763 OG1 THR B 126** 2510 2687 3998 952 -97 -523 -5.076 -15.927 -41.778 1.00 20.54 ATOM 4764 CG2 THR B 126 **ANISOU 4764 CG2 THR B 126** 2145 2327 3333 830 -191 -341 C ATOM 4765 H THR B 126 -6.148 -18.871 -44.155 1.00 26.42 Н ATOM 4766 HA THR B 126 -5.824 -18.535 -41.534 1.00 23.99 Н ATOM 4767 HB THR B 126 -5.574 -16.648 -43.631 1.00 25.45 Н ATOM 4768 HG1 THR B 126 -3.413 -17.034 -43.348 1.00 29.04 Н ATOM 4769 HG21 THR B 126 -4.462 -15.251 -42.105 1.00 24.65 ATOM 4770 HG22 THR B 126 -5.938 -15.514 -41.608 1.00 24.65 ATOM 4771 HG23 THR B 126 -4.732 -16.291 -40.948 1.00 24.65 Н ATOM 4772 N GLN B 127 -7.687 -17.118 -40.729 1.00 16.20 **ANISOU 4772 N GLN B 127** 1936 1617 2604 767 -246 -138 ATOM 4773 CA GLN B 127 -8.883 -16.441 -40.248 1.00 15.77 **ANISOU 4773 CA GLN B 127** 1968 1607 2419 670 -248 -56 ATOM 4774 C GLN B 127 ANISOU 4774 C GLN B 127 -8.501 -15.080 -39.682 1.00 14.33 1709 1532 2205 651 -288 -46 ATOM 4775 O GLN B 127 ANISOU 4775 O GLN B 127 -7.573 -14.984 -38.871 1.00 14.69 0 1698 1588 2294 727 -379 -40 ATOM 4776 CB GLN B 127 -9.594 -17.261 -39.168 1.00 16.82 **ANISOU 4776 CB GLN B 127** 2237 1651 2503 685 -317 46 CCCC ATOM 4777 CG GLN B 127 -10.081 -18.628 -39.610 1.00 18.54 **ANISOU 4777 CG GLN B 127** 2550 1740 2754 689 -281 ATOM 4778 CD GLN B 127 -10.517 -19.504 -38.435 1.00 19.72 **ANISOU 4778 CD GLN B 127** 2836 1786 2871 712 -361 158 ATOM 4779 OE1 GLN B 127 -9.713 -19.831 -37.559 1.00 20.86 **ANISOU 4779 OE1 GLN B 127** 2983 1886 3057 811 -470 207 0 ATOM 4780 NE2 GLN B 127 -11.790 -19.891 -38.420 1.00 19.66 2941 1742 2785 614 -311 **ANISOU 4780 NE2 GLN B 127** ATOM 4781 H GLN B 127 -7.093 -17.238 -40.119 1.00 19.44 Н -9.497 -16.306 -40.987 1.00 18.93 ATOM 4782 HA GLN B 127 н ATOM 4783 HB2 GLN B 127 -8.981 -17.394 -38.429 1.00 20.18 Н -10.368 -16.761 -38.862 1.00 20.18 ATOM 4784 HB3 GLN B 127 Н ATOM 4785 HG2 GLN B 127 -10.841 -18.518 -40.201 1.00 22.25 Н ATOM 4786 HG3 GLN B 127 -9.362 -19.085 -40.074 1.00 22.25 Н ATOM 4787 HE21 GLN B 127 -12.321 -19.647 -39.051 1.00 23.59 Н ATOM 4788 HE22 GLN B 127 -12.082 -20.384 -37.779 1.00 23.59 ATOM 4789 N TYR B 128 -9.218 -14.041 -40.110 1.00 13.48 Ν Ν **ANISOU 4789 N TYR B 128** 1599 1498 2025 551 -228 -45 ATOM 4790 CA TYR B 128 -9.108 -12.691 -39.564 1.00 13.05 **ANISOU 4790 CA TYR B 128** 1496 1526 1937 516 -257 -34 C ATOM 4791 C TYR B 128 -10.324 -12.417 -38.689 1.00 12.77 **ANISOU 4791 C TYR B 128** 1558 1494 1802 467 -281 37 ATOM 4792 O TYR B 128 0 -11.458 -12.675 -39.102 1.00 12.09 **ANISOU 4792 O TYR B 128** 1540 1387 1666 410 -228 59 ATOM 4793 CB TYR B 128 -9.044 -11.632 -40.669 1.00 11.98 **ANISOU 4793 CB TYR B 128** 1290 1457 1804 440 -175 -82 -7.787 -11.612 -41.517 1.00 12.06 ATOM 4794 CG TYR B 128 **ANISOU 4794 CG TYR B 128** 1186 1495 1900 460 -132 -165 ATOM 4795 CD1 TYR B 128 -6.695 -12.428 -41.231 1.00 13.17 ANISOU 4795 CD1 TYR B 128 1263 1606 2134 561 -174 -209 ATOM 4796 CD2 TYR B 128 -7.699 -10.760 -42.613 1.00 12.19

ANISOU 4796 CD2 TYR B 128 1156 1569 1906 376 -47 -199 ATOM 4797 CE1 TYR B 128 -5.560 -12.386 -42.007 1.00 14.27 **ANISOU 4797 CE1 TYR B 128** 1279 1782 2361 576 -121 -302 ATOM 4798 CE2 TYR B 128 -6.574 -10.719 -43.389 1.00 14.06 **ANISOU 4798 CE2 TYR B 128** 1289 1844 2211 375 12 -281 ATOM 4799 CZ TYR B 128 -5.508 -11.527 -43.087 1.00 14.32 **ANISOU 4799 CZ TYR B 128** 1242 1856 2342 474 -19 -341 ATOM 4800 OH TYR B 128 -4.389 -11.472 -43.877 1.00 16.46 0 **ANISOU 4800 OH TYR B 128** 1389 2175 2689 470 0 53 -441 ATOM 4801 H TYR B 128 -9.798 -14.099 -40.742 1.00 16.18 Н ATOM 4802 HA TYR B 128 -8.309 -12.622 -39.019 1.00 15.66 Н ATOM 4803 HB2 TYR B 128 -9.793 -11.775 -41.269 1.00 14.37 Н ATOM 4804 HB3 TYR B 128 -9.127 -10.758 -40.256 1.00 14.37 ATOM 4805 HD1 TYR B 128 -6.731 -13.003 -40.501 1.00 15.80 ATOM 4806 HD2 TYR B 128 -8.417 -10.207 -42.820 1.00 14.63 ATOM 4807 HE1 TYR B 128 -4.835 -12.935 -41.809 1.00 17.12 Н ATOM 4808 HE2 TYR B 128 -6.530 -10.143 -44.117 1.00 16.88 Н ATOM 4809 HH TYR B 128 -4.498 -10.909 -44.491 1.00 19.75 ATOM 4810 N TRP B 129 -10.096 -11.871 -37.498 1.00 12.55 Ν 1527 1500 1743 483 -356 **ANISOU 4810 N TRP B 129** Ν ATOM 4811 CA TRP B 129 -11.174 -11.646 -36.548 1.00 12.64 **ANISOU 4811 CA TRP B 129** 1624 1522 1654 437 -370 113 ATOM 4812 C TRP B 129 ANISOU 4812 C TRP B 129 -11.171 -10.217 -36.029 1.00 12.23 1523 1545 1578 398 -382 86 0 ATOM 4813 O TRP B 129 -10.121 -9.676 -35.676 1.00 13.15 **ANISOU 4813 O TRP B 129** 1565 1699 1733 429 -436 **52** ATOM 4814 CB TRP B 129 -11.059 -12.555 -35.321 1.00 13.90 **ANISOU 4814 CB TRP B 129** 1869 1646 1768 484 -455 ATOM 4815 CG TRP B 129 -10.980 -14.019 -35.562 1.00 14.96 **ANISOU 4815 CG TRP B 129** 2068 1680 1936 534 -465 214 CC ATOM 4816 CD1 TRP B 129 -9.854 -14.749 -35.818 1.00 15.47 2087 1691 2099 630 -514 **ANISOU 4816 CD1 TRP B 129** 197 ATOM 4817 CD2 TRP B 129 -12.061 -14.953 -35.509 1.00 15.55 **ANISOU 4817 CD2 TRP B 129** 2262 1686 1958 490 -427 269 ATOM 4818 NE1 TRP B 129 -10.174 -16.081 -35.946 1.00 16.45 N **ANISOU 4818 NE1 TRP B 129** 2305 1704 2242 239 656 -511 ATOM 4819 CE2 TRP B 129 -11.521 -16.230 -35.759 1.00 16.55 **ANISOU 4819 CE2 TRP B 129** 2424 1704 2158 563 -457 286 CCCCCCC -13.437 -14.834 -35.283 1.00 15.29 ATOM 4820 CE3 TRP B 129 **ANISOU 4820 CE3 TRP B 129** 2303 1670 1836 394 -368 297 ATOM 4821 CZ2 TRP B 129 -12.308 -17.382 -35.790 1.00 17.70 **ANISOU 4821 CZ2 TRP B 129** 2690 1750 2286 534 -428 336 ATOM 4822 CZ3 TRP B 129 -14.215 -15.982 -35.319 1.00 16.36 **ANISOU 4822 CZ3 TRP B 129** 2545 1722 1949 359 -336 344 -13.648 -17.235 -35.572 1.00 17.39 ATOM 4823 CH2 TRP B 129 C **ANISOU 4823 CH2 TRP B 129** 2722 1737 2150 424 -367 366 ATOM 4824 H TRP B 129 -9.322 -11.622 -37.217 1.00 15.07 Н ATOM 4825 HA TRP B 129 -12.026 -11.815 -36.978 1.00 15.16 Н ATOM 4826 HB2 TRP B 129 -10.259 -12.303 -34.834 1.00 16.69 Н ATOM 4827 HB3 TRP B 129 -11.835 -12.401 -34.759 1.00 16.69 Н ATOM 4828 HD1 TRP B 129 -8.997 -14.397 -35.895 1.00 18.56 Н -9.618 -16.715 -36.115 1.00 19.74 ATOM 4829 HE1 TRP B 129 Н ATOM 4830 HE3 TRP B 129 -13.821 -14.004 -35.113 1.00 18.35

ATOM 4831 HZ2 TRP B 129 -11.936 -18.217 -35.965 1.00 21.24 ATOM 4832 HZ3 TRP B 129 -15.131 -15.917 -35.170 1.00 19.63 ATOM 4833 HH2 TRP B 129 -14.196 -17.986 -35.591 1.00 20.87 ATOM 4834 N SER B 130 -12.359 -9.629 -35.964 1.00 11.61 **ANISOU 4834 N SER B 130** 1481 1485 1446 331 -334 ATOM 4835 CA SER B 130 -12.655 -8.525 -35.059 1.00 11.58 **ANISOU 4835 CA SER B 130** 1469 1532 1400 298 -350 ATOM 4836 C SER B 130 -13.719 -9.028 -34.098 1.00 11.39 **ANISOU 4836 C SER B 130** 1542 1510 1275 268 -345 110 ATOM 4837 O SER B 130 -14.821 -9.374 -34.527 1.00 11.79 **ANISOU 4837 O SER B 130** 1632 1542 1308 228 -283 128 ATOM 4838 CB SER B 130 -13.154 -7.284 -35.801 1.00 11.34 **ANISOU 4838 CB SER B 130** 1384 1515 1409 249 -293 ATOM 4839 OG SER B 130 -12.111 -6.623 -36.497 1.00 11.85 ANISOU 4839 OG SER B 130 1364 1586 1552 256 -296 0 ATOM 4840 H SER B 130 -13.030 -9.859 -36.450 1.00 13.93 H ATOM 4841 HA SER B 130 -11.861 -8.290 -34.553 1.00 13.90 н ATOM 4842 HB2 SER B 130 -13.832 -7.555 -36.440 1.00 13.61 ATOM 4843 HB3 SER B 130 -13.538 -6.669 -35.157 1.00 13.61 ATOM 4844 HG SER B 130 -11.516 -6.378 -35.957 1.00 14.22 Н ATOM 4845 N VAL B 131 -13.394 -9.080 -32.809 1.00 11.69 Ν **ANISOU 4845 N VAL B 131** 1619 1581 1241 279 -409 121 ATOM 4846 CA VAL B 131 -14.311 -9.590 -31.796 1.00 12.80 ANISOU 4846 CA VAL B 131 1863 1735 1264 236 -399 161 ATOM 4847 C VAL B 131 -14.618 -8.467 -30.817 1.00 13.13 ANISOU 4847 C VAL B 131 1894 1853 1243 191 -395 C 102 ATOM 4848 O VAL B 131 -13.709 -7.927 -30.179 1.00 15.46 0 ANISOU 4848 O VAL B 131 2158 2190 1526 213 -466 70 ATOM 4849 CB VAL B 131 -13.729 -10.806 -31.058 1.00 14.67 ANISOU 4849 CB VAL B 131 2189 1941 1444 276 -482 241 ATOM 4850 CG1 VAL B 131 -14.721 -11.320 -30.012 1.00 15.96 ANISOU 4850 CG1 VAL B 131 2475 2120 1468 208 -459 293 ATOM 4851 CG2 VAL B 131 -13.341 -11.892 -32.050 1.00 14.31 ANISOU 4851 CG2 VAL B 131 2145 1804 1486 331 -484 278 ATOM 4852 H VAL B 131 -12.637 -8.823 -32.493 1.00 14.03 ATOM 4853 HA VAL B 131 -15.140 -9.859 -32.220 1.00 15.36 Н ATOM 4854 HB VAL B 131 -12.925 -10.532 -30.592 1.00 17.60 Н ATOM 4855 HG11 VAL B 131 -14.334 -12.086 -29.560 1.00 19.15 ATOM 4856 HG12 VAL B 131 -14.898 -10.612 -29.372 1.00 19.15 Н -15.543 -11.578 -30.457 1.00 19.15 -12.977 -12.648 -31.564 1.00 17.17 ATOM 4857 HG13 VAL B 131 ATOM 4858 HG21 VAL B 131 ATOM 4859 HG22 VAL B 131 Н ATOM 4860 HG23 VAL B 131 Н ATOM 4861 N ARG B 132 -15.898 -8.134 -30.687 1.00 13.47 **ANISOU 4861 N ARG B 132** 1953 1915 1249 129 -311 76 N ATOM 4862 CA ARG B 132 -16.304 -7.059 -29.794 1.00 14.13 **ANISOU 4862 CA ARG B 132** 2019 2065 1283 87 -288 -2 ATOM 4863 C ARG B 132 C -15.879 -7.378 -28.363 1.00 15.69 ANISOU 4863 C ARG B 132 2299 2323 1341 70 -350 14 ATOM 4864 O ARG B 132 -16.009 -8.512 -27.891 1.00 14.79 0 ANISOU 4864 O ARG B 132 2286 2200 1133 56 -369 99 ATOM 4865 CB ARG B 132 -17.815 -6.859 -29.876 1.00 13.65 ANISOU 4865 CB ARG B 132 1957 2016 1213 29 -182 -35

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ATOM 4866 CG ARG B 132 -18.276 -5.433 -29.576 1.00 13.66
ANISOU 4866 CG ARG B 132 1886 2052 1250 11 -140 -146
ATOM 4867 CD ARG B 132
                                        -19.745 -5.272 -29.884 1.00 13.08
ANISOU 4867 CD ARG B 132
                                       1782 1981 1208 -25 -44 -180
ATOM 4868 NE ARG B 132
                                       -20.256 -3.913 -29.694 1.00 13.80
ANISOU 4868 NE ARG B 132
                                       1793 2084 1365 -26
                                                                        -3 -292
ATOM 4869 CZ ARG B 132
                                                                                         C
                                        -20.674 -3.405 -28.538 1.00 15.12
ANISOU 4869 CZ ARG B 132
                                       1968 2315 1462 -67 42 -385
ATOM 4870 NH1 ARG B 132
                                        -20.632 -4.121 -27.425 1.00 16.16 N
ANISOU 4870 NH1 ARG B 132 2192 2516 1433 -120 49 -368
ATOM 4871 NH2 ARG B 132 -21.131 -2.160 -28.491 1.00 15.48
ANISOU 4871 NH2 ARG B 132 1933 2351 1599 -55 80 -496
                                                                                        N
ATOM 4872 H ARG B 132 -16.547 -8.514 -31.104 1.00 16.16 H
ATOM 4873 HA ARG B 132 -15.872 -6.235 -30.065 1.00 16.95 H
ATOM 4874 HB2 ARG B 132
                                       -18.111 -7.083 -30.772 1.00 16.38
ATOM 4874 HB2 ARG B 132 -18.111 -7.083 -30.772 1.00 16.38 H
ATOM 4875 HB3 ARG B 132 -18.242 -7.448 -29.234 1.00 16.38 H
ATOM 4876 HG2 ARG B 132 -18.137 -5.239 -28.636 1.00 16.39 H
ATOM 4877 HG3 ARG B 132 -17.777 -4.810 -30.128 1.00 16.39 H
ATOM 4879 HD3 ARG B 132 -19.897 -5.518 -30.811 1.00 15.70 H
ATOM 4880 HE ARG B 132 -20.251 -5.861 -29.303 1.00 15.70 H
ATOM 4881 HH11 ARG B 132 -20.287 -3.402 -30.385 1.00 16.56 H
ATOM 4881 HH11 ARG B 132 -20.341 -4.930 -27.445 1.00 19.40 H
ATOM 4882 HH12 ARG B 132 -20.903 -3.779 -26.684 1.00 19.40
ATOM 4883 HH21 ARG B 132 -21.157 -1.684 -29.207 1.00 18.58
                                                                                          Н
ATOM 4884 HH22 ARG B 132 -21.394 -1.826 -27.743 1.00 18.58
                                                                                       Ν
ATOM 4885 N GLN B 133 -15.356 -6.365 -27.673 1.00 15.82
ANISOU 4885 N GLN B 133 2277 2396 1337 64 -387 -65
                                       -14.805 -6.592 -26.342 1.00 17.19
ATOM 4886 CA GLN B 133
ANISOU 4886 CA GLN B 133 2524 2641 1367 47 -467 -53
                                                                                        C
ATOM 4887 C GLN B 133 -15.882 -6.944 -25.326 1.00 18.40
ANISOU 4887 C GLN B 133 2782 2852 1357 -38 -401 -46
ATOM 4888 O GLN B 133 -15.579 -7.573 -24.305 1.00 18.59
                                                                                        0
ANISOU 4888 O GLN B 133 2910 2924 1230 -62 -467 14
ATOM 4889 CB GLN B 133 -14.030 -5.356 -25.886 1.00 18.43
ANISOU 4889 CB GLN B 133
                                      2609 2851 1544 47 -517 -161
ATOM 4890 CG GLN B 133
                                       -12.755 -5.129 -26.675 1.00 17.59
ANISOU 4890 CG GLN B 133
                                       2406 2705 1573 116 -594 -161
ATOM 4891 CD GLN B 133
ANISOU 4891 CD GLN B 133
                                       -11.939 -3.969 -26.162 1.00 17.87
                                       2370 2793 1626 101 -648 -269
                                                                                          C
                                       -12.467 -3.037 -25.555 1.00 18.59 O 2462 2923 1678 44 -599 -368 O
ATOM 4892 OE1 GLN B 133
ANISOU 4892 OE1 GLN B 133
ATOM 4893 NE2 GLN B 133
                                        -10.632 -4.029 -26.384 1.00 18.18
                                       2343 2834 1731 150 -748 -261
ANISOU 4893 NE2 GLN B 133
                                                                                         Ν
ATOM 4894 H GLN B 133
                                      -15.308 -5.551 -27.948 1.00 18.98 H
                                                                                      H
ATOM 4895 HA GLN B 133
                                       -14.182 -7.334 -26.384 1.00 20.63
ATOM 4896 HB2 GLN B 133 -14.162 -7.334 -26.384 1.00 20.63 H
ATOM 4896 HB2 GLN B 133 -14.592 -4.573 -25.994 1.00 22.12 H
ATOM 4897 HB3 GLN B 133 -13.788 -5.463 -24.952 1.00 22.12 H
ATOM 4898 HG2 GLN B 133 -12.206 -5.927 -26.622 1.00 21.11 H
ATOM 4899 HG3 GLN B 133 -12.986 -4.946 -27.599 1.00 21.11 H
ATOM 4900 HE21 GLN B 133 -10.297 -4.703 -26.799 1.00 21.82 H
ATOM 4901 HE22 GLN B 133 -10.120 -3.393 -26.112 1.00 21.82 H
ATOM 4902 N SER B 134 -17.121 -6.534 -25.573 1.00 19.44 N
ANISOU 4902 N SER B 134 2885 2985 1514 -86 -275 -107 N
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ATOM 4903 CA SER B 134 -18.269 -6.979 -24.806 1.00 20.78 ANISOU 4903 CA SER B 134 3137 3207 1549 -176 -184 -103 ATOM 4904 C SER B 134 -19.396 -7.256 -25.787 1.00 17.89 ANISOU 4904 C SER B 134 2728 2787 1281 -188 -81 -96 ATOM 4905 O SER B 134 -19.471 -6.641 -26.856 1.00 16.16 Ö -19.471 -6.641 -26.856 1.00 16.16 ANISOU 4905 O SER B 134 2404 2516 1219 -138 -66 -136 ATOM 4906 CB SER B 134 -18.703 -5.931 -23.768 1.00 24.84 **ANISOU 4906 CB SER B 134** 3637 3821 1979 -240 -125 -240 ATOM 4907 OG SER B 134 -19.112 -4.746 -24.427 1.00 26.00 **ANISOU 4907 OG SER B 134** 3656 3939 2283 -213 -64 -358 0 ATOM 4908 H SER B 134 -17.324 -5.982 -26.200 1.00 23.32 ATOM 4909 HA SER B 134 -18.052 -7.803 -24.342 1.00 24.93 Н ATOM 4910 HB2 SER B 134 -19.445 -6.281 -23.251 1.00 29.81 ATOM 4911 HB3 SER B 134 -17.954 -5.730 -23.185 1.00 29.81 ATOM 4912 HG SER B 134 -19.350 -4.170 -23.863 1.00 31.20 ATOM 4913 N LYS B 135 -20.270 -8.189 -25.423 1.00 16.15 Ν 2593 2581 962 -263 -14 -40 **ANISOU 4913 N LYS B 135** -21.340 -8.592 -26.327 1.00 15.53 ATOM 4914 CA LYS B 135 C **ANISOU 4914 CA LYS B 135** 2474 2458 970 -285 75 -31 ATOM 4915 C LYS B 135 -22.213 -7.399 -26.701 1.00 15.36 C **ANISOU 4915 C LYS B 135** 2318 2464 1055 -283 159 -164 0 ATOM 4916 O LYS B 135 -22.598 -6.603 -25.841 1.00 16.29 2413 2658 1121 -322 214 -270 **ANISOU 4916 O LYS B 135** ATOM 4917 CB LYS B 135 -22.188 -9.685 -25.675 1.00 16.62 **ANISOU 4917 CB LYS B 135** 2723 2620 971 -391 147 32 ATOM 4918 CG LYS B 135 -21.487 -11.020 -25.584 1.00 17.63 **ANISOU 4918 CG LYS B 135** 2987 2679 1034 -382 63 184 ATOM 4919 CD LYS B 135 -22.352 -12.047 -24.882 1.00 18.45 **ANISOU 4919 CD LYS B 135** 3216 2797 998 -506 141 253 -21.609 -13.354 -24.677 1.00 19.70 ATOM 4920 CE LYS B 135 **ANISOU 4920 CE LYS B 135** 3494 2858 1133 -473 43 405 ATOM 4921 NZ LYS B 135 -22.493 -14.352 -24.027 1.00 20.09 **ANISOU 4921 NZ LYS B 135** 3619 2893 1122 -572 119 459 Ν ATOM 4922 H LYS B 135 -20.265 -8.599 -24.667 1.00 19.38 Н ATOM 4923 HA LYS B 135 -20.953 -8.952 -27.140 1.00 18.64 Н ATOM 4924 HB2 LYS B 135 -22.417 -9.408 -24.774 1.00 19.94 ATOM 4925 HB3 LYS B 135 -22.996 -9.808 -26.197 1.00 19.94 ATOM 4926 HG2 LYS B 135 -21.296 -11.343 -26.479 1.00 21.16 Н ATOM 4927 HG3 LYS B 135 -20.665 -10.918 -25.080 1.00 21.16 ATOM 4928 HD2 LYS B 135 -22.611 -11.705 -24.012 1.00 22.14 ATOM 4929 HD3 LYS B 135 -23.138 -12.226 -25.421 1.00 22.14 ATOM 4930 HE2 LYS B 135 -21.329 -13.705 -25.536 1.00 23.64 Н ATOM 4931 HE3 LYS B 135 -20.841 -13.203 -24.104 1.00 23.64 ATOM 4932 HZ1 LYS B 135 -22.764 -14.048 -23.235 1.00 24.11 ATOM 4933 HZ2 LYS B 135 -23.206 -14.504 -24.537 1.00 24.11 ATOM 4934 HZ3 LYS B 135 -22.053 -15.116 -23.908 1.00 24.11 Н ATOM 4935 N ARG B 136 -22.532 -7.283 -27.981 1.00 15.40 Ν **ANISOU 4935 N ARG B 136** 2237 2406 1210 -238 165 -161 ATOM 4936 CA ARG B 136 -23.355 -6.170 -28.444 1.00 14.63 ANISOU 4936 CA ARG B 136 2010 2316 1234 -220 222 -269 ATOM 4937 C ARG B 136 -24.815 -6.436 -28.101 1.00 14.71 ANISOU 4937 C ARG B 136 1994 2382 1211 -302 341 -320 C ATOM 4938 O ARG B 136 -25.295 -7.546 -28.330 1.00 15.48

ANISOU 4938 O ARG B 136 2142 2472 1270 -355 370 -249 0 ATOM 4939 CB ARG B 136 -23.217 -5.991 -29.956 1.00 14.16 **ANISOU 4939 CB ARG B 136** 1877 2176 1327 -152 177 -233 ATOM 4940 CG ARG B 136 -23.796 -4.689 -30.495 1.00 14.59 **ANISOU 4940 CG ARG B 136** 1806 2216 1522 -110 196 -323 ATOM 4941 CD ARG B 136 -23.490 -4.544 -31.989 1.00 14.33 **ANISOU 4941 CD ARG B 136** 1728 2109 1608 -52 135 -263 ATOM 4942 NE ARG B 136 Ν -23.826 -3.216 -32.503 1.00 14.12 **ANISOU 4942 NE ARG B 136** 1600 2047 1717 126 -325 Ν -3 ATOM 4943 CZ ARG B 136 C -23.467 -2.766 -33.700 1.00 14.15 **ANISOU 4943 CZ ARG B 136** 1570 1988 1819 44 69 -278 -22.759 -3.535 -34.516 1.00 14.39 ATOM 4944 NH1 ARG B 136 Ν ANISOU 4944 NH1 ARG B 136 1647 1994 1824 45 28 -187 ATOM 4945 NH2 ARG B 136 -23.821 -1.542 -34.083 1.00 14.81 Ν ANISOU 4945 NH2 ARG B 136 1575 2028 2025 87 55 -323 Ν ATOM 4946 H ARG B 136 -22.289 -7.828 -28.599 1.00 18.48 Н ATOM 4947 HA ARG B 136 -23.076 -5.351 -28.006 1.00 17.56 Н -22.275 -6.011 -30.185 1.00 16.99 ATOM 4948 HB2 ARG B 136 ATOM 4949 HB3 ARG B 136 -23.677 -6.722 -30.398 1.00 16.99 Н ATOM 4950 HG2 ARG B 136 -24.758 -4.690 -30.377 1.00 17.51 Н H -23.397 -3.940 -30.026 1.00 17.51 ATOM 4951 HG3 ARG B 136 ATOM 4952 HD2 ARG B 136 -22.543 -4.692 -32.134 1.00 17.20 ATOM 4953 HD3 ARG B 136 -24.009 -5.198 -32.483 1.00 17.20 Н ATOM 4954 HE ARG B 136 -24.286 -2.694 -31.998 1.00 16.94 Н -22.530 -4.326 -34.270 1.00 17.26 ATOM 4955 HH11 ARG B 136 Н ATOM 4956 HH12 ARG B 136 -22.528 -3.241 -35.290 1.00 17.26 ATOM 4957 HH21 ARG B 136 -24.280 -1.042 -33.556 1.00 17.77 Н ATOM 4958 HH22 ARG B 136 -23.588 -1.251 -34.858 1.00 17.77 Н ATOM 4959 N PRO B 137 -25.552 -5.453 -27.573 1.00 16.47 **ANISOU 4959 N PRO B 137** 2134 2660 1462 -315 415 -453 -26.993 -5.646 -27.370 1.00 17.33 ATOM 4960 CA PRO B 137 **ANISOU 4960 CA PRO B 137** 2184 2830 1572 -388 536 -521 ATOM 4961 C PRO B 137 -27.670 -6.038 -28.673 1.00 16.49 **ANISOU 4961 C PRO B 137** C 2002 2674 1590 -366 528 -477 ATOM 4962 O PRO B 137 -27.296 -5.569 -29.748 1.00 15.61 0 0 **ANISOU 4962 O PRO B 137** 1835 2490 1605 -279 448 -449 ATOM 4963 CB PRO B 137 -27.474 -4.274 -26.880 1.00 19.39 **ANISOU 4963 CB PRO B 137** 2333 3130 1905 -362 594 -688 ATOM 4964 CG PRO B 137 -26.255 -3.614 -26.324 1.00 19.90 **ANISOU 4964 CG PRO B 137** 2454 3182 1924 -323 522 -705 ATOM 4965 CD PRO B 137 -25.115 -4.105 -27.170 1.00 18.08 **ANISOU 4965 CD PRO B 137** 2284 2870 1717 -266 397 -562 C ATOM 4966 HA PRO B 137 -27.162 -6.318 -26.691 1.00 20.80 Н -27.829 -3.767 -27.627 1.00 23.27 ATOM 4967 HB2 PRO B 137 Н ATOM 4968 HB3 PRO B 137 -28.146 -4.390 -26.191 1.00 23.27 ATOM 4969 HG2 PRO B 137 -26.344 -2.651 -26.396 1.00 23.88 Н ATOM 4970 HG3 PRO B 137 -26.134 -3.879 -25.399 1.00 23.88 Н ATOM 4971 HD2 PRO B 137 -25.002 -3.539 -27.949 1.00 21.70 Н ATOM 4972 HD3 PRO B 137 -24.301 -4.156 -26.645 1.00 21.70 ATOM 4973 N THR B 138 -28.673 -6.903 -28.574 1.00 16.95 Ν ANISOU 4973 N THR B 138 2061 2775 1605 -458 613 -471 ATOM 4974 CA THR B 138 -29.435 -7.317 -29.740 1.00 17.55 ANISOU 4974 CA THR B 138 2058 2821 1787 -456 608 -445 C

ATOM 4975 C THR B 138 -30.885 -6.887 -29.585 1.00 18.96 ANISOU 4975 C THR B 138 2089 3075 2039 -495 711 -572 ATOM 4976 O THR B 138 -31.356 -6.588 -28.484 1.00 20.85 ANISOU 4976 O THR B 138 2311 3395 2215 -552 814 -672 ATOM 4977 CB THR B 138 -29.364 -8.832 -29.953 1.00 17.32 0 ANISOU 4977 CB THR B 138 2146 2764 1672 -534 609 -328 ATOM 4978 OG1 THR B 138 -29.885 -9.508 -28.802 1.00 19.84 0 ANISOU 4978 OG1 THR B 138 2539 3150 1849 -661 715 -337 ATOM 4979 CG2 THR B 138 -27.929 -9.265 -30.189 1.00 15.30 ANISOU 4979 CG2 THR B 138 2013 2427 1374 -477 501 -214 ATOM 4980 H THR B 138 -28.932 -7.266 -27.838 1.00 20.34 ATOM 4981 HA THR B 138 -29.073 -6.883 -30.528 1.00 21.05 Н ATOM 4982 HB THR B 138 Н -29.888 -9.073 -30.733 1.00 20.79 Н ATOM 4983 HG1 THR B 138 -29.435 -9.306 -28.122 1.00 23.81 ATOM 4984 HG21 THR B 138 -27.890 -10.224 -30.324 1.00 18.36 -27.575 -8.821 -30.976 1.00 18.36 ATOM 4985 HG22 THR B 138 Н ATOM 4986 HG23 THR B 138 -27.382 -9.031 -29.423 1.00 18.36 ATOM 4987 N GLY B 139 -31.589 -6.863 -30.713 1.00 18.43 N **ANISOU 4987 N GLY B 139** 1910 2989 2105 -464 682 -575 ATOM 4988 CA GLY B 139 -32.999 -6.534 -30.751 1.00 19.87 ANISOU 4988 CA GLY B 139 1926 3240 2384 -488 760 -691 ATOM 4989 C GLY B 139 -33.307 -5.186 -31.358 1.00 19.69 ANISOU 4989 C GLY B 139 1746 3188 2546 -362 700 -768 ATOM 4990 O GLY B 139 -34.480 -4.905 -31.638 1.00 21.35 C -34.480 -4.905 -31.638 1.00 21.35 0 ANISOU 4990 O GLY B 139 1797 3443 2874 -356 734 -856 0 ATOM 4991 H GLY B 139 -31.258 -7.039 -31.487 1.00 22.12 Н ATOM 4992 HA2 GLY B 139 -33.468 -7.210 -31.266 1.00 23.84 н ATOM 4993 HA3 GLY B 139 -33.352 -6.544 -29.848 1.00 23.84 ATOM 4994 N SER B 140 -32.308 -4.337 -31.545 1.00 18.61 Ν **ANISOU 4994 N SER B 140** 1648 2975 2446 -262 613 -741 ATOM 4995 CA SER B 140 -32.474 -3.053 -32.208 1.00 20.55 ANISOU 4995 CA SER B 140 1773 3163 2872 -139 539 -786 ATOM 4996 C SER B 140 -31.639 -3.043 -33.481 1.00 19.69 ANISOU 4996 C SER B 140 1719 2963 2798 -76 402 -650 ATOM 4997 O SER B 140 -30.787 -3.908 -33.703 1.00 19.49 Ò ANISOU 4997 O SER B 140 1823 2920 2663 -115 373 -545 ATOM 4998 CB SER B 140 -32.065 -1.896 -31.289 1.00 21.20 0 **ANISOU 4998 CB SER B 140** 1847 3228 2981 -88 568 -890 -32.908 -1.832 -30.159 1.00 23.35 ATOM 4999 OG SER B 140 ANISOU 4999 OG SER B 140 2055 3594 3222 -149 706 -1036 ATOM 5000 H SER B 140 -31.501 -4.487 -31.289 1.00 22.33 H ATOM 5001 HA SER B 140 -33.405 -2.935 -32.452 1.00 24.66 ATOM 5002 HB2 SER B 140 -31.151 -2.034 -30.995 1.00 25.44 Н ATOM 5003 HB3 SER B 140 -32.133 -1.063 -31.781 1.00 25.44 ATOM 5004 HG SER B 140 -32.676 -1.196 -29.662 1.00 28.02 ATOM 5005 N ASN B 141 -31.894 -2.057 -34.334 1.00 19.00 Ν ANISOU 5005 N ASN B 141 1534 2817 2867 22 319 -654 ATOM 5006 CA ASN B 141 -31.125 -1.941 -35.561 1.00 17.14 ANISOU 5006 CA ASN B 141 1353 2503 2656 71 197 -528 Ν ATOM 5007 C ASN B 141 -29.665 -1.669 -35.234 1.00 16.87 C ANISOU 5007 C ASN B 141 1442 2412 2555 85 174 -483 C ATOM 5008 O ASN B 141 -29.347 -0.812 -34.400 1.00 16.84 O ANISOU 5008 O ASN B 141 1433 2387 2578 115 202 -561 O

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ATOM 5009 CB ASN B 141 -31.695 -0.833 -36.441 1.00 16.72
ANISOU 5009 CB ASN B 141 1183 2392 2778 170
                                                    107 -532
ATOM 5010 CG ASN B 141
                             -33.042 -1.190 -37.031 1.00 18.10
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-33.578 -2.279 -36.799 1.00 16.91
ANISOU 5010 CG ASN B 141
ATOM 5011 OD1 ASN B 141
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ANISOU 5011 OD1 ASN B 141
                             -33.611 -0.259 -37.792 1.00 18.74
ATOM 5012 ND2 ASN B 141
                            1203 2660 3258 257 -4 -550
ANISOU 5012 ND2 ASN B 141
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ATOM 5013 H ASN B 141 -32.497 -1.453 -34.226 1.00 22.80
                                                                Н
                                                               Н
ATOM 5014 HA ASN B 141 -31.177 -2.776 -36.052 1.00 20.57
ATOM 5015 HB2 ASN B 141 -31.804 -0.030 -35.907 1.00 20.07
ATOM 5016 HB3 ASN B 141
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ATOM 5017 HD21 ASN B 141
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ATOM 5018 HD22 ASN B 141 -33.212 0.492 -37.922 1.00 22.49
ATOM 5019 N ALA B 142 -28.778 -2.417 -35.886 1.00 14.50
ANISOU 5019 N ALA B 142
                           1245 2092 2173 60 127 -371
ATOM 5020 CA ALA B 142
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ANISOU 5020 CA ALA B 142 1344 2044 2108 69 100 -325
ATOM 5021 C ALA B 142 -26.643 -2.234 -37.035 1.00 14.55
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ATOM 5024 H ALA B 142 -28.996 -3.011 -36.469 1.00 17.40
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ATOM 5025 HA ALA B 142
                           -27.146 -1.505 -35.191 1.00 17.36
ATOM 5026 HB1 ALA B 142 -25.852 -3.417 -34.771 1.00 17.69
ATOM 5027 HB2 ALA B 142 -27.248 -3.538 -34.022 1.00 17.69
ATOM 5028 HB3 ALA B 142 -27.002 -4.331 -35.376 1.00 17.69
ATOM 5029 N THR B 143 -25.460 -1.628 -37.032 1.00 14.50
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ATOM 5030 CA THR B 143
                            -24.664 -1.453 -38.238 1.00 14.24
ANISOU 5030 CA THR B 143 1425 1854 2130 137 -88 -107
ATOM 5031 C THR B 143 -23.253 -1.972 -38.005 1.00 11.88
ANISOU 5031 C THR B 143 1210 1555 1751 116 -84 -77
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ATOM 5032 O THR B 143
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ATOM 5033 CB THR B 143
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ANISOU 5033 CB THR B 143
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ATOM 5034 OG1 THR B 143
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ANISOU 5034 OG1 THR B 143
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ATOM 5035 CG2 THR B 143
ANISOU 5035 CG2 THR B 143
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ATOM 5036 H THR B 143 -25.091 -1.303 -36.327 1.00 17.40 H ATOM 5037 HA THR B 143 -25.061 -1.964 -38.961 1.00 17.09 H
ATOM 5041 HG22 THR B 143 -22.823 -0.059 -39.703 1.00 19.76
ATOM 5042 HG23 THR B 143 -24.073 -0.287 -40.640 1.00 19.76
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ATOM 5043 N ILE B 144 -22.704 -2.632 -39.020 1.00 11.03 N ANISOU 5043 N ILE B 144 1142 1444 1603 98 -107 -4 N
ATOM 5044 CA ILE B 144 -21.282 -2.955 -39.086 1.00 11.29
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ATOM 5045 C ILE B 144 -20.719 -2.212 -40.286 1.00 10.91
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                             1173 1377 1594 94 -151
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ATOM 5046 O ILE B 144
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ANISOU 5046 O ILE B 144
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ATOM 5047 CB ILE B 144
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                                                 67 -94
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ATOM 5048 CG1 ILE B 144 -21.433 -5.152 -37.883 1.00 13.04
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ATOM 5049 CG2 ILE B 144
                                                                  C
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ANISOU 5049 CG2 ILE B 144 1249 1414 1426 75 -107 72
ATOM 5050 CD1 ILE B 144
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ATOM 5051 H ILE B 144
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ATOM 5052 HA ILE B 144
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ATOM 5054 HG12 ILE B 144 -20.818 -4.880 -37.184 1.00 15.65
ATOM 5055 HG13 ILE B 144 -22.334 -4.874 -37.654 1.00 15.65
ATOM 5056 HG21 ILE B 144 -19.412 -5.699 -39.545 1.00 12.91 ATOM 5057 HG22 ILE B 144 -19.307 -4.317 -40.322 1.00 12.91
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ATOM 5058 HG23 ILE B 144 -19.010 -4.376 -38.762 1.00 12.91 ATOM 5059 HD11 ILE B 144 -21.688 -7.040 -37.087 1.00 16.09
ATOM 5060 HD12 ILE B 144 -22.039 -6.977 -38.635 1.00 16.09 ATOM 5061 HD13 ILE B 144 -20.522 -6.983 -38.165 1.00 16.09
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ATOM 5062 N THR B 145 -19.859 -1.238 -40.013 1.00 11.76
                                                                   Ν
ANISOU 5062 N THR B 145
                            1273 1446 1750 105 -164
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ATOM 5063 CA THR B 145
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ANISOU 5063 CA THR B 145 1372 1498 1893 90 -189 113
ATOM 5064 C THR B 145
                             -17.936 -1.129 -41.386 1.00 10.53
ANISOU 5064 C THR B 145
                            1144 1272 1584 64 -170 127
ATOM 5065 O THR B 145
                             -16.912 -0.977 -40.719 1.00 10.93
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ANISOU 5065 O THR B 145 1187 1323 1643 66 -165
ATOM 5066 CB THR B 145
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ANISOU 5066 CB THR B 145
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ATOM 5067 OG1 THR B 145
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ANISOU 5067 OG1 THR B 145 1569 1664 2312 144 -216 44
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ATOM 5068 CG2 THR B 145
                                                                   C
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ANISOU 5068 CG2 THR B 145
ATOM 5069 H THR B 145 -19.617 -1.030 -39.214 1.00 14.11
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ATOM 5070 HA THR B 145
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ATOM 5071 HB THR B 145
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ATOM 5073 HG21 THR B 145
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ATOM 5074 HG22 THR B 145 -17.489 1.479 -41.873 1.00 17.03 ATOM 5075 HG23 THR B 145 -18.922 1.912 -42.378 1.00 17.03
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ATOM 5077 CA PHE B 146
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ANISOU 5077 CA PHE B 146 1171 1318 1467 27 -130 160
ATOM 5078 C PHE B 146 -15.620 -2.240 -43.033 1.00 11.30
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ANISOU 5078 C PHE B 146 1265 1419 1611 1 -120 162
ATOM 5079 O PHE B 146 -14.536 -2.778 -42.788 1.00 11.96
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ATOM 5080 CB PHE B 146 -17.334 -3.974 -43.651 1.00 10.64 **ANISOU 5080 CB PHE B 146** 1232 1379 1433 1 -113 186 ATOM 5081 CG PHE B 146 -16.371 -5.123 -43.792 1.00 10.35 1209 1362 1362 3 -77 157 **ANISOU 5081 CG PHE B 146** ATOM 5082 CD1 PHE B 146 -15.863 -5.770 -42.674 1.00 11.02 **ANISOU 5082 CD1 PHE B 146** 1293 1441 1453 47 -80 119 -15.999 -5.576 -45.047 1.00 11.62 ATOM 5083 CD2 PHE B 146 **ANISOU 5083 CD2 PHE B 146** 1384 1545 1484 -37 -45 165 C ATOM 5084 CE1 PHE B 146 -14.996 -6.843 -42.806 1.00 12.12 **ANISOU 5084 CE1 PHE B 146** 1440 1583 1583 66 -59 94 -15.132 -6.644 -45.187 1.00 11.74 ATOM 5085 CE2 PHE B 146 ANISOU 5085 CE2 PHE B 146 1402 1571 1488 -25 -7 121 C -14.627 -7.276 -44.063 1.00 11.85 ATOM 5086 CZ PHE B 146 ATOM 5087 H PHE B 146 -18.635 -2.006 -42.995 1.00 12.64 H ATOM 5088 HA PHE B 146 -16.751 -3.388 -41.783 1.00 12.49 H ATOM 5089 HB2 PHE B 146 -18 194 -4 340 43 200 4 200 4 200 ATOM 5089 HB2 PHE B 146 -18.194 -4.340 -43.392 1.00 12.77
ATOM 5090 HB3 PHE B 146 -17.409 -3.544 -44.518 1.00 12.77
ATOM 5091 HD1 PHE B 146 -16.111 -5.482 -41.825 1.00 13.22
ATOM 5092 HD2 PHE B 146 -16.336 -5.156 -45.805 1.00 13.94 ATOM 5093 HE1 PHE B 146 -14.657 -7.264 -42.050 1.00 13.94 H ATOM 5094 HE2 PHE B 146 -14.885 -6.934 -46.035 1.00 14.09 H ATOM 5095 HZ PHE B 146 -14.041 -7.993 -44.156 1.00 14.22 H ATOM 5096 N SER B 147 -15.698 -1.066 -43.659 1.00 11 50 ANISOU 5096 N SER B 147 1300 1417 1687 -32 -133 204 ATOM 5097 CA SER B 147 -14.464 -0.384 -44.044 1.00 12.12 ANISOU 5097 CA SER B 147 1350 1471 1783 -77 -111 206
ATOM 5098 C SER B 147 -13.570 -0.120 -42.838 1.00 11.70
ANISOU 5098 C SER B 147 1253 1413 1780 -54 -115 133
ATOM 5099 O SER B 147 -12.344 -0.148 -42.963 1.00 11.67 0 ANISOU 5099 O SER B 147 1213 1431 1788 -82 -89 105 ATOM 5100 CB SER B 147 -14.767 0.922 -44.781 1.00 12.14 ANISOU 5100 CB SER B 147 1375 1412 1827 -120 -132 276 ATOM 5101 OG SER B 147 -15.149 1.993 -43.919 1.00 11.98 O ANISOU 5101 OG SER B 147 1338 1318 1895 -90 -168 256 O ATOM 5102 H SER B 147 -16.425 -0.656 -43.866 1.00 13.91 H ATOM 5103 HA SER B 147 -13.972 -0.956 -44.653 1.00 14.54 H ATOM 5104 HB2 SER B 147 -13.972 1.190 -45.269 1.00 14.57 H ATOM 5105 HB3 SER B 147 -15.490 0.760 -45.407 1.00 14.57 H ATOM 5106 HG SER B 147 -14.532 2.156 -43.373 1.00 14.37 H ATOM 5107 N ASN B 148 -14.152 0.143 -41.665 1.00 10.70 N ANISOU 5107 N ASN B 148 1120 1268 1679 -10 -146 94 C ATOM 5108 CA ASN B 148 -13.325 0.378 -40.487 1.00 11.31 ANISOU 5108 CA ASN B 148 1161 1354 1784 5 -160 21 ATOM 5109 C ASN B 148 -12.492 -0.853 -40.150 1.00 10.08 ANISOU 5109 C ASN B 148 990 1261 1580 31 -159 -8 ATOM 5110 O ASN B 148 -11.310 -0.742 -39.813 1.00 9.60 -12.492 -0.853 -40.150 1.00 10.08 ANISOU 5110 O ASN B 148 880 1220 1546 ANISOU 5110 O ASN B 148 880 1220 1546 25 -167 -51 ATOM 5111 CB ASN B 148 -14.195 0.776 -39.301 1.00 11.84 ANISOU 5111 CB ASN B 148 1234 1403 1862 40 -184 -25 ATOM 5112 CG ASN B 148 -14.749 2.183 -39.425 1.00 13.02 ANISOU 5112 CG ASN B 148 1379 1470 2097 27 -193 -25 ATOM 5113 OD1 ASN B 148 -14.162 3.057 -40.082 1.00 12.87

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ANISOU 5113 OD1 ASN B 148 1355 1399 2137 -17 -190
                                                             0
ATOM 5114 ND2 ASN B 148 -15.884 2.419 -38.769 1.00 14.07
                                                             N
ANISOU 5114 ND2 ASN B 148 1514 1586 2244 63 -199 -57
                                                              N
ATOM 5115 H ASN B 148 -15.000 0.189 -41.530 1.00 12.84
                                                            Н
ATOM 5116 HA ASN B 148 -12.716 1.110 -40.671 1.00 13.57
                                                            Н
ATOM 5117 HB2 ASN B 148 -14.944 0.163 -39.238 1.00 14.21
                                                             Н
                           -13.663 0.734 -38.490 1.00 14.21
ATOM 5118 HB3 ASN B 148
ATOM 5119 HD21 ASN B 148 -16.246 3.198 -38.803 1.00 16.88 ATOM 5120 HD22 ASN B 148 -16.255 1.792 -38.312 1.00 16.88
                                                              Н
ATOM 5121 N HIS B 149
                         -13.085 -2.041 -40.265 1.00 10.27
                                                            Ν
                                                            Ν
ANISOU 5121 N HIS B 149
                          1050 1309 1543 61 -152
ATOM 5122 CA HIS B 149
                          -12.356 -3.262 -39.952 1.00 10.06
                                                            C
ANISOU 5122 CA HIS B 149
                          1018 1319 1486
                                             98 -159
ATOM 5123 C HIS B 149
                          -11.298 -3.573 -41.006 1.00 10.21
ANISOU 5123 C HIS B 149
                          997 1354 1527 79 -122 -8
ATOM 5124 O HIS B 149
                          -10.139 -3.849 -40.668 1.00 10.32
                                                            0
ANISOU 5124 O HIS B 149
                         956 1392 1571 102 -136 -52
ATOM 5125 CB HIS B 149
                          -13.346 -4.411 -39.798 1.00 10.41
                                                             CCCC
ANISOU 5125 CB HIS B 149 1123 1365 1468 124 -156
ATOM 5126 CG HIS B 149 -14.328 -4.202 -38.690 1.00 9.92
ANISOU 5126 CG HIS B 149 1090 1301 1376 134 -175
                                                      15
ATOM 5127 ND1 HIS B 149 -14.084 -4.613 -37.400 1.00 10.39
ANISOU 5127 ND1 HIS B 149 1169 1383 1397 163 -209
                           -15.544 -3.603 -38.672 1.00 9.83
ATOM 5128 CD2 HIS B 149
ANISOU 5128 CD2 HIS B 149 1089 1277 1369 118 -163
                                                        21
                           -15.117 -4.302 -36.639 1.00 10.87
ATOM 5129 CE1 HIS B 149
                                                              C
ANISOU 5129 CE1 HIS B 149
                          1254 1449 1426 152 -202 -21
ATOM 5130 NE2 HIS B 149
                           -16.014 -3.680 -37.385 1.00 9.72
                                                             N
ANISOU 5130 NE2 HIS B 149
                          1095 1282 1318 130 -172 -11
                                                            N
ATOM 5131 H HIS B 149
                         -13.897 -2.163 -40.519 1.00 12.33
                                                            Н
ATOM 5132 HA HIS B 149 -11.903 -3.146 -39.102 1.00 12.07
                                                           Н
ATOM 5133 HB2 HIS B 149 -13.845 -4.507 -40.625 1.00 12.49
ATOM 5134 HB3 HIS B 149 -12.855 -5.226 -39.612 1.00 12.49
ATOM 5135 HD1 HIS B 149 -13.378 -5.027 -37.135 1.00 12.47
ATOM 5136 HD2 HIS B 149 -15.981 -3.221 -39.397 1.00 11.80
                                                             Н
ATOM 5137 HE1 HIS B 149 -15.193 -4.475 -35.728 1.00 13.04
                                                             Н
ATOM 5138 N VAL B 150
                          -11.671 -3.530 -42.291 1.00 10.32
                                                            Ν
ANISOU 5138 N VAL B 150
                          1034 1365 1524 33 -77
ATOM 5139 CA VAL B 150
                           -10.688 -3.784 -43.340 1.00 10.63
ANISOU 5139 CA VAL B 150 1036 1431 1570 -2 -23
                                                       13
                           -9.541 -2.784 -43.247 1.00 10.35
ATOM 5140 C VAL B 150
ANISOU 5140 C VAL B 150
ATOM 5141 O VAL B 150
                          930 1404 1598 -40 -14 -20
                           -8.367 -3.151 -43.356 1.00 10.61
                                                             0
ANISOU 5141 O VAL B 150
                          893 1474 1666 -36
                                                10 -75
ATOM 5142 CB VAL B 150
                           -11.349 -3.750 -44.729 1.00 11.12
                                                              C
                           1147 1498 1578 -63 20 64
ANISOU 5142 CB VAL B 150
ATOM 5143 CG1 VAL B 150
                           -10.302 -3.971 -45.819 1.00 11.87
ANISOU 5143 CG1 VAL B 150
                          1207 1636 1665 -115 94
                                                        34
ATOM 5144 CG2 VAL B 150
                           -12.436 -4.795 -44.829 1.00 10.39
ANISOU 5144 CG2 VAL B 150 1113 1404 1429 -34 11 80
                                                            C
ATOM 5145 H VAL B 150 -12.466 -3.361 -42.572 1.00 12.39 H
ATOM 5146 HA VAL B 150 -10.318 -4.671 -43.211 1.00 12.75 H
ATOM 5147 HB VAL B 150 -11.753 -2.879 -44.869 1.00 13.34
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ATOM 5148 HG11 VAL B 150 -10.738 -3.946 -46.685 1.00 14.24 Н ATOM 5149 HG12 VAL B 150 -9.635 -3.268 -45.763 1.00 14.24 Н ATOM 5150 HG13 VAL B 150 -9.884 -4.836 -45.683 1.00 14.24 Н ATOM 5151 HG21 VAL B 150 -12.835 -4.752 -45.712 1.00 12.46 Н ATOM 5152 HG22 VAL B 150 -12.046 -5.671 -44.684 1.00 12.46 Н ATOM 5153 HG23 VAL B 150 -13.109 -4.616 -44.152 1.00 12.46 ATOM 5154 N ASN B 151 -9.857 -1.500 -43.064 1.00 10.72 Ν **ANISOU 5154 N ASN B 151** 988 1413 1673 -81 -32 ATOM 5155 CA ASN B 151 -8.792 -0.504 -43.031 1.00 10.99 **ANISOU 5155 CA ASN B 151** 960 1444 1773 -137 -18 -27 ATOM 5156 C ASN B 151 ANISOU 5156 C ASN B 151 -7.897 -0.707 -41.813 1.00 11.86 995 1584 1926 -88 -64 -106 00 ATOM 5157 O ASN B 151 -6.668 -0.575 -41.906 1.00 11.82 **ANISOU 5157 O ASN B 151** 904 1615 1972 -117 -43 -160 ATOM 5158 CB ASN B 151 -9.388 0.903 -43.052 1.00 11.54 **ANISOU 5158 CB ASN B 151** 1068 1441 1877 -186 -33 17 ATOM 5159 CG ASN B 151 -10.054 1.234 -44.383 1.00 12.75 **ANISOU 5159 CG ASN B 151** 1287 1567 1990 -244 -2 109 ATOM 5160 OD1 ASN B 151 -9.697 0.679 -45.424 1.00 12.53 0 **ANISOU 5160 OD1 ASN B 151** 1264 1587 1910 -286 53 127 ATOM 5161 ND2 ASN B 151 -11.006 2.169 -44.359 1.00 13.34 **ANISOU 5161 ND2 ASN B 151** 1413 1566 2092 -247 -40 165 ATOM 5162 H ASN B 151 -10.653 -1.191 -42.961 1.00 12.87 Н ATOM 5163 HA ASN B 151 -8.242 -0.606 -43.823 1.00 13.19 Н -10.059 0.974 -42.355 1.00 13.85 ATOM 5164 HB2 ASN B 151 Н ATOM 5165 HB3 ASN B 151 -8.681 1.550 -42.900 1.00 13.85 Н ATOM 5166 HD21 ASN B 151 -11.411 2.390 -45.086 1.00 16.01 Н ATOM 5167 HD22 ASN B 151 -11.216 2.551 -43.618 1.00 16.01 ATOM 5168 N ALA B 152 -8.491 -1.039 -40.662 1.00 12.14 Ν **ANISOU 5168 N ALA B 152** 1060 1614 1938 -20 -127 -117 ATOM 5169 CA ALA B 152 -7.688 -1.321 -39.473 1.00 11.04 C C **ANISOU 5169 CA ALA B 152** 865 1513 1817 28 -189 -180 -6.839 -2.567 -39.676 1.00 11.98 ATOM 5170 C ALA B 152 C C O O ANISOU 5170 C ALA B 152 ATOM 5171 O ALA B 152 934 1678 1941 82 -190 -203 -5.642 -2.580 -39.363 1.00 12.13 **ANISOU 5171 O ALA B 152** 857 1738 2015 93 -216 -263 ATOM 5172 CB ALA B 152 C -8.592 -1.493 -38.251 1.00 10.66 C **ANISOU 5172 CB ALA B 152** 879 1457 1714 77 -247 -177 ATOM 5173 H ALA B 152 -9.341 -1.106 -40.547 1.00 14.56 Н Н ATOM 5174 HA ALA B 152 -7.093 -0.573 -39.307 1.00 13.25 ATOM 5175 HB1 ALA B 152 -8.040 -1.679 -37.475 1.00 12.79 Н ATOM 5176 HB2 ALA B 152 -9.094 -0.675 -38.112 1.00 12.79 Н ATOM 5177 HB3 ALA B 152 -9.200 -2.232 -38.409 1.00 12.79 Н ATOM 5178 N TRP B 153 -7.450 -3.632 -40.194 1.00 11.46 Ν **ANISOU 5178 N TRP B 153** 925 1600 1828 118 -165 -163 ATOM 5179 CA TRP B 153 -6.722 -4.876 -40.408 1.00 11.85 C C **ANISOU 5179 CA TRP B 153** 935 1671 1898 180 -164 -190 ATOM 5180 C TRP B 153 -5.463 -4.650 -41.244 1.00 12.43 C **ANISOU 5180 C TRP B 153** 896 1784 2043 143 -106 -251 ATOM 5181 O TRP B 153 -4.367 -5.073 -40.861 1.00 14.33 **ANISOU 5181 O TRP B 153** 1040 2059 2348 195 -141 -312 0 ATOM 5182 CB TRP B 153 -7.640 -5.907 -41.070 1.00 12.22 ANISOU 5182 CB TRP B 153 1066 1688 1890 198 -126 -147

ATOM 5183 CG TRP B 153 -8.748 -6.426 -40.194 1.00 12.04 **ANISOU 5183 CG TRP B 153** 1138 1632 1804 237 -176 -99 ATOM 5184 CD1 TRP B 153 -8.890 -6.263 -38.845 1.00 12.58 **ANISOU 5184 CD1 TRP B 153** 1226 1703 1849 268 -251 -92 -9.880 -7.197 -40.624 1.00 12.47 ATOM 5185 CD2 TRP B 153 C **ANISOU 5185 CD2 TRP B 153** 1279 1655 1802 234 -147 -56 ATOM 5186 NE1 TRP B 153 -10.040 -6.879 -38.415 1.00 12.25 Ν **ANISOU 5186 NE1 TRP B 153** 1280 1636 1739 280 -260 -45 ATOM 5187 CE2 TRP B 153 -10.663 -7.462 -39.486 1.00 11.22 **ANISOU 5187 CE2 TRP B 153** 1187 1480 1595 260 -198 -23 ATOM 5188 CE3 TRP B 153 -10.303 -7.686 -41.863 1.00 13.17 **ANISOU 5188 CE3 TRP B 153** 1396 1735 1871 201 -80 -48 ATOM 5189 CZ2 TRP B 153 -11.853 -8.182 -39.549 1.00 11.83 **ANISOU 5189 CZ2 TRP B 153** 1347 1530 1617 251 -180 17 ATOM 5190 CZ3 TRP B 153 -11.490 -8.407 -41.926 1.00 12.64 **ANISOU 5190 CZ3 TRP B 153** 1412 1640 1749 197 -75 -12 ATOM 5191 CH2 TRP B 153 -12.245 -8.652 -40.773 1.00 11.54 **ANISOU 5191 CH2 TRP B 153** 1328 1481 1575 221 -122 20 ATOM 5192 H TRP B 153 -8.277 -3.659 -40.427 1.00 13.75 Н ATOM 5193 HA TRP B 153 -6.448 -5.230 -39.548 1.00 14.23 Н ATOM 5194 HB2 TRP B 153 -8.049 -5.500 -41.849 1.00 14.67 Н ATOM 5195 HB3 TRP B 153 -7.103 -6.667 -41.344 1.00 14.67 Н ATOM 5196 HD1 TRP B 153 ATOM 5197 HE1 TRP B 153 -8.297 -5.800 -38.298 1.00 15.09 Н -10.321 -6.899 -37.603 1.00 14.70 Н -9.807 -7.521 -42.633 1.00 15.80 ATOM 5198 HE3 TRP B 153 Н ATOM 5199 HZ2 TRP B 153 -12.355 -8.351 -38.785 1.00 14.19 ATOM 5200 HZ3 TRP B 153 -11.782 -8.738 -42.744 1.00 15.16 Н ATOM 5201 HH2 TRP B 153 -13.032 -9.143 -40.841 1.00 13.84 ATOM 5202 N LYS B 154 -5.586 -3.976 -42.389 1.00 12.40 Ν 900 1782 2028 49 -19 -236 Ν **ANISOU 5202 N LYS B 154** ATOM 5203 CA LYS B 154 -4.403 -3.829 -43.228 1.00 13.97 C **ANISOU 5203 CA LYS B 154** 996 2030 2282 -4 57 -298 ATOM 5204 C LYS B 154 C -3.348 -2.947 -42.570 1.00 14.34 933 2106 2408 -32 **ANISOU 5204 C LYS B 154** 26 -356 ATOM 5205 O LYS B 154 -2.152 -3.187 -42.757 1.00 15.50 0 **ANISOU 5205 O LYS B 154** 953 2308 2628 -30 53 -437 ATOM 5206 CB LYS B 154 -4.787 -3.306 -44.613 1.00 15.91 1293 2276 2474 -115 158 -256 **ANISOU 5206 CB LYS B 154** ATOM 5207 CG LYS B 154 -5.202 -1.872 -44.672 1.00 16.34 C **ANISOU 5207 CG LYS B 154** 1394 2294 2521 -205 156 -196 ATOM 5208 CD LYS B 154 -5.406 -1.432 -46.137 1.00 16.56 C **ANISOU 5208 CD LYS B 154** 1474 2330 2489 -320 249 -143 C ATOM 5209 CE LYS B 154 -6.649 -2.072 -46.754 1.00 16.41 C **ANISOU 5209 CE LYS B 154** 1565 2295 2374 -300 247 -77 ATOM 5210 NZ LYS B 154 -6.916 -1.536 -48.119 1.00 16.12 Ν **ANISOU 5210 NZ LYS B 154** 1594 2270 2261 -415 314 -10 Ν ATOM 5211 H LYS B 154 -6.306 -3.612 -42.688 1.00 14.88 Н ATOM 5212 HA LYS B 154 Н -4.008 -4.706 -43.352 1.00 16.77 ATOM 5213 HB2 LYS B 154 Н -4.024 -3.411 -45.202 1.00 19.09 ATOM 5214 HB3 LYS B 154 -5.528 -3.836 -44.946 1.00 19.09 Н ATOM 5215 HG2 LYS B 154 -6.040 -1.758 -44.197 1.00 19.61 ATOM 5216 HG3 LYS B 154 -4.511 -1.318 -44.277 1.00 19.61 Н ATOM 5217 HD2 LYS B 154 -5.514 -0.468 -46.169 1.00 19.87

ATOM 5218 HD3 LYS B 154	-4.635 -1.700 -46.661 1.00 19.87	Н
ATOM 5219 HE2 LYS B 154	-6.515 -3.030 -46.824 1.00 19.69	Н
ATOM 5220 HE3 LYS B 154	-7.419 -1.880 -46.196 1.00 19.69	Н
ATOM 5221 HZ1 LYS B 154	-7.046 -0.657 -48.080 1.00 19.35	Н
ATOM 5222 HZ2 LYS B 154	-6.223 -1.703 -48.652 1.00 19.35	Н
ATOM 5223 HZ3 LYS B 154	-7.642 -1.922 -48.460 1.00 19.35	H
ATOM 5224 N SER B 155	-3.750 -1.954 -41.769 1.00 13.56	N
ANISOU 5224 N SER B 155	870 1977 2307 -58 -32 -331	N
ATOM 5225 CA SER B 155	-2.746 -1.159 -41.069 1.00 16.66	C
ANISOU 5225 CA SER B 155	1157 2398 2775 -90 -70 -400	С
ATOM 5226 C SER B 155	-1.990 -1.986 -40.037 1.00 16.80	С
ANISOU 5226 C SER B 155	1089 2464 2829 16 -168 -461	C
ATOM 5227 O SER B 155	-0.907 -1.578 -39.611 1.00 16.93	ŏ
	983 2531 2921 -3 -200 -538	0
ATOM 5228 CB SER B 155	-3.385 0.076 -40.413 1.00 17.03	C
ANISOU 5228 CB SER B 155	1268 2391 2814 -141 -109 -375	С
ATOM 5229 OG SER B 155	-4.022 -0.222 -39.185 1.00 17.55	0
ANISOU 5229 OG SER B 155	1387 2447 2836 -60 -204 -369	0
ATOM 5230 H SER B 155	-4.567 -1.731 -41.619 1.00 16.28	н
ATOM 5231 HA SER B 155	-2.099 -0.842 -41.718 1.00 19.99	'H
ATOM 5232 HB2 SER B 155	-2.691 0.733 -40.249 1.00 20.44	Н
ATOM 5233 HB3 SER B 155	-4.044 0.443 -41.022 1.00 20.44	Н
ATOM 5234 HG SER B 155	-4.632 -0.787 -39.308 1.00 21.06	Н
ATOM 5235 N HIS B 156 -	-2.531 -3.141 -39.642 1.00 18.11	N
	1318 2615 2947 122 -220 -425	N
ATOM 5236 CA HIS B 156	-1.847 -4.091 -38.774 1.00 21.34	C
ANISOU 5236 CA HIS B 156	1663 3056 3388 235 -322 -460	C
	-1.286 -5.286 -39.548 1.00 20.70	C
	1522 2982 3360 303 -279 -490	C
ATOM 5238 O HIS B 156	-1.007 -6.332 -38.951 1.00 20.96	0
ANISOU 5238 O HIS B 156	1554 3004 3406 414 -360 -485	0
ATOM 5239 CB HIS B 156	-2.795 -4.572 -37.670 1.00 23.00	C
ANISOU 5239 CB HIS B 156	1997 3234 3509 303 -417 -394	C
ATOM 5240 CG HIS B 156	-3.195 -3.497 -36.706 1.00 24.41	
		C
ANISOU 5240 CG HIS B 156	2215 3418 3643 252 -468 -395	C
ATOM 5241 ND1 HIS B 156	-2.412 -3.128 -35.632 1.00 25.89	Ν
ANISOU 5241 ND1 HIS B 156	2330 3658 3848 263 -570 -451	N
ATOM 5242 CD2 HIS B 156	-4.298 -2.713 -36.652 1.00 23.99	C
ANISOU 5242 CD2 HIS B 156	2259 3323 3532 192 -431 -359	C
ATOM 5243 CE1 HIS B 156	-3.014 -2.160 -34.962 1.00 25.68	C
		C
ATOM 5244 NE2 HIS B 156	-4.160 -1.890 -35.560 1.00 24.59	N
ANISOU 5244 NE2 HIS B 156	2324 3423 3596 166 -499 -403	Ν
ATOM 5245 H HIS B 156 -	-3.319 -3.399 -39.872 1.00 21.73	Н
ATOM 5246 HA HIS B 156	-1.101 -3.641 -38.348 1.00 25.60	Н
ATOM 5247 HB2 HIS B 156	-3.603 -4.918 -38.081 1.00 27.60	Н
ATOM 5248 HB3 HIS B 156	-2.356 -5.274 -37.166 1.00 27.60	H
	-5.014 -2.726 -37.245 1.00 28.78	H
	-2.687 -1.742 -34.198 1.00 30.81	Н
	-4.728 -1.297 -35.306 1.00 29.51	Н
ATOM 5252 N GLY B 157	-1.118 -5.153 -40.861 1.00 20.02	N
ANISOU 5252 N GLY B 157	1406 2906 3293 232 -149 -515	Ν
ATOM 5253 CA GLY B 157	-0.480 -6.189 -41.650 1.00 19.92	C
ATOM OLOU OA OLI DIGI	STRUCTION TOUR	•

ANISOU 5253 CA GLY B 157 1318 2909 3341 285 -89 -575 ATOM 5254 C GLY B 157 ANISOU 5254 C GLY B 157 -1.376 -7.331 -42.071 1.00 19.70 C 1408 2819 3256 343 -66 -528 ATOM 5255 O GLY B 157 -0.865 -8.340 -42.565 1.00 21.88 0 **ANISOU 5255 O GLY B 157** 1629 3092 3594 410 -30 -588 0 ATOM 5256 H GLY B 157 -1.367 -4.468 -41.317 1.00 24.02 ATOM 5257 HA2 GLY B 157 -0.113 -5.788 -42.453 1.00 23.90 Н ATOM 5258 HA3 GLY B 157 0.255 -6.561 -41.139 1.00 23.90 Н ATOM 5259 N MET B 158 -2.692 -7.208 -41.900 1.00 17.12 Ν **ANISOU 5259 N MET B 158** 1236 2444 2827 319 -81 -434 ATOM 5260 CA MET B 158 -3.647 -8.242 -42.296 1.00 15.32 **ANISOU 5260 CA MET B 158** 1123 2158 2541 354 -57 -390 ATOM 5261 C MET B 158 -4.298 -7.814 -43.606 1.00 15.06 **ANISOU 5261 C MET B 158** C 1149 2135 2439 243 60 -372 ATOM 5262 O MET B 158 -5.276 -7.058 -43.606 1.00 14.29 1138 2023 2267 178 **ANISOU 5262 O MET B 158** 56 -299 ATOM 5263 CB MET B 158 -4.683 -8.458 -41.203 1.00 15.03 1206 2070 2434 396 -153 -304 **ANISOU 5263 CB MET B 158** ATOM 5264 CG MET B 158 -4.108 -9.021 -39.910 1.00 17.94 1545 2428 2843 504 -280 -304 **ANISOU 5264 CG MET B 158** ATOM 5265 SD MET B 158 ANISOU 5265 SD MET B 158 -5.121 -8.569 -38.488 1.00 18.61 S 1747 2501 2823 495 -376 -219 ATOM 5266 CE MET B 158 ANISOU 5266 CE MET B 158 -6.696 -9.285 -38.937 1.00 17.01 1700 2232 2532 471 -318 -146 C ATOM 5267 H MET B 158 -3.065 -6.518 -41.547 1.00 20.55 Н ATOM 5268 HA MET B 158 -3.173 -9.078 -42.434 1.00 18.39 Н ATOM 5269 HB2 MET B 158 -5.101 -7.607 -40.996 1.00 18.04 Н ATOM 5270 HB3 MET B 158 ATOM 5271 HG2 MET B 158 -5.353 -9.082 -41.525 1.00 18.04 -4.077 -9.988 -39.967 1.00 21.52 -3.216 -8.663 -39.774 1.00 21.52 -4.077 -9.988 -39.967 1.00 21.52 ATOM 5272 HG3 MET B 158 ATOM 5273 HE1 MET B 158 -7.337 -9.103 -38.232 1.00 20.41 Н -6.998 -8.888 -39.769 1.00 20.41 ATOM 5274 HE2 MET B 158 ATOM 5275 HE3 MET B 158 -6.588 -10.243 -39.047 1.00 20.41 Н ATOM 5276 N ASN B 159 -3.745 -8.295 -44.722 1.00 14.62 Ν **ANISOU 5276 N ASN B 159** 1041 2108 2408 221 160 -442 N ATOM 5277 CA ASN B 159 -4.284 -8.019 -46.048 1.00 14.55 1092 2122 2315 111 269 -428 **ANISOU 5277 CA ASN B 159** C ATOM 5278 C ASN B 159 ANISOU 5278 C ASN B 159 -5.220 -9.145 -46.465 1.00 13.98 1124 2004 2185 142 282 -412 ATOM 5279 O ASN B 159 -4.874 -10.325 -46.346 1.00 14.66 1187 2055 2329 233 **ANISOU 5279 O ASN B 159** 277 -472 ATOM 5280 CB ASN B 159 -3.162 -7.880 -47.080 1.00 17.31 **ANISOU 5280 CB ASN B 159** 1331 2544 2701 45 390 -525 ATOM 5281 CG ASN B 159 -2.272 -6.684 -46.824 1.00 18.31 1356 2720 2881 -19 **ANISOU 5281 CG ASN B 159** 395 -542 ATOM 5282 OD1 ASN B 159 -2.747 -5.582 -46.580 1.00 18.35 **ANISOU 5282 OD1 ASN B 159** 1415 2711 2846 -88 364 -463 -0.971 -6.900 -46.886 1.00 19.34 1329 2903 3114 3 437 -654 ATOM 5283 ND2 ASN B 159 Ν Ν **ANISOU 5283 ND2 ASN B 159** ATOM 5284 H ASN B 159 -3.045 -8.794 -44.733 1.00 17.55 Н ATOM 5285 HA ASN B 159 -4.788 -7.190 -46.027 1.00 17.46 ATOM 5286 HB2 ASN B 159 -2.609 -8.676 -47.054 1.00 20.77 Н Н ATOM 5287 HB3 ASN B 159 -3.555 -7.777 -47.961 1.00 20.77

ATOM 5288 HD21 ASN B 159 -0.421 -6.254 -46.748 1.00 23.20 Н ATOM 5289 HD22 ASN B 159 -0.674 -7.687 -47.063 1.00 23.20 ATOM 5290 N LEU B 160 -6.399 -8.777 -46.946 1.00 13.44 -6.399 -8.777 -46.946 1.00 13.44 **ANISOU 5290 N LEU B 160** 1166 1929 2012 68 293 -335 ATOM 5291 CA LEU B 160 -7.340 -9.742 -47.484 1.00 14.18 ANISOU 5291 CA LEU B 160 1355 1992 2042 69 312 -328 ATOM 5292 C LEU B 160 -6.983 -10.103 -48.924 1.00 16.60 ANISOU 5292 C LEU B 160 1649 2352 2308 -2 432 -404 00 ATOM 5293 O LEU B 160 -6.229 -9.402 -49.601 1.00 17.32 **ANISOU 5293 O LEU B 160** 1679 2511 2391 -78 507 -436 ATOM 5294 CB LEU B 160 -8.759 -9.187 -47.418 1.00 14.15 **ANISOU 5294 CB LEU B 160** 1456 1973 1949 19 267 -224 -9.321 -9.080 -45.997 1.00 14.17 ATOM 5295 CG LEU B 160 **ANISOU 5295 CG LEU B 160** 1486 1923 1975 87 165 -165 ATOM 5296 CD1 LEU B 160 -10.506 -8.136 -45.963 1.00 13.18 1423 1799 1788 31 133 -81 **ANISOU 5296 CD1 LEU B 160** ATOM 5297 CD2 LEU B 160 -9.715 -10.453 -45.470 1.00 14.64 ANISOU 5297 CD2 LEU B 160 1595 1922 2046 163 134 -175 ATOM 5298 H LEU B 160 -6.680 -7.964 -46.971 1.00 16.13 ATOM 5299 HA LEU B 160 -7.305 -10.552 -46.951 1.00 17.02 Н ATOM 5300 HB2 LEU B 160 -8.765 -8.298 -47.806 1.00 16.98 ATOM 5301 HB3 LEU B 160 -9.346 -9.770 -47.925 1.00 16.98 Н ATOM 5302 HG LEU B 160 -8.635 -8.720 -45.412 1.00 17.00 ATOM 5303 HD11 LEU B 160 -10.843 -8.086 -45.054 1.00 15.82 -10.843 -8.086 -45.054 1.00 15.82 ATOM 5304 HD12 LEU B 160 ATOM 5305 HD13 LEU B 160 -10.219 -7.259 -46.259 1.00 15.82 -11.197 -8.476 -46.553 1.00 15.82 ATOM 5306 HD21 LEU B 160 -10.066 -10.357 -44.571 1.00 17.57 ATOM 5307 HD22 LEU B 160 -10.392 -10.832 -46.052 1.00 17.57 ATOM 5308 HD23 LEU B 160 -8.930 -11.023 -45.460 1.00 17.57 -10.066 -10.357 -44.571 1.00 17.57 -10.392 -10.832 -46.052 1.00 17.57 ATOM 5309 N GLY B 161 -7.549 -11.213 -49.389 1.00 16.32 ANISOU 5309 N GLY B 161 1677 2286 2239 12 456 -438 ATOM 5310 CA GLY B 161 -7.350 -11.638 -50.758 1.00 18.44 ANISOU 5310 CA GLY B 161 1949 2609 2449 -63 572 -522 ATOM 5311 C GLY B 161 -8.018 -10.696 -51.739 1.00 17.63 ANISOU 5311 C GLY B 161 1915 2578 2204 -202 602 -452 -8.018 -10.696 -51.739 1.00 17.63 C ATOM 5312 O GLY B 161 -8.828 -9.837 -51.384 1.00 16.64 ANISOU 5312 O GLY B 161 1843 2442 2037 -228 527 -336 0 -8.053 -11.734 -48.926 1.00 19.59 ATOM 5313 H GLY B 161 ATOM 5314 HA2 GLY B 161 -6.401 -11.668 -50.955 1.00 22.13 ATOM 5315 HA3 GLY B 161 -7.721 -12.526 -50.880 1.00 22.13 ATOM 5316 N SER B 162 -7.659 -10.871 -53.009 1.00 18.39 Ν **ANISOU 5316 N SER B 162** 2012 2750 2226 -293 715 -527 ATOM 5317 CA SER B 162 -8.131 -9.996 -54.074 1.00 19.70 ANISOU 5317 CA SER B 162 2248 2997 2242 -437 748 -457 ATOM 5318 C SER B 162 -9.425 -10.470 -54.724 1.00 19.92 ANISOU 5318 C SER B 162 2391 3031 2146 -485 718 -423 ATOM 5319 O SER B 162 -10.089 -9.667 -55.387 1.00 19.68 C ANISOU 5319 O SER B 162 2432 3051 1994 -584 692 -326 0 ATOM 5320 CB SER B 162 -7.051 -9.858 -55.149 1.00 22.00 ANISOU 5320 CB SER B 162 2485 3386 2488 -536 893 -552 ATOM 5321 OG SER B 162 -6.648 -11.132 -55.615 1.00 23.82 ANISOU 5321 OG SER B 162 2685 3626 2741 -505 982 -709 ATOM 5322 H SER B 162 -7.136 -11.498 -53.280 1.00 22.07 H

ATOM 5323 HA SER B 162 -8.293 -9.115 -53.703 1.00 23.65 Н ATOM 5324 HB2 SER B 162 -7.408 -9.347 -55.892 1.00 26.40 Н -6.284 -9.401 -54.769 1.00 26.40 ATOM 5325 HB3 SER B 162 Н ATOM 5326 HG SER B 162 -7.305 -11.538 -55.944 1.00 28.59 Н ATOM 5327 N ASN B 163 -9.808 -11.735 -54.545 1.00 19.40 Ν **ANISOU 5327 N ASN B 163** 2346 2912 2114 -420 711 -497 Ν ATOM 5328 CA ASN B 163 -11.033 -12.285 -55.121 1.00 20.10 **ANISOU 5328 CA ASN B 163** 2532 3007 2097 -471 682 -484 C ATOM 5329 C ASN B 163 -12.042 -12.513 -54.001 1.00 18.70 **ANISOU 5329 C ASN B 163** C 2385 2738 1981 -389 565 -407 0 ATOM 5330 O ASN B 163 -11.859 -13.408 -53.170 1.00 18.91 **ANISOU 5330 O ASN B 163** 2392 2677 2117 -291 0 553 -456 ATOM 5331 CB ASN B 163 -10.754 -13.595 -55.849 1.00 21.45 2711 3184 2256 -483 C **ANISOU 5331 CB ASN B 163** 778 -643 ATOM 5332 CG ASN B 163 -9.846 -13.430 -57.033 1.00 24.89 C **ANISOU 5332 CG ASN B 163** 3119 3728 2609 -581 912 -738 ATOM 5333 OD1 ASN B 163 -9.090 -12.467 -57.151 1.00 27.50 0 **ANISOU 5333 OD1 ASN B 163** 3400 4116 2933 -621 950 -704 ATOM 5334 ND2 ASN B 163 -9.910 -14.383 -57.921 1.00 25.77 Ν 3264 3866 2662 -628 987 -864 **ANISOU 5334 ND2 ASN B 163** Ν ATOM 5335 H ASN B 163 -9.362 -12.307 -54.083 1.00 23.28 Н ATOM 5336 HA ASN B 163 -11.409 -11.653 -55.753 1.00 24.12 Н ATOM 5337 HB2 ASN B 163 ATOM 5338 HB3 ASN B 163 -10.332 -14.214 -55.233 1.00 25.74 Н -11.594 -13.964 -56.166 1.00 25.74 Н ATOM 5339 HD21 ASN B 163 -9.415 -14.349 -58.624 1.00 30.92 Н ATOM 5340 HD22 ASN B 163 -10.446 -15.045 -57.804 1.00 30.92 Н ATOM 5341 N TRP B 164 -13.123 -11.743 -54.009 1.00 16.85 **ANISOU 5341 N TRP B 164** 2200 2524 1677 -433 482 -289 N ATOM 5342 CA TRP B 164 -14.081 -11.746 -52.909 1.00 15.79 C **ANISOU 5342 CA TRP B 164** 2080 2319 1599 -367 382 -216 ATOM 5343 C TRP B 164 -15.211 -12.737 -53.171 1.00 14.79 **ANISOU 5343 C TRP B 164** 2013 2179 1428 -393 ATOM 5344 O TRP B 164 -15.775 -12.773 -54.268 1.00 15.94 **ANISOU 5344 O TRP B 164** 2203 2396 1459 -487 367 -253 ATOM 5345 CB TRP B 164 C -14.640 -10.339 -52.702 1.00 15.42 305 -88 **ANISOU 5345 CB TRP B 164** 2035 2293 1531 -387 ATOM 5346 CG TRP B 164 -13.608 -9.416 -52.135 1.00 16.21 **ANISOU 5346 CG TRP B 164** 2076 2379 1703 -353 315 -64 ATOM 5347 CD1 TRP B 164 -12.491 -8.944 -52.765 1.00 18.21 **ANISOU 5347 CD1 TRP B 164** 2297 2681 1942 -403 -92 389 ATOM 5348 CD2 TRP B 164 -13.592 -8.863 -50.815 1.00 15.83 **ANISOU 5348 CD2 TRP B 164** 1991 2272 1752 -274 254 -18 Ν ATOM 5349 NE1 TRP B 164 -11.772 -8.133 -51.906 1.00 18.14 N 2227 2641 2025 -359 **ANISOU 5349 NE1 TRP B 164** 372 -66 ATOM 5350 CE2 TRP B 164 -12.432 -8.071 -50.706 1.00 16.61 Č **ANISOU 5350 CE2 TRP B 164** 2034 2382 1897 -278 -23 286 ATOM 5351 CE3 TRP B 164 -14.447 -8.964 -49.713 1.00 15.64 **ANISOU 5351 CE3 TRP B 164** 1975 2194 1773 -212 182 17 C ATOM 5352 CZ2 TRP B 164 -12.111 -7.381 -49.540 1.00 15.76 **ANISOU 5352 CZ2 TRP B 164** 1881 2232 1878 -219 239 ATOM 5353 CZ3 TRP B 164 C -14.122 -8.280 -48.557 1.00 15.08 **ANISOU 5353 CZ3 TRP B 164** 1865 2086 1780 -153 142 ATOM 5354 CH2 TRP B 164 -12.967 -7.499 -48.480 1.00 15.03

ANISOU 5354 CH2 TRP B 164 1805 2089 1817 -156 166 C 35 ATOM 5355 H TRP B 164 -13.328 -11.203 -54.647 1.00 20.22 Н ATOM 5356 HA TRP B 164 -13.628 -12.014 -52.094 1.00 18.94 Н ATOM 5357 HB2 TRP B 164 -14.931 -9.981 -53.556 1.00 18.50 Н ATOM 5358 HB3 TRP B 164 -15.386 -10.378 -52.083 1.00 18.50 Н -12.242 -9.151 -53.637 1.00 21.85 -11.036 -7.731 -52.095 1.00 21.77 ATOM 5359 HD1 TRP B 164 ATOM 5360 HE1 TRP B 164 ATOM 5361 HE3 TRP B 164 -15.216 -9.486 -49.755 1.00 18.77 Н ATOM 5362 HZ2 TRP B 164 -11.345 -6.856 -49.485 1.00 18.92 Н ATOM 5363 HZ3 TRP B 164 -14.683 -8.341 -47.817 1.00 18.10 ATOM 5364 HH2 TRP B 164 -12.776 -7.047 -47.690 1.00 18.04 ATOM 5365 N ALA B 165 -15.541 -13.533 -52.154 1.00 14.48 N **ANISOU 5365 N ALA B 165** 1979 2051 1474 -321 Ν 333 -257 -16.666 -14.459 -52.225 1.00 13.30 ATOM 5366 CA ALA B 165 **ANISOU 5366 CA ALA B 165** 1882 1874 1298 -353 312 -279 ATOM 5367 C ALA B 165 -17.814 -13.924 -51.367 1.00 13.08 **ANISOU 5367 C ALA B 165** 1852 1834 1283 -341 224 -180 ATOM 5368 O ALA B 165 0 -17.949 -12.703 -51.229 1.00 11.51 **ANISOU 5368 O ALA B 165** 1625 1676 1074 -338 178 -99 ATOM 5369 CB ALA B 165 -16.229 -15.868 -51.797 1.00 13.77 C C **ANISOU 5369 CB ALA B 165** 1960 1830 1442 -296 357 -369 ATOM 5370 H ALA B 165 -15.121 -13.554 -51.404 1.00 17.38 Н ATOM 5371 HA ALA B 165 -16.976 -14.508 -53.143 1.00 15.96 Н ATOM 5372 HB1 ALA B 165 -16.992 -16.465 -51.852 1.00 16.52 Н ATOM 5373 HB2 ALA B 165 -15.525 -16.174 -52.391 1.00 16.52 Н ATOM 5374 HB3 ALA B 165 -15.901 -15.833 -50.885 1.00 16.52 Н ATOM 5375 N TYR B 166 -18.652 -14.796 -50.796 1.00 13.91 N **ANISOU 5375 N TYR B 166** 1988 1883 1416 -339 208 -192 Ν ATOM 5376 CA TYR B 166 -19.841 -14.280 -50.127 1.00 14.29 **ANISOU 5376 CA TYR B 166** 2021 1941 1466 -346 140 -117 ATOM 5377 C TYR B 166 -19.476 -13.485 -48.871 1.00 13.22 **ANISOU 5377 C TYR B 166** 1851 1774 1399 -265 112 -53 ATOM 5378 O TYR B 166 -18.371 -13.575 -48.332 1.00 11.57 0 **ANISOU 5378 O TYR B 166** 1635 1520 1242 -199 134 -65 ATOM 5379 CB TYR B 166 -20.824 -15.405 -49.790 1.00 16.89 **ANISOU 5379 CB TYR B 166** 2388 2224 1807 -382 143 -150 ATOM 5380 CG TYR B 166 -20.365 -16.414 -48.760 1.00 17.11 **ANISOU 5380 CG TYR B 166** 2455 2136 1911 -327 174 -169 CCCC ATOM 5381 CD1 TYR B 166 -20.198 -16.060 -47.427 1.00 16.96 **ANISOU 5381 CD1 TYR B 166** 2426 2076 1943 -259 149 -106 ATOM 5382 CD2 TYR B 166 -20.135 -17.738 -49.118 1.00 18.90 **ANISOU 5382 CD2 TYR B 166** 2737 2287 2156 -345 223 -249 CCC ATOM 5383 CE1 TYR B 166 -19.783 -16.988 -46.488 1.00 18.31 **ANISOU 5383 CE1 TYR B 166** 2647 2142 2169 -211 162 -105 -19.724 -18.672 -48.182 1.00 19.23 ATOM 5384 CE2 TYR B 166 Č **ANISOU 5384 CE2 TYR B 166** 2826 2205 2275 -289 237 -250 ATOM 5385 CZ TYR B 166 -19.552 -18.292 -46.877 1.00 19.09 **ANISOU 5385 CZ TYR B 166** C 2803 2155 2294 -222 202 -169 ATOM 5386 OH TYR B 166 -19.150 -19.218 -45.940 1.00 20.63 0 **ANISOU 5386 OH TYR B 166** 3059 2228 2552 -169 201 -152 0 ATOM 5387 H TYR B 166 -18.558 -15.650 -50.782 1.00 16.70 Н ATOM 5388 HA TYR B 166 -20.293 -13.673 -50.733 1.00 17.14 Н ATOM 5389 HB2 TYR B 166 -21.641 -15.003 -49.455 1.00 20.27

ATOM 5390 HB3 TYR B 166 -21.017 -15.893 -50.606 1.00 20.27 Н ATOM 5391 HD1 TYR B 166 -20.350 -15.181 -47.165 1.00 20.36 Н -20.246 -17.998 -50.004 1.00 22.68 ATOM 5392 HD2 TYR B 166 Н ATOM 5393 HE1 TYR B 166 -19.669 -16.737 -45.600 1.00 21.98 Н ATOM 5394 HE2 TYR B 166 -19.567 -19.552 -48.438 1.00 23.08 Н ATOM 5395 HH TYR B 166 -19.044 -19.968 -46.305 1.00 24.76 ATOM 5396 N GLN B 167 -20.447 -12.690 -48.422 1.00 12.71 N **ANISOU 5396 N GLN B 167** 1460 1814 1556 -152 -26 -395 Ν ATOM 5397 CA GLN B 167 -20.302 -11.765 -47.303 1.00 11.49 C **ANISOU 5397 CA GLN B 167** 1263 1681 1422 -116 -60 -367 ATOM 5398 C GLN B 167 ANISOU 5398 C GLN B 167 -21.677 -11.720 -46.645 1.00 11.56 1305 1649 1437 -137 -74 -318 0 ATOM 5399 O GLN B 167 -22.593 -11.099 -47.191 1.00 11.48 **ANISOU 5399 O GLN B 167** 1283 1640 1437 -202 -84 -289 C ATOM 5400 CB GLN B 167 -19.864 -10.398 -47.814 1.00 11.61 **ANISOU 5400 CB GLN B 167** 1218 1753 1440 -170 -69 -369 ATOM 5401 CG GLN B 167 -19.657 -9.336 -46.768 1.00 11.14 C **ANISOU 5401 CG GLN B 167** 1119 1709 1404 -153 -95 -362 C ATOM 5402 CD GLN B 167 -19.132 -8.056 -47.375 1.00 12.40 **ANISOU 5402 CD GLN B 167** Č 1233 1904 1575 -216 -97 -366 ATOM 5403 OE1 GLN B 167 -19.749 -7.498 -48.281 1.00 12.34 **ANISOU 5403 OE1 GLN B 167** 0 1236 1881 1571 -285 -101 -325 ATOM 5404 NE2 GLN B 167 -17.987 -7.589 -46.893 1.00 12.64 N **ANISOU 5404 NE2 GLN B 167** 1210 1983 1609 -203 -99 -406 N ATOM 5405 H GLN B 167 -21.234 -12.670 -48.768 1.00 15.26 Н ATOM 5406 HA GLN B 167 -19.649 -12.099 -46.668 1.00 13.79 Н ATOM 5407 HB2 GLN B 167 -19.024 -10.504 -48.287 1.00 13.93 Н ATOM 5408 HB3 GLN B 167 -20.540 -10.071 -48.428 1.00 13.93 Н ATOM 5409 HG2 GLN B 167 -20.504 -9.143 -46.336 1.00 13.37 Н ATOM 5410 HG3 GLN B 167 -19.011 -9.650 -46.116 1.00 13.37 ATOM 5411 HE21 GLN B 167 Н -17.581 -8.013 -46.264 1.00 15.17 ATOM 5412 HE22 GLN B 167 -17.651 -6.863 -47.209 1.00 15.17 **ATOM 5413 N AVAL B 168** -21.849 -12.421 -45.524 0.43 11.86 Ν 1383 1653 1471 -86 -75 -303 **ANISOU 5413 N AVAL B 168** Ν ATOM 5414 N BVAL B 168 -21.807 -12.345 -45.472 0.57 11.89 Ν **ANISOU 5414 N BVAL B 168** 1382 1660 1474 -84 -76 -304 **ATOM 5415 CA AVAL B 168** -23.181 -12.532 -44.940 0.43 11.73 C **ANISOU 5415 CA AVAL B 168** 1396 1604 1454 -119 -68 -267 CC **ATOM 5416 CA BVAL B 168** -23.108 -12.648 -44.883 0.57 11.78 ANISOU 5416 CA BVAL B 168 1409 1609 1459 -113 -67 -267 ATOM 5417 C AVAL B 168 -23.144 -12.232 -43.449 0.43 11.13 **ANISOU 5417 C AVAL B 168** 1323 1543 1362 -83 -73 -256 C -23.125 -12.240 -43.414 0.57 11.11 ATOM 5418 C BVAL B 168 **ANISOU 5418 C BVAL B 168** 1322 1541 1359 -81 -73 -256 **ATOM 5419 O AVAL B 168** -22.138 -12.445 -42.763 0.43 10.88 0 **ANISOU 5419 O AVAL B 168** 1298 1532 1306 -24 -94 -261 0 ATOM 5420 O BVAL B 168 -22.124 -12.389 -42.702 0.57 10.64 0 **ANISOU 5420 O BVAL B 168** 1264 1503 1273 -24 -95 -261 CCC **ATOM 5421 CB AVAL B 168** -23.824 -13.921 -45.191 0.43 11.92 ANISOU 5421 CB AVAL B 168 1496 1566 1468 -141 -45 -255 **ATOM 5422 CB BVAL B 168** -23.429 -14.150 -45.046 0.57 12.00 1517 1570 1475 -114 -45 -260 ANISOU 5422 CB BVAL B 168 -23.660 -14.379 -46.651 0.43 12.21 ATOM 5423 CG1AVAL B 168

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ANISOU 5423 CG1AVAL B 168 1544 1594 1500 -183 -32 -289
ATOM 5424 CG1BVAL B 168
                             -24.692 -14.546 -44.305 0.57 12.10
ANISOU 5424 CG1BVAL B 168
                             1569 1549 1478 -155
                                                     -28 -222
                                                                 C
ATOM 5425 CG2AVAL B 168
                             -23.284 -14.968 -44.231 0.43 12.21
ANISOU 5425 CG2AVAL B 168
                             1598 1554 1488 -71 -42 -239
ATOM 5426 CG2BVAL B 168
                             -23.579 -14.501 -46.533 0.57 12.27
                                                                 C
ANISOU 5426 CG2BVAL B 168
                              1560 1596 1508 -173 -31 -290
ATOM 5427 H AVAL B 168
                            -21.228 -12.830 -45.093 0.43 14.23
                                                                н
ATOM 5428 H BVAL B 168
                            -21.143 -12.606 -44.992 0.57 14.26
                                                                Н
ATOM 5429 HA AVAL B 168
                            -23.754 -11.868 -45.355 0.43 14.07
                                                                Н
ATOM 5430 HA BVAL B 168
                             -23.793 -12.141 -45.345 0.57 14.14
ATOM 5431 HB AVAL B 168
                                                                Н
                            -24.777 -13.845 -45.022 0.43 14.31
ATOM 5432 HB BVAL B 168
                             -22.694 -14.671 -44.686 0.57 14.41
ATOM 5433 HG11AVAL B 168
                              -23.177 -13.698 -47.143 0.43 14.65
                                                                Н
ATOM 5434 HG11BVAL B 168
                              -25.058 -13.763 -43.865 0.57 14.52
ATOM 5435 HG12AVAL B 168
                                                                 Н
                              -23.165 -15.213 -46.666 0.43 14.65
ATOM 5436 HG12BVAL B 168
                              -25.334 -14.898 -44.941 0.57 14.52
                                                                  Н
ATOM 5437 HG13AVAL B 168
                              -24.539 -14.509 -47.041 0.43 14.65
ATOM 5438 HG13BVAL B 168
                              -24.472 -15.223 -43.646 0.57 14.52
                                                                  Н
ATOM 5439 HG21AVAL B 168
                             -23.710 -15.818 -44.420 0.43 14.65
                                                                  Н
ATOM 5440 HG21BVAL B 168
                              -23.780 -15.447 -46.615 0.57 14.73
                                                                  Н
ATOM 5441 HG22AVAL B 168
                              -22.325 -15.043 -44.353 0.43 14.65
                                                                  Н
ATOM 5442 HG22BVAL B 168
                              -24.301 -13.975 -46.911 0.57 14.73
                                                                  Н
ATOM 5443 HG23AVAL B 168
                              -23.481 -14.693 -43.321 0.43 14.65
                                                                  Н
ATOM 5444 HG23BVAL B 168
                                                                  Н
                              -22.748 -14.299 -46.991 0.57 14.73
ATOM 5445 N MET B 169
                           -24.270 -11.725 -42.957 1.00 11.54
                                                               Ν
ANISOU 5445 N MET B 169
                            1364 1594 1425 -123 -53 -245
                                                               Ν
ATOM 5446 CA MET B 169
                            -24.475 -11.469 -41.536 1.00 12.22
ANISOU 5446 CA MET B 169
                             1464 1700 1480 -115 -37 -248
ATOM 5447 C MET B 169
                           -25.053 -12.754 -40.965 1.00 12.91
ANISOU 5447 C MET B 169
                            1630 1751 1523 -127 -15 -207
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ATOM 5448 O MET B 169
                           -26.230 -13.061 -41.169 1.00 14.34
ANISOU 5448 O MET B 169
                            1816 1909 1723 -182
                                                   20 -194
                                                                C
ATOM 5449 CB MET B 169
                            -25.403 -10.278 -41.312 1.00 13.68
ANISOU 5449 CB MET B 169
                            1590 1896 1713 -150
                                                    -6 -272
                                                               C
ATOM 5450 CG MET B 169
                            -25.492 -9.867 -39.868 1.00 13.49
                                                               C
ANISOU 5450 CG MET B 169
                            1578 1903 1645 -152
                                                    27 -304
                                                               SS
ATOM 5451 SD MET B 169
ANISOU 5451 SD MET B 169
                            -23.913 -9.278 -39.240 1.00 13.16
                            1535 1915 1550 -119 -18 -343
                                                               Č
ATOM 5452 CE MET B 169
                            -24.077 -9.635 -37.479 1.00 14.31
                             1747 2113 1579 -141
                                                     6 -349
ANISOU 5452 CE MET B 169
ATOM 5453 H MET B 169
                           -24.946 -11.516 -43.446 1.00 13.84
                                                               Н
ATOM 5454 HA MET B 169
                            -23.623 -11.280 -41.113 1.00 14.67
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ATOM 5455 HB2 MET B 169
                            -25.071 -9.521 -41.819 1.00 16.42
                                                                Н
ATOM 5456 HB3 MET B 169
                                                                Н
                            -26.295 -10.513 -41.612 1.00 16.42
ATOM 5457 HG2 MET B 169
                            -26.140 -9.151 -39.780 1.00 16.19
                                                                Н
ATOM 5458 HG3 MET B 169
                            -25.764 -10.631 -39.335 1.00 16.19
                                                                Н
                            -23.268 -9.354 -37.024 1.00 17.18
ATOM 5459 HE1 MET B 169
                                                                Н
                            -24.840 -9.149 -37.128 1.00 17.18
ATOM 5460 HE2 MET B 169
                                                                Н
ATOM 5461 HE3 MET B 169
                            -24.209 -10.588 -37.361 1.00 17.18
                                                               Н
                           -24.216 -13.519 -40.277 1.00 13.27
ATOM 5462 N ALA B 170
                                                               Ν
ANISOU 5462 N ALA B 170
                          1735 1792 1515 -79 -42 -180
                                                              Ν
ATOM 5463 CA ALA B 170
                          -24.459 -14.938 -40.079 1.00 13.74
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ANISOU 5463 CA ALA B 170 1888 1783 1549 -78 -34 -126 C ATOM 5464 C ALA B 170 C -24.725 -15.290 -38.628 1.00 14.34 **ANISOU 5464 C ALA B 170** 2033 1873 1542 -95 -26 -77 ATOM 5465 O ALA B 170 -24.363 -14.569 -37.691 1.00 13.13 0 **ANISOU 5465 O ALA B 170** 1861 1794 1333 -90 -41 -90 ATOM 5466 CB ALA B 170 -23.267 -15.775 -40.553 1.00 13.27 C **ANISOU 5466 CB ALA B 170** 1855 1678 1510 5 -75 -114 ATOM 5467 H ALA B 170 Н -23.492 -13.235 -39.911 1.00 15.92 ATOM 5468 HA ALA B 170 -25.235 -15.201 -40.599 1.00 16.49 -23.462 -16.713 -40.406 1.00 15.93 ATOM 5469 HB1 ALA B 170 ATOM 5470 HB2 ALA B 170 -23.121 -15.610 -41.497 1.00 15.93 -22.480 -15.517 -40.046 1.00 15.93 ATOM 5471 HB3 ALA B 170 Н ATOM 5472 N THR B 171 -25.392 -16.428 -38.483 1.00 14.00 Ν **ANISOU 5472 N THR B 171** 2078 1758 1483 -134 3 -25 ATOM 5473 CA THR B 171 -25.333 -17.257 -37.291 1.00 15.26 C **ANISOU 5473 CA THR B 171** 2344 1898 1558 -139 -6 C ATOM 5474 C THR B 171 -24.396 -18.414 -37.607 1.00 15.64 **ANISOU 5474 C THR B 171** 2460 1847 1638 -51 -60 114 ATOM 5475 O THR B 171 -24.668 -19.199 -38.524 1.00 14.39 0 **ANISOU 5475 O THR B 171** 2335 1588 1545 -59 -34 C ATOM 5476 CB THR B 171 -26.720 -17.774 -36.924 1.00 16.57 **ANISOU 5476 CB THR B 171** 2566 2035 1693 -251 70 ATOM 5477 OG1 THR B 171 -27.604 -16.672 -36.686 1.00 17.42 0 **ANISOU 5477 OG1 THR B 171** 2587 2232 1799 -317 130 ATOM 5478 CG2 THR B 171 -26.652 -18.641 -35.678 1.00 19.14 **ANISOU 5478 CG2 THR B 171** 3020 2339 1915 -274 63 ATOM 5479 H THR B 171 -25.907 -16.753 -39.091 1.00 16.80 Н ATOM 5480 HA THR B 171 -24.974 -16.749 -36.547 1.00 18.32 Н -27.066 -18.313 -37.652 1.00 19.88 ATOM 5481 HB THR B 171 Н ATOM 5482 HG1 THR B 171 -27.664 -16.197 -37.376 1.00 20.90 ATOM 5483 HG21 THR B 171 -27.538 -18.965 -35.451 1.00 22.97 ATOM 5484 HG22 THR B 171 -26.068 -19.400 -35.834 1.00 22.97 ATOM 5485 HG23 THR B 171 -26.306 -18.124 -34.934 1.00 22.97 ATOM 5486 N ALA B 172 -23.286 -18.504 -36.877 1.00 15.35 Ν **ANISOU 5486 N ALA B 172** 2435 1838 1560 34 -136 165 ATOM 5487 CA ALA B 172 -22.291 -19.544 -37.098 1.00 17.43 **ANISOU 5487 CA ALA B 172** 2741 2006 1876 146 -194 ATOM 5488 C ALA B 172 ANISOU 5488 C ALA B 172 -22.032 -20.258 -35.783 1.00 18.62 C 2995 2140 1940 168 -255 353 0 ATOM 5489 O ALA B 172 -22.115 -19.655 -34.710 1.00 19.04 0 **ANISOU 5489 O ALA B 172** 3051 2306 1877 119 -277 379 C ATOM 5490 CB ALA B 172 -20.971 -18.975 -37.648 1.00 18.07 C **ANISOU 5490 CB ALA B 172** 2703 2145 2016 252 -250 164 ATOM 5491 H ALA B 172 -23.085 -17.965 -36.238 1.00 18.42 Н ATOM 5492 HA ALA B 172 -22.635 -20.190 -37.735 1.00 20.91 Н ATOM 5493 HB1 ALA B 172 -20.343 -19.703 -37.778 1.00 21.68 Н ATOM 5494 HB2 ALA B 172 -21.146 -18.533 -38.494 1.00 21.68 Н ATOM 5495 HB3 ALA B 172 -20.612 -18.338 -37.010 1.00 21.68 ATOM 5496 N GLY B 173 -21.717 -21.547 -35.864 1.00 19.30 ANISOU 5496 N GLY B 173 3174 2079 2080 238 -281 437 Ν ATOM 5497 CA GLY B 173 -21.539 -22.319 -34.647 1.00 20.36 ANISOU 5497 CA GLY B 173 3426 2177 2133 254 -347 592 ATOM 5498 C GLY B 173 -20.617 -23.505 -34.807 1.00 23.14

ANISOU 5498 C GLY B 173 3830 2375 2587 403 -416 682 C ATOM 5499 O GLY B 173 -20.308 -23.949 -35.920 1.00 21.45 0 **ANISOU 5499 O GLY B 173** 3585 2050 2514 476 -382 0 611 ATOM 5500 H GLY B 173 -21.604 -21.987 -36.594 1.00 23.16 Н ATOM 5501 HA2 GLY B 173 -21.175 -21.744 -33.956 1.00 24.43 Н ATOM 5502 HA3 GLY B 173 -22.402 -22.644 -34.347 1.00 24.43 Н ATOM 5503 N TYR B 174 -20.181 -24.015 -33.654 1.00 26.44 Ν **ANISOU 5503 N TYR B 174** 4329 2789 2929 444 -515 N ATOM 5504 CA TYR B 174 -19.329 -25.198 -33.573 1.00 29.93 C **ANISOU 5504 CA TYR B 174** 4830 3070 3470 599 -600 C 965 ATOM 5505 C TYR B 174 ANISOU 5505 C TYR B 174 -19.748 -25.988 -32.341 1.00 30.95 C 5139 3138 3482 541 -650 1163 ATOM 5506 O TYR B 174 0 -19.580 -25.511 -31.215 1.00 30.76 **ANISOU 5506 O TYR B 174** 5122 3270 3296 0 498 -731 1247 C ATOM 5507 CB TYR B 174 -17.850 -24.814 -33.499 1.00 33.23 CCCC **ANISOU 5507 CB TYR B 174** 5099 3587 3939 766 -724 968 **ATOM 5508 CG TYR B 174** -16.920 -25.998 -33.421 1.00 38.25 ANISOU 5508 CG TYR B 174 5769 4059 4706 953 -818 1097 ATOM 5509 CD1 TYR B 174 -16.531 -26.675 -34.568 1.00 39.55 C 5901 4051 5075 1075 -760 1016 **ANISOU 5509 CD1 TYR B 174** ATOM 5510 CD2 TYR B 174 -16.430 -26.442 -32.200 1.00 42.00 C **ANISOU 5510 CD2 TYR B 174** 6308 4549 5103 1011 -967 1299 ATOM 5511 CE1 TYR B 174 -15.680 -27.761 -34.501 1.00 42.40 C **ANISOU 5511 CE1 TYR B 174** 6277 4249 5585 1257 -831 1120 ATOM 5512 CE2 TYR B 174 -15.582 -27.527 -32.124 1.00 45.20 C **ANISOU 5512 CE2 TYR B 174** 6679 4830 5664 1160 -1016 1404 ATOM 5513 CZ TYR B 174 C -15.209 -28.182 -33.278 1.00 45.56 **ANISOU 5513 CZ TYR B 174** 6681 4695 5935 1285 -946 1312 C ATOM 5514 OH TYR B 174 -14.361 -29.266 -33.201 1.00 48.98 0 7072 4998 6539 1437 -981 1412 **ANISOU 5514 OH TYR B 174** 0 ATOM 5515 H TYR B 174 -20.372 -23.681 -32.885 1.00 31.73 Н ATOM 5516 HA TYR B 174 -19.466 -25.752 -34.358 1.00 35.91 Н ATOM 5517 HB2 TYR B 174 -17.618 -24.306 -34.293 1.00 39.87 Н Н ATOM 5518 HB3 TYR B 174 -17.707 -24.271 -32.708 1.00 39.87 ATOM 5519 HD1 TYR B 174 -16.848 -26.392 -35.395 1.00 47.46 Н -16.681 -26.002 -31.420 1.00 50.40 Н ATOM 5520 HD2 TYR B 174 ATOM 5521 HE1 TYR B 174 -15.427 -28.206 -35.278 1.00 50.88 Н ATOM 5522 HE2 TYR B 174 -15.262 -27.813 -31.299 1.00 54.24 Н ATOM 5523 HH TYR B 174 -14.152 -29.411 -32.401 1.00 58.77 Н ATOM 5524 N GLN B 175 -20.306 -27.180 -32.554 1.00 30.93 N ANISOU 5524 N GLN B 175 5289 2912 3550 522 -597 1232 N ATOM 5525 CA GLN B 175 -20.674 -28.090 -31.471 1.00 33.30 C **ANISOU 5525 CA GLN B 175** C 5763 3128 3761 462 -632 1430 CC ATOM 5526 C GLN B 175 -21.542 -27.394 -30.425 1.00 32.98 **ANISOU 5526 C GLN B 175** 5766 3275 3489 266 -601 1457 ATOM 5527 O GLN B 175 -21.291 -27.477 -29.220 1.00 33.74 0 0 **ANISOU 5527 O GLN B 175** 5879 3479 3460 244 -671 1582 ATOM 5528 CB GLN B 175 CCCC -19.423 -28.691 -30.827 1.00 35.74 **ANISOU 5528 CB GLN B 175** 6019 3430 4131 631 -769 1575 ATOM 5529 CG GLN B 175 -18.651 -29.627 -31.746 1.00 38.33 **ANISOU 5529 CG GLN B 175** 6305 3548 4710 814 -770 1556 ATOM 5530 CD GLN B 175 -17.448 -30.264 -31.067 1.00 43.30 **ANISOU 5530 CD GLN B 175** 6869 4170 5414 982 -896 1716

ATOM 5531 OE1 GLN B 175 -16.993 -29.806 -30.018 1.00 45.06 0 **ANISOU 5531 OE1 GLN B 175** 7046 4581 5493 982 -1003 1820 0 ATOM 5532 NE2 GLN B 175 -16.935 -31.336 -31.659 1.00 45.38 Ν **ANISOU 5532 NE2 GLN B 175** 7124 4218 5900 1121 -875 1734 Ν ATOM 5533 H GLN B 175 -20.486 -27.490 -33.336 1.00 37.11 ATOM 5534 HA GLN B 175 -21.192 -28.821 -31.843 1.00 39.96 Н ATOM 5535 HB2 GLN B 175 -18.826 -27.970 -30.570 1.00 42.89 Н ATOM 5536 HB3 GLN B 175 -19.686 -29.196 -30.042 1.00 42.89 Н ATOM 5537 HG2 GLN B 175 -19.242 -30.339 -32.038 1.00 45.99 Н ATOM 5538 HG3 GLN B 175 -18.332 -29.125 -32.512 1.00 45.99 Н ATOM 5539 HE21 GLN B 175 -17.285 -31.634 -32.387 1.00 54.46 -16.254 -31.733 -31.315 1.00 54.46 ATOM 5540 HE22 GLN B 175 Н ATOM 5541 N SER B 176 -22.593 -26.720 -30.892 1.00 30.21 **ANISOU 5541 N SER B 176** 5389 2989 3100 120 -471 1312 ATOM 5542 CA SER B 176 -23.443 -25.938 -30.003 1.00 30.64 **ANISOU 5542 CA SER B 176** 5455 3229 2957 -60 -414 1296 C ATOM 5543 C SER B 176 -24.912 -26.134 -30.374 1.00 29.56 ANISOU 5543 C SER B 176 5370 3038 2823 -237 -252 12 C 5370 3038 2823 -237 -252 1225 ATOM 5544 O SER B 176 ANISOU 5544 O SER B 176 -25.263 -26.937 -31.243 1.00 28.71 0 5310 2748 2851 -234 -196 1205 ATOM 5545 CB SER B 176 -23.050 -24.460 -30.061 1.00 28.96 **ANISOU 5545 CB SER B 176** 5060 3239 2704 -41 -427 1148 ATOM 5546 OG SER B 176 ANISOU 5546 OG SER B 176 0 -23.220 -23.957 -31.364 1.00 26.75 4652 2940 2573 -11 -353 974 0 ATOM 5547 H SER B 176 -22.832 -26.700 -31.718 1.00 36.25 Н ATOM 5548 HA SER B 176 -23.319 -26.247 -29.092 1.00 36.76 н ATOM 5549 HB2 SER B 176 -23.614 -23.958 -29.451 1.00 34.75 Н ATOM 5550 HB3 SER B 176 -22.119 -24.369 -29.805 1.00 34.75 Н ATOM 5551 HG SER B 176 -23.003 -23.146 -31.389 1.00 32.10 ATOM 5552 N SER B 177 -25.768 -25.382 -29.680 1.00 29.02 **ANISOU 5552 N SER B 177** 5286 3138 2602 -396 -173 1180 Ν ATOM 5553 CA SER B 177 -27.212 -25.385 -29.865 1.00 28.29 **ANISOU 5553 CA SER B 177** 5206 3046 2496 -576 -18 1106 ATOM 5554 C SER B 177 ANISOU 5554 C SER B 177 -27.705 -23.963 -29.667 1.00 27.05 4902 3107 2269 -646 54 953 ATOM 5555 O SER B 177 -27.006 -23.127 -29.088 1.00 28.06 0 **ANISOU 5555 O SER B 177** 4973 3377 2312 -596 -11 935 ATOM 5556 CB SER B 177 -27.923 -26.301 -28.865 1.00 30.24 **ANISOU 5556 CB SER B 177** 5555 3269 2665 -696 29 1209 ATOM 5557 OG SER B 177 -27.289 -27.556 -28.774 1.00 31.73 **ANISOU 5557 OG SER B 177** 5848 3282 2924 -602 -55 1355 0 ATOM 5558 H SER B 177 -25.516 -24.836 -29.065 1.00 34.82 Н ATOM 5559 HA SER B 177 -27.429 -25.672 -30.766 1.00 33.94 Н ATOM 5560 HB2 SER B 177 -27.912 -25.880 -27.991 1.00 36.28 ATOM 5561 HB3 SER B 177 Н -28.839 -26.433 -29.156 1.00 36.28 ATOM 5562 HG SER B 177 -27.291 -27.934 -29.524 1.00 38.07 Н ATOM 5563 N GLY B 178 -28.915 -23.688 -30.127 1.00 25.17 Ν **ANISOU 5563 N GLY B 178** 4601 2892 2073 -765 186 842 Ν ATOM 5564 CA GLY B 178 -29.525 -22.398 -29.874 1.00 24.06 ANISOU 5564 CA GLY B 178 4326 2935 1883 -833 270 703 ATOM 5565 C GLY B 178 -30.544 -22.041 -30.937 1.00 22.62 ANISOU 5565 C GLY B 178 4013 2743 1838 -880 368 568 ATOM 5566 O GLY B 178 -30.953 -22.873 -31.743 1.00 22.66

ANISOU 5566 O GLY B 178 4050 2618 1941 -905 387 583 0 ATOM 5567 H GLY B 178 -29.401 -24.229 -30.587 1.00 30.21 Н ATOM 5568 HA2 GLY B 178 -29.969 -22.412 -29.012 1.00 28.88 Н ATOM 5569 HA3 GLY B 178 -28.840 -21.712 -29.858 1.00 28.88 Н ATOM 5570 N SER B 179 -30.949 -20.771 -30.913 1.00 20.52 Ν **ANISOU 5570 N SER B 179** 3600 2619 1579 -893 427 434 Ν ATOM 5571 CA SER B 179 -31.856 -20.217 -31.908 1.00 19.40 **ANISOU 5571 CA SER B 179** 3306 2492 1574 -916 498 311 ATOM 5572 C SER B 179 ANISOU 5572 C SER B 179 -31.457 -18.784 -32.217 1.00 18.78 3076 2505 1553 -820 475 192 ATOM 5573 O SER B 179 ANISOU 5573 O SER B 179 -30.890 -18.089 -31.369 1.00 18.27 3015 2531 1395 -795 458 173 ATOM 5574 CB SER B 179 -33.305 -20.223 -31.434 1.00 20.73 **ANISOU 5574 CB SER B 179** 3441 2728 1707 -1082 273 643 ATOM 5575 OG SER B 179 -33.693 -21.508 -30.995 1.00 21.86 **ANISOU 5575 OG SER B 179** 3737 2791 1777 -1199 675 387 0 ATOM 5576 H SER B 179 -30.706 -20.202 -30.316 1.00 24.63 Н ATOM 5577 HA SER B 179 -31.797 -20.737 -32.725 1.00 23.28 Н ATOM 5578 HB2 SER B 179 -33.398 -19.598 -30.698 1.00 24.87 Н ATOM 5579 HB3 SER B 179 Н -33.878 -19.955 -32.169 1.00 24.87 ATOM 5580 HG SER B 179 -33.619 -22.061 -31.623 1.00 26.23 ATOM 5581 N SER B 180 -31.783 -18.345 -33.433 1.00 17.21 Ν **ANISOU 5581 N SER B 180** 2751 2284 1503 -780 472 115 Ν ATOM 5582 CA SER B 180 -31.605 -16.955 -33.822 1.00 16.95 2574 2322 1545 -705 **ANISOU 5582 CA SER B 180** 463 ATOM 5583 C SER B 180 ANISOU 5583 C SER B 180 -32.679 -16.570 -34.831 1.00 17.09 2453 2342 1700 -734 508 -58 ATOM 5584 O SER B 180 -33.275 -17.420 -35.501 1.00 16.84 0 **ANISOU 5584 O SER B 180** 2435 2252 1713 -792 515 -26 ATOM 5585 CB SER B 180 C -30.214 -16.701 -34.418 1.00 16.90 **ANISOU 5585 CB SER B 180** 2567 2280 1574 -571 344 ATOM 5586 OG SER B 180 -30.084 -17.356 -35.678 1.00 16.05 **ANISOU 5586 OG SER B 180** 2461 2076 1562 -537 298 39 ATOM 5587 H SER B 180 ATOM 5588 HA SER B 180 Н -32.111 -18.841 -34.053 1.00 20.65 -31.707 -16.390 -33.040 1.00 20.34 Н ATOM 5589 HB2 SER B 180 -30.092 -15.747 -34.543 1.00 20.28 ATOM 5590 HB3 SER B 180 -29.541 -17.046 -33.810 1.00 20.28 ATOM 5591 HG SER B 180 -29.321 -17.213 -35.998 1.00 19.26 Н ATOM 5592 N ASN B 181 -32.923 -15.264 -34.917 1.00 16.32 N **ANISOU 5592 N ASN B 181** 2221 2310 1671 -695 534 -149 Ν ATOM 5593 CA ASN B 181 -33.779 -14.683 -35.947 1.00 17.39 **ANISOU 5593 CA ASN B 181** 2204 2450 1953 -690 544 -200 CCO ATOM 5594 C ASN B 181 -33.194 -13.317 -36.266 1.00 15.99 **ANISOU 5594 C ASN B 181** 1939 2288 1849 -586 503 -261 -33.051 -12.484 -35.369 1.00 15.75 ATOM 5595 O ASN B 181 **ANISOU 5595 O ASN B 181** 1892 2305 1786 -572 553 -323 ATOM 5596 CB ASN B 181 -35.235 -14.568 -35.476 1.00 18.44 **ANISOU 5596 CB ASN B 181** 2243 2648 2117 -787 665 -245 ATOM 5597 CG ASN B 181 -36.198 -14.182 -36.593 1.00 18.14 2039 2618 2234 -786 654 -272 **ANISOU 5597 CG ASN B 181** ATOM 5598 OD1 ASN B 181 -36.021 -13.171 -37.272 1.00 17.25 ANISOU 5598 OD1 ASN B 181 1827 2502 2226 -696 601 -302 0 ATOM 5599 ND2 ASN B 181 -37.248 -14.980 -36.764 1.00 18.84

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ANISOU 5599 ND2 ASN B 181 2097 2724 2338 -896 700 -253
                                                               Ν
ATOM 5600 H ASN B 181
                          -32.595 -14.681 -34.377 1.00 19.59
                                                              Н
ATOM 5601 HA ASN B 181
                           -33.751 -15.231 -36.746 1.00 20.87
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                           -35.519 -15.425 -35.120 1.00 22.13
ATOM 5602 HB2 ASN B 181
                                                              Н
ATOM 5603 HB3 ASN B 181
                            -35.290 -13.889 -34.786 1.00 22.13
                                                              Н
ATOM 5604 HD21 ASN B 181
                                                              Н
                           -37.823 -14.809 -37.380 1.00 22.61
ATOM 5605 HD22 ASN B 181
                            -37.352 -15.669 -36.259 1.00 22.61
ATOM 5606 N VAL B 182
                          -32.818 -13.102 -37.525 1.00 13.75
ANISOU 5606 N VAL B 182
                           1611 1962 1650 -527 416 -246
                                                             N
ATOM 5607 CA VAL B 182
                           -32.032 -11.935 -37.908 1.00 13.47
ANISOU 5607 CA VAL B 182
                           1525 1924 1671 -437 363 -282
ATOM 5608 C VAL B 182
                          -32.561 -11.408 -39.232 1.00 13.97
ANISOU 5608 C VAL B 182
                          1474 1971 1864 -418 319 -277
ATOM 5609 O VAL B 182
                          -32.822 -12.181 -40.158 1.00 14.06
                                                              0
ANISOU 5609 O VAL B 182
                          1493 1964 1886 -454 276 -231
                                                              CCCCC
ATOM 5610 CB VAL B 182
                           -30.527 -12.274 -38.033 1.00 13.79
ANISOU 5610 CB VAL B 182
                           1663 1936 1639 -382 281 -249
                           -29.710 -11.022 -38.305 1.00 14.00
ATOM 5611 CG1 VAL B 182
ANISOU 5611 CG1 VAL B 182
                           1636 1969 1714 -313 241 -293
ATOM 5612 CG2 VAL B 182
                            -30.012 -12.996 -36.798 1.00 14.01
                                                               C
ANISOU 5612 CG2 VAL B 182
                           1810 1981 1533 -401 297 -220
ATOM 5613 H VAL B 182
                          -33.008 -13.624 -38.181 1.00 16.50
                                                             Н
ATOM 5614 HA VAL B 182
                           -32.136 -11.241 -37.238 1.00 16.17
                                                              Н
ATOM 5615 HB VAL B 182
                           -30.408 -12.870 -38.789 1.00 16.54
                                                              Н
                                                              Н
ATOM 5616 HG11 VAL B 182
                           -28.774 -11.266 -38.379 1.00 16.80
ATOM 5617 HG12 VAL B 182
                           -30.014 -10.622 -39.135 1.00 16.80
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ATOM 5618 HG13 VAL B 182
                            -29.834 -10.399 -37.572 1.00 16.80
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ATOM 5619 HG21 VAL B 182
                            -29.069 -13.190 -36.916 1.00 16.81
                                                               Н
ATOM 5620 HG22 VAL B 182
                            -30.138 -12.425 -36.024 1.00 16.81
                                                               Н
ATOM 5621 HG23 VAL B 182
                            -30.508 -13.822 -36.685 1.00 16.81
ATOM 5622 N THR B 183
                          -32.692 -10.088 -39.332 1.00 13.79
ANISOU 5622 N THR B 183
                          1352 1950 1937 -366
                                                              N
                                                  323 -321
ATOM 5623 CA THR B 183
                           -32.987 -9.425 -40.598 1.00 14.87
ANISOU 5623 CA THR B 183
                           1392 2067 2192 -335 256 -293
ATOM 5624 C THR B 183
                          -31.786 -8.582 -41.009 1.00 13.81
ANISOU 5624 C THR B 183
                           1283 1898 2066 -272
                                                              C
                                                 195 -296
ATOM 5625 O THR B 183
                          -31.219 -7.861 -40.177 1.00 12.85
ANISOU 5625 O THR B 183
                           1179 1770 1931 -240 230 -352
ATOM 5626 CB THR B 183
                           -34.244 -8.561 -40.480 1.00 16.62
ANISOU 5626 CB THR B 183
                           1464 2299 2551 -320
                                                  307 -325
ATOM 5627 OG1 THR B 183
                            -35.346 -9.384 -40.074 1.00 18.01
                                                               0
                           1605 2523 2716 -393 374 -329
ANISOU 5627 OG1 THR B 183
ATOM 5628 CG2 THR B 183
                            -34.573 -7.894 -41.814 1.00 18.04
                                                              C
                           1544 2457 2851 -285 214 -267
ANISOU 5628 CG2 THR B 183
                                                              C
                          -32.614 -9.546 -38.669 1.00 16.55
ATOM 5629 H THR B 183
                                                             Н
ATOM 5630 HA THR B 183
                           -33.140 -10.094 -41.283 1.00 17.85
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ATOM 5631 HB THR B 183
                           -34.098 -7.867 -39.817 1.00 19.94
                                                              Н
ATOM 5632 HG1 THR B 183
                                                             Н
                           -36.042 -8.919 -40.006 1.00 21.62
                           -35.371 -7.350 -41.724 1.00 21.64
ATOM 5633 HG21 THR B 183
ATOM 5634 HG22 THR B 183 -33.835 -7.329 -42.093 1.00 21.64
                                                              Н
ATOM 5635 HG23 THR B 183 -34.727 -8.570 -42.492 1.00 21.64
ATOM 5636 N VAL B 184 -31.407 -8.672 -42.290 1.00 13.48
                                                             Ν
ANISOU 5636 N VAL B 184 1242 1842 2036 -272 109 -240
                                                            Ν
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ATOM 5637 CA VAL B 184 -30.191 -8.066 -42.825 1.00 13.52 **ANISOU 5637 CA VAL B 184** 1280 1826 2030 -236 54 -234 -30.558 -7.131 -43.974 1.00 14.23 ATOM 5638 C VAL B 184 ANISOU 5638 C VAL B 184 ATOM 5639 O VAL B 184 1290 1895 2223 -227 -7 -186 O -31.432 -7.450 -44.789 1.00 15.20 **ANISOU 5639 O VAL B 184** 1363 2037 2377 -261 -46 -133 ATOM 5640 CB VAL B 184 -29.192 -9.138 -43.325 1.00 13.03 **ANISOU 5640 CB VAL B 184** 1311 1773 1866 -253 16 -214 ATOM 5641 CG1 VAL B 184 -27.845 -8.522 -43.633 1.00 12.40 **ANISOU 5641 CG1 VAL B 184** 1253 1690 1769 -220 -19 -226 ATOM 5642 CG2 VAL B 184 -29.049 -10.264 -42.314 1.00 14.21 **ANISOU 5642 CG2 VAL B 184** 1542 1929 1927 -263 59 -228 ATOM 5643 H VAL B 184 -31.859 -9.097 -42.886 1.00 16.17 Н ATOM 5644 HA VAL B 184 -29.758 -7.544 -42.132 1.00 16.22 Н ATOM 5645 HB VAL B 184 -29.535 -9.523 -44.147 1.00 15.63 Н ATOM 5646 HG11 VAL B 184 -27.243 -9.218 -43.942 1.00 14.88 Н ATOM 5647 HG12 VAL B 184 ATOM 5648 HG13 VAL B 184 -27.956 -7.849 -44.322 1.00 14.88 Н -27.492 -8.115 -42.826 1.00 14.88 Н ATOM 5649 HG21 VAL B 184 ATOM 5650 HG22 VAL B 184 -28.419 -10.917 -42.656 1.00 17.05 Н -28.724 -9.897 -41.477 1.00 17.05 Н ATOM 5651 HG23 VAL B 184 ATOM 5652 N TRP B 185 -29.915 -10.679 -42.179 1.00 17.05 Н -29.868 -5.995 -44.059 1.00 13.36 Ν **ANISOU 5652 N TRP B 185** 1173 1747 2157 -190 -23 -195 ATOM 5653 CA TRP B 185 -30.041 -5.097 -45.204 1.00 15.02 **ANISOU 5653 CA TRP B 185** 1331 1925 2451 -186 -92 -125 -28.860 -4.153 -45.399 1.00 15.66 ATOM 5654 C TRP B 185 ANISOU 5654 C TRP B 185 ATOM 5655 O TRP B 185 C 1450 1967 2534 -176 -110 -132 -27.916 -4.119 -44.605 1.00 14.52 **ANISOU 5655 O TRP B 185** 1355 1827 2334 -169 -70 -202 ATOM 5656 CB TRP B 185 -31.338 -4.290 -45.067 1.00 16.31 1381 2049 2767 -145 -83 -108 **ANISOU 5656 CB TRP B 185** ATOM 5657 CG TRP B 185 -31.370 -3.268 -43.962 1.00 16.06 1323 1952 2826 -87 **ANISOU 5657 CG TRP B 185** -3 -191 ATOM 5658 CD1 TRP B 185 -31.116 -1.930 -44.075 1.00 16.81 **ANISOU 5658 CD1 TRP B 185** 1399 1954 3032 -44 -11 -190 ATOM 5659 CD2 TRP B 185 -31.701 -3.499 -42.586 1.00 16.23 **ANISOU 5659 CD2 TRP B 185** 1344 1992 2831 -79 104 -293 Ν ATOM 5660 NE1 TRP B 185 -31.264 -1.312 -42.849 1.00 16.57 1354 1879 3062 -7 **ANISOU 5660 NE1 TRP B 185** 90 -302 Ν -31.623 -2.254 -41.921 1.00 17.00 ATOM 5661 CE2 TRP B 185 **ANISOU 5661 CE2 TRP B 185** 1419 2012 3030 -31 162 -368 ATOM 5662 CE3 TRP B 185 -32.052 -4.636 -41.851 1.00 15.76 C **ANISOU 5662 CE3 TRP B 185** 1310 2003 2675 -118 160 -328 ATOM 5663 CZ2 TRP B 185 -31.874 -2.119 -40.557 1.00 16.86 **ANISOU 5663 CZ2 TRP B 185** 1400 2001 3004 -27 279 -488 ATOM 5664 CZ3 TRP B 185 -32.308 -4.497 -40.494 1.00 16.40 **ANISOU 5664 CZ3 TRP B 185** 1393 2095 2744 -116 270 -428 ATOM 5665 CH2 TRP B 185 -32.215 -3.247 -39.863 1.00 16.07 **ANISOU 5665 CH2 TRP B 185** 1325 1991 2790 -73 331 -514 **ATOM 5666 OXT TRP B 185** -28.822 -3.426 -46.394 1.00 15.92 ANISOU 5666 OXT TRP B 185 1464 1970 2617 -187 -171 -60 ATOM 5667 H TRP B 185 -29.298 -5.721 -43.475 1.00 16.03 Н ATOM 5668 HA TRP B 185 -30.117 -5.636 -46.007 1.00 18.03 Н

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ATOM 5669 HB2 TRP B 185
                                                -31.494 -3.819 -45.901 1.00 19.57
ATOM 5670 HB3 TRP B 185 -32.067 -4.911 -44.907 1.00 19.57 ATOM 5671 HD1 TRP B 185 -30.882 -1.497 -44.865 1.00 20.17
ATOM 5672 HE1 TRP B 185 -31.147 -0.474 -42.693 1.00 19.88
ATOM 5673 HE3 TRP B 185 -32.114 -5.468 -42.263 1.00 18.91
ATOM 5674 HZ2 TRP B 185 -31.816 -1.292 -40.135 1.00 20.23
ATOM 5675 HZ3 TRP B 185 -32.541 -5.245 -39.994 1.00 19.68
ATOM 5676 HH2 TRP B 185 -32.392 -3.183 -38.952 1.00 19.29
TER 5677 TRP B 185
ATOM 5678 N SER C 2
                                           -5.314 3.845 7.444 1.00 37.06
ANISOU 5678 N SER C 2 5183 5326 3570 -107 -810 -522 ATOM 5679 CA SER C 2 -5.781 2.797 6.546 1.00 35.60 ANISOU 5679 CA SER C 2 4945 5114 3467 -37 -800 -453
                                                                                                          C
ATOM 5680 C SER C 2 -7.303 2.707 6.594 1.00 34.03
ANISOU 5680 C SER C 2 4819 4842 3269 23 -738 -385
ATOM 5681 O SER C 2 -7.948 3.370 7.405 1.00 33.51
                                                                                                           C
                                                                                                         0
ANISOU 5681 O SER C 2
ATOM 5682 CB SER C 2
                                            4871 4733 3129 52 -696 -386
                                                                                                           0
                                            -5.146 1.456 6.920 1.00 36.88
ANISOU 5682 CB SER C 2 5104 5274 3635 104 -894 -468
ATOM 5683 OG SER C 2 -5.486 1.083 8.247 1.00 37.59
                                                                                                           0
ANISOU 5683 OG SER C 2 5322 5318 3641 179 -917 -444
ATOM 5684 HA SER C 2
                                                -5.519 3.014 5.638 1.00 42.72
                                                                                                          Н
ATOM 5685 HB2 SER C 2 -5.467 0.774 6.309 1.00 44.26
ATOM 5686 HB3 SER C 2 -4.182 1.534 6.851 1.00 44.26
                                                                                                         Н
                                                                                                           Н
                                            -5.213 1.665 8.787 1.00 45.10
-7.872 1.887 5.716 1.00 33.49
ATOM 5687 HG SER C 2
                                                                                                          Н
ATOM 5688 N THR C 3 -7.872 1.887 5.716 1.00 33.49
ANISOU 5688 N THR C 3 4710 4744 3271 54 -748 -326
ATOM 5689 CA THR C 3 -9.320 1.768 5.630 1.00 32.64
ANISOU 5689 CA THR C 3 4676 4561 3163 95 -731 -241
                                                                                                         Ν
                                                                                                           Ν
                                                                                                          C
                                                                                                             C
C
                                                                                                            C
                                                                                                         0
                                                                                                            0
                                                                                                             C
ATOM 5694 CG2 THR C 3 -9.265 1.839 3.115 1.00 34.42 ANISOU 5694 CG2 THR C 3 4695 4864 3517 -12 -733 -2
                                                4695 4864 3517 -12 -733 -237
                                                                                                             C
ATOM 5695 H THR C 3 -7.442 1.391 5.160 1.00 40.19
ATOM 5696 HA THR C 3 -9.712 2.655 5.609 1.00 39.16
ATOM 5697 HB THR C 3 -10.676 0.937 4.312 1.00 41.10
ATOM 5698 HG1 THR C 3 -8.252 -0.159 4.333 1.00 43.52
ATOM 5699 HG21 THR C 3 -9.519 1.369 2.305 1.00 41.30
ATOM 5700 HG22 THR C 3 -9.684 2.714 3.116 1.00 41.30
ATOM 5701 HG23 THR C 3 -8.302 1.951 3.125 1.00 41.30
ATOM 5702 N ASP C 4 -11.140 1.367 7.194 1.00 25.70
                                                                                                        Н
                                                                                                       Н
                                                                                                         Н
                                                                                                           Н
ANISOU 5702 N ASP C 4 4101 3547 2115 196 -693 -65
ATOM 5703 CA ASP C 4 -11.835 0.708 8.296 1.00 23.97
ANISOU 5703 CA ASP C 4 -11.833 0.708 8.290 1.00 23.97
ANISOU 5703 CA ASP C 4 4079 3267 1762 244 -654 71
ATOM 5704 C ASP C 4 -13.329 0.553 8.022 1.00 20.85
ANISOU 5704 C ASP C 4 3646 2823 1454 189 -539 274
                                                                                                           C
                                                                                                          C
                                                                                                          C
ATOM 5705 O ASP C 4 -14.122 0.479 8.967 1.00 21.84
                                                                                                          0
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ANISOU 5705 O ASP C 4
ATOM 5706 CB ASP C 4
                              3834 2938 1527 195 -356 417
                                                                      0
                             -11.640 1.484 9.605 1.00 26.63
ANISOU 5706 CB ASP C 4
                                                                      C
                             4548 3631 1940 301 -533
                                                               24
ATOM 5707 CG ASP C 4 -12.044 2.940 9.487 1.00 28.54
ANISOU 5707 CG ASP C 4 4808 3887 2149 317 -406 -33
                                                                      C
ATOM 5708 OD1 ASP C 4 -12.723 3.295 8.502 1.00 28.41
ANISOU 5708 OD1 ASP C 4 4665 3858 2274 282 -364
                                                                23
ATOM 5709 OD2 ASP C 4
                              -11.679 3.730 10.379 1.00 30.78
                                                                      0
ANISOU 5709 OD2 ASP C 4 5179 4172 2344 351 -344 -133
                                                                       0
ATOM 5710 H ASP C 4 -11.604 1.978 6.805 1.00 30.84
                                                                    Н
ATOM 5711 HA ASP C 4
                              -11.461 -0.178 8.416 1.00 28.77
                                                                     Н
ATOM 5712 HB2 ASP C 4 -12.183 1.077 10.298 1.00 31.96 ATOM 5713 HB3 ASP C 4 -10.703 1.452 9.856 1.00 31.96
                              -12.183 1.077 10.298 1.00 31.96
                                                                     Н
                                                                     Н
ATOM 5714 N TYR C 5
                             -13.736 0.496 6.752 1.00 18.68
                                                                    Ν
ANISOU 5714 N TYR C 5
ATOM 5715 CA TYR C 5
                              3191 2537 1369 117 -605 292
                                                                     Ν
                              -15.143 0.349 6.416 1.00 18.97
ANISOU 5715 CA TYR C 5
                             3069 2548 1593
                                                  34 -501
                                                              476
                             -15.308 -0.525 5.183 1.00 18.62
ATOM 5716 C TYR C 5
ANISOU 5716 C TYR C 5
ATOM 5717 O TYR C 5
                             2926 2447 1701 -61 -708 489
                                                                     C
                             -14.585 -0.372 4.194 1.00 17.37
                                                                    0
ANISOU 5717 O TYR C 5
ATOM 5718 CB TYR C 5
                            2748 2320 1533 -40 -857
                                                                     0
                                                             344
                            -15.807 1.707 6.168 1.00 19.14
ANISOU 5718 CB TYR C 5 2952 2625 1694 75 -337 483 ATOM 5719 CG TYR C 5 -17.310 1.632 6.203 1.00 20.79
                                                                      C
ANISOU 5719 CG TYR C 5
ATOM 5720 CD1 TYR C 5
                                                                      C
                             2967 2853 2080 34 -184 684
                                                                     30000
                              -17.988 1.580 7.411 1.00 23.55
ANISOU 5720 CD1 TYR C 5
                             3336 3241 2373 68 57 809
ATOM 5721 CD2 TYR C 5
                              -18.053 1.610 5.033 1.00 21.19
ANISOU 5721 CD2 TYR C 5 2797 2911 2343 -36 -282 751
                              -19.364 1.508 7.453 1.00 25.89
ATOM 5722 CE1 TYR C 5
ANISOU 5722 CE1 TYR C 5
                             3390 3601 2846 26 223 1002
                                                                      C
                              -19.435 1.542 5.065 1.00 23.22
                                                                     C
ATOM 5723 CE2 TYR C 5
ANISOU 5723 CE2 TYR C 5
                             2816 3217 2790 -78 -163 936
                                                                      C
ATOM 5724 CZ TYR C 5
ANISOU 5724 CZ TYR C 5
                             -20.082 1.493 6.282 1.00 26.22
                                                                     C
                             3173 3654 3136 -50 102 1063
                                                                      C
ATOM 5725 OH TYR C 5
                              -21.455 1.419 6.330 1.00 29.58
                                                                     0
ANISOU 5725 OH TYR C 5
                             3302 4174 3764 -97 247 1256
                                                                      0
ATOM 5726 H TYR C 5
ATOM 5727 HA TYR C 5
                             -13.213 0.540 6.071 1.00 22.41
                                                                    Н
                              -15.602 -0.081 7.155 1.00 22.77
                                                                     Η
ATOM 5727 HA TYR C 5 -15.502 -0.061 7.133 1.00 22.77
ATOM 5728 HB2 TYR C 5 -15.522 2.329 6.855 1.00 22.97
ATOM 5729 HB3 TYR C 5 -15.543 2.033 5.294 1.00 22.97
ATOM 5730 HD1 TYR C 5 -17.506 1.591 8.206 1.00 28.26
ATOM 5731 HD2 TYR C 5 -17.615 1.646 4.213 1.00 25.43
                                                                     Н
                                                                     Н
                                                                     Н
                                                                     Н
ATOM 5732 HE1 TYR C 5
ATOM 5733 HE2 TYR C 5
                              -19.805 1.474 8.272 1.00 31.07
-19.923 1.529 4.273 1.00 27.87
                                                                     Н
                              -21.771 1.418 5.552 1.00 35.50
ATOM 5734 HH TYR C 5
                                                                     Н
                             -16.280 -1.432 5.251 1.00 20.15
ATOM 5735 N TRP C 6
                                                                    N
ANISOU 5735 N TRP C 6
                              3065 2563 2027 -178 -712 666
                                                                     N
                                                                     C
ATOM 5736 CA TRP C 6
                              -16.615 -2.338 4.155 1.00 20.50
ANISOU 5736 CA TRP C 6 3045 2519 2227 -294 -933 681
                                                                      C
ATOM 5737 C TRP C 6 -18.070 -2.099 3.791 1.00 22.02
                                                                    C
ANISOU 5737 C TRP C 6 2978 2749 2641 -417 -855 854
                                                                     C
ATOM 5738 O TRP C 6 -18.968 -2.357 4.602 1.00 23.83
                                                                    0
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ANISOU 5738 O TRP C 6 3128 2980 2948 -506 -691 1050 ATOM 5739 CB TRP C 6 -16.373 -3.795 4.559 1.00 21.87 ANISOU 5739 CB TRP C 6 3413 2517 2381 -356 -1079 730
                                                                                    0
                                                                                   C
ATOM 5740 CG TRP C 6 -16.895 -4.838 3.601 1.00 23.09
ANISOU 5740 CG TRP C 6 3544 2521 2709 -506 -1314 758
                                                                                   C
ATOM 5741 CD1 TRP C 6
                                    -17.747 -5.864 3.901 1.00 26.23
ANISOU 5741 CD1 TRP C 6 3962 2754 3251 -705 -1361
ATOM 5742 CD2 TRP C 6
                                    -16.575 -4.981 2.213 1.00 22.75
ANISOU 5742 CD2 TRP C 6 3482 2467 2694 -482 -1545 582
                                                                                   C
ATOM 5743 NE1 TRP C 6
                                    -17.979 -6.633 2.787 1.00 26.72
                                                                                   Ν
ANISOU 5743 NE1 TRP C 6 4029 2677 3447 -814 -1638
                                                                                     N
ATOM 5744 CE2 TRP C 6
                                    -17.275 -6.110 1.736 1.00 25.67
                                                                                   C
ANISOU 5744 CE2 TRP C 6 3882 2645 3227 -660 -1751
                                                                                   C
                                    -15.775 -4.261 1.322 1.00 20.87
ATOM 5745 CE3 TRP C 6
ANISOU 5745 CE3 TRP C 6 3208 2365 2357 -339 -1559
ATOM 5746 CZ2 TRP C 6
                                    -17.197 -6.532 0.412 1.00 25.67
ANISOU 5746 CZ2 TRP C 6 3908 2586 3261 -670 -2012 495
ATOM 5747 CZ3 TRP C 6
                                    -15.698 -4.688 0.008 1.00 20.85
ANISOU 5747 CZ3 TRP C 6 3184 2327 2412 -322 -1619
ATOM 5748 CH2 TRP C 6
                                    -16.406 -5.807 -0.434 1.00 23.74
ANISOU 5748 CH2 TRP C 6 3612 2500 2907 -460 -1836 279 C
                                                                            Н
ATOM 5749 H TRP C 6 -16.775 -1.545 5.945 1.00 24.18
ATOM 5749 H TRP C 6 -16.775 -1.545 5.945 1.00 24.18

ATOM 5750 HA TRP C 6 -16.064 -2.135 3.383 1.00 24.61

ATOM 5751 HB2 TRP C 6 -15.417 -3.933 4.645 1.00 26.25

H ATOM 5752 HB3 TRP C 6 -16.800 -3.949 5.416 1.00 26.25

H ATOM 5753 HD1 TRP C 6 -18.109 -6.025 4.742 1.00 31.48

ATOM 5754 HE1 TRP C 6 -18.490 -7.324 2.753 1.00 32.07

ATOM 5755 HE3 TRP C 6 -15.299 -3.515 1.608 1.00 25.05

ATOM 5756 HZ2 TRP C 6 -17.668 -7.276 0.114 1.00 30.81

ATOM 5757 HZ3 TRP C 6 -15.167 -4.217 -0.594 1.00 25.02
ATOM 5758 HH2 TRP C 6 -16.335 -6.068 -1.323 1.00 28.48
ATOM 5759 N LEUC 7 -18.294 -1.596 2.582 1.00 21.12
ANISOU 5759 N LEU C 7 2721 2688 2617 -417 -969 792
ATOM 5760 CA LEU C 7 -19.624 -1.335 2.059 1.00 22.58
ANISOU 5760 CA LEU C 7 2630 2928 3023 -507 -962 936
                                                                                 Ν
                                                                                   C
ATOM 5761 C LEU C 7
ANISOU 5761 C LEU C 7
                                  -19.959 -2.410 1.041 1.00 24.30
                                    2823 3043 3367 -672 -1261
                                                                           934
ATOM 5762 O LEUC 7
ANISOU 5762 O LEUC 7
ATOM 5763 CB LEUC 7
                                   -19.181 -2.653 0.113 1.00 22.61
                                  2750 2789 3051 -630 -1473 758
                                                                                    0
                                    -19.697 0.052 1.414 1.00 21.61
ANISOU 5763 CB LEU C 7
                                   2396 2917 2898 -374 -914 883
ATOM 5764 CG LEU C 7
                                    -21.041 0.422 0.775 1.00 23.48
ANISOU 5764 CG LEU C 7 2330 3229 3364 -414 -949 1024
ATOM 5765 CD1 LEU C 7 -22.158 0.414 1.804 1.00 25.69
ANISOU 5765 CD1 LEU C 7 2389 3577 3796 -443 -708 1218
ATOM 5766 CD2 LEU C 7 -20.976 1.761 0.094 1.00 22.97 C ANISOU 5766 CD2 LEU C 7 2231 3228 3269 -258 -941 975 C
ATOM 5769 HB2 LEU C 7 -17.667 -1.391 2.030 1.00 25.35 H
ATOM 5768 HA LEU C 7 -20.272 -1.376 2.780 1.00 27.10 H
ATOM 5769 HB2 LEU C 7 -19.507 0.717 2.094 1.00 25.93 H
ATOM 5770 HB3 LEU C 7 -19.022 0.101 0.718 1.00 25.93 H
ATOM 5771 HG LEU C 7 -21.257 -0.241 0.101 1.00 28.18 H
ATOM 5772 HD11 LEU C 7 -22.991 0.652 1.368 1.00 30.83
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ATOM 5773 HD12 LEU C
                      7
                          -22.227 -0.474 2.188 1.00 30.83
                                                           Н
ATOM 5774 HD13 LEU C
                       7
                          -21.952 1.060 2.498 1.00 30.83
                                                           Н
ATOM 5775 HD21 LEU C
                       7
                          -21.842 1.959 -0.296 1.00 27.57
ATOM 5776 HD22 LEU C
                          7
                                                           Н
ATOM 5777 HD23 LEU C
ATOM 5778 N ASNC 8
                         -21.113 -3.059 1.219 1.00 27.88
ANISOU 5778 N ASN C
                         3096 3461 4034 -867 -1278 1123
                                                            N
ATOM 5779 CA ASN C 8
                         -21.475 -4.192 0.372 1.00 32.06
ANISOU 5779 CA ASN C 8
                          3636 3848 4699 -1067 -1594 1118
ATOM 5780 C ASN C 8
                         -22.999 -4.194 0.208 1.00 36.48
                                                         C
ANISOU 5780 C ASN C 8
                         3825 4487 5548 -1262 -1603 1328
ATOM 5781 O ASN C 8
                         -23.728 -4.988 0.814 1.00 39.42
ANISOU 5781 O ASN C 8
                         4099 4794 6086 -1489 -1564 1516
ATOM 5782 CB ASN C 8
                         -20.965 -5.502 0.966 1.00 33.97
ANISOU 5782 CB ASN C 8
                         4155 3861 4891 -1168 -1678 1122
ATOM 5783 CG ASN C 8
                         -21.438 -6.709 0.200 1.00 36.78
                                                           C
ANISOU 5783 CG ASN C 8
                         4555 4012 5409 -1400 -2012 1122
ATOM 5784 OD1 ASN C
                       8
                         -21.822 -6.613 -0.961 1.00 36.94
                                                           0
ANISOU 5784 OD1 ASN C 8 4477 4065 5495 -1420 -2207 1036
ATOM 5785 ND2 ASN C 8
                          -21.410 -7.864 0.853 1.00 39.92
                                                           Ν
                       8
ANISOU 5785 ND2 ASN C
                          5147 4175 5847 -1555 -2067 1218
                         -21.697 -2.863 1.819 1.00 33.45
ATOM 5786 H ASN C 8
                                                          Н
ATOM 5787 HA ASN C 8
ATOM 5788 HB2 ASN C 8
                         -21.074 -4.078 -0.504 1.00 38.48
                                                         Н
                          -19.995 -5.499 0.953 1.00 40.76
                                                          Н
ATOM 5789 HB3 ASN C 8
                          -21.285 -5.581 1.878 1.00 40.76
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ATOM 5790 HD21 ASN C
                      8 -21.669 -8.585 0.462 1.00 47.91
                          -21.133 -7.891 1.666 1.00 47.91
ATOM 5791 HD22 ASN C 8
                                                           Н
ATOM 5792 N PHE C 9
                         -23.485 -3.300 -0.648 1.00 36.54
ANISOU 5792 N PHE C 9
                         3614 4645 5624 -1179 -1667 1308
ATOM 5793 CA PHEC 9
                         -24.913 -3.073 -0.808 1.00 40.59
ANISOU 5793 CA PHE C 9
                          3718 5292 6412 -1292 -1662 1493
ATOM 5794 C PHE C 9
                        -25.378 -3.534 -2.180 1.00 42.64
ANISOU 5794 C PHE C 9
                         4049 5469 6682 -1321 -1914 1369
                         -24.746 -3.234 -3.199 1.00 41.65
ATOM 5795 O PHE C 9
ANISOU 5795 O PHE C 9
                         4146 5312 6366 -1165 -2014 1165
ATOM 5796 CB PHE C 9
                         -25.265 -1.594 -0.620 1.00 40.53
                                                           C
ANISOU 5796 CB PHE C
                      9
                          3489 5497 6415 -1045 -1425 1542
                                                             C
ATOM 5797 CG PHE C 9
                         -26.646 -1.227 -1.117 1.00 44.34
                          3617 6113 7119 -1045 -1446 1647
                                                             C
ANISOU 5797 CG PHE C
                      9
                                                           C
ATOM 5798 CD1 PHE C 9
                          -27.710 -1.109 -0.237 1.00 47.35
                                                              C
ANISOU 5798 CD1 PHE C 9
                          3630 6652 7708 -1086 -1196 1854
ATOM 5799 CD2 PHE C 9
                          -26.877 -0.996 -2.466 1.00 45.28
ANISOU 5799 CD2 PHE C
                          3810 6204 7189 -974 -1668 1512
                                                             C
ATOM 5800 CE1 PHE C 9
                                                           C
                          -28.974 -0.771 -0.694 1.00 50.90
                                                             C
ANISOU 5800 CE1 PHE C
                          3772 7231 8335 -1048 -1216 1911
ATOM 5801 CE2 PHE C 9
                          -28.138 -0.666 -2.926 1.00 48.43
                                                             C
ANISOU 5801 CE2 PHE C 9
                          3912 6723 7766 -958 -1707 1586
ATOM 5802 CZ PHE C 9
                         -29.185 -0.549 -2.040 1.00 51.31
                                                          C
ANISOU 5802 CZ PHE C 9
                          3891 7246 8360 -990 -1499 1780
ATOM 5803 H PHE C 9 -22.997 -2.805 -1.155 1.00 43.84
ATOM 5804 HA PHE C 9 -25.393 -3.585 -0.138 1.00 48.71
ATOM 5805 HB2 PHE C 9 -25.224 -1.380 0.325 1.00 48.64
ATOM 5806 HB3 PHE C 9 -24.622 -1.055 -1.107 1.00 48.64
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ATOM 5807 HD1 PHE C 9 -27.574 -1.257 0.671 1.00 56.82 H
ATOM 5808 HD2 PHE C 9 -26.175 -1.073 -3.071 1.00 54.34 H
ATOM 5809 HE1 PHE C 9 -29.681 -0.696 -0.095 1.00 61.07 H
ATOM 5810 HE2 PHE C 9 -28.277 -0.514 -3.833 1.00 58.12 H
ATOM 5811 HZ PHE C 9 -30.033 -0.324 -2.348 1.00 61.58 H
ATOM 5812 N THR C 10 -26.503 -4.244 -2.190 1.00 45.55
ANISOU 5812 N THR C 10 4217 5824 7267 -1528 -1981 1498
ATOM 5813 CA THR C 10 -27.217 -4.605 -3.406 1.00 48.28 C
ANISOU 5813 CA THR C 10 4536 6138 7669 -1582 -2219 1420 C
ATOM 5814 C THR C 10 -28.695 -4.603 -3.051 1.00 52.34 C
ANISOU 5814 C THR C 10 4622 6799 8464 -1729 -2153 1627 C ATOM 5815 O THR C 10 -29.071 -5.137 -2.005 1.00 53.43 O
ANISOU 5815 O THR C 10 4621 6941 8740 -1910 -2000 1805 O
ATOM 5816 CB THR C 10 -26.781 -5.983 -3.934 1.00 50.32 C ANISOU 5816 CB THR C 10 5119 6141 7861 -1721 -2465 1292 ATOM 5817 OG1 THR C 10 -27.270 -6.173 -5.269 1.00 53.17 O
ANISOU 5817 OG1 THR C 10 5500 6490 8214 -1722 -2695 1171 O
ATOM 5818 CG2 THR C 10 -27.302 -7.112 -3.037 1.00 53.77
                                                                                    C
ANISOU 5818 CG2 THR C 10 5491 6454 8484 -2011 -2471 1472
ATOM 5819 H THR C 10 -26.883 -4.538 -1.476 1.00 54.66 H
ATOM 5819 H THR C 10 -20.683 -4.536 -1.476 1.00 54.66 H
ATOM 5820 HA THR C 10 -27.057 -3.940 -4.093 1.00 57.93 H
ATOM 5821 HB THR C 10 -25.812 -6.027 -3.942 1.00 60.39 H
ATOM 5822 HG1 THR C 10 -27.032 -6.925 -5.558 1.00 63.81 H
ATOM 5823 HG21 THR C 10 -27.017 -7.971 -3.386 1.00 64.52 H
ATOM 5824 HG22 THR C 10 -26.955 -7.007 -2.137 1.00 64.52 H
ATOM 5825 HG23 THR C 10 -28.271 -7.090 -3.006 1.00 64.52 H
ATOM 5826 N ASP C 11 -29.527 -3.996 -3.895 1.00 55.41 N
ATOM 5828 C ASP C 11 -31.624 -5.256 -3.983 1.00 65.88 C
ANISOU 5828 C ASP C 11 5657 8707 10666 -2071 -2420 1800
ATOM 5829 O ASP C 11 -32.638 -5.253 -4.686 1.00 68.98 O
ANISOU 5829 O ASP C 11 5809 9199 11202 -2133 -2586 1804
ATOM 5830 CB ASP C 11 -31.620 -2.760 -4.290 1.00 60.96 C
ANISOU 5830 CB ASP C 11 4824 8402 9936 -1533 -2208 1754
ATOM 5831 CG ASP C 11 -31.617 -2.886 -5.800 1.00 61.37
ANISOU 5831 CG ASP C 11 5055 8385 9877 -1512 -2543 1579
ATOM 5832 OD1 ASP C 11 -30.822 -3.689 -6.334 1.00 60.04 O
ANISOU 5832 OD1 ASP C 11 5251 8016 9545 -1592 -2707 1437
ATOM 5833 OD2 ASP C 11 -32.407 -2.175 -6.456 1.00 63.63 O
ANISOU 5833 OD2 ASP C 11 5122 8828 10228 -1392 -2635 1579 O
ATOM 5834 H ASP C 11 -29.299 -3.616 -4.631 1.00 66.50 H
ATOM 5835 HA ASP C 11 -31.064 -3.831 -2.634 1.00 72.92 H
ATOM 5836 HB2 ASP C 11 -32.543 -2.700 -3.997 1.00 73.15 H
ATOM 5837 HB3 ASP C 11 -31.145 -1.947 -4.057 1.00 73.15 H
ATOM 5838 N GLY C 12 -31.056 -6.381 -3.542 1.00 67.09 N
ANISOU 5838 N GLY C 12 6072 8636 10782 -2263 -2460 1807 N
ATOM 5839 CA GLY C 12 -31.629 -7.692 -3.777 1.00 71.89 C
ANISOU 5839 CA GLY C 12 6699 9084 11531 -2575 -2680 1838
ATOM 5840 C GLY C 12 -31.650 -8.162 -5.218 1.00 72.87 C ANISOU 5840 C GLY C 12 7018 9078 11589 -2591 -3053 1637 C
ATOM 5841 O GLY C 12 -31.882 -9.353 -5.450 1.00 77.69 O
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ANISOU 5841 O GLY C 12 7750 9491 12279 -2836 -3268 1624
ATOM 5842 H GLY C 12 -30.321 -6.403 -3.095 1.00 80.50 H
ATOM 5843 HA2 GLY C 12 -31.131 -8.346 -3.262 1.00 86.27
ATOM 5844 HA3 GLY C 12 -32.544 -7.694 -3.454 1.00 86.27
ATOM 5845 N GLY C 13
                        -31.410 -7.283 -6.192 1.00 67.47
                       6391 8493 10751 -2339 -3129 1482 N
ANISOU 5845 N GLY C 13
ATOM 5846 CA GLY C 13
                         -31.581 -7.656 -7.586 1.00 65.86 C
ANISOU 5846 CA GLY C 13 6329 8219 10475 -2352 -3456 1305
ATOM 5847 C GLY C 13
                        -30.407 -8.453 -8.116 1.00 61.07
ANISOU 5847 C GLY C 13 6223 7350 9631 -2304 -3595 1100 C
ATOM 5848 O GLY C 13
                        -29.248 -8.052 -7.969 1.00 56.85
ANISOU 5848 O GLY C 13 5940 6785 8875 -2089 -3445 1004
ATOM 5849 H GLY C 13
                        -31.150 -6.473 -6.068 1.00 80.96 H
ATOM 5850 HA2 GLY C 13 -32.385 -8.190 -7.682 1.00 79.03
ATOM 5851 HA3 GLY C 13 -31.677 -6.855 -8.125 1.00 79.03
ATOM 5852 N GLY C 14
                        -30.709 -9.589 -8.737 1.00 63.62
ANISOU 5852 N GLY C 14 6681 7487 10003 -2498 -3883 1023 N
ATOM 5853 CA GLY C 14 -29.692 -10.339 -9.459 1.00 62.93
ANISOU 5853 CA GLY C 14 7058 7168 9685 -2408 -4042 794
ATOM 5854 C GLY C 14
                        -28.648 -10.938 -8.538 1.00 60.75
                                                         C
ANISOU 5854 C GLY C 14 7062 6685 9337 -2384 -3915 799
ATOM 5855 O GLY C 14 -28.952 -11.431 -7.446 1.00 62.11
                                                         0
ANISOU 5855 O GLY C 14 7135 6775 9689 -2586 -3840 986 O
ATOM 5856 H GLY C 14 -31.492 -9.945 -8.754 1.00 76.34
ATOM 5857 HA2 GLY C 14 -30.113 -11.058 -9.956 1.00 75.52
                                                       Н
ATOM 5858 HA3 GLY C 14 -29.245 -9.752 -10.089 1.00 75.52
ATOM 5859 N ILE C 15 -27.397 -10.912 -8.994 1.00 58.87
ANISOU 5859 N ILE C 15
                       7171 6374 8825 -2132 -3884 591
                                                       N
ATOM 5860 CA ILE C 15
                        -26.268 -11.471 -8.258 1.00 57.69
ANISOU 5860 CA ILE C 15 7315 6034 8573 -2051 -3795 551
                                                        С
ATOM 5861 C ILE C 15 -25.214 -10.384 -8.092 1.00 52.84
ANISOU 5861 C ILE C 15 6743 5592 7741 -1759 -3523 475
ATOM 5862 O ILE C 15
                       -24.713 -9.838 -9.083 1.00 51.25
                                                       0
ANISOU 5862 O ILE C 15 6628 5512 7334 -1552 -3496
                                                   300
ATOM 5863 CB ILE C 15 -25.667 -12.696 -8.967 1.00 60.71
ANISOU 5863 CB ILE C 15 8091 6137 8839 -2015 -4037 344 C
ATOM 5864 H ILE C 15 -27.173 -10.565 -9.748 1.00 70.65
                                                        Н
                       -26.564 -11.745 -7.376 1.00 69.23
ATOM 5865 HA ILE C 15
ATOM 5866 N VAL C 16
                        -24.878 -10.072 -6.848 1.00 50.23
ANISOU 5866 N VAL C 16 6350 5284 7451 -1760 -3320 612
ATOM 5867 CA VAL C 16 -23.764 -9.190 -6.528 1.00 45.99
ANISOU 5867 CA VAL C 16 5887 4870 6716 -1510 -3081
                                                     С
ATOM 5868 C VAL C 16
                        -22.860 -9.964 -5.580 1.00 44.24
ANISOU 5868 C VAL C 16
                       5912 4447 6452 -1497 -3067 531
ATOM 5869 O VAL C 16
                        -23.212 -10.179 -4.412 1.00 43.36
                                                         0
ANISOU 5869 O VAL C 16
                        5710 4281 6485 -1674 -3022 736
                                                         0
ATOM 5870 CB VAL C 16 -24.231 -7.866 -5.905 1.00 44.46
ANISOU 5870 CB VAL C 16 5371 4926 6596 -1495 -2859 698 C
ATOM 5871 H VAL C 16 -25.292 -10.367 -6.154 1.00 60.28
                                                     Н
ATOM 5872 HA VAL C 16 -23.266 -8.990 -7.335 1.00 55.18
ATOM 5873 N ASN C 17 -21.714 -10.410 -6.082 1.00 44.04
                                                        Н
ANISOU 5873 N ASN C 17 6185 4321 6226 -1286 -3099 308 N
ATOM 5874 CA ASN C 17 -20.781 -11.230 -5.313 1.00 44.60
                                                          C
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ANISOU 5874 CA ASN C 17 6524 4181 6239 -1218 -3129 272
ATOM 5875 C ASN C 17 -19.585 -10.360 -4.943 1.00 40.47
                                                                                 C
ANISOU 5875 C ASN C 17 6020 3829 5528 -965 -2879 172
                                                                                C
ATOM 5876 O ASN C 17 -18.702 -10.114 -5.772 1.00 39.34
ANISOU 5876 O ASN C 17 5950 3795 5201 -732 -2790 -36
ATOM 5877 CB ASN C 17 -20.359 -12.466 -6.107 1.00 47.17
ANISOU 5877 CB ASN C 17 7156 4267 6500 -1135 -3359
ATOM 5878 H ASN C 17 -21.448 -10.248 -6.884 1.00 52.84 H
ATOM 5879 HA ASN C 17 -21.210 -11.525 -4.495 1.00 53.52
ATOM 5880 N ALA C 18 -19.558 -9.906 -3.691 1.00 38.63
ANISOU 5880 N ALA C 18 5702 3638 5338 -1033 -2759
                                                                                  Ν
ATOM 5881 CA ALA C 18 -18.544 -8.987 -3.195 1.00 34.63
ANISOU 5881 CA ALA C 18 5180 3311 4668 -829 -2525
                                                                                  C
ATOM 5882 C ALA C 18 -17.569 -9.721 -2.286 1.00 33.91
                                                                                C
ANISOU 5882 C ALA C 18 5345 3042 4498 -734 -2570 2 ATOM 5883 O ALA C 18 -17.982 -10.505 -1.430 1.00 36.15
                                                                                  C
                                                                                 0
ANISOU 5883 O ALA C 18 5745 3104 4885 -925 -2729 379 ATOM 5884 CB ALA C 18 -19.189 -7.836 -2.423 1.00 33.10
                                                                                0
ANISOU 5884 CB ALA C 18 4715 3313 4549 -943 -2370 449
ATOM 5885 H ALA C 18 -20.137 -10.125 -3.094 1.00 46.36
ATOM 5886 HA ALA C 18 -18.049 -8.617 -3.942 1.00 41.56
ATOM 5887 HB1 ALA C 18 -18.492 -7.240 -2.105 1.00 39.72
                                                                                Н
ATOM 5888 HB2 ALA C 18 -19.789 -7.357 -3.015 1.00 39.72 ATOM 5889 HB3 ALA C 18 -19.683 -8.198 -1.672 1.00 39.72
                                                                                Н
                                                                                Н
ATOM 5890 N VAL C 19 -16.277 -9.456 -2.465 1.00 32.00 ANISOU 5890 N VAL C 19 5170 2911 4077 -452 -2420
                                                                               Ν
ATOM 5891 CA VAL C 19 -15.224 -10.129 -1.710 1.00 32.86
                                                                                 C
ANISOU 5891 CA VAL C 19 5505 2878 4101 -290 -2459
ATOM 5892 C VAL C 19 -14.468 -9.087 -0.896 1.00 29.13
ANISOU 5892 C VAL C 19 4912 2646 3511 -172 -2204 -62
ATOM 5893 O VAL C 19 -13.820 -8.195 -1.458 1.00 27.80
ANISOU 5893 O VAL C 19 4571 2741 3250 -38 -1986 -180 ATOM 5894 CB VAL C 19 -14.268 -10.904 -2.630 1.00 34.63
ANISOU 5894 CB VAL C 19 5877 3035 4244 -39 -2525 -281 ATOM 5895 CG1 VAL C 19 -13.139 -11.548 -1.830 1.00 35.10
ANISOU 5895 CG1 VAL C 19 6140 2965 4232 180 -2573 -357
ATOM 5896 CG2 VAL C 19
                                    -15.026 -11.966 -3.412 1.00 37.69
ANISOU 5896 CG2 VAL C 19 6417 3176 4727 -145 -2798 -281
ATOM 5897 H VAL C 19 -15.980 -8.879 -3.030 1.00 38.40
                                                                               Н
                                                                              Н
ATOM 5898 HA VAL C 19 -15.627 -10.760 -1.093 1.00 39.43
ATOM 5899 HB VAL C 19 -13.872 -10.288 -3.266 1.00 41.55
ATOM 5899 HB VAL C 19 -13.872 -10.288 -3.266 1.00 41.55

ATOM 5900 HG11 VAL C 19 -12.556 -12.028 -2.439 1.00 42.12 H

ATOM 5901 HG12 VAL C 19 -12.641 -10.853 -1.372 1.00 42.12 H

ATOM 5902 HG13 VAL C 19 -13.521 -12.163 -1.184 1.00 42.12 H

ATOM 5903 HG21 VAL C 19 -14.403 -12.440 -3.984 1.00 45.23 H

ATOM 5904 HG22 VAL C 19 -15.438 -12.583 -2.787 1.00 45.23 H
ATOM 5905 HG23 VAL C 19 -15.708 -11.534 -3.950 1.00 45.23
ATOM 5906 N ASN C 20 -14.536 -9.216 0.426 1.00 28.37
                                                                                Ν
ANISOU 5906 N ASN C 20 4921 2459 3400 -243 -2243 80
                                                                               Ν
ATOM 5907 CA ASN C 20 -13.776 -8.382 1.354 1.00 26.05
ANISOU 5907 CA ASN C 20 4558 2366 2972 -113 -2022 70
ATOM 5908 C ASN C 20 -12.348 -8.921 1.412 1.00 26.63
ANISOU 5908 C ASN C 20 4743 2417 2959 154 -2009 -123
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ATOM 5909 O ASN C 20 -12.034 -9.853 2.156 1.00 26.90 ANISOU 5909 O ASN C 20 5020 2234 2966 212 -2161 -103 0 ATOM 5910 CB ASN C 20 -14.443 -8.388 2.726 1.00 27.27 C ANISOU 5910 CB ASN C 20 4804 2457 3099 -267 -2050 342 ATOM 5911 CG ASN C 20 -13.718 -7.530 3.746 1.00 25.68 C C ANISOU 5911 CG ASN C 20 4563 2454 2741 -120 -1812 ATOM 5912 OD1 ASN C 20 -12.515 -7.268 3.635 1.00 24.42 0 **ANISOU 5912 OD1 ASN C 20** 4351 2415 2514 82 -1710 115 0 ATOM 5913 ND2 ASN C 20 -14.453 -7.099 4.767 1.00 25.69 Ν 4557 2494 2711 -233 -1669 576 N -15.031 -9.798 0.822 1.00 34.04 H **ANISOU 5913 ND2 ASN C 20** ATOM 5914 H ASN C 20 -13.750 -7.470 1.026 1.00 31.26 ATOM 5915 HA ASN C 20 Н -15.346 -8.047 2.637 1.00 32.72 -14.464 -9.297 3.061 1.00 32.72 ATOM 5916 HB2 ASN C 20 ATOM 5917 HB3 ASN C 20 Н ATOM 5918 HD21 ASN C 20 -14.096 -6.609 5.377 1.00 30.83 ATOM 5919 HD22 ASN C 20 -15.285 -7.310 4.818 1.00 30.83 Н Н -11.471 -8.329 0.610 1.00 34.47 N ATOM 5920 N GLY C 21 ANISOU 5920 N GLY C 21 3964 4963 4170 1746 -1731 -5 ATOM 5921 CA GLY C 21 -10.107 -8.794 0.507 1.00 35.74 4134 5184 4260 1906 -1724 ANISOU 5921 CA GLY C 21 -98 ATOM 5922 C GLY C 21 ANISOU 5922 C GLY C 21 -9.278 -8.405 1.715 1.00 37.99 4276 5627 4533 1841 -1636 7 ATOM 5923 O GLY C 21 ANISOU 5923 O GLY C 21 -9.724 -7.723 2.638 1.00 34.29 0 3728 5211 4089 1683 -1581 ATOM 5924 H GLY C 21 -11.648 -7.650 0.113 1.00 41.37 Н ATOM 5925 HA2 GLY C 21 -10.099 -9.761 0.426 1.00 42.88 ATOM 5926 HA3 GLY C 21 -9.694 -8.415 -0.285 1.00 42.88 Н ATOM 5927 N SER C 22 -8.033 -8.863 1.704 1.00 44.35 Ν ANISOU 5927 N SER C 22 5056 6505 5289 1982 -1635 -45 N ATOM 5928 CA SER C 22 -7.143 -8.572 2.815 1.00 47.99 ANISOU 5928 CA SER C 22 5383 7109 5743 1932 -1583 ATOM 5929 C SER C 22 ANISOU 5929 C SER C 22 -6.830 -7.082 2.835 1.00 46.45 C 5129 7079 5443 1849 -1432 10 ATOM 5930 O SER C 22 ANISOU 5930 O SER C 22 -6.609 -6.460 1.791 1.00 47.29 0 5264 7253 5449 1916 -1345 -104 ATOM 5931 CB SER C 22 -5.860 -9.399 2.711 1.00 50.91 ANISOU 5931 CB SER C 22 5720 7533 6090 2118 -1620 C ATOM 5932 OG SER C 22 ANISOU 5932 OG SER C 22 -4.824 -8.676 2.077 1.00 51.35 0 5717 7776 6019 2213 -1498 ATOM 5933 H SER C 22 -7.686 -9.338 1.077 1.00 53.22 Н ATOM 5934 HA SER C 22 -7.585 -8.800 3.648 1.00 57.59 -5.571 -9.642 3.604 1.00 61.09 -6.044 -10.199 2.195 1.00 61.09 ATOM 5935 HB2 SER C 22 Н ATOM 5936 HB3 SER C 22 Н -4.131 -9.148 2.031 1.00 61.62 ATOM 5937 HG SER C 22 Н ATOM 5938 N GLY C 23 -6.846 -6.505 4.031 1.00 43.55 Ν ANISOU 5938 N GLY C 23 4691 6769 5089 1710 -1411 111 ATOM 5939 CA GLY C 23 -6.581 -5.092 4.187 1.00 40.73 C ANISOU 5939 CA GLY C 23 4294 6546 4635 1624 -1296 ATOM 5940 C GLY C 23 ANISOU 5940 C GLY C 23 -7.499 -4.214 3.365 1.00 39.80 C 4255 6398 4468 1582 -1216 C ATOM 5941 O GLY C 23 -8.641 -3.946 3.756 1.00 38.96 0 ANISOU 5941 O GLY C 23 4196 6211 4398 1485 -1222 68 0 ATOM 5942 H GLY C 23 -7.009 -6.917 4.768 1.00 52.27 Н

ATOM 5943 HA2 GLY C 23 -6.684 -4.849 5.120 1.00 48.87 H ATOM 5944 HA3 GLY C 23 -5.667 -4.907 3.922 1.00 48.87 H ATOM 5945 N GLY C 24 -7.012 -3.760 2.214 1.00 39.02 N ANISOU 5945 N GLY C 24 4164 6377 4284 1666 -1142 -86 N ATOM 5946 CA GLY C 24 -7.745 -2.781 1.438 1.00 36.18 C ANISOU 5946 CA GLY C 24 3872 6009 3865 1629 -1062 -147 C ATOM 5947 C GLY C 24 -8.287 -3.313 0.133 1.00 34.96 C ANISOU 5947 C GLY C 24 3826 5757 3702 1744 -1090 -244 C ATOM 5948 O GLY C 24 -9.019 -2.608 -0.566 1.00 33.89 O ANISOU 5948 O GLY C 24 3758 5591 3526 1722 -1042 -294 O ATOM 5949 H GLY C 24 -6.264 -4.003 1.867 1.00 46.82 H ATOM 5950 HA2 GLY C 24 -8.492 -2.454 1.963 1.00 43.41 ATOM 5951 HA3 GLY C 24 -7.163 -2.032 1.240 1.00 43.41 ATOM 5951 HA3 GLY C 24 -7.163 -2.032 1.240 1.00 43.41 H
ATOM 5952 N ASN C 25 -7.930 -4.542 -0.219 1.00 35.96 N
ANISOU 5952 N ASN C 25 3982 5824 3858 1879 -1179 -278 N
ATOM 5953 CA ASN C 25 -8.421 -5.133 -1.450 1.00 37.05 C ANISOU 5953 CA ASN C 25
ANISOU 5953 CA ASN C 25
ATOM 5954 C ASN C 25
ANISOU 5954 C ASN C 25
ATOM 5955 O ASN C 25
ATOM 5955 O ASN C 25
ANISOU 5955 O ASN C 25
ATOM 5956 CB ASN C 25 ANISOU 5958 OD1 ASN C 25 5261 6161 4727 2342 -1589 -581 O ATOM 5959 ND2 ASN C 25 -7.659 -6.658 -4.264 1.00 41.43 N ANISOU 5959 ND2 ASN C 25 5106 6334 4300 2530 -1349 -710 N ATOM 5960 H ASN C 25 -7.407 -5.050 0.237 1.00 43.15 H ATOM 5961 HA ASN C 25 -8.390 -4.468 -2.156 1.00 44.46 H ATOM 5962 HB2 ASN C 25 -6.662 -5.984 -2.103 1.00 44.46 H
ATOM 5963 HB3 ASN C 25 -7.483 -6.941 -1.136 1.00 47.27 H
ATOM 5964 HD21 ASN C 25 -7.944 -7.046 -4.977 1.00 49.71 H
ATOM 5965 HD22 ASN C 25 -7.089 -6.017 -4.322 1.00 49.71 H
ATOM 5966 N TYR C 26 -10.609 -5.485 -2.382 1.00 32.50 N
ANISOU 5966 N TYR C 26 3879 4970 3500 1956 -1394 -442 N ATOM 5967 CA TYR C 26 -11.922 -6.092 -2.476 1.00 31.46 ANISOU 5967 CA TYR C 26 3817 4637 3500 1886 -1544 -400 ATOM 5968 C TYR C 26 -12.155 -6.448 -3.935 1.00 32.51 C ANISOU 5968 C TYR C 26 4132 4652 3567 2041 -1637 -576 C ATOM 5969 O TYR C 26 -11.488 -5.929 -4.830 1.00 32.44 O ANISOU 5969 O TYR C 26 4181 4750 3395 2180 -1540 -706 O ATOM 5970 CB TYR C 26 -13.023 -5.162 -1.945 1.00 29.89 ANISOU 5970 CB TYR C 26 3546 4450 3359 1699 -1486 -277 ATOM 5971 CG TYR C 26 -13.319 -3.959 -2.825 1.00 28.66 C ANISOU 5971 CG TYR C 26 3446 4347 3096 1710 -1380 -372 C ATOM 5972 CD1 TYR C 26 -14.243 -4.040 -3.855 1.00 29.17 ANISOU 5972 CD1 TYR C 26 3623 4283 3179 1738 -1470 -441 ATOM 5973 CD2 TYR C 26 -12.684 -2.744 -2.612 1.00 27.34 ANISOU 5973 CD2 TYR C 26 3222 4350 2816 1689 -1208 -386 C ATOM 5974 CE1 TYR C 26 -14.523 -2.946 -4.654 1.00 28.06 C ANISOU 5974 CE1 TYR C 26 3534 4188 2940 1757 -1376 -518

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ATOM 5975 CE2 TYR C 26 -12.960 -1.639 -3.408 1.00 26.92
ANISOU 5975 CE2 TYR C 26 3218 4341 2669 1703 -1114 -456 C
ATOM 5976 CZ TYR C 26 -13.881 -1.752 -4.429 1.00 26.70
ANISOU 5976 CZ TYR C 26 3299 4189 2655 1742 -1193 -520 C ATOM 5977 OH TYR C 26 -14.165 -0.670 -5.232 1.00 25.88 O
ANISOU 5977 OH TYR C 26 3248 4124 2461 1766 -1105 -582 O
ATOM 5978 H TYR C 26
                                      -10.369 -5.065 -3.093 1.00 39.00
ATOM 5979 HA TYR C 26 -11.936 -6.911 -1.955 1.00 37.75
                                                                                      Н
ATOM 5980 HB2 TYR C 26 -11.936 -6.911 -1.955 1.00 37.75 H
ATOM 5981 HB3 TYR C 26 -12.753 -4.829 -1.074 1.00 35.86 H
ATOM 5982 HD1 TYR C 26 -14.681 -4.845 -4.012 1.00 35.01 H
ATOM 5983 HD2 TYR C 26 -12.064 -2.668 -1.924 1.00 32.81 H
ATOM 5984 HE1 TYR C 26 -15.143 -3.018 -5.343 1.00 33.67 H
ATOM 5985 HE2 TYR C 26 -12.524 -0.832 -3.257 1.00 32.30 H
ATOM 5986 HH TYR C 26 -13.709 -0.006 -4.992 1.00 31.05 H
ATOM 5987 N SER C 27 -13.108 -7.343 -4.164 1.00 33.98 N
ANISOU 5987 N SER C 27 4411 4622 3877 2018 -1835 -569 N ATOM 5988 CA SER C 27 -13.425 -7.799 -5.508 1.00 35.60 C
ANISOU 5988 CA SER C 27 4832 4665 4030 2163 -1980 -751
ATOM 5989 C SER C 27 -14.932 -7.851 -5.669 1.00 35.33
ANISOU 5989 C SER C 27 4827 4451 4145 2015 -2127 -683 C ATOM 5990 O SER C 27 -15.668 -8.017 -4.695 1.00 35.11 O
ANISOU 5990 O SER C 27 4659 4403 4278 1834 -2161 -481
ATOM 5991 CB SER C 27 -12.811 -9.182 -5.797 1.00 39.55
ANISOU 5991 CB SER C 27 5480 5031 4518 2345 -2155 -861
ATOM 5992 OG SER C 27 -11.397 -9.113 -5.808 1.00 40.72
ANISOU 5992 OG SER C 27 5592 5374 4505 2516 -2013 -920 O ATOM 5993 H SER C 27 -13.591 -7.704 -3.550 1.00 40.77 H
ATOM 5994 HA SER C 27
                                       -13.070 -7.167 -6.153 1.00 42.72
ATOM 5995 HB2 SER C 27 -13.092 -9.802 -5.107 1.00 47.46
ATOM 5996 HB3 SER C 27 -13.119 -9.489 -6.664 1.00 47.46
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ATOM 5998 N VAL C 28 -15.387 -7.707 -6.912 1.00 35.96
ATOM 5998 N VAL C 28 5083 4419 4161 2400 6616
ANISOU 5998 N VAL C 28 5083 4419 4161 2102 -2212 -838 N
ATOM 5999 CA VAL C 28 -16.807 -7.747 -7.220 1.00 36.92
ANISOU 5999 CA VAL C 28 5238 4365 4426 1972 -2375 -783 C
ATOM 6000 C VAL C 28 -17.000 -8.487 -8.535 1.00 39.57
                                                                                  C
ANISOU 6000 C VAL C 28 5859 4454 4720 2131 -2618 -1002
ATOM 6001 O VAL C 28 -16.218 -8.317 -9.476 1.00 40.21 O
ANISOU 6001 O VAL C 28 6103 4585 4590 2354 -2562 -1203 ATOM 6002 CB VAL C 28 -17.411 -6.330 -7.301 1.00 34.76
ANISOU 6002 CB VAL C 28 4859 4235 4114 1871 -2201 -713
ATOM 6003 CG1 VAL C 28
                                       -18.914 -6.393 -7.125 1.00 35.51
ANISOU 6004 CG2 VAL C 28 4420 4251 3815 1798 -1938 -592
ATOM 6005 H VAL C 28 -14.885 -7.583 -7.599 1.00 43.15 H
ATOM 6006 HA VAL C 28 -17.273 -8.237 -6.524 1.00 44.31 H
ATOM 6007 HB VAL C 28 -17.227 -5.958 -8.177 1.00 41.71 H
ATOM 6008 HG11 VAL C 28 -19.276 -5.494 -7.179 1.00 42.62 H
ATOM 6009 HG12 VAL C 28 -19.291 -6.944 -7.829 1.00 42.62 H
ATOM 6010 HG13 VAL C 28 -19.115 -6.779 -6.258 1.00 42.62 H
ATOM 6011 HG21 VAL C 28 -17.169 -4.524 -6.322 1.00 39.43 H
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ATOM 6012 HG22 VAL C 28 -16.937 -5.773 -5.367 1.00 39.43
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ATOM 6015 CA ASN C 29
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ANISOU 6015 CA ASN C 29 6677 4362 5372 2126 -3185 -1149
ATOM 6016 C ASN C 29
ANISOU 6016 C ASN C 29
                          -20.014 -9.971 -9.754 1.00 43.95
                          6703 4293 5704 1892 -3369 -991
                                                              C
ATOM 6017 O ASN C 29
                          -20.585 -10.526 -8.811 1.00 44.78
ANISOU 6017 O ASN C 29
                           6651 4339 6024 1699 -3463 -780
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ATOM 6018 CB ASN C 29
                           -17.943 -11.395 -9.957 1.00 46.01
ANISOU 6018 CB ASN C 29
                          7260 4488 5732 2269 -3445 -1296
ATOM 6019 CG ASN C 29
                           -16.421 -11.443 -10.078 1.00 46.32
ANISOU 6019 CG ASN C 29
                            7378 4711 5512 2547 -3286 -1462
                                                               C
ATOM 6020 OD1 ASN C 29
                           -15.850 -11.047 -11.091 1.00 46.68
ANISOU 6020 OD1 ASN C 29
                           7611 4828 5296 2803 -3230 -1686
                            -15.761 -11.962 -9.049 1.00 47.35
ATOM 6021 ND2 ASN C 29
ANISOU 6021 ND2 ASN C 29
                           7363 4930 5699 2513 -3217 -1340
ATOM 6022 H ASN C 29
                          -18.498 -9.546 -7.895 1.00 49.36 H
ATOM 6023 HA ASN C 29
                           -18.213 -9.441 -10.582 1.00 51.83
                                                             Н
ATOM 6024 HB2 ASN C 29 -18.198 -11.909 -9.175 1.00 55.21 ATOM 6025 HB3 ASN C 29 -18.319 -11.798 -10.755 1.00 55.21
                            -18.319 -11.798 -10.755 1.00 55.21
ATOM 6026 HD21 ASN C 29
ATOM 6027 HD22 ASN C 29
                          -14.903 -12.011 -9.069 1.00 56.82
                           -16.192 -12.249 -8.362 1.00 56.82
ATOM 6028 N TRP C 30
                          -20.676 -9.351 -10.733 1.00 44.13
ANISOU 6028 N TRP C 30
                           6825 4257 5687 1913 -3414 -1071
ATOM 6029 CA TRP C 30
                           -22.115 -9.138 -10.641 1.00 44.71
ANISOU 6029 CA TRP C 30 6774 4243 5969 1689 -3541 -887
                                                                C
ATOM 6030 C TRP C 30
                          -22.780 -9.333 -11.999 1.00 47.27
                                                             C
ANISOU 6030 C TRP C 30
                          7369 4287 6303 1757 -3820 -1056
ATOM 6031 O TRP C 30
                          -22.129 -9.295 -13.047 1.00 47.58
ANISOU 6031 O TRP C 30
                          7679 4267 6134 2005 -3833 -1316
ATOM 6032 CB TRP C 30
                          -22.422 -7.739 -10.096 1.00 41.87
ANISOU 6032 CB TRP C 30 6143 4207 5560 1590 -3224 -711
                                                                C
ATOM 6033 CG TRP C 30
                           -22.152 -6.614 -11.067 1.00 40.77
                                                                C
ANISOU 6033 CG TRP C 30
                          6106 4179 5204 1738 -3062 -870
ATOM 6034 CD1 TRP C 30
                           -23.070 -5.977 -11.855 1.00 41.03
ANISOU 6034 CD1 TRP C 30 ATOM 6035 CD2 TRP C 30
                           6179 4164 5245 1714 -3124 -877
                           -20.889 -5.991 -11.341 1.00 38.87
ANISOU 6035 CD2 TRP C 30
                           5930 4124 4716 1932 -2813 -1024
ATOM 6036 NE1 TRP C 30
                           -22.458 -4.997 -12.601 1.00 39.76
ANISOU 6036 NE1 TRP C 30
                           6117 4136 4852 1885 -2926 -1028
ATOM 6037 CE2 TRP C 30
                           -21.121 -4.984 -12.304 1.00 38.50
ANISOU 6037 CE2 TRP C 30
                            5967 4124 4536 2017 -2731 -1114
                                                               C
ATOM 6038 CE3 TRP C 30
                           -19.589 -6.177 -10.862 1.00 38.18
ANISOU 6038 CE3 TRP C 30
                           5822 4175 4509 2039 -2655 -1075
ATOM 6039 CZ2 TRP C 30
                           -20.102 -4.176 -12.799 1.00 36.98
ANISOU 6039 CZ2 TRP C 30
                           5836 4110 4104 2204 -2493 -1242
ATOM 6040 CZ3 TRP C 30
                           -18.576 -5.368 -11.356 1.00 36.71
ANISOU 6040 CZ3 TRP C 30
                           5684 4179 4086 2217 -2422 -1201
ATOM 6041 CH2 TRP C 30
                           -18.841 -4.379 -12.312 1.00 36.23
ANISOU 6041 CH2 TRP C 30 5701 4160 3903 2296 -2340 -1277
ATOM 6042 H TRP C 30 -20.316 -9.047 -11.453 1.00 52.96
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ATOM 6043 HA TRP C 30 -22.491 -9.788 -10.027 1.00 53.65
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ATOM 6044 HB2 TRP C 30 -23.361 -7.700 -9.855 1.00 50.25 H ATOM 6045 HB3 TRP C 30 -21.876 -7.586 -9.309 1.00 50.25 H
                                      -23.978 -6.179 -11.884 1.00 49.23 H

-22.850 -4.479 -13.165 1.00 47.71 H

-19.408 -6.829 -10.224 1.00 45.82 H

-20.274 -3.518 -13.435 1.00 44.37 H

-17.706 -5.484 -11.048 1.00 44.05 H
ATOM 6046 HD1 TRP C 30
ATOM 6047 HE1 TRP C 30
ATOM 6048 HE3 TRP C 30
ATOM 6049 HZ2 TRP C 30
ATOM 6050 HZ3 TRP C 30
ATOM 6051 HH2 TRP C 30 -18.142 -3.855 -12.629 1.00 43.47
                                    -24.100 -9.535 -11.961 1.00 49.62
ATOM 6052 N SER C 31
ANISOU 6052 N SER C 31
                                    7587 4422 6842 1545 -4042 -890 N
ATOM 6053 CA SER C 31
                                     -24.870 -9.765 -13.175 1.00 54.74
ANISOU 6053 CA SER C 31 8482 4771 7546 1574 -4354 -1015 C
ATOM 6054 C SER C 31
                                    -26.351 -9.500 -12.924 1.00 62.71
ANISOU 6054 C SER C 31 9265 5756 8803 1308 -4470 -750 ATOM 6055 O SER C 31 -26.880 -9.847 -11.864 1.00 59.47
ANISOU 6055 O SER C 31 8599 5390 8608 1090 -4484 -485 ATOM 6056 CB SER C 31 -24.672 -11.198 -13.687 1.00 56.06
ANISOU 6056 CB SER C 31 9016 4483 7803 1667 -4795 -1218
ATOM 6057 H SER C 31
                                    -24.570 -9.543 -11.241 1.00 59.54 H
ATOM 6059 N ASN C 32 -27.010 -8.894 -13.864 1.00 65.69 N ASN C 32 10937 7475 10074.36 N
ANISOU 6059 N ASN C 32 10837 7175 10242 1344 -4549 -813 N ATOM 6060 CA ASN C 32 -28.455 -8.654 -13.889 1.00 83.45 C
ANISOU 6060 CA ASN C 32 11798 8289 11618 1120 -4697 -581 C
ATOM 6061 C ASN C 32
ANISOU 6061 C ASN C 32
                                     -28.891 -8.031 -12.566 1.00 84.87 C
                                   11549 8819 11878 943 -4415 -263 C
ATOM 6062 O ASN C 32
                                     -29.962 -8.331 -12.034 1.00 86.86
ANISOU 6062 O ASN C 32 11581 9033 12387 724 -4551 2
                                                                                    0
ATOM 6063 CB ASN C 32 -29.226 -9.947 -14.159 1.00 89.42 C
ANISOU 6063 CB ASN C 32 12696 8607 12673 967 -5182 -531 C
                                     -26.631 -8.607 -14.634 1.00 89.23 H
ATOM 6064 H ASN C 32
ATOM 6065 HA ASN C 32 -28.678 -8.027 -14.595 1.00100.13
ATOM 6066 N THR C 33 -28.059 -7.139 -12.040 1.00 82.53
ANISOU 6066 N THR C 33 11139 8862 11357 1053 -4021 -284
                                   11139 8862 11357 1053 -4021 -284
ATOM 6067 CA THR C 33 -28.307 -6.545 -10.737 1.00 79.70
ANISOU 6067 CA THR C 33 10426 8835 11023 945 -3738 -16 C
ATOM 6068 C THR C 33 -29.487 -5.580 -10.802 1.00 75.15 C ANISOU 6068 C THR C 33 9644 8425 10483 872 -3673 159 C
ATOM 6069 O THR C 33 -30.105 -5.367 -11.848 1.00 78.52
                                                                               0
ANISOU 6069 O THR C 33 10189 8714 10929 884 -3851
ATOM 6070 CB THR C 33 -27.063 -5.808 -10.246 1.00 78.07 C ANISOU 6070 CB THR C 33 10196 8903 10563 1087 -3373 -102 C
ATOM 6071 OG1 THR C 33 -26.765 -4.721 -11.134 1.00 76.84
ANISOU 6071 OG1 THR C 33
                                      10162 8840 10195 1228 -3229 -269
ANISOU 6071 OGT THR C 33 10162 8840 10193 1228 -3229 -269 O ATOM 6072 CG2 THR C 33 -25.874 -6.748 -10.189 1.00 78.86 C ANISOU 6072 CG2 THR C 33 10480 8868 10617 1184 -3428 -270 C ATOM 6073 H THR C 33 -27.340 -6.861 -12.421 1.00 99.04 H ATOM 6074 HA THR C 33 -28.519 -7.245 -10.100 1.00 95.64 H ATOM 6075 HB THR C 33 -27.223 -5.462 -9.354 1.00 93.68 H ATOM 6076 HG1 THR C 33 -27.412 -4.185 -11.158 1.00 92.21 H ATOM 6077 HG21 THR C 33 -25.090 -6.271 -9.877 1.00 94.63 H ATOM 6078 HG22 THR C 33 -26.060 -7.481 -9.582 1.00 94.63
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ATOM 6079 HG23 THR C 33 -25.694 -7.107 -11.072 1.00 94.63 ATOM 6080 N GLY C 34 -29.815 -5.011 -9.648 1.00 66.61 ANISOU 6080 N GLY C 34 8259 7646 9403 817 -3424 396 8259 7646 9403 817 -3424 396 Ν ATOM 6081 CA GLY C 34 -30.565 -3.775 -9.597 1.00 59.96 ANISOU 6081 CA GLY C 34 7237 7063 8482 843 -3239 516 C ATOM 6082 C GLY C 34 -29.578 -2.650 -9.365 1.00 52.91 ANISOU 6082 C GLY C 34 6366 6428 7310 990 -2890 419 ATOM 6083 O GLY C 34 -28.682 -2.430 -10.185 1.00 50.84 O ANISOU 6083 O GLY C 34 6342 6074 6900 1093 -2871 178 O ATOM 6084 H GLY C 34 -29.611 -5.328 -8.875 1.00 79.93 Н ATOM 6085 HA2 GLY C 34 -31.031 -3.627 -10.434 1.00 71.95 Н ATOM 6086 HA3 GLY C 34 -31.206 -3.797 -8.869 1.00 71.95 Н -29.713 -1.948 -8.248 1.00 46.55 ATOM 6087 N SER C 35 ANISOU 6087 N SER C 35 4451 6710 6525 -38 -1724 1778 N ATOM 6088 CA SER C 35 -28.699 -1.010 -7.793 1.00 42.53 ANISOU 6088 CA SER C 35 4166 6184 5809 205 -1324 1614 ATOM 6089 C SER C 35 -27.803 -1.688 -6.768 1.00 38.46 ANISOU 6089 C SER C 35 3852 5436 5325 77 -1342 1532 ATOM 6090 O SER C 35 -28.277 -2.469 -5.937 1.00 41.14 ANISOU 6090 O SER C 35 4080 5726 5823 -163 -1448 1756 0 ATOM 6091 CB SER C 35 -29.339 0.233 -7.182 1.00 44.12 ANISOU 6091 CB SER C 35 4209 6636 5920 382 -867 1861 C ATOM 6092 OG SER C 35 -29.494 1.247 -8.158 1.00 45.24 O ANISOU 6092 OG SER C 35 4337 6921 5929 634 -744 1798 O H H ATOM 6093 H SER C 35 -30.395 -1.999 -7.727 1.00 55.86 ATOM 6094 HA SER C 35 -28.152 -0.735 -8.545 1.00 51.04 ATOM 6095 HB2 SER C 35 -30.212 -0.002 -6.829 1.00 52.95 ATOM 6096 HB3 SER C 35 -28.771 0.564 -6.469 1.00 52.95 -30.212 -0.002 -6.829 1.00 52.95 Н Н ATOM 6097 HG SER C 35 -29.847 1.927 -7.812 1.00 54.28 ATOM 6098 N PHE C 36 -26.504 -1.392 -6.836 1.00 32.44 ANISOU 6098 N PHE C 36 3365 4547 4414 232 -1246 1243 N ATOM 6099 CA PHE C 36 -25.549 -1.892 -5.855 1.00 29.00 ANISOU 6099 CA PHE C 36 3120 3916 3983 151 -1242 1162 ATOM 6100 C PHE C 36 -24.360 -0.945 -5.775 1.00 25.99 ANISOU 6100 C PHE C 36 2938 3527 3409 356 -974 962 C C ATOM 6101 O PHE C 36 -24.021 -0.261 -6.745 1.00 25.02 ANISOU 6101 O PHE C 36 2850 3484 3172 538 -905 819 0 ATOM 6102 CB PHE C 36 -25.050 -3.296 -6.211 1.00 29.43 ANISOU 6102 CB PHE C 36 3309 3714 4157 24 -1684 984 ATOM 6103 CG PHE C 36 ANISOU 6103 CG PHE C 36 -24.090 -3.311 -7.359 1.00 28.54 3376 3548 3919 240 -1806 638 ATOM 6104 CD1 PHE C 36 ANISOU 6104 CD1 PHE C 36 -24.554 -3.333 -8.659 1.00 30.32 C 3563 3849 4109 330 -1993 543 ATOM 6105 CD2 PHE C 36 ANISOU 6105 CD2 PHE C 36 -22.728 -3.278 -7.139 1.00 26.99 C 3370 3264 3620 369 -1726 ATOM 6106 CE1 PHE C 36 ANISOU 6106 CE1 PHE C 36 -23.679 -3.333 -9.718 1.00 29.75 C 3660 3774 3871 572 -2071 C ATOM 6107 CE2 PHE C 36 -21.848 -3.275 -8.194 1.00 26.70 ANISOU 6107 CE2 PHE C 36 3454 3244 3448 599 -1795 159 C ATOM 6108 CZ PHE C 36 -22.328 -3.305 -9.488 1.00 27.86 C ANISOU 6108 CZ PHE C 36 3580 3476 3530 715 -1954 63 C ATOM 6109 H PHE C 36 -26.151 -0.900 -7.447 1.00 38.93 H ATOM 6110 HA PHE C 36 -25.972 -1.929 -4.983 1.00 34.80 Н

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ATOM 6111 HB2 PHE C 36
                           -24.598 -3.674 -5.440 1.00 35.31
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ATOM 6112 HB3 PHE C 36
                           -25.810 -3.848 -6.452 1.00 35.31
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ATOM 6113 HD1 PHE C 36
                           -25.470 -3.351 -8.820 1.00 36.39
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                           -22.403 -3.256 -6.268 1.00 32.39
ATOM 6114 HD2 PHE C 36
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ATOM 6115 HE1 PHE C 36
                           -24.002 -3.353 -10.589 1.00 35.70
                                                            Н
                           -20.932 -3.258 -8.037 1.00 32.04
ATOM 6116 HE2 PHE C 36
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                          -21.734 -3.307 -10.204 1.00 33.43
ATOM 6117 HZ PHE C 36
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ATOM 6118 N AVAL C 37
                          -23.738 -0.905 -4.600 0.64 25.51
                                                            N
ANISOU 6118 N AVAL C 37
                                                            Ν
                           3003 3377 3314
                                            307 -841
ATOM 6119 N BVAL C 37
                          -23.727 -0.919 -4.608 0.36 25.46
                                                            Ν
ANISOU 6119 N BVAL C 37
                           2997 3368 3308 306 -846
                                                      977
                                                             N
ATOM 6120 CA AVAL C 37
                           -22.507 -0.154 -4.374 0.64 23.56
                                                             C
                                                              C
ANISOU 6120 CA AVAL C 37
                           2945 3085 2922 427 -664
                                                             C
ATOM 6121 CA BVAL C 37
                           -22.492 -0.168 -4.410 0.36 23.51
ANISOU 6121 CA BVAL C 37
                           2939 3078 2916 429 -670
                                                       804
                                                            C
ATOM 6122 C AVAL C 37
                          -21.643 -0.978 -3.430 0.64 22.88
                                                             C
ANISOU 6122 C AVAL C 37
                           2995 2824 2875 308 -797 755
ATOM 6123 C BVAL C 37
                          -21.633 -0.945 -3.426 0.36 22.97
ANISOU 6123 C BVAL C 37
                           3008 2837 2882 311 -789
                                                             C
ATOM 6124 O AVAL C 37
                          -22.108 -1.391 -2.363 0.64 23.82
                                                            0
ANISOU 6124 O AVAL C 37
                           3103 2908 3038
                                           171 -787
                                                             0
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ATOM 6125 O BVAL C 37
                          -22.090 -1.300 -2.335 0.36 23.73
                                                            0
ANISOU 6125 O BVAL C 37
                           3098 2904 3016 180 -764
                                                      937
                                                             0
ATOM 6126 CB AVAL C 37
                           -22.773 1.245 -3.775 0.64 22.97
ANISOU 6126 CB AVAL C 37
                           2912 3109 2706 533 -295 922
                                                             C
ATOM 6127 CB BVAL C 37
                           -22.763 1.270 -3.914 0.36 22.93
                                                             C
ANISOU 6127 CB BVAL C 37
                            2902 3111 2702 544 -302 910
ATOM 6128 CG1AVAL C 37
                           -21.463 1.997 -3.580 0.64 21.48
                                                             C
ANISOU 6128 CG1AVAL C 37
                            2929 2835 2399 594 -187 758
ATOM 6129 CG1BVAL C 37
                           -23.612 1.262 -2.645 0.36 24.21
                            3025 3318 2857 479 -151 1151
ANISOU 6129 CG1BVAL C 37
                                                             C
                                                             C
ATOM 6130 CG2AVAL C 37
                           -23.724 2.070 -4.646 0.64 23.53
ANISOU 6130 CG2AVAL C 37
                            2844 3353 2745 679 -159 1014
                                                             C
                           -21.453 2.018 -3.687 0.36 21.49
                                                             C
ATOM 6131 CG2BVAL C 37
ANISOU 6131 CG2BVAL C 37
                            2924 2842 2400 602 -190
                                                              C
ATOM 6132 H AVAL C 37
                          -24.019 -1.316 -3.899 0.64 30.62
                                                            Н
ATOM 6133 H BVAL C 37
                          -23.996 -1.335 -3.905 0.36 30.55
                                                            Н
ATOM 6134 HA AVAL C 37
                           -22.033 -0.046 -5.213 0.64 28.27
                                                            Н
ATOM 6135 HA BVAL C 37
                           -22.014 -0.112 -5.252 0.36 28.21
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ATOM 6136 HB AVAL C 37
                           -23.185 1.139 -2.904 0.64 27.56
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ATOM 6137 HB BVAL C 37
                           -23.259 1.746 -4.597 0.36 27.52
                                                            Н
ATOM 6138 HG11AVAL C 37
                           -21.653 2.870 -3.204 0.64 25.78
                                                             Н
ATOM 6139 HG11BVAL C 37
                            -23.763 2.177 -2.361 0.36 29.05
                                                             Н
                            -20.897 1.492 -2.975 0.64 25.78
                                                             Н
ATOM 6140 HG12AVAL C 37
                            -24.459 0.830 -2.836 0.36 29.05
ATOM 6141 HG12BVAL C 37
ATOM 6142 HG13AVAL C 37
                            -21.024 2.095 -4.440 0.64 25.78
                                                             Н
ATOM 6143 HG13BVAL C 37
                            -23.140 0.774 -1.953 0.36 29.05
                                                             Н
ATOM 6144 HG21AVAL C 37
                            -23.980 1.543 -5.419 0.64 28.24
                                                             Н
ATOM 6145 HG21BVAL C 37
                            -20.713 1.430 -3.903 0.36 25.79
ATOM 6146 HG22AVAL C 37
                            -24.510 2.298 -4.125 0.64 28.24
                                                             Н
                            -21.433 2.800 -4.260 0.36 25.79
ATOM 6147 HG22BVAL C 37
                            -23.270 2.878 -4.931 0.64 28.24
ATOM 6148 HG23AVAL C 37
                                                             Н
ATOM 6149 HG23BVAL C 37
                          -21.401 2.287 -2.756 0.36 25.79
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ATOM 6150 N VAL C 38	-20.395 -1.227 -3.820 1.00 22.04	N
	2998 2635 2741 376 -914 533	N
	-19.481 -2.043 -3.027 1.00 22.13	Ċ
	3128 2488 2793 300 -1070 472	C
ATOM 6152 C VAL C 38		C
	3057 2357 2527 397 -961 333	C
		_
	-17.632 -0.866 -3.990 1.00 20.44	0
ANISOU 6153 O VAL C 38		0
	-19.332 -3.464 -3.614 1.00 23.46	C
ANISOU 6154 CB VAL C 38		C
	-18.352 -4.270 -2.789 1.00 24.17	C
	3539 2426 3220 255 -1597 303	C
	-20.683 -4.162 -3.695 1.00 25.17	C
ANISOU 6156 CG2 VAL C 38		_
ATOM 6157 HA VAL C 38		Н
ATOM 6158 HB VAL C 38		Н
ATOM 6159 HG11 VAL C 38	-18.272 -5.157 -3.173 1.00 29.01	Н
	-17.490 -3.826 -2.799 1.00 29.01	Н
ATOM 6161 HG13 VAL C 38	-18.683 -4.332 -1.879 1.00 29.01	Н
ATOM 6162 HG21 VAL C 38	-20.558 -5.049 -4.067 1.00 30.20	Н
ATOM 6163 HG22 VAL C 38	-21.059 -4.226 -2.804 1.00 30.20	Н
ATOM 6164 HG23 VAL C 38	-21.272 -3.644 -4.266 1.00 30.20	Н
	-17.494 -1.380 -1.806 1.00 20.79	N
	3150 2263 2485 310 -948 367	N
	-16.137 -0.881 -1.732 1.00 20.22	C
ANISOU 6166 CA GLY C 39		C
	-15.612 -0.837 -0.318 1.00 20.88	C
	3343 2205 2383 235 -927 318	C
	-16.337 -1.048 0.661 1.00 21.00	o
	3440 2163 2377 139 -900 452	o
	-17.822 -1.666 -1.064 1.00 24.94	Н
	-15.555 -1.452 -2.257 1.00 24.26	"н
	-16.102 0.015 -2.101 1.00 24.26	H
	-14.311 -0.572 -0.244 1.00 20.42	
ATOM 6172 N LYS C 40		N
ANISOU 6172 N LYS C 40	3292 2167 2301 245 -975 236	N
ATOM 6173 CA LYS C 40	-13.592 -0.345 0.997 1.00 20.91	C
	3486 2160 2297 129 -1017 270	C
ATOM 6174 C LYS C 40	-13.350 1.145 1.165 1.00 20.86	C
	3570 2177 2179 74 -845 280	C
ATOM 6175 O LYS C 40	-13.181 1.885 0.191 1.00 20.43	0
ANISOU 6175 O LYS C 40	3421 2209 2134 126 -740 253	0
ATOM 6176 CB LYS C 40	-12.248 -1.069 0.996 1.00 22.66	С
ANISOU 6176 CB LYS C 40	3631 2392 2588 162 -1234 197	С
ATOM 6177 CG LYS C 40	-12.321 -2.577 1.164 1.00 24.60	С
ANISOU 6177 CG LYS C 40	3882 2531 2934 212 -1461 186	С
ATOM 6178 CD LYS C 40	-12.334 -2.968 2.625 1.00 24.77	C
ANISOU 6178 CD LYS C 40	4067 2429 2913 75 -1559 296	С
ATOM 6179 CE LYS C 40	-12.356 -4.478 2.794 1.00 24.99	С
ANISOU 6179 CE LYS C 40	4121 2313 3061 111 -1812 316	С
ATOM 6180 NZ LYS C 40	-11.024 -5.135 2.607 1.00 25.24	N
ANISOU 6180 NZ LYS C 40	4087 2347 3157 251 -2023 215	N
ATOM 6181 H LYS C 40	-13.804 -0.518 -0.936 1.00 24.51	Η
ATOM 6182 HA LYS C 40		 H
0.02 11/1 2100 40	3.331 111 13 1100 20100	••

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ATOM 6183 HB2 LYS C 40
                           -11.803 -0.892 0.152 1.00 27.19
                                                              Н
                           -11.711 -0.721 1.725 1.00 27.19
-13.137 -2.905 0.753 1.00 29.52
ATOM 6184 HB3 LYS C 40
                                                              Н
ATOM 6185 HG2 LYS C 40
                                                              Н
                           -11.547 -2.984 0.746 1.00 29.52

-11.535 -2.625 3.056 1.00 29.72

-13.127 -2.603 3.048 1.00 29.72

-12.666 -4.687 3.689 1.00 29.99

-12.966 -4.855 2.140 1.00 29.99

-11.100 -6.014 2.717 1.00 30.29
ATOM 6186 HG3 LYS C 40
                                                              Н
ATOM 6187 HD2 LYS C 40
                                                              Н
ATOM 6188 HD3 LYS C 40
                                                              Н
ATOM 6189 HE2 LYS C 40
                                                              Н
ATOM 6190 HE3 LYS C 40
                                                              Н
ATOM 6191 HZ1 LYS C 40
                                                              Н
                           -10.717 -4.971 1.787 1.00 30.29
ATOM 6192 HZ2 LYS C 40
                           -10.443 -4.818 3.202 1.00 30.29
ATOM 6193 HZ3 LYS C 40
                          -13.316 1.578 2.410 1.00 21.52
ATOM 6194 N GLY C 41
                           3867 2165 2143 -29 -837 323
ANISOU 6194 N GLY C 41
                                                             Ν
ATOM 6195 CA GLY C 41
                           -12.994 2.954 2.662 1.00 22.33
                                                              C
                                                              C
ANISOU 6195 CA GLY C 41 4128 2219 2139 -94 -746
                                                        309
                          -12.900 3.246 4.132 1.00 24.20
ATOM 6196 C GLY C 41
                                                             C
ANISOU 6196 C GLY C 41
                                                              C
                           4658 2331 2208 -183 -799
ATOM 6197 O GLY C 41
                          -12.480 2.410 4.937 1.00 23.98
                                                             0
ANISOU 6197 O GLY C 41
                           4660 2282 2167 -237 -970
                                                              0
ATOM 6198 H GLY C 41
                          -13.473 1.103 3.110 1.00 25.82
                                                             Н
                          -12.143 3.169 2.249 1.00 26.80
ATOM 6199 HA2 GLY C 41
                                                              Н
                           -13.678 3.524 2.277 1.00 26.80
ATOM 6200 HA3 GLY C 41
                                                              Н
ATOM 6201 N TRP C 42
                          -13.307 4.451 4.479 1.00 25.48
                                                             Ν
ANISOU 6201 N TRP C 42
                           5066 2397 2217 -170 -660
                                                             Ν
ATOM 6202 CA TRP C 42
                           -13.194 4.960 5.827 1.00 27.26
                                                              C
                                                               C
ANISOU 6202 CA TRP C 42
                          5650 2485 2223 -218 -712
                          -14.591 5.137 6.392 1.00 26.64
ATOM 6203 C TRP C 42
ANISOU 6203 C TRP C 42
                           5754 2419 1951
                                            -33 -463
                                                              C
ATOM 6204 O TRP C 42
                          -15.515 5.534 5.677 1.00 26.03
ANISOU 6204 O TRP C 42
                                                              0
                           5593 2399 1899 106 -242
                                                        381
ATOM 6205 CB TRP C 42
                           -12.397 6.271 5.818 1.00 29.07
ANISOU 6205 CB TRP C 42 6075 2556 2413 -343 -803
                                                              C
                                                        205
ATOM 6206 CG TRP C 42
                                                              C
                           -10.992 6.010 5.371 1.00 29.79
ANISOU 6206 CG TRP C 42 5918 2703 2696 -535 -1045
                                                         210
                                                                C
ATOM 6207 CD1 TRP C 42
                           -9.923 5.716 6.167 1.00 32.48
                                                              C
ANISOU 6207 CD1 TRP C 42
                           6297 3016 3028 -700 -1325
                                                                C
                                                          200
ATOM 6208 CD2 TRP C 42
                            -10.516 5.945 4.024 1.00 29.24
                                                              C
ANISOU 6208 CD2 TRP C 42
                           5489 2779 2840 -547 -1018
                                                          254
ATOM 6209 NE1 TRP C 42
                            -8.807 5.491 5.400 1.00 33.00
                                                              Ν
                           6016 3215 3307 -811 -1463
ANISOU 6209 NE1 TRP C 42
                                                         249
                                                                N
ATOM 6210 CE2 TRP C 42
                            -9.145 5.628 4.079 1.00 31.15
                                                              C
ANISOU 6210 CE2 TRP C 42
                            5541 3095 3197 -708 -1264
                                                                C
                                                         282
ATOM 6211 CE3 TRP C 42
                            -11.113 6.129 2.777 1.00 26.65
                                                              C
ANISOU 6211 CE3 TRP C 42
                            4978 2552 2597 -418 -810
                                                              C
                                                         283
                                                              C
ATOM 6212 CZ2 TRP C 42
                            -8.364 5.494 2.934 1.00 31.23
                           5176 3300 3389 -717 -1271
ANISOU 6212 CZ2 TRP C 42
                                                         349
                                                                C
ATOM 6213 CZ3 TRP C 42
                           -10.336 5.996 1.643 1.00 27.21
                                                              C
ANISOU 6213 CZ3 TRP C 42
                           4717 2793 2829 -437 -834
                                                              C
                                                         331
ATOM 6214 CH2 TRP C 42 -8.979 5.682 1.727 1.00 29.24
                                                              C
ANISOU 6214 CH2 TRP C 42 4781 3144 3184 -572 -1045
                                                          367
                          -13.664 5.009 3.931 1.00 30.57
ATOM 6215 H TRP C 42
                                                             Н
ATOM 6216 HA TRP C 42 -12.720 4.317 6.376 1.00 32.71
ATOM 6217 HB2 TRP C 42 -12.806 6.897 5.200 1.00 34.88
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ATOM 6218 HB3 TRP C 42 -12.372 6.643 6.714 1.00 34.88
                                                                                                                                                                                                            Н
ATOM 6219 HD1 TRP C 42 -9.946 5.677 7.096 1.00 38.97 H
ATOM 6220 HE1 TRP C 42 -8.023 5.302 5.699 1.00 39.60 H
ATOM 6221 HE3 TRP C 42 -12.018 6.334 2.710 1.00 31.98 H
ATOM 6220 HET TRP C 42 -8.023 5.302 5.099 1.00 39.00 H
ATOM 6221 HE3 TRP C 42 -12.018 6.334 2.710 1.00 31.98 H
ATOM 6222 HZ2 TRP C 42 -7.459 5.289 2.989 1.00 37.47 H
ATOM 6223 HZ3 TRP C 42 -10.724 6.120 0.807 1.00 32.66 H
ATOM 6224 HH2 TRP C 42 -8.480 5.606 0.946 1.00 35.08 H
ATOM 6225 N THR C 43 -14.759 4.787 7.663 1.00 28.15 N
ANISOU 6225 N THR C 43 6161 2594 1941 -14 -491 375 N
ATOM 6226 CA THR C 43 -16.044 5.035 8.292 1.00 29.48
ANISOU 6226 CA THR C 43 6497 2823 1880 196 -220 463
ATOM 6227 C THR C 43 -16.343 6.534 8.346 1.00 31.39
 ANISOU 6227 C THR C 43 7061 2929 1935 345 -71 356
ANISOU 6227 C THR C 43 7061 2929 1935 345 -71 356
ATOM 6228 O THR C 43 -17.516 6.912 8.446 1.00 31.90
ANISOU 6228 O THR C 43 7107 3083 1930 579 209 407
ATOM 6229 CB THR C 43 -16.077 4.406 9.689 1.00 33.49
ANISOU 6229 CB THR C 43 7140 3372 2213 200 -267 520
ATOM 6230 OG1 THR C 43 -15.392 3.138 9.668 1.00 31.45
ANISOU 6231 CG2 THR C 43 -17.522 4.172 10.125 1.00 34.70
ANISOU 6231 CG2 THR C 43 7179 3723 2284 397 39 686 C ATOM 6232 H THR C 43 -14.166 4.417 8.165 1.00 33.78 H
ATOM 6232 H THR C 43 -14.166 4.417 8.165 1.00 33.78 H
ATOM 6233 HA THR C 43 -16.738 4.613 7.761 1.00 35.37 H
ATOM 6234 HB THR C 43 -15.651 5.000 10.327 1.00 40.19 H
ATOM 6235 HG1 THR C 43 -14.593 3.248 9.435 1.00 37.74 H
ATOM 6236 HG21 THR C 43 -17.541 3.774 11.010 1.00 41.64 H
ATOM 6237 HG22 THR C 43 -18.002 5.014 10.148 1.00 41.64 H
ATOM 6238 HG23 THR C 43 -17.963 3.574 9.501 1.00 41.64 H
ATOM 6239 N THR C 44 -15.313 7.386 8.217 1.00 32.87 N
ANISOU 6239 N THR C 44 7442 2908 2141 203 -269 207 N
ATOM 6240 CA THR C 44 -15.443 8.845 8.277 1.00 33.37 C
 ANISOU 6240 CA THR C 44 7884 2751 2044 306 -207 93 C
ATOM 6241 C THR C 44 -14.607 9.478 7.166 1.00 32.92 (ANISOU 6241 C THR C 44 7694 2575 2240 106 -346 54 ATOM 6242 O THR C 44 -13.375 9.388 7.182 1.00 32.92
                                                                                                                                                                                                             C
ANISOU 6242 O THR C 44 7641 2508 2361 -165 -633 21 O ATOM 6243 CB THR C 44 -14.985 9.385 9.646 1.00 36.58 C ANISOU 6243 CB THR C 44 8735 2949 2215 298 -370 -40 C ATOM 6244 OG1 THR C 44 -15.787 8.817 10.691 1.00 37.88 O
ANISOU 6244 OG1 THR C 44 8884 3266 2241 502 -198 18
ATOM 6245 CG2 THR C 44 -15.085 10.919 9.708 1.00 39.18
ANISOU 6245 CG2 THR C 44 -15.085 10.919 9.708 1.00 39.18 C ATOM 6246 H THR C 44 -14.502 7.128 8.090 1.00 39.45 H ATOM 6247 HA THR C 44 -16.371 9.002 9.444 1.00 (2.25)
ATOM 6246 H THR C 44 -14.502 7.128 8.090 1.00 39.45 H
ATOM 6247 HA THR C 44 -16.371 9.093 8.144 1.00 40.04 H
ATOM 6248 HB THR C 44 -14.058 9.139 9.789 1.00 43.90 H
ATOM 6249 HG1 THR C 44 -16.594 9.018 10.575 1.00 45.45 H
ATOM 6250 HG21 THR C 44 -14.793 11.236 10.577 1.00 47.01 H
ATOM 6251 HG22 THR C 44 -14.525 11.316 9.023 1.00 47.01 H
ATOM 6252 HG23 THR C 44 -16.004 11.198 9.564 1.00 47.01 H
ATOM 6253 N GLY C 45 -15.267 10.148 6.224 1.00 31.91 N
ANISOU 6253 N GLY C 45 7499 2442 2184 245 -142 89 N ATOM 6254 CA GLY C 45 -14.549 10.819 5.160 1.00 31.81 C ANISOU 6254 CA GLY C 45 7370 2332 2383 71 -241 97 C
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ATOM 6255 C GLY C 45 -13.846 12.077 5.640 1.00 34.49 ANISOU 6255 C GLY C 45 8158 2317 2629 -70 -446 -4 ATOM 6256 O GLY C 45 -14.192 12.676 6.664 1.00 37.06 ATOM 6256 O GLY C 45 -14.192 12.070 0.004 1.00 0.104 ANISOU 6256 O GLY C 45 8969 2432 2681 67 -454 -120 ATOM 6257 H GLY C 45 -16.122 10.225 6.183 1.00 38.30 -13.885 10.218 4.789 1.00 38.17 0 ATOM 6258 HA2 GLY C 45 -13.885 10.218 4.789 1.00 38.17 ATOM 6259 HA3 GLY C 45 -15.170 11.064 4.456 1.00 38.17 ATOM 6260 N SER C 46 -12.824 12.475 4.878 1.00 34.60 N
ANISOU 6260 N SER C 46 8012 2266 2867 -351 -629 53 N
ATOM 6261 CA SER C 46 -12.050 13.677 5.152 1.00 37.79 C
ANISOU 6261 CA SER C 46 8786 2314 3260 -578 -885 8 C ATOM 6262 C SER C 46 -11.922 14.470 3.858 1.00 37.94 ANISOU 6262 C SER C 46 8638 2291 3485 -659 -818 144 C ANISOU 6262 C SER C 46 6638 2291 3465 -659 -818 144 C
ATOM 6263 O SER C 46 -11.609 13.883 2.801 1.00 35.60 O
ANISOU 6263 O SER C 46 7842 2282 3401 -728 -742 287 O
ATOM 6264 CB SER C 46 -10.658 13.333 5.696 1.00 39.01 C
ANISOU 6264 CB SER C 46 8839 2481 3503 -936 -1254 14 O
ANISOU 6265 OG SER C 46 9414 2733 3975 -1164 -1500 37 ATOM 6266 H SER C 46 -12.557 12.050 4.179 1.00 41.52 H ATOM 6266 H SER C 46 -12.557 12.050 4.179 1.00 41.52 H ATOM 6267 HA SER C 46 -12.514 14.222 5.807 1.00 45.35 H ATOM 6268 HB2 SER C 46 -10.755 12.912 6.565 1.00 46.81 H ATOM 6270 HG SER C 46 -10.221 12.725 5.080 1.00 46.81 H ATOM 6271 N PRO C 47 -12.147 15.788 3.878 1.00 40.61 N ANISOU 6271 N PRO C 47 9264 2415 3751 -611 -829 108 N ATOM 6272 CA PRO C 47 9163 2441 4029 -731 -800 267 ATOM 6273 C PRO C 47 -10.416 16.705 2.347 1.00 42.54 ATOM 6273 C PRO C 47 -10.416 16.705 2.347 1.00 42.54 ATOM 6273 C PRO C 47 -10.416 16.705 2.347 1.00 42.54

ANISOU 6273 C PRO C 47 9098 2624 4442 -1177 -1094 416

ATOM 6274 O PRO C 47 -10.063 17.158 1.253 1.00 42.92

ANISOU 6274 O PRO C 47 8916 2706 4685 -1316 -1059 615

ATOM 6275 CB PRO C 47 10012 2588 4280 -548 -776 171

ATOM 6276 CG PRO C 47 10715 2758 4227 511 056 10 ANISOU 6276 CG PRO C 47 10715 2758 4327 -511 -956 -10 C ATOM 6277 CD PRO C 47 -12.566 16.640 5.011 1.00 43.97 ATOM 6277 CD PRO C 47
ANISOU 6277 CD PRO C 47
ANISOU 6277 CD PRO C 47
ATOM 6278 HA PRO C 47
ATOM 6279 HB2 PRO C 47
ATOM 6280 HB3 PRO C 47
ATOM 6281 HG2 PRO C 47
ATOM 6282 HG3 PRO C 47
ATOM 6283 HD2 PRO C 47
ATOM 6284 HD3 PRO C 47
ATOM 6285 N PHE C 48
ANISOU 6285 N PHE C 48
ANISOU 6285 N PHE C 48
ANISOU 6287 CD PRO C 47
10195 2621 3891 -447 -892 -52
C
11.961 16.176 1.902 1.00 49.37
H
-12.035 18.645 2.557 1.00 53.31
H
-11.616 18.438 4.716 1.00 56.22
H
-11.961 16.525 5.760 1.00 56.22
H
-13.482 16.442 5.260 1.00 52.76
H
ANISOU 6285 N PHE C 48
-9.544 16.291 3.265 1.00 43.60
N
-9.544 16.291 3.265 1.00 43.60
N ANISOU 6285 N PHE C 48 9242 2767 4556 -1394 -1372 359 N ATOM 6286 CA PHE C 48 -8.109 16.345 3.044 1.00 45.47 C ANISOU 6286 CA PHE C 48 9183 3072 5020 -1809 -1658 531 C ATOM 6287 C PHE C 48 -7.537 15.040 2.516 1.00 42.92 C ANISOU 6287 C PHE C 48 8368 3076 4865 -1918 -1634 667 C ATOM 6288 O PHE C 48 -6.409 15.034 2.011 1.00 44.21 O ANISOU 6288 O PHE C 48 8158 3393 5246 -2224 -1790 884 O

ATOM 6289 CB PHE C 48	-7.397 16.713 4.349 1.00 48.92 C
ANISOU 6289 CB PHE C 48	9890 3353 5345 -1980 -2014 427 C
ATOM 6290 CG PHE C 48	-7.912 17.977 4.975 1.00 52.49 C
ANISOU 6290 CG PHE C 48	10879 3466 5597 -1860 -2079 291 C
ATOM 6291 CD1 PHE C 48	-7.872 19.168 4.273 1.00 54.93 C
ANISOU 6291 CD1 PHE C 48	11264 3585 6023 -1956 -2097 390 C
ATOM 6292 CD2 PHE C 48	-8.440 17.976 6.256 1.00 53.60 C
ANISOU 6292 CD2 PHE C 48	11456 3484 5427 -1636 -2118 85 C
ATOM 6293 CE1 PHE C 48	-8.344 20.332 4.831 1.00 58.69 C
ANISOU 6293 CE1 PHE C 48	12256 3727 6316 -1832 -2179 261 C
ATOM 6294 CE2 PHE C 48	-8.913 19.143 6.823 1.00 57.36 C
ANISOU 6294 CE2 PHE C 48	12444 3650 5698 -1493 -2181 -31 C
ATOM 6295 CZ PHE C 48	-8.865 20.324 6.108 1.00 59.93 C
ANISOU 6295 CZ PHE C 48	12857 3765 6147 -1590 -2223 43 C
ATOM 6296 H PHE C 48	-9.766 15.971 4.032 1.00 52.32 H
ATOM 6297 HA PHE C 48	-7.918 17.039 2.393 1.00 54.56 H
	-7.520 15.994 4.988 1.00 58.70 H
	-6.452 16.835 4.167 1.00 58.70 H
ATOM 6300 HD1 PHE C 48	-7.522 19.181 3.412 1.00 65.92 H
	-8.473 17.182 6.739 1.00 64.32 H
ATOM 6302 HE1 PHE C 48	-8.309 21.127 4.348 1.00 70.42 H
ATOM 6303 HE2 PHE C 48	-9.265 19.133 7.684 1.00 68.83 H
ATOM 6304 HZ PHE C 48	-9.184 21.111 6.487 1.00 71.91 H
ATOM 6305 N ARG C 49	-8.286 13.948 2.601 1.00 40.27 N
ANISOU 6305 N ARG C 49	7931 2945 4424 -1617 -1418 557 N
ATOM 6306 CA ARG C 49	
ANISOU 6306 CA ARG C 49	7352 3299 4478 -1600 -1401 618 C
ATOM 6307 C ARG C 49	-7.376 12.549 0.810 1.00 41.68 C
ANISOU 6307 C ARG C 49	7092 3842 4901 -1595 -1234 826 C
	1002 00 12 1001 1000 1201 020
ATOM 6308 O ARG C 49	-8 093 13 059 -0 053 1 00 39 47 O
ATOM 6308 O ARG C 49 ANISOU 6308 O ARG C 49	-8.093 13.059 -0.053 1.00 39.47 O
ANISOU 6308 O ARG C 49	6835 3550 4613 -1445 -1003 877 O
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ANISOU 6310 CG ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ANISOU 6310 CG ARG C 49 ATOM 6311 CD ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C -9.086 9.124 2.979 1.00 31.46 C
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ANISOU 6310 CG ARG C 49 ATOM 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C -9.086 9.124 2.979 1.00 31.46 C 5921 2789 3245 -968 -1121 368 C
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ANISOU 6310 CG ARG C 49 ATOM 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ATOM 6312 NE ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C -9.086 9.124 2.979 1.00 31.46 C 5921 2789 3245 -968 -1121 368 C -8.765 9.017 4.398 1.00 34.60 N
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ANISOU 6310 CG ARG C 49 ATOM 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ATOM 6312 NE ARG C 49 ANISOU 6312 NE ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C -9.086 9.124 2.979 1.00 31.46 C 5921 2789 3245 -968 -1121 368 C -8.765 9.017 4.398 1.00 34.60 N 6613 3028 3507 -1078 -1351 282 N
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ANISOU 6310 CG ARG C 49 ATOM 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ATOM 6312 NE ARG C 49 ANISOU 6312 NE ARG C 49 ATOM 6313 CZ ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C -9.086 9.124 2.979 1.00 31.46 C 5921 2789 3245 -968 -1121 368 C -8.765 9.017 4.398 1.00 34.60 N 6613 3028 3507 -1078 -1351 282 N -9.621 9.201 5.402 1.00 35.11 C
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ANISOU 6310 CG ARG C 49 ATOM 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ATOM 6312 NE ARG C 49 ANISOU 6313 CZ ARG C 49 ANISOU 6313 CZ ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C -9.086 9.124 2.979 1.00 31.46 C 5921 2789 3245 -968 -1121 368 C -8.765 9.017 4.398 1.00 34.60 N 6613 3028 3507 -1078 -1351 282 N -9.621 9.201 5.402 1.00 35.11 C 7094 2912 3334 -953 -1299 169 C
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ATOM 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ATOM 6312 NE ARG C 49 ANISOU 6312 NE ARG C 49 ANISOU 6313 CZ ARG C 49 ANISOU 6313 CZ ARG C 49 ANISOU 6314 NH1 ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C -9.086 9.124 2.979 1.00 31.46 C 5921 2789 3245 -968 -1121 368 C -8.765 9.017 4.398 1.00 34.60 N 6613 3028 3507 -1078 -1351 282 N -9.621 9.201 5.402 1.00 35.11 C 7094 2912 3334 -953 -1299 169 C -10.901 9.501 5.183 1.00 34.49 N
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ANISOU 6310 CG ARG C 49 ATOM 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ANISOU 6312 NE ARG C 49 ANISOU 6312 NE ARG C 49 ATOM 6313 CZ ARG C 49 ANISOU 6314 NH1 ARG C 49 ANISOU 6314 NH1 ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C -9.086 9.124 2.979 1.00 31.46 C 5921 2789 3245 -968 -1121 368 C -8.765 9.017 4.398 1.00 34.60 N 6613 3028 3507 -1078 -1351 282 N -9.621 9.201 5.402 1.00 35.11 C 7094 2912 3334 -953 -1299 169 C -10.901 9.501 5.183 1.00 34.49 N 7165 2796 3145 -705 -1013 140 N
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ANISOU 6310 CG ARG C 49 ATOM 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ATOM 6312 NE ARG C 49 ANISOU 6312 NE ARG C 49 ANISOU 6313 CZ ARG C 49 ANISOU 6314 NH1 ARG C 49 ANISOU 6314 NH1 ARG C 49 ANISOU 6315 NH2 ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C -9.086 9.124 2.979 1.00 31.46 C 5921 2789 3245 -968 -1121 368 C -8.765 9.017 4.398 1.00 34.60 N 6613 3028 3507 -1078 -1351 282 N -9.621 9.201 5.402 1.00 35.11 C 7094 2912 3334 -953 -1299 169 C -10.901 9.501 5.183 1.00 34.49 N 7165 2796 3145 -705 -1013 140 N -9.185 9.069 6.643 1.00 36.25 N
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ANISOU 6310 CG ARG C 49 ATOM 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ATOM 6312 NE ARG C 49 ANISOU 6312 NE ARG C 49 ANISOU 6313 CZ ARG C 49 ANISOU 6314 NH1 ARG C 49 ANISOU 6314 NH1 ARG C 49 ANISOU 6315 NH2 ARG C 49 ANISOU 6315 NH2 ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C -9.086 9.124 2.979 1.00 31.46 C 5921 2789 3245 -968 -1121 368 C -8.765 9.017 4.398 1.00 34.60 N 6613 3028 3507 -1078 -1351 282 N -9.621 9.201 5.402 1.00 35.11 C 7094 2912 3334 -953 -1299 169 C -10.901 9.501 5.183 1.00 34.49 N 7165 2796 3145 -705 -1013 140 N -9.185 9.069 6.643 1.00 36.25 N 7495 2946 3334 -1054 -1534 100 N
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ANISOU 6310 CG ARG C 49 ATOM 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ANISOU 6312 NE ARG C 49 ANISOU 6312 NE ARG C 49 ANISOU 6313 CZ ARG C 49 ANISOU 6314 NH1 ARG C 49 ANISOU 6314 NH1 ARG C 49 ANISOU 6315 NH2 ARG C 49 ANISOU 6315 NH2 ARG C 49 ANISOU 6316 H ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C -9.086 9.124 2.979 1.00 31.46 C 5921 2789 3245 -968 -1121 368 C -8.765 9.017 4.398 1.00 34.60 N 6613 3028 3507 -1078 -1351 282 N -9.621 9.201 5.402 1.00 35.11 C 7094 2912 3334 -953 -1299 169 C -10.901 9.501 5.183 1.00 34.49 N 7165 2796 3145 -705 -1013 140 N -9.185 9.069 6.643 1.00 36.25 N 7495 2946 3334 -1054 -1534 100 N -9.113 13.935 2.837 1.00 48.32 H
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ATOM 6311 CD ARG C 49 ATOM 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ATOM 6312 NE ARG C 49 ANISOU 6312 NE ARG C 49 ANISOU 6313 CZ ARG C 49 ANISOU 6313 CZ ARG C 49 ANISOU 6314 NH1 ARG C 49 ANISOU 6315 NH2 ARG C 49 ANISOU 6315 NH2 ARG C 49 ANISOU 6316 H ARG C 49 ATOM 6316 H ARG C 49 ATOM 6317 HA ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C -9.086 9.124 2.979 1.00 31.46 C 5921 2789 3245 -968 -1121 368 C -8.765 9.017 4.398 1.00 34.60 N 6613 3028 3507 -1078 -1351 282 N -9.621 9.201 5.402 1.00 35.11 C 7094 2912 3334 -953 -1299 169 C -10.901 9.501 5.183 1.00 34.49 N 7165 2796 3145 -705 -1013 140 N -9.185 9.069 6.643 1.00 36.25 N 7495 2946 3334 -1054 -1534 100 N -9.113 13.935 2.837 1.00 48.32 H -6.913 12.519 2.800 1.00 47.78 H
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ATOM 6310 CG ARG C 49 ATOM 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ANISOU 6312 NE ARG C 49 ANISOU 6312 NE ARG C 49 ANISOU 6313 CZ ARG C 49 ANISOU 6314 NH1 ARG C 49 ATOM 6314 NH1 ARG C 49 ATOM 6315 NH2 ARG C 49 ATOM 6315 NH2 ARG C 49 ATOM 6316 H ARG C 49 ATOM 6317 HA ARG C 49 ATOM 6318 HB2 ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C -9.086 9.124 2.979 1.00 31.46 C 5921 2789 3245 -968 -1121 368 C -8.765 9.017 4.398 1.00 34.60 N 6613 3028 3507 -1078 -1351 282 N -9.621 9.201 5.402 1.00 35.11 C 7094 2912 3334 -953 -1299 169 C -10.901 9.501 5.183 1.00 34.49 N 7165 2796 3145 -705 -1013 140 N -9.185 9.069 6.643 1.00 36.25 N 7495 2946 3334 -1054 -1534 100 N -9.113 13.935 2.837 1.00 48.32 H -6.913 12.519 2.800 1.00 47.78 H -8.861 11.580 3.620 1.00 42.89 H
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ANISOU 6310 CG ARG C 49 ATOM 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ANISOU 6312 NE ARG C 49 ANISOU 6312 NE ARG C 49 ANISOU 6313 CZ ARG C 49 ATOM 6313 CZ ARG C 49 ANISOU 6314 NH1 ARG C 49 ANISOU 6315 NH2 ARG C 49 ANISOU 6315 NH2 ARG C 49 ANISOU 6316 H ARG C 49 ATOM 6316 H ARG C 49 ATOM 6317 HA ARG C 49 ATOM 6318 HB2 ARG C 49 ATOM 6319 HB3 ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C -9.086 9.124 2.979 1.00 31.46 C 5921 2789 3245 -968 -1121 368 C -8.765 9.017 4.398 1.00 34.60 N 6613 3028 3507 -1078 -1351 282 N -9.621 9.201 5.402 1.00 35.11 C 7094 2912 3334 -953 -1299 169 C -10.901 9.501 5.183 1.00 34.49 N 7165 2796 3145 -705 -1013 140 N -9.185 9.069 6.643 1.00 36.25 N 7495 2946 3334 -1054 -1534 100 N -9.113 13.935 2.837 1.00 48.32 H -6.913 12.519 2.800 1.00 47.78 H -8.861 11.580 3.620 1.00 42.89 H -9.543 11.702 2.191 1.00 42.89
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ATOM 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ATOM 6312 NE ARG C 49 ANISOU 6312 NE ARG C 49 ANISOU 6313 CZ ARG C 49 ANISOU 6313 CZ ARG C 49 ANISOU 6314 NH1 ARG C 49 ANISOU 6315 NH2 ARG C 49 ATOM 6315 NH2 ARG C 49 ATOM 6316 H ARG C 49 ATOM 6317 HA ARG C 49 ATOM 6318 HB2 ARG C 49 ATOM 6319 HB3 ARG C 49 ATOM 6319 HB3 ARG C 49 ATOM 6320 HG2 ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C -9.086 9.124 2.979 1.00 31.46 C 5921 2789 3245 -968 -1121 368 C -8.765 9.017 4.398 1.00 34.60 N 6613 3028 3507 -1078 -1351 282 N -9.621 9.201 5.402 1.00 35.11 C 7094 2912 3334 -953 -1299 169 C -10.901 9.501 5.183 1.00 34.49 N 7165 2796 3145 -705 -1013 140 N -9.185 9.069 6.643 1.00 36.25 N 7495 2946 3334 -1054 -1534 100 N -9.113 13.935 2.837 1.00 48.32 H -6.913 12.519 2.800 1.00 47.78 H -8.861 11.580 3.620 1.00 42.89 H -9.543 11.702 2.191 1.00 42.89 H -9.543 11.702 2.191 1.00 42.89 H -8.276 10.051 1.354 1.00 40.32 H
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ATOM 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ANISOU 6312 NE ARG C 49 ANISOU 6312 NE ARG C 49 ANISOU 6313 CZ ARG C 49 ANISOU 6314 NH1 ARG C 49 ANISOU 6314 NH1 ARG C 49 ANISOU 6315 NH2 ARG C 49 ATOM 6315 NH2 ARG C 49 ATOM 6316 H ARG C 49 ATOM 6317 HA ARG C 49 ATOM 6318 HB2 ARG C 49 ATOM 6319 HB3 ARG C 49 ATOM 6320 HG2 ARG C 49 ATOM 6321 HG3 ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C -9.086 9.124 2.979 1.00 31.46 C 5921 2789 3245 -968 -1121 368 C -8.765 9.017 4.398 1.00 34.60 N 6613 3028 3507 -1078 -1351 282 N -9.621 9.201 5.402 1.00 35.11 C 7094 2912 3334 -953 -1299 169 C -10.901 9.501 5.183 1.00 34.49 N 7165 2796 3145 -705 -1013 140 N -9.185 9.069 6.643 1.00 36.25 N 7495 2946 3334 -1054 -1534 100 N -9.113 13.935 2.837 1.00 48.32 H -6.913 12.519 2.800 1.00 47.78 H -8.861 11.580 3.620 1.00 42.89 H -9.543 11.702 2.191 1.00 42.89 H -9.543 11.702 2.191 1.00 42.89 H -8.276 10.051 1.354 1.00 40.32 H
ANISOU 6308 O ARG C 49 ATOM 6309 CB ARG C 49 ANISOU 6309 CB ARG C 49 ATOM 6310 CG ARG C 49 ATOM 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ANISOU 6311 CD ARG C 49 ATOM 6312 NE ARG C 49 ANISOU 6312 NE ARG C 49 ANISOU 6313 CZ ARG C 49 ANISOU 6313 CZ ARG C 49 ANISOU 6314 NH1 ARG C 49 ANISOU 6315 NH2 ARG C 49 ATOM 6315 NH2 ARG C 49 ATOM 6316 H ARG C 49 ATOM 6317 HA ARG C 49 ATOM 6318 HB2 ARG C 49 ATOM 6319 HB3 ARG C 49 ATOM 6319 HB3 ARG C 49 ATOM 6320 HG2 ARG C 49	6835 3550 4613 -1445 -1003 877 O -8.709 11.551 2.662 1.00 35.74 C 6845 2922 3814 -1265 -1210 462 C -8.227 10.176 2.314 1.00 33.60 C 6105 3010 3652 -1205 -1209 501 C -9.086 9.124 2.979 1.00 31.46 C 5921 2789 3245 -968 -1121 368 C -8.765 9.017 4.398 1.00 34.60 N 6613 3028 3507 -1078 -1351 282 N -9.621 9.201 5.402 1.00 35.11 C 7094 2912 3334 -953 -1299 169 C -10.901 9.501 5.183 1.00 34.49 N 7165 2796 3145 -705 -1013 140 N -9.185 9.069 6.643 1.00 36.25 N 7495 2946 3334 -1054 -1534 100 N -9.113 13.935 2.837 1.00 48.32 H -6.913 12.519 2.800 1.00 47.78 H -8.861 11.580 3.620 1.00 42.89 H -9.543 11.702 2.191 1.00 42.89 H -9.543 11.702 2.191 1.00 42.89 H -8.276 10.051 1.354 1.00 40.32 H

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ATOM 6324 HE ARG C 49 -7.955 8.817 4.603 1.00 41.52
ATOM 6325 HH11 ARG C 49 -11.190 9.587 4.378 1.00 41.39
ATOM 6326 HH12 ARG C 49
                                 -11.435 9.614 5.847 1.00 41.39
                                  -8.361 8.873 6.791 1.00 43.50
-9.725 9.182 7.303 1.00 43.50
ATOM 6327 HH21 ARG C 49
                                                                            Н
ATOM 6328 HH22 ARG C 49
                                                                            Н
ATOM 6329 N THR C 50 -6.254 11.895 0.527 1.00 45.99
ANISOU 6329 N THR C 50
                                7191 4688 5595 -1730 -1349
                                                                     957
ATOM 6330 CA THR C 50
                                -5.913 11.458 -0.820 1.00 48.01
ANISOU 6330 CA THR C 50 6938 5337 5967 -1618 -1158 1127
ATOM 6331 C THR C 50 -6.151 9.955 -0.876 1.00 43.45
                                                                          C
ANISOU 6331 C THR C 50 6134 5032 5341 -1315 -1066
                                                                      989
ATOM 6332 O THR C 50 -5.393 9.177 -0.284 1.00 45.46
                                                                          0
ANISOU 6332 O THR C 50 6235 5400 5636 -1367 -1250 ATOM 6333 CB THR C 50 -4.465 11.797 -1.168 1.00 54.36
ANISOU 6333 CB THR C 50 7368 6326 6960 -1936 -1328 1406
ATOM 6334 OG1 THR C 50 -4.271 13.215 -1.086 1.00 58.27
ANISOU 6334 OG1 THR C 50 8115 6503 7523 -2270 -1464 1552 O
ATOM 6335 CG2 THR C 50 -4.117 11.314 -2.580 1.00 54.80
                                                                          С
ANISOU 6335 CG2 THR C 50 6897 6847 7077 -1746 -1086 1588
ATOM 6336 H THR C 50 -5.661 11.688 1.115 1.00 55.19
ATOM 6337 HA THR C 50 -6.497 11.890 -1.463 1.00 57.61 ATOM 6338 HB THR C 50 -3.872 11.356 -0.540 1.00 65.23
ATOM 6339 HG1 THR C 50 -4.783 13.606 -1.625 1.00 69.93 ATOM 6340 HG21 THR C 50 -3.196 11.535 -2.789 1.00 65.76 ATOM 6342 HG23 THR C 50 -4.698 11.740 -3.229 1.00 65.76
                                                                           Н
ATOM 6343 N ILE C 51
ANISOU 6343 N ILE C 51
                             -7.215 9.550 -1.561 1.00 35.58
                                5138 4115 4266 -1007 -815
                                                                            N
ATOM 6344 CA ILE C 51
                              -7.525 8.135 -1.693 1.00 30.01
                                                                          C
ANISOU 6344 CA ILE C 51 4261 3610 3529 -737 -764
                                                                            C
ATOM 6345 C ILE C 51 -6.579 7.530 -2.717 1.00 30.08
ANISOU 6345 C ILE C 51 3807 3998 3623 -638 -733 886
                                                                           C
ATOM 6346 O ILE C 51 -6.345 8.107 -3.790 1.00 30.61
                                                                         0
ANISOU 6346 O ILE C 51 3681 4236 3714 -625 -591 1045 ATOM 6347 CB ILE C 51 -8.995 7.925 -2.097 1.00 26.83
                               4005 3161 3027 -476 -553 658 -9.932 8.357 -0.963 1.00 26.13
ANISOU 6347 CB ILE C 51
                                                                            C
ATOM 6348 CG1 ILE C 51
ANISOU 6348 CG1 ILE C 51 4340 2763 2825 -502 -556
ATOM 6349 CG2 ILE C 51 -9.264 6.462 -2.429 1.00 24.96
ANISOU 6349 CG2 ILE C 51 3580 3114 2790 -232 -544
ATOM 6350 CD1 ILE C 51
                                 -10.312 9.815 -1.001 1.00 28.17
ANISOU 6350 CD1 ILE C 51
                                 4878 2789 3037 -582 -478 611
ATOM 6351 H ILE C 51
                                -7.771 10.074 -1.957 1.00 42.70
                                                                         Н
ATOM 6352 HA ILE C 51
                                -7.376 7.694 -0.842 1.00 36.01
-9.185 8.463 -2.881 1.00 32.19
                                                                        Н
ATOM 6353 HB ILE C 51
ATOM 6354 HG12 ILE C 51
                                -10.749 7.837 -1.018 1.00 31.36
                                                                         Н
ATOM 6356 HG21 ILE C 51 -9.492 8.188 -0.115 1.00 31.36 H ATOM 6356 HG21 ILE C 51 -8.692 6.196 -3.166 1.00 29.95 H ATOM 6358 HG23 ILE C 51 -9.070 5.921 -1.648 1.00 29.95 H ATOM 6359 HD11 ILE C 51 -10.902 10.006 -0.255 1.00 33.81 H ATOM 6360 HD12 ILE C 51 -9.507 10.352 -0.933 1.00 33.81 H ATOM 6361 HD13 ILE C 51 -10.765 10.001 -1.838 1.00 33.81 H
ATOM 6355 HG13 ILE C 51
                               -9.492 8.188 -0.115 1.00 31.36
                                                                           Н
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ATOM 6362 N ASN C 52 -6.020 6.376 -2.379 1.00 29.21 ANISOU 6362 N ASN C 52 3528 4029 3542 -540 -861 819 ATOM 6363 CA ASN C 52 -5.181 5.616 -3.284 1.00 30.20 ANISOU 6363 CA ASN C 52 3240 4526 3707 -339 -822 888 ATOM 6364 C ASN C 52 -5.902 4.330 -3.640 1.00 28.27 ANISOU 6364 C ASN C 52 -5.902 4.330 -3.040 1.00 26.27 C ANISOU 6364 C ASN C 52 3025 4324 3393 10 -776 683 C ATOM 6365 O ASN C 52 -6.613 3.753 -2.813 1.00 26.74 O ANISOU 6365 C ASN C 52 3081 3904 3176 20 -870 534 O ATOM 6366 CB ASN C 52 -3.830 5.282 -2.650 1.00 32.63 C ANISOU 6366 CB ASN C 52 3311 4971 4117 -471 -1041 991 C ATOM 6367 CG ASN C 52 -3.068 6.513 -2.227 1.00 35.11 С ANISOU 6367 CG ASN C 52 3598 5216 4527 -880 -1166 1207 ATOM 6368 OD1 ASN C 52 -2.240 7.032 -2.975 1.00 37.42 O ANISOU 6368 OD1 ASN C 52 3548 5770 4901 -970 -1107 1456 ATOM 6369 ND2 ASN C 52 -3.350 6.996 -1.021 1.00 34.91 N ANISOU 6369 ND2 ASN C 52 3946 4834 4483 -1133 -1354 1126 N ATOM 6370 H ASN C 52 -6.117 6.006 -1.609 1.00 35.05 ATOM 6371 HA ASN C 52 -5.029 6.124 -4.096 1.00 36.23 ATOM 6372 HB2 ASN C 52 -3.975 4.734 -1.863 1.00 39.16 ATOM 6373 HB3 ASN C 52 -3.288 4.801 -3.295 1.00 39.16 Н Н Н ATOM 6374 HD21 ASN C 52 -2.943 7.697 -0.733 1.00 41.89 H
ATOM 6375 HD22 ASN C 52 -3.939 6.608 -0.530 1.00 41.89 H ATOM 6376 N TYR C 53 -5.706 3.868 -4.869 1.00 28.82 ANISOU 6376 N TYR C 53 2849 4682 3418 296 -648 689 N ATOM 6377 CA TYR C 53 -6.317 2.605 -5.231 1.00 27.66 ANISOU 6377 CA TYR C 53 2766 4534 3209 619 -672 479 ATOM 6378 C TYR C 53 -5.663 2.061 -6.489 1.00 29.47

ANISOU 6378 C TYR C 53 2708 5126 3362 967 -578 486

ATOM 6379 O TYR C 53 -4.972 2.777 -7.216 1.00 31.29

ANISOU 6379 O TYR C 53 2682 5640 3567 965 -426 682

ATOM 6380 CB TYR C 53 -7.834 2.757 -5.434 1.00 25.46 C 0 0 ANISOU 6382 CD1 TYR C 53 2763 4242 2831 568 -239 602 C ATOM 6383 CD2 TYR C 53 -8.433 2.624 -7.881 1.00 26.05 C 2676 4476 2745 1107 -344 -8.654 5.367 -8.089 1.00 26.33 ANISOU 6383 CD2 TYR C 53 ATOM 6384 CE1 TYR C 53 ANISOU 6384 CE1 TYR C 53 2750 4461 2794 692 -52 687 C ATOM 6385 CE2 TYR C 53 -8.757 3.199 -9.100 1.00 26.55 2677 4724 2688 1243 -163 -8.869 4.566 -9.200 1.00 26.61 ANISOU 6385 CE2 TYR C 53 ATOM 6386 CZ TYR C 53 ANISOU 6386 CZ TYR C 53 ATOM 6387 OH TYR C 53 2688 4716 2706 1032 -8 580 C -9.200 5.122 -10.416 1.00 27.32 0 ANISOU 6387 OH TYR C 53 2723 4991 2667 1176 167 668 ATOM 6388 H TYR C 53 -5.244 4.250 -5.485 1.00 34.58 H H ATOM 6389 HA TYR C 53 -6.172 1.966 -4.516 1.00 33.19 ATOM 6390 HB2 TYR C 53 -8.244 1.879 -5.405 1.00 30.55 H
ATOM 6391 HB3 TYR C 53 -8.191 3.311 -4.722 1.00 30.55 H
ATOM 6392 HD1 TYR C 53 -8.171 5.315 -6.131 1.00 31.06 H
ATOM 6393 HD2 TYR C 53 -8.354 1.700 -7.820 1.00 31.26 H
ATOM 6394 HE1 TYR C 53 -8.726 6.292 -8.156 1.00 31.60 H

ATOM 6396 HH TYR C 53 -9.239 5.959 -10.349 1.00 31.86 H ATOM 6397 N ASN C 54 -5.898 0.775 -6.727 1.00 29.37 N ANISOU 6397 N ASN C 54 2760 5006 2202 1077 ANISOU 6397 N ASN C 54 2760 5096 3302 1277 -678 280 N ATOM 6398 CA ASN C 54 -5.491 0.124 -7.966 1.00 33.19 C ANISOU 6400 O ASN C 54 3336 5218 3465 1934 -937 -197 O ATOM 6401 CB ASN C 54 -4.140 -0.580 -7.821 1.00 35.34 C ANISOU 6401 CB ASN C 54
ANISOU 6401 CB ASN C 54
ATOM 6402 CG ASN C 54
ANISOU 6402 CG ASN C 54
ANISOU 6402 CG ASN C 54
ATOM 6403 OD1 ASN C 54 ANISOU 6403 OD1 ASN C 54 3745 6962 4080 2448 -494 -41 O ATOM 6404 ND2 ASN C 54 -2.361 -1.279 -9.322 1.00 41.53 N ANISOU 6404 ND2 ASN C 54 3551 7687 4541 2369 -423 305 N ATOM 6405 H ASN C 54 -6.300 0.250 -6.177 1.00 35.24 H ATOM 6406 HA ASN C 54 -5.421 0.785 -8.672 1.00 39.83 H ATOM 6407 HB2 ASN C 54
ATOM 6408 HB3 ASN C 54
ATOM 6409 HD21 ASN C 54
ATOM 6410 HD22 ASN C 54 H ATOM 6411 N ALA C 55 -7.300 -0.569 -9.415 1.00 33.71 N ANISOU 6411 N ALA C 55 3478 5819 3512 2061 -591 -100 N ATOM 6412 CA ALA C 55 -8.344 -1.453 -9.927 1.00 34.93 ANISOU 6412 CA ALA C 55 3913 5759 3601 2182 -705 -341 C ATOM 6413 C ALA C 55 -7.679 -2.454 -10.864 1.00 35.91 C ANISOU 6413 C ALA C 55 4071 6014 3560 2499 -707 -505 C ATOM 6414 O ALA C 55 -7.583 -2.239 -12.072 1.00 37.87 ANISOU 6414 O ALA C 55 4291 6508 3591 2695 -562 -512 C ATOM 6415 CB ALA C 55 -9.434 -0.657 -10.637 1.00 34.28 C ANISOU 6415 CB ALA C 55 3889 5702 3434 2153 -596 -305 ATOM 6416 H ALA C 55 -7.193 0.145 -9.883 1.00 40.46 H ATOM 6417 HA ALA C 55 -8.747 -1.940 -9.191 1.00 41.92 ATOM 6418 HB1 ALA C 55 -10.111 -1.270 -10.964 1.00 41.14 Н ATOM 6419 HB2 ALA C 55 -9.830 -0.033 -10.008 1.00 41.14 ATOM 6420 HB3 ALA C 55 -9.039 -0.173 -11.379 1.00 41.14 Н Н ATOM 6421 N GLY C 56 -7.209 -3.559 -10.290 1.00 34.40 ANISOU 6421 N GLY C 56 3965 5665 3441 2566 -883 -626 N ATOM 6422 CA GLY C 56 -6.558 -4.585 -11.086 1.00 37.71 ANISOU 6422 CA GLY C 56 4459 6190 3679 2906 -918 -795 C ATOM 6423 C GLY C 56 -7.495 -5.234 -12.080 1.00 37.81 C ANISOU 6423 C GLY C 56 4763 6094 3511 3084 -1050 -1039 ATOM 6424 O GLY C 56 -7.054 -5.768 -13.101 1.00 41.28 O ANISOU 6424 O GLY C 56 5274 6718 3691 3411 -1049 -1161 O ATOM 6425 H GLY C 56 -7.256 -3.735 -9.450 1.00 41.28 H ATOM 6426 HA2 GLY C 56 -5.817 -4.192 -11.574 1.00 45.25 ATOM 6427 HA3 GLY C 56 -6.207 -5.273 -10.499 1.00 45.25 ATOM 6428 N VAL C 57 -8.791 -5.216 -11.791 1.00 35.57 N
ANISOU 6428 N VAL C 57 4646 5521 3347 2879 -1194 -1099 N
ATOM 6429 CA VAL C 57 -9.807 -5.720 -12.708 1.00 36.51 C

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ANISOU 6429 CA VAL C 57 5016 5526 3331 3002 -1364 -1309
ATOM 6430 C VALC 57
                         -10.934 -4.701 -12.760 1.00 34.16
                                                           C
ANISOU 6430 C VAL C 57
                          4665 5209 3107 2777 -1274 -1182
                                                              C
ATOM 6431 O VAL C 57
                         -11.510 -4.353 -11.721 1.00 31.41
ANISOU 6431 O VAL C 57
                          4278 4661 2993 2472 -1299 -1048
ATOM 6432 CB VAL C 57
                          -10.344 -7.099 -12.288 1.00 37.72
                                                            C
                         5466 5264 3601 2991 -1735 -1532
ANISOU 6432 CB VAL C 57
ATOM 6433 CG1 VAL C 57
                          -11.532 -7.517 -13.173 1.00 38.92
ANISOU 6433 CG1 VAL C 57
                          5870 5247 3673 3065 -1966 -1735
ATOM 6434 CG2 VAL C 57
                           -9.207 -8.135 -12.352 1.00 40.79
ANISOU 6434 CG2 VAL C 57
                           5934 5691 3872 3271 -1838 -1663
ATOM 6435 H VAL C 57
                          -9.114 -4.910 -11.055 1.00 42.68
ATOM 6436 HA VAL C 57
                          -9.426 -5.799 -13.596 1.00 43.81
ATOM 6437 HB VAL C 57
                          -10.656 -7.051 -11.371 1.00 45.26
ATOM 6438 HG11 VAL C 57
                          -11.848 -8.388 -12.885 1.00 46.71
ATOM 6439 HG12 VAL C 57
                          -12.240 -6.861 -13.081 1.00 46.71
ATOM 6440 HG13 VAL C 57
                          -11.238 -7.560 -14.096 1.00 46.71
                          -9.553 -9.001 -12.087 1.00 48.95
ATOM 6441 HG21 VAL C 57
ATOM 6442 HG22 VAL C 57
                           -8.870 -8.177 -13.261 1.00 48.95
                                                             Н
ATOM 6443 HG23 VAL C 57
                          -8.498 -7.863 -11.749 1.00 48.95
                                                             Н
ATOM 6444 N TRP C 58
                         -11.239 -4.218 -13.967 1.00 34.96
ANISOU 6444 N TRP C 58
                          4769 5538 2977 2943 -1173 -1203
                                                             Ν
ATOM 6445 CA TRP C 58
                          -12.354 -3.298 -14.202 1.00 33.50
ANISOU 6445 CA TRP C 58
                          4545 5353 2829 2784 -1095 -1091
                                                              C
ATOM 6446 C TRP C 58
                         -13.054 -3.727 -15.488 1.00 35.40
ANISOU 6446 C TRP C 58
                          4976 5616 2859 3026 -1230 -1302
                                                             C
ATOM 6447 O TRP C 58
                         -12.665 -3.318 -16.584 1.00 36.98
                                                            0
ANISOU 6447 O TRP C 58
                         5138 6146 2768 3256 -1091 -1275
                                                              0
ATOM 6448 CB TRP C 58
                         -11.888 -1.856 -14.294 1.00 34.23
                                                            C
ANISOU 6448 CB TRP C 58 4386 5749 2870 2712 -763 -811
                                                             C
ATOM 6449 CG TRP C 58
                          -13.040 -0.935 -14.495 1.00 33.62
ANISOU 6449 CG TRP C 58 4295 5657 2823 2572 -696 -690
ATOM 6450 CD1 TRP C 58
                          -13.247 -0.090 -15.546 1.00 34.90
                                                              C
ANISOU 6450 CD1 TRP C 58
                          4403 6075 2783 2686 -523 -590
ATOM 6451 CD2 TRP C 58
                          -14.174 -0.795 -13.635 1.00 32.36
                                                              C
ANISOU 6451 CD2 TRP C 58
                          4179 5230 2886 2299 -806 -628
ATOM 6452 NE1 TRP C 58
                          -14.435 0.580 -15.384 1.00 33.85
                                                             Ν
ANISOU 6452 NE1 TRP C 58
                           4276 5831 2755 2512 -518 -485
                                                              N
ATOM 6453 CE2 TRP C 58
                          -15.021 0.169 -14.214 1.00 32.16
                                                              C
ANISOU 6453 CE2 TRP C 58
                           4115 5314 2792 2272 -684 -498
ATOM 6454 CE3 TRP C 58
                          -14.550 -1.383 -12.423 1.00 31.47
                                                              C
ANISOU 6454 CE3 TRP C 58
                           4133 4824 3003 2077 -987 -637
ATOM 6455 CZ2 TRP C 58
                          -16.224 0.557 -13.625 1.00 31.21
                                                              C
ANISOU 6455 CZ2 TRP C 58
                          4004 5034 2819 2052 -729 -383
ATOM 6456 CZ3 TRP C 58
                          -15.740 -1.000 -11.841 1.00 30.39
ANISOU 6456 CZ3 TRP C 58
                          4002 4548 2995 1851 -1026 -511
                                                              C
                                                             C
ATOM 6457 CH2 TRP C 58
                          -16.565 -0.038 -12.441 1.00 30.46
ANISOU 6457 CH2 TRP C 58
                          3956 4688 2928 1853 -892 -388
                                                              C
ATOM 6458 H TRP C 58
                         -10.804 -4.415 -14.682 1.00 41.95
ATOM 6459 HA TRP C 58
                          -12.988 -3.368 -13.472 1.00 40.20
                                                           Н
ATOM 6460 HB2 TRP C 58 -11.440 -1.610 -13.469 1.00 41.07
ATOM 6461 HB3 TRP C 58 -11.285 -1.760 -15.047 1.00 41.07
                                                            Н
ATOM 6462 HD1 TRP C 58 -12.666 0.020 -16.264 1.00 41.88
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A T O L A A A O A L L A T D D O T O	
ATOM 6463 HE1 TRP C 58	-14.755 1.168 -15.924 1.00 40.62 H
ATOM 6464 HE3 TRP C 58	-14.007 -2.020 -12.017 1.00 37.77 H
ATOM 6465 HZ2 TRP C 58	-16.774 1.193 -14.022 1.00 37.45 H
ATOM 6466 HZ3 TRP C 58	-15.998 -1.383 -11.034 1.00 36.46 H
ATOM 6467 HH2 TRP C 58	-17.361 0.202 -12.024 1.00 36.55 H
ATOM 6468 N ALA C 59	-14.102 -4.531 -15.346 1.00 35.52 N
ANISOU 6468 N ALA C 59	5174 5264 3059 2936 -1520 -1446 N
ATOM 6469 CA ALA C 59	-14.825 -5.092 -16.484 1.00 38.11 C
ANISOU 6469 CA ALA C 59	5682 5488 3309 3156 -1714 -1641 C
ATOM 6470 C ALA C 59	-16.318 -4.907 -16.264 1.00 37.76 C
ANISOU 6470 C ALA C 59	5627 5242 3477 2791 -1858 -1506 C
ATOM 6471 O ALA C 59	-17.051 -5.871 -16.009 1.00 38.02 O
ANISOU 6471 O ALA C 59	5812 4930 3702 2636 -2177 -1574 O
ATOM 6472 CB ALA C 59	-14.472 -6.569 -16.682 1.00 41.36 C
ANISOU 6472 CB ALA C 59	6317 5642 3755 3340 -2016 -1843 C
ATOM 6473 H ALA C 59	-14.421 -4.771 -14.584 1.00 42.63 H
ATOM 6474 HA ALA C 59	-14.575 -4.611 -17.289 1.00 45.73 H
ATOM 6475 HB1 ALA C 59	-14.967 -6.912 -17.443 1.00 49.63 H
ATOM 6476 HB2 ALA C 59	-13.519 -6.646 -16.844 1.00 49.63 H
ATOM 6477 HB3 ALA C 59	-14.713 -7.061 -15.882 1.00 49.63 H
ATOM 6478 N PRO C 60	-16.800 -3.667 -16.330 1.00 37.86 N
ANISOU 6478 N PRO C 60	5456 5476 3454 2640 -1631 -1285 N
ATOM 6479 CA PRO C 60	-18.244 -3.434 -16.293 1.00 39.71 C
ANISOU 6479 CA PRO C 60	5657 5606 3826 2361 -1752 -1156 C
ATOM 6480 C PRO C 60	-18.883 -3.689 -17.646 1.00 45.38 C
ANISOU 6480 C PRO C 60	6488 6353 4401 2526 -1906 -1285 C
ATOM 6481 O PRO C 60	-18.297 -3.431 -18.699 1.00 47.90 O
	0000 0004 4400 0000 4775 4000 0
ANISOU 6481 O PRO C 60	6838 6894 4466 2863 -1775 -1383 O
ATOM 6482 CB PRO C 60	-18.349 -1.953 -15.909 1.00 36.49 C
ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C
ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60 ATOM 6483 CG PRO C 60	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C -17.105 -1.347 -16.496 1.00 35.80 C
ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60 ATOM 6483 CG PRO C 60	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C
ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60 ATOM 6483 CG PRO C 60 ANISOU 6483 CG PRO C 60	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C -17.105 -1.347 -16.496 1.00 35.80 C 4890 5636 3075 2519 -1156 -894 C
ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60 ATOM 6483 CG PRO C 60 ANISOU 6483 CG PRO C 60 ATOM 6484 CD PRO C 60	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C -17.105 -1.347 -16.496 1.00 35.80 C 4890 5636 3075 2519 -1156 -894 C -16.036 -2.403 -16.344 1.00 35.85 C
ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60 ATOM 6483 CG PRO C 60 ANISOU 6483 CG PRO C 60 ATOM 6484 CD PRO C 60 ANISOU 6484 CD PRO C 60	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C -17.105 -1.347 -16.496 1.00 35.80 C 4890 5636 3075 2519 -1156 -894 C -16.036 -2.403 -16.344 1.00 35.85 C 5004 5566 3051 2701 -1261 -1104 C
ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60 ATOM 6483 CG PRO C 60 ANISOU 6483 CG PRO C 60 ATOM 6484 CD PRO C 60 ANISOU 6484 CD PRO C 60 ATOM 6485 HA PRO C 60	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C -17.105 -1.347 -16.496 1.00 35.80 C 4890 5636 3075 2519 -1156 -894 C -16.036 -2.403 -16.344 1.00 35.85 C 5004 5566 3051 2701 -1261 -1104 C -18.667 -3.984 -15.616 1.00 47.66 H
ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60 ATOM 6483 CG PRO C 60 ANISOU 6483 CG PRO C 60 ATOM 6484 CD PRO C 60 ANISOU 6484 CD PRO C 60	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C -17.105 -1.347 -16.496 1.00 35.80 C 4890 5636 3075 2519 -1156 -894 C -16.036 -2.403 -16.344 1.00 35.85 C 5004 5566 3051 2701 -1261 -1104 C
ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60 ATOM 6483 CG PRO C 60 ANISOU 6483 CG PRO C 60 ATOM 6484 CD PRO C 60 ANISOU 6484 CD PRO C 60 ATOM 6485 HA PRO C 60 ATOM 6486 HB2 PRO C 60	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C -17.105 -1.347 -16.496 1.00 35.80 C 4890 5636 3075 2519 -1156 -894 C -16.036 -2.403 -16.344 1.00 35.85 C 5004 5566 3051 2701 -1261 -1104 C -18.667 -3.984 -15.616 1.00 47.66 H -19.145 -1.564 -16.304 1.00 43.79 H
ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60 ATOM 6483 CG PRO C 60 ANISOU 6483 CG PRO C 60 ATOM 6484 CD PRO C 60 ANISOU 6484 CD PRO C 60 ATOM 6485 HA PRO C 60 ATOM 6486 HB2 PRO C 60 ATOM 6487 HB3 PRO C 60	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C -17.105 -1.347 -16.496 1.00 35.80 C 4890 5636 3075 2519 -1156 -894 C -16.036 -2.403 -16.344 1.00 35.85 C 5004 5566 3051 2701 -1261 -1104 C -18.667 -3.984 -15.616 1.00 47.66 H -19.145 -1.564 -16.304 1.00 43.79 H -18.358 -1.861 -14.944 1.00 43.79
ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60 ATOM 6483 CG PRO C 60 ANISOU 6483 CG PRO C 60 ATOM 6484 CD PRO C 60 ANISOU 6484 CD PRO C 60 ATOM 6485 HA PRO C 60 ATOM 6486 HB2 PRO C 60 ATOM 6487 HB3 PRO C 60 ATOM 6488 HG2 PRO C 60	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C -17.105 -1.347 -16.496 1.00 35.80 C 4890 5636 3075 2519 -1156 -894 C -16.036 -2.403 -16.344 1.00 35.85 C 5004 5566 3051 2701 -1261 -1104 C -18.667 -3.984 -15.616 1.00 47.66 H -19.145 -1.564 -16.304 1.00 43.79 H -18.358 -1.861 -14.944 1.00 43.79 H -17.253 -1.141 -17.432 1.00 42.96
ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60 ATOM 6483 CG PRO C 60 ANISOU 6483 CG PRO C 60 ATOM 6484 CD PRO C 60 ANISOU 6484 CD PRO C 60 ATOM 6485 HA PRO C 60 ATOM 6486 HB2 PRO C 60 ATOM 6487 HB3 PRO C 60 ATOM 6488 HG2 PRO C 60 ATOM 6489 HG3 PRO C 60	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C -17.105 -1.347 -16.496 1.00 35.80 C 4890 5636 3075 2519 -1156 -894 C -16.036 -2.403 -16.344 1.00 35.85 C 5004 5566 3051 2701 -1261 -1104 C -18.667 -3.984 -15.616 1.00 47.66 H -19.145 -1.564 -16.304 1.00 43.79 H -18.358 -1.861 -14.944 1.00 43.79
ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60 ATOM 6483 CG PRO C 60 ANISOU 6483 CG PRO C 60 ATOM 6484 CD PRO C 60 ANISOU 6484 CD PRO C 60 ATOM 6485 HA PRO C 60 ATOM 6486 HB2 PRO C 60 ATOM 6487 HB3 PRO C 60 ATOM 6488 HG2 PRO C 60 ATOM 6489 HG3 PRO C 60	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C -17.105 -1.347 -16.496 1.00 35.80 C 4890 5636 3075 2519 -1156 -894 C -16.036 -2.403 -16.344 1.00 35.85 C 5004 5566 3051 2701 -1261 -1104 C -18.667 -3.984 -15.616 1.00 47.66 H -19.145 -1.564 -16.304 1.00 43.79 H -18.358 -1.861 -14.944 1.00 43.79 H -17.253 -1.141 -17.432 1.00 42.96 H
ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60 ATOM 6483 CG PRO C 60 ANISOU 6483 CG PRO C 60 ATOM 6484 CD PRO C 60 ANISOU 6484 CD PRO C 60 ATOM 6485 HA PRO C 60 ATOM 6486 HB2 PRO C 60 ATOM 6487 HB3 PRO C 60 ATOM 6488 HG2 PRO C 60 ATOM 6489 HG3 PRO C 60 ATOM 6489 HG3 PRO C 60	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C -17.105 -1.347 -16.496 1.00 35.80 C 4890 5636 3075 2519 -1156 -894 C -16.036 -2.403 -16.344 1.00 35.85 C 5004 5566 3051 2701 -1261 -1104 C -18.667 -3.984 -15.616 1.00 47.66 H -19.145 -1.564 -16.304 1.00 43.79 H -18.358 -1.861 -14.944 1.00 43.79 H -17.253 -1.141 -17.432 1.00 42.96 H -16.868 -0.546 -16.002 1.00 42.96 H -15.430 -2.383 -17.101 1.00 43.02
ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60 ATOM 6483 CG PRO C 60 ANISOU 6483 CG PRO C 60 ATOM 6484 CD PRO C 60 ANISOU 6484 CD PRO C 60 ATOM 6485 HA PRO C 60 ATOM 6486 HB2 PRO C 60 ATOM 6487 HB3 PRO C 60 ATOM 6488 HG2 PRO C 60 ATOM 6489 HG3 PRO C 60 ATOM 6490 HD2 PRO C 60 ATOM 6491 HD3 PRO C 60	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C -17.105 -1.347 -16.496 1.00 35.80 C 4890 5636 3075 2519 -1156 -894 C -16.036 -2.403 -16.344 1.00 35.85 C 5004 5566 3051 2701 -1261 -1104 C -18.667 -3.984 -15.616 1.00 47.66 H -19.145 -1.564 -16.304 1.00 43.79 H -18.358 -1.861 -14.944 1.00 43.79 H -17.253 -1.141 -17.432 1.00 42.96 H -15.430 -2.383 -17.101 1.00 43.02 H -15.562 -2.286 -15.505 1.00 43.02
ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60 ATOM 6483 CG PRO C 60 ANISOU 6483 CG PRO C 60 ATOM 6484 CD PRO C 60 ANISOU 6484 CD PRO C 60 ATOM 6485 HA PRO C 60 ATOM 6486 HB2 PRO C 60 ATOM 6487 HB3 PRO C 60 ATOM 6488 HG2 PRO C 60 ATOM 6489 HG3 PRO C 60 ATOM 6490 HD2 PRO C 60 ATOM 6491 HD3 PRO C 60 ATOM 6491 N ASN C 61	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C -17.105 -1.347 -16.496 1.00 35.80 C 4890 5636 3075 2519 -1156 -894 C -16.036 -2.403 -16.344 1.00 35.85 C 5004 5566 3051 2701 -1261 -1104 C -18.667 -3.984 -15.616 1.00 47.66 H -19.145 -1.564 -16.304 1.00 43.79 H -18.358 -1.861 -14.944 1.00 43.79 H -17.253 -1.141 -17.432 1.00 42.96 H -16.868 -0.546 -16.002 1.00 42.96 H -15.430 -2.383 -17.101 1.00 43.02 H -15.562 -2.286 -15.505 1.00 43.02 H -20.112 -4.199 -17.602 1.00 48.64 N
ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60 ATOM 6483 CG PRO C 60 ANISOU 6483 CG PRO C 60 ATOM 6484 CD PRO C 60 ANISOU 6484 CD PRO C 60 ATOM 6485 HA PRO C 60 ATOM 6486 HB2 PRO C 60 ATOM 6487 HB3 PRO C 60 ATOM 6488 HG2 PRO C 60 ATOM 6489 HG3 PRO C 60 ATOM 6490 HD2 PRO C 60 ATOM 6491 HD3 PRO C 60	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C -17.105 -1.347 -16.496 1.00 35.80 C 4890 5636 3075 2519 -1156 -894 C -16.036 -2.403 -16.344 1.00 35.85 C 5004 5566 3051 2701 -1261 -1104 C -18.667 -3.984 -15.616 1.00 47.66 H -19.145 -1.564 -16.304 1.00 43.79 H -18.358 -1.861 -14.944 1.00 43.79 H -17.253 -1.141 -17.432 1.00 42.96 H -15.430 -2.383 -17.101 1.00 43.02 H -15.562 -2.286 -15.505 1.00 43.02
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ATOM 6482 CB PRO C 60 ANISOU 6482 CB PRO C 60 ATOM 6483 CG PRO C 60 ANISOU 6483 CG PRO C 60 ATOM 6484 CD PRO C 60 ATOM 6484 CD PRO C 60 ATOM 6485 HA PRO C 60 ATOM 6486 HB2 PRO C 60 ATOM 6487 HB3 PRO C 60 ATOM 6488 HG2 PRO C 60 ATOM 6489 HG3 PRO C 60 ATOM 6490 HD2 PRO C 60 ATOM 6491 HD3 PRO C 60 ATOM 6492 N ASN C 61 ANISOU 6492 N ASN C 61 ANISOU 6493 CA ASN C 61 ANISOU 6494 C ASN C 61 ANISOU 6494 C ASN C 61 ANISOU 6495 O ASN C 61 ATOM 6496 CB ASN C 61 ANISOU 6496 CB ASN C 61	-18.349 -1.953 -15.909 1.00 36.49 C 5031 5431 3402 2239 -1430 -881 C -17.105 -1.347 -16.496 1.00 35.80 C 4890 5636 3075 2519 -1156 -894 C -16.036 -2.403 -16.344 1.00 35.85 C 5004 5566 3051 2701 -1261 -1104 C -18.667 -3.984 -15.616 1.00 47.66 H -19.145 -1.564 -16.304 1.00 43.79 H -18.358 -1.861 -14.944 1.00 43.79 H -17.253 -1.141 -17.432 1.00 42.96 H -15.430 -2.383 -17.101 1.00 43.02 H -15.562 -2.286 -15.505 1.00 43.02 H -20.112 -4.199 -17.602 1.00 48.64 N 6943 6557 4979 2281 -2191 -1255 N -20.917 -4.436 -18.803 1.00 53.07 C 7604 7121 5437 2359 -2395 -1344 C -22.249 -3.722 -18.588 1.00 51.90 C 7250 7061 5408 2048 -2403 -1077 C -23.191 -4.304 -18.041 1.00 54.41 O 7529 7191 5954 1747 -2657 -981 O -21.101 -5.932 -19.062 1.00 57.80 C 8470 7364 6127 2384 -2809 -1566 C

ATOM 6499 N GLY C 62 -22.317 -2.460 -19.013 1.00 47.32 ANISOU 6499 N GLY C 62 6522 6778 4678 2140 -2120 -930 ATOM 6500 CA GLY C 62 -23.486 -1.628 -18.788 1.00 42.85 ANISOU 6500 CA GLY C 62 5742 6328 4213 1929 -2077 -651 ATOM 6501 C GLY C 62 -23.190 -0.477 -17.846 1.00 37.68 ANISOU 6501 C GLY C 62 4912 5795 3611 1884 -1720 -425 ATOM 6502 O GLY C 62 -22.058 0.018 -17.804 1.00 33.83 ANISOU 6502 O GLY C 62 4454 5404 2996 2051 -1456 -465 0 0 ATOM 6503 H GLY C 62 -21.687 -2.062 -19.441 1.00 56.78 ATOM 6504 HA2 GLY C 62 -23.793 -1.264 -19.633 1.00 51.42 ATOM 6505 HA3 GLY C 62 -24.198 -2.165 -18.406 1.00 51.42 ATOM 6506 N TRP C 63 -24.183 -0.035 -17.079 1.00 38.02 Ν ANISOU 6506 N TRP C 63 4766 5843 3836 1678 -1707 -172 ATOM 6507 CA TRP C 63 -23.963 1.078 -16.159 1.00 37.36 ANISOU 6507 CA TRP C 63 4564 5837 3794 1674 -1366 29 ATOM 6508 C TRP C 63 -23.263 0.534 -14.921 1.00 34.14 ANISOU 6508 C TRP C 63 4197 5260 3516 1568 -1371 -10 ATOM 6509 O TRP C 63 -23.893 -0.014 -14.014 1.00 34.79 C ANISOU 6509 O TRP C 63 4205 5220 3795 1372 -1530 89 ATOM 6510 CB TRP C 63 -25.267 1.782 -15.806 1.00 41.11 0 ANISOU 6510 CB TRP C 63 4833 6397 4389 1580 -1308 307 ATOM 6511 CG TRP C 63 -25.026 3.199 -15.359 1.00 41.90 ANISOU 6511 CG TRP C 63 4893 6592 4436 1678 -894 476 ATOM 6512 CD1 TRP C 63 -25.284 4.343 -16.064 1.00 43.57 C ANISOU 6512 CD1 TRP C 63 5084 6945 4526 1811 -679 583 ATOM 6513 CD2 TRP C 63 -24.447 3.618 -14.116 1.00 40.75 C ANISOU 6513 CD2 TRP C 63 4766 6367 4351 1643 -667 557 ATOM 6514 NE1 TRP C 63 -24.913 5.447 -15.329 1.00 42.19 ANISOU 6514 NE1 TRP C 63 4931 6753 4347 1849 -344 723 N ATOM 6515 CE2 TRP C 63 -24.395 5.027 -14.131 1.00 40.48 ANISOU 6515 CE2 TRP C 63 4744 6400 4236 1748 -333 705 ATOM 6516 CE3 TRP C 63 -23.974 2.938 -12.989 1.00 40.10 ANISOU 6516 CE3 TRP C 63 4720 6127 4387 1508 -721 513 C ATOM 6517 CZ2 TRP C 63 -23.889 5.765 -13.061 1.00 38.70 ANISOU 6517 CZ2 TRP C 63 4588 6078 4040 1738 -82 804 -23.889 5.765 -13.061 1.00 38.70 C -23.474 3.674 -11.927 1.00 38.27 ATOM 6518 CZ3 TRP C 63 ANISOU 6518 CZ3 TRP C 63 4546 5808 4188 1454 -433 595 ATOM 6519 CH2 TRP C 63 -23.434 5.072 -11.973 1.00 37.76 ANISOU 6519 CH2 TRP C 63 4514 5797 4035 1565 -130 725 C

ATOM 6532 C GLY C 64 -20.048 1.355 -13.658 1.00 26.03 ANISOU 6532 C GLY C 64 3293 4245 2353 1741 -864 -96 ATOM 6533 O GLY C 64 -19.491 1.747 -14.685 1.00 26.56 ANISOU 6533 O GLY C 64 3372 4484 2234 1922 -748 -146 O ATOM 6534 H GLY C 64 -21.483 0.943 -15.575 1.00 36.14 H ATOM 6535 HA2 GLY C 64 -21.689 0.361 -12.944 1.00 33.73 H ATOM 6536 HA3 GLY C 64 -20.761 -0.555 -13.845 1.00 33.73 ATOM 6537 N ALA C 65 -19.734 1.811 -12.454 1.00 23.88 ANISOU 6537 N ALA C 65 3002 3875 2195 1590 -696 20 N ATOM 6538 CA ALA C 65 -18.841 2.938 -12.274 1.00 22.96 ANISOU 6538 CA ALA C 65 2879 3831 2016 1603 -399 121 ATOM 6539 C ALA C 65 -17.832 2.648 -11.176 1.00 22.50 ANISOU 6539 C ALA C 65 2857 3640 2051 1472 -387 84 ANISOU 6539 C ALA C 65 267 3040 2051 1472 -367 64 C ATOM 6540 O ALA C 65 -18.141 1.994 -10.172 1.00 21.54 O ANISOU 6540 O ALA C 65 2776 3343 2067 1320 -506 69 O ATOM 6541 CB ALA C 65 -19.633 4.213 -11.935 1.00 22.39 C ANISOU 6541 CB ALA C 65 2791 3746 1969 1535 -171 333 C ATOM 6542 H ALA C 65 -20.030 1.479 -11.718 1.00 28.65 H ATOM 6543 HA ALA C 65 -18.354 3.094 -13.099 1.00 27.56 ATOM 6544 HB1 ALA C 65 -19.012 4.949 -11.820 1.00 26.87 Н ATOM 6545 HB2 ALA C 65 -20.246 4.406 -12.662 1.00 26.87 H ATOM 6546 HB3 ALA C 65 -20.129 4.067 -11.114 1.00 26.87 H ATOM 6547 N LEU C 66 -16.623 3.138 -11.394 1.00 23.35 N ANISOU 6547 N LEU C 66 2932 3857 2082 1526 -250 102 N ATOM 6548 CA LEU C 66 -15.528 3.074 -10.438 1.00 24.29 C ANISOU 6549 C LEU C 66 -15.366 4.492 0.995 4.00 23.53 ATOM 6549 C LEU C 66 -15.366 4.482 -9.885 1.00 22.53 ANISOU 6549 C LEU C 66 2860 3620 2079 1237 -14 288 ATOM 6550 O LEU C 66 -14.933 5.383 -10.609 1.00 24.26 ANISOU 6550 O LEU C 66 3022 3978 2216 1284 140 404 ATOM 6551 CB LEU C 66 -14.262 2.582 -11.134 1.00 27.22 ANISOU 6551 CB LEU C 66 3325 4462 2554 1587 -260 20 ATOM 6552 CG LEU C 66 -12.937 2.590 -10.379 1.00 30.02 ANISOU 6552 CG LEU C 66 3606 4824 2977 1491 -239 60 ANISOU 6553 CD1 LEU C 66 3606 4824 2977 1491 -239 60 ANISOU 6553 CD1 LEU C 66 -12.978 1.596 -9.225 1.00 29.95 ANISOU 6553 CD1 LEU C 66 3692 4585 3104 1381 -445 -47 C ATOM 6554 CD2 LEU C 66 -11.792 2.260 -11.342 1.00 32.79 ATOM 6554 CD2 LEU C 66 -11.792 2.260 -11.342 1.00 32.79

ANISOU 6554 CD2 LEU C 66 3793 5472 3193 1752 -203 31

ATOM 6555 H LEU C 66 -16.403 3.533 -12.125 1.00 28.02

ATOM 6556 HA LEU C 66 -15.750 2.469 -9.713 1.00 29.15

ATOM 6557 HB2 LEU C 66 -14.418 1.665 -11.409 1.00 32.66

ATOM 6558 HB3 LEU C 66 -14.132 3.127 -11.926 1.00 32.66

ATOM 6559 HG LEU C 66 -12.782 3.475 -10.013 1.00 36.03

ATOM 6560 HD11 LEU C 66 -12.127 1.618 -8.760 1.00 35.94

ATOM 6561 HD12 LEU C 66 -13.693 1.845 -8.619 1.00 35.94

ATOM 6562 HD13 LEU C 66 -13.138 0.708 -9.580 1.00 35.94

ATOM 6563 HD21 LEU C 66 -10.955 2.268 -10.852 1.00 39.35

ATOM 6564 HD22 LEU C 66 -11.944 1.381 -11.724 1.00 39.35

ATOM 6565 HD23 LEU C 66 -11.770 2.927 -12.046 1.00 39.35

ATOM 6566 N ALA C 67 -15.748 4.687 -8.621 1.00 20.32

N ANISOU 6566 N ALA C 67 2696 3129 1895 1056 -9 325 ANISOU 6566 N ALA C 67 2696 3129 1895 1056 -9 325 N ATOM 6567 CA ALA C 67 -15.912 6.041 -8.123 1.00 20.28 C ANISOU 6567 CA ALA C 67 2807 3014 1885 946 167 466 C

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ATOM 6568 C ALA C 67 -15.697 6.126 -6.621 1.00 20.88
ANISOU 6568 C ALA C 67 3036 2878 2020 763 136 461 C ATOM 6569 O ALA C 67 -16.029 5.209 -5.867 1.00 19.40 O ANISOU 6569 O ALA C 67 2873 2620 1879 726 22 393 O ATOM 6570 CB ALA C 67 -17.312 6.588 -8.436 1.00 20.38 C ANISOU 6570 CB ALA C 67 2862 3018 1862 1043 274 542 C
ATOM 6571 H ALA C 67 -15.914 4.068 -8.048 1.00 24.38
ATOM 6572 HA ALA C 67 -15.261 6.617 -8.553 1.00 24.34
ATOM 6573 HB1 ALA C 67 -17.382 7.491 -8.088 1.00 24.45
ATOM 6574 HB2 ALA C 67 -17.441 6.592 -9.397 1.00 24.45
ATOM 6575 HB3 ALA C 67 -17.974 6.018 -8.014 1.00 24.45
ATOM 6576 N LEU C 68 -15.158 7.262 -6.199 1.00 20.92
ANISOU 6576 N LEU C 68 3166 2769 2012 641 219 545
                                                                                                                             N
ATOM 6577 CA LEU C 68 -15.269 7.653 -4.804 1.00 21.31
ANISOU 6577 CA LEU C 68 3451 2589 2057 511 212 538
ATOM 6578 C LEU C 68 -16.727 7.974 -4.513 1.00 20.60
ANISOU 6578 C LEU C 68 3485 2435 1909 639 345
                                                                                                                               C
ATOM 6579 O LEU C 68 -17.346 8.772 -5.221 1.00 21.06
ANISOU 6579 O LEU C 68 3556 2518 1930 760 481 651 ATOM 6580 CB LEU C 68 -14.390 8.868 -4.518 1.00 22.79
                                                                                                                                 0
ANISOU 6580 CB LEU C 68 3790 2628 2240 345 222 613 ATOM 6581 CG LEU C 68 -14.247 9.276 -3.061 1.00 25.03
ANISOU 6581 CG LEU C 68 4370 2655 2484 205 152 569
ATOM 6582 CD1 LEU C 68 -13.477 8.208 -2.280 1.00 24.49
ANISOU 6582 CD1 LEU C 68 4229 2620 2458 90 -36 489
ATOM 6583 CD2 LEU C 68 -13.552 10.627 -2.903 1.00 20.02 ANISOU 6583 CD2 LEU C 68 4803 2699 2729 36 127 650 CATOM 6584 H LEU C 68 -14.727 7.818 -6.694 1.00 25.10 H
ATOM 6585 HA LEU C 68 -14.989 6.921 -4.233 1.00 25.57 H
ATOM 6586 HB2 LEU C 68 -13.499 8.683 -4.853 1.00 27.35 H
ATOM 6587 HB3 LEU C 68 -14.760 9.628 -4.993 1.00 27.35 H
ATOM 6588 HG LEU C 68 -15.128 9.364 -2.666 1.00 30.03 H
ATOM 6589 HD11 LEU C 68 -13.398 8.489 -1.355 1.00 29.39 H
ATOM 6590 HD12 LEU C 68 -13.962 7.369 -2.331 1.00 29.39 H
ATOM 6591 HD13 LEU C 68 -12.595 8.105 -2.671 1.00 29.39 H
ATOM 6592 HD21 LEU C 68 -13.463 10.882 -2.052 1.00 32.31 H
ATOM 6594 HD23 I FIL C 68 -14.086 11 283 -3.457 1.00 32.31 H
ATOM 6594 HD23 LEU C 68 -14.086 11.283 -3.457 1.00 32.31 ATOM 6595 N VAL C 69 -17.289 7.323 -3.504 1.00 20.35
ANISOU 6595 N VAL C 69 3514 2350 1866 630 313 541
ATOM 6596 CA VAL C 69 -18.676 7.524 -3.103 1.00 20.79
ANISOU 6596 CA VAL C 69 3631 2406 1863 766 458 614
ATOM 6597 C VAL C 69 -18.689 7.810 -1.608 1.00 22.16
                                                                                                                                C
ANISOU 6597 C VAL C 69 4072 2417 1931 726 495 602
ATOM 6598 O VAL C 69 -18.055 7.092 -0.830 1.00 21.45
                                                                                                                              C
ATOM 6598 O VAL C 69 -18.055 7.092 -0.830 1.00 21.45 O ANISOU 6598 O VAL C 69 4013 2283 1852 590 353 547 O ATOM 6599 CB VAL C 69 -19.545 6.294 -3.435 1.00 20.61 C ANISOU 6599 CB VAL C 69 3364 2546 1919 806 386 645 ATOM 6600 CG1 VAL C 69 -20.980 6.502 -2.985 1.00 21.68 O ANISOU 6600 CG1 VAL C 69 3487 2742 2008 933 548 784 ATOM 6601 CG2 VAL C 69 -19.500 5.997 -4.927 1.00 19.89 ANISOU 6601 CG2 VAL C 69 3068 2604 1886 871 311 618 ATOM 6602 H VAL C 69 -16.876 6.743 -3.022 1.00 24.42 H
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ATOM 6603 HA VAL C 69 -19.040 8.294 -3.568 1.00 24.95
                                                              Н
ATOM 6604 HB VALC 69
                           -19.192 5.522 -2.965 1.00 24.73
                                                              Н
ATOM 6605 HG11 VAL C 69
                           -21.498 5.712 -3.208 1.00 26.02
                                                             Н
                           -20.992 6.646 -2.026 1.00 26.02
-21.344 7.277 -3.441 1.00 26.02
ATOM 6606 HG12 VAL C 69
ATOM 6607 HG13 VAL C 69
                                                               Н
                            -20.052 5.221 -5.111 1.00 23.87
-19.838 6.767 -5.412 1.00 23.87
-18.582 5.820 -5.186 1.00 23.87
ATOM 6608 HG21 VAL C 69
ATOM 6609 HG22 VAL C 69
ATOM 6610 HG23 VAL C 69
                                                               Н
                          -19.389 8.860 -1.209 1.00 23.91
ATOM 6611 N GLY C 70
ANISOU 6611 N GLY C 70
                           4510 2547 2027 877 677 650
                                                              Ν
ATOM 6612 CA GLY C 70
                           -19.434 9.182 0.204 1.00 26.51
                            5149 2728 2196 899 719 617
ANISOU 6612 CA GLY C 70
                                                              C
ATOM 6613 C GLY C 70
ANISOU 6613 C GLY C 70
                                                              C
                           -20.621 10.065 0.495 1.00 29.99
                           5754 3157 2482 1185 968 691
                                                              C
ATOM 6614 O GLY C 70
                           -21.344 10.500 -0.405 1.00 28.33
                                                              0
ANISOU 6614 O GLY C 70
                          5413 3038 2312 1346 1093 776
                                                                0
ATOM 6615 H GLY C 70
                          -19.834 9.389 -1.720 1.00 28.69
                                                              Н
ATOM 6616 HA2 GLY C 70
                           -19.511 8.368 0.727 1.00 31.81
                                                               н
ATOM 6617 HA3 GLY C 70
                            -18.624 9.647 0.464 1.00 31.81
                                                              Н
ATOM 6618 N TRP C 71
                          -20.813 10.323 1.781 1.00 33.06
                                                              Ν
ANISOU 6618 N TRP C 71
                           6424 3451 2686 1275 1034
                                                               N
                                                         652
ATOM 6619 CA TRP C 71
                           -21.889 11.181 2.235 1.00 36.13
                                                               C
ANISOU 6619 CA TRP C 71
                          6940 3826 2963 1588 1247
                                                                C
ATOM 6620 C TRP C 71
                          -21.352 12.167 3.258 1.00 36.95
ANISOU 6620 C TRP C 71
                           7586 3611 2842 1652 1219
                                                              C
ATOM 6621 O TRP C 71
                           -20.362 11.902 3.946 1.00 37.27
                                                              0
ANISOU 6621 O TRP C 71
                           7842 3518 2801 1441 1035 423
                                                                0
ATOM 6622 CB TRP C 71
                           -23.045 10.373 2.872 1.00 37.53
ANISOU 6622 CB TRP C 71
                          6836 4276 3149 1711 1372
                                                         804
ATOM 6623 CG TRP C 71
                           -23.670 9.337 1.968 1.00 34.70
                                                              C
ANISOU 6623 CG TRP C 71
                          5998 4202 2986 1627 1359
                                                                C
                                                          967
ATOM 6624 CD1 TRP C 71
                            -23.125 8.146 1.581 1.00 33.06
                                                               C
ANISOU 6624 CD1 TRP C 71
                            5599 4069 2892 1370 1183 1000
ATOM 6625 CD2 TRP C 71
                            -24.970 9.396 1.364 1.00 34.83
ANISOU 6625 CD2 TRP C 71
                           5704 4440 3090 1815 1496 1136
ATOM 6626 NE1 TRP C 71
                            -24.002 7.464 0.765 1.00 32.00
ANISOU 6626 NE1 TRP C 71
                            5091 4168 2901 1376 1192 1170
ATOM 6627 CE2 TRP C 71
                            -25.143 8.208 0.620 1.00 32.89
ANISOU 6627 CE2 TRP C 71
                            5102 4393 3003 1628 1382 1259
                                                                 C
                                                               C
ATOM 6628 CE3 TRP C 71
                            -26.003 10.339 1.375 1.00 37.11
ANISOU 6628 CE3 TRP C 71
                            5998 4769 3333 2137 1677 1217
                                                                 C
ATOM 6629 CZ2 TRP C 71
                           -26.301 7.942 -0.104 1.00 32.54
ANISOU 6629 CZ2 TRP C 71
                                                                 C
                            4697 4597 3069 1719 1436 1457
ATOM 6630 CZ3 TRP C 71
                            -27.157 10.070 0.652 1.00 36.96
                                                               C
                            5592 5018 3435 2241 1737 1423
ANISOU 6630 CZ3 TRP C 71
ATOM 6631 CH2 TRP C 71
                            -27.293 8.883 -0.077 1.00 34.37
ANISOU 6631 CH2 TRP C 71
                            4900 4897 3263 2017 1616 1537
                          -20.326 10.008 2.416 1.00 39.67
ATOM 6632 H TRP C 71
                                                              Н
ATOM 6633 HA TRP C 71
                          -22.242 11.681 1.482 1.00 43.36
ATOM 6634 HB2 TRP C 71 -22.705 9.912 3.654 1.00 45.04
                                                              Н
ATOM 6635 HB3 TRP C 71 -23.744 10.991 3.137 1.00 45.04 H
ATOM 6636 HD1 TRP C 71 -22.284 7.839 1.831 1.00 39.67 H
ATOM 6637 HE1 TRP C 71 -23.859 6.694 0.409 1.00 38.40
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ATOM 6638 HE3 TRP C 71 -25.918 11.129 1.858 1.00 44.53
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ATOM 6639 HZ2 TRP C 71 -26.395 7.156 -0.592 1.00 39.05
ATOM 6640 HZ3 TRP C 71 -27.852 10.688 0.653 1.00 44.36
                                                                   Н
                                                                  Н
ATOM 6641 HH2 TRP C 71 -28.078 8.729 -0.552 1.00 41.25 ATOM 6642 N THR C 72 -22.008 13.316 3.334 1.00 37.66
                                                                   Н
ANISOU 6642 N THR C 72
                             7923 3558 2827 1953 1365 520
                                                                   Ν
ATOM 6643 CA THR C 72
                             -21.984 14.138 4.530 1.00 39.32
ANISOU 6643 CA THR C 72
                                                                     C
                             8626 3514 2801 2122 1357
ATOM 6644 C THR C 72
                            -23.417 14.300 5.008 1.00 41.75
ANISOU 6644 C THR C 72
                             8798 4017 3050 2500 1582 571
                                                                   C
ATOM 6645 O THR C 72 -24.373 14.055 4.265 1.00 40.43
ANISOU 6645 O THR C 72 8226 4108 3028 2626 1723 734
                                                                    0
ATOM 6646 CB THR C 72 -21.355 15.520 4.290 1.00 40.66
ANISOU 6646 CB THR C 72 9309 3304 2835 2106 1246
                                                              345
                                                                     C
ATOM 6647 OG1 THR C 72 -22.121 16.229 3.311 1.00 40.87
                                                                    0
ANISOU 6647 OG1 THR C 72
                             9234 3398 2897 2305 1403 468
                                                                     0
ATOM 6648 CG2 THR C 72
                             -19.898 15.382 3.830 1.00 38.65
ANISOU 6648 CG2 THR C 72
                             9129 2874 2683 1685 986 214
                                                                     C
ATOM 6649 H THR C 72 -22.481 13.645 2.696 1.00 45.19
                             -21.478 13.686 5.223 1.00 47.19
ATOM 6650 HA THR C 72
ATOM 6651 HB THR C 72 -21.362 16.020 5.121 1.00 48.79
ATOM 6652 HG1 THR C 72 -22.131 15.800 2.589 1.00 49.05
                                                                  Н
ATOM 6653 HG21 THR C 72 -19.512 16.260 3.682 1.00 46.38
ATOM 6654 HG22 THR C 72 -19.379 14.919 4.507 1.00 46.38
ATOM 6655 HG23 THR C 72 -19.858 14.877 3.002 1.00 46.38
ATOM 6656 N ARG C 73
                             -23.554 14.683 6.271 1.00 44.58
                                                                  Ν
ANISOU 6656 N ARG C 73
                            9486 4272 3179 2674 1593 521
                                                                    Ν
ATOM 6657 CA ARG C 73
                            -24.825 15.117 6.826 1.00 48.55
                                                                    C
ANISOU 6657 CA ARG C 73 9977 4919 3549 3085 1803
                                                              652
ATOM 6658 C ARG C 73 -24.753 16.609 7.125 1.00 51.88 ANISOU 6658 C ARG C 73 10977 5013 3722 3308 1764
                                                                    C
ATOM 6659 O ARG C 73
                             -23.688 17.230 7.066 1.00 51.60
                                                                   0
ANISOU 6659 O ARG C 73
                             11347 4648 3611 3094 1548
                                                              420
                                                                     0
ATOM 6660 CB ARG C 73
                            -25.174 14.311 8.086 1.00 51.08
                                                                    C
ANISOU 6660 CB ARG C 73 10194 5457 3758 3152 1878
                                                                     C
ATOM 6661 CG ARG C 73
                              -25.374 12.825 7.833 1.00 48.44
                                                                    C
ANISOU 6661 CG ARG C 73
                             9295 5480 3629 2909 1905
                                                                     C
                                                              804
ATOM 6662 CD ARG C 73
                              -25.748 12.102 9.118 1.00 52.75
ANISOU 6662 CD ARG C 73
                             9772 6245 4026 2970 1990
                                                                     C
                                                                   Ν
ATOM 6663 NE ARG C 73
                              -26.440 10.841 8.853 1.00 52.85
ANISOU 6663 NE ARG C 73
                              9215 6648 4216 2828 2068 1106
                                                                      N
ATOM 6664 CZ ARG C 73
                              -25.886 9.632 8.895 1.00 51.62
ANISOU 6664 CZ ARG C 73
                                                                      C
                             8862 6593 4159 2473 1937 1133
ATOM 6665 NH1 ARG C 73
                              -24.604 9.477 9.200 1.00 50.78
                                                                    Ν
ANISOU 6665 NH1 ARG C 73
                              9042 6256 3994 2234 1725
                                                               944
                                                                      N
ATOM 6666 NH2 ARG C 73
                              -26.631 8.563 8.633 1.00 51.28
                                                                   Ν
                                                                      Ν
ANISOU 6666 NH2 ARG C 73
                              8342 6869 4272 2351 1991 1378
                             -22.909 14.699 6.839 1.00 53.49
ATOM 6667 H ARG C 73
ATOM 6668 HA ARG C 73 -25.526 14.972 0.170 1.00 50.25

ATOM 6669 HB2 ARG C 73 -24.453 14.408 8.728 1.00 61.30 H

ATOM 6670 HB3 ARG C 73 -25.997 14.661 8.462 1.00 61.30 H

ATOM 6671 HG2 ARG C 73 -26.092 12.701 7.192 1.00 58.12 H
                                                                 Н
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ATOM 6673 HD2 ARG C 73 -24.941 11.905 9.619 1.00 63.30 H
ATOM 6674 HD3 ARG C 73 -26.338 12.667 9.641 1.00 63.30 H
ATOM 6675 HE ARG C 73 -27.275 10.885 8.653 1.00 63.42 H
ATOM 6676 HH11 ARG C 73 -24.117 10.164 9.371 1.00 60.93 H
ATOM 6677 HH12 ARG C 73 -24.260 8.689 9.224 1.00 60.93 H
ATOM 6678 HH21 ARG C 73 -27.463 8.656 8.435 1.00 61.53 H
ATOM 6679 HH22 ARG C 73 -26.281 7.778 8.659 1.00 61.53 H
ATOM 6680 N SER C 74 -25.910 17.191 7.421 1.00 55.18 N
                                                                                                                                                                       Н
 ANISOU 6680 N SER C 74 11417 5551 3998 3721 1955 704 N
ATOM 6681 CA SER C 74 -26.011 18.603 7.771 1.00 59.60 C ANISOU 6681 CA SER C 74 12526 5843 4275 3986 1931 635
 ATOM 6682 C SER C 74 -25.328 19.482 6.723 1.00 58.56
ANISOU 6682 C SER C 74 12622 5447 4181 3778 1783 553 C ATOM 6683 O SER C 74 -24.351 20.181 7.031 1.00 59.97 O ANISOU 6683 O SER C 74 13274 5283 4230 3598 1550 355 C ATOM 6684 CB SER C 74 -25.425 18.851 9.153 1.00 62.79 C
ANISOU 6684 CB SER C 74 13420 6023 4415 4023 1794 454 C
ATOM 6685 OG SER C 74 -26.187 18.192 10.145 1.00 64.71 O
 ANISOU 6685 OG SER C 74 13473 6548 4565 4278 1977 542 O
 ATOM 6686 H SER C 74 -26.665 16.780 7.428 1.00 66.22 H
ATOM 6687 HA SER C 74 -26.949 18.850 7.798 1.00 71.52 H
ATOM 6688 HB2 SER C 74 -24.516 18.514 9.176 1.00 75.35 H
ATOM 6689 HB3 SER C 74 -25.430 19.805 9.332 1.00 75.35 H
ATOM 6690 HG SER C 74 -25.856 18.335 10.904 1.00 77.65 H
                                                                                                                                                                       Н
ATOM 6691 N PRO C 75 -25.812 19.480 5.470 1.00 56.50 N
ANISOU 6691 N PRO C 75 12013 5354 4100 3774 1894 696 N
 ATOM 6692 CA PRO C 75 -26.979 18.730 4.996 1.00 55.30 C
ANISOU 6696 CG PRO C 75 11930 5430 4221 3864 2003 813 C
                                                                           -25.213 20.248 4.370 1.00 55.56
 ATOM 6697 CD PRO C 75
ATOM 6697 CD PRO C 75
ANISOU 6697 CD PRO C 75
ATOM 6698 HA PRO C 75
ATOM 6698 HA PRO C 75
ATOM 6699 HB2 PRO C 75
ATOM 6700 HB3 PRO C 75
ATOM 6701 HG2 PRO C 75
ATOM 6702 HG3 PRO C 75
ATOM 6703 HD2 PRO C 75
ATOM 6704 HD3 PRO C 75
ATOM 6705 N LEIL C 76
ATOM 6705 N LEIL C 76
ATOM 6706 N LEIL C 76
ATOM 6707 CD PRO C 75
12023 5049 4037 3568 1791 618
C
-27.633 18.627 5.705 1.00 66.36
H
-27.633 18.627 5.705 1.00 66.36
ATOM 6705 N LEU C 76 -27.601 16.519 4.177 1.00 49.68
 ANISOU 6705 N LEU C 76 9522 5460 3896 3702 2183 1160 N
ATOM 6706 CA LEU C 76 -27.354 15.198 3.615 1.00 45.66
ANISOU 6706 CA LEU C 76 8524 5162 3662 3389 2118 1177
 ATOM 6707 C LEU C 76 -26.958 15.334 2.150 1.00 44.14 C
 ANISOU 6707 C LEU C 76 8206 4920 3644 3219 2037 1183 C
 ATOM 6708 O LEU C 76 -27.782 15.701 1.303 1.00 44.79 O
 ANISOU 6708 O LEU C 76 8098 5148 3773 3374 2110 1352 O
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ATOM 6709 CB LEU C 76 -28.589 14.315 3.753 1.00 46.49
ANISOU 6709 CB LEU C 76 8106 5696 3863 3495 2246 1402 ATOM 6710 CG LEU C 76 -28.349 12.859 3.334 1.00 43.03 C ANISOU 6710 CG LEU C 76 7212 5482 3654 3136 2150 1424 ATOM 6711 CD1 LEU C 76 -27.339 12.192 4.250 1.00 41.80 C
ANISOU 6711 CD1 LEU C 76 7229 5220 3432 2886 2052 1256 C ATOM 6712 CD2 LEU C 76 -29.658 12.080 3.316 1.00 44.79 C
ANISOU 6712 CD2 LEU C 76 6927 6121 3972 3212 2251 1703 C
ATOM 6713 H LEU C 76 -28.432 16.689 4.322 1.00 59.62 H
ATOM 6714 HA LEU C 76 -26.622 14.777 4.092 1.00 54.79
ATOM 6715 HB2 LEU C 76 -28.872 14.315 4.681 1.00 55.79
ATOM 6715 HB2 LEU C 76 -28.872 14.315 4.681 1.00 55.79 H
ATOM 6716 HB3 LEU C 76 -29.295 14.674 3.193 1.00 55.79 H
ATOM 6717 HG LEU C 76 -27.985 12.848 2.435 1.00 51.63 H
ATOM 6718 HD11 LEU C 76 -27.208 11.275 3.961 1.00 50.16 H
ATOM 6720 HD13 LEU C 76 -26.501 12.677 4.203 1.00 50.16 H
ATOM 6721 HD21 LEU C 76 -29.478 11.165 3.048 1.00 53.75 H
ATOM 6722 HD22 LEU C 76 -30.046 12.094 4.205 1.00 53.75 H
ATOM 6723 HD23 LEU C 76 -30.264 12.496 2.684 1.00 53.75 H
ATOM 6723 HD23 LEU C 76 -30.264 12.496 2.684 1.00 53.75 ATOM 6724 N ILE C 77 -25.697 15.043 1.852 1.00 40.77
ANISOU 6724 N ILE C 77 7888 4312 3291 2905 1887 1011
                                                                                                  N
ATOM 6725 CA ILE C 77 -25.159 15.121 0.500 1.00 38.23
ANISOU 6725 CA ILE C 77 7452 3956 3120 2737 1817 997 ATOM 6726 C ILE C 77 -24.533 13.774 0.179 1.00 35.93
ANISOU 6726 C ILE C 77 6805 3845 3002 2401 1697 931
ATOM 6727 O ILE C 77
                                          -23.858 13.182 1.026 1.00 34.11
ANISOU 6727 O ILE C 77 6674 3570 2716 2209 1604 829
                                                                                                      0
ATOM 6728 CB ILE C 77
                                           -24.113 16.251 0.359 1.00 38.47
ANISOU 6728 CB ILE C 77 7957 3667 2991 2592 1737 831 ATOM 6729 CG1 ILE C 77 -24.758 17.622 0.604 1.00 42.63
ANISOU 6729 CG1 ILE C 77 8845 4077 3274 2874 1842 870
ATOM 6730 CG2 ILE C 77 -23.446 16.211 -1.016 1.00 36.33
ANISOU 6730 CG2 ILE C 77 7513 3421 2871 2400 1700 786
ATOM 6731 CD1 ILE C 77 -23.755 18.758 0.761 1.00 45.06
ANISOU 6731 CD1 ILE C 77 9669 3999 3454 2738 1699 662 C
ATOM 6732 H ILE C 77 -25.116 14.791 2.434 1.00 48.92 H ATOM 6733 HA ILE C 77 -25.880 15.285 -0.129 1.00 45.88 H
ATOM 6734 HB ILE C 77 -23.427 16.114 1.032 1.00 46.16 H
ATOM 6735 HG12 ILE C 77 -25.332 17.836 -0.148 1.00 51.15 H
ATOM 6736 HG13 ILE C 77 -25.285 17.578 1.418 1.00 51.15 H
ATOM 6737 HG21 ILE C 77 -22.797 16.930 -1.073 1.00 43.60 H
ATOM 6738 HG22 ILE C 77 -23.003 15.355 -1.127 1.00 43.60
ATOM 6739 HG23 ILE C 77 -24.125 16.324 -1.699 1.00 43.60
                                                                                                    Н
                                            -24.237 19.586 0.912 1.00 43.60 H

-23.178 18.568 1.518 1.00 54.08 H

-23.226 18.826 -0.050 1.00 54.08
                                                                                                    Н
ATOM 6740 HD11 ILE C 77
ATOM 6741 HD12 ILE C 77
ATOM 6742 HD13 ILE C 77 -23.226 18.826 -0.050 1.00 54.08 ATOM 6743 N ALA C 78 -24.775 13.281 -1.032 1.00 35.13
ANISOU 6743 N ALA C 78 6313 3962 3073 2320 1665 1020
ATOM 6744 CA ALA C 78 -24.065 12.130 -1.573 1.00 33.94
                                                                                                   c c
ANISOU 6744 CA ALA C 78 5901 3948 3047 1994 1496 993
ATOM 6745 C ALA C 78 -23.182 12.626 -2.703 1.00 32.72
ANISOU 6745 C ALA C 78 5802 3685 2945 1868 1406 955
                                                                                                    C
ATOM 6746 O ALA C 78 -23.664 13.307 -3.609 1.00 34.76
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ANISOU 6746 O ALA C 78 5999 3977 3231 2024 1480 1024 0 ATOM 6747 CB ALA C 78 -25.027 11.061 -2.090 1.00 34.13 C ANISOU 6747 CB ALA C 78 5460 4310 3199 1992 1486 1149 C -25.361 13.606 -1.571 1.00 42.16 ATOM 6748 H ALA C 78 Н ATOM 6749 HA ALA C 78 -23.503 11.739 -0.886 1.00 40.73 н -24.512 10.317 -2.440 1.00 40.96 -25.588 10.761 -1.358 1.00 40.96 ATOM 6750 HB1 ALA C 78 Н ATOM 6751 HB2 ALA C 78 ATOM 6752 HB3 ALA C 78 -25.575 11.444 -2.793 1.00 40.96 Н -21.893 12.326 -2.629 1.00 30.75 ATOM 6753 N TYR C 79 Ν **ANISOU 6753 N TYR C 79** 5657 3315 2711 1596 1240 N 872 ATOM 6754 CA TYR C 79 -20.949 12.808 -3.619 1.00 29.79 C ANISOU 6754 CA TYR C 79 5556 3104 2659 1454 1145 C 880 ATOM 6755 C TYR C 79 -20.277 11.635 -4.313 1.00 26.28 C **ANISOU 6755 C TYR C 79** 4785 2861 2338 1255 986 860 C ATOM 6756 O TYR C 79 -20.176 10.533 -3.760 1.00 23.80 0 **ANISOU 6756 O TYR C 79** 4350 2635 2059 1155 0 891 800 ATOM 6757 CB TYR C 79 -19.899 13.738 -2.988 1.00 32.36 ANISOU 6757 CB TYR C 79 6282 3081 2932 1303 1058 C 807 ATOM 6758 CG TYR C 79 -19.026 13.122 -1.907 1.00 31.49 ANISOU 6758 CG TYR C 79 6269 2888 2808 1076 895 685 ATOM 6759 CD1 TYR C 79 -17.806 12.547 -2.224 1.00 30.04 **ANISOU 6759 CD1 TYR C 79** 5902 2760 2752 792 704 660 ATOM 6760 CD2 TYR C 79 -19.401 13.167 -0.568 1.00 33.39 **ANISOU 6760 CD2 TYR C 79** 6790 3012 2885 1177 935 607 ATOM 6761 CE1 TYR C 79 -16.993 11.997 -1.248 1.00 29.90 **ANISOU 6761 CE1 TYR C 79** 5955 2677 2727 596 536 564 C ATOM 6762 CE2 TYR C 79 -18.591 12.620 0.423 1.00 32.87 **ANISOU 6762 CE2 TYR C 79** 6826 2875 2786 973 C 765 504 ATOM 6763 CZ TYR C 79 -17.386 12.039 0.074 1.00 30.92 6378 2675 2696 673 ANISOU 6763 CZ TYR C 79 C ATOM 6764 OH TYR C 79 -16.565 11.497 1.041 1.00 31.51 0 ANISOU 6764 OH TYR C 79 6535 2692 2745 482 0 367 400 -21.540 11.843 -2.011 1.00 36.90 ATOM 6765 H TYR C 79 Н ATOM 6766 HA TYR C 79 -21.431 13.316 -4.290 1.00 35.75 Н ATOM 6767 HB2 TYR C 79 -19.310 14.053 -3.691 1.00 38.83 Н ATOM 6768 HB3 TYR C 79 -20.360 14.494 -2.592 1.00 38.83 Н ATOM 6769 HD1 TYR C 79 -17.536 12.515 -3.114 1.00 36.05 ATOM 6770 HD2 TYR C 79 ATOM 6771 HE1 TYR C 79 -20.212 13.557 -0.332 1.00 40.07 -16.181 11.609 -1.482 1.00 35.87 Н Н ATOM 6772 HE2 TYR C 79 -18.856 12.649 1.314 1.00 39.44 Н -16.917 11.587 1.799 1.00 37.81 ATOM 6773 HH TYR C 79 Н ATOM 6774 N TYR C 80 -19.835 11.899 -5.541 1.00 25.38 N ANISOU 6774 N TYR C 80 4543 2822 2280 1225 958 912 Ν ATOM 6775 CA TYR C 80 -19.230 10.914 -6.418 1.00 24.29 C 4109 2900 2219 1124 829 ANISOU 6775 CA TYR C 80 C 880 ATOM 6776 C TYR C 80 -18.046 11.542 -7.139 1.00 25.38 ANISOU 6776 C TYR C 80 4253 3012 2378 998 798 C ATOM 6777 O TYR C 80 -18.142 12.667 -7.638 1.00 26.00 **ANISOU 6777 O TYR C 80** 4452 2999 2427 1053 893 1054 0 ATOM 6778 CB TYR C 80 -20.230 10.403 -7.468 1.00 24.77 C ANISOU 6778 CB TYR C 80 3919 3211 2284 1301 C 847 ATOM 6779 CG TYR C 80 -21.553 9.948 -6.911 1.00 24.39 C ANISOU 6779 CG TYR C 80 3801 3229 2238 1418 892 C 966

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ATOM 6780 CD1 TYR C 80 -22.600 10.839 -6.747 1.00 26.41
ANISOU 6780 CD1 TYR C 80 4143 3460 2431 1627 1071 1085 C
ATOM 6781 CD2 TYR C 80
                                        -21.761 8.622 -6.556 1.00 24.46
ANISOU 6781 CD2 TYR C 80 3643 3334 2317 1327 753 911
ATOM 6782 CE1 TYR C 80
                                        -23.815 10.430 -6.238 1.00 27.35
ANISOU 6782 CE1 TYR C 80 4133 3705 2553 1745 1138 1170 C
                                       -22.971 8.202 -6.044 1.00 25.45
ATOM 6783 CE2 TYR C 80
ANISOU 6783 CE2 TYR C 80 3657 3548 2464 1394 793 1007 ATOM 6784 CZ TYR C 80 -23.993 9.110 -5.888 1.00 27.47
ANISOU 6784 CZ TYR C 80 3949 3835 2652 1605 999 1147
ATOM 6785 OH TYR C 80 -25.204 8.704 -5.379 1.00 30.26
ANISOU 6785 OH TYR C 80 4130 4341 3026 1685 1065 1294 O
ATOM 6786 H TYR C 80 -19.880 12.680 -5.898 1.00 30.46 H
                                                                                     Н
ATOM 6787 HA TYR C 80 -18.913 10.161 -5.896 1.00 29.15
ATOM 6788 HB2 TYR C 80 -20.408 11.118 -8.099 1.00 29.73 H
ATOM 6789 HB3 TYR C 80 -19.833 9.650 -7.933 1.00 29.73 H
ATOM 6790 HD1 TYR C 80 -22.480 11.731 -6.981 1.00 31.69 H
ATOM 6791 HD2 TYR C 80 -21.070 8.008 -6.659 1.00 29.35 H
ATOM 6790 HD1 ITR C 00 -21.070 8.008 -6.659 1.00 25.50 ATOM 6791 HD2 TYR C 80 -24.507 11.041 -6.130 1.00 32.82 ATOM 6793 HE2 TYR C 80 -23.096 7.311 -5.807 1.00 30.54 HA TYR C 80 -25.182 7.882 -5.207 1.00 36.31 H
                                                                                        Н
ANISOU 6795 N VAL C 81 4073 3075 2400 842 668 874 ATOM 6796 CA VAL C 81 -15.840 11.116 -8.115 1.00 26.24
                                                                                       Ν
                                                                                         C
ANISOU 6796 CA VAL C 81 4081 3330 2558 754 655 969
ATOM 6797 C VAL C 81 -15.662 9.901 -9.013 1.00 25.47
ANISOU 6797 C VAL C 81 3696 3541 2442 870 595 897
ATOM 6798 O VAL C 81 -15.160 8.860 -8.570 1.00 23.98
                                                                                         C
ANISOU 6798 O VAL C 81 -13.100 0.000 -0.370 1.00 23.90 O ANISOU 6798 O VAL C 81 3418 3399 2295 820 466 774 O ATOM 6799 CB VAL C 81 -14.542 11.454 -7.370 1.00 28.02 C
ANISOU 6799 CB VAL C 81 4383 3410 2853 483 550 992
ATOM 6800 CG1 VAL C 81 -13.415 11.755 -8.355 1.00 29.83
ANISOU 6800 CG1 VAL C 81 4395 3827 3111 389
                                                                        561 1159
ATOM 6801 CG2 VAL C 81 -14.765 12.632 -6.436 1.00 29.38
ANISOU 6801 CG2 VAL C 81 4927 3220 3018 383 557 1018
ATOM 6802 H VAL C 81 -16.804 10.106 -6.731 1.00 30.15 H
ATOM 6803 HA VAL C 81 -16.081 11.874 -8.669 1.00 31.48 H
ATOM 6804 HB VAL C 81 -14.276 10.691 -6.833 1.00 33.62 H
ATOM 6805 HG11 VAL C 81 -12.609 11.964 -7.858 1.00 35.80 H
ATOM 6806 HG12 VAL C 81 -13.267 10.975 -8.912 1.00 35.80 H
ATOM 6808 HG21 VAL C 81 -13.671 12.511 -8.905 1.00 35.80 H
ATOM 6808 HG21 VAL C 81
ATOM 6809 HG22 VAL C 81
                                      -13.935 12.831 -5.975 1.00 35.26
                                      -15.046 13.400 -6.959 1.00 35.26
ATOM 6810 HG23 VAL C 81 -15.454 12.399 -5.794 1.00 35.26
ATOM 6811 N VAL C 82
                                      -16.067 10.032 -10.271 1.00 23.43
                                                                                         Ν
ANISOU 6811 N VAL C 82 3323 3477 2102 1046 670 967
ATOM 6812 CA VAL C 82 -16.151 8.903 -11.191 1.00 23.27
ANISOU 6812 CA VAL C 82 3106 3721 2015 1219 591 862
ATOM 6813 C VAL C 82 -14.926 8.902 -12.096 1.00 24.46
ANISOU 6813 C VAL C 82 3087 4113 2094 1251 627 936
ATOM 6814 O VAL C 82 -14.752 9.805 -12.930 1.00 26.20
                                                                                        C
ANISOU 6814 O VAL C 82 3278 4439 2239 1288 761 1124
                                                                                        0
ATOM 6815 CB VAL C 82 -17.439 8.958 -12.026 1.00 23.30
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ANISOU 6815 CB VAL C 82 3095 3821 1938 1422 619 882
ATOM 6816 CG1 VAL C 82 -17.568 7.703 -12.873 1.00 23.98
ANISOU 6816 CG1 VAL C 82 3044 4122 1947 1584 463 729
 ATOM 6817 CG2 VAL C 82 -18.653 9.139 -11.137 1.00 22.65 C ANISOU 6817 CG2 VAL C 82 3127 3554 1925 1409 635 884 C
ANISOU 6817 CG2 VAL C 82 3127 3554 1925 1409 635 884 C ATOM 6818 H VAL C 82 -16.304 10.780 -10.623 1.00 28.12 H ATOM 6819 HA VAL C 82 -16.153 8.077 -10.683 1.00 27.93 H ATOM 6820 HB VAL C 82 -17.392 9.719 -12.626 1.00 27.96 H ATOM 6821 HG11 VAL C 82 -18.386 7.755 -13.392 1.00 28.78 H ATOM 6822 HG12 VAL C 82 -16.802 7.643 -13.466 1.00 28.78 H ATOM 6823 HG13 VAL C 82 -17.596 6.929 -12.289 1.00 28.78 H ATOM 6824 HG21 VAL C 82 -19.449 9.170 -11.691 1.00 27.18 H ATOM 6825 HG22 VAL C 82 -18.708 8.392 -10.520 1.00 27.18 H ATOM 6826 HG23 VAL C 82 -18.562 9.970 -10.643 1.00 27.18 H ATOM 6827 N ASP C 83 -14.111 7.856 -11.975 1.00 24.40 N ANISOU 6827 N ASP C 83 2957 4217 2097 1269 515 808 N
 ANISOU 6827 N ASP C 83 2957 4217 2097 1269 515 808 N ATOM 6828 CA ASP C 83 -12.913 7.691 -12.789 1.00 26.08 C ANISOU 6828 CA ASP C 83 2964 4724 2222 1361 565 879 C
 ATOM 6829 C ASP C 83 -13.125 6.830 -14.025 1.00 26.94 C ANISOU 6829 C ASP C 83 2988 5108 2139 1694 536 755 C
ANISOU 6829 C ASP C 83 2988 5108 2139 1694 536 755 C ATOM 6830 O ASP C 83 -12.457 7.053 -15.041 1.00 28.95 O ANISOU 6830 O ASP C 83 3097 5666 2238 1850 661 876 O ATOM 6831 CB ASP C 83 -11.792 7.075 -11.942 1.00 28.61 C ANISOU 6831 CB ASP C 83 3191 5030 2648 1240 462 822 C ATOM 6832 CG ASP C 83 -10.924 8.123 -11.271 1.00 29.90 C ANISOU 6832 CG ASP C 83 3334 5092 2933 934 510 1037 C ATOM 6833 OD1 ASP C 83 -11.226 9.330 -11.416 1.00 30.31 O ANISOU 6834 OD2 ASP C 83 3490 5032 2996 811 615 1215 O ATOM 6834 OD2 ASP C 83 3392 5271 3188 814 412 1031 O ATOM 6835 H ASP C 83 -14.235 7.215 -11.415 1.00 29.28 H ATOM 6836 HA ASP C 83 -12.615 8.565 -13.085 1.00 31.30 H
 ATOM 6836 HA ASP C 83 -12.615 8.565 -13.085 1.00 31.30 H
ATOM 6837 HB2 ASP C 83 -12.185 6.522 -11.249 1.00 34.33 H
ATOM 6838 HB3 ASP C 83 -11.223 6.536 -12.514 1.00 34.33 H
ATOM 6839 N SER C 84 -14.025 5.857 -13.977 1.00 25.94 N
ANISOU 6839 N SER C 84 2959 4889 2006 1805 361 531 N
ATOM 6840 CA SER C 84 -14.301 5.045 -15.154 1.00 27.22 C
 ANISOU 6840 CA SER C 84 3112 5260 1971 2117 269 380 C ATOM 6841 C SER C 84 -15.690 4.452 -15.004 1.00 26.70 C
 ANISOU 6841 C SER C 84 3177 5006 1961 2111 67 231 ATOM 6842 O SER C 84 -16.309 4.518 -13.934 1.00 24.61
                                                                                                                                                                                                                                                                                                                 C
ATOM 6842 O SER C 84 -16.309 4.518 -13.934 1.00 24.61 O ANISOU 6842 O SER C 84 2974 4494 1883 1892 23 248 O ATOM 6843 CB SER C 84 -13.238 3.953 -15.349 1.00 28.55 C ANISOU 6843 CB SER C 84 3204 5581 2061 2315 179 219 ATOM 6844 OG SER C 84 -13.492 3.182 -16.515 1.00 30.36 O ANISOU 6844 OG SER C 84 3533 5945 2058 2572 57 46 O ATOM 6845 H SER C 84 -14.486 5.647 -13.282 1.00 31.12 H ATOM 6846 HA SER C 84 -14.298 5.613 -15.940 1.00 32.67 H ATOM 6847 HB2 SER C 84 -12.368 4.373 -15.434 1.00 34.25 H ATOM 6848 HB3 SER C 84 -13.246 3.366 -14.576 1.00 34.25 H ATOM 6849 HG SER C 84 -12.901 2.592 -16.603 1.00 36.43 H ATOM 6850 N TRP C 85 -16.170 3.875 -16.099 1.00 29.08 N ANISOU 6850 N TRP C 85 3518 5444 2086 2347 -61 99 N
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ATOM 6851 CA TRP C 85 -17.514 3.332 -16.151 1.00 28.78 ANISOU 6851 CA TRP C 85 3574 5239 2122 2278 -266 -18 ATOM 6852 C TRP C 85 -17.614 2.425 -17.369 1.00 31.04 ANISOU 6852 C TRP C 85 3945 5610 2237 2492 -428 -251 ATOM 6853 O TRP C 85 -16.700 2.352 -18.194 1.00 32.55 C **ANISOU 6853 O TRP C 85** 4127 6023 2218 2739 -329 -309 0 ATOM 6854 CB TRP C 85 -18.556 4.453 -16.215 1.00 27.66 ANISOU 6854 CB TRP C 85 3403 5098 2010 2202 -140 193 ATOM 6855 CG TRP C 85 -18.368 5.333 -17.414 1.00 29.56 ANISOU 6855 CG TRP C 85 3609 5577 2047 2372 312 ATOM 6856 CD1 TRP C 85 -18.969 5.195 -18.630 1.00 31.09 ANISOU 6856 CD1 TRP C 85 3823 5891 2101 2521 -15 C ATOM 6857 CD2 TRP C 85 -17.511 6.479 -17.519 1.00 29.31 C ANISOU 6857 CD2 TRP C 85 3506 5666 1963 2388 313 552 ATOM 6858 NE1 TRP C 85 -18.548 6.186 -19.483 1.00 32.28 ANISOU 6858 NE1 TRP C 85 3898 6238 2129 2659 207 414 Ν ATOM 6859 CE2 TRP C 85 -17.649 6.985 -18.827 1.00 30.82 ANISOU 6859 CE2 TRP C 85 3643 6026 2041 2552 C 625 ATOM 6860 CE3 TRP C 85 -16.644 7.125 -16.636 1.00 27.86 C ANISOU 6860 CE3 TRP C 85 3302 5402 1880 2206 473 706 ATOM 6861 CZ2 TRP C 85 -16.958 8.108 -19.270 1.00 31.87 ANISOU 6861 CZ2 TRP C 85 3700 6225 2184 2518 566 C 880 ATOM 6862 CZ3 TRP C 85 -15.957 8.237 -17.074 1.00 29.08 ANISOU 6862 CZ3 TRP C 85 3383 5605 2061 2141 654 932 ATOM 6863 CH2 TRP C 85 -16.118 8.721 -18.384 1.00 31.32 ANISOU 6863 CH2 TRP C 85 3612 6044 2243 2294 694 1027 ATOM 6864 H TRP C 85 -15.729 3.787 -16.833 1.00 34.89 ATOM 6865 HA TRP C 85 -17.680 2.801 -15.356 1.00 34.53 ATOM 6866 HB2 TRP C 85 -19.442 4.062 -16.263 1.00 33.20 -19.442 4.062 -16.263 1.00 33.20 H -18.477 5.005 -15.421 1.00 33.20 H -19.579 4.528 -18.849 1.00 37.31 H -18.803 6.285 -20.298 1.00 38.74 H -16.533 6.812 -15.768 1.00 33.43 H -17.063 8.430 -20.137 1.00 38.24 H -15.377 8.675 -16.493 1.00 34.90 H -15.641 9.472 -18.654 1.00 37.59 ATOM 6867 HB3 TRP C 85 ATOM 6868 HD1 TRP C 85 ATOM 6869 HE1 TRP C 85 ATOM 6870 HE3 TRP C 85 ATOM 6871 HZ2 TRP C 85 ATOM 6872 HZ3 TRP C 85 ATOM 6873 HH2 TRP C 85 -15.641 9.472 -18.654 1.00 37.58 ATOM 6874 N GLY C 86 -18.745 1.734 -17.474 1.00 29.41 Ν ANISOU 6874 N GLY C 86 3766 3632 3776 1889 -652 14 Ν ATOM 6875 CA GLY C 86 -19.021 0.924 -18.641 1.00 31.88 ANISOU 6875 CA GLY C 86 4102 3872 4140 2035 -819 -191 C ATOM 6876 C GLY C 86 ANISOU 6876 C GLY C 86 ATOM 6877 O GLY C 86 -19.733 1.749 -19.687 1.00 32.16 4053 3991 4175 1991 -781 -263 C -19.093 2.450 -20.476 1.00 32.37 0 ANISOU 6877 O GLY C 86 3986 4352 3962 2055 -704 -278 0 ATOM 6878 H GLY C 86 -19.367 1.722 -16.880 1.00 35.29 ATOM 6879 HA2 GLY C 86 -18.191 0.589 -19.014 1.00 38.26 ATOM 6880 HA3 GLY C 86 -19.583 0.172 -18.396 1.00 38.26 Η Н ATOM 6881 N THR C 87 -21.060 1.689 -19.679 1.00 32.52 Ν ANISOU 6881 N THR C 87 4128 3727 4500 1870 -830 -287 Ν ATOM 6882 CA THR C 87 -21.910 2.498 -20.544 1.00 33.71 C ANISOU 6882 CA THR C 87 4211 3908 4691 1810 -809 -353 ATOM 6883 C THR C 87 -22.678 3.464 -19.656 1.00 34.55 C ANISOU 6883 C THR C 87 4267 3925 4937 1551 -624 -191

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ATOM 6884 O THR C 87 -23.400 3.030 -18.752 1.00 34.08
ATOM 6887 CG2 THR C 87 -23.574 2.429 -22.441 1.00 36.72 C
ANISOU 6887 CG2 THR C 87 4605 4112 5235 1796 -1026 -617 C
ATOM 6888 H THR C 87 -21.506 1.167 -19.161 1.00 39.02 H
ATOM 6889 HA THR C 87 -21.306 1.167-19.161 1.00 39.02 H
ATOM 6889 HA THR C 87 -21.363 3.006 -21.164 1.00 40.46 H
ATOM 6890 HB THR C 87 -23.565 1.283 -20.740 1.00 43.48 H
ATOM 6891 HG1 THR C 87 -21.821 0.057 -21.315 1.00 47.13 H
ATOM 6892 HG21 THR C 87 -24.185 1.859 -22.933 1.00 44.07 H
ATOM 6893 HG22 THR C 87 -24.073 3.163 -22.050 1.00 44.07 H
ATOM 6894 HG23 THR C 87 -22.913 2.787 -23.054 1.00 44.07 H
ATOM 6895 N ALA C 88 -22.515 4.764 -19.902 1.00 36.22 N
ANISOU 6895 N ALA C 88 4403 4390 4969 1473 -477 -133
ATOM 6896 CA ALA C 88 -23.247 5.767 -19.142 1.00 36.18
ANISOU 6896 CA ALA C 88 4379 4324 5043 1206 -296 1
ATOM 6897 C ALA C 88 -23.318 7.059 -19.943 1.00 33.48
                                                                                                            CC
ANISOU 6897 C ALA C 88 3975 4191 4555 1185 -247 -14
ATOM 6898 O ALA C 88 -22.423 7.371 -20.733 1.00 35.70
ATOM 6900 H ALA C 88 -21.990 5.086 -20.502 1.00 43.47 H ATOM 6901 HA ALA C 88 -24.153 5.454 -18.993 1.00 43.42 H ATOM 6902 HB1 ALA C 88 -23.117 6.695 -17.306 1.00 44.68 H ATOM 6903 HB2 ALA C 88 -22.593 5.196 -17.272 1.00 44.68 H ATOM 6904 HB3 ALA C 88 -21.693 6.338 -17.913 1.00 44.68 H ATOM 6905 N ARG C 89 -24.392 7.807 -19.719 1.00 28.03 N ANISOU 6905 N ARG C 89 3274 3377 4000 1022 -169 12 N ATOM 6906 CA ARG C 89 -24.646 9.067 -20.414 1.00 25.54 C
ANISOU 6906 CA ARG C 89 2929 3196 3579 988 -144 0
ATOM 6907 C ARG C 89 -24.879 10.117 -19.335 1.00 24.15
                                                                                                            CC
ANISOU 6907 C ARG C 89 2795 3001 3381 784 13 141
ATOM 6908 O ARG C 89 -25.948 10.162 -18.722 1.00 24.81
ANISOU 6908 O ARG C 89 2882 2894 3649 694 85 152
ATOM 6909 CB ARG C 89 -25.839 8.937 -21.356 1.00 25.04
                                                                                                             0
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ATOM 6910 CG ARG C 89 -25.881 9.953 -22.483 1.00 24.37
ANISOU 6910 CG ARG C 89 2744 3060 3457 1125 -308 -213 ATOM 6911 CD ARG C 89 -26.915 9.555 -23.520 1.00 23.81
ANISOU 6911 CD ARG C 89 2660 2830 3559 1261 -498 -414 C
                                                -26.417 8.495 -24.387 1.00 24.19
ATOM 6912 NE ARG C 89
                                                                                                             Ν
ANISOU 6912 NE ARG C 89 2751 2915 3524 1486 -664 -547
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ATOM 6913 CZ ARG C 89 -25.746 8.701 -25.518 1.00 24.52
ANISOU 6913 CZ ARG C 89 2850 3201 3264 1641 -697 -586 C ATOM 6914 NH1 ARG C 89 -25.484 9.939 -25.935 1.00 22.97 N
ANISOU 6914 NH1 ARG C 89 2639 3223 2864 1662 -612 -498 N
ATOM 6915 NH2 ARG C 89 -25.346 7.663 -26.241 1.00 25.33
ANISOU 6915 NH2 ARG C 89 3034 3329 3262 1791 -821 -706 N
ATOM 6916 H ARG C 89 -25.007 7.601 -19.153 1.00 33.64 H
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ATOM 6917 HA ARG C 89
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ATOM 6918 HB2 ARG C 89
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                           -26.652 9.040 -20.838 1.00 30.05
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ATOM 6920 HG2 ARG C 89
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ATOM 6921 HG3 ARG C 89
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                                                              Н
                           -27.711 9.231 -23.070 1.00 28.58
ATOM 6922 HD2 ARG C 89
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                           -27.129 10.324 -24.071 1.00 28.58
ATOM 6923 HD3 ARG C 89
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ATOM 6924 HE ARG C 89
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ATOM 6925 HH11 ARG C 89
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ATOM 6926 HH12 ARG C 89
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ATOM 6927 HH21 ARG C 89
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                           -24.910 7.790 -26.971 1.00 30.40
ATOM 6928 HH22 ARG C 89
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ATOM 6929 N TRP C 90
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ANISOU 6929 N TRP C 90
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ATOM 6930 CA TRP C 90
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                                                              C
ANISOU 6930 CA TRP C 90
                           2723 2975 2921 570 138
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ATOM 6931 C TRP C 90
ANISOU 6931 C TRP C 90
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ATOM 6932 O TRP C 90
ANISOU 6932 O TRP C 90
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                         2682 3045 2847 552
                                                  60
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ATOM 6933 CB TRP C 90
                          -22.508 12.310 -17.597 1.00 23.29
ANISOU 6933 CB TRP C 90
                         2814 3234 2801 521
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ATOM 6934 CG TRP C 90
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ANISOU 6934 CG TRP C 90
                          2935 3448 2937 625
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ATOM 6935 CD1 TRP C 90
                           -20.715 10.527 -18.195 1.00 26.33
ANISOU 6935 CD1 TRP C 90
                           3049 3879 3075 764
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ATOM 6936 CD2 TRP C 90
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ANISOU 6936 CD2 TRP C 90
                           3053 3331 3018 631
                                                  131 529
ATOM 6937 NE1 TRP C 90
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ATOM 6938 CE2 TRP C 90
                                                              C
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ANISOU 6938 CE2 TRP C 90
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                                            765
ATOM 6939 CE3 TRP C 90
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ANISOU 6939 CE3 TRP C 90
                           3091 3050 2984 562
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                           -20.435 8.226 -15.435 1.00 25.75
ATOM 6940 CZ2 TRP C 90
ANISOU 6940 CZ2 TRP C 90
                           3213 3442 3130 810
                                                      544
                                                   62
ATOM 6941 CZ3 TRP C 90
                           -22.087 9.291 -14.030 1.00 25.12
                                                              C
ANISOU 6941 CZ3 TRP C 90
                           3312 3097 3136 606 260 635
                                                              C
ATOM 6942 CH2 TRP C 90
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ANISOU 6942 CH2 TRP C 90
                                                              C
                           3412 3307 3251 717
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                          -23.131 10.952 -19.529 1.00 27.88
ATOM 6943 H TRP C 90
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ATOM 6944 HA TRP C 90
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ATOM 6945 HB2 TRP C 90
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ATOM 6946 HB3 TRP C 90
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ATOM 6947 HD1 TRP C 90
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ATOM 6948 HE1 TRP C 90
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                           -22.976 10.930 -14.799 1.00 28.82
ATOM 6949 HE3 TRP C 90
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                           -19.805 7.559 -15.588 1.00 30.90
-22.554 9.296 -13.225 1.00 30.15
ATOM 6950 HZ2 TRP C 90
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ATOM 6951 HZ3 TRP C 90
                                                             Н
                           -20.991 7.636 -13.616 1.00 31.49
ATOM 6952 HH2 TRP C 90
                                                             Н
                          -25.613 13.597 -17.573 1.00 22.28 N
ATOM 6953 N THR C 91
ANISOU 6953 N THR C 91 2770 2749 2949 449 217 348
                                                             Ν
ATOM 6954 CA THR C 91 -26.550 14.655 -17.924 1.00 21.18
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ANISOU 6954 CA THR C 91 2656 2552 2840 431 204 294
 ATOM 6955 C THR C 91 -27.144 15.226 -16.645 1.00 20.19
ANISOU 6955 C THR C 91 2648 2320 2702 403 310 336
                                                                                                                                                                                                                    Č
 ANISOU 6955 C THR C 91 2040 2320 2702 403 310 330 ATOM 6956 O THR C 91 2669 2262 2765 422 434 386 ATOM 6957 CB THR C 91 2669 2262 2765 422 434 386 ATOM 6957 CB THR C 91 2800 2730 3318 512 172 161 ATOM 6958 OG1 THR C 91 2800 2730 3318 512 172 161 28.491 15.170 -19.305 1.00 23.96 ANISOU 6958 OG1 THR C 91 2907 2776 3420 517 134 98
                                                                                                                                                                                                                    Ö
 ATOM 6959 CG2 THR C 91 -28.481 13.055 -18.142 1.00 24.62 C ANISOU 6959 CG2 THR C 91 2892 2736 3725 518 273 160 C
  ATOM 6960 H THR C 91 -25.679 13.324 -16.760 1.00 26.74 H
ATOM 6960 H THR C 91 -25.679 13.324 -16.760 1.00 26.74 H ATOM 6961 HA THR C 91 -26.078 15.364 -18.388 1.00 25.42 H ATOM 6962 HB THR C 91 -27.226 13.691 -19.621 1.00 27.95 H ATOM 6963 HG1 THR C 91 -29.087 14.866 -19.812 1.00 28.75 H ATOM 6964 HG21 THR C 91 -29.168 12.720 -18.739 1.00 29.54 H ATOM 6965 HG22 THR C 91 -27.917 12.317 -17.864 1.00 29.54 H ATOM 6966 HG23 THR C 91 -28.904 13.441 -17.359 1.00 29.54 H ATOM 6967 N GLY C 92 -27.420 16.536 -16.657 1.00 17.71 N ANISOU 6967 N GLY C 92 -27.420 16.536 -16.523 1.00 18.73 C ANISOU 6968 CA GLY C 92 -27.447 18.617 -15.386 1.00 18.86 C
                                                                                                                                                                                                                    C
 ATOM 6969 C GLY C 92 -27.447 18.617 -15.386 1.00 18.86
ANISOU 6969 C GLY C 92 2927 2039 2200 376 164 349
ANISOU 6969 C GLY C 92 2927 2039 2200 376 164 349 C ATOM 6970 O GLY C 92 -26.818 19.154 -16.298 1.00 18.25 O ANISOU 6970 O GLY C 92 2834 2017 2082 286 12 376 O ATOM 6971 H GLY C 92 -27.272 17.052 -17.329 1.00 21.25 H ATOM 6972 HA2 GLY C 92 -28.966 17.270 -15.633 1.00 22.48 H ATOM 6973 HA3 GLY C 92 -27.811 16.721 -14.710 1.00 22.48 H ATOM 6974 N THR C 93 -27.710 19.230 -14.234 1.00 20.19 N ANISOU 6974 N THR C 93 3290 2128 2251 449 184 344 N ATOM 6975 CA THR C 93 -27.140 20.540 -13.941 1.00 21.23 C ANISOU 6975 CA THR C 93 3652 2194 2219 410 -36 352 C ATOM 6976 C THR C 93 -25.619 20.458 -13.985 1.00 21.10 C
ANISOU 6975 CA THR C 93  3652 2194 2219 410 -36 352 C ATOM 6976 C THR C 93 -25.619 20.458 -13.985 1.00 21.10 C ANISOU 6976 C THR C 93 3633 2243 2140 250 -189 469 C ATOM 6977 O THR C 93 -25.021 19.552 -13.400 1.00 21.88 O ANISOU 6977 O THR C 93 3694 2400 2219 252 -114 523 O ATOM 6978 CB THR C 93 -27.617 21.031 -12.565 1.00 22.15 C ANISOU 6978 CB THR C 93 4014 2217 2185 581 O 306 C ATOM 6979 OG1 THR C 93 -29.029 21.258 -12.607 1.00 22.26 O ANISOU 6979 OG1 THR C 93 3995 2205 2259 745 141 212 O ATOM 6980 CG2 THR C 93 -26.907 22.321 -12.160 1.00 22.78 C
  ANISOU 6980 CG2 THR C 93 4376 2178 2102 547 -305 297 C
ATOM 6989 CA TYR C 94 -23.576 21.391 -14.995 1.00 21.27 C
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ANISOU 6989 CA TYR C 94 3587 2361 2133 -67 -542 C ATOM 6990 C TYR C 94 -22.926 22.684 -14.510 1.00 23.37 Č ANISOU 6990 C TYR C 94 4058 2485 2337 -189 -842 748 Ö ATOM 6991 O TYR C 94 -23.386 23.781 -14.850 1.00 22.80 0 **ANISOU 6991 O TYR C 94** 4119 2280 2265 -214 -989 725 ATOM 6992 CB TYR C 94 -23.357 21.217 -16.508 1.00 19.92 SOOOOG ANISOU 6992 CB TYR C 94 3188 2352 2030 -141 -510 ATOM 6993 CG TYR C 94 -21.927 21.447 -16.940 1.00 20.81 ANISOU 6993 CG TYR C 94 3173 2607 2126 -320 -638 ATOM 6994 CD1 TYR C 94 -20.914 20.598 -16.519 1.00 20.91 **ANISOU 6994 CD1 TYR C 94** 3061 2756 2129 -338 -605 1029 ATOM 6995 CD2 TYR C 94 -21.586 22.518 -17.752 1.00 21.90 ANISOU 6995 CD2 TYR C 94 3302 2750 2270 -471 -792 1099 ATOM 6996 CE1 TYR C 94 -19.604 20.803 -16.904 1.00 22.14 3045 3076 2290 -494 -710 1235 ANISOU 6996 CE1 TYR C 94 -20.279 22.731 -18.140 1.00 23.25 ATOM 6997 CE2 TYR C 94 C ANISOU 6997 CE2 TYR C 94 3304 3077 2453 -651 -885 1338 ATOM 6998 CZ TYR C 94 -19.288 21.870 -17.709 1.00 23.40 ANISOU 6998 CZ TYR C 94 3161 3257 2472 -659 -838 1403 C ATOM 6999 OH TYR C 94 -17.975 22.065 -18.084 1.00 25.13 0 ANISOU 6999 OH TYR C 94 0 3158 3667 2723 -829 -917 1659 ATOM 7000 H TYR C 94 -25.404 22.099 -15.002 1.00 25.47 Н ATOM 7001 HA TYR C 94 -23.155 20.646 -14.538 1.00 25.52 Н ATOM 7002 HB2 TYR C 94 -23.602 20.312 -16.759 1.00 23.91 Н ATOM 7003 HB3 TYR C 94 -23.916 21.853 -16.981 1.00 23.91 ATOM 7004 HD1 TYR C 94 -21.122 19.875 -15.972 1.00 25.10 ATOM 7005 HD2 TYR C 94 ATOM 7006 HE1 TYR C 94 -22.250 23.101 -18.043 1.00 26.28 Н -18.936 20.224 -16.614 1.00 26.57 Н ATOM 7007 HE2 TYR C 94 -20.066 23.453 -18.686 1.00 27.90 Н ATOM 7008 HH TYR C 94 -17.914 22.746 -18.573 1.00 30.16 ATOM 7009 N LYS C 95 -21.847 22.557 -13.727 1.00 25.38 Ν 4345 2744 2555 -264 -970 ANISOU 7009 N LYS C 95 N ATOM 7010 CA LYS C 95 -21.240 23.703 -13.052 1.00 29.57 C ANISOU 7010 CA LYS C 95 5101 3086 3050 -366 -1314 ATOM 7011 C LYS C 95 -19.854 24.085 -13.557 1.00 32.95 **ANISOU 7011 C LYS C 95** 5350 3586 3585 -642 -1533 1094 C ATOM 7012 O LYS C 95 -19.463 25.242 -13.404 1.00 34.91 0 **ANISOU 7012 O LYS C 95** 5699 3660 3905 -783 -1805 1114 0 ATOM 7013 CB LYS C 95 -21.148 23.435 -11.544 1.00 31.89 ANISOU 7013 CB LYS C 95 5629 3276 3211 -207 -1363 768 ATOM 7014 CG LYS C 95 -22.499 23.222 -10.870 1.00 32.11 C ANISOU 7014 CG LYS C 95 5847 3239 3114 80 -1146 589 C ATOM 7015 CD LYS C 95 -23.335 24.487 -10.862 1.00 33.33 ANISOU 7015 CD LYS C 95 6248 3199 3215 168 -1304 478 C ATOM 7016 H LYS C 95 -21.447 21.811 -13.572 1.00 30.46 Н ATOM 7017 HA LYS C 95 -21.817 24.473 -13.177 1.00 35.49 Н ATOM 7018 HB2 LYS C 95 -20.617 22.636 -11.401 1.00 38.27 Н -20.721 24.194 -11.118 1.00 38.27 ATOM 7019 HB3 LYS C 95 Н ATOM 7020 HG2 LYS C 95 -22.991 22.537 -11.350 1.00 38.53 Н ATOM 7021 HG3 LYS C 95 -22.356 22.948 -9.950 1.00 38.53 Н ATOM 7022 N GLY C 96 -19.090 23.159 -14.125 1.00 34.91 Ν ANISOU 7022 N GLY C 96 5285 4094 3883 -705 -1380 1221 Ν ATOM 7023 CA GLY C 96 -17.772 23.497 -14.638 1.00 36.94 C

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ANISOU 7023 CA GLY C 96 5303 4477 4255 -950 -1533 1461
ATOM 7024 C GLY C 96
                         -16.877 22.269 -14.677 1.00 35.69
                                                            C
ANISOU 7024 C GLY C 96
                          4871 4593 4095 -918 -1388 1546
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ATOM 7025 O GLY C 96
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ANISOU 7025 O GLY C 96
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ATOM 7026 H GLY C 96
ATOM 7027 HA2 GLY C 96
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ATOM 7028 HA3 GLY C 96
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ATOM 7029 N THR C 97
                         -15.568 22.523 -14.675 1.00 35.45
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ANISOU 7029 N THR C 97
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ATOM 7030 CA THR C 97
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ANISOU 7030 CA THR C 97
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ATOM 7031 C THR C 97
                         -13.538 21.626 -13.640 1.00 35.09
                                                            C
ANISOU 7031 C THR C 97
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ATOM 7032 O THR C 97
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ANISOU 7032 O THR C 97
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ATOM 7033 CB THR C 97
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ANISOU 7033 CB THR C 97 3617 4941 3890 -1177 -1334 2106
                                                              C
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ATOM 7042 HG23 THR C 97
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ATOM 7045 C VAL C 98
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ATOM 7049 CG2 VAL C 98
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ANISOU 7049 CG2 VAL C 98
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ATOM 7051 HA VAL C 98
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ATOM 7052 HB VAL C 98
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ATOM 7053 HG11 VAL C 98 -13.089 18.743 -9.999 1.00 37.01
ATOM 7054 HG12 VAL C 98 -13.667 19.007 -11.456 1.00 37.01
ATOM 7055 HG13 VAL C 98
                          -12.313 18.197 -11.274 1.00 37.01
ATOM 7056 HG21 VAL C 98 -11.106 19.942 -9.197 1.00 43.56
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ATOM 7057 HG22 VAL C 98 -10.241 19.448 -10.435 1.00 43.56
ATOM 7058 HG23 VAL C 98 -10.375 21.002 -10.128 1.00 43.56
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ATOM 7059 N LYS C 99 -9.396 19.915 -12.906 1.00 37.38
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ANISOU 7059 N LYS C 99 3727 5711 4766 -1268 -1930 2249 ATOM 7060 CA LYS C 99 -8.292 19.030 -13.235 1.00 39.30 ANISOU 7060 CA LYS C 99 3598 6295 5039 -1187 -1804 2357 ATOM 7061 C LYS C 99 -7.725 18.469 -11.944 1.00 39.85 ANISOU 7061 C LYS C 99 3799 6241 5104 -1074 -1990 2202 ATOM 7062 O LYS C 99 -7.554 19.198 -10.962 1.00 41.97 **ANISOU 7062 O LYS C 99** 4292 6204 5451 -1188 -2294 2144 ATOM 7063 CB LYS C 99 -7.201 19.772 -14.013 1.00 43.04 ANISOU 7063 CB LYS C 99 3698 6951 5703 -1437 -1827 2690 C -9.145 20.698 -12.654 1.00 44.86 ATOM 7064 H LYS C 99 Н ATOM 7065 HA LYS C 99 -8.615 18.294 -13.778 1.00 47.16 ATOM 7066 N SER C 100 -7.437 17.169 -11.943 1.00 38.31 **ANISOU 7066 N SER C 100** 3491 6264 4803 -823 -1823 2120 Ν ATOM 7067 CA SER C 100 -6.939 16.547 -10.725 1.00 38.96 **ANISOU 7067 CA SER C 100** 3720 6233 4851 -683 -1999 1972 ATOM 7068 C SER C 100 -6.420 15.144 -11.008 1.00 39.06 **ANISOU 7068 C SER C 100** C 3526 6533 4782 -421 -1810 1932 ATOM 7069 O SER C 100 -7.062 14.366 -11.724 1.00 36.76 0 **ANISOU 7069 O SER C 100** 3218 6383 4364 -239 -1542 1878 0 ATOM 7070 CB SER C 100 -8.041 16.519 -9.664 1.00 36.99 **ANISOU 7070 CB SER C 100** 3974 5645 4435 -561 -2077 1753 ATOM 7071 OG SER C 100 -7.639 15.779 -8.529 1.00 37.81 0 **ANISOU 7071 OG SER C 100** 4250 5663 4451 -375 -2201 1620 -7.519 16.640 -12.615 1.00 45.98 ATOM 7072 H SER C 100 Н ATOM 7073 HA SER C 100 -6.203 17.075 -10.378 1.00 46.75 Н ATOM 7074 HB2 SER C 100 -8.239 17.429 -9.392 1.00 44.38 ATOM 7075 HB3 SER C 100 -8.833 16.107 -10.044 1.00 44.38 Н ATOM 7076 HG SER C 100 -7.465 14.988 -8.749 1.00 45.37 Н ATOM 7077 N ASP C 101 -5.248 14.830 -10.461 1.00 41.29 3662 6883 5144 -387 -1969 1942 **ANISOU 7077 N ASP C 101** N ATOM 7078 CA ASP C 101 -4.632 13.521 -10.633 1.00 41.71 C 3543 7178 5126 -118 -1838 1881 C **ANISOU 7078 CA ASP C 101** -4.556 13.131 -12.110 1.00 41.60 ATOM 7079 C ASP C 101 C ANISOU 7079 C ASP C 101 ATOM 7080 O ASP C 101 3215 7510 5079 -35 -1506 1980 C -4.914 12.022 -12.508 1.00 40.16 0 **ANISOU 7080 O ASP C 101** 3077 7432 4752 238 -1309 1851 0 ATOM 7081 CB ASP C 101 -5.390 12.472 -9.820 1.00 39.68 C **ANISOU 7081 CB ASP C 101** 3658 6743 4675 150 -1829 1666 ATOM 7082 CG ASP C 101 -5.589 12.898 -8.381 1.00 39.75 **ANISOU 7082 CG ASP C 101** 4049 6414 4642 114 -2112 1569 ATOM 7083 OD1 ASP C 101 -4.661 12.694 -7.571 1.00 42.17 0 4348 6696 4980 174 -2333 1528 **ANISOU 7083 OD1 ASP C 101** ATOM 7084 OD2 ASP C 101 -6.662 13.458 -8.065 1.00 38.05 0 4152 5960 4347 50 -2107 1521 **ANISOU 7084 OD2 ASP C 101** 0 ATOM 7085 H ASP C 101 -4.784 15.369 -9.978 1.00 49.55 ATOM 7086 HA ASP C 101 -3.725 13.558 -10.292 1.00 50.05 Н ATOM 7087 HB2 ASP C 101 -6.263 12.333 -10.217 1.00 47.61 Н ATOM 7088 HB3 ASP C 101 -4.886 11.644 -9.823 1.00 47.61 -4.081 14.067 -12.932 1.00 43.65 ATOM 7089 N GLY C 102 Ν **ANISOU 7089 N GLY C 102** 3191 7931 5463 -263 -1453 2217 N ATOM 7090 CA GLY C 102 -3.813 13.806 -14.334 1.00 44.43 ANISOU 7090 CA GLY C 102 3001 8391 5490 -167 -1144 2348 -5.023 13.743 -15.243 1.00 41.76 ATOM 7091 C GLY C 102 C

ANISOU 7091 C GLY C 102 2793 8074 5000 -82 -909 2296 C ATOM 7092 O GLY C 102 -4.849 13.607 -16.463 1.00 42.58 0 **ANISOU 7092 O GLY C 102** 2706 8470 5003 19 -665 2402 0 ATOM 7093 H GLY C 102 -3.905 14.874 -12.691 1.00 52.38 Н ATOM 7094 HA2 GLY C 102 -3.226 14.500 -14.673 1.00 53.32 Н ATOM 7095 HA3 GLY C 102 -3.345 12.959 -14.408 1.00 53.32 Н ATOM 7096 N GLY C 103 -6.244 13.826 -14.703 1.00 38.54 Ν **ANISOU 7096 N GLY C 103** 2721 7371 4552 -94 -979 2136 Ν ATOM 7097 CA GLY C 103 -7.445 13.856 -15.508 1.00 37.52 C **ANISOU 7097 CA GLY C 103** 2715 7228 4314 -31 -796 2080 C ATOM 7098 C GLY C 103 ANISOU 7098 C GLY C 103 -8.195 15.173 -15.353 1.00 37.30 C 2840 6965 4367 -319 -926 2166 C ATOM 7099 O GLY C 103 -7.886 15.999 -14.485 1.00 38.36 0 **ANISOU 7099 O GLY C 103** 3058 6887 4630 -547 -1183 2225 0 ATOM 7100 H GLY C 103 -6.394 13.866 -13.857 1.00 46.25 Н ATOM 7101 HA2 GLY C 103 -7.214 13.739 -16.443 1.00 45.03 Н ATOM 7102 HA3 GLY C 103 -8.033 13.132 -15.242 1.00 45.03 Н -9.185 15.365 -16.224 1.00 35.39 ATOM 7103 N THR C 104 Ν **ANISOU 7103 N THR C 104** 2661 6741 4044 -284 -770 2151 N ATOM 7104 CA THR C 104 -10.097 16.498 -16.158 1.00 34.15 C C **ANISOU 7104 CA THR C 104** 2709 6337 3928 -498 -878 2186 ATOM 7105 C THR C 104 -11.512 15.982 -15.923 1.00 30.76 ANISOU 7105 C THR C 104 ATOM 7106 O THR C 104 C 2647 5643 3398 -328 -759 1898 -11.939 15.010 -16.557 1.00 29.26 0 **ANISOU 7106 O THR C 104** 2441 5564 3113 -87 -559 1771 0 ATOM 7107 CB THR C 104 -10.054 17.334 -17.445 1.00 35.86 C **ANISOU 7107 CB THR C 104** 2713 6751 4162 -629 -772 2417 ATOM 7108 OG1 THR C 104 -8.715 17.782 -17.692 1.00 38.42 **ANISOU 7108 OG1 THR C 104** 2721 7279 4599 -796 -800 2691 0 -10.957 18.543 -17.327 1.00 35.52 ATOM 7109 CG2 THR C 104 C 2938 6383 4175 -848 -900 2414 **ANISOU 7109 CG2 THR C 104** C ATOM 7110 H THR C 104 -9.351 14.834 -16.880 1.00 42.47 Н ATOM 7111 HA THR C 104 -9.851 17.069 -15.413 1.00 40.98 Н ATOM 7112 HB THR C 104 -10.358 16.794 -18.192 1.00 43.04 Н ATOM 7113 HG1 THR C 104 -8.691 18.239 -18.397 1.00 46.11 Н ATOM 7114 HG21 THR C 104 -10.922 19.064 -18.144 1.00 42.62 Н ATOM 7115 HG22 THR C 104 -11.872 18.260 -17.172 1.00 42.62 Н ATOM 7116 HG23 THR C 104 -10.670 19.100 -16.586 1.00 42.62 Н ATOM 7117 N TYR C 105 -12.245 16.637 -15.024 1.00 28.51 Ν **ANISOU 7117 N TYR C 105** 2686 5007 3139 -442 -894 1798 N ATOM 7118 CA TYR C 105 -13.537 16.140 -14.553 1.00 26.82 **ANISOU 7118 CA TYR C 105** 2794 4544 2853 -290 -781 1556 C ATOM 7119 C TYR C 105 -14.617 17.193 -14.757 1.00 26.62 C **ANISOU 7119 C TYR C 105** C 2965 4310 2841 -399 -790 1518 ATOM 7120 O TYR C 105 -14.420 18.356 -14.398 1.00 27.23 **ANISOU 7120 O TYR C 105** 3126 4248 2970 -593 -1002 1607 0 ATOM 7121 CB TYR C 105 -13.480 15.774 -13.067 1.00 26.23 C **ANISOU 7121 CB TYR C 105** 2964 4258 2742 -230 -901 1450 ATOM 7122 CG TYR C 105 -12.555 14.637 -12.683 1.00 27.02 **ANISOU 7122 CG TYR C 105** 2942 4505 2817 -84 -911 1447 ATOM 7123 CD1 TYR C 105 -11.178 14.815 -12.633 1.00 29.57 **ANISOU 7123 CD1 TYR C 105** 3010 5020 3204 -171 -1086 1604 C ATOM 7124 CD2 TYR C 105 -13.065 13.398 -12.320 1.00 25.98

ANISOU 7124 CD2 TYR C 105 2951 4301 2618 135 -769 1300 C ATOM 7125 CE1 TYR C 105 -10.332 13.785 -12.262 1.00 30.34 **ANISOU 7125 CE1 TYR C 105** 2998 5254 3275 -9 -1113 1588 ATOM 7126 CE2 TYR C 105 -12.224 12.354 -11.941 1.00 26.82 C **ANISOU 7126 CE2 TYR C 105** 2982 4513 2695 287 -807 1290 ATOM 7127 CZ TYR C 105 -10.858 12.555 -11.915 1.00 29.06 **ANISOU 7127 CZ TYR C 105** 3018 5005 3020 231 -979 1420 C ATOM 7128 OH TYR C 105 -10.010 11.531 -11.541 1.00 30.57 0 **ANISOU 7128 OH TYR C 105** 3128 5309 3179 408 -1033 1399 0 ATOM 7129 H TYR C 105 -12.012 17.384 -14.667 1.00 34.21 Н ATOM 7130 HA TYR C 105 -13.781 15.347 -15.056 1.00 32.19 Н -13.191 16.558 -12.573 1.00 31.47 ATOM 7131 HB2 TYR C 105 Н ATOM 7132 HB3 TYR C 105 -14.373 15.527 -12.781 1.00 31.47 -10.817 15.640 -12.865 1.00 35.48 ATOM 7133 HD1 TYR C 105 ATOM 7134 HD2 TYR C 105 -13.984 13.261 -12.336 1.00 31.17 Н ATOM 7135 HE1 TYR C 105 -9.413 13.921 -12.243 1.00 36.41 Н ATOM 7136 HE2 TYR C 105 -12.580 11.527 -11.709 1.00 32.18 Н ATOM 7137 HH TYR C 105 -10.454 10.842 -11.357 1.00 36.69 Н ATOM 7138 N ASP C 106 -15.763 16.777 -15.304 1.00 26.74 Ν **ANISOU 7138 N ASP C 106** 3060 4277 2823 -264 -595 1378 N ATOM 7139 CA ASP C 106 -16.946 17.630 -15.368 1.00 26.58 C **ANISOU 7139 CA ASP C 106** 3245 4042 2811 -311 -593 1298 ATOM 7140 C ASP C 106 -17.706 17.588 -14.045 1.00 27.08 3612 3839 2839 -239 -610 1152 C **ANISOU 7140 C ASP C 106** ATOM 7141 O ASP C 106 -17.839 16.528 -13.426 1.00 24.81 0 **ANISOU 7141 O ASP C 106** 3375 3530 2523 -97 -504 1072 00000 ATOM 7142 CB ASP C 106 -17.877 17.178 -16.493 1.00 25.71 **ANISOU 7142 CB ASP C 106** 3074 3994 2702 -183 -401 1204 ATOM 7143 CG ASP C 106 -17.274 17.367 -17.871 1.00 27.06 **ANISOU 7143 CG ASP C 106** 2997 4437 2849 -205 -368 1349 ATOM 7144 OD1 ASP C 106 0 -16.744 18.460 -18.140 1.00 27.88 **ANISOU 7144 OD1 ASP C 106** 3042 4582 2970 -396 -486 1536 -17.331 16.417 -18.686 1.00 27.11 ATOM 7145 OD2 ASP C 106 0 **ANISOU 7145 OD2 ASP C 106** 0 2879 4610 2813 -18 -233 1285 ATOM 7146 H ASP C 106 -15.878 15.998 -15.648 1.00 32.09 Н ATOM 7147 HA ASP C 106 -16.676 18.546 -15.539 1.00 31.89 Н ATOM 7148 HB2 ASP C 106 -18.074 16.235 -16.379 1.00 30.86 Н ATOM 7149 HB3 ASP C 106 -18.697 17.695 -16.451 1.00 30.86 Н ATOM 7150 N ILE C 107 -18.245 18.736 -13.635 1.00 26.85 N **ANISOU 7150 N ILE C 107** 3798 3608 2796 -313 -736 1126 -18.936 18.870 -12.355 1.00 27.13 ATOM 7151 CA ILE C 107 4141 3420 2748 -203 -754 1001 **ANISOU 7151 CA ILE C 107** ATOM 7152 C ILE C 107 -20.437 18.935 -12.604 1.00 25.09 3974 3066 2494 -89 -568 875 **ANISOU 7152 C ILE C 107** 00 ATOM 7153 O ILE C 107 -20.911 19.816 -13.331 1.00 24.77 **ANISOU 7153 O ILE C 107** 3936 2984 2490 -153 -620 870 ATOM 7154 CB ILE C 107 -18.466 20.121 -11.597 1.00 30.16 **ANISOU 7154 CB ILE C 107** 4738 3629 3093 -307 -1075 1031 ATOM 7155 CG1 ILE C 107 -16.974 20.023 -11.265 1.00 32.20 **ANISOU 7155 CG1 ILE C 107** 4876 3970 3390 -430 -1292 1160 ATOM 7156 CG2 ILE C 107 -19.299 20.322 -10.316 1.00 30.55 ANISOU 7156 CG2 ILE C 107 5148 3468 2994 -114 -1077 880 C ATOM 7157 CD1 ILE C 107 -16.379 21.322 -10.726 1.00 35.18

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ATOM 7159 HA ILE C 107
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                                                            Н
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ATOM 7160 HB ILE C 107
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ATOM 7162 HG13 ILE C 107 -16.489 19.785 -12.070 1.00 38.65
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ATOM 7163 HG21 ILE C 107
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ATOM 7164 HG22 ILE C 107
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ATOM 7165 HG23 ILE C 107
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ATOM 7166 HD11 ILE C 107
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ATOM 7167 HD12 ILE C 107
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ATOM 7168 HD13 ILE C 107
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ATOM 7169 N TYR C 108
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ATOM 7170 CA TYR C 108
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ANISOU 7170 CA TYR C 108
ATOM 7171 C TYR C 108
ANISOU 7171 C TYR C 108
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ATOM 7172 O TYR C 108 -22.715 17.656 -9.680 1.00 22.60
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ATOM 7173 CB TYR C 108
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ANISOU 7173 CB TYR C 108
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                                                   30 672
ATOM 7174 CG TYR C 108
ANISOU 7174 CG TYR C 108
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ATOM 7175 CD1 TYR C 108
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ANISOU 7175 CD1 TYR C 108
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ATOM 7176 CD2 TYR C 108
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ATOM 7177 CE1 TYR C 108
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ANISOU 7177 CE1 TYR C 108
                           2540 2488 1934 102
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ATOM 7178 CE2 TYR C 108
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ANISOU 7178 CE2 TYR C 108
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ATOM 7179 CZ TYR C 108
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ATOM 7180 OH TYR C 108
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ANISOU 7180 OH TYR C 108
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ATOM 7181 H TYR C 108
ATOM 7182 HA TYR C 108
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-24.142 16.887 -12.898 1.00 24.44 H
ATOM 7183 HB2 TYR C 108
ATOM 7184 HB3 TYR C 108
ATOM 7185 HD1 TYR C 108
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H
H
ATOM 7186 HD2 TYR C 108
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ATOM 7187 HE1 TYR C 108
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ATOM 7188 HE2 TYR C 108
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ATOM 7189 HH TYR C 108
ATOM 7190 N THR C 109
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ANISOU 7190 N THR C 109
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ATOM 7191 CA THR C 109
                          -25.439 18.254 -9.551 1.00 26.35
ANISOU 7191 CA THR C 109 4701 2861 2450 659 227 559
ATOM 7192 C THR C 109 -26.722 17.635 -10.071 1.00 26.33
ANISOU 7192 C THR C 109 4483 2884 2636 702 490 549
ATOM 7193 O THR C 109 -27.258 18.060 -11.100 1.00 25.92
ANISOU 7193 O THR C 109 4300 2831 2717 648 454 483
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ATOM 7195 OG1 THR C 109
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ANISOU 7195 OG1 THR C 109
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                                                       391
ATOM 7196 CG2 THR C 109
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ANISOU 7196 CG2 THR C 109
ATOM 7197 H THR C 109
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ATOM 7198 HA THR C 109
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ATOM 7202 HG22 THR C 109
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ATOM 7203 HG23 THR C 109
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ATOM 7204 N THR C 110
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ANISOU 7204 N THR C 110
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ATOM 7205 CA THR C 110
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ANISOU 7205 CA THR C 110
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ATOM 7206 C THR C 110
ANISOU 7206 C THR C 110 5249 3785 3578 1039 1228 ATOM 7207 O THR C 110 -28.485 16.194 -7.185 1.00 34.35
                                                              C
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ANISOU 7207 O THR C 110
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ATOM 7208 CB THR C 110
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ANISOU 7208 CB THR C 110
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ATOM 7209 OG1 THR C 110
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ANISOU 7209 OG1 THR C 110
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ATOM 7210 CG2 THR C 110
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ANISOU 7210 CG2 THR C 110
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ATOM 7211 H THR C 110
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ATOM 7212 HA THR C 110
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ATOM 7213 HB THR C 110
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ATOM 7214 HG1 THR C 110
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ATOM 7215 HG21 THR C 110
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ATOM 7216 HG22 THR C 110
                            -28.325 15.445 -12.234 1.00 29.78
                                                              Н
ATOM 7217 HG23 THR C 110
                          -26.903 15.166 -11.606 1.00 29.78
ATOM 7218 N THR C 111
                          -30.396 15.567 -8.164 1.00 37.06
                           5547 4298 4236 1102 1487 826
ANISOU 7218 N THR C 111
                                                              Ν
ATOM 7219 CA THR C 111
                           -31.076 15.458 -6.887 1.00 42.95
ANISOU 7219 CA THR C 111
                           6390 5106 4823 1319 1777
ATOM 7220 C THR C 111
                          -31.919 14.200 -6.891 1.00 46.07
                                                              C
ANISOU 7220 C THR C 111
                         6478 5507 5521 1244 2059 1162
ATOM 7221 O THR C 111
                          -32.483 13.816 -7.922 1.00 45.27
                                                            0
ANISOU 7221 O THR C 111
                                                              0
                         6076 5357 5769 1089 2031 1134
ATOM 7222 CB THR C 111
                           -31.940 16.694 -6.593 1.00 45.08
                                                             C
                                                              C
ANISOU 7222 CB THR C 111
                          6763 5434 4931 1553 1830 864
ATOM 7223 OG1 THR C 111
                           -32.406 16.641 -5.237 1.00 48.83
                                                              0
                           7391 6009 5152 1830 2112 999
ANISOU 7223 OG1 THR C 111
                                                              0
                                                              C
ATOM 7224 CG2 THR C 111
                           -33.123 16.778 -7.549 1.00 45.29
ANISOU 7224 CG2 THR C 111 6454 5475 5278 1499 1910 823
                                                              C
ATOM 7225 H THR C 111
                          -30.881 15.379 -8.850 1.00 44.47
                                                           Н
                         -30.416 15.377 -6.181 1.00 51.54
ATOM 7226 HA THR C 111
                                                            Н
ATOM 7227 HB THR C 111 -31.402 17.492 -6.712 1.00 54.09
ATOM 7228 HG1 THR C 111 -31.753 16.629 -4.709 1.00 58.59
ATOM 7229 HG21 THR C 111 -33.656 17.563 -7.348 1.00 54.35
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ATOM 7230 HG22 THR C 111 -32.806 16.837 -8.464 1.00 54.35 ATOM 7231 HG23 THR C 111 -33.679 15.988 -7.458 1.00 54.35 H ATOM 7232 N ARG C 112 -31.967 13.552 -5.735 1.00 49.71 N ANISOU 7232 N ARG C 112 7031 6008 5849 1354 2301 1373 N ATOM 7233 CA ARG C 112 -32.742 12.341 -5.527 1.00 52.98 C ANISOU 7233 CA ARG C 112 7165 6395 6570 1259 2491 1581 ATOM 7234 C ARG C 112 -33.839 12.650 -4.521 1.00 56.48 ANISOU 7234 C ARG C 112 7580 6958 6923 1468 2717 1691 ATOM 7235 O ARG C 112 -33.567 13.215 -3.458 1.00 58.43 ANISOU 7235 O ARG C 112 8117 7279 6807 1701 2731 1674 ATOM 7236 CB ARG C 112 -31.843 11.204 -5.029 1.00 53.88 ANISOU 7236 CB ARG C 112 7378 6430 6665 1173 2429 1685 C ATOM 7237 CG ARG C 112 -31.629 10.055 -6.019 1.00 52.98 ANISOU 7237 CG ARG C 112 7041 6170 6920 919 2330 1728 ATOM 7238 CD ARG C 112 -31.381 10.540 -7.437 1.00 49.74 ANISOU 7238 CD ARG C 112 6530 5716 6651 801 2105 1518 C ATOM 7239 H ARG C 112 -31.542 13.806 -5.031 1.00 59.66 H ATOM 7240 HA ARG C 112 -33.153 12.069 -6.363 1.00 63.57 H ATOM 7241 HB2 ARG C 112 -30.970 11.572 -4.818 1.00 64.66 ATOM 7242 HB3 ARG C 112 -32.238 10.828 -4.227 1.00 64.66 ATOM 7242 HB3 ARG C 112 -30.870 11.572 -4.818 1.00 64.66 H
ATOM 7242 HB3 ARG C 112 -32.238 10.828 -4.227 1.00 64.66 H
ATOM 7243 HG2 ARG C 112 -30.859 9.537 -5.740 1.00 63.58 H
ATOM 7244 HG3 ARG C 112 -32.421 9.495 -6.028 1.00 63.58 H
ATOM 7245 N TYR C 113 -35.078 12.335 -4.889 1.00 70.74 N
ANISOU 7245 CA TYR C 113 9081 7809 9986 866 2745 1775 N ATOM 7246 CA TYR C 113 -36.218 12.411 -3.987 1.00 74.62 C ANISOU 7246 CA TYR C 113 9147 8621 10584 1059 2973 2128 ATOM 7247 C TYR C 113 -36.951 11.081 -4.033 1.00 80.14 C ANISOU 7247 C TYR C 113 9438 9384 11627 711 2854 2411 C ATOM 7248 O TYR C 113 -37.178 10.527 -5.113 1.00 78.27 O ANISOU 7248 O TYR C 113 9132 9034 11574 392 2513 2390 O ATOM 7249 CB TYR C 113 -37.172 13.549 -4.367 1.00 75.14 C ANISOU 7249 CB TYR C 113 9035 8884 10632 1350 2984 2225 C ATOM 7250 H TYR C 113 -35.287 12.068 -5.679 1.00 84.89 H ATOM 7251 HA TYR C 113 -35.905 12.560 -3.081 1.00 89.55 H ATOM 7252 N ASN C 114 -37.323 10.569 -2.862 1.00 87.62 N ANISOU 7252 N ASN C 114 10142 10496 12653 773 3132 2679 N ATOM 7253 CA ASN C 114 -37.826 9.203 -2.785 1.00 93.96 C ANISOU 7253 CA ASN C 114 10613 11313 13776 414 3050 2931 ATOM 7254 C ASN C 114 -36.690 8.264 -3.161 1.00 90.54 C ANISOU 7254 C ASN C 114 10536 10562 13302 78 2866 2683 C ATOM 7255 O ASN C 114 -36.789 7.509 -4.135 1.00 92.53 O ANISOU 7255 O ASN C 114 10760 10659 13738 -290 2539 2656 O ATOM 7256 CB ASN C 114 -39.030 9.000 -3.712 1.00 99.47 C ANISOU 7256 CB ASN C 114 10871 12121 14804 205 2763 3149 C ATOM 7257 H ASN C 114 -37.295 10.985 -2.110 1.00105.14 H ATOM 7258 HA ASN C 114 -38.100 9.008 -1.876 1.00112.76 H ATOM 7259 N ALA C 115 -35.597 8.327 -2.400 1.00 84.12 N ANISOU 7259 N ALA C 115 10080 9642 12239 217 3067 2502 N ATOM 7262 O ALA C 115 -33.882 7.656 -0.341 1.00 72.43 O

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ANISOU 7262 O ALA C 115 9060 8031 10428 387 3497 2389
ATOM 7263 CB ALA C 115
                             -33.343 8.433 -3.382 1.00 73.68
                                                                   C
ANISOU 7263 CB ALA C 115 9562 7819 10613 73 2824 1884
                                                                  C
ATOM 7264 H ALA C 115 -35.532 8.819 -1.697 1.00100.94
ATOM 7265 HA ALA C 115
                             -34.620 6.824 -3.268 1.00 91.78
                              -33.710 8.764 -4.216 1.00 88.41
-33.113 9.177 -2.803 1.00 88.41
-32.557 7.894 -3.556 1.00 88.41
ATOM 7266 HB1 ALA C 115
                                                                  Н
ATOM 7267 HB2 ALA C 115
ATOM 7268 HB3 ALA C 115
                                                                   Н
ATOM 7269 N PRO C 116
                             -33.236 5.804 -1.444 1.00 60.02
ANISOU 7269 N PRO C 116
                              7591 6105 9108 -255 3131 2298
                                                                    Ν
ATOM 7270 CA PRO C 116
                              -32.545 5.272 -0.265 1.00 55.56
                                                                   C
                             7169 5529 8414 -167 3337 2302
ANISOU 7270 CA PRO C 116
ATOM 7271 C PRO C 116
ANISOU 7271 C PRO C 116
                             -31.226 5.987 -0.032 1.00 51.95
                             7136 4939 7662 44 3367 1982
                                                                  C
ATOM 7272 O PRO C 116
                             -30.499 6.312 -0.974 1.00 48.11
                                                                  0
                            6905 4243 7131 -44 3203 1742
ANISOU 7272 O PRO C 116
                                                                    0
ATOM 7273 CB PRO C 116
                              -32.323 3.799 -0.622 1.00 54.42
                                                                   C
                             7026 5248 8405 -539 3091 2271
ANISOU 7273 CB PRO C 116
ATOM 7274 CG PRO C 116
                             -32.245 3.800 -2.120 1.00 53.62
ANISOU 7274 CG PRO C 116
                             7032 4933 8408 -798 2810 2145
                                                                   C
ATOM 7275 CD PRO C 116
                              -33.189 4.869 -2.580 1.00 56.42
ANISOU 7275 CD PRO C 116
                             7167 5430 8839 -666 2817 2250
                             -33.104 5.340 0.524 1.00 66.67

-31.492 3.486 -0.231 1.00 65.31

-33.074 3.267 -0.314 1.00 65.31

-31.339 4.003 -2.398 1.00 64.34

-32.520 2.933 -2.460 1.00 64.34

-32.838 5.312 -3.368 1.00 67.70
ATOM 7276 HA PRO C 116
                                                                   Н
ATOM 7277 HB2 PRO C 116
                                                                  Н
ATOM 7278 HB3 PRO C 116
ATOM 7279 HG2 PRO C 116
ATOM 7280 HG3 PRO C 116
                                                                   Н
ATOM 7281 HD2 PRO C 116
ATOM 7282 HD3 PRO C 116 -34.069 4.494 -2.745 1.00 67.70
                                                                   Н
ATOM 7283 N SER C 117 -30.916 6.220 1.236 1.00 53.73
ANISOU 7283 N SER C 117 7443 5275 7696 322 3547 1974
ATOM 7284 CA SER C 117
                             -29.680 6.892 1.613 1.00 51.91
ANISOU 7284 CA SER C 117 7590 4926 7208 517 3557 1695
ATOM 7285 C SER C 117 -29.198 6.242 2.905 1.00 52.56 ANISOU 7285 C SER C 117 7738 5041 7189 617 3620
                            7738 5041 7189 617 3620 1707
ATOM 7286 O SER C 117
                             -29.549 5.098 3.220 1.00 53.37
ANISOU 7286 O SER C 117 7662 5193 7424 461 3605 1858
ATOM 7287 CB SER C 117
                             -29.905 8.408 1.732 1.00 52.13
ANISOU 7287 CB SER C 117
                            7717 5042 7046 846 3700 1650
ATOM 7288 H SER C 117
                             -31.410 5.997 1.904 1.00 64.47
                                                                Н
ATOM 7289 HA SER C 117
                              -29.011 6.738 0.928 1.00 62.29
ATOM 7290 N ILE C 118
                           -28.378 6.971 3.659 1.00 52.25
ANISOU 7290 N ILE C 118
                            7981 4958 6912 872 3674 1546
ATOM 7291 CA ILE C 118
                            -27.971 6.537 4.991 1.00 53.71
ANISOU 7291 CA ILE C 118
                            8268 5167 6971 1022 3743 1576
ATOM 7292 C ILE C 118
                           -28.853 7.158 6.071 1.00 56.56
                                                                C
ANISOU 7292 C ILE C 118
                            8570 5713 7206 1350 3927 1753
ATOM 7293 O ILE C 118
                            -28.886 6.642 7.200 1.00 57.25
                                                              0
ANISOU 7293 O ILE C 118 8680 5844 7227 1468 4014 1858
ATOM 7294 CB ILE C 118 -26.483 6.864 5.244 1.00 51.35 C ANISOU 7294 CB ILE C 118 8330 4679 6501 1084 3648 1314 ATOM 7295 CG1 ILE C 118 -26.230 8.373 5.149 1.00 50.23 C
ANISOU 7295 CG1 ILE C 118 8412 4495 6180 1295 3634 1163
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ATOM 7296 CG2 ILE C 118 -25.614 6.108 4.240 1.00 49.23
ANISOU 7296 CG2 ILE C 118 8086 4245 6373 778 3463 1149
ATOM 7297 CD1 ILE C 118
                                                   -24.796 8.781 5.450 1.00 48.41
ANISOU 7297 CD1 ILE C 118 8524 4069 5801 1331 3509 947
ATOM 7298 H ILE C 118 -28.041 7.725 3.419 1.00 62.69 H
ATOM 7299 HA ILE C 118
                                                  -28.074 5.574 5.047 1.00 64.45
                                                                                                                Н
                                                  -26.250 6.567 6.138 1.00 61.62
ATOM 7300 HB ILE C 118
ATOM 7301 HG12 ILE C 118 -26.438 8.668 4.249 1.00 60.28 H
ATOM 7302 HG13 ILE C 118 -26.805 8.826 5.785 1.00 60.28 H
ATOM 7303 HG21 ILE C 118 -24.682 6.320 4.407 1.00 59.07 H
ATOM 7304 HG22 ILE C 118 -25.762 5.156 4.349 1.00 59.07 H
                                                    -25.859 6.381 3.342 1.00 59.07
-24.719 9.744 5.369 1.00 58.09
ATOM 7305 HG23 ILE C 118
                                                                                                                    Н
ATOM 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 N ASP C 119 -29.563 8.238 5 750 1 00 5730 ANISOU 7309 AN
ATOM 7306 HD11 ILE C 118
                                                                                                                   Н
ANISOU 7309 N ASP C 119
                                                  8671 5971 7326 1512 3982 1787 N
                                                    -30.650 8.754 6.593 1.00 60.35
ATOM 7310 CA ASP C 119
                                                                                                                     C
                                                   8865 6481 7585 1802 4150 1999
ANISOU 7310 CA ASP C 119
                                                  -32.006 8.340 6.041 1.00 62.12
ATOM 7311 C ASP C 119
ANISOU 7311 C ASP C 119 8644 6884 8075 1686 4245 2278 ATOM 7312 O ASP C 119 -32.891 9.180 5.878 1.00 65.13
ANISOU 7312 O ASP C 119
ATOM 7313 CB ASP C 119
                                                 8884 7403 8460 1865 4328 2391
                                                    -30.575 10.273 6.698 1.00 60.09
ANISOU 7313 CB ASP C 119
                                                   9065 6441 7327 2081 4121 1870
ATOM 7314 CG ASP C 119
                                                    -29.311 10.755 7.363 1.00 58.14
                                                                                                                      C
                                                    9240 6019 6831 2179 3987 1638
ANISOU 7314 CG ASP C 119
ATOM 7315 OD1 ASP C 119
                                                   -28.560 9.912 7.898 1.00 57.58
                                                                                                                      0
ANISOU 7315 OD1 ASP C 119 9274 5858 6747 2097 3964 1602
                                                     -29.082 11.988 7.368 1.00 57.11
ATOM 7316 OD2 ASP C 119
                                                                                                                  0
ANISOU 7316 OD2 ASP C 119 9328 5848 6524 2324 3887 1510 O
                                                  -29.430 8.704 5.048 1.00 69.38
ATOM 7317 H ASP C 119
ATOM 7318 HA ASP C 119
                                                  -30.564 8.386 7.486 1.00 72.43
ATOM 7319 HB2 ASP C 119
                                                   -30.608 10.653 5.806 1.00 72.11
-31.328 10.590 7.221 1.00 72.11
ATOM 7320 HB3 ASP C 119
ATOM 7321 N GLY C 120
                                                  -32.195 7.065 5.727 1.00 60.50
ANISOU 7321 N GLY C 120
                                                    8209 6672 8105 1375 4206 2399
ATOM 7322 CA GLY C 120
                                                    -33.512 6.552 5.403 1.00 62.59
ANISOU 7322 CA GLY C 120
                                                   8030 7100 8652 1241 4270 2703 C
ATOM 7323 C GLY C 120
ANISOU 7323 C GLY C 120
                                                                                                                   C
                                                   -33.547 5.790 4.089 1.00 62.36
                                                    7828 6982 8886 807 4073 2704
ATOM 7324 O GLY C 120
ANISOU 7324 O GLY C 120
                                                   -32.626 5.830 3.273 1.00 57.91
                                                   7496 6228 8278 640 3904 2464 O
ATOM 7325 H GLY C 120
                                                   -31.571 6.474 5.696 1.00 72.60
ATOM 7326 HA2 GLY C 120
                                                   -33.807 5.956 6.109 1.00 75.11
                                                                                                                 Н
                                                  -34.138 7.290 5.345 1.00 75.11
ATOM 7327 HA3 GLY C 120
                                                                                                                    Н
                                                  -34.677 5.098 3.894 1.00 68.76
ATOM 7328 N ASP C 121
                                                 8230 7913 9984 624 4080 2989
ANISOU 7328 N ASP C 121
ATOM 7329 CA ASP C 121
                                                 -34.899 4.236 2.736 1.00 71.86
ANISOU 7329 CA ASP C 121 8442 8208 10655 181 3845 3032
ATOM 7330 C ASP C 121 -35.563 4.961 1.574 1.00 75.38 C ANISOU 7330 C ASP C 121 8679 8695 11268 106 3763 3114 C
ATOM 7331 O ASP C 121 -35.421 4.532 0.423 1.00 74.42
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ANISOU 7331 O ASP C 121 8568 8402 11306 -240 3509 3049 ATOM 7332 CB ASP C 121 -35.767 3.038 3.135 1.00 75.30 C ANISOU 7332 CB ASP C 121 8550 8727 11332 -17 3849 3294 CATOM 7333 H ASP C 121 -35.344 5.116 4.437 1.00 82.52 H ATOM 7335 N ARG C 122 -36.308 6.030 1.850 1.00 80.41 N ANISOU 7335 N ARG C 122 9142 9545 11867 433 3954 3258 N ATOM 7336 CA ARG C 122 36.862 6.808 0.840 4.00 82.73 ATOM 7336 CA ARG C 122 -36.862 6.898 0.810 1.00 83.72 C ANISOU 7336 CA ARG C 122 9391 10028 12392 442 3884 3311 C ATOM 7337 C ARG C 122 -36.620 8.330 1.279 1.00 84.36 C
ANISOU 7337 C ARG C 122 9712 10201 12140 918 4083 3172 C
ATOM 7338 O ARG C 122 -37.353 8.841 2.132 1.00 86.98 O
ANISOU 7338 O ARG C 122 9891 10743 12416 1251 4299 3352 O
ATOM 7339 CB ARG C 122 -38.343 6.623 0.576 1.00 89.12 C ANISOU 7339 CB ARG C 122 9485 10928 13447 331 3869 3700 C ATOM 7340 H ARG C 122 -36.510 6.279 2.647 1.00 96.50 H ATOM 7341 HA ARG C 122 -36.384 6.758 -0.022 1.00100.47 H
ATOM 7342 N THR C 123 -35.586 8.969 0.731 1.00 81.71 N
ANISOU 7342 N THR C 123 9800 9675 11570 951 3912 2789 N
ATOM 7343 CA THR C 123 -35.115 10.248 1.239 1.00 79.95 C ANISOU 7343 CA THR C 123 9902 9474 11003 1361 4079 2609 C ATOM 7344 C THR C 123 -34.784 11.184 0.086 1.00 74.06 C ANISOU 7344 C THR C 123 9354 8615 10170 1369 3832 2320 C ATOM 7345 O THR C 123 -34.728 10.783 -1.080 1.00 76.14 O ANISOU 7345 O THR C 123 9579 8749 10602 1059 3529 2222 O ATOM 7346 CB THR C 123 -33.879 10.073 2.132 1.00 79.32 C ANISOU 7349 N THR C 124 8581 7615 8856 1740 3974 2184 N ATOM 7350 CA THR C 124 -34.157 13.488 -0.504 1.00 58.20 C ANISOU 7350 CA THR C 124 7851 6516 7746 1809 3800 1901 C ATOM 7351 C THR C 124 -32.759 13.961 -0.135 1.00 55.25 C ANISOU 7351 C THR C 124 7977 5925 7090 1896 3813 1572 C ATOM 7352 O THR C 124 -32.541 14.443 0.982 1.00 53.37 O ANISOU 7352 O THR C 124 7916 5718 6644 2136 3913 1560 O ATOM 7353 CB THR C 124 -35.125 14.680 -0.504 1.00 56.91 C ANISOU 7353 CB THR C 124 7565 6560 7499 2175 3941 2024 C ATOM 7354 OG1 THR C 124 -36.385 14.278 -1.053 1.00 59.04 O ANISOU 7354 OG1 THR C 124 7337 7020 8077 2060 3861 2319 O ATOM 7355 CG2 THR C 124 -34.564 15.853 -1.303 1.00 53.86 C ANISOU 7355 CG2 THR C 124 7528 6021 6914 2295 3810 1705 C ATOM 7356 H THR C 124 -34.620 12.733 1.248 1.00 79.12 H ATOM 7357 HA THR C 124 -34.128 13.116 -1.400 1.00 69.84 H ATOM 7357 HA THR C 124 -34.126 13.116 -1.400 1.00 69.64 H ATOM 7358 HB THR C 124 -35.259 14.977 0.410 1.00 68.29 H ATOM 7360 HG21 THR C 124 -36.918 14.927 -1.054 1.00 70.85 H ATOM 7361 HG22 THR C 124 -35.191 16.593 -1.289 1.00 64.63 H ATOM 7362 HG23 THR C 124 -34.413 15.585 -2.223 1.00 64.63 H ATOM 7363 N PHE C 125 -31.821 13.829 -1.069 1.00 47.59 N ANISOU 7363 N PHE C 125 7566 6057 4461 3107 1905 1311 N ATOM 7364 CA PHE C 125 -30,473 14,336 -0,875 1.00 49,35 C

ANISOU 7364 CA PHE C 125 8163 5984 4602 2965 1776 1031 ATOM 7365 C PHE C 125 -29.986 14.976 -2.166 1.00 47.94 C ANISOU 7365 C PHE C 125 8039 5665 4510 2844 1690 C ATOM 7366 O PHE C 125 -30.555 14.781 -3.244 1.00 47.36 ANISOU 7366 O PHE C 125 7684 5735 4575 2828 1716 1096 ATOM 7367 CB PHE C 125 -29.501 13.231 -0.432 1.00 48.99 0 ANISOU 7367 CB PHE C 125 8092 5941 4583 2736 1662 -29.581 11.981 -1.261 1.00 47.46 ATOM 7368 CG PHE C 125 **ANISOU 7368 CG PHE C 125** 7520 5946 4565 2567 1623 1031 C C ATOM 7369 CD1 PHE C 125 -28.646 11.729 -2.254 1.00 45.19 **ANISOU 7369 CD1 PHE C 125** 7227 5583 4359 2349 1491 917 ATOM 7370 CD2 PHE C 125 -30.584 11.049 -1.039 1.00 48.45 ANISOU 7370 CD2 PHE C 125 7299 6351 4760 2607 1700 1265 C -28.719 10.573 -3.019 1.00 43.79 ATOM 7371 CE1 PHE C 125 ANISOU 7371 CE1 PHE C 125 6707 5560 4370 2132 1361 1018 ATOM 7372 CE2 PHE C 125 -30.662 9.894 -1.796 1.00 46.80 C ANISOU 7372 CE2 PHE C 125 6773 6307 4700 2396 1614 1392 C ATOM 7373 CZ PHE C 125 -29.730 9.655 -2.788 1.00 44.47 ANISOU 7373 CZ PHE C 125 6497 5889 4511 2157 1422 1258 ATOM 7374 H PHE C 125 -31.945 13.446 -1.829 1.00 57.11 H ATOM 7375 HA PHE C 125 -30.487 15.019 -0.186 1.00 59.22 H ATOM 7376 HB2 PHE C 125 -28.594 13.570 -0.494 1.00 58.79 H -29.699 12.991 0.486 1.00 58.79 -27.967 12.344 -2.414 1.00 54.23 -31.216 11.205 -0.374 1.00 58.14 -28.089 10.414 -3.685 1.00 52.54 ATOM 7377 HB3 PHE C 125 ATOM 7378 HD1 PHE C 125 ATOM 7379 HD2 PHE C 125 ATOM 7380 HE1 PHE C 125 ATOM 7381 HE2 PHE C 125 -31.341 9.279 -1.638 1.00 56.16 Н ATOM 7382 HZ PHE C 125 -29.780 8.879 -3.297 1.00 53.37 Н ATOM 7383 N THR C 126 -28.926 15.762 -2.030 1.00 46.26 ANISOU 7383 N THR C 126 8185 5177 4214 2746 1571 741 N ATOM 7384 CA THR C 126 -28.250 16.366 -3.164 1.00 42.98 C ANISOU 7384 CA THR C 126 7839 4604 3886 2597 1456 ATOM 7385 C THR C 126 -27.094 15.474 -3.585 1.00 38.74 ANISOU 7385 C THR C 126 7220 4048 3450 2330 1304 5 ATOM 7386 O THR C 126 -26.423 14.869 -2.743 1.00 36.66 ANISOU 7386 O THR C 126 7046 3767 3117 2230 1244 458 ATOM 7387 CB THR C 126 -27.746 17.763 -2.798 1.00 45.69 ANISOU 7387 CB THR C 126 8618 4649 4093 2623 1379 505 ATOM 7388 OG1 THR C 126 -28.869 18.634 -2.618 1.00 48.91 ANISOU 7388 OG1 THR C 126 9087 5073 4424 2907 1522 591 ATOM 7389 CG2 THR C 126 -26.814 18.336 -3.879 1.00 44.22 ANISOU 7389 CG2 THR C 126 8522 4267 4013 2410 1207 427 ATOM 7390 H THR C 126 -28.572 15.964 -1.273 1.00 55.51 ATOM 7391 HA THR C 126 -28.868 16.444 -3.908 1.00 51.57 ATOM 7392 HB THR C 126 -27.248 17.712 -1.967 1.00 54.83 ATOM 7393 HG1 THR C 126 -28.604 19.405 -2.417 1.00 58.69 ATOM 7394 HG21 THR C 126 -26.511 19.220 -3.620 1.00 53.07 ATOM 7395 HG22 THR C 126 -26.042 17.759 -3.991 1.00 53.07 ATOM 7396 HG23 THR C 126 -27.286 18.400 -4.724 1.00 53.07 ATOM 7397 N GLN C 127 -26.879 15.386 -4.894 1.00 36.33 N ANISOU 7397 N GLN C 127 6736 3759 3310 2221 1230 599 ATOM 7398 CA GLN C 127 -25.789 14.608 -5.462 1.00 32.27 ANISOU 7398 CA GLN C 127 6060 3310 2891 1882 1033 531 C

ATOM 7399 C GLN C 127 -24.784 15.548 -6.113 1.00 30.62 ANISOU 7399 C GLN C 127 6032 2916 2687 1699 ATOM 7400 O GLN C 127 -25.128 16.277 -7.048 1.0 878 459 -25.128 16.277 -7.048 1.00 30.58 0 ANISOU 7400 O GLN C 127 6004 2876 2741 1737 885 549 ATOM 7401 CB GLN C 127 -26.317 13.590 -6.469 1.00 31.26 C **ANISOU 7401 CB GLN C 127** 5510 3443 2922 1805 1017 658 C ATOM 7402 CG GLN C 127 -27.149 12.498 -5.829 1.00 31.89 C **ANISOU 7402 CG GLN C 127** 5386 3710 3019 1891 1105 ATOM 7403 CD GLN C 127 -27.578 11.445 -6.824 1.00 31.71 C **ANISOU 7403 CD GLN C 127** 4997 3898 3155 1764 1023 872 ATOM 7404 OE1 GLN C 127 -28.113 11.763 -7.881 1.00 32.95 0 5013 4123 3385 1784 1025 974 **ANISOU 7404 OE1 GLN C 127** 0 Ν ATOM 7405 NE2 GLN C 127 -27.332 10.180 -6.496 1.00 31.57 4845 3964 3186 1626 925 853 **ANISOU 7405 NE2 GLN C 127** Ν ATOM 7406 H GLN C 127 -27.364 15.779 -5.486 1.00 43.60 Н ATOM 7407 HA GLN C 127 -25.337 14.126 -4.752 1.00 38.72 Н ATOM 7408 HB2 GLN C 127 -26.873 14.048 -7.118 1.00 37.51 Н ATOM 7409 HB3 GLN C 127 -25.565 13.169 -6.915 1.00 37.51 ATOM 7410 HG2 GLN C 127 ATOM 7411 HG3 GLN C 127 -26.626 12.064 -5.137 1.00 38.27 -27.948 12.892 -5.445 1.00 38.27 Н ATOM 7412 HE21 GLN C 127 -26.948 9.996 -5.749 1.00 37.88 Н -27.558 9.545 -7.031 1.00 37.88 ATOM 7413 HE22 GLN C 127 ATOM 7414 N TYR C 128 ANISOU 7414 N TYR C 128 Ν -23.568 15.561 -5.578 1.00 30.99 6256 2852 2669 1494 730 Ν ATOM 7415 CA TYR C 128 -22.420 16.205 -6.198 1.00 30.90 ANISOU 7415 CA TYR C 128 6330 2737 2674 1234 544 ATOM 7416 C TYR C 128 -21.688 15.176 -7.045 1.00 27.59 **ANISOU 7416 C TYR C 128** C 5545 2579 2361 1008 447 ATOM 7417 O TYR C 128 -21.433 14.062 -6.578 1.00 25.38 **ANISOU 7417 O TYR C 128** 5122 2428 2095 972 430 250 ATOM 7418 CB TYR C 128 -21.453 16.751 -5.144 1.00 34.60 ANISOU 7418 CB TYR C 128 7166 2970 3009 1109 408 ATOM 7419 CG TYR C 128 -21.933 17.930 -4.326 1.00 39.98 **ANISOU 7419 CG TYR C 128** 8315 3328 3547 1316 453 -23.222 18.430 -4.452 1.00 42.52 ATOM 7420 CD1 TYR C 128 ANISOU 7420 CD1 TYR C 128 8693 3600 3863 1655 646 182 ATOM 7421 CD2 TYR C 128 -21.075 18.547 -3.421 1.00 42.85 **ANISOU 7421 CD2 TYR C 128** 9078 3432 3770 1184 287 ATOM 7422 CE1 TYR C 128 -23.647 19.520 -3.692 1.00 46.39 **ANISOU 7422 CE1 TYR C 128** 9493 3931 4203 1803 669 118 ATOM 7423 CE2 TYR C 128 -21.486 19.633 -2.661 1.00 46.36 C **ANISOU 7423 CE2 TYR C 128** 9903 3653 4060 1344 295 ATOM 7424 CZ TYR C 128 -22.773 20.119 -2.798 1.00 48.13 **ANISOU 7424 CZ TYR C 128 ATOM 7425 OH TYR C 128** C 10087 3926 4275 1657 491 -10 -23.189 21.207 -2.044 1.00 51.24 0 **ANISOU 7425 OH TYR C 128** 10813 4146 4508 1824 493 -68 0 ATOM 7426 H TYR C 128 -23.379 15.187 -4.826 1.00 37.19 -22.714 16.934 -6.767 1.00 37.08 Н ATOM 7427 HA TYR C 128 ATOM 7428 HB2 TYR C 128 -21.247 16.035 -4.523 1.00 41.51 ATOM 7428 HB2 TYR C 128 -21.247 16.035 -4.523 1.00 41.51 H
ATOM 7429 HB3 TYR C 128 -20.639 17.027 -5.595 1.00 41.51 H
ATOM 7430 HD1 TYR C 128 -23.811 18.033 -5.051 1.00 51.03 H
ATOM 7431 HD2 TYR C 128 -20.208 18.226 -3.325 1.00 51.42 H
ATOM 7432 HE1 TYR C 128 -24.512 19.845 -3.788 1.00 55.67 ATOM 7432 HE1 TYR C 128 -24.512 19.845 -3.788 1.00 55.67

ATOM 7433 HE2 TYR C 128 -20.897 20.033 -2.062 1.00 55.64 ATOM 7434 HH TYR C 128 -23.987 21.396 -2.228 1.00 61.48 Н ATOM 7435 N TRP C 129 -21.323 15.553 -8.271 1.00 26.41 Ν **ANISOU 7435 N TRP C 129** 5259 2505 2269 870 378 380 Ν -20.557 14.681 -9.149 1.00 24.94 ATOM 7436 CA TRP C 129 C 4751 2583 2144 693 **ANISOU 7436 CA TRP C 129** 296 374 ATOM 7437 C TRP C 129 ANISOU 7437 C TRP C 129 ATOM 7438 O TRP C 129 -19.308 15.382 -9.662 1.00 26.13 4925 2739 2265 436 148 413 C -19.353 16.555 -10.049 1.00 27.28 0 **ANISOU 7438 O TRP C 129** 5232 2742 2393 383 112 510 ATOM 7439 CB TRP C 129 -21.368 14.234 -10.384 1.00 24.10 **ANISOU 7439 CB TRP C 129** 4363 2684 2112 770 366 454 ATOM 7440 CG TRP C 129 -22.692 13.579 -10.139 1.00 23.62 **ANISOU 7440 CG TRP C 129** 4211 2664 2100 980 488 486 ATOM 7441 CD1 TRP C 129 -23.882 14.198 -9.901 1.00 24.67 **ANISOU 7441 CD1 TRP C 129** 4443 2698 2234 1188 614 C 587 ATOM 7442 CD2 TRP C 129 -22.971 12.178 -10.176 1.00 22.39 3827 2675 2004 996 **ANISOU 7442 CD2 TRP C 129** 479 449 ATOM 7443 NE1 TRP C 129 -24.883 13.268 -9.761 1.00 24.35 4212 2791 2248 1311 691 **ANISOU 7443 NE1 TRP C 129** 642 N ATOM 7444 CE2 TRP C 129 -24.346 12.018 -9.923 1.00 22.76 C **ANISOU 7444 CE2 TRP C 129** 3828 2731 2090 1175 C 592 **558** CC ATOM 7445 CE3 TRP C 129 -22.187 11.042 -10.383 1.00 21.49 **ANISOU 7445 CE3 TRP C 129** 3552 2696 1919 886 374 ATOM 7446 CZ2 TRP C 129 -24.953 10.769 -9.876 1.00 22.42 C **ANISOU 7446 CZ2 TRP C 129** 3585 2816 2117 1194 576 585 ATOM 7447 CZ3 TRP C 129 -22.789 9.802 -10.331 1.00 20.74 **ANISOU 7447 CZ3 TRP C 129** 3302 2683 1895 C 937 356 ATOM 7448 CH2 TRP C 129 -24.159 9.675 -10.084 1.00 21.94 **ANISOU 7448 CH2 TRP C 129** 3414 2831 2090 1062 443 465 ATOM 7449 H TRP C 129 -21.511 16.318 -8.618 1.00 31.69 Н ATOM 7450 HA TRP C 129 -20.285 13.889 -8.659 1.00 29.93 Н ATOM 7451 HB2 TRP C 129 -21.535 15.016 -10.932 1.00 28.93 н -20.828 13.604 -10.886 1.00 28.93 ATOM 7452 HB3 TRP C 129 Н ATOM 7453 HD1 TRP C 129 -23.998 15.118 -9.834 1.00 29.60 Н ATOM 7454 HE1 TRP C 129 -25.709 13.441 -9.596 1.00 29.22 Н ATOM 7455 HE3 TRP C 129 -21.276 11.120 -10.549 1.00 25.79 Н ATOM 7456 HZ2 TRP C 129 -25.864 10.680 -9.707 1.00 26.90 Н ATOM 7457 HZ3 TRP C 129 -22.276 9.038 -10.468 1.00 24.89 Н ATOM 7458 HH2 TRP C 129 -24.538 8.826 -10.053 1.00 26.33 Н ATOM 7459 N SER C 130 -18.210 14.636 -9.708 1.00 25.77 Ν **ANISOU 7459 N SER C 130** 4694 2876 2220 281 57 363 Ν ATOM 7460 CA SER C 130 -17.084 14.911 -10.591 1.00 26.97 **ANISOU 7460 CA SER C 130** 4678 3214 2356 55 -48 444 ATOM 7461 C SER C 130 ANISOU 7461 C SER C 130 ATOM 7462 O SER C 130 C -16.909 13.689 -11.476 1.00 26.48 4253 3486 2323 109 -5 394 -16.687 12.586 -10.967 1.00 25.20 0 **ANISOU 7462 O SER C 130** 3997 3390 2188 177 -11 278 ATOM 7463 CB SER C 130 -15.803 15.196 -9.805 1.00 28.94 5031 3404 2561 -167 -209 447 **ANISOU 7463 CB SER C 130** C ATOM 7464 OG SER C 130 -15.821 16.497 -9.255 1.00 30.22 ANISOU 7464 OG SER C 130 5559 3246 2676 -267 -300 504 0 ATOM 7465 H SER C 130 -18.091 13.939 -9.218 1.00 30.92 Н

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ATOM 7466 HA SER C 130
                           -17.285 15.677 -11.151 1.00 32.37
                                                              Н
ATOM 7467 HB2 SER C 130
                           -15.724 14.551 -9.085 1.00 34.73
                                                              Н
ATOM 7468 HB3 SER C 130
                           -15.043 15.118 -10.403 1.00 34.73
                                                              Н
ATOM 7469 HG SER C 130
                           -15.888 17.068 -9.868 1.00 36.26
                                                              Н
ATOM 7470 N VAL C 131
                          -17.019 13.879 -12.789 1.00 24.87
                                                             Ν
ANISOU 7470 N VAL C 131
                           3871 3479 2101
                                           89
                                                 26 478
ATOM 7471 CA VAL C 131
                           -16.993 12.782 -13.750 1.00 24.14
ANISOU 7471 CA VAL C 131
                            3487 3686 1999 175 66 408
ATOM 7472 C VAL C 131
                          -15.842 13.019 -14.718 1.00 25.70
                                                             C
ANISOU 7472 C VAL C 131
                           3469 4190 2108
                                           23
                                                 27
                                                     495
ATOM 7473 O VAL C 131
                                                             0
                          -15.850 14.001 -15.474 1.00 26.61
ANISOU 7473 O VAL C 131
                           3582 4354 2174 -95
                                                 22 660
ATOM 7474 CB VAL C 131
                           -18.323 12.660 -14.509 1.00 23.57
ANISOU 7474 CB VAL C 131
                            3383 3624 1949 318 147 429
ATOM 7475 CG1 VAL C 131
                           -18.316 11.423 -15.395 1.00 23.12
                                                               CC
ANISOU 7475 CG1 VAL C 131
                            3090 3829 1866 407 150 317
ATOM 7476 CG2 VAL C 131
                           -19.507 12.638 -13.532 1.00 22.85
ANISOU 7476 CG2 VAL C 131
                            3479 3266 1936 463 203 412
ATOM 7477 H VAL C 131
                          -17.113 14.652 -13.154 1.00 29.85
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ATOM 7478 HA VAL C 131
                           -16.832 11.949 -13.281 1.00 28.97
                                                              Н
ATOM 7479 HB VAL C 131
                           -18.427 13.435 -15.083 1.00 28.29
                                                              Н
ATOM 7480 HG11 VAL C 131
                            -19.164 11.366 -15.864 1.00 27.74
                                                             Н
ATOM 7481 HG12 VAL C 131
                            -17.589 11.496 -16.033 1.00 27.74
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ATOM 7482 HG13 VAL C 131
                           -18.192 10.638 -14.839 1.00 27.74
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ATOM 7483 HG21 VAL C 131
                            -20.332 12.561 -14.038 1.00 27.42
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ATOM 7484 HG22 VAL C 131
                            -19.411 11.878 -12.937 1.00 27.42
ATOM 7485 HG23 VAL C 131
                            -19.509 13.462 -13.020 1.00 27.42
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ATOM 7486 N ARG C 132
                           -14.880 12.100 -14.733 1.00 25.59
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ANISOU 7486 N ARG C 132
                           3254 4402 2068
                                            41
                                                 4 404
                           -13.738 12.238 -15.629 1.00 27.38
ATOM 7487 CA ARG C 132
                                                              C
ANISOU 7487 CA ARG C 132
                            3223 4992 2188 -67 -6 502
ATOM 7488 C ARG C 132
ANISOU 7488 C ARG C 132
                                                             C
                           -14.201 12.288 -17.081 1.00 28.02
                           3164 5313 2170
                                            -9
                                                 72
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ATOM 7489 O ARG C 132
                           -15.067 11.514 -17.500 1.00 26.77
                                                              0
ANISOU 7489 O ARG C 132
                           3003 5153 2016 176 119 405
                                                              C
ATOM 7490 CB ARG C 132
                           -12.764 11.077 -15.415 1.00 27.54
ANISOU 7490 CB ARG C 132
                            3037 5228 2197
                                            36 -19
                                                       373
                                                              C
ATOM 7491 CG ARG C 132
                           -11.325 11.329 -15.888 1.00 29.96
ANISOU 7491 CG ARG C 132
                            3066 5914 2405
                                            -96
                                                  -38 520
                                                              C
ATOM 7492 CD ARG C 132
                           -10.413 10.218 -15.381 1.00 30.19
ANISOU 7492 CD ARG C 132
                            2926 6089 2457
                                              39
                                                  -62
                                                              Ν
ATOM 7493 NE ARG C 132
                            -8.994 10.488 -15.592 1.00 33.14
ANISOU 7493 NE ARG C 132
                            3009 6829 2753 -93
                                                             Ν
                                                  -89 580
                            -8.310 10.140 -16.679 1.00 36.01
                                                              C
ATOM 7494 CZ ARG C 132
ANISOU 7494 CZ ARG C 132
                            3048 7659 2976 21
                                                   9 613
ATOM 7495 NH1 ARG C 132
                            -8.904 9.501 -17.678 1.00 34.35
                                                              Ν
ANISOU 7495 NH1 ARG C 132
                            2804 7576 2672 269
                                                   123
                                                              Ν
ATOM 7496 NH2 ARG C 132
                            -7.019 10.432 -16.765 1.00 39.19
                                                              Ν
                             3155 8422 3315 -112 -14 827
ANISOU 7496 NH2 ARG C 132
                                                              Ν
ATOM 7497 H ARG C 132 -14.865 11.396 -14.240 1.00 30.71
                                                             Н
ATOM 7498 HA ARG C 132 -13.273 13.066 -15.429 1.00 32.86
ATOM 7499 HB2 ARG C 132 -12.728 10.877 -14.467 1.00 33.04
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ATOM 7500 HB3 ARG C 132 -13.098 10.304 -15.897 1.00 33.04
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ATOM 7501 HG2 ARG C 132
                                    -11.297 11.333 -16.858 1.00 35.96
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ATOM 7502 HG3 ARG C 132 -11.009 12.170 ATOM 7503 HD2 ARG C 132 -10.556 10.106 -14.428 1.00 36.23 ATOM 7504 HD3 ARG C 132 -10.632 9.395 -15.846 1.00 36.23 H ATOM 7505 HE ARG C 132 -8.569 10.903 -14.970 1.00 39.77 H -9.740 9.307 -17.627 1.00 41.22 H -2.152 0.280 -18.376 1.00 41.22 H
                                                                                    Н
                                                                                    Н
ATOM 7506 HH11 ARG C 132
ATOM 7507 HH12 ARG C 132
ATOM 7508 HH21 ARG C 132
ATOM 7509 HH22 ARG C 132
-6.628 10.847 -16.122 1.00 47.03
ATOM 7510 N GLN C 133
                                    -13.591 13.195 -17.855 1.00 30.19
                                                                                    Ν
ANISOU 7510 N GLN C 133
                                     3319 5806 2344 -193
                                                                    63 756
ATOM 7511 CA GLN C 133
                                     -14.019 13.456 -19.228 1.00 30.92
ANISOU 7511 CA GLN C 133 3299 6131 2318 -179 126 846
ATOM 7512 C GLN C 133
                                    -13.756 12.285 -20.160 1.00 32.21
ANISOU 7512 C GLN C 133 3225 6673 2341 25 205 682
ATOM 7513 O GLN C 133 -14.391 12.195 -21.216 1.00 31.25
                                                                                    0
ANISOU 7513 O GLN C 133 3063 6696 2114 99 250 675
ATOM 7514 CB GLN C 133
                                     -13.315 14.694 -19.769 1.00 32.70
ANISOU 7514 CB GLN C 133
                                     3442 6519 2463 -453 81 1149
ATOM 7515 CG GLN C 133
                                     -13.750 15.972 -19.083 1.00 33.03
ANISOU 7515 CG GLN C 133
                                    3787 6139 2625 -639 -22 1309
                                                                                     CCO
ATOM 7516 CD GLN C 133
                                     -13.218 17.199 -19.781 1.00 35.35
ANISOU 7516 CD GLN C 133
                                     4024 6559 2848 -926 -99 1635
                                    -12.212 17.131 -20.485 1.00 37.22
ATOM 7517 OE1 GLN C 133
                                    3961 7229 2952 -1044 -85 1776
ANISOU 7517 OE1 GLN C 133
                                      -13.896 18.327 -19.601 1.00 35.79
ATOM 7518 NE2 GLN C 133
ANISOU 7518 NE2 GLN C 133 4364 6248 2987 -1030 -183 1774
ATOM 7519 H GLN C 133 -12.922 13.673 -17.603 1.00 36.22
                                    -12.922 13.6.2
-14.973 13.631 -19.231 1.00 3...
-12.359 14.595 -19.637 1.00 39.24
-13.511 14.780 -20.715 1.00 39.24
-14.719 16.020 -19.085 1.00 39.64
-13.417 15.975 -18.172 1.00 39.64
-14.599 18.332 -19.107 1.00 42.95
-13 631 19.053 -19.979 1.00 42.95
H
ATOM 7520 HA GLN C 133 -14.973 13.631 -19.231 1.00 37.10
ATOM 7521 HB2 GLN C 133
ATOM 7522 HB3 GLN C 133
ATOM 7523 HG2 GLN C 133
ATOM 7524 HG3 GLN C 133
ATOM 7525 HE21 GLN C 133
ATOM 7526 HE22 GLN C 133
ATOM 7527 N SER C 134 -12.812 11.418 -19.816 1.00 33.07
ANISOU 7527 N SER C 134
                                     3187 6945 2432 126 212 555
ATOM 7528 CA SER C 134
                                     -12.693 10.126 -20.465 1.00 34.80
ANISOU 7528 CA SER C 134 3270 7408 2544 398 270 322
ATOM 7529 C SER C 134 -12.192 9.142 -19.422 1.00 32.93
ANISOU 7529 C SER C 134 3044 7044 2423 533 227 142
ATOM 7530 O SER C 134
                                    -11.616 9.528 -18.399 1.00 31.16
ANISOU 7530 O SER C 134 2843 6691 2305 390
                                                                    169 239
ATOM 7531 CB SER C 134 -11.772 10.179 -21.690 1.00 39.08
ANISOU 7531 CB SER C 134 3518 8491 2841 426 362 411
ATOM 7532 OG SER C 134 -10.434 10.447 -21.323 1.00 41.84 O ANISOU 7532 OG SER C 134 3649 9077 3172 320 366 565 O ATOM 7533 H SER C 134 -12.226 11.557 -19.203 1.00 39.68 H ATOM 7534 HA SER C 134 -13.570 9.835 -20.759 1.00 41.76 H
ATOM 7535 HB2 SER C 134 -13.570 9.835 -20.759 1.00 41.76 H
ATOM 7535 HB2 SER C 134 -11.807 9.324 -22.146 1.00 46.90 H
ATOM 7536 HB3 SER C 134 -12.081 10.882 -22.284 1.00 46.90 H
ATOM 7537 HG SER C 134 -10.151 9.845 -20.809 1.00 50.21 H
ATOM 7538 N LYS C 135 -12.433 7.862 -19.695 1.00 32.78 N
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ANISOU 7538 N LYS C 135 3032 7044 2380 802 230 -117 Ν ATOM 7539 CA LYS C 135 -12.201 6.821 -18.708 1.00 31.53 **ANISOU 7539 CA LYS C 135** 2932 6691 2358 948 162 -296 ATOM 7540 C LYS C 135 -10.730 6.745 -18.330 1.00 32.92 **ANISOU 7540 C LYS C 135** 2881 7116 2511 958 C 174 -231 ATOM 7541 O LYS C 135 -9.843 6.766 -19.189 1.00 35.02 2891 7815 2602 1034 **ANISOU 7541 O LYS C 135** 0 ATOM 7542 CB LYS C 135 -12.677 5.477 -19.250 1.00 31.57 **ANISOU 7542 CB LYS C 135** 2999 6671 2324 1230 133 -576 ATOM 7543 CG LYS C 135 -14.129 5.504 -19.701 1.00 30.31 **ANISOU 7543 CG LYS C 135** 3027 6307 2181 1196 -14.606 4.149 -20.169 1.00 31.08 ATOM 7544 CD LYS C 135 **ANISOU 7544 CD LYS C 135** 3227 6331 2252 1427 7 -878 ATOM 7545 CE LYS C 135 -16.072 4.205 -20.553 1.00 31.06 **ANISOU 7545 CE LYS C 135** 3385 6136 2281 1345 -62 -861 ATOM 7546 NZ LYS C 135 -16.615 2.873 -20.910 1.00 32.15 N **ANISOU 7546 NZ LYS C 135** 3664 6135 2415 1513 -208 -1105 Ν ATOM 7547 H LYS C 135 -12.732 7.573 -20.448 1.00 39.34 Н ATOM 7548 HA LYS C 135 -12.709 7.022 -17.907 1.00 37.84 Н ATOM 7549 HB2 LYS C 135 -12.130 5.234 -20.014 1.00 37.88 Н ATOM 7550 HB3 LYS C 135 -12.591 4.808 -18.554 1.00 37.88 ATOM 7551 HG2 LYS C 135 -14.687 5.781 -18.957 1.00 36.37 -14.221 6.128 -20.437 1.00 36.37 -14.094 3.877 -20.948 1.00 37.30 ATOM 7552 HG3 LYS C 135 ATOM 7553 HD2 LYS C 135 Н -14.501 3.504 -19.453 1.00 37.30 -16.583 4.548 -19.804 1.00 37.27 ATOM 7554 HD3 LYS C 135 Н ATOM 7555 HE2 LYS C 135 ATOM 7556 HE3 LYS C 135 -16.176 4.788 -21.322 1.00 37.27 Н -16.167 2.537 -21.601 1.00 38.57 -16.538 2.319 -20.218 1.00 38.57 ATOM 7557 HZ1 LYS C 135 ATOM 7558 HZ2 LYS C 135 ATOM 7559 HZ3 LYS C 135 -17.475 2.945 -21.129 1.00 38.57 -10.480 6.644 -17.037 1.00 31.35 ATOM 7560 N ARG C 136 Ν **ANISOU 7560 N ARG C 136** 2763 6673 2477 886 Ν 88 -215 ATOM 7561 CA ARG C 136 -9.120 6.573 -16.531 1.00 32.81 C **ANISOU 7561 CA ARG C 136** 2731 7069 2666 869 65 -123 -8.561 5.166 -16.725 1.00 34.03 ATOM 7562 C ARG C 136 **ANISOU 7562 C ARG C 136** 2755 7377 2799 1223 C 76 -342 ATOM 7563 O ARG C 136 -9.279 4.186 -16.514 1.00 32.96 0 **ANISOU 7563 O ARG C 136** 2809 6966 2747 1407 19 -567 0 ATOM 7564 CB ARG C 136 -9.089 6.931 -15.056 1.00 31.27 **ANISOU 7564 CB ARG C 136** 2701 6543 2637 667 -56 -38 ATOM 7565 CG ARG C 136 -7.715 7.190 -14.489 1.00 33.10 **ANISOU 7565 CG ARG C 136** 2718 6984 2873 539 -118 C 137 ATOM 7566 CD ARG C 136 -7.862 7.637 -13.031 1.00 32.31 **ANISOU 7566 CD ARG C 136** C 2862 6509 2906 315 -258 204 -6.607 8.094 -12.444 1.00 35.11 ATOM 7567 NE ARG C 136 Ν **ANISOU 7567 NE ARG C 136** 3046 7032 3261 104 -365 Ν 415 -6.520 8.804 -11.320 1.00 36.16 ATOM 7568 CZ ARG C 136 C **ANISOU 7568 CZ ARG C 136** 3385 6904 3452 -168 -511 C 527 ATOM 7569 NH1 ARG C 136 -7.613 9.152 -10.657 1.00 34.22 **ANISOU 7569 NH1 ARG C 136** 3515 6232 3253 -222 -535 Ν ATOM 7570 NH2 ARG C 136 -5.334 9.177 -10.861 1.00 38.69 N 3531 7403 3766 -382 -640 **ANISOU 7570 NH2 ARG C 136** 736 Ν ATOM 7571 H ARG C 136 -11.085 6.615 -16.426 1.00 37.63 Н

ATOM	7572 HA ARG C 136	-8.558 7.200 -17.014 1.00 39.37	Н
ATOM		-9.617 7.734 -14.923 1.00 37.52	Н
ATOM			Ĥ
ATOM			Ĥ
ATOM		-7.280 7.898 -14.990 1.00 39.72	H
ATOM			H
	7577 HD2 ARG C 136		H
ATOM		-5.876 7.892 -12.849 1.00 42.13	H
ATOM			
_			Н
ATOM			H
ATOM			H
	7583 HH22 ARG C 136		Н
	7584 N PRO C 137		N .
	J 7584 N PRO C 137	2781 8163 3036 1332 141 -268	N
		-6.683 3.702 -17.171 1.00 38.78	С
ANISO	J 7585 CA PRO C 137	2922 8532 3281 1715 145 -477	С
ATOM	7586 C PRO C 137	-6.599 3.094 -15.782 1.00 37.97	C
ANISO	J 7586 C PRO C 137	2945 8082 3401 1717 -6 -524	С
ATOM	7587 O PRO C 137	-6.235 3.758 -14.807 1.00 36.71	0
ANISO	J 7587 O PRO C 137	2771 7838 3340 1443 -85 -321	0
	7588 CB PRO C 137	-5.287 3.959 -17.749 1.00 42.30	C
_	J 7588 CB PRO C 137		C
	7589 CG PRO C 137		C
		2969 9782 3509 1433 309 -27	Č
	7590 CD PRO C 137	-6.336 6.076 -17.536 1.00 39.07	C
	J 7590 CD PRO C 137		C
	7591 HA PRO C 137	-7.181 3.114 -17.760 1.00 46.54	H.
	7592 HB2 PRO C 137		H
		-5.080 3.285 -18.416 1.00 50.76	H
ATOM			H
ATOM			Н
		-5.893 6.454 -16.761 1.00 46.89	Н
ATOM	7597 HD3 PRO C 137	-6.780 6.758 -18.063 1.00 46.89	Н
ATOM	7598 N THR C 138	-6.937 1.815 -15.709 1.00 38.26	N
ANISO	J 7598 N THR C 138	3125 7909 3505 2021 -66 -789	N
ATOM	7599 CA THR C 138	-6.852 1.031 -14.490 1.00 36.79	С
ANISO	J 7599 CA THR C 138	3051 7408 3518 2073 -217 -844	С
ATOM	7600 C THR C 138	-5.619 0.129 -14.538 1.00 40.05	С
	J 7600 C THR C 138	3279 8023 3916 2351 -217 -886	C
	7601 O THR C 138	-4.923 0.035 -15.554 1.00 42.67	0
	J 7601 O THR C 138	3477 8665 4071 2479 -101 -885	0
	7602 CB THR C 138	-8.127 0.201 -14.323 1.00 35.15	c
	J 7602 CB THR C 138	3186 6750 3421 2152 -323 -1059	C
	7603 OG1 THR C 138	-8.355 -0.563 -15.519 1.00 36.71	_
			0
	J 7603 OG1 THR C 138	3447 7007 3493 2414 -293 -1279	_
	7604 CG2 THR C 138	-9.328 1.111 -14.074 1.00 32.14	C
	J 7604 CG2 THR C 138		
	7605 H THR C 138	-7.229 1.364 -16.380 1.00 45.92	н.
ATOM		-6.769 1.625 -13.728 1.00 44.14	H
ATOM	7607 HB THR C 138	-8.030 -0.398 -13.567 1.00 42.18	H.
ATOM	7608 HG1 THR C 138	-9.053 -1.022 -15.438 1.00 44.05	H
ATOM	7609 HG21 THR C 138	-10.131 0.578 -13.970 1.00 38.57	Н
ATOM	7610 HG22 THR C 138	-9.187	Н

ATOM 7611 HG23 THR C 138 -9.446 1.716 -14.823 1.00 38.57 ATOM 7612 N GLY C 139 -5.351 -0.542 -13.417 1.00 39.81 ANISOU 7612 N GLY C 139 3295 7765 4066 2401 -358 -893 ATOM 7613 CA GLY C 139 -4.284 -1.513 -13.322 1.00 42.89 C ANISOU 7613 CA GLY C 139 3597 8222 4479 2630 -377 -924 C ATOM 7614 C GLY C 139 -3.030 -1.014 -12.628 1.00 44.32 C ANISOU 7614 C GLY C 139 3465 8679 4695 2506 -382 -652 C ATOM 7615 O GLY C 139 -2.294 -1.823 -12.047 1.00 46.20 O ANISOU 7615 O GLY C 139 3652 8863 5038 2653 -456 -644 O ATOM 7616 H GLY C 139 -5.789 -0.443 -12.684 1.00 47.77 H ATOM 7617 HA2 GLY C 139 -4.607 -2.288 -12.835 1.00 51.47 H ATOM 7617 HA2 GLY C 139 -4.607 -2.288 -12.835 1.00 51.47 ATOM 7618 HA3 GLY C 139 -4.039 -1.800 -14.215 1.00 51.47 Н ATOM 7619 N SER C 140 -2.755 0.286 -12.698 1.00 43.89 ANISOU 7619 N SER C 140 3205 8913 4559 2218 -325 -411 N ATOM 7620 CA SER C 140 -1.616 0.898 -12.028 1.00 45.44 C ANISOU 7620 CA SER C 140 3123 9357 4786 2000 -375 -107 C ATOM 7621 C SER C 140 -2.105 1.721 -10.848 1.00 42.70 C ANISOU 7621 C SER C 140 2874 8809 4541 1639 -560 38 C ANISOU 7621 C SER C 140 2874 8809 4541 1639 -560 38 C ATOM 7622 O SER C 140 -3.290 2.031 -10.727 1.00 39.79 O ANISOU 7622 O SER C 140 -0.813 1.787 -12.987 1.00 47.93 C ANISOU 7623 CB SER C 140 3156 10145 4911 1873 -220 112 C ATOM 7624 OG SER C 140 -0.313 1.050 -14.086 1.00 50.92 O ANISOU 7625 H SEP C 140 3462 10742 5141 2213 -63 -12 O ATOM 7625 H SER C 140 -3.230 0.849 -13.142 1.00 52.67 H
ATOM 7626 HA SER C 140 -1.028 0.203 -11.692 1.00 54.53 H ATOM 7626 HA SER C 140
ATOM 7627 HB2 SER C 140
ATOM 7628 HB3 SER C 140
ATOM 7629 HG SER C 140
ATOM 7630 N ASN C 141
ANISOU 7630 N ASN C 141
ANISOU 7631 CA ASN C 141
ATOM 7632 C ASN C 141 ANISOU 7631 CA ASN C 141
ATOM 7632 C ASN C 141
ATOM 7632 C ASN C 141
ATOM 7633 O ASN C 141
ATOM 7634 CB ASN C 141
ATOM 7635 CG ASN C 141
ATOM 7636 OD1 ASN C 141
ATOM 7637 ND2 ASN C 141
ATOM 7638 H ASN C 141
ATOM 7639 HA ASN C 141
ATOM 7639 HA ASN C 141
ATOM 7639 HA ASN C 141
ATOM 7644 HB3 ASN C 141
ATOM 7644 N ALA C 142
ANISOU 7655 ASN C 141
ATOM 7645 ASN C 141
ATOM 7646 ASN C 141
ATOM 7647 ANISOU 7464 N ALA C 142
ANISOU 7658 ASN C 141
ATOM 7648 ASN

ATOM 7645 CA ALA C 142 -3.905 5.788 -8.840 1.00 36.58 ANISOU 7648 CB ALA C 142 2884 6733 3455 424 -661 238 C -3.540 4.124 -7.880 1.00 45.51 H ATOM 7649 H ALA C 142 ATOM 7650 HA ALA C 142
ATOM 7651 HB1 ALA C 142
ATOM 7652 HB2 ALA C 142
ATOM 7653 HB3 ALA C 142
ATOM 7654 N THR C 143
ANISOU 7654 N THR C 143
ANISOU 7655 ON THR C 143
ATOM 7655 ON THR C 143
ATOM 7655 ON THR C 143
ANISOU 7655 ON THR C 143 ATOM 7655 CA THR C 143 -4.682 8.754 -6.596 1.00 35.34 C ANISOU 7655 CA THR C 143 3665 6246 3518 -716 -1160 733 C ATOM 7656 C THR C 143 -5.916 9.552 -6.977 1.00 33.93 C ANISOU 7656 C THR C 143 3801 5794 3295 -744 -1054 648 C ATOM 7657 O THR C 143 -6.081 9.952 -8.136 1.00 33.73 O ANISOU 7657 O THR C 143 3647 5935 3233 -727 -936 691 C ATOM 7658 CB THR C 143 -3.534 9.724 -6.260 1.00 38.71 C ANISOU 7658 CB THR C 143 3998 6810 3898 -1108 -1370 1015 C ATOM 7659 OG1 THR C 143 -3.242 10.554 -7.395 1.00 39.83 O ANISOU 7668 N ILE C 144 3987 5185 3075 -762 -1086 539 N ATOM 7669 CA ILE C 144 -7.871 10.732 -6.114 1.00 31.29 ANISOU 7669 CA ILE C 144 4204 4779 2905 -816 -1021 500 C ATOM 7670 C ILE C 144 -7.604 11.757 -5.022 1.00 32.80 ANISOU 7670 C ILE C 144 4738 4703 3021 -1108 -1220 580 ATOM 7671 O ILE C 144 -7.919 11.535 -3.849 1.00 32.45 0 ANISOU 7671 O ILE C 144 4958 4425 2945 -1079 -1278 486 O ATOM 7672 CB ILE C 144 -9.263 10.104 -5.981 1.00 28.86 C ANISOU 7672 CB ILE C 144 4074 4260 2631 -536 -860 302 ATOM 7673 CG1 ILE C 144 -9.561 9.256 -7.223 1.00 27.84 C ANISOU 7673 CG1 ILE C 144 3657 4363 2558 -293 -703 225 ATOM 7674 CG2 ILE C 144 -10.333 11.194 -5.794 1.00 28.44 ANISOU 7674 CG2 ILE C 144 4397 3892 2517 -579 -809 283 C ATOM 7675 CD1 ILE C 144 -10.981 8.762 -7.325 1.00 26.22 C ANISOU 7675 CD1 ILE C 144 3596 3977 2391 -73 -568 80 C ATOM 7676 H ILE C 144 -6.789 9.333 -5.257 1.00 38.68 H ATOM 7677 HA ILE C 144 -7.817 11.177 -6.973 1.00 37.55 H ATOM 7678 HB ILE C 144 -9.270 9.526 -5.202 1.00 34.63

ATOM 7679 HG12 ILE C 144 -9.378 9.789 -8.012 1.00 33.41 H
ATOM 7680 HG13 ILE C 144 -8.980 8.479 -7.213 1.00 33.41 H
ATOM 7681 HG21 ILE C 144 -11.202 10.772 -5.713 1.00 34.13 H
ATOM 7682 HG22 ILE C 144 -10.133 11.698 -4.990 1.00 34.13 H
ATOM 7683 HG23 ILE C 144 -10.321 11.783 -6.565 1.00 34.13 H
ATOM 7684 HD11 ILE C 144 -11.579 9.525 -7.352 1.00 31.47 H
ATOM 7685 HD12 ILE C 144 -11.076 8.239 -8.136 1.00 31.47 H
ATOM 7686 HD13 ILE C 144 -11.180 8.212 -6.551 1.00 31.47 H
ATOM 7687 N THR C 145 -7.000 12.876 -5.405 1.00 34.83 N
ANISOU 7687 N THR C 145 5002 4998 3235 -1400 -1343 765 N
ATOM 7688 CA THR C 145 -6.743 13.968 -4.474 1.00 36.83 C
ANISOU 7688 CA THR C 145 5636 4951 3405 -1708 -1577 839 C
ATOM 7689 C THR C 145 -8.049 14.698 -4.180 1.00 36.24 C
ANISOU 7689 C THR C 145 -6.049 14.098 -4.160 1.00 30.24 C
ATOM 7690 O THR C 145
ATOM 7691 CB THR C 145 -5.701 14.918 -5.062 1.00 39.68 C
ANISOU 7691 CB THR C 145 5843 5479 3755 -2080 -1762 1117 C
ATOM 7692 OG1 THR C 145 -4.553 14.166 -5.473 1.00 40.65 O
ANISOU 7692 OG1 THR C 145 5441 6076 3929 -2110 -1781 1273 O
ATOM 7693 CG2 THR C 145 -5.279 15.953 -4.035 1.00 42.33 C
ANISOU 7693 CG2 THR C 145 6586 5490 4006 -2441 -2075 1201 C
ATOM 7694 H THR C 145 -6.728 13.028 -6.206 1.00 41.80 H
ATOM 7695 HA THR C 145 -6.397 13.609 -3.642 1.00 44.19 H
ATOM 7696 HB THR C 145 -6.078 15.379 -5.827 1.00 47.62 H
ATOM 7697 HG1 THR C 145 -4.772 13.601 -6.055 1.00 48.78 H
ATOM 7698 HG21 THR C 145 -4.618 16.550 -4.419 1.00 50.79 H
ATOM 7699 HG22 THR C 145 -6.048 16.473 -3.753 1.00 50.79 H
ATOM 7700 HG23 THR C 145 -4.895 15.513 -3.260 1.00 50.79 H
ATOM 7701 N PHE C 146 -8.778 14.226 -3.161 1.00 34.79 N
ANISOU 7701 N PHE C 146 6119 4057 3041 -1403 -1433 506 N
ATOM 7702 CA PHE C 146 -10.139 14.697 -2.920 1.00 33.93 C
ANISOU 7702 CA PHE C 146 6388 3630 2874 -1197 -1286 360 C
ATOM 7703 C PHE C 146 -10.179 16.188 -2.606 1.00 36.41 C
ANISOU 7703 C PHE C 146 7158 3594 3081 -1395 -1447 393 C
ATOM 7704 O PHE C 146 -11.189 16.845 -2.873 1.00 36.26 O
ANISOU 7704 O PHE C 146 7383 3355 3038 -1236 -1323 331 O
ATOM 7705 CB PHE C 146 -10.775 13.887 -1.780 1.00 33.32 C
ANISOU 7705 CB PHE C 146 6471 3448 2742 -977 -1205 202 C
ATOM 7706 CG PHE C 146 -12.259 14.112 -1.613 1.00 32.74 C
ANISOU 7706 CG PHE C 146 6665 3160 2617 -694 -992 77 C
ATOM 7707 CD1 PHE C 146 -13.112 14.068 -2.705 1.00 30.37 C
ANISOU 7707 CD1 PHE C 146 6194 2936 2409 -510 -792 82 C
ATOM 7708 CD2 PHE C 146 -12.803 14.345 -0.359 1.00 32.88 C
ANISOU 7709 CE1 PHE C 146 6327 2710 2304 -246 -600 7 C
ATOM 7710 CE2 PHE C 146 -14.167 14.544 -0.203 1.00 32.45 C
ANISOU 7710 CE2 PHE C 146 7229 2737 2362 -303 -768 -117 C
ATOM 7711 CZ PHE C 146 -14.999 14.514 -1.298 1.00 30.94 C
ANISOU 7711 CZ PHE C 146 6837 2630 2290 -132 -577 -86 C
ATOM 7712 H PHE C 146 -8.505 13.635 -2.600 1.00 41.74 H
ATOM 7713 HA PHE C 146 -10.667 14.548 -3.720 1.00 40.72 H

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ATOM 7714 HB2 PHE C 146
                           -10.638 12.943 -1.955 1.00 39.99
ATOM 7715 HB3 PHE C 146
                           -10.344 14.132 -0.946 1.00 39.99
                           -12.764 13.913 -3.554 1.00 36.44
ATOM 7716 HD1 PHE C 146
                           -12.247 14.373 0.385 1.00 39.45
ATOM 7717 HD2 PHE C 146
                           -15.035 14.247 -3.292 1.00 35.82
ATOM 7718 HE1 PHE C 146
                           -14.519 14.706 0.643 1.00 38.94
ATOM 7719 HE2 PHE C 146
                                                            Н
ATOM 7720 HZ PHE C 146
                          -15.914 14.646 -1.193 1.00 37.13
                                                            Н
ATOM 7721 N SER C 147
                          -9.100 16.750 -2.058 1.00 39.03
ANISOU 7721 N SER C 147
                          7620 3858 3351 -1741 -1741
                                                             Ν
                                                       500
ATOM 7722 CA SER C 147
                          -9.079 18.197 -1.844 1.00 41.90
                                                            C
ANISOU 7722 CA SER C 147
                           8451 3848 3622 -1963 -1946
ATOM 7723 C SER C 147
                          -9.225 18.958 -3.159 1.00 42.23
                                                           C
                          8377 3917 3753 -2035 -1908
ANISOU 7723 C SER C 147
                                                       685
ATOM 7724 O SER C 147
                          -9.799 20.056 -3.184 1.00 43.79
                                                           0
ANISOU 7724 O SER C 147
                          8988 3749 3901 -2036 -1958
                                                       660
ATOM 7725 CB SER C 147
                          -7.792 18.623 -1.131 1.00 45.03
                                                            C
ANISOU 7725 CB SER C 147
                          8963 4195 3949 -2390 -2322
ATOM 7726 OG SER C 147
                          -6.643 18.302 -1.885 1.00 45.47
                                                         0
ANISOU 7726 OG SER C 147
                           8493 4661 4121 -2643 -2418
ATOM 7727 H SER C 147
                          -8.391 16.332 -1.809 1.00 46.84
                          -9.827 18.440 -1.277 1.00 50.28
ATOM 7728 HA SER C 147
                          -7.816 19.582 -0.990 1.00 54.03
ATOM 7729 HB2 SER C 147
ATOM 7730 HB3 SER C 147
                          -7.743 18.166 -0.276 1.00 54.03
                                                           Н
ATOM 7731 HG SER C 147
                          -6.606 17.473 -2.013 1.00 54.56
                                                           Н
ATOM 7732 N ASN C 148
                          -8.719 18.400 -4.260 1.00 41.15
ANISOU 7732 N ASN C 148
                          7695 4208 3732 -2077 -1822
                                                      841
ATOM 7733 CA ASN C 148
                          -8.897 19.053 -5.553 1.00 41.63
ANISOU 7733 CA ASN C 148
                          7619 4344 3855 -2135 -1766
                                                            C
ATOM 7734 C ASN C 148
                          -10.376 19.224 -5.875 1.00 40.44
                                                           C
                          7671 3983 3712 -1778 -1521
ANISOU 7734 C ASN C 148
ATOM 7735 O ASN C 148
                          -10.805 20.296 -6.321 1.00 41.13
ANISOU 7735 O ASN C 148
                          8003 3826 3798 -1828 -1565
ATOM 7736 CB ASN C 148
                          -8.199 18.255 -6.657 1.00 40.77
ANISOU 7736 CB ASN C 148
                           6882 4783 3827 -2156 -1661
                                                       1149
ATOM 7737 CG ASN C 148
                          -6.678 18.353 -6.590 1.00 43.12
ANISOU 7737 CG ASN C 148
                           6916 5344 4124 -2543 -1911 1399
ATOM 7738 OD1 ASN C 148
                          -6.122 19.253 -5.952 1.00 45.97
ANISOU 7738 OD1 ASN C 148
                           7569 5459 4439 -2889 -2210 1517
ATOM 7739 ND2 ASN C 148
                           -5.998 17.430 -7.270 1.00 42.54
                                                            Ν
ANISOU 7739 ND2 ASN C 148 6290 5779 4094 -2481 -1799 1490
ATOM 7740 H ASN C 148
                          -8.279 17.661 -4.285 1.00 49.38
                                                         Н
ATOM 7741 HA ASN C 148
                          -8.493 19.935 -5.520 1.00 49.96
                                                          Н
ATOM 7742 HB2 ASN C 148
                          -8.443 17.320 -6.572 1.00 48.93
                                                           Н
ATOM 7743 HB3 ASN C 148
                          -8.483 18.595 -7.520 1.00 48.93
                          -5.138 17.439 -7.266 1.00 51.05
ATOM 7744 HD21 ASN C 148
                          -6.419 16.825 -7.713 1.00 51.05
ATOM 7745 HD22 ASN C 148
ATOM 7746 N HIS C 149
                        -11.175 18.178 -5.638 1.00 36.95
ANISOU 7746 N HIS C 149
                          7125 3629 3284 -1424 -1278 650
                                                            Ν
ATOM 7747 CA HIS C 149
                          -12.603 18.225 -5.936 1.00 35.44
                                                            C
ANISOU 7747 CA HIS C 149 7055 3302 3107 -1084 -1040
ATOM 7748 C HIS C 149
                         -13.365 19.055 -4.920 1.00 36.93
ANISOU 7748 C HIS C 149 7807 3034 3190 -958 -1066 408
                                                           C
ATOM 7749 O HIS C 149 -14.293 19.790 -5.272 1.00 37.45
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ANISOU 7749 O HIS C 149 8082 2890 3257 -790 -973 402
                                                           0
ATOM 7750 CB HIS C 149 -13.162 16.808 -5.972 1.00 32.50
ANISOU 7750 CB HIS C 149 6382 3180 2787 -793 -814 414
                                                            C
ATOM 7751 CG HIS C 149
                          -12.467 15.940 -6.964 1.00 31.40
ANISOU 7751 CG HIS C 149
                         5737 3465 2728 -847 -780 494
                                                            C
ATOM 7752 ND1 HIS C 149
                          -12.896 15.817 -8.268 1.00 30.45
ANISOU 7752 ND1 HIS C 149
                          5360 3550 2661 -749 -641
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ATOM 7753 CD2 HIS C 149
                          -11.345 15.191 -6.861 1.00 31.53
ANISOU 7753 CD2 HIS C 149
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                          5468 3749 2763 -969 -870
ATOM 7754 CE1 HIS C 149
                          -12.080 15.007 -8.918 1.00 30.09
ANISOU 7754 CE1 HIS C 149
                          4913 3878 2643 -789 -634
ATOM 7755 NE2 HIS C 149
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                          -11.130 14.615 -8.088 1.00 30.76
                          4961 4009 2718 -908 -765 585
ANISOU 7755 NE2 HIS C 149
                         -10.910 17.431 -5.305 1.00 44.34
ATOM 7756 H HIS C 149
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ATOM 7757 HA HIS C 149
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                         -13.058 16.405 -5.096 1.00 39.00
ATOM 7758 HB2 HIS C 149
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ATOM 7759 HB3 HIS C 149 -14.101 16.844 -6.212 1.00 39.00
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ATOM 7760 HD1 HIS C 149 -13.591 16.198 -8.602 1.00 36.54
ATOM 7761 HD2 HIS C 149 -10.824 15.079 -6.099 1.00 37.84
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ATOM 7762 HE1 HIS C 149 -12.160 14.757 -9.811 1.00 36.11
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ATOM 7763 N VAL C 150
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ANISOU 7763 N VAL C 150
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ATOM 7764 CA VAL C 150
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ANISOU 7764 CA VAL C 150 9031 2851 3322 -880 -1221
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                         -13.501 21.219 -3.016 1.00 42.93
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ATOM 7765 C VAL C 150
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ANISOU 7765 C VAL C 150
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ATOM 7766 O VAL C 150 -14.496 21.948 -3.064 1.00 43.91
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ANISOU 7767 CB VAL C 150
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ATOM 7768 CG1 VAL C 150
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ATOM 7769 CG2 VAL C 150
                           -13.311 17.981 -0.856 1.00 38.28
ANISOU 7769 CG2 VAL C 150 8713 2853 2980 -771 -1176 -20
ATOM 7770 H VAL C 150 -12.421 18.363 -3.360 1.00 45.44
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ATOM 7771 HA VAL C 150
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                                                          Н
                          -12.011 19.528 -1.348 1.00 49.34
ATOM 7772 HB VAL C 150
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ATOM 7773 HG11 VAL C 150
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ATOM 7774 HG12 VAL C 150
                          -13.181 21.341 -0.512 1.00 52.95
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ATOM 7775 HG13 VAL C 150
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ATOM 7776 HG21 VAL C 150
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ATOM 7777 HG22 VAL C 150
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                          -12.959 17.378 -1.529 1.00 45.94
ATOM 7778 HG23 VAL C 150
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ATOM 7779 N ASN C 151
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ATOM 7780 CA ASN C 151
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ANISOU 7780 CA ASN C 151 10625 3275 4353 -1700 -1933
                          -12.832 23.480 -4.900 1.00 47.29
ATOM 7781 C ASN C 151
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ANISOU 7781 C ASN C 151
                         10398 3193 4378 -1557 -1771
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ATOM 7782 O ASN C 151
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ATOM 7783 CB ASN C 151 -10.583 23.364 -3.846 1.00 51.19
ANISOU 7783 CB ASN C 151 10849 3818 4782 -2217 -2267
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	-9.823 23.381 -2.557 1.00 55.03 C 11545 4242 5122 -2367 -2496 705 C
ANISOU 7784 CG ASN C 151	
	-10.208 24.052 -1.598 1.00 57.42 O
ANISOU 7785 OD1 ASN C 151	12289 4266 5264 -2198 -2549 551 O
	-8.735 22.638 -2.518 1.00 55.26 N
	11235 4562 5200 -2667 -2621 852 N
	11.575 21.179 -3.366 1.00 53.77 H
ATOM 7788 HA ASN C 151	-12.386 23.624 -2.913 1.00 57.65 H
	-10.200 22.674 -4.410 1.00 61.43 H
ATOM 7790 HB3 ASN C 151	-10.480 24.232 -4.266 1.00 61.43 H
ATOM 7791 HD21 ASN C 151	-8.259 22.609 -1.802 1.00 66.31 H
ATOM 7792 HD22 ASN C 151	-8.501 22.182 -3.208 1.00 66.31 H
ATOM 7793 N ALA C 152 -	12.663 22.715 -5.981 1.00 44.76 N
ANISOU 7793 N ALA C 152	9539 3293 4176 -1593 -1626 795 N
ATOM 7794 CA ALA C 152	-13.383 23.002 -7.216 1.00 44.15 C
ANISOU 7794 CA ALA C 152	9285 3298 4192 -1457 -1468 909 C
	14.877 23.130 -6.952 1.00 43.31 C
	9442 2949 4064 -993 -1233 731 C
	15.518 24.097 -7.379 1.00 44.98 O
	9855 2928 4306 -890 -1235 773 O
	-13.105 21.905 -8.244 1.00 41.22 C
	8269 3494 3901 -1454 -1292 1003 C
	12.143 22.032 -6.021 1.00 53.72 H
	-13.067 23.844 -7.580 1.00 52.98 H
	-13.589 22.107 -9.060 1.00 49.47 H
	-12.152 21.874 -8.422 1.00 49.47 H
	-13.402 21.054 -7.885 1.00 49.47 H
	15.448 22.154 -6.248 1.00 41.13 N
	9096 2785 3745 -697 -1022 536 N
	-16.861 22.214 -5.900 1.00 40.81 C
	9259 2576 3669 -251 -785 398 C
ATOM 7805 C TRP C 153 -	17.166 23.487 -5.119 1.00 44.43 C
ANISOU 7805 C TRP C 153 1	10222 2642 4016 -155 -892 279 C
ATOM 7806 O TRP C 153 -	18.121 24.208 -5.435 1.00 45.68 O
ANISOU 7806 O TRP C 153	10465 2695 4196 98 -782 271 O
ATOM 7807 CB TRP C 153	-17.257 20.966 -5.096 1.00 39.11 C
	8885 2571 3407 -21 -588 239 C
ATOM 7808 CG TRP C 153	-17.240 19.655 -5.876 1.00 35.18 C
	7805 2537 3026 -14 -441 294 C
ATOM 7809 CD1 TRP C 153	-17.100 19.489 -7.228 1.00 34.05 C
	7286 2655 2996 -115 -418 440 C
ATOM 7810 CD2 TRP C 153	-17.370 18.338 -5.326 1.00 33.03 C
ANISOU 7810 CD2 TRP C 153	7304 2495 2749 107 -319 197 C
ATOM 7811 NE1 TRP C 153	
	-17.135 18.141 -7.549 1.00 31.42 N
ANISOU 7811 NE1 TRP C 153	6535 2681 2722 -46 -293 408 N
ATOM 7812 CE2 TRP C 153	-17.297 17.420 -6.396 1.00 31.25 C
ANISOU 7812 CE2 TRP C 153	6597 2629 2647 81 -242 269 C
ATOM 7813 CE3 TRP C 153	-17.537 17.846 -4.029 1.00 33.09 C 7485 2436 2651 231 -280 62 C
ANISOU 7813 CE3 TRP C 153	7485 2436 2651 231 -280 62 C
ATOM 7814 CZ2 TRP C 153	-17.394 16.044 -6.207 1.00 28.66 C
	5985 2545 2359 175 -150 204 C
ATOM 7815 CZ3 TRP C 153	-17.630 16.468 -3.844 1.00 31.19 C
ANISOU 7815 CZ3 TRP C 153	6923 2469 2457 304 -180 31 C

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ATOM 7816 CH2 TRP C 153 -17.557 15.590 -4.928 1.00 29.11
ANISOU 7816 CH2 TRP C 153 6209 2513 2339 274 -128 98 C
ATOM 7817 H TRP C 153 -15.040 21.452 -5.963 1.00 49.35 H ATOM 7818 HA TRP C 153 -17.388 22.227 -6.714 1.00 48.97 H
ATOM 7819 HB2 TRP C 153 -17.388 22.227 -6.714 1.00 48.97
ATOM 7819 HB2 TRP C 153 -16.642 20.871 -4.353 1.00 46.94
ATOM 7820 HB3 TRP C 153 -18.158 21.092 -4.758 1.00 46.94
ATOM 7821 HD1 TRP C 153 -16.996 20.180 -7.842 1.00 40.86
ATOM 7822 HE1 TRP C 153 -10.990 20.180 -7.842 1.00 40.86 H
ATOM 7822 HE1 TRP C 153 -17.065 17.812 -8.341 1.00 37.70 H
ATOM 7823 HE3 TRP C 153 -17.587 18.426 -3.305 1.00 39.71 H
ATOM 7824 HZ2 TRP C 153 -17.344 15.455 -6.925 1.00 34.39 H
ATOM 7825 HZ3 TRP C 153 -17.742 16.128 -2.985 1.00 37.42 H
ATOM 7826 HH2 TRP C 153 -17.621 14.675 -4.775 1.00 34.93 H
ATOM 7827 N LYS C 154 -16.343 23.796 -4.111 1.00 46.50
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ATOM 7828 CA LYS C 154 -16.552 25.012 -3.330 1.00 50.51
ANISOU 7828 CA LYS C 154 11697 2987 4507 -265 -1237
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ATOM 7829 C LYS C 154 -16.692 26.228 -4.239 1.00 53.78
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ATOM 7830 O LYS C 154 -17.619 27.031 -4.087 1.00 55.13
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ATOM 7831 CB LYS C 154 -15.400 25.219 -2.345 1.00 52.74 ANISOU 7831 CB LYS C 154 12214 3175 4648 -573 -1536
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ATOM 7832 CG LYS C 154 -15.370 24.225 -1.182 1.00 51.51
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ATOM 7833 CD LYS C 154 -14.183 24.465 -0.235 1.00 53.99
ANISOU 7833 CD LYS C 154 12595 3373 4546 -779 -1755 -62
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ATOM 7834 CE LYS C 154
                                               -14.024 25.937 0.118 1.00 58.93
ANISOU 7834 CE LYS C 154 13662 3677 5053 -850 -2002
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ATOM 7835 NZ LYS C 154 -13.286 26.155 1.397 1.00 62.06
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ANISOU 7835 NZ LYS C 154 14365 3952 5264 -998 -2235 -96 N
ATOM 7836 H LYS C 154 -15.668 23.324 -3.865 1.00 55.80 H
ATOM 7836 H LYS C 154 -15.668 23.324 -3.865 1.00 55.80 H
ATOM 7837 HA LYS C 154 -17.372 24.923 -2.819 1.00 60.61 H
ATOM 7838 HB2 LYS C 154 -14.562 25.134 -2.826 1.00 63.29 H
ATOM 7840 HG2 LYS C 154 -15.471 26.110 -1.968 1.00 63.29 H
ATOM 7841 HG3 LYS C 154 -16.188 24.314 -0.668 1.00 61.81 H
ATOM 7842 HD2 LYS C 154 -15.295 23.325 -1.536 1.00 61.81 H
ATOM 7843 HD3 LYS C 154 -14.327 23.971 0.587 1.00 64.79 H
ATOM 7844 HE2 LYS C 154 -13.366 24.167 -0.666 1.00 64.79 H
ATOM 7845 HE3 LYS C 154 -13.532 26.380 -0.591 1.00 70.72 H
ATOM 7846 HZ1 LYS C 154 -13.217 27.027 1.563 1.00 74.48 H
ATOM 7847 HZ2 LYS C 154 -13.720 25.766 2.069 1.00 74.48 H
                                               -13.720 25.766 2.069 1.00 74.48
-12.469 25.806 1.340 1.00 74.48
ATOM 7847 HZ2 LYS C 154
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ATOM 7848 HZ3 LYS C 154
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ATOM 7849 N SER C 155 -15.781 26.370 -5.207 1.00 54.29
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ANISOU 7849 N SER C 155
ATOM 7850 CA SER C 155 -15.765 27.544 -6.074 1.00 56.53
ANISOU 7850 CA SER C 155 12387 3495 5596 -866 -1696
ATOM 7851 C SER C 155 -17.025 27.679 -6.919 1.00 55.09 C ANISOU 7851 C SER C 155 12079 3328 5524 -519 -1437 602
ATOM 7852 O SER C 155 -17.181 28.701 -7.599 1.00 56.86
ANISOU 7852 O SER C 155 12379 3395 5828 -571 -1543 722 O ATOM 7853 CB SER C 155 -14.537 27.503 -6.990 1.00 55.85 C ANISOU 7853 CB SER C 155 11988 3611 5621 -1367 -1916 841 C
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ATOM 7854 OG SER C 155 -14.681 26.519 -8.002 1.00 51.59
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ATOM 7855 H SER C 155 -15.163 25.797 -5.380 1.00 65.15 H
ATOM 7856 HA SER C 155 -15.694 28.338 -5.521 1.00 67.83
ATOM 7857 HB2 SER C 155 -14.429 28.371 -7.409 1.00 67.02
ATOM 7858 HB3 SER C 155 -13.754 27.294 -6.457 1.00 67.02 ATOM 7859 HG SER C 155 -14.000 26.511 -8.493 1.00 61.91
ATOM 7860 N HIS C 156 -17.919 26.685 -6.899 1.00 51.16
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ATOM 7861 CA HIS C 156 -19.156 26.712 -7.675 1.00 50.57
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ATOM 7862 C HIS C 156 -20.385 26.625 -6.775 1.00 52.51
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ATOM 7863 O HIS C 156 -21.443 26.156 -7.201 1.00 48.99
ANISOU 7863 O HIS C 156 10840 2953 4821 932 -370 423
ATOM 7864 CB HIS C 156 -19.176 25.581 -8.702 1.00 46.34
ANISOU 7864 CB HIS C 156 10129 2845 4633 103 -725 750
ATOM 7865 CG HIS C 156 -18.133 25.711 -9.767 1.00 46.31
ANISOU 7865 CG HIS C 156 9906 2986 4705 -329 -918 1001 ATOM 7866 ND1 HIS C 156 -18.178 26.688 -10.739 1.00 48.38
ANISOU 7866 ND1 HIS C 156 10142 3182 5056 -448 -1024 1194
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ATOM 7867 CD2 HIS C 156 -17.022 24.980 -10.021 1.00 44.79
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ANISOU 7867 CD2 HIS C 156 9469 3053 4496 -667 -1014 1114
ATOM 7868 CE1 HIS C 156 -17.137 26.556 -11.542 1.00 48.15
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                                 -16.420 25.526 -11.128 1.00 46.47
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ANISOU 7869 NE2 HIS C 156 9487 3398 4772 -979 -1158 1372
ATOM 7870 H HIS C 156 -17.826 25.969 -6.431 1.00 61.39
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ATOM 7872 HB2 HIS C 156 -19.027 24.740 -8.243 1.00 55.61
ATOM 7872 HB2 HIS C 156 -19.027 24.740 -8.243 1.00 55.61 -20.043 25.570 -9.137 1.00 55.61 ATOM 7874 HD2 HIS C 156 -16.721 24.246 -9.535 1.00 53.75 ATOM 7875 HE1 HIS C 156 -16.942 27.096 -12.273 1.00 57.78 ATOM 7877 N GLY C 157 -20.261 27.077 -5.529 1.00 57.97 ANISOU 7877 N GLY C 157 12601 3715 5712 703 -705 200
                                                                            Н
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ATOM 7878 CA GLY C 157 -21.389 27.053 -4.623 1.00 61.94
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ATOM 7879 C GLY C 157 -21.784 25.675 -4.155 1.00 58.51
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ATOM 7880 O GLY C 157
                                 -22.898 25.499 -3.655 1.00 62.21
ANISOU 7880 O GLY C 157 12975 4680 5982 1690 27 -43 O ATOM 7881 H GLY C 157 -19.538 27.398 -5.192 1.00 69.57 H
ATOM 7882 HA2 GLY C 157 -21.178 27.587 -3.841 1.00 74.33
ATOM 7883 HA3 GLY C 157 -22.156 27.453 -5.062 1.00 74.33
ATOM 7884 N MET C 158 -20.899 24.687 -4.310 1.00 50.82 ANISOU 7884 N MET C 158 11354 3284 4673 1039 -286 3
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ATOM 7885 CA MET C 158 -21.161 23.310 -3.910 1.00 44.84
ANISOU 7885 CA MET C 158 10339 2803 3896 1159 -87 1
                                                                             C
ATOM 7886 C MET C 158 -20.413 23.048 -2.605 1.00 46.36
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ATOM 7887 O MET C 158 -19.247 22.649 -2.602 1.00 45.92
ANISOU 7887 O MET C 158 10680 2888 3879 701 -402 -117
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ATOM 7888 CB MET C 158
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ANISOU 7888 CB MET C 158
                            9493 2558 3624 969 -78 141
ATOM 7889 CG MET C 158
                            -21.643 22.416 -6.244 1.00 40.37
ANISOU 7889 CG MET C 158
                            9105 2572 3664 1126 69 297
ATOM 7890 SD MET C 158
                            -20.996 21.556 -7.687 1.00 37.22
ANISOU 7890 SD MET C 158
                            8252 2470 3420 842
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ATOM 7891 CE MET C 158
                            -21.046 19.850 -7.110 1.00 34.14
ANISOU 7891 CE MET C 158
                                                                C
                            7509 2441 3019 901 165 387
ATOM 7892 H MET C 158
                           -20.119 24.798 -4.654 1.00 60.99 H
                          -22.113 23.199 -3.758 1.00 53.81
ATOM 7893 HA MET C 158
ATOM 7894 HB2 MET C 158
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                            -20.778 21.437 -4.669 1.00 49.51 H

-22.501 22.020 -6.025 1.00 48.45 H

-21.764 23.347 -6.486 1.00 48.45 H
ATOM 7895 HB3 MET C 158
ATOM 7896 HG2 MET C 158
ATOM 7897 HG3 MET C 158
ATOM 7898 HE1 MET C 158
ATOM 7899 HE2 MET C 158
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ATOM 7900 HE3 MET C 158
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ATOM 7901 N ASN C 159 -21.098 23.257 -1.490 1.00 47.73
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ANISOU 7901 N ASN C 159 11143 3090 3903 1321 -89 -222
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ATOM 7902 CA ASN C 159
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ATOM 7903 C ASN C 159
ANISOU 7903 C ASN C 159 10944 3161 3551 1384 13 -311 ATOM 7904 O ASN C 159 -22.045 21.268 0.199 1.00 45.48
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ANISOU 7904 O ASN C 159 10581 3229 3468 1674 276 -252
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ATOM 7905 CB ASN C 159
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ATOM 7906 CG ASN C 159
ANISOU 7906 CG ASN C 159 13215 3626 4653 1316 -457 -408 C
ATOM 7907 OD1 ASN C 159
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ATOM 7908 ND2 ASN C 159 -21.554 26.388 0.029 1.00 59.51
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ATOM 7909 H ASN C 159 -21.920 23.512 -1.469 1.00 57.28
ATOM 7910 HA ASN C 159 -19.540 23.089 -0.253 1.00 58.77
                                                              Н
ATOM 7911 HB2 ASN C 159 -21.897 24.156 0.884 1.00 64.28
ATOM 7912 HB3 ASN C 159
                           -20.499 24.049 1.635 1.00 64.28
ATOM 7913 HD21 ASN C 159 -21.386 27.178 -0.265 1.00 71.41 ATOM 7914 HD22 ASN C 159 -22.367 26.144 0.168 1.00 71.41
                           -21.386 27.178 -0.265 1.00 71.41
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                           -19.976 21.072 1.072 1.00 45.71
ATOM 7915 N LEU C 160
                           10865 3094 3410 1159 -125 -348
ANISOU 7915 N LEU C 160
                                                                 N
ATOM 7916 CA LEU C 160
                            -20.233 19.782 1.689 1.00 43.69
                                                                C
ANISOU 7916 CA LEU C 160 10365 3079 3156 1251 27 -341
ATOM 7917 C LEU C 160 -20.682 19.969 3.134 1.00 46.59
ANISOU 7917 C LEU C 160 10970 3404 3328 1459 93 -394
                                                               C
                                                               C
ATOM 7918 O LEU C 160 -20.339 20.956 3.790 1.00 50.01
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ANISOU 7918 O LEU C 160 11796 3599 3609 1431
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ATOM 7919 CB LEU C 160 -18.984 18.904 1.635 1.00 41.49
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ATOM 7920 CG LEU C 160
                            -18.683 18.287 0.269 1.00 38.45
ANISOU 7920 CG LEU C 160 9230 2622 2757 758 -159 -302
ATOM 7921 CD1 LEU C 160 -17.272 17.723 0.270 1.00 37.53
ANISOU 7921 CD1 LEU C 160 9035 2557 2667 381 -405 -317 C
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ATOM 7922 CD2 LEU C 160 -19.705 17.209 -0.051 1.00 35.90 C
ANISOU 7922 CD2 LEU C 160 8552 2566 2521 1010 112 -259 C
ATOM 7923 H LEU C 160 -19.176 21.364 1.194 1.00 54.86 H
ATOM 7924 HA LEU C 160 -19.176 21.304 1.194 1.00 34.86 H
ATOM 7925 HB2 LEU C 160 -18.218 19.443 1.888 1.00 49.79 H
ATOM 7926 HB3 LEU C 160 -19.092 18.177 2.267 1.00 49.79 H
ATOM 7927 HG LEU C 160 -18.738 18.974 -0.414 1.00 46.14 H
ATOM 7928 HD11 LEU C 160 -17.087 17.333 -0.599 1.00 45.04 H
ATOM 7929 HD12 LEU C 160 -16.645 18.441 0.451 1.00 45.04 H
ATOM 7930 HD13 LEU C 160 -17.205 17.043 0.959 1.00 45.04 H
ATOM 7931 HD21 LEU C 160 -20.590 17.607 -0.064 1.00 43.07 H
ATOM 7932 HD22 LEU C 160 -19.500 16.828 -0.919 1.00 43.07 H
ATOM 7933 HD23 LEU C 160 -19.662 16.521 0.631 1.00 43.07 H
ATOM 7934 N GLY C 161 -21.462 19.011 3.617 1.00 45.49 N
ATOM 7935 CA GLY C 161 -21.979 19.071 4.970 1.00 48.60 C
ANISOU 7935 CA GLY C 161 11169 3895 3403 1885 405 -390 C
ATOM 7936 C GLY C 161 -20.879 19.044 6.017 1.00 49.80 C
ANISOU 7936 C GLY C 161 11568 3921 3432 1654 184 -484 C
ATOM 7937 O GLY C 161 -19.697 18.840 5.742 1.00 48.26 O
ANISOU 7937 O GLY C 161 11356 3673 3309 1309 -43 -496 O
ATOM 7938 H GLY C 161 -21.706 18.313 3.177 1.00 54.59 H
ATOM 7939 HA2 GLY C 161 -22.490 19.888 5.083 1.00 58.32 H
ATOM 7940 HA3 GLY C 161 -22.568 18.316 5.124 1.00 58.32 H
ATOM 7941 N SER C 162 -21.306 19.245 7.264 1.00 52.84 N
ANISOU 7941 N SER C 162 12175 4283 3620 1856 256 -539 N
ATOM 7942 CA SER C 162 -20.391 19.325 8.393 1.00 54.97 C
ANISOU 7942 CA SER C 162 12724 4427 3736 1676 56 -631 C
ATOM 7943 C SER C 162 -20.152 17.981 9.070 1.00 53.15 C
ANISOU 7943 C SER C 162 12240 4438 3518 1580 91 -608 C
ATOM 7944 O SER C 162 -19.147 17.829 9.776 1.00 53.95 O
ANISOU 7944 O SER C 162 12478 4473 3546 1332 -118 -657 O
ATOM 7945 CB SER C 162 -20.934 20.315 9.425 1.00 60.03 C
ANISOU 7945 CB SER C 162 13788 4901 4119 1952 99 -727 C
ATOM 7946 OG SER C 162 -22.249 19.953 9.806 1.00 60.80 O
ANISOU 7946 OG SER C 162 13728 5221 4154 2336 411 -686 O
ATOM 7947 H SER C 162 -22.133 19.338 7.481 1.00 63.41 H
ATOM 7948 HA SER C 162 -19.536 19.658 8.080 1.00 65.97 H
ATOM 7950 HB3 SER C 162 -20.949 21.204 9.036 1.00 72.03 H
ATOM 7951 HG SER C 162 -22.544 20.498 10.372 1.00 72.96 H
ATOM 7952 N ASN C 163 -21.052 17.017 8.887 1.00 51.07 N
ANISOU 7952 N ASN C 163 11612 4456 3336 1759 332 -520 N
ATOM 7953 CA ASN C 163 -20.943 15.695 9.500 1.00 49.58 C
ANISOU 7953 CA ASN C 163 11172 4518 3148 1680 370 -476 C
ATOM 7954 C ASN C 163 -20.589 14.687 8.404 1.00 45.21 C
ANISOU 7954 C ASN C 163 10226 4117 2835 1484 334 -391 C
ATOM 7955 O ASN C 163 -21.440 14.280 7.609 1.00 43.37 O
ANISOU 7955 O ASN C 163 9710 4038 2731 1631 513 -297 O
ATOM 7956 CB ASN C 163 -22.235 15.335 10.226 1.00 51.29 C
ANISOU 7956 CB ASN C 163 11283 4961 3245 2016 649 -414 C
ANISOU 7957 CG ASN C 163 10790 5059 3054 1924 693 -324 C

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ATOM 7963 HB3 ASN C 163
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ATOM 7965 HD22 ASN C 163
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ANISOU 7966 N TRP C 164
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ANISOU 7967 CA TRP C 164
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ANISOU 7968 C TRP C 164
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ATOM 7980 H TRP C 164
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ATOM 7986 HE3 TRP C 164
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ANISOU 7992 C ALA C 165 7564 3667 2170 859 85 -13 ATOM 7993 O ALA C 165 -18.023 9.545 6.019 1.00 34.02 ANISOU 7993 O ALA C 165 7517 3382 2026 665 -115 -104 0 ATOM 7994 CB ALA C 165 -21.599 9.505 6.554 1.00 37.86 C ANISOU 7994 CB ALA C 165 7831 4136 2419 1328 548 105 C ATOM 7995 H ALA C 165 -20.255 11.618 6.194 1.00 47.18 ATOM 7996 HA ALA C 165 -20.091 9.570 7.946 1.00 46.19 ATOM 7997 HB1 ALA C 165 -21.751 8.552 6.650 1.00 45.44 ATOM 7998 HB2 ALA C 165 -22.229 9.998 7.103 1.00 45.44 Н ATOM 7999 HB3 ALA C 165 -21.696 9.765 5.625 1.00 45.44 ATOM 8000 N TYR C 166 -19.502 7.874 5.713 1.00 34.15 ANISOU 8000 N TYR C 166 7111 3688 2178 867 107 121 Ν ATOM 8001 CA TYR C 166 -18.487 7.016 5.122 1.00 32.94 ANISOU 8001 CA TYR C 166 6694 3557 2263 663 -113 130 ATOM 8002 C TYR C 166 -17.994 7.587 3.795 1.00 30.94 ANISOU 8002 C TYR C 166 6338 3245 2172 599 -160 44 C ATOM 8003 O TYR C 166 -18.622 8.440 3.162 1.00 30.02 ANISOU 8003 O TYR C 166 6284 3078 2044 709 -19 12 ATOM 8004 CB TYR C 166 -18.997 5.578 4.939 1.00 33.14 ANISOU 8004 CB TYR C 166 6390 3718 2482 680 -116 ATOM 8005 CG TYR C 166 ANISOU 8005 CG TYR C 166 -19.996 5.328 3.816 1.00 31.73 5966 3603 2488 787 343 15 ATOM 8006 CD1 TYR C 166 -19.648 5.502 2.478 1.00 30.15 ANISOU 8006 CD1 TYR C 166 5616 3374 2466 751 -30 258 ATOM 8007 CD2 TYR C 166 -21.273 4.860 4.094 1.00 32.12 ANISOU 8007 CD2 TYR C 166 5910 3770 2523 905 166 514 ATOM 8008 CE1 TYR C 166 -20.555 5.264 1.464 1.00 28.80 **ANISOU 8008 CE1 TYR C 166** 5238 3264 2441 62 316 832 ATOM 8009 CE2 TYR C 166 -22.186 4.615 3.077 1.00 30.22 5435 3594 2451 970 249 596 -21.815 4.814 1.768 1.00 29.20 **ANISOU 8009 CE2 TYR C 166** ATOM 8010 CZ TYR C 166 ANISOU 8010 CZ TYR C 166 5197 3409 2488 931 188 485 C ATOM 8011 OH TYR C 166 -22.705 4.580 0.744 1.00 28.80 0 ANISOU 8011 OH TYR C 166 4933 3424 2585 979 245 564 ATOM 8012 H TYR C 166 -20.300 7.555 5.707 1.00 40.98 H 4933 3424 200 -20.300 7.555 5.707 1.00 40.90 -17.728 6.981 5.724 1.00 39.52 H -18.232 5.007 4.772 1.00 39.76 H -19.425 5.303 5.766 1.00 39.76 H -18.796 5.809 2.265 1.00 36.18 H -21.527 4.727 4.979 1.00 38.54 H 0 ATOM 8013 HA TYR C 166 ATOM 8014 HB2 TYR C 166 ATOM 8015 HB3 TYR C 166 ATOM 8016 HD1 TYR C 166 ATOM 8017 HD2 TYR C 166 -21.527 4.727 4.979 1.00 38.54 ATOM 8018 HE1 TYR C 166 -20.308 5.397 0.577 1.00 34.56 ATOM 8019 HE2 TYR C 166 -23.042 4.313 3.280 1.00 36.26 ATOM 8020 HH TYR C 166 -23.437 4.310 1.055 1.00 34.56 N 25 N ((Н ATOM 8021 N GLN C 167 -16.836 7.092 3.391 1.00 29.08 ANISOU 8021 N GLN C 167 5930 3038 2082 428 -359 ATOM 8022 CA GLN C 167 -16.130 7.572 2.214 1.00 28.16 ANISOU 8022 CA GLN C 167 5690 2921 2089 336 -426 ANISOU 8022 CA GLN C 167 5090 2921 2069 330 1426 131 C
ATOM 8023 C GLN C 167 -15.439 6.330 1.680 1.00 25.96 C
ANISOU 8023 C GLN C 167 5075 2769 2019 288 -554 -5 C
ATOM 8024 O GLN C 167 -14.495 5.836 2.303 1.00 26.06 O
ANISOU 8024 O GLN C 167 5061 2808 2032 181 -724 16 O
ATOM 8025 CB GLN C 167 -15.144 8.687 2.582 1.00 29.88 C
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-12.477 10.107 2.843 1.00 33.75 O
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ATOM 8029 NE2 GLN C 167
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ATOM 8030 H GLN C 167 -16.424 6.455 3.797 1.00 34.90 H
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ATOM 8031 HA GLN C 167
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ATOM 8031 HA GLN C 167
ATOM 8032 HB2 GLN C 167
ATOM 8033 HB3 GLN C 167
ATOM 8034 HG2 GLN C 167
ATOM 8035 HG3 GLN C 167
ATOM 8036 HE21 GLN C 167
ATOM 8037 HE22 GLN C 167
ATOM 8038 N AVAL C 168
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ANISOU 8039 N BVAL C 168
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 ATOM 8048 CG1AVAL C 168 -16.645 3.080 1.728 0.46 24.20
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 ATOM 8049 CG1BVAL C 168 -16.380 2.247 -0.647 0.54 22.64
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 ATOM 8050 CG2AVAL C 168 -17.761 3.698 -0.429 0.46 22.48
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ATOM 8053 H BVAL C 168 -16.509 6.233 0.061 0.54 28.86 H
ATOM 8054 HA AVAL C 168 -14.610 4.285 0.526 0.46 28.15 H
ATOM 8055 HA BVAL C 168 -14.778 4.194 0.523 0.54 28.08 H
ATOM 8056 HB AVAL C 168 -16.085 2.569 -0.171 0.46 27.77 H
ATOM 8057 HB BVAL C 168 -17.493 3.905 -0.247 0.54 27.62 H
ATOM 8058 HG11AVAL C 168 -17.285 2.358 1.822 0.46 29.04 H
ATOM 8059 HG11BVAL C 168 -17.124 1.632 -0.556 0.54 27.16 H
ATOM 8060 HG12AVAL C 168 -15.795 2.823 2.120 0.46 29.04 H
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ANISOU 8083 SD BMET C 169
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ATOM 8084 CE AMET C 169
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ATOM 8085 CE BMET C 169
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ATOM 8092 HB3AMET C 169
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ATOM 8094 HG2AMET C 169
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ATOM 8095 HG2BMET C 169
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ATOM 8096 HG3AMET C 169
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ATOM 8097 HG3BMET C 169
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ATOM 8099 HE1BMET C 169 -11.146 6.434 -4.493 0.54 28.78 ATOM 8100 HE2AMET C 169 -12.304 5.993 -7.760 0.46 28.77
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ATOM 8110 HB1 ALA C 170
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                             -17.731 -0.220 -7.613 1.00 21.85
ANISOU 8114 CA THR C 171 3105 2624 2571 988 -768 -439
ATOM 8115 C THR C 171 -19.243 -0.131 -7.454 1.00 21.46
ANISOU 8115 C THR C 171 3103 2499 2552 909 -729 -286
                                                                 C
ATOM 8116 O THR C 171 -19.807 -0.735 -6.536 1.00 21.81
                                                                  0
ANISOU 8116 O THR C 171 3195 2424 2669 856 -799 -162
ATOM 8117 CB THR C 171 -17.277 -1.650 -7.908 1.00 23.20
                                                                   0
ANISOU 8117 CB THR C 171
                            3264 2701 2849 1108 -970 -572
ATOM 8118 OG1 THR C 171
                             -15.850 -1.667 -8.009 1.00 23.88
ANISOU 8118 OG1 THR C 171 3265 2907 2899 1216 -977 -685
ATOM 8119 CG2 THR C 171 -17.887 -2.167 -9.206 1.00 24.37
ANISOU 8119 CG2 THR C 171 3412 2838 3009 1174 -1039 -683
ATOM 8120 H THR C 171 -17.217 -0.325 -5.732 1.00 25.94 H
ATOM 8121 HA THR C 171
                            -17.457 0.355 -8.345 1.00 26.21
ATOM 8122 HB THR C 171
                             -17.556 -2.232 -7.184 1.00 27.83
                            -15.582 -2.447 -8.171 1.00 28.65
ATOM 8123 HG1 THR C 171
ATOM 8124 HG21 THR C 171
                             -17.588 -3.074 -9.374 1.00 29.24
ATOM 8125 HG22 THR C 171
                              -18.855 -2.162 -9.142 1.00 29.24
ATOM 8126 HG23 THR C 171
                             -17.617 -1.603 -9.947 1.00 29.24
ATOM 8127 N ALA C 172 -19.894 0.644 -8.323 1.00 20.99
ANISOU 8127 N ALA C 172
                             3008 2536 2432 899 -615 -263
                                                                 Ν
ATOM 8128 CA ALA C 172
                             -21.329 0.873 -8.248 1.00 20.89
ANISOU 8128 CA ALA C 172
                             2995 2504 2440 843 -555 -87
ATOM 8129 C ALA C 172 -21.945 0.663 -9.624 1.00 22.60
ANISOU 8129 C ALA C 172
                            3143 2775 2670 850 -611 -127
ATOM 8130 O ALA C 172
                            -21.312 0.931 -10.647 1.00 22.13
ANISOU 8130 O ALA C 172 3050 2820 2537 904 -598 -274
                                                                   0
ATOM 8131 CB ALA C 172 -21.652 2.291 -7.740 1.00 20.24
                                                                  C
ANISOU 8131 CB ALA C 172 2961 2479 2252 835 -339 28
ATOM 8132 H ALA C 172 -19.514 1.055 -8.976 1.00 25.19
                                                                 C
                                                                 Н
ATOM 8133 HA ALA C 172 -21.725 0.233 -7.636 1.00 25.07
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ATOM 8134 HB1 ALA C 172 -22.615 2.402 -7.705 1.00 24.29 ATOM 8135 HB2 ALA C 172 Н ATOM 8136 HB3 ALA C 172 Н ATOM 8137 N GLY C 173 -23.179 0.171 -9.646 1.00 24.75 N **ANISOU 8137 N GLY C 173** 3383 3000 3022 782 -685 N ATOM 8138 CA GLY C 173 -23.811 -0.123 -10.922 1.00 27.86 **ANISOU 8138 CA GLY C 173** 3728 3432 3424 758 -787 ATOM 8139 C GLY C 173 -25.320 -0.110 -10.844 1.00 30.37 **ANISOU 8139 C GLY C 173** 3962 3773 3805 657 -795 C ATOM 8140 O GLY C 173 -25.915 0.001 -9.771 1.00 30.53 0 **ANISOU 8140 O GLY C 173** 3950 3788 3863 624 -715 471 0 ATOM 8141 H GLY C 173 -23.661 0.003 -8.954 1.00 29.70 ATOM 8142 HA2 GLY C 173 -23.533 0.534 -11.578 1.00 33.43 Н ATOM 8143 HA3 GLY C 173 -23.528 -1.000 -11.226 1.00 33.43 ATOM 8144 N TYR C 174 -25.936 -0.221 -12.023 1.00 34.22 Ν **ANISOU 8144 N TYR C 174** 4401 4317 4287 612 -892 264 Ν -27.387 -0.251 -12.160 1.00 37.21 ATOM 8145 CA TYR C 174 **ANISOU 8145 CA TYR C 174** 4657 4751 4729 499 -936 538 ATOM 8146 C TYR C 174 ANISOU 8146 C TYR C 174 -27.755 -1.218 -13.274 1.00 40.17 C 5060 5064 5140 392 -1229 468 ATOM 8147 O TYR C 174 -27.265 -1.078 -14.398 1.00 39.68 **ANISOU 8147 O TYR C 174** 5054 5051 4972 451 -1262 0 256 ATOM 8148 CB TYR C 174 -27.950 1.138 -12.474 1.00 36.86 C **ANISOU 8148 CB TYR C 174** 4510 4890 4604 562 -697 679 ATOM 8149 CG TYR C 174 -29.458 1.174 -12.584 1.00 38.16 C **ANISOU 8149 CG TYR C 174** 4502 5160 4837 474 -720 999 ATOM 8150 H TYR C 174 -25.521 -0.282 -12.774 1.00 41.07 Н ATOM 8151 HA TYR C 174 -27.786 -0.566 -11.334 1.00 44.65 Н ATOM 8152 HB2 TYR C 174 -27.689 1.748 -11.766 1.00 44.23 Н -27.583 1.440 -13.320 1.00 44.23 ATOM 8153 HB3 TYR C 174 ATOM 8154 N GLN C 175 -28.627 -2.180 -12.960 1.00 43.20 Ν **ANISOU 8154 N GLN C 175** 5410 5347 5656 226 -1452 Ν -29.034 -3.230 -13.891 1.00 45.45 ATOM 8155 CA GLN C 175 C **ANISOU 8155 CA GLN C 175** 5773 5509 5988 83 -1801 604 ATOM 8156 C GLN C 175 -27.925 -3.525 -14.893 1.00 41.49 **ANISOU 8156 C GLN C 175** 5463 4934 5366 222 -1889 199 C ATOM 8157 O GLN C 175 -28.103 -3.329 -16.099 1.00 45.19 0 0 **ANISOU 8157 O GLN C 175** 5951 5495 5724 220 -1949 103 ATOM 8158 CB GLN C 175 -30.327 -2.836 -14.620 1.00 48.55 **ANISOU 8158 CB GLN C 175** 5999 6069 6380 -55 -1843 861 ATOM 8159 CG GLN C 175 -31.274 -1.976 -13.800 1.00 48.83 **ANISOU 8159 CG GLN C 175** 5788 6305 6458 -63 -1595 1239 -29.005 -2.244 -12.190 1.00 51.84 ATOM 8160 H GLN C 175 Н ATOM 8161 HA GLN C 175 -29.209 -4.043 -13.391 1.00 54.54 Н ATOM 8162 HB2 GLN C 175 -30.093 -2.336 -15.418 1.00 58.26 Н ATOM 8163 HB3 GLN C 175 -30.802 -3.644 -14.868 1.00 58.26 Н ATOM 8164 N ASER C 176 -26.772 -3.974 -14.412 0.51 37.13 Ν **ANISOU 8164 N ASER C 176** 5039 4250 4818 358 -1888 -28 Ν ATOM 8165 N BSER C 176 -26.781 -3.984 -14.395 0.49 37.12 Ν 5038 4246 4821 356 -1890 -24 Ν **ANISOU 8165 N BSER C 176 ATOM 8166 CA ASER C 176** -25.641 -4.261 -15.289 0.51 35.44 ANISOU 8166 CA ASER C 176 4977 4013 4477 543 -1935 -401 C ATOM 8167 CA BSER C 176 -25.601 -4.207 -15.218 0.49 35.29

ANISOU 8167 CA BSER C 176 4950 4000 4459 549 -1915 -396 ATOM 8168 C ASER C 176 -25.006 -5.566 -14.827 0.51 35.71 **ANISOU 8168 C ASER C 176** 5194 3761 4614 601 -2174 -568 C ATOM 8169 C BSER C 176 -25.005 -5.559 -14.830 0.49 35.70 **ANISOU 8169 C BSER C 176** C 5191 3761 4611 601 -2173 -568 ATOM 8170 O ASER C 176 -25.609 -6.358 -14.094 0.51 35.96 0 **ANISOU 8170 O ASER C 176** 5260 3587 4815 441 -2379 -389 0 ATOM 8171 O BSER C 176 -25.632 -6.383 -14.151 0.49 36.07 0 **ANISOU 8171 O BSER C 176** 0 5280 3598 4827 438 -2390 -394 ATOM 8172 CB ASER C 176 -24.651 -3.086 -15.304 0.51 32.32 C ANISOU 8172 CB ASER C 176 4495 3843 3942 716 -1601 -502 **ATOM 8173 CB BSER C 176** -24.610 -3.046 -15.048 0.49 32.06 C **ANISOU 8173 CB BSER C 176** 4451 3801 3929 715 -1577 -476 **ATOM 8174 OG ASER C 176** -23.981 -2.958 -14.063 0.51 30.51 ANISOU 8174 OG ASER C 176 4245 3567 3782 769 -1475 -466 0 ATOM 8175 OG BSER C 176 -23.720 -2.955 -16.148 0.49 32.12 0 **ANISOU 8175 OG BSER C 176** 0 4512 3928 3763 879 -1550 -756 **ATOM 8176 HA ASER C 176** -25.967 -4.389 -16.193 0.51 42.53 Н **ATOM 8177 HA BSER C 176** -25.864 -4.247 -16.151 0.49 42.35 Н **ATOM 8178 HB2ASER C 176** -23.993 -3.239 -16.001 0.51 38.78 Н Н **ATOM 8179 HB2BSER C 176** -25.108 -2.216 -14.979 0.49 38.47 **ATOM 8180 HB3ASER C 176** -25.138 -2.267 -15.484 0.51 38.78 ATOM 8181 HB3BSER C 176 -24.094 -3.190 -14.239 0.49 38.47 Н **ATOM 8182 HG ASER C 176** -23.445 -2.312 -14.091 0.51 36.61 Н **ATOM 8183 HG BSER C 176** -23.279 -3.667 -16.220 0.49 38.54 ATOM 8184 N SER C 177 -23.770 -5.797 -15.264 1.00 36.30 **ANISOU 8184 N SER C 177** 5374 3833 4584 840 -2152 -892 ATOM 8185 CA SER C 177 -23.072 -7.045 -15.004 1.00 39.01 5912 3902 5010 964 -2386 -1094 **ANISOU 8185 CA SER C 177** ATOM 8186 C SER C 177 ANISOU 8186 C SER C 177 -21.581 -6.769 -15.131 1.00 39.11 5900 4063 4899 1262 -2190 -1349 ATOM 8187 O SER C 177 -21.178 -5.816 -15.804 1.00 36.99 0 **ANISOU 8187 O SER C 177** 5514 4090 4452 1351 -1953 -1415 0 ATOM 8188 CB SER C 177 -23.510 -8.135 -15.995 1.00 42.44 C **ANISOU 8188 CB SER C 177** 6592 4104 5429 946 -2751 -1272 ATOM 8189 OG SER C 177 -24.899 -8.416 -15.889 1.00 43.09 0 6669 4065 5637 628 -2969 -992 **ANISOU 8189 OG SER C 177** 0 ATOM 8190 HA SER C 177 -23.260 -7.346 -14.101 1.00 46.82 Н ATOM 8191 HB2 SER C 177 -23.319 -7.833 -16.896 1.00 50.93 ATOM 8192 HB3 SER C 177 -23.012 -8.946 -15.807 1.00 50.93 Н ATOM 8193 HG SER C 177 -25.345 -7.723 -16.052 1.00 51.70 ATOM 8194 N GLY C 178 -20.768 -7.595 -14.475 1.00 41.73 **ANISOU 8194 N GLY C 178** 6323 4203 5328 1404 -2298 -1456 Ν -19.339 -7.591 -14.732 1.00 42.98 ATOM 8195 CA GLY C 178 **ANISOU 8195 CA GLY C 178** 6458 4498 5374 1719 -2172 -1709 ATOM 8196 C GLY C 178 -18.530 -7.955 -13.500 1.00 42.58 **ANISOU 8196 C GLY C 178** 6375 4336 5466 1792 -2177 -1655 ATOM 8197 O GLY C 178 -19.053 -8.501 -12.532 1.00 43.14 0 6509 4159 5723 1627 -2341 -1474 **ANISOU 8197 O GLY C 178** 0 ATOM 8198 H GLY C 178 -21.021 -8.163 -13.881 1.00 50.07 H ATOM 8199 HA2 GLY C 178 -19.134 -8.228 -15.434 1.00 51.57 Н ATOM 8200 HA3 GLY C 178 -19.066 -6.708 -15.029 1.00 51.57 ATOM 8201 N SER C 179 -17.236 -7.621 -13.573 1.00 40.58 N

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ANISOU 8201 N SER C 179 5991 4320 5108 2016 -1988 -1770
ATOM 8202 CA SER C 179 -16.247 -7.996 -12.574 1.00 39.51
ANISOU 8202 CA SER C 179 5789 4161 5061 2089 -1984 -1718
ATOM 8203 C SER C 179 -15.374 -6.806 -12.216 1.00 36.16
ANISOU 8203 C SER C 179 5134 4052 4554 2125 -1705 -1652
ATOM 8204 O SER C 179 -15.034 -5.987 -13.075 1.00 35.34
                                                                    0
ANISOU 8204 O SER C 179 4906 4250 4273 2194 -1512 -1719
ATOM 8205 CB SER C 179
                              -15.332 -9.102 -13.077 1.00 42.68
ANISOU 8205 CB SER C 179
                             6254 4550 5414 2317 -2089 -1896 C
                              -16.064 -10.273 -13.369 1.00 45.89
ATOM 8206 OG SER C 179
ANISOU 8206 OG SER C 179
                              6896 4640 5901 2287 -2382 -1949
ATOM 8207 H SER C 179 -16.904 -7.161 -14.219 1.00 48.70 H
ATOM 8208 HA SER C 179
                             -16.695 -8.304 -11.771 1.00 47.41
ATOM 8209 HB2 SER C 179
                              -14.886 -8.800 -13.883 1.00 51.22
ATOM 8210 HB3 SER C 179
                              -14.675 -9.304 -12.392 1.00 51.22
ATOM 8211 HG SER C 179
                              -16.456 -10.547 -12.679 1.00 55.07
                              -14.978 -6.748 -10.945 0.49 34.58
ATOM 8212 N ASER C 180
ANISOU 8212 N ASER C 180
                               4879 3788 4471 2062 -1706 -1499 N
ATOM 8213 N BSER C 180
                              -14.995 -6.724 -10.942 0.51 34.52 N
                              4870 3782 4463 2059 -1704 -1496 N
ANISOU 8213 N BSER C 180
ATOM 8214 CA ASER C 180
                              -14.105 -5.696 -10.452 0.49 32.79
ANISOU 8214 CA ASER C 180 4449 3838 4173 2036 -1493 -1394
ATOM 8215 CA BSER C 180
                              -14.072 -5.690 -10.503 0.51 32.84
ANISOU 8215 CA BSER C 180 4452 3855 4173 2046 -1489 -1402
ATOM 8216 C ASER C 180
                              -13.207 -6.253 -9.358 0.49 33.52
                              4510 3848 4380 2101 -1589 -1336
ANISOU 8216 C ASER C 180
ATOM 8217 C BSER C 180
                              -13.219 -6.219 -9.360 0.51 33.47 C
ANISOU 8217 C BSER C 180
                              4501 3845 4371 2098 -1585 -1333 C
ATOM 8218 O ASER C 180
                              -13.637 -7.084 -8.555 0.49 34.25 O
                              4737 3660 4617 2010 -1768 -1253
ANISOU 8218 O ASER C 180
ATOM 8219 O BSER C 180
                              -13.691 -6.993 -8.523 0.51 34.05 O
ANISOU 8219 O BSER C 180
                              4708 3639 4589 1997 -1759 -1240
ATOM 8220 CB ASER C 180
                              -14.900 -4.512 -9.892 0.49 29.92 C
ANISOU 8220 CB ASER C 180 4056 3534 3779 1735 -1343 -1165
ATOM 8221 CB BSER C 180 -14.810 -4.419 -10.055 0.51 29.98 C
ANISOU 8221 CB BSER C 180 4045 3582 3762 1753 -1320 -1183 C
ATOM 8222 OG ASER C 180
                               -14.028 -3.577 -9.278 0.49 28.50
                                                                  0
ANISOU 8222 OG ASER C 180 3738 3554 3536 1674 -1196 -1060
ATOM 8223 OG BSER C 180
                               -15.476 -4.612 -8.818 0.51 28.43
                                                                     0
                              3939 3172 3690 1569 -1403 -995 -15.208 -7.318 -10.343 0.49 41.49
                                                                      0
ANISOU 8223 OG BSER C 180
ATOM 8224 H ASER C 180
                                                                 H
H
ATOM 8225 HA ASER C 180
                              -13.544 -5.375 -11.176 0.49 39.35
ATOM 8226 HA BSER C 180
                              -13.484 -5.455 -11.237 0.51 39.41
                                                                     Н
ATOM 8226 HA BSER C 180 -13.484 -5.455 -11.237 0.51 39.41 H
ATOM 8227 HB2ASER C 180 -15.373 -4.076 -10.618 0.49 35.91 H
ATOM 8228 HB2BSER C 180 -14.166 -3.701 -9.956 0.51 35.97 H
ATOM 8230 HB3BSER C 180 -15.466 -4.183 -10.730 0.51 35.97 H
ATOM 8231 HG ASER C 180 -13.475 -3.288 -9.841 0.49 34.20 H
ATOM 8232 HG BSER C 180 -14 921 -4 816 -8 222 0.51 34 11
ATOM 8232 HG BSER C 180 -14.921 -4.816 -8.222 0.51 34.11 H
ATOM 8233 N ASN C 181 -11.960 -5.790 -9.340 1.00 32.70 N
ANISOU 8233 N ASN C 181 4209 4018 4197 2212 -1467 -1340 N ATOM 8234 CA ASN C 181 -11.050 -6.014 -8.227 1.00 33.78 C
ANISOU 8234 CA ASN C 181 4268 4149 4419 2216 -1528 -1226 C
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ATOM 8235 C ASN C 181 -10.376 -4.686 -7.971 1.00 32.32
ANISOU 8235 C ASN C 181 3881 4278 4121 2087 -1353 -1089 ATOM 8236 O ASN C 181 -9.799 -4.101 -8.893 1.00 32.44
ANISOU 8236 O ASN C 181 3727 4598 4001 2174 -1205 -1147 ATOM 8237 CB ASN C 181 -9.988 -7.080 -8.506 1.00 37.39 C
ANISOU 8237 CB ASN C 181 4687 4630 4890 2444 -1581 -1344
ATOM 8238 CG ASN C 181
                                     -8.920 -7.135 -7.399 1.00 39.35
ANISOU 8238 CG ASN C 181 4796 4939 5216 2452 -1622 -1195
ATOM 8239 OD1 ASN C 181 -9.040 -7.900 -6.446 1.00 39.76 O
ANISOU 8239 OD1 ASN C 181 4963 4737 5409 2393 -1785 -1113
ATOM 8240 ND2 ASN C 181 -7.889 -6.298 -7.517 1.00 40.21 N
ANISOU 8240 ND2 ASN C 181 4643 5406 5230 2497 -1487 -1130
ATOM 8241 H ASN C 181 -11.603 -5.340 -9.980 1.00 39.24 H
ATOM 8242 HA ASN C 181
                                   -11.552 -6.269 -7.436 1.00 40.54
ATOM 8244 HB3 ASN C 181 -9.545 -6.876 -9.344 1.00 44.87 H
ATOM 8245 HD21 ASN C 181 -7.268 -6.294 -6.922 1.00 48.26 H
ATOM 8246 HD22 ASN C 181 -7.844 -5.763 -8.189 1.00 48.26 H
ATOM 8247 N VAL C 182 -10.469 -4.205 -6.737 1.00 30.64 N
ANISOU 8247 N VAL C 182 3706 3994 3941 1945 4274 201
ATOM 8243 HB2 ASN C 181
                                     -10.416 -7.949 -8.557 1.00 44.87
                                      3706 3994 3941 1845 -1371 -894 N
ANISOU 8247 N VAL C 182
ATOM 8248 CA VAL C 182
                                   -9.898 -2.922 -6.367 1.00 29.74
ANISOU 8248 CA VAL C 182 3473 4111 3714 1649 -1246 -750
ATOM 8249 C VAL C 182 -9.254 -3.056 -5.001 1.00 31.72 C ANISOU 8249 C VAL C 182 3719 4309 4025 1552 -1369 -599 C
ATOM 8250 O VAL C 182 -9.738 -3.773 -4.119 1.00 32.35
ANISOU 8250 O VAL C 182 3949 4137 4206 1519 -1504 -548
                                     -10.949 -1.790 -6.341 1.00 27.90
ATOM 8251 CB VAL C 182
ANISOU 8251 CB VAL C 182 3369 3840 3392 1400 -1113 -671 C
ATOM 8252 CG1 VAL C 182 -10.273 -0.432 -6.124 1.00 27.28
ANISOU 8252 CG1 VAL C 182 3203 3970 3190 1209 -1015 -545 C
ATOM 8253 CG2 VAL C 182 -11.779 -1.792 -7.613 1.00 27.03 C
ANISOU 8253 CG2 VAL C 182 3287 3742 3241 1480 -1029 -795 C
ATOM 8254 H VAL C 182 -10.864 -4.610 -6.089 1.00 36.76 H
ATOM 8255 HA VAL C 182 -9.210 -2.682 -7.007 1.00 35.68
ATOM 8256 HB VAL C 182 -11.551 -1.942 -5.596 1.00 33.48
ATOM 8256 HB VAL C 182 -11.551 -1.942 -5.596 1.00 33.48

ATOM 8257 HG11 VAL C 182 -10.953 0.260 -6.111 1.00 32.73

ATOM 8258 HG12 VAL C 182 -9.800 -0.447 -5.277 1.00 32.73

ATOM 8259 HG13 VAL C 182 -9.650 -0.271 -6.849 1.00 32.73

ATOM 8260 HG21 VAL C 182 -12.428 -1.072 -7.567 1.00 32.43

ATOM 8261 HG22 VAL C 182 -11.191 -1.659 -8.373 1.00 32.43

ATOM 8263 N THP C 183 -8.149 -2.354 -4.846 1.00 32.16
                                     -8.149 -2.354 -4.846 1.00 32.16 N
ATOM 8263 N THR C 183
                                      3591 4621 4009 1485 -1337 -503
ANISOU 8263 N THR C 183
ATOM 8264 CA THR C 183 -7.441 -2.242 -3.588 1.00 32.44 C
                                      3607 4657 4061 1341 -1460 -337
ANISOU 8264 CA THR C 183
                                     -7.378 -0.769 -3.240 1.00 30.73 C
ATOM 8265 C THR C 183
ANISOU 8265 C THR C 183
                                      3433 4543 3700 1032 -1384 -210 C
ATOM 8266 O THR C 183 -7.175 0.070 -4.120 1.00 30.64 O
ANISOU 8266 O THR C 183 3312 4733 3599 988 -1260 -217 O
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ATOM 8269 CG2 THR C 183 -5.201 -2.591 -2.487 1.00 35.32 ANISOU 8269 CG2 THR C 183 3634 5300 4487 1365 -1686 -111 ATOM 8270 H THR C 183 -7.774 -1.915 -5.483 1.00 38.60 H
ATOM 8271 HA THR C 183 -7.932 -2.707 -2.892 1.00 38.92 H
ATOM 8272 HB THR C 183 -5.594 -2.478 -4.475 1.00 41.23 H
ATOM 8273 HG1 THR C 183 -6.623 -4.425 -4.605 1.00 42.67 H
ATOM 8274 HG21 THR C 183 -4.326 -2.995 -2.594 1.00 42.38 H ATOM 8275 HG22 THR C 183 -5.094 -1.635 -2.364 1.00 42.38 ATOM 8276 HG23 THR C 183 -5.627 -2.964 -1.700 1.00 42.38 ATOM 8277 N VAL C 184 -7.607 -0.462 -1.965 1.00 30.26 3564 4327 3605 821 -1467 -97 N **ANISOU 8277 N VAL C 184** ATOM 8278 CA VAL C 184 -7.775 0.905 -1.494 1.00 29.53 ANISOU 8278 CA VAL C 184
ANISOU 8278 CA VAL C 184
ATOM 8279 C VAL C 184
ANISOU 8279 C VAL C 184
ANISOU 8279 C VAL C 184
ATOM 8280 O VAL C 184
ANISOU 8280 O VAL C 184
ANISOU 8280 O VAL C 184
ATOM 8281 CB VAL C 184
ANISOU 8281 CB VAL C 184 ANISOU 8281 CB VAL C 184 3751 3799 3123 474 -1328 -42 ATOM 8282 CG1 VAL C 184 -9.408 2.660 -0.747 1.00 27.40 ANISOU 8282 CG1 VAL C 184 3854 3688 2870 247 -1266 8 ATOM 8283 CG2 VAL C 184 -10.221 0.747 -2.140 1.00 26.72 ANISOU 8283 CG2 VAL C 184 3558 3574 3020 649 -1203 -165 C ATOM 8284 H VAL C 184 -7.671 -1.048 -1.339 1.00 36.31 H ATOM 8285 HA VAL C 184 -7.531 1.524 -2.200 1.00 35.44 ATOM 8286 HB VAL C 184 -9.425 0.693 -0.261 1.00 33.71 ATOM 8294 CA TRP C 185 -5.451 2.681 0.907 1.00 34.29 C ANISOU 8294 CA TRP C 185 4304 4997 3727 -118 -1815 383 ATOM 8295 C TRP C 185 -5.156 4.172 0.963 1.00 34.89 C ANISOU 8295 C TRP C 185 4509 5097 3651 -426 -1849 461 ATOM 8296 O TRP C 185 -5.572 4.938 0.085 1.00 33.17 0 ANISOU 8296 O TRP C 185 4319 4889 3397 -448 -1709 412 ATOM 8297 CB TRP C 185 -4.135 1.901 0.812 1.00 36.99 **ANISOU 8297 CB TRP C 185** 4277 5592 4185 -18 -1951 489 -3.203 2.374 -0.283 1.00 38.65 ATOM 8298 CG TRP C 185 C **ANISOU 8298 CG TRP C 185** 4143 6139 4403 -21 -1902 561 ATOM 8299 CD1 TRP C 185 -2.238 3.339 -0.182 1.00 41.03 C **ANISOU 8299 CD1 TRP C 185** 4322 6642 4626 -310 -2017 ATOM 8300 CD2 TRP C 185 -3.142 1.890 -1.631 1.00 37.76 C 3763 6221 4362 267 -1737 463 C **ANISOU 8300 CD2 TRP C 185** -1.586 3.487 -1.384 1.00 41.78 N ATOM 8301 NE1 TRP C 185

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ANISOU 8303 CE3 TRP C 185
                             3508 5875 4193
                                               601 -1610
                                                          266
ATOM 8304 CZ2 TRP C 185
                             -1.792 2.388 -3.625 1.00 40.05
                                                               C
ANISOU 8304 CZ2 TRP C 185
                                                          579
                                                                 C
                             3436 7170 4612
                                               386 -1569
ATOM 8305 CZ3 TRP C 185
                                                               C
                             -3.521 0.702 -3.672 1.00 36.54
                                                                 C
ANISOU 8305 CZ3 TRP C 185
                             3344 6237 4304 836 -1472
                                                          194
ATOM 8306 CH2 TRP C 185
                             -2.501 1.432 -4.297 1.00 38.53
                                                               C
ANISOU 8306 CH2 TRP C 185
                             3283 6876 4480 743 -1435
                                                                 C
                                                           347
ATOM 8307 OXT TRP C 185
                             -4.485 4.620 1.898 1.00 35.70
                                                               0
ANISOU 8307 OXT TRP C 185
                             4704 5194 3665 -669 -2044
                                                           585
                                                                  0
ATOM 8308 H TRP C 185
                            -6.471 2.990 -0.755 1.00 38.35
                                                              Н
ATOM 8309 HA TRP C 185
                            -5.886 2.433 1.738 1.00 41.15
                                                              Н
ATOM 8310 HB2 TRP C 185
                             -3.664 1.984 1.656 1.00 44.39
                                                               Н
ATOM 8311 HB3 TRP C 185
                             -4.339 0.968 0.642 1.00 44.39
                                                               Н
ATOM 8312 HD1 TRP C 185
                             -2.052 3.827 0.588 1.00 49.24
                                                               Н
ATOM 8313 HE1 TRP C 185
                             -0.946 4.040 -1.541 1.00 50.14
                                                               Н
ATOM 8314 HE3 TRP C 185
                                                               Н
                             -4.526 0.428 -1.936 1.00 42.88
                             -1.117 2.872 -4.043 1.00 48.06
-3.986 0.059 -4.157 1.00 43.85
ATOM 8315 HZ2 TRP C 185
                                                               Н
ATOM 8316 HZ3 TRP C 185
                                                               Н
ATOM 8317 HH2 TRP C 185
                             -2.305 1.266 -5.190 1.00 46.23
                                                               Н
             TRP C 185
TER 8318
HETATM 8319 K
                 K A 201
                           -7.319 -5.472 -26.177 1.00 17.24
                                                              K
HETATM 8320 K
                 K B 201
                                                               K
                           -37.692 -16.388 -48.771 1.00 21.22
                K C 201
HETATM 8321 K
                           -10.727 -9.394 4.518 1.00 41.96
                                                              Κ
HETATM 8322 O
               HOH A 301
                             -9.339 -21.157 -3.388 1.00 44.07
                                                                0
                             -9.599 -8.614 -15.360 1.00 39.39
HETATM 8323 O HOH A 302
                                                                 0
HETATM 8324 O
               HOH A 303
                             -10.229 -11.531 -6.671 0.89 37.20
                                                                 0
HETATM 8325 O HOH A 304
                             -12.049 -22.967 -15.288 1.00 44.18
HETATM 8326 O
               HOH A 305
                             -14.217 -21.490 -16.673 1.00 47.88
                                                                 0
HETATM 8327 O HOH A 306
                             2.746 -31.536 -32.761 0.91 27.90
                                                                 0
                             -0.009 -7.455 -27.526 0.80 19.09
HETATM 8328 O
               HOH A 307
                                                                0
HETATM 8329 O HOH A 308
                                                                 0
                             20.715 -27.009 -13.296 1.00 30.75
HETATM 8330 O
               HOH A 309
                              6.080 -1.039 -15.852 1.00 41.13
HETATM 8331 O HOH A 310
                              8.790 -14.535 -31.973 1.00 39.94
                                                                 0
HETATM 8332 O HOH A 311
                              4.588 -12.892 -5.108 0.91 22.51
HETATM 8333 O
               HOH A 312
                              9.940 -34.355 -34.551 1.00 29.08
                                                                 0
HETATM 8334 O
                             11.827 -19.020 -32.206 1.00 29.41
               HOH A 313
HETATM 8335 O AHOH A 314
                             14.338 -38.591 -15.199 0.59 20.58
                                                                  0
HETATM 8336 O BHOH A 314
                              15.495 -40.071 -14.302 0.41 20.16
                                                                  0
HETATM 8337 O HOH A 315
                             18.292 -10.734 -19.392 1.00 36.16
                                                                 0
HETATM 8338 O HOH A 316
                              6.134 -7.517 -11.228 0.96 19.21
HETATM 8339 O
               HOH A 317
                              7.346 -35.849 -11.658 0.97 32.98
                                                                 0
HETATM 8340 O
                                                                 0
               HOH A 318
                             10.748 -9.066 -24.574 1.00 27.77
HETATM 8341 O
                                                                 0
               HOH A 319
                              6.902 -22.110 -35.275 1.00 25.32
                             -7.045 -23.930 -4.819 1.00 35.53
HETATM 8342 O
               HOH A 320
                                                                0
HETATM 8343 O
               HOH A 321
                              3.695 -5.808 -25.176 1.00 17.43
HETATM 8344 O
               HOH A 322
                             9.220 -23.279 -4.612 1.00 35.34
                                                                0
HETATM 8345 O
               HOH A 323
                              3.232 -10.643 -4.755 1.00 33.11
                                                                0
HETATM 8346 O HOH A 324
                             10.043 -25.867 -5.523 1.00 18.98
                                                                 0
HETATM 8347 O
               HOH A 325
                             6.040 -35.026 -24.918 1.00 13.30
HETATM 8348 O HOH A 326
                             13.860 -16.283 -14.386 1.00 13.60
                                                                 0
HETATM 8349 O
               HOH A 327
                             14.470 -11.621 -8.460 1.00 43.82
                                                                 0
HETATM 8350 O
               HOH A 328
                             14.660 -25.758 -29.578 1.00 22.80
                                                                 0
HETATM 8351 O HOH A 329 -3.440 -38.841 -24.807 1.00 32.52
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LIETATM 0252 O	11011 4 220	7 004 04 075 00 005 4 00 44 07	_
HETATM 8352 O	HOH A 330	7.224 -21.375 -26.865 1.00 11.67	0
HETATM 8353 O	HOH A 331	1.862 -6.239 -31.443 1.00 38.15	0
HETATM 8354 O	HOH A 332	18.375 -35.866 -16.322 1.00 26.84	0
HETATM 8355 O	HOH A 333	-1.264 -41.662 -22.983 1.00 39.83	0
HETATM 8356 O	HOH A 334	-6.685 -40.337 -18.540 0.96 37.26	0
HETATM 8357 O	HOH A 335	5.447 -15.242 -35.003 0.94 28.85	Ŏ
HETATM 8358 O	HOH A 336	16.487 -29.292 -28.867 1.00 34.14	Ö
HETATM 8359 O	HOH A 337	-3.543 -3.248 -28.058 1.00 22.47	Õ
HETATM 8360 O	HOH A 338	20.756 -34.427 -14.549 1.00 27.81	0
HETATM 8361 O	HOH A 339	-8.889 -4.528 -16.234 0.96 30.70	0
HETATM 8362 O	HOH A 340	-0.186 -28.229 -4.681 1.00 44.82	0
HETATM 8363 O	HOH A 341	18.119 -28.503 -27.065 1.00 24.60	0
HETATM 8364 O	HOH A 342	21.608 -21.574 -17.078 0.95 19.25	0
HETATM 8365 O	HOH A 343	16.047 -26.957 -22.810 1.00 11.78	0
HETATM 8366 O	HOH A 344	13,231 -31,946 -33,367 0,99 29,44	0
HETATM 8367 O	HOH A 345	21.961 -19.591 -15.022 0.93 34.32	Ŏ
HETATM 8368 O	HOH A 346	-5.321 -2.742 -16.824 1.00 31.19	Õ
HETATM 8369 O	HOH A 347	8.587 -6.955 -8.551 0.84 28.84	Õ
	HOH A 347	16.106 -27.123 -25.646 1.00 11.73	
HETATM 8370 O			0
HETATM 8371 O	HOH A 349	1.688 -6.705 -7.287 0.99 24.53	0
HETATM 8372 O	HOH A 350	7.950 -17.721 -0.792 1.00 33.81	0
HETATM 8373 O	HOH A 351	7.301 -9.966 -10.420 1.00 20.38	0
HETATM 8374 O	HOH A 352	9.746 -22.444 -34.690 1.00 21.86	0
HETATM 8375 O	HOH A 353	19.223 -22.052 -2.552 1.00 45.23	0
HETATM 8376 O	HOH A 354	-5.367 -2.216 -20.679 1.00 24.47	0
HETATM 8377 O	HOH A 355	13.575 -14.416 -10.127 1.00 17.91	0
HETATM 8378 O	HOH A 356	14,228 -8.577 -13.012 1.00 32.37	0
HETATM 8379 O	HOH A 357	1.277 -2.788 -7.310 1.00 51.44	o
HETATM 8380 O	HOH A 358	4.439 -25.016 -33.453 1.00 44.52	o
HETATM 8381 O	HOH A 359	19.220 -14.310 -23.437 0.99 25.38	ŏ
HETATM 8382 O	HOH A 360	18.863 -25.383 -3.736 1.00 27.33	
			0
HETATM 8383 O	HOH A 361	16.711 -15.208 -22.683 1.00 24.81	0
HETATM 8384 O	HOH A 362	-6.930 -0.824 -26.575 0.78 26.97	0
HETATM 8385 O	HOH A 363	11.343 -23.750 -36.390 0.95 32.94	0
HETATM 8386 O	HOH A 364	-16.270 -16.989 -16.969 0.95 29.18	0
HETATM 8387 O	HOH A 365	12.073 -2.654 -20.584 1.00 40.69	0
HETATM 8388 O	HOH A 366	-6.634 -5.427 -18.517 0.93 29.57	0
HETATM 8389 O	HOH A 367	9.738 -0.969 -11.967 1.00 33.88	0
HETATM 8390 O	HOH A 368	-0.272 -7.349 -5.806 1.00 29.70	0
HETATM 8391 O	HOH A 369	11.681 -5.625 -16.951 1.00 41.30	O
HETATM 8392 O	HOH A 370	-6.693 -38.863 -28.231 0.98 36.57	Ŏ
HETATM 8393 O	HOH A 371	14.543 -10.553 -25.957 1.00 25.19	Ö
HETATM 8394 O	HOH A 371	18.013 -36.112 -23.943 1.00 11.72	ŏ
			_
HETATM 8395 O	HOH A 373	12.520 -9.147 -9.416 0.96 37.22	0
HETATM 8396 O	HOH A 374	22.436 -21.756 -12.398 0.87 30.32	0
HETATM 8397 O	HOH A 375	1.793 -2.833 -23.207 1.00 24.39	0
HETATM 8398 O	HOH A 376	20.122 -13.660 -14.791 1.00 27.65	0
HETATM 8399 O	HOH A 377	-11.446 -9.848 -22.944 0.98 29.92	0
HETATM 8400 O	HOH A 378	-11.476 -22.435 -23.453 1.00 34.04	0
HETATM 8401 O	HOH A 379	-9.055 -33.801 -21.449 0.99 41.65	0
HETATM 8402 O	HOH A 380	-2.472 -36.198 -16.262 0.93 26.71	0
HETATM 8403 O	HOH A 381	21.815 -14.028 -16.971 1.00 42.55	O
HETATM 8404 O	HOH A 382	21.949 -17.989 -21.275 0.91 40.88	Ŏ
			•

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HETATM 8405 O
                HOH A 383
                             -12.721 -13.104 -7.895 1.00 38.02
                                                                 0
HETATM 8406 O
                HOH A 384
                              18.738 -23.129 -27.295 1.00 40.05
                                                                 0
HETATM 8407 O
                HOH A 385
                              -3.577 -18.517 -1.327 1.00 32.32
                                                                 0
HETATM 8408 O
                                                                 0
               HOH A 386
                              3.971 -36.958 -13.855 1.00 38.44
HETATM 8409 O
                                                                 0
               HOH A 387
                             -3.354 -19.765 -32.165 1.00 38.19
HETATM 8410 O
                                                                 0
               HOH A 388
                             4.873 -32.402 -32.587 1.00 21.44
                                                                 0
HETATM 8411 O
               HOH A 389
                             -15.990 -19.972 -17.420 1.00 48.45
                             4.302 -20.300 -34.234 1.00 35.10
HETATM 8412 O
               HOH A 390
                                                                 0
HETATM 8413 O
               HOH A 391
                              12.917 -13.524 -2.798 1.00 32.89
                                                                 0
                              19.895 -15.574 -7.940 1.00 49.91
HETATM 8414 O HOH A 392
                                                                 0
HETATM 8415 O
                              14.860 -17.419 -4.970 1.00 25.91
               HOH A 393
HETATM 8416 O
                                                                 0
               HOH A 394
                              5.931 -13.899 -32.187 1.00 20.30
               HOH A 395
                                                                 0
HETATM 8417 O
                              19.847 -34.591 -12.273 0.97 34.00
HETATM 8418 O
               HOH A 396
                             -6.928 -32.588 -32.809 1.00 42.51
                                                                 0
                                                                 0
HETATM 8419 O
               HOH A 397
                              18.913 -20.727 -25.028 1.00 33.02
HETATM 8420 O
               HOH A 398
                              3.669 -39.747 -14.394 0.98 39.60
                                                                 0
HETATM 8421 O
                              5.683 -24.024 -1.735 1.00 51.54
               HOH A 399
                              2.691 -22.028 -0.542 1.00 39.51
                                                                0
HETATM 8422 O
                HOH A 400
HETATM 8423 O
               HOH A 401
                              10.969 -7.160 -9.786 1.00 42.94
HETATM 8424 O
                                                                 0
                HOH A 402
                              21.626 -28.369 -10.530 1.00 37.94
                                                                 0
HETATM 8425 O
               HOH A 403
                              20.958 -13.872 -11.324 1.00 42.63
HETATM 8426 O
                HOH A 404
                              7.177 -37.720 -12.729 1.00 32.85
                                                                 0
HETATM 8427 O
                                                                 0
               HOH A 405
                              -3.398 -29.127 -19.642 1.00 37.76
HETATM 8428 O
                                                                 0
               HOH A 406
                             -9.694 -21.699 -25.663 1.00 39.07
HETATM 8429 O
                             5.030 -8.904 -3.424 0.92 32.51
               HOH A 407
                                                                0
HETATM 8430 O
                HOH A 408
                             2.803 -3.123 -25.301 0.97 36.94
                                                                0
                                                                 0
HETATM 8431 O
               HOH A 409
                             3.080 -13.694 -35.828 1.00 53.04
HETATM 8432 O
               HOH A 410
                              0.989 -14.435 -2.873 1.00 33.30
                                                                0
HETATM 8433 O
               HOH A 411
                              2.478 -4.432 -5.943 1.00 42.21
                                                                0
                                                                 0
HETATM 8434 O
                HOH A 412
                              18.376 -23.493 -0.915 0.97 37.09
HETATM 8435 O
                                                                 0
               HOH A 413
                              14.047 -11.745 -3.444 1.00 48.80
HETATM 8436 O
                             -9.150 -2.817 -22.592 0.88 31.56
               HOH A 414
                                                                0
HETATM 8437 O
               HOH A 415
                              11.225 -38.674 -15.291 0.93 38.19
                                                                 0
                                                                 0
HETATM 8438 O
               HOH A 416
                              16.468 -28.030 -30.885 1.00 46.91
HETATM 8439 O
                                                                 0
               HOH A 417
                              1.692 -31.198 -35.344 0.91 38.08
                                                                 0
HETATM 8440 O
                              -2.520 -39.832 -26.932 1.00 40.06
               HOH A 418
HETATM 8441 O
                              20.190 -32.355 -7.758 1.00 42.70
                                                                 0
                HOH A 419
                                                                 0
HETATM 8442 O
               HOH A 420
                              20.339 -10.973 -13.983 1.00 42.20
HETATM 8443 O
                                                                 0
               HOH A 421
                             20.488 -12.289 -21.491 0.95 37.72
                                                                 0
HETATM 8444 O
               HOH A 422
                             9.787 -38.480 -17.080 0.97 35.85
                                                                 0
HETATM 8445 O
                HOH A 423
                              15.944 -25.038 -27.298 1.00 16.52
                                                                 0
HETATM 8446 O
               HOH A 424
                              11.789 -20.592 -34.506 1.00 37.90
HETATM 8447 O
               HOH B 301
                                                                 0
                             -8.721 -20.561 -53.439 1.00 43.62
HETATM 8448 O
                                                                 0
               HOH B 302
                              0.249 -23.246 -40.752 0.96 37.32
                                                                 0
HETATM 8449 O
                HOH B 303
                              -5.106 -19.264 -46.225 1.00 36.83
                                                                 0
HETATM 8450 O
               HOH B 304
                             -15.221 -14.617 -24.431 1.00 50.95
HETATM 8451 O
                                                                 0
               HOH B 305
                             -32.482 -10.989 -49.681 0.94 31.59
HETATM 8452 O
               HOH B 306
                             -20.994 3.176 -44.263 0.97 20.02
                                                                 0
                                                                 0
                             -16.427 -30.072 -39.891 1.00 43.93
HETATM 8453 O
               HOH B 307
HETATM 8454 O HOH B 308
                             -25.077 -36.208 -38.675 1.00 36.47
                                                                 0
HETATM 8455 O
               HOH B 309
                             -32.015 -23.527 -47.337 1.00 27.22
                                                                 0
               HOH B 310
HETATM 8456 O
                             -26.236 -2.194 -46.938 1.00 27.50
                                                                 0
                           -25.261 -26.022 -48.205 1.00 24.83
                                                                 0
HETATM 8457 O HOH B 311
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HETATM 8458 O
                HOH B 312
                              -10.899 -7.012 -24.616 1.00 20.48
                                                                   0
HETATM 8459 O
                HOH B 313
                              -13.134 3.067 -42.478 1.00 11.62
                                                                    0
HETATM 8460 O
                HOH B 314
                              -17.443 -26.362 -48.090 1.00 34.48
HETATM 8461 O HOH B 315
                                                                   0
                              -0.799 -12.805 -38.145 0.83 32.26
                                                                    0
HETATM 8462 O
                HOH B 316
                              -33.087 -22.723 -28.732 1.00 36.22
HETATM 8463 O HOH B 317
                             -2.987 -11.552 -47.729 1.00 36.76
                                                                   0
HETATM 8464 O
                HOH B 318
                              -4.910 -8.728 -51.798 1.00 43.85
                                                                   0
                                                                   0
HETATM 8465 O HOH B 319
                              -30.621 1.117 -33.099 1.00 24.81
HETATM 8466 O
                HOH B 320
                              -26.410 -30.408 -39.467 1.00 25.60
                                                                    0
                              -20.350 -2.421 -32.208 1.00 12.77
HETATM 8467 O HOH B 321
                                                                   0
                                                                   0
HETATM 8468 O
                HOH B 322
                              -32.453 -9.849 -29.427 1.00 26.53
                                                                   0
                              -16.373 -11.528 -48.896 1.00 12.68
HETATM 8469 O HOH B 323
HETATM 8470 O
                HOH B 324
                                                                    0
                              -30.523 -32.817 -30.709 0.95 34.12
HETATM 8471 O HOH B 325
                              -22.885 2.552 -36.526 0.92 22.48
HETATM 8472 O
                HOH B 326
                              -1.141 -4.985 -44.506 0.92 37.45
                                                                   0
HETATM 8473 O
                HOH B 327
                                                                    0
                              -28.284 -10.560 -26.911 1.00 19.48
HETATM 8474 O
                HOH B 328
                             -5.639 1.751 -38.319 0.99 15.33
                                                                  0
                HOH B 329
                              -29.911 -6.410 -33.171 0.96 13.20
HETATM 8475 O
                                                                   0
HETATM 8476 O
                HOH B 330
                              -21.648 3.464 -41.448 1.00 22.54
                                                                   0
HETATM 8477 O
                HOH B 331
                              -18.525 -2.948 -36.275 0.94 7.74
                                                                   0
                                                                   0
HETATM 8478 O HOH B 332
                              -23.224 -29.008 -38.096 1.00 23.17
HETATM 8479 O
                HOH B 333
                              -26.391 2.321 -42.328 0.92 24.07
                                                                   0
                                                                   0
HETATM 8480 O HOH B 334
                              -23.792 -20.115 -23.920 1.00 33.08
HETATM 8481 O
                HOH B 335
                              -35.888 -7.606 -45.331 1.00 27.03
                                                                   0
                                                                   0
HETATM 8482 O HOH B 336
                              -11.851 -10.336 -27.394 1.00 22.43
                              -22.469 -0.545 -30.462 1.00 23.61
                                                                   0
HETATM 8483 O
                HOH B 337
                              -14.340 5.394 -38.662 1.00 29.94

-7.179 -20.461 -31.671 0.89 38.19

-25.606 -9.955 -27.046 1.00 15.20
HETATM 8484 O HOH B 338
                                                                   0
HETATM 8485 O
                HOH B 339
                                                                   0
HETATM 8486 O HOH B 340
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                              -25.000 -3.000

-32.102 -7.156 -47.453 1.00 20.1-

-20.363 -16.098 -53.747 1.00 30.54

-4.644 -10.720 -57.484 0.99 29.08
                                                                   0
HETATM 8487 O
                HOH B 341
HETATM 8488 O HOH B 342
                                                                   0
HETATM 8489 O
                                                                   0
                HOH B 343
                                                                   0
HETATM 8490 O HOH B 344
                                                                    0
HETATM 8491 O
                HOH B 345
                              -11.933 -16.238 -58.357 1.00 44.04
                              -35.703 -10.661 -36.120 1.00 26.22
HETATM 8492 O
                                                                    0
                HOH B 346
HETATM 8493 O HOH B 347
                              -16.652 2.619 -30.703 0.92 43.10
HETATM 8494 O
                HOH B 348
                              -16.419 1.338 -27.692 1.00 37.88
                                                                   0
                                                                   0
HETATM 8495 O
                HOH B 349
                              -27.050 -6.390 -32.405 0.92 15.61
                                                                    0
HETATM 8496 O
                HOH B 350
                              -22.192 -31.336 -30.959 1.00 46.35
                                                                    0
HETATM 8497 O HOH B 351
                              -38.191 -20.305 -47.364 1.00 23.52
HETATM 8498 O
                                                                    0
                HOH B 352
                              -37.442 -16.834 -40.343 1.00 44.83
HETATM 8499 O
                HOH B 353
                              -39.053 -14.598 -39.108 1.00 42.25
                                                                    0
HETATM 8500 O
                HOH B 354
                              -5.005 -4.677 -47.990 1.00 20.31
                                                                   0
HETATM 8501 O HOH B 355
                                                                   0
                              -35.873 -3.572 -37.788 0.92 48.31
                                                                    0
HETATM 8502 O
                HOH B 356
                              -36.033 -22.030 -45.983 1.00 25.63
HETATM 8503 O HOH B 357
                              -29.937 -12.416 -26.010 1.00 36.72
                                                                    0
HETATM 8504 O
                HOH B 358
                              -21.592 0.905 -48.101 0.99 17.96
                                                                   0
HETATM 8505 O HOH B 359
                              1.227 -1.184 -41.433 1.00 35.34
                                                                   0
HETATM 8506 O
                HOH B 360
                              -29.525 -3.958 -30.467 1.00 21.06
HETATM 8507 O HOH B 361
                              -18.098 -13.537 -55.891 0.87 27.53
                                                                    0
HETATM 8508 O
                HOH B 362
                              -20.222 -25.297 -27.703 0.97 24.68
                                                                    0
HETATM 8509 O HOH B 363
                              -31.601 -21.141 -27.044 1.00 40.96
                                                                    0
                            -7.682 -5.800 -44.492 1.00 12.52
HETATM 8510 O HOH B 364
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HETATM 8511 O HOH B 365
                             -39.712 -13.822 -42.772 0.94 22.58
                                                                  0
HETATM 8512 O
               HOH B 366
                             -15.063 -2.052 -24.817 0.75 23.06
                                                                  0
HETATM 8513 O
                HOH B 367
                             -13.646 -9.849 -56.106 0.78 13.61
                                                                  0
HETATM 8514 O HOH B 368
                             -9.528 -2.182 -49.151 1.00 29.53
HETATM 8515 O
                             -10.163 -6.789 -55.207 1.00 39.82
                                                                  0
                HOH B 369
HETATM 8516 O HOH B 370
                            -0.693 -6.652 -30.164 1.00 24.46
HETATM 8517 O
                HOH B 371
                             -10.202 -21.531 -35.273 0.88 28.53
                                                                  0
HETATM 8518 O HOH B 372
                             -8.698 -6.945 -51.201 0.99 27.01
                                                                 0
HETATM 8519 O
                HOH B 373
                             -14.842 -11.640 -56.774 1.00 37.71
                                                                  0
HETATM 8520 O HOH B 374
                            -4.623 -19.198 -50.899 1.00 28.44
                                                                  0
HETATM 8521 O
                                                                  0
                HOH B 375
                             -19.774 -9.416 -22.825 0.95 17.69
HETATM 8522 O HOH B 376
                                                                  0
                             -32.385 -25.759 -43.221 0.92 23.58
                                                                  0
HETATM 8523 O HOH B 377
                             -18.112 3.722 -36.769 1.00 22.70
                             -36.262 -6.896 -33.086 1.00 32.74
HETATM 8524 O HOH B 378
                                                                  0
HETATM 8525 O
               HOH B 379
                             -29.366 -7.754 -25.859 1.00 32.03
HETATM 8526 O
               HOH B 380
                                                                  0
                             -24.916 0.509 -32.299 1.00 44.52
                                                                  0
HETATM 8527 O HOH B 381
                             -17.507 4.848 -39.075 1.00 28.66
HETATM 8528 O
                HOH B 382
                             -7.179 -5.951 -47.238 1.00 15.87
HETATM 8529 O HOH B 383
                             -10.928 -14.105 -25.593 0.93 25.76
                                                                  0
HETATM 8530 O
                HOH B 384
                             -21.993 -6.694 -54.358 0.95 31.60
                                                                  0
HETATM 8531 O HOH B 385
                             -29.880 -29.219 -27.765 1.00 35.10
HETATM 8532 O AHOH B 386
                              -13.292 -21.320 -36.293 0.55 20.93
                                                                   0
HETATM 8533 O BHOH B 386
                              -14.747 -22.571 -35.858 0.45 21.18
                                                                   0
HETATM 8534 O HOH B 387
                             -23.130 -1.468 -48.494 1.00 19.70
                                                                  0
HETATM 8535 O HOH B 388
                                                                  0
                             -14.113 -21.257 -26.739 1.00 33.87
                                                                  0
HETATM 8536 O
                HOH B 389
                             -31.920 -25.835 -29.754 1.00 41.10
HETATM 8537 O HOH B 390
                             -8.037 -3.066 -25.283 0.94 15.70
                                                                 0
HETATM 8538 O
                HOH B 391
                             -22.937 -19.982 -54.251 1.00 43.71
                                                                  0
HETATM 8539 O HOH B 392
                            -8.022 -26.343 -36.885 1.00 38.24
                                                                  0
                                                                  0
HETATM 8540 O
                HOH B 393
                             -25.721 -1.456 -30.999 1.00 32.96
HETATM 8541 O HOH B 394
                                                                  0
                             -17.352 3.730 -32.951 1.00 24.92
HETATM 8542 O
                             -6.522 -18.821 -52.994 1.00 25.38
-2.424 -16.472 -37.310 1.00 34.48
                                                                  0
               HOH B 395
                            -6.522 -18.821 -52.994 1.00 25.38
HETATM 8543 O HOH B 396
                                                                  0
                                                                  0
HETATM 8544 O
                HOH B 397
                             -11.467 -1.047 -47.160 0.84 18.70
HETATM 8545 O
               HOH B 398
                                                                  0
                             -16.621 -22.697 -26.340 1.00 35.34
                             -19.677 -6.328 -54.606 1.00 33.61
HETATM 8546 O HOH B 399
                                                                  0
                                                                  0
HETATM 8547 O
                HOH B 400
                             -25.102 1.013 -35.086 1.00 20.09
                                                                  0
HETATM 8548 O HOH B 401
                             -24.576 -27.887 -46.124 0.99 21.00
HETATM 8549 O AHOH B 402
                                                                  0
                             -38.154 -8.419 -40.697 0.57 20.10
                                                                  0
HETATM 8550 O BHOH B 402
                              -38.942 -6.503 -40.774 0.43 20.61
HETATM 8551 O HOH B 403
                                                                  0
                              -1.343 -10.158 -44.949 0.97 23.70
HETATM 8552 O HOH B 404
                             -34.567 -0.658 -33.990 1.00 30.55
                                                                  0
                                                                  0
HETATM 8553 O
                HOH B 405
                             -12.842 -7.774 -22.995 0.99 30.77
                             -4.227 -20.634 -34.943 1.00 29.24
-16.997 -2.685 -23.656 0.71 30.73
HETATM 8554 O HOH B 406
                                                                  0
HETATM 8555 O
                                                                  0
                HOH B 407
                             -2.347 -10.013 -36.702 1.00 42.32
-23.165 -9.218 -54.577 1.00 18.92
HETATM 8556 O HOH B 408
                                                                  0
HETATM 8557 O
                                                                  0
                HOH B 409
                             -27.502 -3.640 -50.553 1.00 38.28
HETATM 8558 O HOH B 410
                                                                  0
                                                                  0
HETATM 8559 O
                HOH B 411
                             -4.061 -17.750 -55.751 1.00 35.19
HETATM 8560 O HOH B 412
                              0.252 -4.587 -35.211 1.00 34.18
HETATM 8561 O
                HOH B 413
                             -35.791 -19.131 -34.448 1.00 48.06
                                                                  0
HETATM 8562 O
                            -22.482 -10.298 -57.122 1.00 33.19
               HOH B 414
                                                                  0
                            -5.388 -19.961 -32.493 0.99 38.13
HETATM 8563 O HOH B 415
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HETATM 8564 O
                HOH B 416
                             -19.126 -17.366 -52.486 1.00 29.58
                                                                  0
HETATM 8565 O
                 HOH B 417
                             -30.966 1.579 -41.711 0.96 35.62
                                                                  0
HETATM 8566 O
                 HOH B 418
                             -19.144 -0.002 -26.071 1.00 35.48
                                                                  0
                                                                  0
                             -14.103 -10.245 -26.101 1.00 30.63
HETATM 8567 O
                HOH B 419
HETATM 8568 O
                HOH B 420
                             -24.994 -2.995 -49.561 1.00 21.71
                                                                  0
                                                                  0
HETATM 8569 O
                HOH B 421
                             -35.573 -8.763 -36.809 1.00 31.32
HETATM 8570 O
                                                                  0
                HOH B 422
                             -23.533 -26.624 -26.049 1.00 42.19
HETATM 8571 O
                HOH B 423
                             -13.439 -13.935 -20.326 0.79 28.32
                                                                  0
HETATM 8572 O
                HOH B 424
                             -6.169 1.083 -31.899 1.00 39.35
                                                                 0
                             -37.429 -17.391 -34.727 0.93 21.00
HETATM 8573 O
                HOH B 425
                                                                  0
HETATM 8574 O
                HOH B 426
                             -17.372 -2.762 -26.935 0.88 18.76
                                                                  0
HETATM 8575 O
                HOH B 427
                             -4.448 -0.992 -32.108 1.00 27.38
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HETATM 8576 O
                                                                  0
                HOH B 428
                             -18.065 -16.183 -23.206 1.00 32.03
HETATM 8577 O
                HOH B 429
                             -1.542 -2.407 -31.750 0.98 37.62
                                                                 0
HETATM 8578 O
                HOH B 430
                             -31.800 -9.576 -54.647 1.00 42.35
                                                                  0
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HETATM 8579 O
                HOH B 431
                             -30.490 -32.822 -27.801 1.00 32.01
                                                                  0
                HOH B 432
                             -15.533 -10.680 -23.410 1.00 49.55
HETATM 8580 O
HETATM 8581 O
                             -8.618 1.737 -31.495 1.00 39.57
                 HOH B 433
                                                                 0
HETATM 8582 O
                HOH B 434
                             -38.343 -8.412 -44.107 1.00 49.16
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HETATM 8583 O
                HOH B 435
                             -28.060 -6.490 -54.609 0.95 34.19
HETATM 8584 O
                HOH B 436
                             -26.447 1.750 -45.260 0.95 36.33
HETATM 8585 O
                 HOH B 437
                             -2.234 -18.026 -34.320 0.94 25.50
                                                                  0
HETATM 8586 O
                HOH B 438
                              -4.834 -1.547 -28.501 0.83 23.60
                                                                 0
HETATM 8587 O
                HOH B 439
                             -17.002 -14.059 -22.782 1.00 40.14
                                                                  0
HETATM 8588 O
                             -18.629 -15.798 -55.060 0.81 31.55
                                                                  0
                HOH B 440
HETATM 8589 O
                HOH B 441
                              -2.579 -15.474 -45.582 1.00 35.94
                                                                  0
                                                                  0
HETATM 8590 O
                HOH B 442
                             -19.629 -0.627 -51.741 0.87 29.07
HETATM 8591 O
                HOH B 443
                             -40.611 -17.429 -45.222 1.00 31.49
                                                                  0
HETATM 8592 O
                HOH B 444
                             -36.911 -7.260 -37.603 0.88 35.66
                                                                  0
                                                                  0
HETATM 8593 O
                HOH B 445
                             -34.533 -10.111 -51.085 1.00 35.39
HETATM 8594 O
                HOH B 446
                             -1.524 -4.260 -29.854 1.00 28.78
                                                                 0
HETATM 8595 O
                HOH B 447
                             -23.206 -33.309 -44.925 1.00 42.72
                                                                  0
HETATM 8596 O
                HOH B 448
                             -23.751 -5.599 -54.530 1.00 31.81
                                                                  0
                                                                  0
HETATM 8597 O
                HOH B 449
                             -16.522 -20.480 -19.488 1.00 48.74
HETATM 8598 O
                                                                  0
                HOH B 450
                             -26.028 -13.783 -25.194 0.97 30.86
HETATM 8599 O
                HOH B 451
                             -11.636 -11.582 -24.865 1.00 58.48
                                                                  0
HETATM 8600 O
                 HOH B 452
                             -7.521 1.385 -35.943 1.00 20.72
                                                                 0
HETATM 8601 O
                HOH B 453
                             -25.363 -11.068 -57.989 1.00 39.59
                                                                  0
HETATM 8602 O
                HOH B 454
                             -13.987 -5.839 -21.069 1.00 41.75
                                                                  0
HETATM 8603 O
                HOH B 455
                              1.394 -4.367 -33.121 1.00 42.14
HETATM 8604 O
                 HOH B 456
                              -6.644 -6.413 -52.359 1.00 45.60
                                                                 0
HETATM 8605 O
                HOH B 457
                              1.488 -3.748 -36.754 0.93 34.91
                                                                 0
HETATM 8606 O
                             -39.313 -16.470 -33.315 1.00 51.22
                HOH B 458
                                                                  0
                             -26.251 -8.051 -24.119 1.00 42.34
HETATM 8607 O
                HOH B 459
                                                                  0
HETATM 8608 O
                                                                  0
                HOH B 460
                             -35.180 -5.567 -46.888 1.00 41.98
HETATM 8609 O
                HOH B 461
                             -18.987 -19.527 -53.034 1.00 37.25
                                                                  0
HETATM 8610 O
                HOH B 462
                             -22.662 -25.066 -49.073 0.91 39.52
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HETATM 8611 O
                HOH B 463
                             -9.299 -5.298 -49.015 0.95 17.18
                                                                 0
HETATM 8612 O
                HOH B 464
                             -21.402 -22.977 -48.897 1.00 36.99
                                                                  0
                HOH C 301
                             -10.221 15.844 -20.793 0.89 33.78
                                                                  0
HETATM 8613 O
HETATM 8614 O
                HOH C 302
                             -14.358 24.235 -11.214 0.93 29.35
                                                                  0
HETATM 8615 O
                             -26.426 -2.508 -17.706 0.94 45.14
                 HOH C 303
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HETATM 8616 O
                HOH C 304
                            -6.161 0.922 -11.054 0.97 30.41
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HETATM 8617 O HOH C 305
                               -19.697 5.670 8.380 1.00 30.80
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HETATM 8618 O HOH C 306
                               -30.948 15.266 -18.689 0.84 21.75
                                                                     0
HETATM 8619 O
                HOH C 307
                               -7.296 3.716 -12.502 1.00 32.75
                                                                    0
HETATM 8620 O HOH C 308
                                                                     0
                               -31.653 15.868 -10.351 1.00 51.62
HETATM 8621 O
                HOH C 309
                              -7.341 -2.826 -14.881 0.91 24.72
                                                                    0
HETATM 8622 O HOH C 310
                               -19.540 2.336 -23.007 0.93 33.75
                                                                     0
                HOH C 311
                               -16.822 24.351 -18.489 1.00 21.73
                                                                     0
HETATM 8623 O
HETATM 8624 O HOH C 312
                               -17.546 11.281 3.444 1.00 32.54
                                                                     0
HETATM 8625 O
                HOH C 313
                              -2.040 14.507 -1.512 1.00 43.38
                                                                    0
HETATM 8626 O HOH C 314
                               -18.701 16.766 12.137 0.85 26.70
                                                                    0
                               -23.887 26.202 -6.227 0.92 31.34
HETATM 8627 O
                                                                     0
                HOH C 315
HETATM 8628 O HOH C 316
                              -5.934 -0.217 2.996 0.82 22.43
HETATM 8629 O
                             -9.487 12.836 -9.134 1.00 25.03
-3.558 14.426 1.155 1.00 53.36
                HOH C 317
                                                                    0
HETATM 8630 O HOH C 318
                                                                    0
HETATM 8631 O
                                                                    0
                HOH C 319
                               -28.299 8.677 -8.468 1.00 41.11
HETATM 8632 O
                HOH C 320
                              -13.581 -11.943 2.738 1.00 30.98
                                                                     0
                             HETATM 8633 O
                HOH C 321
HETATM 8634 O
                HOH C 322
HETATM 8635 O
                HOH C 323
                              -11.120 2.532 -17.668 0.89 21.44
-17.340 21.731 1.161 0.98 28.57
                HOH C 324
HETATM 8636 O
                                                                     0
                              -28.530 9.258 -18.765 0.88 28.62
-2.714 5.515 -12.352 0.98 32.06
                                                                     0
HETATM 8637 O HOH C 325
HETATM 8638 O
                HOH C 326
                                                                    0
HETATM 8639 O HOH C 327
                               -18.510 8.789 10.368 1.00 31.69
                                                                     0
                               -17.280 -8.005 -17.748 1.00 39.06
HETATM 8640 O
                HOH C 328
                                                                     0
                             0.998 4.527 -11.152 0.90 31.85
-6.756 15.370 -0.832 0.96 32.99
HETATM 8641 O HOH C 329
                                                                    0
                HOH C 330
                                                                    0
HETATM 8642 O
                             -7.683 11.551 -13.098 1.00 41.83
-9.936 0.228 -17.712 1.00 34.43
-25.672 25.052 -3.133 1.00 38.05
HETATM 8643 O HOH C 331
                                                                    0
HETATM 8644 O
                HOH C 332
HETATM 8645 O HOH C 333
                                                                     0
                               -19.804 -9.162 2.829 1.00 50.74
HETATM 8646 O
                HOH C 334
                                                                    0
                              -8.671 -2.593 7.939 1.00 38.67 C
-13.485 14.905 8.318 1.00 48.32
-24.587 6.183 -28.601 1.00 22.74
                               -8.671 -2.593 7.939 1.00 38.67
HETATM 8647 O HOH C 335
                                                                    0
HETATM 8648 O
                HOH C 336
HETATM 8649 O HOH C 337
HETATM 8650 O
                HOH C 338
                               -29.874 13.818 -14.430 1.00 42.76
HETATM 8651 O
                HOH C 339
                               -13.147 7.410 -22.482 0.90 34.71
                                                                     0
                               -14.453 24.928 -17.483 1.00 37.66
HETATM 8652 O
                HOH C 340
                                                                     0
HETATM 8653 O
                HOH C 341
                              -8.675 22.599 -12.002 0.84 28.58
                             -2.001 14.020 -4.056 1.00 46.99
-7.362 12.990 6.057 0.86 29.23
-4.288 11.468 2.667 0.91 27.78
-5.707 7.317 2.142 0.94 36.15
HETATM 8654 O
                HOH C 342
HETATM 8655 O
                HOH C 343
                                                                    0
                                                                    0
HETATM 8656 O
                HOH C 344
                 HOH C 345
HETATM 8657 O
                                                                    0
HETATM 8658 O
                HOH C 346
                               -4.891 9.971 -14.661 1.00 51.24
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HETATM 8659 O
                HOH C 347
                              -5.724 12.215 -18.947 1.00 41.21
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HETATM 8660 O HOH C 348
                              -3.300 16.320 -8.754 1.00 40.17
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                HOH C 349
HETATM 8661 O
                               -17.434 12.173 -19.203 0.99 30.30
                                                                    0
HETATM 8662 O HOH C 350
                               -2.328 9.448 -10.020 0.92 33.87
                                                                    0
                HOH C 351
HETATM 8663 O
                               -20.512 5.587 -22.193 0.97 38.84
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HETATM 8664 O HOH C 352
                               -10.744 15.647 8.460 1.00 39.55
                                                                     0
HETATM 8665 O
                HOH C 353
                               -21.129 -10.655 1.957 1.00 51.25
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HETATM 8666 O HOH C 354
                               -12.608 6.547 9.667 0.99 31.91
                                                                    0
                             -1.025 5.846 -5.522 1.00 34.17
                HOH C 355
HETATM 8667 O
                                                                    0
HETATM 8668 O HOH C 356 -14.441 21.003 -20.999 1.00 30.68 HETATM 8669 O HOH C 357 -2.963 16.847 -12.226 1.00 40.60
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HETATM 8670 O HOH C 358
                            -5.873 7.995 4.690 1.00 49.57
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HETATM 8671 O HOH C 359
                            -18.779 7.132 -22.435 1.00 35.65
                                                               0
               HOH C 360
                             -3.681 7.690 -13.454 1.00 46.34
HETATM 8672 O
                                                              0
HETATM 8673 O HOH C 361
                             -4.067 -4.260 0.984 1.00 38.16
                                                              0
HETATM 8674 O HOH C 362
                            -26.451 20.503 -1.510 1.00 42.31
                                                               0
                            -1.919 -0.704 -16.585 1.00 43.51
HETATM 8675 O HOH C 363
                                                               0
HETATM 8676 O
               HOH C 364
                            -21.638 6.080 7.439 0.92 37.65
                                                              0
HETATM 8677 O HOH C 365
                            -9.226 13.384 -18.848 1.00 32.76
                                                               0
HETATM 8678 O HOH C 366
                            -21.571 10.943 -21.441 1.00 36.57
                                                               0
HETATM 8679 O HOH C 367
                             -6.529 10.110 -20.019 1.00 35.49
                                                               0
HETATM 8680 O HOH C 368
                            -2.265 2.568 -16.308 1.00 44.15
                                                              0
HETATM 8681 O HOH C 369
                            -6.360 -8.018 7.012 1.00 27.50
                                                              0
HETATM 8682 O HOH C 370
                            -29.234 5.795 -4.066 1.00 37.18
                                                              0
                            -4.212 -1.951 2.876 0.96 36.60
HETATM 8683 O HOH C 371
                                                              0
HETATM 8684 O HOH C 372
                            -26.492 5.093 -23.726 0.97 37.58
                                                               0
HETATM 8685 O HOH C 373
                            -14.098 -13.773 -6.449 0.90 38.20
                                                               0
HETATM 8686 O HOH C 374
                                                               0
                            -0.521 15.092 -12.369 1.00 41.29
HETATM 8687 O HOH C 375
                            -21.356 8.069 10.448 1.00 38.21
                                                               0
HETATM 8688 O HOH C 376
                            -26.885 4.285 -27.201 1.00 50.44
                                                               0
HETATM 8689 O HOH C 377
                            -18.035 -10.580 3.042 1.00 46.13
                                                               0
HETATM 8690 O HOH C 378
                           -23.877 4.610 6.578 0.99 37.49
                                                              0
HETATM 8691 O HOH C 379 -11.086 1.974 -20.823 1.00 42.99
CONECT 283 8319
CONECT 286 8319
CONECT 297 8319
CONECT 3166 8320
CONECT 3169 8320
CONECT 3180 8320
CONECT 4290 8319
CONECT 4459 8319
CONECT 5909 8321
CONECT 5912 8321
CONECT 5923 8321
CONECT 8319 283 286 297 4290
CONECT 8319 4459 8537
CONECT 8320 3166 3169 3180
CONECT 8321 5909 5912 5923
CONECT 8537 8319
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MASTER

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