

Class 11 Structural Bioinformatics pt 2

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AlphaFold has changed the game for protein structure prediction and allows anyone with sufficient bioinformatics skills to predict the structure of any protein.

Using GoogleColab we ran AlphaFold from our notebook, and to be specific we used their AlphaFold2_mmseqs2 version that uses mmseqs rather than HMMer for searching sequences.

The main outputs include a set of **PDB structure** files along with matching **JSON format files** that tell us how good the resulting models might be.

Let's begin by loading the PDB structures in Mol*

```
library(bio3d)

results_dir <- "hivprdimer"

pdb_files <- list.files(path=results_dir,
                        pattern="*.pdb",
                        full.names = TRUE)

basename(pdb_files)

## [1] "hivprdimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_5_seed_000.pdb"
## [2] "hivprdimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_1_seed_000.pdb"
## [3] "hivprdimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb"
## [4] "hivprdimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000.pdb"
## [5] "hivprdimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb"
```

Alignment of files:

```
pdbas <- pdbaln(pdb_files, fit=TRUE, exefile="msa")

## Reading PDB files:
## hivprdimer/hivprdimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_5_seed_000.pdb
## hivprdimer/hivprdimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_1_seed_000.pdb
## hivprdimer/hivprdimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb
## hivprdimer/hivprdimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_seed_000.pdb
## hivprdimer/hivprdimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb
## .....
```

```
##
## Extracting sequences
##
## pdb/seq: 1   name: hivprdimer/hivprdimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_5_see
## pdb/seq: 2   name: hivprdimer/hivprdimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_1_see
## pdb/seq: 3   name: hivprdimer/hivprdimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_see
## pdb/seq: 4   name: hivprdimer/hivprdimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_2_see
## pdb/seq: 5   name: hivprdimer/hivprdimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_see
```

Now, we download the BiocManager file to use specific functions. Downloaded in console.

```
rd <- rmsd(pdb, fit=T)
```

```
## Warning in rmsd(pdb, fit = T): No indices provided, using the 198 non NA positions
```

```
range(rd)
```

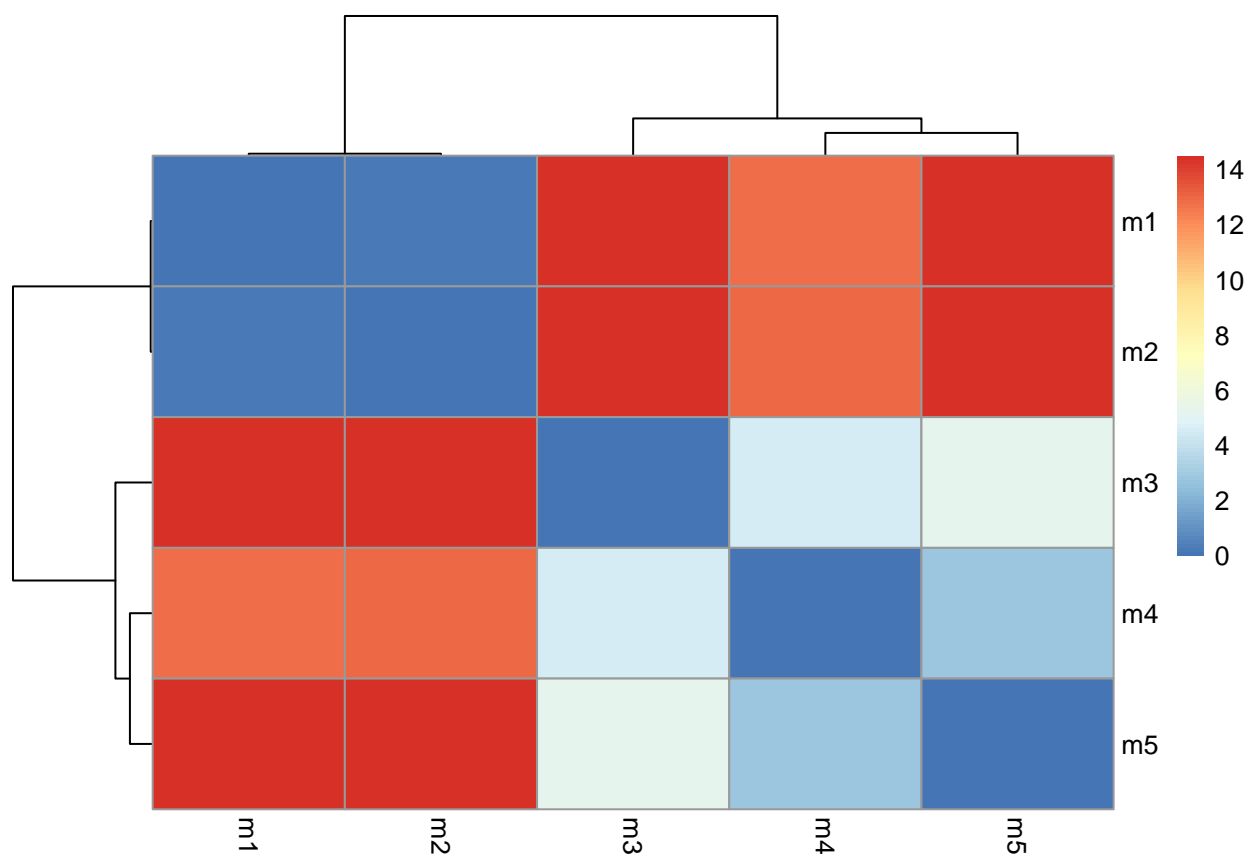
```
## [1] 0.000 14.507
```

```
library(pheatmap)
```

```
colnames(rd) <- paste0("m",1:5)
```

```
rownames(rd) <- paste0("m",1:5)
```

```
pheatmap(rd)
```



```
# Read a reference PDB structure
```

```
pdb <- read.pdb("1hsg")
```

```
## Note: Accessing on-line PDB file
```

```
pdb$atom
```

```
##      type eleno elety  alt resid chain resno insert      x      y      z o
## 1  ATOM      1      N <NA>  PRO      A      1 <NA> 29.361 39.686  5.862 1
## 2  ATOM      2      CA <NA>  PRO      A      1 <NA> 30.307 38.663  5.319 1
## 3  ATOM      3      C  <NA>  PRO      A      1 <NA> 29.760 38.071  4.022 1
## 4  ATOM      4      O  <NA>  PRO      A      1 <NA> 28.600 38.302  3.676 1
## 5  ATOM      5      CB <NA>  PRO      A      1 <NA> 30.508 37.541  6.342 1
## 6  ATOM      6      CG <NA>  PRO      A      1 <NA> 29.296 37.591  7.162 1
## 7  ATOM      7      CD <NA>  PRO      A      1 <NA> 28.778 39.015  7.019 1
## 8  ATOM      8      N  <NA>  GLN      A      2 <NA> 30.607 37.334  3.305 1
## 9  ATOM      9      CA <NA>  GLN      A      2 <NA> 30.158 36.492  2.199 1
## 10 ATOM     10      C  <NA>  GLN      A      2 <NA> 30.298 35.041  2.643 1
## 11 ATOM     11      O  <NA>  GLN      A      2 <NA> 31.401 34.494  2.763 1
## 12 ATOM     12      CB <NA>  GLN      A      2 <NA> 30.970 36.738  0.926 1
## 13 ATOM     13      CG <NA>  GLN      A      2 <NA> 30.625 35.783 -0.201 1
## 14 ATOM     14      CD <NA>  GLN      A      2 <NA> 31.184 36.217 -1.549 1
```

## 15	ATOM	15	OE1 <NA>	GLN	A	2	<NA>	32.006	35.518	-2.156	1
## 16	ATOM	16	NE2 <NA>	GLN	A	2	<NA>	30.684	37.339	-2.061	1
## 17	ATOM	17	N <NA>	ILE	A	3	<NA>	29.160	34.436	2.919	1
## 18	ATOM	18	CA <NA>	ILE	A	3	<NA>	29.123	33.098	3.397	1
## 19	ATOM	19	C <NA>	ILE	A	3	<NA>	28.968	32.155	2.198	1
## 20	ATOM	20	O <NA>	ILE	A	3	<NA>	28.088	32.330	1.368	1
## 21	ATOM	21	CB <NA>	ILE	A	3	<NA>	27.977	32.995	4.409	1
## 22	ATOM	22	CG1 <NA>	ILE	A	3	<NA>	28.341	33.820	5.652	1
## 23	ATOM	23	CG2 <NA>	ILE	A	3	<NA>	27.692	31.548	4.745	1
## 24	ATOM	24	CD1 <NA>	ILE	A	3	<NA>	27.264	33.884	6.696	1
## 25	ATOM	25	N <NA>	THR	A	4	<NA>	29.891	31.210	2.066	1
## 26	ATOM	26	CA <NA>	THR	A	4	<NA>	29.774	30.143	1.062	1
## 27	ATOM	27	C <NA>	THR	A	4	<NA>	28.986	28.975	1.658	1
## 28	ATOM	28	O <NA>	THR	A	4	<NA>	28.690	28.948	2.875	1
## 29	ATOM	29	CB <NA>	THR	A	4	<NA>	31.165	29.618	0.634	1
## 30	ATOM	30	OG1 <NA>	THR	A	4	<NA>	31.866	29.209	1.815	1
## 31	ATOM	31	CG2 <NA>	THR	A	4	<NA>	31.980	30.688	-0.085	1
## 32	ATOM	32	N <NA>	LEU	A	5	<NA>	28.641	28.019	0.803	1
## 33	ATOM	33	CA <NA>	LEU	A	5	<NA>	27.644	27.003	1.144	1
## 34	ATOM	34	C <NA>	LEU	A	5	<NA>	28.204	25.559	1.071	1
## 35	ATOM	35	O <NA>	LEU	A	5	<NA>	27.446	24.583	0.969	1
## 36	ATOM	36	CB <NA>	LEU	A	5	<NA>	26.411	27.139	0.226	1
## 37	ATOM	37	CG <NA>	LEU	A	5	<NA>	25.676	28.479	0.352	1
## 38	ATOM	38	CD1 <NA>	LEU	A	5	<NA>	24.624	28.624	-0.753	1
## 39	ATOM	39	CD2 <NA>	LEU	A	5	<NA>	25.088	28.590	1.745	1
## 40	ATOM	40	N <NA>	TRP	A	6	<NA>	29.528	25.436	1.146	1
## 41	ATOM	41	CA <NA>	TRP	A	6	<NA>	30.177	24.150	1.279	1
## 42	ATOM	42	C <NA>	TRP	A	6	<NA>	29.837	23.488	2.611	1
## 43	ATOM	43	O <NA>	TRP	A	6	<NA>	29.706	22.271	2.673	1
## 44	ATOM	44	CB <NA>	TRP	A	6	<NA>	31.685	24.301	1.109	1
## 45	ATOM	45	CG <NA>	TRP	A	6	<NA>	32.152	24.955	-0.189	1
## 46	ATOM	46	CD1 <NA>	TRP	A	6	<NA>	32.681	26.216	-0.345	1
## 47	ATOM	47	CD2 <NA>	TRP	A	6	<NA>	32.274	24.314	-1.478	1
## 48	ATOM	48	NE1 <NA>	TRP	A	6	<NA>	33.102	26.385	-1.655	1
## 49	ATOM	49	CE2 <NA>	TRP	A	6	<NA>	32.864	25.258	-2.369	1
## 50	ATOM	50	CE3 <NA>	TRP	A	6	<NA>	31.949	23.035	-1.986	1
## 51	ATOM	51	CZ2 <NA>	TRP	A	6	<NA>	33.093	24.968	-3.717	1
## 52	ATOM	52	CZ3 <NA>	TRP	A	6	<NA>	32.195	22.755	-3.294	1
## 53	ATOM	53	CH2 <NA>	TRP	A	6	<NA>	32.754	23.722	-4.169	1
## 54	ATOM	54	N <NA>	GLN	A	7	<NA>	29.667	24.280	3.667	1
## 55	ATOM	55	CA <NA>	GLN	A	7	<NA>	29.141	23.799	4.960	1
## 56	ATOM	56	C <NA>	GLN	A	7	<NA>	27.747	24.395	5.208	1
## 57	ATOM	57	O <NA>	GLN	A	7	<NA>	27.349	25.330	4.547	1
## 58	ATOM	58	CB <NA>	GLN	A	7	<NA>	30.072	24.227	6.100	1
## 59	ATOM	59	CG <NA>	GLN	A	7	<NA>	31.512	23.694	5.995	1
## 60	ATOM	60	CD <NA>	GLN	A	7	<NA>	32.521	24.750	5.469	1
## 61	ATOM	61	OE1 <NA>	GLN	A	7	<NA>	32.666	25.860	6.038	1
## 62	ATOM	62	NE2 <NA>	GLN	A	7	<NA>	33.268	24.374	4.419	1
## 63	ATOM	63	N <NA>	ARG	A	8	<NA>	26.992	23.877	6.169	1
## 64	ATOM	64	CA <NA>	ARG	A	8	<NA>	25.757	24.566	6.593	1
## 65	ATOM	65	C <NA>	ARG	A	8	<NA>	26.029	26.025	6.996	1
## 66	ATOM	66	O <NA>	ARG	A	8	<NA>	26.947	26.291	7.775	1
## 67	ATOM	67	CB <NA>	ARG	A	8	<NA>	25.087	23.849	7.776	1
## 68	ATOM	68	CG <NA>	ARG	A	8	<NA>	24.646	22.409	7.505	1

## 69	ATOM	69	CD <NA>	ARG	A	8	<NA>	23.728	21.896	8.637	1
## 70	ATOM	70	NE <NA>	ARG	A	8	<NA>	22.952	20.730	8.230	1
## 71	ATOM	71	CZ <NA>	ARG	A	8	<NA>	22.367	19.871	9.064	1
## 72	ATOM	72	NH1 <NA>	ARG	A	8	<NA>	22.376	20.074	10.370	1
## 73	ATOM	73	NH2 <NA>	ARG	A	8	<NA>	21.776	18.789	8.589	1
## 74	ATOM	74	N <NA>	PRO	A	9	<NA>	25.123	26.955	6.645	1
## 75	ATOM	75	CA <NA>	PRO	A	9	<NA>	25.491	28.352	6.938	1
## 76	ATOM	76	C <NA>	PRO	A	9	<NA>	25.127	28.763	8.364	1
## 77	ATOM	77	O <NA>	PRO	A	9	<NA>	24.136	29.472	8.578	1
## 78	ATOM	78	CB <NA>	PRO	A	9	<NA>	24.719	29.176	5.916	1
## 79	ATOM	79	CG <NA>	PRO	A	9	<NA>	23.625	28.254	5.407	1
## 80	ATOM	80	CD <NA>	PRO	A	9	<NA>	24.096	26.855	5.591	1
## 81	ATOM	81	N <NA>	LEU	A	10	<NA>	25.905	28.285	9.330	1
## 82	ATOM	82	CA <NA>	LEU	A	10	<NA>	25.653	28.510	10.750	1
## 83	ATOM	83	C <NA>	LEU	A	10	<NA>	26.383	29.770	11.208	1
## 84	ATOM	84	O <NA>	LEU	A	10	<NA>	27.567	29.927	10.938	1
## 85	ATOM	85	CB <NA>	LEU	A	10	<NA>	26.120	27.284	11.573	1
## 86	ATOM	86	CG <NA>	LEU	A	10	<NA>	25.161	26.082	11.544	1
## 87	ATOM	87	CD1 <NA>	LEU	A	10	<NA>	25.895	24.743	11.662	1
## 88	ATOM	88	CD2 <NA>	LEU	A	10	<NA>	24.206	26.196	12.696	1
## 89	ATOM	89	N <NA>	VAL	A	11	<NA>	25.667	30.672	11.872	1
## 90	ATOM	90	CA <NA>	VAL	A	11	<NA>	26.267	31.854	12.497	1
## 91	ATOM	91	C <NA>	VAL	A	11	<NA>	25.818	31.957	13.955	1
## 92	ATOM	92	O <NA>	VAL	A	11	<NA>	24.929	31.184	14.402	1
## 93	ATOM	93	CB <NA>	VAL	A	11	<NA>	25.824	33.131	11.791	1
## 94	ATOM	94	CG1 <NA>	VAL	A	11	<NA>	26.270	33.089	10.323	1
## 95	ATOM	95	CG2 <NA>	VAL	A	11	<NA>	24.333	33.275	11.879	1
## 96	ATOM	96	N <NA>	THR	A	12	<NA>	26.397	32.913	14.700	1
## 97	ATOM	97	CA <NA>	THR	A	12	<NA>	26.001	33.143	16.102	1
## 98	ATOM	98	C <NA>	THR	A	12	<NA>	24.915	34.200	16.204	1
## 99	ATOM	99	O <NA>	THR	A	12	<NA>	25.010	35.279	15.610	1
## 100	ATOM	100	CB <NA>	THR	A	12	<NA>	27.201	33.565	16.998	1
## 101	ATOM	101	OG1 <NA>	THR	A	12	<NA>	28.330	32.709	16.751	1
## 102	ATOM	102	CG2 <NA>	THR	A	12	<NA>	26.827	33.430	18.450	1
## 103	ATOM	103	N <NA>	ILE	A	13	<NA>	23.848	33.868	16.909	1
## 104	ATOM	104	CA <NA>	ILE	A	13	<NA>	22.842	34.875	17.206	1
## 105	ATOM	105	C <NA>	ILE	A	13	<NA>	22.770	35.114	18.707	1
## 106	ATOM	106	O <NA>	ILE	A	13	<NA>	23.328	34.363	19.500	1
## 107	ATOM	107	CB <NA>	ILE	A	13	<NA>	21.413	34.460	16.661	1
## 108	ATOM	108	CG1 <NA>	ILE	A	13	<NA>	20.878	33.229	17.431	1
## 109	ATOM	109	CG2 <NA>	ILE	A	13	<NA>	21.510	34.194	15.162	1
## 110	ATOM	110	CD1 <NA>	ILE	A	13	<NA>	19.353	33.201	17.603	1
## 111	ATOM	111	N <NA>	LYS	A	14	<NA>	22.106	36.199	19.087	1
## 112	ATOM	112	CA <NA>	LYS	A	14	<NA>	21.894	36.545	20.492	1
## 113	ATOM	113	C <NA>	LYS	A	14	<NA>	20.442	36.943	20.615	1
## 114	ATOM	114	O <NA>	LYS	A	14	<NA>	19.960	37.808	19.873	1
## 115	ATOM	115	CB <NA>	LYS	A	14	<NA>	22.777	37.724	20.896	1
## 116	ATOM	116	CG <NA>	LYS	A	14	<NA>	22.727	38.056	22.383	1
## 117	ATOM	117	CD <NA>	LYS	A	14	<NA>	23.270	39.450	22.678	1
## 118	ATOM	118	CE <NA>	LYS	A	14	<NA>	24.814	39.490	22.755	1
## 119	ATOM	119	NZ <NA>	LYS	A	14	<NA>	25.394	40.891	22.572	1
## 120	ATOM	120	N <NA>	ILE	A	15	<NA>	19.739	36.267	21.512	1
## 121	ATOM	121	CA <NA>	ILE	A	15	<NA>	18.345	36.563	21.813	1
## 122	ATOM	122	C <NA>	ILE	A	15	<NA>	18.224	36.327	23.316	1

## 123	ATOM	123	O <NA>	ILE	A	15	<NA>	18.886	35.449	23.864	1
## 124	ATOM	124	CB <NA>	ILE	A	15	<NA>	17.380	35.592	21.022	1
## 125	ATOM	125	CG1 <NA>	ILE	A	15	<NA>	15.935	35.812	21.435	1
## 126	ATOM	126	CG2 <NA>	ILE	A	15	<NA>	17.745	34.137	21.266	1
## 127	ATOM	127	CD1 <NA>	ILE	A	15	<NA>	14.929	35.116	20.526	1
## 128	ATOM	128	N <NA>	GLY	A	16	<NA>	17.446	37.139	24.012	1
## 129	ATOM	129	CA <NA>	GLY	A	16	<NA>	17.356	36.968	25.459	1
## 130	ATOM	130	C <NA>	GLY	A	16	<NA>	18.711	36.871	26.160	1
## 131	ATOM	131	O <NA>	GLY	A	16	<NA>	18.866	36.162	27.153	1
## 132	ATOM	132	N <NA>	GLY	A	17	<NA>	19.671	37.659	25.697	1
## 133	ATOM	133	CA <NA>	GLY	A	17	<NA>	20.970	37.660	26.340	1
## 134	ATOM	134	C <NA>	GLY	A	17	<NA>	21.680	36.316	26.278	1
## 135	ATOM	135	O <NA>	GLY	A	17	<NA>	22.785	36.163	26.794	1
## 136	ATOM	136	N <NA>	GLN	A	18	<NA>	21.093	35.361	25.572	1
## 137	ATOM	137	CA <NA>	GLN	A	18	<NA>	21.780	34.106	25.263	1
## 138	ATOM	138	C <NA>	GLN	A	18	<NA>	22.500	34.159	23.907	1
## 139	ATOM	139	O <NA>	GLN	A	18	<NA>	21.937	34.624	22.915	1
## 140	ATOM	140	CB <NA>	GLN	A	18	<NA>	20.776	32.957	25.228	1
## 141	ATOM	141	CG <NA>	GLN	A	18	<NA>	19.599	33.116	26.176	1
## 142	ATOM	142	CD <NA>	GLN	A	18	<NA>	19.556	31.997	27.179	1
## 143	ATOM	143	OE1 <NA>	GLN	A	18	<NA>	20.393	31.944	28.082	1
## 144	ATOM	144	NE2 <NA>	GLN	A	18	<NA>	18.647	31.035	26.975	1
## 145	ATOM	145	N <NA>	LEU	A	19	<NA>	23.733	33.672	23.848	1
## 146	ATOM	146	CA <NA>	LEU	A	19	<NA>	24.334	33.365	22.552	1
## 147	ATOM	147	C <NA>	LEU	A	19	<NA>	23.896	31.963	22.106	1
## 148	ATOM	148	O <NA>	LEU	A	19	<NA>	23.975	31.020	22.863	1
## 149	ATOM	149	CB <NA>	LEU	A	19	<NA>	25.869	33.432	22.625	1
## 150	ATOM	150	CG <NA>	LEU	A	19	<NA>	26.561	34.761	22.968	1
## 151	ATOM	151	CD1 <NA>	LEU	A	19	<NA>	28.007	34.629	22.620	1
## 152	ATOM	152	CD2 <NA>	LEU	A	19	<NA>	25.983	35.913	22.194	1
## 153	ATOM	153	N <NA>	LYS	A	20	<NA>	23.416	31.855	20.876	1
## 154	ATOM	154	CA <NA>	LYS	A	20	<NA>	23.006	30.584	20.266	1
## 155	ATOM	155	C <NA>	LYS	A	20	<NA>	23.626	30.463	18.874	1
## 156	ATOM	156	O <NA>	LYS	A	20	<NA>	24.024	31.460	18.283	1
## 157	ATOM	157	CB <NA>	LYS	A	20	<NA>	21.494	30.523	20.107	1
## 158	ATOM	158	CG <NA>	LYS	A	20	<NA>	20.778	29.875	21.264	1
## 159	ATOM	159	CD <NA>	LYS	A	20	<NA>	19.868	30.857	21.939	1
## 160	ATOM	160	CE <NA>	LYS	A	20	<NA>	19.112	30.168	23.043	1
## 161	ATOM	161	NZ <NA>	LYS	A	20	<NA>	18.467	28.892	22.571	1
## 162	ATOM	162	N <NA>	GLU	A	21	<NA>	23.725	29.250	18.342	1
## 163	ATOM	163	CA <NA>	GLU	A	21	<NA>	24.053	29.117	16.931	1
## 164	ATOM	164	C <NA>	GLU	A	21	<NA>	22.822	28.761	16.150	1
## 165	ATOM	165	O <NA>	GLU	A	21	<NA>	21.879	28.136	16.672	1
## 166	ATOM	166	CB <NA>	GLU	A	21	<NA>	25.197	28.130	16.679	1
## 167	ATOM	167	CG <NA>	GLU	A	21	<NA>	25.035	26.716	17.168	1
## 168	ATOM	168	CD <NA>	GLU	A	21	<NA>	25.878	25.743	16.334	1
## 169	ATOM	169	OE1 <NA>	GLU	A	21	<NA>	27.022	26.130	15.972	1
## 170	ATOM	170	OE2 <NA>	GLU	A	21	<NA>	25.379	24.639	15.983	1
## 171	ATOM	171	N <NA>	ALA	A	22	<NA>	22.778	29.268	14.927	1
## 172	ATOM	172	CA <NA>	ALA	A	22	<NA>	21.553	29.189	14.165	1
## 173	ATOM	173	C <NA>	ALA	A	22	<NA>	21.870	29.183	12.682	1
## 174	ATOM	174	O <NA>	ALA	A	22	<NA>	22.975	29.578	12.252	1
## 175	ATOM	175	CB <NA>	ALA	A	22	<NA>	20.625	30.359	14.524	1
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## 177	ATOM	177	CA <NA>	LEU	A	23	<NA>	21.047	28.473	10.476	1
## 178	ATOM	178	C <NA>	LEU	A	23	<NA>	20.381	29.596	9.664	1
## 179	ATOM	179	O <NA>	LEU	A	23	<NA>	19.231	29.943	9.912	1
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## 182	ATOM	182	CD1 <NA>	LEU	A	23	<NA>	21.939	26.039	8.621	1
## 183	ATOM	183	CD2 <NA>	LEU	A	23	<NA>	19.490	25.490	8.627	1
## 184	ATOM	184	N <NA>	LEU	A	24	<NA>	21.122	30.163	8.715	1
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## 189	ATOM	189	CG <NA>	LEU	A	24	<NA>	22.647	32.673	8.359	1
## 190	ATOM	190	CD1 <NA>	LEU	A	24	<NA>	23.698	33.581	7.738	1
## 191	ATOM	191	CD2 <NA>	LEU	A	24	<NA>	21.797	33.496	9.368	1
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## 193	ATOM	193	CA <NA>	ASP	A	25	<NA>	17.853	29.516	5.837	1
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## 197	ATOM	197	CG <NA>	ASP	A	25	<NA>	16.316	27.513	6.146	1
## 198	ATOM	198	OD1 <NA>	ASP	A	25	<NA>	16.236	27.458	4.905	1
## 199	ATOM	199	OD2 <NA>	ASP	A	25	<NA>	15.762	26.696	6.882	1
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## 205	ATOM	205	OG1 <NA>	THR	A	26	<NA>	17.693	30.177	0.863	1
## 206	ATOM	206	CG2 <NA>	THR	A	26	<NA>	18.601	32.197	1.773	1
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## 222	ATOM	222	OD1 <NA>	ASP	A	29	<NA>	8.591	31.192	3.104	1
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##	234	ATOM	234	C <NA>	THR	A	31	<NA>	11.707	31.128	13.318	1
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##	236	ATOM	236	CB <NA>	THR	A	31	<NA>	12.896	33.338	12.795	1
##	237	ATOM	237	OG1 <NA>	THR	A	31	<NA>	13.451	34.082	11.707	1
##	238	ATOM	238	CG2 <NA>	THR	A	31	<NA>	14.027	32.992	13.816	1
##	239	ATOM	239	N <NA>	VAL	A	32	<NA>	12.390	30.005	13.537	1
##	240	ATOM	240	CA <NA>	VAL	A	32	<NA>	11.893	28.983	14.419	1
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##	245	ATOM	245	CG2 <NA>	VAL	A	32	<NA>	10.805	27.963	12.423	1
##	246	ATOM	246	N <NA>	LEU	A	33	<NA>	12.899	28.904	16.576	1
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##	252	ATOM	252	CD1 <NA>	LEU	A	33	<NA>	15.091	32.156	18.733	1
##	253	ATOM	253	CD2 <NA>	LEU	A	33	<NA>	16.139	30.718	16.927	1
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##	278	ATOM	278	SD <NA>	MET	A	36	<NA>	15.123	31.051	22.667	1
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##	290	ATOM	290	CB <NA>	LEU	A	38	<NA>	10.409	34.626	24.500	1
##	291	ATOM	291	CG <NA>	LEU	A	38	<NA>	11.559	34.187	23.577	1
##	292	ATOM	292	CD1 <NA>	LEU	A	38	<NA>	11.171	34.399	22.132	1
##	293	ATOM	293	CD2 <NA>	LEU	A	38	<NA>	12.807	34.964	23.875	1
##	294	ATOM	294	N <NA>	PRO	A	39	<NA>	9.929	36.666	26.880	1
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##	309	ATOM	309	CB <NA>	ARG	A	41	<NA>	0.956	36.719	25.748	1
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##	311	ATOM	311	CD <NA>	ARG	A	41	<NA>	0.118	36.953	28.169	1
##	312	ATOM	312	NE <NA>	ARG	A	41	<NA>	1.356	37.143	28.933	1
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##	314	ATOM	314	NH1 <NA>	ARG	A	41	<NA>	1.161	39.450	29.040	1
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##	325	ATOM	325	CE2 <NA>	TRP	A	42	<NA>	1.966	30.246	25.193	1
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##	327	ATOM	327	CZ2 <NA>	TRP	A	42	<NA>	1.117	29.219	25.618	1
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##	329	ATOM	329	CH2 <NA>	TRP	A	42	<NA>	0.305	28.651	24.686	1
##	330	ATOM	330	N <NA>	LYS	A	43	<NA>	0.781	33.465	20.639	1
##	331	ATOM	331	CA <NA>	LYS	A	43	<NA>	-0.305	32.776	19.928	1
##	332	ATOM	332	C <NA>	LYS	A	43	<NA>	0.220	31.412	19.477	1
##	333	ATOM	333	O <NA>	LYS	A	43	<NA>	1.400	31.270	19.145	1
##	334	ATOM	334	CB <NA>	LYS	A	43	<NA>	-0.739	33.603	18.700	1
##	335	ATOM	335	CG <NA>	LYS	A	43	<NA>	-1.311	34.967	19.027	1
##	336	ATOM	336	CD <NA>	LYS	A	43	<NA>	-1.066	35.945	17.886	1
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## 341	ATOM	341	C <NA>	PRO	A	44	<NA>	-0.275	29.085	17.454	1
## 342	ATOM	342	O <NA>	PRO	A	44	<NA>	-1.185	29.721	16.929	1
## 343	ATOM	343	CB <NA>	PRO	A	44	<NA>	-0.893	28.021	19.667	1
## 344	ATOM	344	CG <NA>	PRO	A	44	<NA>	-2.170	28.683	20.012	1
## 345	ATOM	345	CD <NA>	PRO	A	44	<NA>	-1.825	30.129	20.325	1
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## 347	ATOM	347	CA <NA>	LYS	A	45	<NA>	0.634	28.302	15.290	1
## 348	ATOM	348	C <NA>	LYS	A	45	<NA>	1.025	26.869	14.873	1
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## 355	ATOM	355	N <NA>	MET	A	46	<NA>	0.570	26.438	13.707	1
## 356	ATOM	356	CA <NA>	MET	A	46	<NA>	1.091	25.232	13.081	1
## 357	ATOM	357	C <NA>	MET	A	46	<NA>	1.899	25.638	11.874	1
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## 359	ATOM	359	CB <NA>	MET	A	46	<NA>	-0.047	24.319	12.624	1
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## 362	ATOM	362	CE <NA>	MET	A	46	<NA>	-0.585	21.081	13.426	1
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## 365	ATOM	365	C <NA>	ILE	A	47	<NA>	4.420	24.140	10.114	1
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## 367	ATOM	367	CB <NA>	ILE	A	47	<NA>	5.234	26.259	10.953	1
## 368	ATOM	368	CG1 <NA>	ILE	A	47	<NA>	5.959	25.628	12.127	1
## 369	ATOM	369	CG2 <NA>	ILE	A	47	<NA>	4.898	27.703	11.148	1
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## 377	ATOM	377	C <NA>	GLY	A	49	<NA>	8.221	20.379	6.232	1
## 378	ATOM	378	O <NA>	GLY	A	49	<NA>	7.177	20.197	5.583	1
## 379	ATOM	379	N <NA>	ILE	A	50	<NA>	9.309	19.619	6.155	1
## 380	ATOM	380	CA <NA>	ILE	A	50	<NA>	9.537	18.544	5.194	1
## 381	ATOM	381	C <NA>	ILE	A	50	<NA>	8.802	17.261	5.658	1
## 382	ATOM	382	O <NA>	ILE	A	50	<NA>	8.143	16.589	4.863	1
## 383	ATOM	383	CB <NA>	ILE	A	50	<NA>	11.095	18.362	5.046	1
## 384	ATOM	384	CG1 <NA>	ILE	A	50	<NA>	11.553	18.874	3.682	1
## 385	ATOM	385	CG2 <NA>	ILE	A	50	<NA>	11.521	16.945	5.317	1
## 386	ATOM	386	CD1 <NA>	ILE	A	50	<NA>	10.910	18.225	2.567	1
## 387	ATOM	387	N <NA>	GLY	A	51	<NA>	8.865	16.952	6.945	1
## 388	ATOM	388	CA <NA>	GLY	A	51	<NA>	8.174	15.771	7.405	1
## 389	ATOM	389	C <NA>	GLY	A	51	<NA>	6.812	16.062	7.983	1
## 390	ATOM	390	O <NA>	GLY	A	51	<NA>	6.408	15.342	8.870	1
## 391	ATOM	391	N <NA>	GLY	A	52	<NA>	6.141	17.132	7.563	1
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## 393	ATOM	393	C <NA>	GLY	A	52	<NA>	4.884	18.624	9.170	1
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## 395	ATOM	395	N <NA>	PHE	A	53	<NA>	3.806	18.788	9.925	1
## 396	ATOM	396	CA <NA>	PHE	A	53	<NA>	3.593	19.996	10.731	1
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## 398	ATOM	398	O <NA>	PHE	A	53	<NA>	3.930	18.810	12.781	1
## 399	ATOM	399	CB <NA>	PHE	A	53	<NA>	2.121	20.351	10.670	1
## 400	ATOM	400	CG <NA>	PHE	A	53	<NA>	1.760	21.152	9.484	1
## 401	ATOM	401	CD1 <NA>	PHE	A	53	<NA>	1.725	20.567	8.216	1
## 402	ATOM	402	CD2 <NA>	PHE	A	53	<NA>	1.556	22.518	9.607	1
## 403	ATOM	403	CE1 <NA>	PHE	A	53	<NA>	1.500	21.332	7.075	1
## 404	ATOM	404	CE2 <NA>	PHE	A	53	<NA>	1.327	23.302	8.496	1
## 405	ATOM	405	CZ <NA>	PHE	A	53	<NA>	1.290	22.718	7.212	1
## 406	ATOM	406	N <NA>	ILE	A	54	<NA>	4.483	20.969	12.792	1
## 407	ATOM	407	CA <NA>	ILE	A	54	<NA>	4.689	21.005	14.248	1
## 408	ATOM	408	C <NA>	ILE	A	54	<NA>	3.921	22.179	14.858	1
## 409	ATOM	409	O <NA>	ILE	A	54	<NA>	3.575	23.139	14.182	1
## 410	ATOM	410	CB <NA>	ILE	A	54	<NA>	6.199	21.155	14.625	1
## 411	ATOM	411	CG1 <NA>	ILE	A	54	<NA>	6.796	22.408	13.939	1
## 412	ATOM	412	CG2 <NA>	ILE	A	54	<NA>	6.967	19.888	14.203	1
## 413	ATOM	413	CD1 <NA>	ILE	A	54	<NA>	8.110	22.821	14.465	1
## 414	ATOM	414	N <NA>	LYS	A	55	<NA>	3.632	22.095	16.145	1
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## 416	ATOM	416	C <NA>	LYS	A	55	<NA>	4.038	24.093	17.449	1
## 417	ATOM	417	O <NA>	LYS	A	55	<NA>	4.949	23.610	18.157	1
## 418	ATOM	418	CB <NA>	LYS	A	55	<NA>	2.021	22.661	17.895	1
## 419	ATOM	419	CG <NA>	LYS	A	55	<NA>	0.974	23.665	18.300	1
## 420	ATOM	420	CD <NA>	LYS	A	55	<NA>	0.006	23.101	19.304	1
## 421	ATOM	421	CE <NA>	LYS	A	55	<NA>	-0.580	24.217	20.149	1
## 422	ATOM	422	NZ <NA>	LYS	A	55	<NA>	0.439	24.751	21.104	1
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## 425	ATOM	425	C <NA>	VAL	A	56	<NA>	4.225	27.378	18.556	1
## 426	ATOM	426	O <NA>	VAL	A	56	<NA>	3.023	27.557	18.455	1
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## 431	ATOM	431	CA <NA>	ARG	A	57	<NA>	4.459	29.271	20.026	1
## 432	ATOM	432	C <NA>	ARG	A	57	<NA>	5.038	30.502	19.335	1
## 433	ATOM	433	O <NA>	ARG	A	57	<NA>	6.242	30.596	19.138	1
## 434	ATOM	434	CB <NA>	ARG	A	57	<NA>	4.824	29.245	21.505	1
## 435	ATOM	435	CG <NA>	ARG	A	57	<NA>	4.168	28.102	22.260	1
## 436	ATOM	436	CD <NA>	ARG	A	57	<NA>	4.656	28.068	23.693	1
## 437	ATOM	437	NE <NA>	ARG	A	57	<NA>	6.032	27.573	23.790	1
## 438	ATOM	438	CZ <NA>	ARG	A	57	<NA>	7.027	28.273	24.317	1
## 439	ATOM	439	NH1 <NA>	ARG	A	57	<NA>	6.825	29.532	24.678	1
## 440	ATOM	440	NH2 <NA>	ARG	A	57	<NA>	8.223	27.723	24.467	1
## 441	ATOM	441	N <NA>	GLN	A	58	<NA>	4.171	31.431	18.958	1
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## 443	ATOM	443	C <NA>	GLN	A	58	<NA>	4.681	33.818	19.085	1
## 444	ATOM	444	O <NA>	GLN	A	58	<NA>	3.694	34.242	19.683	1
## 445	ATOM	445	CB <NA>	GLN	A	58	<NA>	3.539	32.859	17.094	1
## 446	ATOM	446	CG <NA>	GLN	A	58	<NA>	3.736	34.104	16.321	1

##	447	ATOM	447	CD <NA>	GLN	A	58	<NA>	2.500	34.473	15.541	1
##	448	ATOM	448	OE1 <NA>	GLN	A	58	<NA>	1.530	33.703	15.489	1
##	449	ATOM	449	NE2 <NA>	GLN	A	58	<NA>	2.508	35.651	14.940	1
##	450	ATOM	450	N <NA>	TYR	A	59	<NA>	5.883	34.378	19.196	1
##	451	ATOM	451	CA <NA>	TYR	A	59	<NA>	6.097	35.658	19.896	1
##	452	ATOM	452	C <NA>	TYR	A	59	<NA>	6.304	36.752	18.835	1
##	453	ATOM	453	O <NA>	TYR	A	59	<NA>	6.923	36.513	17.800	1
##	454	ATOM	454	CB <NA>	TYR	A	59	<NA>	7.354	35.588	20.765	1
##	455	ATOM	455	CG <NA>	TYR	A	59	<NA>	7.213	34.624	21.955	1
##	456	ATOM	456	CD1 <NA>	TYR	A	59	<NA>	7.479	33.237	21.805	1
##	457	ATOM	457	CD2 <NA>	TYR	A	59	<NA>	6.795	35.087	23.223	1
##	458	ATOM	458	CE1 <NA>	TYR	A	59	<NA>	7.345	32.365	22.871	1
##	459	ATOM	459	CE2 <NA>	TYR	A	59	<NA>	6.638	34.224	24.268	1
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##	462	ATOM	462	N <NA>	ASP	A	60	<NA>	5.767	37.940	19.049	1
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##	466	ATOM	466	CB <NA>	ASP	A	60	<NA>	4.719	39.777	17.832	1
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##	468	ATOM	468	OD1 <NA>	ASP	A	60	<NA>	3.989	38.368	16.050	1
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##	472	ATOM	472	C <NA>	GLN	A	61	<NA>	9.535	41.630	19.179	1
##	473	ATOM	473	O <NA>	GLN	A	61	<NA>	9.777	42.191	20.264	1
##	474	ATOM	474	CB <NA>	GLN	A	61	<NA>	7.471	43.051	19.131	1
##	475	ATOM	475	CG <NA>	GLN	A	61	<NA>	7.718	44.555	18.814	1
##	476	ATOM	476	CD <NA>	GLN	A	61	<NA>	7.182	45.552	19.907	1
##	477	ATOM	477	OE1 <NA>	GLN	A	61	<NA>	7.936	46.461	20.398	1
##	478	ATOM	478	NE2 <NA>	GLN	A	61	<NA>	5.892	45.377	20.306	1
##	479	ATOM	479	N <NA>	ILE	A	62	<NA>	10.283	40.645	18.676	1
##	480	ATOM	480	CA <NA>	ILE	A	62	<NA>	11.484	40.115	19.328	1
##	481	ATOM	481	C <NA>	ILE	A	62	<NA>	12.745	40.584	18.614	1
##	482	ATOM	482	O <NA>	ILE	A	62	<NA>	12.830	40.485	17.396	1
##	483	ATOM	483	CB <NA>	ILE	A	62	<NA>	11.465	38.545	19.309	1
##	484	ATOM	484	CG1 <NA>	ILE	A	62	<NA>	10.152	38.035	19.930	1
##	485	ATOM	485	CG2 <NA>	ILE	A	62	<NA>	12.688	37.973	20.027	1
##	486	ATOM	486	CD1 <NA>	ILE	A	62	<NA>	9.966	38.380	21.363	1
##	487	ATOM	487	N <NA>	LEU	A	63	<NA>	13.722	41.086	19.369	1
##	488	ATOM	488	CA <NA>	LEU	A	63	<NA>	15.038	41.476	18.822	1
##	489	ATOM	489	C <NA>	LEU	A	63	<NA>	16.033	40.304	18.862	1
##	490	ATOM	490	O <NA>	LEU	A	63	<NA>	16.195	39.661	19.897	1
##	491	ATOM	491	CB <NA>	LEU	A	63	<NA>	15.631	42.666	19.619	1
##	492	ATOM	492	CG <NA>	LEU	A	63	<NA>	16.776	43.426	18.914	1
##	493	ATOM	493	CD1 <NA>	LEU	A	63	<NA>	16.560	44.922	18.993	1
##	494	ATOM	494	CD2 <NA>	LEU	A	63	<NA>	18.103	43.062	19.558	1
##	495	ATOM	495	N <NA>	ILE	A	64	<NA>	16.686	40.036	17.738	1
##	496	ATOM	496	CA <NA>	ILE	A	64	<NA>	17.760	39.039	17.653	1
##	497	ATOM	497	C <NA>	ILE	A	64	<NA>	18.991	39.753	17.116	1
##	498	ATOM	498	O <NA>	ILE	A	64	<NA>	18.862	40.632	16.288	1
##	499	ATOM	499	CB <NA>	ILE	A	64	<NA>	17.390	37.875	16.634	1
##	500	ATOM	500	CG1 <NA>	ILE	A	64	<NA>	16.127	37.137	17.110	1

## 501	ATOM	501	CG2 <NA>	ILE	A	64	<NA>	18.551	36.857	16.518	1
## 502	ATOM	502	CD1 <NA>	ILE	A	64	<NA>	16.194	35.643	16.885	1
## 503	ATOM	503	N <NA>	GLU	A	65	<NA>	20.181	39.387	17.573	1
## 504	ATOM	504	CA <NA>	GLU	A	65	<NA>	21.406	39.983	17.036	1
## 505	ATOM	505	C <NA>	GLU	A	65	<NA>	22.192	39.019	16.135	1
## 506	ATOM	506	O <NA>	GLU	A	65	<NA>	22.866	38.128	16.631	1
## 507	ATOM	507	CB <NA>	GLU	A	65	<NA>	22.307	40.439	18.180	1
## 508	ATOM	508	CG <NA>	GLU	A	65	<NA>	21.987	41.843	18.676	1
## 509	ATOM	509	CD <NA>	GLU	A	65	<NA>	23.228	42.558	19.187	1
## 510	ATOM	510	OE1 <NA>	GLU	A	65	<NA>	24.094	42.925	18.348	1
## 511	ATOM	511	OE2 <NA>	GLU	A	65	<NA>	23.348	42.730	20.429	1
## 512	ATOM	512	N <NA>	ILE	A	66	<NA>	22.148	39.215	14.823	1
## 513	ATOM	513	CA <NA>	ILE	A	66	<NA>	22.818	38.327	13.863	1
## 514	ATOM	514	C <NA>	ILE	A	66	<NA>	24.123	38.945	13.303	1
## 515	ATOM	515	O <NA>	ILE	A	66	<NA>	24.114	39.903	12.521	1
## 516	ATOM	516	CB <NA>	ILE	A	66	<NA>	21.831	37.964	12.694	1
## 517	ATOM	517	CG1 <NA>	ILE	A	66	<NA>	20.481	37.516	13.278	1
## 518	ATOM	518	CG2 <NA>	ILE	A	66	<NA>	22.444	36.880	11.799	1
## 519	ATOM	519	CD1 <NA>	ILE	A	66	<NA>	19.263	38.072	12.560	1
## 520	ATOM	520	N <NA>	CYS	A	67	<NA>	25.251	38.396	13.731	1
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## 522	ATOM	522	C <NA>	CYS	A	67	<NA>	26.798	40.370	13.560	1
## 523	ATOM	523	O <NA>	CYS	A	67	<NA>	27.461	41.045	12.763	1
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## 527	ATOM	527	CA <NA>	GLY	A	68	<NA>	26.319	42.307	14.938	1
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## 529	ATOM	529	O <NA>	GLY	A	68	<NA>	24.371	43.518	15.561	1
## 530	ATOM	530	N <NA>	HIS	A	69	<NA>	24.449	42.689	13.479	1
## 531	ATOM	531	CA <NA>	HIS	A	69	<NA>	23.251	43.368	13.013	1
## 532	ATOM	532	C <NA>	HIS	A	69	<NA>	22.009	43.025	13.836	1
## 533	ATOM	533	O <NA>	HIS	A	69	<NA>	21.626	41.865	13.958	1
## 534	ATOM	534	CB <NA>	HIS	A	69	<NA>	22.975	43.009	11.568	1
## 535	ATOM	535	CG <NA>	HIS	A	69	<NA>	24.157	43.172	10.639	1
## 536	ATOM	536	ND1 <NA>	HIS	A	69	<NA>	25.294	42.398	10.762	1
## 537	ATOM	537	CD2 <NA>	HIS	A	69	<NA>	24.283	43.886	9.518	1
## 538	ATOM	538	CE1 <NA>	HIS	A	69	<NA>	26.075	42.630	9.723	1
## 539	ATOM	539	NE2 <NA>	HIS	A	69	<NA>	25.505	43.532	8.946	1
## 540	ATOM	540	N <NA>	LYS	A	70	<NA>	21.364	44.050	14.376	1
## 541	ATOM	541	CA <NA>	LYS	A	70	<NA>	20.030	43.883	14.945	1
## 542	ATOM	542	C <NA>	LYS	A	70	<NA>	18.929	43.698	13.882	1
## 543	ATOM	543	O <NA>	LYS	A	70	<NA>	19.000	44.197	12.761	1
## 544	ATOM	544	CB <NA>	LYS	A	70	<NA>	19.667	45.075	15.840	1
## 545	ATOM	545	CG <NA>	LYS	A	70	<NA>	20.422	45.141	17.154	1
## 546	ATOM	546	CD <NA>	LYS	A	70	<NA>	19.885	46.281	18.036	1
## 547	ATOM	547	CE <NA>	LYS	A	70	<NA>	20.905	46.699	19.095	1
## 548	ATOM	548	NZ <NA>	LYS	A	70	<NA>	20.376	47.817	19.946	1
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## 551	ATOM	551	C <NA>	ALA	A	71	<NA>	15.600	42.546	14.556	1
## 552	ATOM	552	O <NA>	ALA	A	71	<NA>	15.880	42.175	15.705	1
## 553	ATOM	553	CB <NA>	ALA	A	71	<NA>	16.937	41.464	12.683	1
## 554	ATOM	554	N <NA>	ILE	A	72	<NA>	14.366	42.881	14.219	1

## 555	ATOM	555	CA <NA>	ILE	A	72	<NA>	13.233	42.663	15.111	1
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## 557	ATOM	557	O <NA>	ILE	A	72	<NA>	12.083	42.266	13.025	1
## 558	ATOM	558	CB <NA>	ILE	A	72	<NA>	12.635	44.019	15.609	1
## 559	ATOM	559	CG1 <NA>	ILE	A	72	<NA>	13.664	44.777	16.446	1
## 560	ATOM	560	CG2 <NA>	ILE	A	72	<NA>	11.353	43.782	16.409	1
## 561	ATOM	561	CD1 <NA>	ILE	A	72	<NA>	13.437	46.286	16.451	1
## 562	ATOM	562	N <NA>	GLY	A	73	<NA>	11.457	41.034	14.821	1
## 563	ATOM	563	CA <NA>	GLY	A	73	<NA>	10.359	40.420	14.090	1
## 564	ATOM	564	C <NA>	GLY	A	73	<NA>	9.750	39.238	14.835	1
## 565	ATOM	565	O <NA>	GLY	A	73	<NA>	10.019	39.007	16.009	1
## 566	ATOM	566	N <NA>	THR	A	74	<NA>	8.853	38.524	14.181	1
## 567	ATOM	567	CA <NA>	THR	A	74	<NA>	8.224	37.361	14.786	1
## 568	ATOM	568	C <NA>	THR	A	74	<NA>	9.169	36.194	14.895	1
## 569	ATOM	569	O <NA>	THR	A	74	<NA>	9.964	35.908	14.007	1
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## 571	ATOM	571	OG1 <NA>	THR	A	74	<NA>	6.030	38.013	14.001	1
## 572	ATOM	572	CG2 <NA>	THR	A	74	<NA>	6.287	35.760	14.688	1
## 573	ATOM	573	N <NA>	VAL	A	75	<NA>	9.085	35.534	16.025	1
## 574	ATOM	574	CA <NA>	VAL	A	75	<NA>	9.944	34.420	16.291	1
## 575	ATOM	575	C <NA>	VAL	A	75	<NA>	9.018	33.325	16.795	1
## 576	ATOM	576	O <NA>	VAL	A	75	<NA>	8.104	33.576	17.594	1
## 577	ATOM	577	CB <NA>	VAL	A	75	<NA>	11.002	34.791	17.336	1
## 578	ATOM	578	CG1 <NA>	VAL	A	75	<NA>	11.638	33.561	17.884	1
## 579	ATOM	579	CG2 <NA>	VAL	A	75	<NA>	12.070	35.661	16.648	1
## 580	ATOM	580	N <NA>	LEU	A	76	<NA>	9.200	32.127	16.258	1
## 581	ATOM	581	CA <NA>	LEU	A	76	<NA>	8.353	30.995	16.628	1
## 582	ATOM	582	C <NA>	LEU	A	76	<NA>	9.229	30.084	17.483	1
## 583	ATOM	583	O <NA>	LEU	A	76	<NA>	10.409	29.923	17.194	1
## 584	ATOM	584	CB <NA>	LEU	A	76	<NA>	7.937	30.247	15.365	1
## 585	ATOM	585	CG <NA>	LEU	A	76	<NA>	7.222	30.919	14.207	1
## 586	ATOM	586	CD1 <NA>	LEU	A	76	<NA>	6.909	29.914	13.139	1
## 587	ATOM	587	CD2 <NA>	LEU	A	76	<NA>	5.961	31.526	14.713	1
## 588	ATOM	588	N <NA>	VAL	A	77	<NA>	8.689	29.507	18.538	1
## 589	ATOM	589	CA <NA>	VAL	A	77	<NA>	9.519	28.691	19.405	1
## 590	ATOM	590	C <NA>	VAL	A	77	<NA>	8.852	27.309	19.499	1
## 591	ATOM	591	O <NA>	VAL	A	77	<NA>	7.621	27.241	19.608	1
## 592	ATOM	592	CB <NA>	VAL	A	77	<NA>	9.648	29.353	20.800	1
## 593	ATOM	593	CG1 <NA>	VAL	A	77	<NA>	10.306	28.419	21.773	1
## 594	ATOM	594	CG2 <NA>	VAL	A	77	<NA>	10.426	30.686	20.648	1
## 595	ATOM	595	N <NA>	GLY	A	78	<NA>	9.637	26.227	19.375	1
## 596	ATOM	596	CA <NA>	GLY	A	78	<NA>	9.027	24.918	19.185	1
## 597	ATOM	597	C <NA>	GLY	A	78	<NA>	10.005	23.782	18.984	1
## 598	ATOM	598	O <NA>	GLY	A	78	<NA>	11.215	24.012	19.065	1
## 599	ATOM	599	N <NA>	PRO	A	79	<NA>	9.538	22.542	18.758	1
## 600	ATOM	600	CA <NA>	PRO	A	79	<NA>	10.442	21.388	18.731	1
## 601	ATOM	601	C <NA>	PRO	A	79	<NA>	11.136	21.242	17.389	1
## 602	ATOM	602	O <NA>	PRO	A	79	<NA>	10.748	20.397	16.559	1
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## 604	ATOM	604	CG <NA>	PRO	A	79	<NA>	8.239	20.616	18.339	1
## 605	ATOM	605	CD <NA>	PRO	A	79	<NA>	8.170	22.144	18.383	1
## 606	ATOM	606	N <NA>	THR	A	80	<NA>	12.138	22.078	17.162	1
## 607	ATOM	607	CA <NA>	THR	A	80	<NA>	12.910	22.043	15.936	1
## 608	ATOM	608	C <NA>	THR	A	80	<NA>	14.280	21.503	16.325	1

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## 611	ATOM	611	OG1 <NA>	THR	A	80	<NA>	13.971	23.419	14.244	1
## 612	ATOM	612	CG2 <NA>	THR	A	80	<NA>	13.542	24.478	16.300	1
## 613	ATOM	613	N <NA>	PRO	A	81	<NA>	14.915	20.725	15.449	1
## 614	ATOM	614	CA <NA>	PRO	A	81	<NA>	16.233	20.170	15.766	1
## 615	ATOM	615	C <NA>	PRO	A	81	<NA>	17.352	21.205	15.795	1
## 616	ATOM	616	O <NA>	PRO	A	81	<NA>	18.306	21.085	16.567	1
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## 618	ATOM	618	CG <NA>	PRO	A	81	<NA>	15.477	19.489	13.607	1
## 619	ATOM	619	CD <NA>	PRO	A	81	<NA>	14.331	20.114	14.238	1
## 620	ATOM	620	N <NA>	VAL	A	82	<NA>	17.220	22.219	14.948	1
## 621	ATOM	621	CA <NA>	VAL	A	82	<NA>	18.236	23.243	14.762	1
## 622	ATOM	622	C <NA>	VAL	A	82	<NA>	17.549	24.626	14.801	1
## 623	ATOM	623	O <NA>	VAL	A	82	<NA>	16.328	24.735	14.569	1
## 624	ATOM	624	CB <NA>	VAL	A	82	<NA>	18.969	23.017	13.388	1
## 625	ATOM	625	CG1 <NA>	VAL	A	82	<NA>	18.009	22.769	12.263	1
## 626	ATOM	626	CG2 <NA>	VAL	A	82	<NA>	19.843	24.144	13.080	1
## 627	ATOM	627	N <NA>	ASN	A	83	<NA>	18.292	25.671	15.167	1
## 628	ATOM	628	CA <NA>	ASN	A	83	<NA>	17.731	27.051	15.193	1
## 629	ATOM	629	C <NA>	ASN	A	83	<NA>	17.799	27.628	13.799	1
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## 631	ATOM	631	CB <NA>	ASN	A	83	<NA>	18.508	27.950	16.161	1
## 632	ATOM	632	CG <NA>	ASN	A	83	<NA>	18.236	27.600	17.636	1
## 633	ATOM	633	OD1 <NA>	ASN	A	83	<NA>	17.102	27.381	18.051	1
## 634	ATOM	634	ND2 <NA>	ASN	A	83	<NA>	19.287	27.475	18.398	1
## 635	ATOM	635	N <NA>	ILE	A	84	<NA>	16.729	28.283	13.370	1
## 636	ATOM	636	CA <NA>	ILE	A	84	<NA>	16.588	28.651	11.955	1
## 637	ATOM	637	C <NA>	ILE	A	84	<NA>	16.190	30.132	11.811	1
## 638	ATOM	638	O <NA>	ILE	A	84	<NA>	15.178	30.600	12.384	1
## 639	ATOM	639	CB <NA>	ILE	A	84	<NA>	15.504	27.755	11.242	1
## 640	ATOM	640	CG1 <NA>	ILE	A	84	<NA>	16.049	26.365	11.040	1
## 641	ATOM	641	CG2 <NA>	ILE	A	84	<NA>	15.081	28.324	9.932	1
## 642	ATOM	642	CD1 <NA>	ILE	A	84	<NA>	14.957	25.345	11.321	1
## 643	ATOM	643	N <NA>	ILE	A	85	<NA>	16.991	30.863	11.053	1
## 644	ATOM	644	CA <NA>	ILE	A	85	<NA>	16.710	32.257	10.821	1
## 645	ATOM	645	C <NA>	ILE	A	85	<NA>	16.155	32.252	9.420	1
## 646	ATOM	646	O <NA>	ILE	A	85	<NA>	16.857	31.950	8.464	1
## 647	ATOM	647	CB <NA>	ILE	A	85	<NA>	17.999	33.119	10.844	1
## 648	ATOM	648	CG1 <NA>	ILE	A	85	<NA>	18.724	32.983	12.207	1
## 649	ATOM	649	CG2 <NA>	ILE	A	85	<NA>	17.653	34.600	10.517	1
## 650	ATOM	650	CD1 <NA>	ILE	A	85	<NA>	17.830	33.204	13.418	1
## 651	ATOM	651	N <NA>	GLY	A	86	<NA>	14.888	32.608	9.302	1
## 652	ATOM	652	CA <NA>	GLY	A	86	<NA>	14.238	32.655	8.011	1
## 653	ATOM	653	C <NA>	GLY	A	86	<NA>	14.181	34.034	7.393	1
## 654	ATOM	654	O <NA>	GLY	A	86	<NA>	14.714	34.991	7.894	1
## 655	ATOM	655	N <NA>	ARG	A	87	<NA>	13.398	34.131	6.334	1
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## 660	ATOM	660	CG <NA>	ARG	A	87	<NA>	13.030	34.044	3.318	1
## 661	ATOM	661	CD <NA>	ARG	A	87	<NA>	12.310	34.101	1.966	1
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## 663	ATOM	663	CZ <NA>	ARG	A	87	<NA>	9.899	34.575	2.137	1
## 664	ATOM	664	NH1 <NA>	ARG	A	87	<NA>	10.126	35.860	1.922	1
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## 666	ATOM	666	N <NA>	ASN	A	88	<NA>	12.063	36.352	7.198	1
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## 668	ATOM	668	C <NA>	ASN	A	88	<NA>	12.511	38.266	8.653	1
## 669	ATOM	669	O <NA>	ASN	A	88	<NA>	12.419	39.481	8.723	1
## 670	ATOM	670	CB <NA>	ASN	A	88	<NA>	10.359	36.959	8.863	1
## 671	ATOM	671	CG <NA>	ASN	A	88	<NA>	10.892	36.309	10.125	1
## 672	ATOM	672	OD1 <NA>	ASN	A	88	<NA>	11.577	35.273	10.065	1
## 673	ATOM	673	ND2 <NA>	ASN	A	88	<NA>	10.446	36.809	11.283	1
## 674	ATOM	674	N <NA>	LEU	A	89	<NA>	13.551	37.601	9.136	1
## 675	ATOM	675	CA <NA>	LEU	A	89	<NA>	14.633	38.337	9.729	1
## 676	ATOM	676	C <NA>	LEU	A	89	<NA>	15.802	38.487	8.783	1
## 677	ATOM	677	O <NA>	LEU	A	89	<NA>	16.580	39.394	8.941	1
## 678	ATOM	678	CB <NA>	LEU	A	89	<NA>	15.096	37.687	11.029	1
## 679	ATOM	679	CG <NA>	LEU	A	89	<NA>	14.146	37.555	12.221	1
## 680	ATOM	680	CD1 <NA>	LEU	A	89	<NA>	14.939	37.022	13.434	1
## 681	ATOM	681	CD2 <NA>	LEU	A	89	<NA>	13.508	38.913	12.527	1
## 682	ATOM	682	N <NA>	LEU	A	90	<NA>	15.910	37.651	7.761	1
## 683	ATOM	683	CA <NA>	LEU	A	90	<NA>	17.078	37.773	6.865	1
## 684	ATOM	684	C <NA>	LEU	A	90	<NA>	17.048	39.068	6.049	1
## 685	ATOM	685	O <NA>	LEU	A	90	<NA>	18.098	39.613	5.652	1
## 686	ATOM	686	CB <NA>	LEU	A	90	<NA>	17.200	36.561	5.913	1
## 687	ATOM	687	CG <NA>	LEU	A	90	<NA>	17.754	35.226	6.440	1
## 688	ATOM	688	CD1 <NA>	LEU	A	90	<NA>	17.798	34.207	5.340	1
## 689	ATOM	689	CD2 <NA>	LEU	A	90	<NA>	19.138	35.441	7.022	1
## 690	ATOM	690	N <NA>	THR	A	91	<NA>	15.835	39.547	5.808	1
## 691	ATOM	691	CA <NA>	THR	A	91	<NA>	15.653	40.738	4.985	1
## 692	ATOM	692	C <NA>	THR	A	91	<NA>	16.137	41.999	5.772	1
## 693	ATOM	693	O <NA>	THR	A	91	<NA>	16.848	42.870	5.252	1
## 694	ATOM	694	CB <NA>	THR	A	91	<NA>	14.157	40.860	4.594	1
## 695	ATOM	695	OG1 <NA>	THR	A	91	<NA>	13.342	40.810	5.786	1
## 696	ATOM	696	CG2 <NA>	THR	A	91	<NA>	13.740	39.709	3.681	1
## 697	ATOM	697	N <NA>	GLN	A	92	<NA>	15.842	42.001	7.064	1
## 698	ATOM	698	CA <NA>	GLN	A	92	<NA>	16.170	43.099	7.967	1
## 699	ATOM	699	C <NA>	GLN	A	92	<NA>	17.650	43.315	8.126	1
## 700	ATOM	700	O <NA>	GLN	A	92	<NA>	18.071	44.440	8.459	1
## 701	ATOM	701	CB <NA>	GLN	A	92	<NA>	15.580	42.837	9.347	1
## 702	ATOM	702	CG <NA>	GLN	A	92	<NA>	14.081	42.603	9.325	1
## 703	ATOM	703	CD <NA>	GLN	A	92	<NA>	13.318	43.811	8.800	1
## 704	ATOM	704	OE1 <NA>	GLN	A	92	<NA>	12.836	43.807	7.683	1
## 705	ATOM	705	NE2 <NA>	GLN	A	92	<NA>	13.349	44.892	9.543	1
## 706	ATOM	706	N <NA>	ILE	A	93	<NA>	18.444	42.266	7.913	1
## 707	ATOM	707	CA <NA>	ILE	A	93	<NA>	19.887	42.417	8.035	1
## 708	ATOM	708	C <NA>	ILE	A	93	<NA>	20.530	42.555	6.677	1
## 709	ATOM	709	O <NA>	ILE	A	93	<NA>	21.744	42.639	6.577	1
## 710	ATOM	710	CB <NA>	ILE	A	93	<NA>	20.557	41.231	8.872	1
## 711	ATOM	711	CG1 <NA>	ILE	A	93	<NA>	20.472	39.878	8.113	1
## 712	ATOM	712	CG2 <NA>	ILE	A	93	<NA>	19.926	41.182	10.272	1
## 713	ATOM	713	CD1 <NA>	ILE	A	93	<NA>	21.520	38.796	8.533	1
## 714	ATOM	714	N <NA>	GLY	A	94	<NA>	19.713	42.563	5.636	1
## 715	ATOM	715	CA <NA>	GLY	A	94	<NA>	20.226	42.870	4.327	1
## 716	ATOM	716	C <NA>	GLY	A	94	<NA>	20.843	41.689	3.611	1

## 717	ATOM	717	O <NA>	GLY	A	94	<NA>	21.680	41.866	2.723	1
## 718	ATOM	718	N <NA>	CYS	A	95	<NA>	20.294	40.507	3.844	1
## 719	ATOM	719	CA <NA>	CYS	A	95	<NA>	20.890	39.296	3.297	1
## 720	ATOM	720	C <NA>	CYS	A	95	<NA>	20.407	39.005	1.897	1
## 721	ATOM	721	O <NA>	CYS	A	95	<NA>	19.217	39.101	1.606	1
## 722	ATOM	722	CB <NA>	CYS	A	95	<NA>	20.585	38.134	4.215	1
## 723	ATOM	723	SG <NA>	CYS	A	95	<NA>	21.505	36.663	3.848	1
## 724	ATOM	724	N <NA>	THR	A	96	<NA>	21.339	38.698	1.005	1
## 725	ATOM	725	CA <NA>	THR	A	96	<NA>	20.969	38.276	-0.346	1
## 726	ATOM	726	C <NA>	THR	A	96	<NA>	21.721	37.024	-0.758	1
## 727	ATOM	727	O <NA>	THR	A	96	<NA>	22.753	36.645	-0.178	1
## 728	ATOM	728	CB <NA>	THR	A	96	<NA>	21.298	39.331	-1.459	1
## 729	ATOM	729	OG1 <NA>	THR	A	96	<NA>	22.688	39.698	-1.364	1
## 730	ATOM	730	CG2 <NA>	THR	A	96	<NA>	20.405	40.560	-1.303	1
## 731	ATOM	731	N <NA>	LEU	A	97	<NA>	21.183	36.413	-1.805	1
## 732	ATOM	732	CA <NA>	LEU	A	97	<NA>	21.718	35.228	-2.473	1
## 733	ATOM	733	C <NA>	LEU	A	97	<NA>	22.314	35.753	-3.779	1
## 734	ATOM	734	O <NA>	LEU	A	97	<NA>	21.616	36.396	-4.577	1
## 735	ATOM	735	CB <NA>	LEU	A	97	<NA>	20.518	34.349	-2.810	1
## 736	ATOM	736	CG <NA>	LEU	A	97	<NA>	20.318	32.897	-2.464	1
## 737	ATOM	737	CD1 <NA>	LEU	A	97	<NA>	21.285	32.388	-1.422	1
## 738	ATOM	738	CD2 <NA>	LEU	A	97	<NA>	18.896	32.782	-2.010	1
## 739	ATOM	739	N <NA>	ASN	A	98	<NA>	23.577	35.469	-4.026	1
## 740	ATOM	740	CA <NA>	ASN	A	98	<NA>	24.207	35.904	-5.257	1
## 741	ATOM	741	C <NA>	ASN	A	98	<NA>	24.863	34.748	-5.999	1
## 742	ATOM	742	O <NA>	ASN	A	98	<NA>	25.635	33.982	-5.396	1
## 743	ATOM	743	CB <NA>	ASN	A	98	<NA>	25.229	36.991	-4.938	1
## 744	ATOM	744	CG <NA>	ASN	A	98	<NA>	24.609	38.190	-4.212	1
## 745	ATOM	745	OD1 <NA>	ASN	A	98	<NA>	24.263	38.112	-3.019	1
## 746	ATOM	746	ND2 <NA>	ASN	A	98	<NA>	24.354	39.252	-4.955	1
## 747	ATOM	747	N <NA>	PHE	A	99	<NA>	24.539	34.602	-7.287	1
## 748	ATOM	748	CA <NA>	PHE	A	99	<NA>	25.376	33.754	-8.172	1
## 749	ATOM	749	C <NA>	PHE	A	99	<NA>	25.726	34.383	-9.544	1
## 750	ATOM	750	O <NA>	PHE	A	99	<NA>	24.797	34.890	-10.226	1
## 751	ATOM	751	CB <NA>	PHE	A	99	<NA>	24.743	32.354	-8.375	1
## 752	ATOM	752	CG <NA>	PHE	A	99	<NA>	23.328	32.389	-8.856	1
## 753	ATOM	753	CD1 <NA>	PHE	A	99	<NA>	22.303	32.588	-7.961	1
## 754	ATOM	754	CD2 <NA>	PHE	A	99	<NA>	23.029	32.118	-10.181	1
## 755	ATOM	755	CE1 <NA>	PHE	A	99	<NA>	21.000	32.515	-8.357	1
## 756	ATOM	756	CE2 <NA>	PHE	A	99	<NA>	21.730	32.028	-10.613	1
## 757	ATOM	757	CZ <NA>	PHE	A	99	<NA>	20.700	32.221	-9.700	1
## 758	ATOM	759	N <NA>	PRO	B	1	<NA>	22.659	36.727	-10.823	1
## 759	ATOM	760	CA <NA>	PRO	B	1	<NA>	21.708	37.741	-10.269	1
## 760	ATOM	761	C <NA>	PRO	B	1	<NA>	21.931	37.939	-8.779	1
## 761	ATOM	762	O <NA>	PRO	B	1	<NA>	22.755	37.283	-8.190	1
## 762	ATOM	763	CB <NA>	PRO	B	1	<NA>	20.263	37.289	-10.512	1
## 763	ATOM	764	CG <NA>	PRO	B	1	<NA>	20.385	35.811	-10.891	1
## 764	ATOM	765	CD <NA>	PRO	B	1	<NA>	21.753	35.755	-11.555	1
## 765	ATOM	766	N <NA>	GLN	B	2	<NA>	21.203	38.873	-8.191	1
## 766	ATOM	767	CA <NA>	GLN	B	2	<NA>	21.156	39.043	-6.744	1
## 767	ATOM	768	C <NA>	GLN	B	2	<NA>	19.698	38.882	-6.389	1
## 768	ATOM	769	O <NA>	GLN	B	2	<NA>	18.850	39.538	-6.975	1
## 769	ATOM	770	CB <NA>	GLN	B	2	<NA>	21.625	40.447	-6.329	1
## 770	ATOM	771	CG <NA>	GLN	B	2	<NA>	21.353	40.777	-4.865	1

## 771	ATOM	772	CD <NA>	GLN	B	2	<NA>	22.139	41.975	-4.358	1
## 772	ATOM	773	OE1 <NA>	GLN	B	2	<NA>	21.577	42.881	-3.752	1
## 773	ATOM	774	NE2 <NA>	GLN	B	2	<NA>	23.450	41.976	-4.586	1
## 774	ATOM	775	N <NA>	ILE	B	3	<NA>	19.405	38.008	-5.448	1
## 775	ATOM	776	CA <NA>	ILE	B	3	<NA>	18.037	37.742	-5.100	1
## 776	ATOM	777	C <NA>	ILE	B	3	<NA>	17.832	38.164	-3.660	1
## 777	ATOM	778	O <NA>	ILE	B	3	<NA>	18.457	37.631	-2.746	1
## 778	ATOM	779	CB <NA>	ILE	B	3	<NA>	17.694	36.224	-5.238	1
## 779	ATOM	780	CG1 <NA>	ILE	B	3	<NA>	17.788	35.772	-6.692	1
## 780	ATOM	781	CG2 <NA>	ILE	B	3	<NA>	16.284	35.967	-4.750	1
## 781	ATOM	782	CD1 <NA>	ILE	B	3	<NA>	18.183	34.327	-6.802	1
## 782	ATOM	783	N <NA>	THR	B	4	<NA>	16.960	39.132	-3.461	1
## 783	ATOM	784	CA <NA>	THR	B	4	<NA>	16.635	39.571	-2.117	1
## 784	ATOM	785	C <NA>	THR	B	4	<NA>	15.555	38.634	-1.627	1
## 785	ATOM	786	O <NA>	THR	B	4	<NA>	15.066	37.784	-2.372	1
## 786	ATOM	787	CB <NA>	THR	B	4	<NA>	16.147	41.074	-2.110	1
## 787	ATOM	788	OG1 <NA>	THR	B	4	<NA>	15.093	41.256	-3.079	1
## 788	ATOM	789	CG2 <NA>	THR	B	4	<NA>	17.283	42.019	-2.472	1
## 789	ATOM	790	N <NA>	LEU	B	5	<NA>	15.157	38.761	-0.379	1
## 790	ATOM	791	CA <NA>	LEU	B	5	<NA>	14.466	37.636	0.259	1
## 791	ATOM	792	C <NA>	LEU	B	5	<NA>	13.125	38.065	0.821	1
## 792	ATOM	793	O <NA>	LEU	B	5	<NA>	12.585	37.446	1.733	1
## 793	ATOM	794	CB <NA>	LEU	B	5	<NA>	15.340	37.047	1.374	1
## 794	ATOM	795	CG <NA>	LEU	B	5	<NA>	16.622	36.365	0.892	1
## 795	ATOM	796	CD1 <NA>	LEU	B	5	<NA>	17.455	35.953	2.080	1
## 796	ATOM	797	CD2 <NA>	LEU	B	5	<NA>	16.248	35.136	-0.006	1
## 797	ATOM	798	N <NA>	TRP	B	6	<NA>	12.567	39.127	0.262	1
## 798	ATOM	799	CA <NA>	TRP	B	6	<NA>	11.260	39.582	0.682	1
## 799	ATOM	800	C <NA>	TRP	B	6	<NA>	10.196	38.601	0.218	1
## 800	ATOM	801	O <NA>	TRP	B	6	<NA>	9.192	38.404	0.903	1
## 801	ATOM	802	CB <NA>	TRP	B	6	<NA>	11.004	40.992	0.135	1
## 802	ATOM	803	CG <NA>	TRP	B	6	<NA>	12.065	42.014	0.478	1
## 803	ATOM	804	CD1 <NA>	TRP	B	6	<NA>	13.157	42.366	-0.279	1
## 804	ATOM	805	CD2 <NA>	TRP	B	6	<NA>	12.209	42.716	1.739	1
## 805	ATOM	806	NE1 <NA>	TRP	B	6	<NA>	13.979	43.196	0.470	1
## 806	ATOM	807	CE2 <NA>	TRP	B	6	<NA>	13.433	43.441	1.686	1
## 807	ATOM	808	CE3 <NA>	TRP	B	6	<NA>	11.443	42.805	2.913	1
## 808	ATOM	809	CZ2 <NA>	TRP	B	6	<NA>	13.914	44.211	2.785	1
## 809	ATOM	810	CZ3 <NA>	TRP	B	6	<NA>	11.903	43.585	3.953	1
## 810	ATOM	811	CH2 <NA>	TRP	B	6	<NA>	13.148	44.273	3.896	1
## 811	ATOM	812	N <NA>	GLN	B	7	<NA>	10.396	38.008	-0.958	1
## 812	ATOM	813	CA <NA>	GLN	B	7	<NA>	9.518	36.960	-1.516	1
## 813	ATOM	814	C <NA>	GLN	B	7	<NA>	10.321	35.670	-1.433	1
## 814	ATOM	815	O <NA>	GLN	B	7	<NA>	11.546	35.694	-1.298	1
## 815	ATOM	816	CB <NA>	GLN	B	7	<NA>	9.215	37.238	-3.000	1
## 816	ATOM	817	CG <NA>	GLN	B	7	<NA>	8.278	38.433	-3.326	1
## 817	ATOM	818	CD <NA>	GLN	B	7	<NA>	7.629	38.332	-4.744	1
## 818	ATOM	819	OE1 <NA>	GLN	B	7	<NA>	8.319	38.100	-5.754	1
## 819	ATOM	820	NE2 <NA>	GLN	B	7	<NA>	6.307	38.532	-4.814	1
## 820	ATOM	821	N <NA>	ARG	B	8	<NA>	9.661	34.528	-1.525	1
## 821	ATOM	822	CA <NA>	ARG	B	8	<NA>	10.385	33.251	-1.642	1
## 822	ATOM	823	C <NA>	ARG	B	8	<NA>	11.348	33.305	-2.780	1
## 823	ATOM	824	O <NA>	ARG	B	8	<NA>	10.964	33.682	-3.906	1
## 824	ATOM	825	CB <NA>	ARG	B	8	<NA>	9.435	32.061	-1.862	1

##	825	ATOM	826	CG <NA>	ARG	B	8	<NA>	8.623	31.716	-0.644	1
##	826	ATOM	827	CD <NA>	ARG	B	8	<NA>	7.828	30.471	-0.844	1
##	827	ATOM	828	NE <NA>	ARG	B	8	<NA>	7.143	30.102	0.378	1
##	828	ATOM	829	CZ <NA>	ARG	B	8	<NA>	6.523	28.938	0.561	1
##	829	ATOM	830	NH1 <NA>	ARG	B	8	<NA>	6.476	28.028	-0.411	1
##	830	ATOM	831	NH2 <NA>	ARG	B	8	<NA>	5.925	28.688	1.719	1
##	831	ATOM	832	N <NA>	PRO	B	9	<NA>	12.533	32.711	-2.598	1
##	832	ATOM	833	CA <NA>	PRO	B	9	<NA>	13.443	32.743	-3.746	1
##	833	ATOM	834	C <NA>	PRO	B	9	<NA>	13.174	31.592	-4.703	1
##	834	ATOM	835	O <NA>	PRO	B	9	<NA>	13.897	30.587	-4.698	1
##	835	ATOM	836	CB <NA>	PRO	B	9	<NA>	14.813	32.658	-3.125	1
##	836	ATOM	837	CG <NA>	PRO	B	9	<NA>	14.564	31.823	-1.917	1
##	837	ATOM	838	CD <NA>	PRO	B	9	<NA>	13.238	32.289	-1.373	1
##	838	ATOM	839	N <NA>	LEU	B	10	<NA>	12.134	31.727	-5.504	1
##	839	ATOM	840	CA <NA>	LEU	B	10	<NA>	11.816	30.740	-6.534	1
##	840	ATOM	841	C <NA>	LEU	B	10	<NA>	12.459	31.075	-7.877	1
##	841	ATOM	842	O <NA>	LEU	B	10	<NA>	12.274	32.150	-8.406	1
##	842	ATOM	843	CB <NA>	LEU	B	10	<NA>	10.303	30.637	-6.738	1
##	843	ATOM	844	CG <NA>	LEU	B	10	<NA>	9.483	30.307	-5.497	1
##	844	ATOM	845	CD1 <NA>	LEU	B	10	<NA>	8.028	30.334	-5.876	1
##	845	ATOM	846	CD2 <NA>	LEU	B	10	<NA>	9.845	28.975	-4.951	1
##	846	ATOM	847	N <NA>	VAL	B	11	<NA>	13.225	30.141	-8.420	1
##	847	ATOM	848	CA <NA>	VAL	B	11	<NA>	13.759	30.227	-9.768	1
##	848	ATOM	849	C <NA>	VAL	B	11	<NA>	13.103	29.153	-10.641	1
##	849	ATOM	850	O <NA>	VAL	B	11	<NA>	12.381	28.285	-10.135	1
##	850	ATOM	851	CB <NA>	VAL	B	11	<NA>	15.253	29.988	-9.735	1
##	851	ATOM	852	CG1 <NA>	VAL	B	11	<NA>	15.898	31.108	-8.939	1
##	852	ATOM	853	CG2 <NA>	VAL	B	11	<NA>	15.573	28.635	-9.104	1
##	853	ATOM	854	N <NA>	THR	B	12	<NA>	13.346	29.214	-11.949	1
##	854	ATOM	855	CA <NA>	THR	B	12	<NA>	12.809	28.220	-12.873	1
##	855	ATOM	856	C <NA>	THR	B	12	<NA>	13.951	27.253	-13.210	1
##	856	ATOM	857	O <NA>	THR	B	12	<NA>	15.089	27.656	-13.442	1
##	857	ATOM	858	CB <NA>	THR	B	12	<NA>	12.259	28.907	-14.158	1
##	858	ATOM	859	OG1 <NA>	THR	B	12	<NA>	11.693	27.933	-15.028	1
##	859	ATOM	860	CG2 <NA>	THR	B	12	<NA>	13.341	29.639	-14.925	1
##	860	ATOM	861	N <NA>	ILE	B	13	<NA>	13.684	25.961	-13.124	1
##	861	ATOM	862	CA <NA>	ILE	B	13	<NA>	14.708	24.966	-13.446	1
##	862	ATOM	863	C <NA>	ILE	B	13	<NA>	14.230	24.165	-14.639	1
##	863	ATOM	864	O <NA>	ILE	B	13	<NA>	13.014	24.057	-14.918	1
##	864	ATOM	865	CB <NA>	ILE	B	13	<NA>	14.993	23.953	-12.269	1
##	865	ATOM	866	CG1 <NA>	ILE	B	13	<NA>	13.699	23.190	-11.870	1
##	866	ATOM	867	CG2 <NA>	ILE	B	13	<NA>	15.564	24.705	-11.094	1
##	867	ATOM	868	CD1 <NA>	ILE	B	13	<NA>	13.900	22.077	-10.834	1
##	868	ATOM	869	N <NA>	LYS	B	14	<NA>	15.186	23.630	-15.378	1
##	869	ATOM	870	CA <NA>	LYS	B	14	<NA>	14.828	22.733	-16.464	1
##	870	ATOM	871	C <NA>	LYS	B	14	<NA>	15.482	21.387	-16.141	1
##	871	ATOM	872	O <NA>	LYS	B	14	<NA>	16.690	21.305	-15.886	1
##	872	ATOM	873	CB <NA>	LYS	B	14	<NA>	15.340	23.256	-17.814	1
##	873	ATOM	874	CG <NA>	LYS	B	14	<NA>	14.868	22.447	-18.992	1
##	874	ATOM	875	CD <NA>	LYS	B	14	<NA>	14.687	23.295	-20.194	1
##	875	ATOM	876	CE <NA>	LYS	B	14	<NA>	15.979	23.453	-20.922	1
##	876	ATOM	877	NZ <NA>	LYS	B	14	<NA>	15.739	23.451	-22.389	1
##	877	ATOM	878	N <NA>	ILE	B	15	<NA>	14.660	20.354	-16.136	1
##	878	ATOM	879	CA <NA>	ILE	B	15	<NA>	15.108	18.999	-15.906	1

## 879	ATOM	880	C <NA>	ILE	B	15	<NA>	14.188	18.067	-16.702	1
## 880	ATOM	881	O <NA>	ILE	B	15	<NA>	12.968	18.199	-16.719	1
## 881	ATOM	882	CB <NA>	ILE	B	15	<NA>	15.090	18.663	-14.360	1
## 882	ATOM	883	CG1 <NA>	ILE	B	15	<NA>	15.694	17.283	-14.101	1
## 883	ATOM	884	CG2 <NA>	ILE	B	15	<NA>	13.682	18.760	-13.780	1
## 884	ATOM	885	CD1 <NA>	ILE	B	15	<NA>	16.011	17.036	-12.625	1
## 885	ATOM	886	N <NA>	GLY	B	16	<NA>	14.799	17.159	-17.438	1
## 886	ATOM	887	CA <NA>	GLY	B	16	<NA>	14.024	16.279	-18.286	1
## 887	ATOM	888	C <NA>	GLY	B	16	<NA>	13.311	17.029	-19.391	1
## 888	ATOM	889	O <NA>	GLY	B	16	<NA>	12.318	16.549	-19.924	1
## 889	ATOM	890	N <NA>	GLY	B	17	<NA>	13.887	18.145	-19.823	1
## 890	ATOM	891	CA <NA>	GLY	B	17	<NA>	13.243	18.938	-20.850	1
## 891	ATOM	892	C <NA>	GLY	B	17	<NA>	12.009	19.638	-20.345	1
## 892	ATOM	893	O <NA>	GLY	B	17	<NA>	11.392	20.369	-21.084	1
## 893	ATOM	894	N <NA>	GLN	B	18	<NA>	11.676	19.486	-19.073	1
## 894	ATOM	895	CA <NA>	GLN	B	18	<NA>	10.572	20.249	-18.515	1
## 895	ATOM	896	C <NA>	GLN	B	18	<NA>	11.056	21.466	-17.699	1
## 896	ATOM	897	O <NA>	GLN	B	18	<NA>	12.196	21.494	-17.175	1
## 897	ATOM	898	CB <NA>	GLN	B	18	<NA>	9.708	19.388	-17.619	1
## 898	ATOM	899	CG <NA>	GLN	B	18	<NA>	8.936	18.297	-18.309	1
## 899	ATOM	900	CD <NA>	GLN	B	18	<NA>	9.088	16.973	-17.566	1
## 900	ATOM	901	OE1 <NA>	GLN	B	18	<NA>	9.813	16.078	-18.014	1
## 901	ATOM	902	NE2 <NA>	GLN	B	18	<NA>	8.488	16.884	-16.371	1
## 902	ATOM	903	N <NA>	LEU	B	19	<NA>	10.186	22.475	-17.590	1
## 903	ATOM	904	CA <NA>	LEU	B	19	<NA>	10.450	23.647	-16.749	1
## 904	ATOM	905	C <NA>	LEU	B	19	<NA>	9.631	23.511	-15.483	1
## 905	ATOM	906	O <NA>	LEU	B	19	<NA>	8.432	23.277	-15.551	1
## 906	ATOM	907	CB <NA>	LEU	B	19	<NA>	10.010	24.932	-17.474	1
## 907	ATOM	908	CG <NA>	LEU	B	19	<NA>	10.775	25.419	-18.723	1
## 908	ATOM	909	CD1 <NA>	LEU	B	19	<NA>	10.226	26.727	-19.190	1
## 909	ATOM	910	CD2 <NA>	LEU	B	19	<NA>	12.241	25.543	-18.395	1
## 910	ATOM	911	N <NA>	LYS	B	20	<NA>	10.273	23.619	-14.329	1
## 911	ATOM	912	CA <NA>	LYS	B	20	<NA>	9.576	23.583	-13.044	1
## 912	ATOM	913	C <NA>	LYS	B	20	<NA>	10.018	24.784	-12.260	1
## 913	ATOM	914	O <NA>	LYS	B	20	<NA>	10.998	25.429	-12.605	1
## 914	ATOM	915	CB <NA>	LYS	B	20	<NA>	9.970	22.364	-12.236	1
## 915	ATOM	916	CG <NA>	LYS	B	20	<NA>	10.281	21.123	-13.051	1
## 916	ATOM	917	CD <NA>	LYS	B	20	<NA>	9.037	20.289	-13.305	1
## 917	ATOM	918	CE <NA>	LYS	B	20	<NA>	9.400	18.836	-13.595	1
## 918	ATOM	919	NZ <NA>	LYS	B	20	<NA>	9.672	18.102	-12.328	1
## 919	ATOM	920	N <NA>	GLU	B	21	<NA>	9.324	25.048	-11.162	1
## 920	ATOM	921	CA <NA>	GLU	B	21	<NA>	9.705	26.075	-10.199	1
## 921	ATOM	922	C <NA>	GLU	B	21	<NA>	10.311	25.408	-8.990	1
## 922	ATOM	923	O <NA>	GLU	B	21	<NA>	9.847	24.351	-8.547	1
## 923	ATOM	924	CB <NA>	GLU	B	21	<NA>	8.468	26.848	-9.767	1
## 924	ATOM	925	CG <NA>	GLU	B	21	<NA>	8.676	28.343	-9.687	1
## 925	ATOM	926	CD <NA>	GLU	B	21	<NA>	7.419	29.111	-10.041	1
## 926	ATOM	927	OE1 <NA>	GLU	B	21	<NA>	6.374	28.877	-9.383	1
## 927	ATOM	928	OE2 <NA>	GLU	B	21	<NA>	7.461	29.911	-11.004	1
## 928	ATOM	929	N <NA>	ALA	B	22	<NA>	11.348	26.008	-8.443	1
## 929	ATOM	930	CA <NA>	ALA	B	22	<NA>	12.025	25.431	-7.271	1
## 930	ATOM	931	C <NA>	ALA	B	22	<NA>	12.472	26.569	-6.331	1
## 931	ATOM	932	O <NA>	ALA	B	22	<NA>	12.709	27.701	-6.765	1
## 932	ATOM	933	CB <NA>	ALA	B	22	<NA>	13.248	24.643	-7.708	1

## 933	ATOM	934	N <NA>	LEU	B	23	<NA>	12.560	26.257	-5.054	1
## 934	ATOM	935	CA <NA>	LEU	B	23	<NA>	13.017	27.151	-4.001	1
## 935	ATOM	936	C <NA>	LEU	B	23	<NA>	14.518	27.005	-3.822	1
## 936	ATOM	937	O <NA>	LEU	B	23	<NA>	15.008	25.915	-3.588	1
## 937	ATOM	938	CB <NA>	LEU	B	23	<NA>	12.330	26.721	-2.741	1
## 938	ATOM	939	CG <NA>	LEU	B	23	<NA>	12.592	27.472	-1.469	1
## 939	ATOM	940	CD1 <NA>	LEU	B	23	<NA>	12.006	28.877	-1.562	1
## 940	ATOM	941	CD2 <NA>	LEU	B	23	<NA>	11.917	26.658	-0.379	1
## 941	ATOM	942	N <NA>	LEU	B	24	<NA>	15.266	28.090	-3.963	1
## 942	ATOM	943	CA <NA>	LEU	B	24	<NA>	16.672	28.114	-3.511	1
## 943	ATOM	944	C <NA>	LEU	B	24	<NA>	16.809	28.098	-1.992	1
## 944	ATOM	945	O <NA>	LEU	B	24	<NA>	16.417	29.019	-1.338	1
## 945	ATOM	946	CB <NA>	LEU	B	24	<NA>	17.416	29.342	-4.065	1
## 946	ATOM	947	CG <NA>	LEU	B	24	<NA>	17.444	29.528	-5.585	1
## 947	ATOM	948	CD1 <NA>	LEU	B	24	<NA>	18.151	30.843	-5.884	1
## 948	ATOM	949	CD2 <NA>	LEU	B	24	<NA>	18.170	28.385	-6.270	1
## 949	ATOM	950	N <NA>	ASP	B	25	<NA>	17.407	27.054	-1.437	1
## 950	ATOM	951	CA <NA>	ASP	B	25	<NA>	17.227	26.751	-0.026	1
## 951	ATOM	952	C <NA>	ASP	B	25	<NA>	18.555	26.446	0.653	1
## 952	ATOM	953	O <NA>	ASP	B	25	<NA>	19.003	25.309	0.692	1
## 953	ATOM	954	CB <NA>	ASP	B	25	<NA>	16.258	25.572	0.084	1
## 954	ATOM	955	CG <NA>	ASP	B	25	<NA>	15.759	25.336	1.493	1
## 955	ATOM	956	OD1 <NA>	ASP	B	25	<NA>	16.399	25.780	2.453	1
## 956	ATOM	957	OD2 <NA>	ASP	B	25	<NA>	14.731	24.675	1.645	1
## 957	ATOM	958	N <NA>	THR	B	26	<NA>	19.163	27.455	1.257	1
## 958	ATOM	959	CA <NA>	THR	B	26	<NA>	20.441	27.290	1.920	1
## 959	ATOM	960	C <NA>	THR	B	26	<NA>	20.319	26.393	3.168	1
## 960	ATOM	961	O <NA>	THR	B	26	<NA>	21.316	25.867	3.637	1
## 961	ATOM	962	CB <NA>	THR	B	26	<NA>	21.063	28.678	2.282	1
## 962	ATOM	963	OG1 <NA>	THR	B	26	<NA>	20.188	29.407	3.146	1
## 963	ATOM	964	CG2 <NA>	THR	B	26	<NA>	21.279	29.499	1.024	1
## 964	ATOM	965	N <NA>	GLY	B	27	<NA>	19.106	26.199	3.688	1
## 965	ATOM	966	CA <NA>	GLY	B	27	<NA>	18.957	25.372	4.876	1
## 966	ATOM	967	C <NA>	GLY	B	27	<NA>	18.845	23.903	4.520	1
## 967	ATOM	968	O <NA>	GLY	B	27	<NA>	18.660	23.054	5.417	1
## 968	ATOM	969	N <NA>	ALA	B	28	<NA>	18.819	23.600	3.217	1
## 969	ATOM	970	CA <NA>	ALA	B	28	<NA>	18.721	22.211	2.738	1
## 970	ATOM	971	C <NA>	ALA	B	28	<NA>	20.089	21.661	2.292	1
## 971	ATOM	972	O <NA>	ALA	B	28	<NA>	20.749	22.243	1.403	1
## 972	ATOM	973	CB <NA>	ALA	B	28	<NA>	17.682	22.117	1.578	1
## 973	ATOM	974	N <NA>	ASP	B	29	<NA>	20.536	20.559	2.918	1
## 974	ATOM	975	CA <NA>	ASP	B	29	<NA>	21.779	19.912	2.496	1
## 975	ATOM	976	C <NA>	ASP	B	29	<NA>	21.693	19.374	1.107	1
## 976	ATOM	977	O <NA>	ASP	B	29	<NA>	22.642	19.502	0.361	1
## 977	ATOM	978	CB <NA>	ASP	B	29	<NA>	22.169	18.827	3.447	1
## 978	ATOM	979	CG <NA>	ASP	B	29	<NA>	22.272	19.337	4.844	1
## 979	ATOM	980	OD1 <NA>	ASP	B	29	<NA>	22.714	20.482	5.029	1
## 980	ATOM	981	OD2 <NA>	ASP	B	29	<NA>	21.836	18.647	5.778	1
## 981	ATOM	982	N <NA>	ASP	B	30	<NA>	20.524	18.868	0.719	1
## 982	ATOM	983	CA <NA>	ASP	B	30	<NA>	20.355	18.227	-0.584	1
## 983	ATOM	984	C <NA>	ASP	B	30	<NA>	19.212	18.807	-1.371	1
## 984	ATOM	985	O <NA>	ASP	B	30	<NA>	18.383	19.523	-0.846	1
## 985	ATOM	986	CB <NA>	ASP	B	30	<NA>	20.084	16.745	-0.413	1
## 986	ATOM	987	CG <NA>	ASP	B	30	<NA>	21.023	16.088	0.586	1

## 987	ATOM	988	OD1 <NA>	ASP	B	30	<NA>	22.233	15.970	0.265	1
## 988	ATOM	989	OD2 <NA>	ASP	B	30	<NA>	20.531	15.682	1.672	1
## 989	ATOM	990	N <NA>	THR	B	31	<NA>	19.152	18.428	-2.643	1
## 990	ATOM	991	CA <NA>	THR	B	31	<NA>	18.113	18.843	-3.603	1
## 991	ATOM	992	C <NA>	THR	B	31	<NA>	17.019	17.743	-3.682	1
## 992	ATOM	993	O <NA>	THR	B	31	<NA>	17.342	16.586	-3.904	1
## 993	ATOM	994	CB <NA>	THR	B	31	<NA>	18.810	19.051	-4.967	1
## 994	ATOM	995	OG1 <NA>	THR	B	31	<NA>	19.740	20.123	-4.831	1
## 995	ATOM	996	CG2 <NA>	THR	B	31	<NA>	17.844	19.330	-6.078	1
## 996	ATOM	997	N <NA>	VAL	B	32	<NA>	15.750	18.102	-3.440	1
## 997	ATOM	998	CA <NA>	VAL	B	32	<NA>	14.628	17.162	-3.514	1
## 998	ATOM	999	C <NA>	VAL	B	32	<NA>	13.618	17.726	-4.436	1
## 999	ATOM	1000	O <NA>	VAL	B	32	<NA>	13.169	18.861	-4.263	1
## 1000	ATOM	1001	CB <NA>	VAL	B	32	<NA>	13.781	17.005	-2.245	1
## 1001	ATOM	1002	CG1 <NA>	VAL	B	32	<NA>	13.297	15.592	-2.184	1
## 1002	ATOM	1003	CG2 <NA>	VAL	B	32	<NA>	14.518	17.455	-1.007	1
## 1003	ATOM	1004	N <NA>	LEU	B	33	<NA>	13.199	16.926	-5.401	1
## 1004	ATOM	1005	CA <NA>	LEU	B	33	<NA>	12.141	17.335	-6.327	1
## 1005	ATOM	1006	C <NA>	LEU	B	33	<NA>	10.876	16.500	-6.065	1
## 1006	ATOM	1007	O <NA>	LEU	B	33	<NA>	10.948	15.389	-5.534	1
## 1007	ATOM	1008	CB <NA>	LEU	B	33	<NA>	12.618	17.139	-7.766	1
## 1008	ATOM	1009	CG <NA>	LEU	B	33	<NA>	13.889	17.846	-8.247	1
## 1009	ATOM	1010	CD1 <NA>	LEU	B	33	<NA>	13.942	17.794	-9.731	1
## 1010	ATOM	1011	CD2 <NA>	LEU	B	33	<NA>	13.897	19.266	-7.782	1
## 1011	ATOM	1012	N <NA>	GLU	B	34	<NA>	9.719	17.083	-6.361	1
## 1012	ATOM	1013	CA <NA>	GLU	B	34	<NA>	8.442	16.392	-6.346	1
## 1013	ATOM	1014	C <NA>	GLU	B	34	<NA>	8.514	15.172	-7.224	1
## 1014	ATOM	1015	O <NA>	GLU	B	34	<NA>	9.413	15.013	-8.040	1
## 1015	ATOM	1016	CB <NA>	GLU	B	34	<NA>	7.316	17.305	-6.819	1
## 1016	ATOM	1017	CG <NA>	GLU	B	34	<NA>	6.914	18.362	-5.808	1
## 1017	ATOM	1018	CD <NA>	GLU	B	34	<NA>	6.205	19.552	-6.439	1
## 1018	ATOM	1019	OE1 <NA>	GLU	B	34	<NA>	6.323	19.742	-7.666	1
## 1019	ATOM	1020	OE2 <NA>	GLU	B	34	<NA>	5.613	20.369	-5.715	1
## 1020	ATOM	1021	N <NA>	GLU	B	35	<NA>	7.526	14.309	-7.044	1
## 1021	ATOM	1022	CA <NA>	GLU	B	35	<NA>	7.425	13.006	-7.682	1
## 1022	ATOM	1023	C <NA>	GLU	B	35	<NA>	7.528	13.141	-9.172	1
## 1023	ATOM	1024	O <NA>	GLU	B	35	<NA>	6.660	13.711	-9.819	1
## 1024	ATOM	1025	CB <NA>	GLU	B	35	<NA>	6.100	12.361	-7.297	1
## 1025	ATOM	1026	CG <NA>	GLU	B	35	<NA>	5.907	10.953	-7.838	1
## 1026	ATOM	1027	CD <NA>	GLU	B	35	<NA>	7.182	10.093	-7.854	1
## 1027	ATOM	1028	OE1 <NA>	GLU	B	35	<NA>	7.743	9.853	-6.766	1
## 1028	ATOM	1029	OE2 <NA>	GLU	B	35	<NA>	7.521	9.561	-8.946	1
## 1029	ATOM	1030	N <NA>	MET	B	36	<NA>	8.627	12.651	-9.705	1
## 1030	ATOM	1031	CA <NA>	MET	B	36	<NA>	8.791	12.578	-11.145	1
## 1031	ATOM	1032	C <NA>	MET	B	36	<NA>	9.583	11.322	-11.483	1
## 1032	ATOM	1033	O <NA>	MET	B	36	<NA>	10.100	10.637	-10.616	1
## 1033	ATOM	1034	CB <NA>	MET	B	36	<NA>	9.546	13.808	-11.654	1
## 1034	ATOM	1035	CG <NA>	MET	B	36	<NA>	10.867	14.095	-11.014	1
## 1035	ATOM	1036	SD <NA>	MET	B	36	<NA>	11.575	15.547	-11.778	1
## 1036	ATOM	1037	CE <NA>	MET	B	36	<NA>	11.710	15.108	-13.551	1
## 1037	ATOM	1038	N <NA>	SER	B	37	<NA>	9.657	11.016	-12.763	1
## 1038	ATOM	1039	CA <NA>	SER	B	37	<NA>	10.411	9.858	-13.218	1
## 1039	ATOM	1040	C <NA>	SER	B	37	<NA>	11.673	10.374	-13.825	1
## 1040	ATOM	1041	O <NA>	SER	B	37	<NA>	11.636	11.272	-14.685	1

##	1041	ATOM	1042	CB <NA>	SER	B	37	<NA>	9.573	9.049	-14.221	1
##	1042	ATOM	1043	OG <NA>	SER	B	37	<NA>	8.330	8.594	-13.579	1
##	1043	ATOM	1044	N <NA>	LEU	B	38	<NA>	12.793	9.884	-13.330	1
##	1044	ATOM	1045	CA <NA>	LEU	B	38	<NA>	14.091	10.261	-13.857	1
##	1045	ATOM	1046	C <NA>	LEU	B	38	<NA>	14.818	9.018	-14.330	1
##	1046	ATOM	1047	O <NA>	LEU	B	38	<NA>	14.416	7.898	-13.995	1
##	1047	ATOM	1048	CB <NA>	LEU	B	38	<NA>	14.866	10.942	-12.759	1
##	1048	ATOM	1049	CG <NA>	LEU	B	38	<NA>	14.480	12.376	-12.556	1
##	1049	ATOM	1050	CD1 <NA>	LEU	B	38	<NA>	15.159	12.900	-11.300	1
##	1050	ATOM	1051	CD2 <NA>	LEU	B	38	<NA>	14.955	13.131	-13.766	1
##	1051	ATOM	1052	N <NA>	PRO	B	39	<NA>	15.767	9.161	-15.261	1
##	1052	ATOM	1053	CA <NA>	PRO	B	39	<NA>	16.525	8.031	-15.798	1
##	1053	ATOM	1054	C <NA>	PRO	B	39	<NA>	17.366	7.241	-14.777	1
##	1054	ATOM	1055	O <NA>	PRO	B	39	<NA>	17.943	7.817	-13.847	1
##	1055	ATOM	1056	CB <NA>	PRO	B	39	<NA>	17.407	8.673	-16.857	1
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##	1057	ATOM	1058	CD <NA>	PRO	B	39	<NA>	16.150	10.405	-15.968	1
##	1058	ATOM	1059	N <NA>	GLY	B	40	<NA>	17.477	5.932	-14.999	1
##	1059	ATOM	1060	CA <NA>	GLY	B	40	<NA>	18.494	5.171	-14.302	1
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##	1061	ATOM	1062	O <NA>	GLY	B	40	<NA>	16.865	4.438	-12.729	1
##	1062	ATOM	1063	N <NA>	ARG	B	41	<NA>	19.000	3.939	-12.313	1
##	1063	ATOM	1064	CA <NA>	ARG	B	41	<NA>	18.722	3.282	-11.042	1
##	1064	ATOM	1065	C <NA>	ARG	B	41	<NA>	18.615	4.306	-9.916	1
##	1065	ATOM	1066	O <NA>	ARG	B	41	<NA>	19.168	5.390	-10.018	1
##	1066	ATOM	1067	CB <NA>	ARG	B	41	<NA>	19.852	2.333	-10.662	1
##	1067	ATOM	1068	CG <NA>	ARG	B	41	<NA>	20.359	1.417	-11.726	1
##	1068	ATOM	1069	CD <NA>	ARG	B	41	<NA>	20.905	0.188	-11.023	1
##	1069	ATOM	1070	NE <NA>	ARG	B	41	<NA>	19.927	-0.864	-11.169	1
##	1070	ATOM	1071	CZ <NA>	ARG	B	41	<NA>	19.354	-1.538	-10.177	1
##	1071	ATOM	1072	NH1 <NA>	ARG	B	41	<NA>	19.839	-1.513	-8.939	1
##	1072	ATOM	1073	NH2 <NA>	ARG	B	41	<NA>	18.333	-2.314	-10.472	1
##	1073	ATOM	1074	N <NA>	TRP	B	42	<NA>	17.989	3.918	-8.810	1
##	1074	ATOM	1075	CA <NA>	TRP	B	42	<NA>	17.920	4.766	-7.634	1
##	1075	ATOM	1076	C <NA>	TRP	B	42	<NA>	18.295	3.969	-6.380	1
##	1076	ATOM	1077	O <NA>	TRP	B	42	<NA>	18.163	2.742	-6.361	1
##	1077	ATOM	1078	CB <NA>	TRP	B	42	<NA>	16.525	5.338	-7.459	1
##	1078	ATOM	1079	CG <NA>	TRP	B	42	<NA>	15.444	4.372	-7.312	1
##	1079	ATOM	1080	CD1 <NA>	TRP	B	42	<NA>	14.681	3.834	-8.299	1
##	1080	ATOM	1081	CD2 <NA>	TRP	B	42	<NA>	14.840	3.957	-6.079	1
##	1081	ATOM	1082	NE1 <NA>	TRP	B	42	<NA>	13.640	3.121	-7.756	1
##	1082	ATOM	1083	CE2 <NA>	TRP	B	42	<NA>	13.719	3.166	-6.402	1
##	1083	ATOM	1084	CE3 <NA>	TRP	B	42	<NA>	15.154	4.180	-4.715	1
##	1084	ATOM	1085	CZ2 <NA>	TRP	B	42	<NA>	12.881	2.589	-5.411	1
##	1085	ATOM	1086	CZ3 <NA>	TRP	B	42	<NA>	14.300	3.625	-3.745	1
##	1086	ATOM	1087	CH2 <NA>	TRP	B	42	<NA>	13.168	2.842	-4.106	1
##	1087	ATOM	1088	N <NA>	LYS	B	43	<NA>	18.801	4.689	-5.365	1
##	1088	ATOM	1089	CA <NA>	LYS	B	43	<NA>	19.180	4.182	-4.032	1
##	1089	ATOM	1090	C <NA>	LYS	B	43	<NA>	18.127	4.736	-3.089	1
##	1090	ATOM	1091	O <NA>	LYS	B	43	<NA>	17.442	5.729	-3.400	1
##	1091	ATOM	1092	CB <NA>	LYS	B	43	<NA>	20.561	4.731	-3.581	1
##	1092	ATOM	1093	CG <NA>	LYS	B	43	<NA>	21.777	4.400	-4.445	1
##	1093	ATOM	1094	CD <NA>	LYS	B	43	<NA>	22.996	5.295	-4.048	1
##	1094	ATOM	1095	CE <NA>	LYS	B	43	<NA>	24.193	5.280	-5.063	1

##	1095	ATOM	1096	NZ <NA>	LYS	B	43	<NA>	25.251	6.324	-4.725	1
##	1096	ATOM	1097	N <NA>	PRO	B	44	<NA>	18.053	4.208	-1.878	1
##	1097	ATOM	1098	CA <NA>	PRO	B	44	<NA>	17.102	4.804	-0.946	1
##	1098	ATOM	1099	C <NA>	PRO	B	44	<NA>	17.754	5.853	-0.023	1
##	1099	ATOM	1100	O <NA>	PRO	B	44	<NA>	18.929	5.769	0.330	1
##	1100	ATOM	1101	CB <NA>	PRO	B	44	<NA>	16.596	3.610	-0.171	1
##	1101	ATOM	1102	CG <NA>	PRO	B	44	<NA>	17.803	2.676	-0.117	1
##	1102	ATOM	1103	CD <NA>	PRO	B	44	<NA>	18.649	2.962	-1.335	1
##	1103	ATOM	1104	N <NA>	LYS	B	45	<NA>	16.974	6.847	0.381	1
##	1104	ATOM	1105	CA <NA>	LYS	B	45	<NA>	17.443	7.812	1.371	1
##	1105	ATOM	1106	C <NA>	LYS	B	45	<NA>	16.334	8.328	2.257	1
##	1106	ATOM	1107	O <NA>	LYS	B	45	<NA>	15.192	8.470	1.828	1
##	1107	ATOM	1108	CB <NA>	LYS	B	45	<NA>	18.177	8.988	0.701	1
##	1108	ATOM	1109	CG <NA>	LYS	B	45	<NA>	19.183	9.659	1.670	1
##	1109	ATOM	1110	CD <NA>	LYS	B	45	<NA>	20.095	10.640	1.011	1
##	1110	ATOM	1111	CE <NA>	LYS	B	45	<NA>	20.751	11.491	2.069	1
##	1111	ATOM	1112	NZ <NA>	LYS	B	45	<NA>	21.413	12.705	1.509	1
##	1112	ATOM	1113	N <NA>	MET	B	46	<NA>	16.672	8.585	3.514	1
##	1113	ATOM	1114	CA <NA>	MET	B	46	<NA>	15.755	9.281	4.404	1
##	1114	ATOM	1115	C <NA>	MET	B	46	<NA>	16.373	10.584	4.732	1
##	1115	ATOM	1116	O <NA>	MET	B	46	<NA>	17.542	10.636	5.104	1
##	1116	ATOM	1117	CB <NA>	MET	B	46	<NA>	15.562	8.530	5.708	1
##	1117	ATOM	1118	CG <NA>	MET	B	46	<NA>	14.763	7.266	5.540	1
##	1118	ATOM	1119	SD <NA>	MET	B	46	<NA>	13.357	7.367	6.566	1
##	1119	ATOM	1120	CE <NA>	MET	B	46	<NA>	14.146	6.922	8.167	1
##	1120	ATOM	1121	N <NA>	ILE	B	47	<NA>	15.582	11.636	4.604	1
##	1121	ATOM	1122	CA <NA>	ILE	B	47	<NA>	16.003	12.986	4.955	1
##	1122	ATOM	1123	C <NA>	ILE	B	47	<NA>	15.018	13.507	5.961	1
##	1123	ATOM	1124	O <NA>	ILE	B	47	<NA>	13.822	13.222	5.884	1
##	1124	ATOM	1125	CB <NA>	ILE	B	47	<NA>	16.040	13.915	3.699	1
##	1125	ATOM	1126	CG1 <NA>	ILE	B	47	<NA>	14.745	13.761	2.918	1
##	1126	ATOM	1127	CG2 <NA>	ILE	B	47	<NA>	17.229	13.534	2.782	1
##	1127	ATOM	1128	CD1 <NA>	ILE	B	47	<NA>	14.742	14.561	1.698	1
##	1128	ATOM	1129	N <NA>	GLY	B	48	<NA>	15.542	14.239	6.941	1
##	1129	ATOM	1130	CA <NA>	GLY	B	48	<NA>	14.714	14.799	8.014	1
##	1130	ATOM	1131	C <NA>	GLY	B	48	<NA>	14.762	16.314	8.114	1
##	1131	ATOM	1132	O <NA>	GLY	B	48	<NA>	15.803	16.952	7.888	1
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##	1134	ATOM	1135	C <NA>	GLY	B	49	<NA>	12.647	18.565	9.672	1
##	1135	ATOM	1136	O <NA>	GLY	B	49	<NA>	12.880	17.976	10.721	1
##	1136	ATOM	1137	N <NA>	ILE	B	50	<NA>	11.850	19.611	9.584	1
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##	1138	ATOM	1139	C <NA>	ILE	B	50	<NA>	9.707	18.988	10.393	1
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##	1141	ATOM	1142	CG1 <NA>	ILE	B	50	<NA>	11.556	22.421	10.394	1
##	1142	ATOM	1143	CG2 <NA>	ILE	B	50	<NA>	9.299	21.862	11.270	1
##	1143	ATOM	1144	CD1 <NA>	ILE	B	50	<NA>	11.936	22.850	11.773	1
##	1144	ATOM	1145	N <NA>	GLY	B	51	<NA>	9.164	18.455	11.474	1
##	1145	ATOM	1146	CA <NA>	GLY	B	51	<NA>	8.011	17.583	11.313	1
##	1146	ATOM	1147	C <NA>	GLY	B	51	<NA>	8.360	16.130	11.054	1
##	1147	ATOM	1148	O <NA>	GLY	B	51	<NA>	7.494	15.283	11.167	1
##	1148	ATOM	1149	N <NA>	GLY	B	52	<NA>	9.638	15.842	10.818	1

##	1149	ATOM	1150	CA <NA>	GLY	B	52	<NA>	10.123	14.474	10.792	1
##	1150	ATOM	1151	C <NA>	GLY	B	52	<NA>	10.860	14.080	9.524	1
##	1151	ATOM	1152	O <NA>	GLY	B	52	<NA>	11.419	14.930	8.826	1
##	1152	ATOM	1153	N <NA>	PHE	B	53	<NA>	10.878	12.788	9.221	1
##	1153	ATOM	1154	CA <NA>	PHE	B	53	<NA>	11.638	12.302	8.079	1
##	1154	ATOM	1155	C <NA>	PHE	B	53	<NA>	10.739	11.914	6.924	1
##	1155	ATOM	1156	O <NA>	PHE	B	53	<NA>	9.601	11.543	7.137	1
##	1156	ATOM	1157	CB <NA>	PHE	B	53	<NA>	12.458	11.126	8.531	1
##	1157	ATOM	1158	CG <NA>	PHE	B	53	<NA>	13.464	11.471	9.564	1
##	1158	ATOM	1159	CD1 <NA>	PHE	B	53	<NA>	13.092	11.697	10.886	1
##	1159	ATOM	1160	CD2 <NA>	PHE	B	53	<NA>	14.789	11.625	9.189	1
##	1160	ATOM	1161	CE1 <NA>	PHE	B	53	<NA>	14.036	12.076	11.825	1
##	1161	ATOM	1162	CE2 <NA>	PHE	B	53	<NA>	15.753	12.001	10.078	1
##	1162	ATOM	1163	CZ <NA>	PHE	B	53	<NA>	15.392	12.225	11.421	1
##	1163	ATOM	1164	N <NA>	ILE	B	54	<NA>	11.204	12.078	5.695	1
##	1164	ATOM	1165	CA <NA>	ILE	B	54	<NA>	10.538	11.431	4.563	1
##	1165	ATOM	1166	C <NA>	ILE	B	54	<NA>	11.513	10.453	3.866	1
##	1166	ATOM	1167	O <NA>	ILE	B	54	<NA>	12.727	10.529	4.052	1
##	1167	ATOM	1168	CB <NA>	ILE	B	54	<NA>	9.923	12.446	3.500	1
##	1168	ATOM	1169	CG1 <NA>	ILE	B	54	<NA>	10.968	13.414	2.964	1
##	1169	ATOM	1170	CG2 <NA>	ILE	B	54	<NA>	8.754	13.195	4.090	1
##	1170	ATOM	1171	CD1 <NA>	ILE	B	54	<NA>	10.571	14.020	1.616	1
##	1171	ATOM	1172	N <NA>	LYS	B	55	<NA>	10.983	9.503	3.111	1
##	1172	ATOM	1173	CA <NA>	LYS	B	55	<NA>	11.816	8.478	2.482	1
##	1173	ATOM	1174	C <NA>	LYS	B	55	<NA>	11.862	8.988	1.074	1
##	1174	ATOM	1175	O <NA>	LYS	B	55	<NA>	10.827	9.256	0.525	1
##	1175	ATOM	1176	CB <NA>	LYS	B	55	<NA>	11.062	7.136	2.489	1
##	1176	ATOM	1177	CG <NA>	LYS	B	55	<NA>	11.699	5.963	3.273	1
##	1177	ATOM	1178	CD <NA>	LYS	B	55	<NA>	13.070	5.502	2.689	1
##	1178	ATOM	1179	CE <NA>	LYS	B	55	<NA>	12.949	4.923	1.253	1
##	1179	ATOM	1180	NZ <NA>	LYS	B	55	<NA>	13.964	5.445	0.291	1
##	1180	ATOM	1181	N <NA>	VAL	B	56	<NA>	13.024	9.137	0.474	1
##	1181	ATOM	1182	CA <NA>	VAL	B	56	<NA>	13.072	9.652	-0.897	1
##	1182	ATOM	1183	C <NA>	VAL	B	56	<NA>	13.885	8.719	-1.786	1
##	1183	ATOM	1184	O <NA>	VAL	B	56	<NA>	14.547	7.817	-1.279	1
##	1184	ATOM	1185	CB <NA>	VAL	B	56	<NA>	13.757	11.033	-0.959	1
##	1185	ATOM	1186	CG1 <NA>	VAL	B	56	<NA>	12.766	12.134	-0.523	1
##	1186	ATOM	1187	CG2 <NA>	VAL	B	56	<NA>	15.032	11.016	-0.119	1
##	1187	ATOM	1188	N <NA>	ARG	B	57	<NA>	13.889	8.977	-3.102	1
##	1188	ATOM	1189	CA <NA>	ARG	B	57	<NA>	14.697	8.220	-4.083	1
##	1189	ATOM	1190	C <NA>	ARG	B	57	<NA>	15.894	9.023	-4.591	1
##	1190	ATOM	1191	O <NA>	ARG	B	57	<NA>	15.735	10.066	-5.210	1
##	1191	ATOM	1192	CB <NA>	ARG	B	57	<NA>	13.862	7.854	-5.298	1
##	1192	ATOM	1193	CG <NA>	ARG	B	57	<NA>	12.767	6.845	-5.041	1
##	1193	ATOM	1194	CD <NA>	ARG	B	57	<NA>	12.224	6.316	-6.354	1
##	1194	ATOM	1195	NE <NA>	ARG	B	57	<NA>	10.944	6.937	-6.617	1
##	1195	ATOM	1196	CZ <NA>	ARG	B	57	<NA>	10.717	7.776	-7.614	1
##	1196	ATOM	1197	NH1 <NA>	ARG	B	57	<NA>	11.534	7.792	-8.658	1
##	1197	ATOM	1198	NH2 <NA>	ARG	B	57	<NA>	9.555	8.403	-7.678	1
##	1198	ATOM	1199	N <NA>	GLN	B	58	<NA>	17.095	8.516	-4.388	1
##	1199	ATOM	1200	CA <NA>	GLN	B	58	<NA>	18.306	9.218	-4.819	1
##	1200	ATOM	1201	C <NA>	GLN	B	58	<NA>	18.742	8.833	-6.226	1
##	1201	ATOM	1202	O <NA>	GLN	B	58	<NA>	19.157	7.694	-6.438	1
##	1202	ATOM	1203	CB <NA>	GLN	B	58	<NA>	19.465	8.920	-3.861	1

##	1203	ATOM	1204	CG <NA>	GLN	B	58	<NA>	20.738	9.622	-4.271	1
##	1204	ATOM	1205	CD <NA>	GLN	B	58	<NA>	21.825	9.463	-3.248	1
##	1205	ATOM	1206	OE1 <NA>	GLN	B	58	<NA>	21.554	9.424	-2.048	1
##	1206	ATOM	1207	NE2 <NA>	GLN	B	58	<NA>	23.045	9.365	-3.692	1
##	1207	ATOM	1208	N <NA>	TYR	B	59	<NA>	18.705	9.773	-7.167	1
##	1208	ATOM	1209	CA <NA>	TYR	B	59	<NA>	19.361	9.587	-8.464	1
##	1209	ATOM	1210	C <NA>	TYR	B	59	<NA>	20.689	10.330	-8.544	1
##	1210	ATOM	1211	O <NA>	TYR	B	59	<NA>	20.860	11.368	-7.943	1
##	1211	ATOM	1212	CB <NA>	TYR	B	59	<NA>	18.472	10.082	-9.563	1
##	1212	ATOM	1213	CG <NA>	TYR	B	59	<NA>	17.116	9.383	-9.609	1
##	1213	ATOM	1214	CD1 <NA>	TYR	B	59	<NA>	16.157	9.612	-8.615	1
##	1214	ATOM	1215	CD2 <NA>	TYR	B	59	<NA>	16.814	8.484	-10.637	1
##	1215	ATOM	1216	CE1 <NA>	TYR	B	59	<NA>	14.959	8.977	-8.640	1
##	1216	ATOM	1217	CE2 <NA>	TYR	B	59	<NA>	15.647	7.851	-10.673	1
##	1217	ATOM	1218	CZ <NA>	TYR	B	59	<NA>	14.704	8.066	-9.679	1
##	1218	ATOM	1219	OH <NA>	TYR	B	59	<NA>	13.561	7.307	-9.711	1
##	1219	ATOM	1220	N <NA>	ASP	B	60	<NA>	21.665	9.797	-9.258	1
##	1220	ATOM	1221	CA <NA>	ASP	B	60	<NA>	22.959	10.470	-9.336	1
##	1221	ATOM	1222	C <NA>	ASP	B	60	<NA>	23.303	10.921	-10.737	1
##	1222	ATOM	1223	O <NA>	ASP	B	60	<NA>	22.793	10.396	-11.707	1
##	1223	ATOM	1224	CB <NA>	ASP	B	60	<NA>	24.042	9.554	-8.834	1
##	1224	ATOM	1225	CG <NA>	ASP	B	60	<NA>	23.843	9.184	-7.407	1
##	1225	ATOM	1226	OD1 <NA>	ASP	B	60	<NA>	23.463	10.074	-6.620	1
##	1226	ATOM	1227	OD2 <NA>	ASP	B	60	<NA>	24.107	8.012	-7.044	1
##	1227	ATOM	1228	N <NA>	GLN	B	61	<NA>	24.189	11.897	-10.837	1
##	1228	ATOM	1229	CA <NA>	GLN	B	61	<NA>	24.622	12.478	-12.111	1
##	1229	ATOM	1230	C <NA>	GLN	B	61	<NA>	23.474	12.903	-13.022	1
##	1230	ATOM	1231	O <NA>	GLN	B	61	<NA>	23.492	12.665	-14.229	1
##	1231	ATOM	1232	CB <NA>	GLN	B	61	<NA>	25.596	11.549	-12.869	1
##	1232	ATOM	1233	CG <NA>	GLN	B	61	<NA>	26.892	12.283	-13.369	1
##	1233	ATOM	1234	CD <NA>	GLN	B	61	<NA>	28.007	11.392	-13.985	1
##	1234	ATOM	1235	OE1 <NA>	GLN	B	61	<NA>	28.747	11.845	-14.875	1
##	1235	ATOM	1236	NE2 <NA>	GLN	B	61	<NA>	28.197	10.173	-13.442	1
##	1236	ATOM	1237	N <NA>	ILE	B	62	<NA>	22.493	13.589	-12.452	1
##	1237	ATOM	1238	CA <NA>	ILE	B	62	<NA>	21.380	14.141	-13.224	1
##	1238	ATOM	1239	C <NA>	ILE	B	62	<NA>	21.710	15.575	-13.686	1
##	1239	ATOM	1240	O <NA>	ILE	B	62	<NA>	22.247	16.373	-12.924	1
##	1240	ATOM	1241	CB <NA>	ILE	B	62	<NA>	20.090	14.147	-12.331	1
##	1241	ATOM	1242	CG1 <NA>	ILE	B	62	<NA>	19.709	12.702	-11.952	1
##	1242	ATOM	1243	CG2 <NA>	ILE	B	62	<NA>	18.950	14.826	-13.045	1
##	1243	ATOM	1244	CD1 <NA>	ILE	B	62	<NA>	19.068	11.933	-13.057	1
##	1244	ATOM	1245	N <NA>	LEU	B	63	<NA>	21.400	15.900	-14.931	1
##	1245	ATOM	1246	CA <NA>	LEU	B	63	<NA>	21.600	17.263	-15.431	1
##	1246	ATOM	1247	C <NA>	LEU	B	63	<NA>	20.386	18.085	-15.052	1
##	1247	ATOM	1248	O <NA>	LEU	B	63	<NA>	19.260	17.703	-15.355	1
##	1248	ATOM	1249	CB <NA>	LEU	B	63	<NA>	21.769	17.265	-16.962	1
##	1249	ATOM	1250	CG <NA>	LEU	B	63	<NA>	21.792	18.587	-17.759	1
##	1250	ATOM	1251	CD1 <NA>	LEU	B	63	<NA>	22.903	19.529	-17.300	1
##	1251	ATOM	1252	CD2 <NA>	LEU	B	63	<NA>	21.997	18.246	-19.205	1
##	1252	ATOM	1253	N <NA>	ILE	B	64	<NA>	20.626	19.203	-14.381	1
##	1253	ATOM	1254	CA <NA>	ILE	B	64	<NA>	19.548	20.111	-14.029	1
##	1254	ATOM	1255	C <NA>	ILE	B	64	<NA>	20.089	21.523	-14.223	1
##	1255	ATOM	1256	O <NA>	ILE	B	64	<NA>	21.175	21.858	-13.763	1
##	1256	ATOM	1257	CB <NA>	ILE	B	64	<NA>	19.107	19.880	-12.540	1

##	1257	ATOM	1258	CG1 <NA>	ILE	B	64	<NA>	18.216	20.990	-12.036	1
##	1258	ATOM	1259	CG2 <NA>	ILE	B	64	<NA>	20.311	19.766	-11.655	1
##	1259	ATOM	1260	CD1 <NA>	ILE	B	64	<NA>	17.324	20.544	-10.930	1
##	1260	ATOM	1261	N <NA>	GLU	B	65	<NA>	19.327	22.330	-14.953	1
##	1261	ATOM	1262	CA <NA>	GLU	B	65	<NA>	19.661	23.719	-15.251	1
##	1262	ATOM	1263	C <NA>	GLU	B	65	<NA>	18.938	24.686	-14.338	1
##	1263	ATOM	1264	O <NA>	GLU	B	65	<NA>	17.700	24.745	-14.345	1
##	1264	ATOM	1265	CB <NA>	GLU	B	65	<NA>	19.282	24.017	-16.688	1
##	1265	ATOM	1266	CG <NA>	GLU	B	65	<NA>	20.180	25.011	-17.326	1
##	1266	ATOM	1267	CD <NA>	GLU	B	65	<NA>	19.960	25.126	-18.805	1
##	1267	ATOM	1268	OE1 <NA>	GLU	B	65	<NA>	19.601	24.094	-19.445	1
##	1268	ATOM	1269	OE2 <NA>	GLU	B	65	<NA>	20.214	26.241	-19.314	1
##	1269	ATOM	1270	N <NA>	ILE	B	66	<NA>	19.709	25.427	-13.547	1
##	1270	ATOM	1271	CA <NA>	ILE	B	66	<NA>	19.159	26.431	-12.654	1
##	1271	ATOM	1272	C <NA>	ILE	B	66	<NA>	19.519	27.864	-13.127	1
##	1272	ATOM	1273	O <NA>	ILE	B	66	<NA>	20.684	28.254	-13.167	1
##	1273	ATOM	1274	CB <NA>	ILE	B	66	<NA>	19.663	26.199	-11.203	1
##	1274	ATOM	1275	CG1 <NA>	ILE	B	66	<NA>	19.566	24.717	-10.848	1
##	1275	ATOM	1276	CG2 <NA>	ILE	B	66	<NA>	18.824	27.018	-10.232	1
##	1276	ATOM	1277	CD1 <NA>	ILE	B	66	<NA>	20.510	24.280	-9.745	1
##	1277	ATOM	1278	N <NA>	CYS	B	67	<NA>	18.504	28.630	-13.516	1
##	1278	ATOM	1279	CA <NA>	CYS	B	67	<NA>	18.684	29.971	-14.104	1
##	1279	ATOM	1280	C <NA>	CYS	B	67	<NA>	19.685	29.990	-15.245	1
##	1280	ATOM	1281	O <NA>	CYS	B	67	<NA>	20.565	30.852	-15.294	1
##	1281	ATOM	1282	CB <NA>	CYS	B	67	<NA>	19.124	30.970	-13.037	1
##	1282	ATOM	1283	SG <NA>	CYS	B	67	<NA>	17.736	31.542	-12.037	1
##	1283	ATOM	1284	N <NA>	GLY	B	68	<NA>	19.562	29.010	-16.143	1
##	1284	ATOM	1285	CA <NA>	GLY	B	68	<NA>	20.485	28.891	-17.256	1
##	1285	ATOM	1286	C <NA>	GLY	B	68	<NA>	21.899	28.603	-16.811	1
##	1286	ATOM	1287	O <NA>	GLY	B	68	<NA>	22.843	28.970	-17.493	1
##	1287	ATOM	1288	N <NA>	HIS	B	69	<NA>	22.059	28.002	-15.633	1
##	1288	ATOM	1289	CA <NA>	HIS	B	69	<NA>	23.354	27.479	-15.197	1
##	1289	ATOM	1290	C <NA>	HIS	B	69	<NA>	23.178	25.984	-15.087	1
##	1290	ATOM	1291	O <NA>	HIS	B	69	<NA>	22.307	25.523	-14.354	1
##	1291	ATOM	1292	CB <NA>	HIS	B	69	<NA>	23.711	27.993	-13.810	1
##	1292	ATOM	1293	CG <NA>	HIS	B	69	<NA>	23.976	29.473	-13.740	1
##	1293	ATOM	1294	ND1 <NA>	HIS	B	69	<NA>	25.177	29.994	-13.361	1
##	1294	ATOM	1295	CD2 <NA>	HIS	B	69	<NA>	23.114	30.512	-13.920	1
##	1295	ATOM	1296	CE1 <NA>	HIS	B	69	<NA>	25.058	31.325	-13.286	1
##	1296	ATOM	1297	NE2 <NA>	HIS	B	69	<NA>	23.849	31.652	-13.613	1
##	1297	ATOM	1298	N <NA>	LYS	B	70	<NA>	23.995	25.240	-15.820	1
##	1298	ATOM	1299	CA <NA>	LYS	B	70	<NA>	23.935	23.791	-15.800	1
##	1299	ATOM	1300	C <NA>	LYS	B	70	<NA>	24.749	23.243	-14.652	1
##	1300	ATOM	1301	O <NA>	LYS	B	70	<NA>	25.875	23.676	-14.403	1
##	1301	ATOM	1302	CB <NA>	LYS	B	70	<NA>	24.423	23.212	-17.115	1
##	1302	ATOM	1303	CG <NA>	LYS	B	70	<NA>	23.463	23.445	-18.279	1
##	1303	ATOM	1304	CD <NA>	LYS	B	70	<NA>	24.261	23.524	-19.576	1
##	1304	ATOM	1305	CE <NA>	LYS	B	70	<NA>	23.377	23.737	-20.816	1
##	1305	ATOM	1306	NZ <NA>	LYS	B	70	<NA>	22.863	22.443	-21.404	1
##	1306	ATOM	1307	N <NA>	ALA	B	71	<NA>	24.104	22.353	-13.909	1
##	1307	ATOM	1308	CA <NA>	ALA	B	71	<NA>	24.689	21.612	-12.802	1
##	1308	ATOM	1309	C <NA>	ALA	B	71	<NA>	24.391	20.156	-13.159	1
##	1309	ATOM	1310	O <NA>	ALA	B	71	<NA>	23.339	19.865	-13.735	1
##	1310	ATOM	1311	CB <NA>	ALA	B	71	<NA>	23.991	21.992	-11.485	1

##	1311	ATOM	1312	N <NA>	ILE	B	72	<NA>	25.330	19.253	-12.902	1
##	1312	ATOM	1313	CA <NA>	ILE	B	72	<NA>	25.048	17.816	-13.016	1
##	1313	ATOM	1314	C <NA>	ILE	B	72	<NA>	25.312	17.246	-11.637	1
##	1314	ATOM	1315	O <NA>	ILE	B	72	<NA>	26.442	17.315	-11.167	1
##	1315	ATOM	1316	CB <NA>	ILE	B	72	<NA>	26.029	17.094	-13.983	1
##	1316	ATOM	1317	CG1 <NA>	ILE	B	72	<NA>	26.092	17.805	-15.333	1
##	1317	ATOM	1318	CG2 <NA>	ILE	B	72	<NA>	25.615	15.649	-14.171	1
##	1318	ATOM	1319	CD1 <NA>	ILE	B	72	<NA>	27.241	17.224	-16.197	1
##	1319	ATOM	1320	N <NA>	GLY	B	73	<NA>	24.303	16.690	-10.975	1
##	1320	ATOM	1321	CA <NA>	GLY	B	73	<NA>	24.545	16.248	-9.616	1
##	1321	ATOM	1322	C <NA>	GLY	B	73	<NA>	23.470	15.337	-9.095	1
##	1322	ATOM	1323	O <NA>	GLY	B	73	<NA>	22.674	14.852	-9.881	1
##	1323	ATOM	1324	N <NA>	THR	B	74	<NA>	23.517	15.041	-7.794	1
##	1324	ATOM	1325	CA <NA>	THR	B	74	<NA>	22.568	14.162	-7.116	1
##	1325	ATOM	1326	C <NA>	THR	B	74	<NA>	21.280	14.889	-6.829	1
##	1326	ATOM	1327	O <NA>	THR	B	74	<NA>	21.299	16.005	-6.275	1
##	1327	ATOM	1328	CB <NA>	THR	B	74	<NA>	23.128	13.638	-5.748	1
##	1328	ATOM	1329	OG1 <NA>	THR	B	74	<NA>	24.323	12.880	-5.961	1
##	1329	ATOM	1330	CG2 <NA>	THR	B	74	<NA>	22.071	12.763	-5.030	1
##	1330	ATOM	1331	N <NA>	VAL	B	75	<NA>	20.177	14.227	-7.192	1
##	1331	ATOM	1332	CA <NA>	VAL	B	75	<NA>	18.832	14.773	-7.068	1
##	1332	ATOM	1333	C <NA>	VAL	B	75	<NA>	17.989	13.688	-6.360	1
##	1333	ATOM	1334	O <NA>	VAL	B	75	<NA>	17.993	12.504	-6.743	1
##	1334	ATOM	1335	CB <NA>	VAL	B	75	<NA>	18.229	15.113	-8.501	1
##	1335	ATOM	1336	CG1 <NA>	VAL	B	75	<NA>	16.760	15.421	-8.434	1
##	1336	ATOM	1337	CG2 <NA>	VAL	B	75	<NA>	18.967	16.317	-9.099	1
##	1337	ATOM	1338	N <NA>	LEU	B	76	<NA>	17.295	14.086	-5.303	1
##	1338	ATOM	1339	CA <NA>	LEU	B	76	<NA>	16.390	13.196	-4.575	1
##	1339	ATOM	1340	C <NA>	LEU	B	76	<NA>	14.972	13.423	-5.073	1
##	1340	ATOM	1341	O <NA>	LEU	B	76	<NA>	14.652	14.514	-5.518	1
##	1341	ATOM	1342	CB <NA>	LEU	B	76	<NA>	16.450	13.476	-3.067	1
##	1342	ATOM	1343	CG <NA>	LEU	B	76	<NA>	17.787	13.595	-2.330	1
##	1343	ATOM	1344	CD1 <NA>	LEU	B	76	<NA>	17.591	13.640	-0.845	1
##	1344	ATOM	1345	CD2 <NA>	LEU	B	76	<NA>	18.678	12.463	-2.705	1
##	1345	ATOM	1346	N <NA>	VAL	B	77	<NA>	14.135	12.391	-5.049	1
##	1346	ATOM	1347	CA <NA>	VAL	B	77	<NA>	12.749	12.509	-5.485	1
##	1347	ATOM	1348	C <NA>	VAL	B	77	<NA>	11.826	11.894	-4.472	1
##	1348	ATOM	1349	O <NA>	VAL	B	77	<NA>	12.052	10.766	-3.999	1
##	1349	ATOM	1350	CB <NA>	VAL	B	77	<NA>	12.502	11.835	-6.868	1
##	1350	ATOM	1351	CG1 <NA>	VAL	B	77	<NA>	11.065	12.148	-7.398	1
##	1351	ATOM	1352	CG2 <NA>	VAL	B	77	<NA>	13.593	12.322	-7.843	1
##	1352	ATOM	1353	N <NA>	GLY	B	78	<NA>	10.778	12.616	-4.125	1
##	1353	ATOM	1354	CA <NA>	GLY	B	78	<NA>	10.004	12.229	-2.965	1
##	1354	ATOM	1355	C <NA>	GLY	B	78	<NA>	8.832	13.128	-2.672	1
##	1355	ATOM	1356	O <NA>	GLY	B	78	<NA>	8.614	14.117	-3.393	1
##	1356	ATOM	1357	N <NA>	PRO	B	79	<NA>	8.032	12.814	-1.646	1
##	1357	ATOM	1358	CA <NA>	PRO	B	79	<NA>	6.887	13.664	-1.350	1
##	1358	ATOM	1359	C <NA>	PRO	B	79	<NA>	7.292	14.915	-0.550	1
##	1359	ATOM	1360	O <NA>	PRO	B	79	<NA>	7.007	15.036	0.638	1
##	1360	ATOM	1361	CB <NA>	PRO	B	79	<NA>	5.951	12.742	-0.594	1
##	1361	ATOM	1362	CG <NA>	PRO	B	79	<NA>	6.838	11.781	0.040	1
##	1362	ATOM	1363	CD <NA>	PRO	B	79	<NA>	8.096	11.665	-0.739	1
##	1363	ATOM	1364	N <NA>	THR	B	80	<NA>	7.997	15.816	-1.220	1
##	1364	ATOM	1365	CA <NA>	THR	B	80	<NA>	8.324	17.137	-0.702	1

##	1365	ATOM	1366	C <NA>	THR	B	80	<NA>	7.227	18.114	-1.090	1
##	1366	ATOM	1367	O <NA>	THR	B	80	<NA>	6.528	17.896	-2.080	1
##	1367	ATOM	1368	CB <NA>	THR	B	80	<NA>	9.677	17.594	-1.299	1
##	1368	ATOM	1369	OG1 <NA>	THR	B	80	<NA>	9.952	18.951	-0.924	1
##	1369	ATOM	1370	CG2 <NA>	THR	B	80	<NA>	9.688	17.449	-2.825	1
##	1370	ATOM	1371	N <NA>	PRO	B	81	<NA>	6.922	19.074	-0.214	1
##	1371	ATOM	1372	CA <NA>	PRO	B	81	<NA>	5.896	20.066	-0.556	1
##	1372	ATOM	1373	C <NA>	PRO	B	81	<NA>	6.244	20.969	-1.727	1
##	1373	ATOM	1374	O <NA>	PRO	B	81	<NA>	5.343	21.294	-2.509	1
##	1374	ATOM	1375	CB <NA>	PRO	B	81	<NA>	5.694	20.874	0.729	1
##	1375	ATOM	1376	CG <NA>	PRO	B	81	<NA>	6.274	19.954	1.831	1
##	1376	ATOM	1377	CD <NA>	PRO	B	81	<NA>	7.387	19.243	1.190	1
##	1377	ATOM	1378	N <NA>	VAL	B	82	<NA>	7.520	21.355	-1.868	1
##	1378	ATOM	1379	CA <NA>	VAL	B	82	<NA>	7.990	22.207	-2.983	1
##	1379	ATOM	1380	C <NA>	VAL	B	82	<NA>	9.255	21.636	-3.581	1
##	1380	ATOM	1381	O <NA>	VAL	B	82	<NA>	9.973	20.911	-2.929	1
##	1381	ATOM	1382	CB <NA>	VAL	B	82	<NA>	8.375	23.616	-2.484	1
##	1382	ATOM	1383	CG1 <NA>	VAL	B	82	<NA>	7.122	24.513	-2.361	1
##	1383	ATOM	1384	CG2 <NA>	VAL	B	82	<NA>	9.101	23.485	-1.163	1
##	1384	ATOM	1385	N <NA>	ASN	B	83	<NA>	9.588	21.960	-4.812	1
##	1385	ATOM	1386	CA <NA>	ASN	B	83	<NA>	10.914	21.521	-5.319	1
##	1386	ATOM	1387	C <NA>	ASN	B	83	<NA>	11.922	22.373	-4.576	1
##	1387	ATOM	1388	O <NA>	ASN	B	83	<NA>	11.716	23.574	-4.429	1
##	1388	ATOM	1389	CB <NA>	ASN	B	83	<NA>	11.068	21.763	-6.823	1
##	1389	ATOM	1390	CG <NA>	ASN	B	83	<NA>	10.096	20.950	-7.647	1
##	1390	ATOM	1391	OD1 <NA>	ASN	B	83	<NA>	10.013	19.733	-7.494	1
##	1391	ATOM	1392	ND2 <NA>	ASN	B	83	<NA>	9.305	21.627	-8.498	1
##	1392	ATOM	1393	N <NA>	ILE	B	84	<NA>	12.983	21.755	-4.066	1
##	1393	ATOM	1394	CA <NA>	ILE	B	84	<NA>	13.979	22.449	-3.233	1
##	1394	ATOM	1395	C <NA>	ILE	B	84	<NA>	15.345	22.255	-3.870	1
##	1395	ATOM	1396	O <NA>	ILE	B	84	<NA>	15.779	21.111	-4.072	1
##	1396	ATOM	1397	CB <NA>	ILE	B	84	<NA>	14.041	21.833	-1.837	1
##	1397	ATOM	1398	CG1 <NA>	ILE	B	84	<NA>	12.754	22.151	-1.088	1
##	1398	ATOM	1399	CG2 <NA>	ILE	B	84	<NA>	15.323	22.264	-1.122	1
##	1399	ATOM	1400	CD1 <NA>	ILE	B	84	<NA>	12.438	21.217	0.060	1
##	1400	ATOM	1401	N <NA>	ILE	B	85	<NA>	16.044	23.346	-4.167	1
##	1401	ATOM	1402	CA <NA>	ILE	B	85	<NA>	17.441	23.243	-4.575	1
##	1402	ATOM	1403	C <NA>	ILE	B	85	<NA>	18.305	23.504	-3.345	1
##	1403	ATOM	1404	O <NA>	ILE	B	85	<NA>	18.262	24.613	-2.802	1
##	1404	ATOM	1405	CB <NA>	ILE	B	85	<NA>	17.805	24.332	-5.644	1
##	1405	ATOM	1406	CG1 <NA>	ILE	B	85	<NA>	16.809	24.299	-6.827	1
##	1406	ATOM	1407	CG2 <NA>	ILE	B	85	<NA>	19.271	24.191	-6.067	1
##	1407	ATOM	1408	CD1 <NA>	ILE	B	85	<NA>	16.672	22.956	-7.581	1
##	1408	ATOM	1409	N <NA>	GLY	B	86	<NA>	19.121	22.530	-2.936	1
##	1409	ATOM	1410	CA <NA>	GLY	B	86	<NA>	19.857	22.642	-1.690	1
##	1410	ATOM	1411	C <NA>	GLY	B	86	<NA>	21.324	22.800	-1.940	1
##	1411	ATOM	1412	O <NA>	GLY	B	86	<NA>	21.750	22.958	-3.056	1
##	1412	ATOM	1413	N <NA>	ARG	B	87	<NA>	22.117	22.755	-0.887	1
##	1413	ATOM	1414	CA <NA>	ARG	B	87	<NA>	23.533	23.126	-0.985	1
##	1414	ATOM	1415	C <NA>	ARG	B	87	<NA>	24.413	22.356	-1.973	1
##	1415	ATOM	1416	O <NA>	ARG	B	87	<NA>	25.398	22.903	-2.461	1
##	1416	ATOM	1417	CB <NA>	ARG	B	87	<NA>	24.171	23.147	0.403	1
##	1417	ATOM	1418	CG <NA>	ARG	B	87	<NA>	23.646	24.256	1.283	1
##	1418	ATOM	1419	CD <NA>	ARG	B	87	<NA>	24.429	24.306	2.576	1

##	1419	ATOM	1420	NE <NA>	ARG	B	87	<NA>	24.362	23.068	3.371	1
##	1420	ATOM	1421	CZ <NA>	ARG	B	87	<NA>	25.357	22.185	3.495	1
##	1421	ATOM	1422	NH1 <NA>	ARG	B	87	<NA>	26.467	22.303	2.795	1
##	1422	ATOM	1423	NH2 <NA>	ARG	B	87	<NA>	25.255	21.190	4.368	1
##	1423	ATOM	1424	N <NA>	ASN	B	88	<NA>	24.074	21.101	-2.275	1
##	1424	ATOM	1425	CA <NA>	ASN	B	88	<NA>	24.950	20.312	-3.132	1
##	1425	ATOM	1426	C <NA>	ASN	B	88	<NA>	24.980	20.893	-4.527	1
##	1426	ATOM	1427	O <NA>	ASN	B	88	<NA>	26.015	20.853	-5.202	1
##	1427	ATOM	1428	CB <NA>	ASN	B	88	<NA>	24.512	18.849	-3.197	1
##	1428	ATOM	1429	CG <NA>	ASN	B	88	<NA>	23.126	18.649	-3.777	1
##	1429	ATOM	1430	OD1 <NA>	ASN	B	88	<NA>	22.167	19.280	-3.351	1
##	1430	ATOM	1431	ND2 <NA>	ASN	B	88	<NA>	23.020	17.775	-4.767	1
##	1431	ATOM	1432	N <NA>	LEU	B	89	<NA>	23.863	21.490	-4.949	1
##	1432	ATOM	1433	CA <NA>	LEU	B	89	<NA>	23.811	22.125	-6.273	1
##	1433	ATOM	1434	C <NA>	LEU	B	89	<NA>	24.018	23.645	-6.231	1
##	1434	ATOM	1435	O <NA>	LEU	B	89	<NA>	24.321	24.242	-7.236	1
##	1435	ATOM	1436	CB <NA>	LEU	B	89	<NA>	22.457	21.815	-6.962	1
##	1436	ATOM	1437	CG <NA>	LEU	B	89	<NA>	22.219	20.372	-7.436	1
##	1437	ATOM	1438	CD1 <NA>	LEU	B	89	<NA>	20.937	20.300	-8.243	1
##	1438	ATOM	1439	CD2 <NA>	LEU	B	89	<NA>	23.408	19.901	-8.273	1
##	1439	ATOM	1440	N <NA>	LEU	B	90	<NA>	23.819	24.255	-5.075	1
##	1440	ATOM	1441	CA <NA>	LEU	B	90	<NA>	24.020	25.701	-4.954	1
##	1441	ATOM	1442	C <NA>	LEU	B	90	<NA>	25.511	26.005	-5.072	1
##	1442	ATOM	1443	O <NA>	LEU	B	90	<NA>	25.907	26.959	-5.732	1
##	1443	ATOM	1444	CB <NA>	LEU	B	90	<NA>	23.430	26.234	-3.624	1
##	1444	ATOM	1445	CG <NA>	LEU	B	90	<NA>	21.900	26.309	-3.475	1
##	1445	ATOM	1446	CD1 <NA>	LEU	B	90	<NA>	21.487	26.779	-2.081	1
##	1446	ATOM	1447	CD2 <NA>	LEU	B	90	<NA>	21.358	27.241	-4.506	1
##	1447	ATOM	1448	N <NA>	THR	B	91	<NA>	26.336	25.143	-4.491	1
##	1448	ATOM	1449	CA <NA>	THR	B	91	<NA>	27.785	25.304	-4.546	1
##	1449	ATOM	1450	C <NA>	THR	B	91	<NA>	28.270	25.184	-5.969	1
##	1450	ATOM	1451	O <NA>	THR	B	91	<NA>	29.168	25.903	-6.378	1
##	1451	ATOM	1452	CB <NA>	THR	B	91	<NA>	28.501	24.261	-3.669	1
##	1452	ATOM	1453	OG1 <NA>	THR	B	91	<NA>	27.898	22.990	-3.894	1
##	1453	ATOM	1454	CG2 <NA>	THR	B	91	<NA>	28.366	24.579	-2.208	1
##	1454	ATOM	1455	N <NA>	GLN	B	92	<NA>	27.619	24.323	-6.741	1
##	1455	ATOM	1456	CA <NA>	GLN	B	92	<NA>	28.009	24.110	-8.150	1
##	1456	ATOM	1457	C <NA>	GLN	B	92	<NA>	27.823	25.361	-8.999	1
##	1457	ATOM	1458	O <NA>	GLN	B	92	<NA>	28.719	25.701	-9.794	1
##	1458	ATOM	1459	CB <NA>	GLN	B	92	<NA>	27.226	22.956	-8.793	1
##	1459	ATOM	1460	CG <NA>	GLN	B	92	<NA>	27.720	21.588	-8.406	1
##	1460	ATOM	1461	CD <NA>	GLN	B	92	<NA>	27.313	20.496	-9.421	1
##	1461	ATOM	1462	OE1 <NA>	GLN	B	92	<NA>	27.138	20.746	-10.620	1
##	1462	ATOM	1463	NE2 <NA>	GLN	B	92	<NA>	27.230	19.281	-8.941	1
##	1463	ATOM	1464	N <NA>	ILE	B	93	<NA>	26.683	26.043	-8.820	1
##	1464	ATOM	1465	CA <NA>	ILE	B	93	<NA>	26.362	27.233	-9.606	1
##	1465	ATOM	1466	C <NA>	ILE	B	93	<NA>	26.904	28.524	-8.963	1
##	1466	ATOM	1467	O <NA>	ILE	B	93	<NA>	26.574	29.627	-9.385	1
##	1467	ATOM	1468	CB <NA>	ILE	B	93	<NA>	24.838	27.349	-9.857	1
##	1468	ATOM	1469	CG1 <NA>	ILE	B	93	<NA>	24.103	27.648	-8.559	1
##	1469	ATOM	1470	CG2 <NA>	ILE	B	93	<NA>	24.300	26.092	-10.460	1
##	1470	ATOM	1471	CD1 <NA>	ILE	B	93	<NA>	22.672	28.017	-8.785	1
##	1471	ATOM	1472	N <NA>	GLY	B	94	<NA>	27.741	28.369	-7.949	1
##	1472	ATOM	1473	CA <NA>	GLY	B	94	<NA>	28.481	29.498	-7.421	1

##	1473	ATOM	1474	C <NA>	GLY	B	94	<NA>	27.749	30.439	-6.488	1
##	1474	ATOM	1475	O <NA>	GLY	B	94	<NA>	28.177	31.555	-6.261	1
##	1475	ATOM	1476	N <NA>	CYS	B	95	<NA>	26.808	29.899	-5.748	1
##	1476	ATOM	1477	CA <NA>	CYS	B	95	<NA>	25.895	30.718	-5.004	1
##	1477	ATOM	1478	C <NA>	CYS	B	95	<NA>	26.408	30.993	-3.598	1
##	1478	ATOM	1479	O <NA>	CYS	B	95	<NA>	26.769	30.065	-2.870	1
##	1479	ATOM	1480	CB <NA>	CYS	B	95	<NA>	24.578	29.989	-4.978	1
##	1480	ATOM	1481	SG <NA>	CYS	B	95	<NA>	23.221	30.929	-4.410	1
##	1481	ATOM	1482	N <NA>	THR	B	96	<NA>	26.473	32.277	-3.244	1
##	1482	ATOM	1483	CA <NA>	THR	B	96	<NA>	26.794	32.734	-1.882	1
##	1483	ATOM	1484	C <NA>	THR	B	96	<NA>	25.672	33.544	-1.205	1
##	1484	ATOM	1485	O <NA>	THR	B	96	<NA>	24.760	34.079	-1.852	1
##	1485	ATOM	1486	CB <NA>	THR	B	96	<NA>	28.051	33.660	-1.858	1
##	1486	ATOM	1487	OG1 <NA>	THR	B	96	<NA>	27.888	34.689	-2.857	1
##	1487	ATOM	1488	CG2 <NA>	THR	B	96	<NA>	29.316	32.870	-2.141	1
##	1488	ATOM	1489	N <NA>	LEU	B	97	<NA>	25.759	33.617	0.119	1
##	1489	ATOM	1490	CA <NA>	LEU	B	97	<NA>	24.902	34.468	0.963	1
##	1490	ATOM	1491	C <NA>	LEU	B	97	<NA>	25.714	35.689	1.398	1
##	1491	ATOM	1492	O <NA>	LEU	B	97	<NA>	26.854	35.558	1.870	1
##	1492	ATOM	1493	CB <NA>	LEU	B	97	<NA>	24.489	33.718	2.236	1
##	1493	ATOM	1494	CG <NA>	LEU	B	97	<NA>	23.211	32.901	2.344	1
##	1494	ATOM	1495	CD1 <NA>	LEU	B	97	<NA>	23.114	32.358	3.719	1
##	1495	ATOM	1496	CD2 <NA>	LEU	B	97	<NA>	22.037	33.773	2.076	1
##	1496	ATOM	1497	N <NA>	ASN	B	98	<NA>	25.121	36.868	1.264	1
##	1497	ATOM	1498	CA <NA>	ASN	B	98	<NA>	25.870	38.101	1.449	1
##	1498	ATOM	1499	C <NA>	ASN	B	98	<NA>	25.102	39.038	2.370	1
##	1499	ATOM	1500	O <NA>	ASN	B	98	<NA>	23.889	39.124	2.261	1
##	1500	ATOM	1501	CB <NA>	ASN	B	98	<NA>	26.140	38.756	0.086	1
##	1501	ATOM	1502	CG <NA>	ASN	B	98	<NA>	27.048	37.921	-0.814	1
##	1502	ATOM	1503	OD1 <NA>	ASN	B	98	<NA>	28.268	37.895	-0.630	1
##	1503	ATOM	1504	ND2 <NA>	ASN	B	98	<NA>	26.455	37.192	-1.754	1
##	1504	ATOM	1505	N <NA>	PHE	B	99	<NA>	25.809	39.706	3.283	1
##	1505	ATOM	1506	CA <NA>	PHE	B	99	<NA>	25.267	40.855	4.034	1
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##	1507	ATOM	1508	O <NA>	PHE	B	99	<NA>	27.448	41.208	5.013	1
##	1508	ATOM	1509	CB <NA>	PHE	B	99	<NA>	24.284	40.418	5.127	1
##	1509	ATOM	1510	CG <NA>	PHE	B	99	<NA>	24.859	39.479	6.130	1
##	1510	ATOM	1511	CD1 <NA>	PHE	B	99	<NA>	25.061	38.150	5.808	1
##	1511	ATOM	1512	CD2 <NA>	PHE	B	99	<NA>	25.071	39.890	7.436	1
##	1512	ATOM	1513	CE1 <NA>	PHE	B	99	<NA>	25.450	37.240	6.756	1
##	1513	ATOM	1514	CE2 <NA>	PHE	B	99	<NA>	25.473	38.988	8.409	1
##	1514	ATOM	1515	CZ <NA>	PHE	B	99	<NA>	25.658	37.663	8.073	1
##	1515	HETATM	1517	N1 <NA>	MK1	B	902	<NA>	9.280	23.763	3.004	1
##	1516	HETATM	1518	C1 <NA>	MK1	B	902	<NA>	9.498	23.983	4.459	1
##	1517	HETATM	1519	C2 <NA>	MK1	B	902	<NA>	10.591	24.905	4.962	1
##	1518	HETATM	1520	C3 <NA>	MK1	B	902	<NA>	10.591	24.864	6.466	1
##	1519	HETATM	1521	O1 <NA>	MK1	B	902	<NA>	10.937	23.849	7.057	1
##	1520	HETATM	1522	N2 <NA>	MK1	B	902	<NA>	10.193	25.953	7.094	1
##	1521	HETATM	1523	C4 <NA>	MK1	B	902	<NA>	10.145	26.250	8.490	1
##	1522	HETATM	1524	C5 <NA>	MK1	B	902	<NA>	9.379	27.577	8.641	1
##	1523	HETATM	1525	C6 <NA>	MK1	B	902	<NA>	11.398	26.347	9.074	1
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##	1525	HETATM	1527	N3 <NA>	MK1	B	902	<NA>	11.819	24.282	4.355	1
##	1526	HETATM	1528	C8 <NA>	MK1	B	902	<NA>	11.753	23.776	2.961	1

##	1527	HETATM	1529	C9 <NA>	MK1	B	902	<NA>	10.440	23.182	2.493	1
##	1528	HETATM	1530	C10 <NA>	MK1	B	902	<NA>	13.083	24.963	4.552	1
##	1529	HETATM	1531	C11 <NA>	MK1	B	902	<NA>	14.203	24.064	5.078	1
##	1530	HETATM	1532	O2 <NA>	MK1	B	902	<NA>	15.242	24.884	4.634	1
##	1531	HETATM	1533	C12 <NA>	MK1	B	902	<NA>	14.440	23.761	6.569	1
##	1532	HETATM	1534	C13 <NA>	MK1	B	902	<NA>	15.573	22.821	7.005	1
##	1533	HETATM	1535	C14 <NA>	MK1	B	902	<NA>	15.644	22.664	8.534	1
##	1534	HETATM	1536	C15 <NA>	MK1	B	902	<NA>	16.733	21.750	8.961	1
##	1535	HETATM	1537	C16 <NA>	MK1	B	902	<NA>	18.058	21.916	8.553	1
##	1536	HETATM	1538	C17 <NA>	MK1	B	902	<NA>	19.037	21.016	8.947	1
##	1537	HETATM	1539	C18 <NA>	MK1	B	902	<NA>	18.673	19.939	9.758	1
##	1538	HETATM	1540	C19 <NA>	MK1	B	902	<NA>	17.347	19.773	10.176	1
##	1539	HETATM	1541	C20 <NA>	MK1	B	902	<NA>	16.374	20.687	9.772	1
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##	1541	HETATM	1543	O3 <NA>	MK1	B	902	<NA>	14.367	20.831	6.397	1
##	1542	HETATM	1544	N4 <NA>	MK1	B	902	<NA>	16.583	20.913	5.924	1
##	1543	HETATM	1545	C22 <NA>	MK1	B	902	<NA>	16.692	19.500	5.604	1
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##	1548	HETATM	1550	C26 <NA>	MK1	B	902	<NA>	17.500	17.363	2.496	1
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##	1579	HETATM	1581	O <NA>	HOH	A	373	<NA>	27.561	43.155	19.015	1
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##	1639	HETATM	1641	0	<NA>	HOH	B	370	<NA>	13.975	15.741	12.070	1
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##	1647	HETATM	1649	0	<NA>	HOH	B	387	<NA>	16.904	27.594	-15.938	1
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##	1665	HETATM	1667	0	<NA>	HOH	B	471	<NA>	5.749	25.785	-19.792	1
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##	1670	HETATM	1672	0	<NA>	HOH	B	509	<NA>	19.882	3.986	-18.136	1
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##	1677	HETATM	1679	0	<NA>	HOH	B	532	<NA>	19.507	45.215	1.709	1
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##	1679	HETATM	1681	0	<NA>	HOH	B	549	<NA>	19.908	8.718	-19.215	1
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##	1682	HETATM	1684	0	<NA>	HOH	B	568	<NA>	2.817	28.133	2.191	1
##	1683	HETATM	1685	0	<NA>	HOH	B	591	<NA>	15.835	40.105	-5.971	1
##	1684	HETATM	1686	0	<NA>	HOH	B	595	<NA>	4.515	36.451	-4.499	1
##	1685	HETATM	1687	0	<NA>	HOH	B	613	<NA>	24.127	-10.994	-0.982	1
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##		b segid elesy charge											
##	1	38.10	<NA>	N	<NA>								

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##	1369	13.16	<NA>	C	<NA>
##	1370	24.57	<NA>	N	<NA>
##	1371	24.68	<NA>	C	<NA>
##	1372	26.51	<NA>	C	<NA>
##	1373	32.43	<NA>	O	<NA>
##	1374	22.89	<NA>	C	<NA>
##	1375	24.08	<NA>	C	<NA>
##	1376	21.46	<NA>	C	<NA>
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##	1380	26.47	<NA>	O	<NA>
##	1381	26.47	<NA>	C	<NA>
##	1382	26.39	<NA>	C	<NA>
##	1383	24.12	<NA>	C	<NA>
##	1384	16.61	<NA>	N	<NA>
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##	1386	19.55	<NA>	C	<NA>
##	1387	18.36	<NA>	O	<NA>
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##	1390	23.24	<NA>	O	<NA>
##	1391	22.85	<NA>	N	<NA>
##	1392	17.31	<NA>	N	<NA>
##	1393	13.51	<NA>	C	<NA>
##	1394	19.87	<NA>	C	<NA>
##	1395	20.54	<NA>	O	<NA>
##	1396	10.82	<NA>	C	<NA>
##	1397	13.42	<NA>	C	<NA>
##	1398	11.48	<NA>	C	<NA>
##	1399	20.08	<NA>	C	<NA>
##	1400	19.47	<NA>	N	<NA>
##	1401	19.69	<NA>	C	<NA>
##	1402	22.78	<NA>	C	<NA>
##	1403	24.74	<NA>	O	<NA>
##	1404	18.51	<NA>	C	<NA>
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##	1406	14.76	<NA>	C	<NA>
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##	1424	17.41	<NA>	C	<NA>
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##	1426	20.40	<NA>	O	<NA>
##	1427	19.90	<NA>	C	<NA>
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##	1430	16.65	<NA>	N	<NA>
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##	1436	17.87	<NA>	C	<NA>
##	1437	20.88	<NA>	C	<NA>
##	1438	17.17	<NA>	C	<NA>
##	1439	20.01	<NA>	N	<NA>
##	1440	22.17	<NA>	C	<NA>
##	1441	19.95	<NA>	C	<NA>
##	1442	21.08	<NA>	O	<NA>
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##	1448	23.96	<NA>	C	<NA>
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##	1450	26.72	<NA>	O	<NA>
##	1451	21.26	<NA>	C	<NA>
##	1452	25.49	<NA>	O	<NA>
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##	1454	25.95	<NA>	N	<NA>
##	1455	27.31	<NA>	C	<NA>
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##	1460	27.56	<NA>	C	<NA>
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##	1462	27.50	<NA>	N	<NA>
##	1463	28.73	<NA>	N	<NA>
##	1464	28.11	<NA>	C	<NA>
##	1465	30.61	<NA>	C	<NA>
##	1466	32.40	<NA>	O	<NA>
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##	1468	25.74	<NA>	C	<NA>
##	1469	21.29	<NA>	C	<NA>
##	1470	27.65	<NA>	C	<NA>
##	1471	30.93	<NA>	N	<NA>
##	1472	31.94	<NA>	C	<NA>
##	1473	30.20	<NA>	C	<NA>
##	1474	31.24	<NA>	O	<NA>
##	1475	27.82	<NA>	N	<NA>
##	1476	26.76	<NA>	C	<NA>
##	1477	27.20	<NA>	C	<NA>
##	1478	27.85	<NA>	O	<NA>
##	1479	27.09	<NA>	C	<NA>
##	1480	36.34	<NA>	S	<NA>
##	1481	26.04	<NA>	N	<NA>
##	1482	25.60	<NA>	C	<NA>
##	1483	24.26	<NA>	C	<NA>
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##	1487	24.73	<NA>	C	<NA>
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##	1489	27.92	<NA>	C	<NA>
##	1490	30.25	<NA>	C	<NA>
##	1491	29.52	<NA>	O	<NA>
##	1492	27.18	<NA>	C	<NA>
##	1493	22.23	<NA>	C	<NA>
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##	1501	33.93	<NA>	C	<NA>
##	1502	37.15	<NA>	O	<NA>
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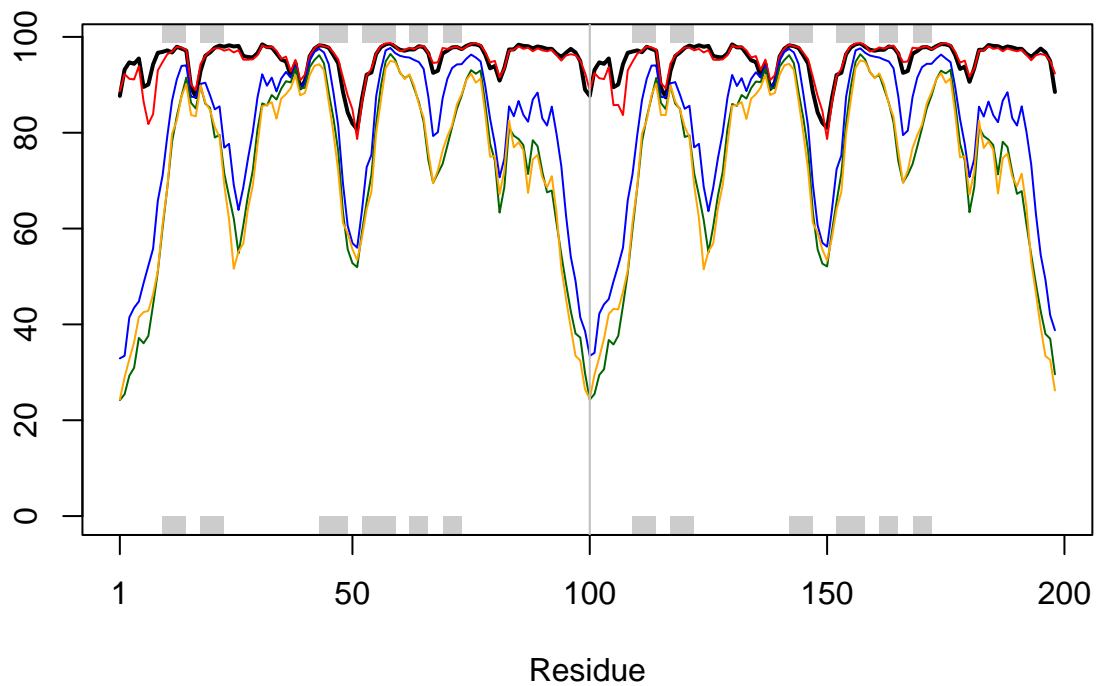
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##	1541	32.66	<NA>	O	<NA>
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##	1571	41.93	<NA>	0	<NA>
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##	1673	78.93	<NA>	0	<NA>
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##	1675	78.14	<NA>	0	<NA>

```
## 1676 54.05 <NA>    0 <NA>
## 1677 72.78 <NA>    0 <NA>
## 1678 58.40 <NA>    0 <NA>
## 1679 58.78 <NA>    0 <NA>
## 1680 68.40 <NA>    0 <NA>
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## 1684 49.41 <NA>    0 <NA>
## 1685 64.49 <NA>    0 <NA>
## 1686 54.09 <NA>    0 <NA>
```

```
plotb3(pdbb$b[1,], typ="l", lwd=2, sse=pdbb)
points(pdbb$b[2,], typ="l", col="red")
points(pdbb$b[3,], typ="l", col="blue")
points(pdbb$b[4,], typ="l", col="darkgreen")
points(pdbb$b[5,], typ="l", col="orange")
abline(v=100, col="gray")
```



Finding the rigid core to improve the superposition:

```
core <- core.find(pdb)
```

```
## core size 197 of 198 vol = 5017.583
## core size 196 of 198 vol = 4299.462
## core size 195 of 198 vol = 4030.786
## core size 194 of 198 vol = 3797.241
## core size 193 of 198 vol = 3567.126
## core size 192 of 198 vol = 3378.469
## core size 191 of 198 vol = 3249.342
## core size 190 of 198 vol = 3149.254
## core size 189 of 198 vol = 3070.29
## core size 188 of 198 vol = 2993.999
## core size 187 of 198 vol = 2917.618
## core size 186 of 198 vol = 2865.321
## core size 185 of 198 vol = 2835.031
## core size 184 of 198 vol = 2825.584
## core size 183 of 198 vol = 2833.979
## core size 182 of 198 vol = 2894.691
## core size 181 of 198 vol = 2975.843
## core size 180 of 198 vol = 3026.495
## core size 179 of 198 vol = 3070.895
## core size 178 of 198 vol = 3121.204
## core size 177 of 198 vol = 3127.656
## core size 176 of 198 vol = 3102.311
## core size 175 of 198 vol = 3060.45
## core size 174 of 198 vol = 2993.84
## core size 173 of 198 vol = 2902.747
## core size 172 of 198 vol = 2841.824
## core size 171 of 198 vol = 2771.39
## core size 170 of 198 vol = 2708.164
## core size 169 of 198 vol = 2616.115
## core size 168 of 198 vol = 2540.663
## core size 167 of 198 vol = 2471.823
## core size 166 of 198 vol = 2396.567
## core size 165 of 198 vol = 2324.756
## core size 164 of 198 vol = 2258.532
## core size 163 of 198 vol = 2189.811
## core size 162 of 198 vol = 2118.531
## core size 161 of 198 vol = 2048.541
## core size 160 of 198 vol = 1964.22
## core size 159 of 198 vol = 1878.019
## core size 158 of 198 vol = 1802.026
## core size 157 of 198 vol = 1719.543
## core size 156 of 198 vol = 1640.479
## core size 155 of 198 vol = 1561.746
## core size 154 of 198 vol = 1490.107
## core size 153 of 198 vol = 1416.211
## core size 152 of 198 vol = 1345.494
## core size 151 of 198 vol = 1287.606
## core size 150 of 198 vol = 1225.523
## core size 149 of 198 vol = 1168.6
## core size 148 of 198 vol = 1123.809
## core size 147 of 198 vol = 1069.607
```

```

## core size 146 of 198 vol = 1028.33
## core size 145 of 198 vol = 986.295
## core size 144 of 198 vol = 947.191
## core size 143 of 198 vol = 910.624
## core size 142 of 198 vol = 868.922
## core size 141 of 198 vol = 829.982
## core size 140 of 198 vol = 788.548
## core size 139 of 198 vol = 749.234
## core size 138 of 198 vol = 713.554
## core size 137 of 198 vol = 679.035
## core size 136 of 198 vol = 639.012
## core size 135 of 198 vol = 599.236
## core size 134 of 198 vol = 556.226
## core size 133 of 198 vol = 521.307
## core size 132 of 198 vol = 484.526
## core size 131 of 198 vol = 453.614
## core size 130 of 198 vol = 422.947
## core size 129 of 198 vol = 404.641
## core size 128 of 198 vol = 397.064
## core size 127 of 198 vol = 371.629
## core size 126 of 198 vol = 355.609
## core size 125 of 198 vol = 334.859
## core size 124 of 198 vol = 313.691
## core size 123 of 198 vol = 291.489
## core size 122 of 198 vol = 268.734
## core size 121 of 198 vol = 245.865
## core size 120 of 198 vol = 236.559
## core size 119 of 198 vol = 218.641
## core size 118 of 198 vol = 201.313
## core size 117 of 198 vol = 183.861
## core size 116 of 198 vol = 167.249
## core size 115 of 198 vol = 151.276
## core size 114 of 198 vol = 137.843
## core size 113 of 198 vol = 124.983
## core size 112 of 198 vol = 112.07
## core size 111 of 198 vol = 101.394
## core size 110 of 198 vol = 91.994
## core size 109 of 198 vol = 82.201
## core size 108 of 198 vol = 74.644
## core size 107 of 198 vol = 70.256
## core size 106 of 198 vol = 64.859
## core size 105 of 198 vol = 58.745
## core size 104 of 198 vol = 54.966
## core size 103 of 198 vol = 49.885
## core size 102 of 198 vol = 45.389
## core size 101 of 198 vol = 41.648
## core size 100 of 198 vol = 38.714
## core size 99 of 198 vol = 36.289
## core size 98 of 198 vol = 33.698
## core size 97 of 198 vol = 28.156
## core size 96 of 198 vol = 23.583
## core size 95 of 198 vol = 19.899
## core size 94 of 198 vol = 16.637
## core size 93 of 198 vol = 12.448

```

```
## core size 92 of 198 vol = 9.42
## core size 91 of 198 vol = 8.296
## core size 90 of 198 vol = 5.783
## core size 89 of 198 vol = 4.006
## core size 88 of 198 vol = 2.903
## core size 87 of 198 vol = 2.24
## core size 86 of 198 vol = 1.765
## core size 85 of 198 vol = 1.408
## core size 84 of 198 vol = 1.164
## core size 83 of 198 vol = 0.969
## core size 82 of 198 vol = 0.833
## core size 81 of 198 vol = 0.675
## core size 80 of 198 vol = 0.579
## core size 79 of 198 vol = 0.529
## core size 78 of 198 vol = 0.456
## FINISHED: Min vol ( 0.5 ) reached
```

```
core.inds <- print(core, vol=0.5)
```

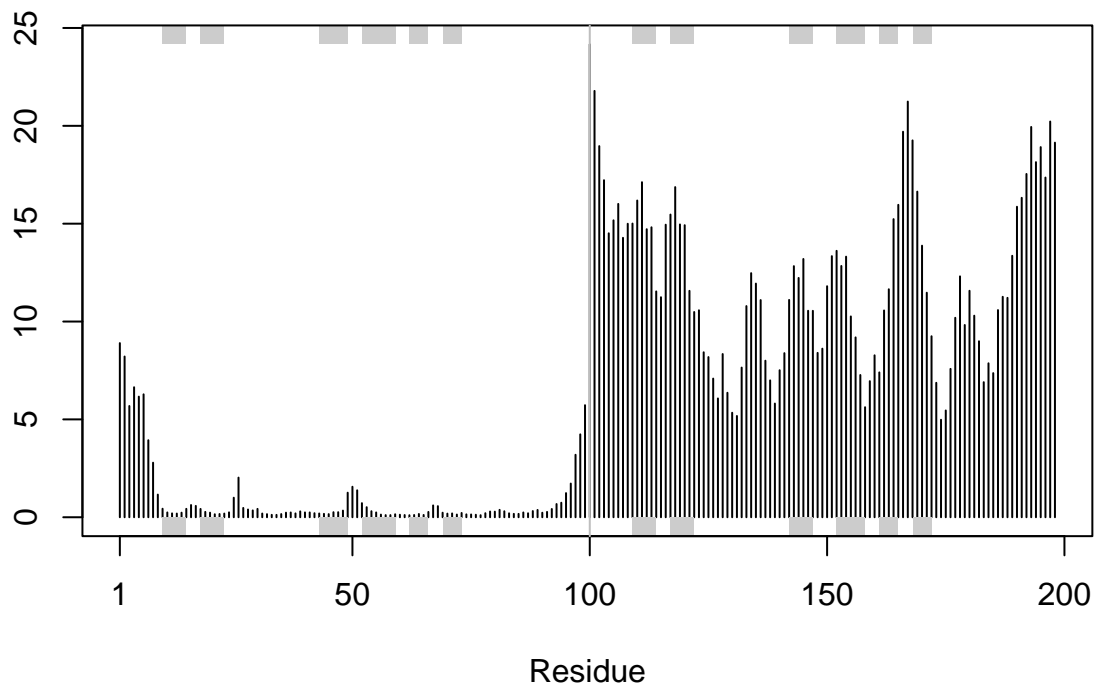
```
## # 79 positions (cumulative volume <= 0.5 Angstrom^3)
## start end length
## 1 10 24 15
## 2 27 48 22
## 3 53 94 42
```

```
xyz <- pdbfit(pdb, core.inds, outpath="corefit_structures")
```

```
rf <- rmsf(xyz)
```

```
plotb3(rf, sse=pdb)
```

```
abline(v=100, col="gray", ylab="RMSF")
```



Predicted Alignment Errors for Domains

Inter domain prediction for model 1 and 2

```
library(jsonlite)

# Listing of all PAE JSON files

pae_files <- list.files(path=results_dir,
                        pattern=".*model.*\\.json",
                        full.names = TRUE)
```

Inter domain prediction for model 1 and 5

```
pae1 <- read_json(pae_files[1],simplifyVector = TRUE)
pae5 <- read_json(pae_files[5],simplifyVector = TRUE)

attributes(pae1)
```

```
## $names
## [1] "plddt" "max_pae" "pae" "ptm" "iptm"
```

```
head(pae1$plddt)
```

```
## [1] 87.69 93.19 94.69 94.38 95.50 89.56
```

Now to figure out the max PAE scores of the other models (helps determine model ranks)

```
pae1$max_pae
```

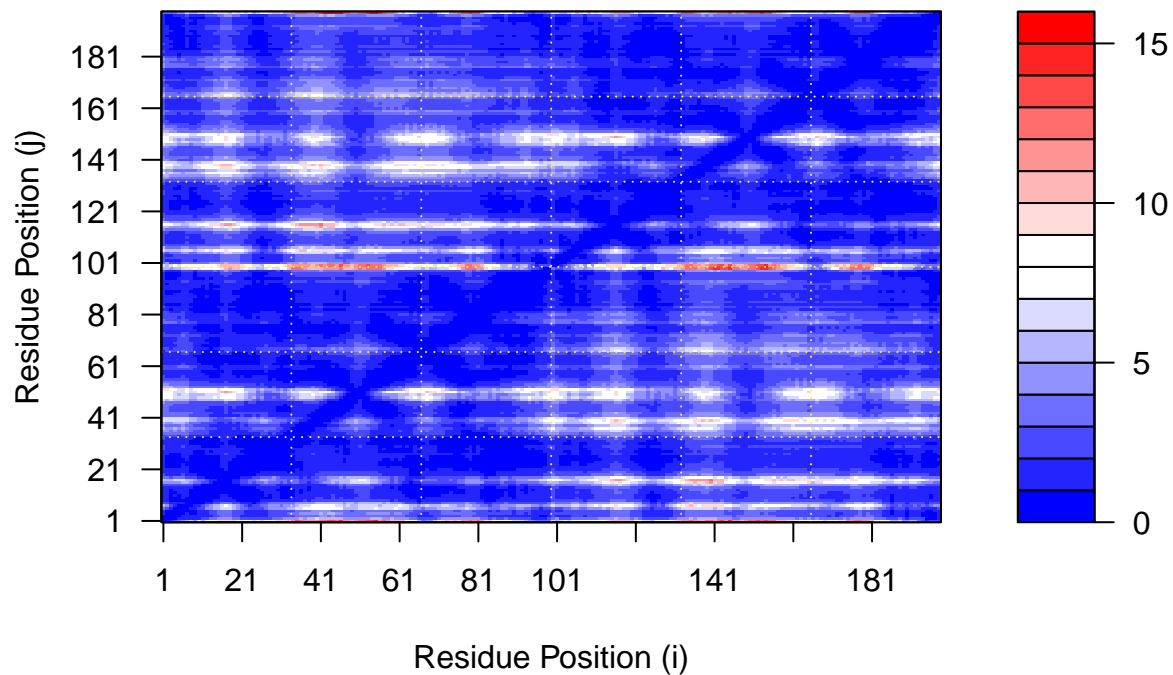
```
## [1] 15.89844
```

```
pae5$max_pae
```

```
## [1] 29.25
```

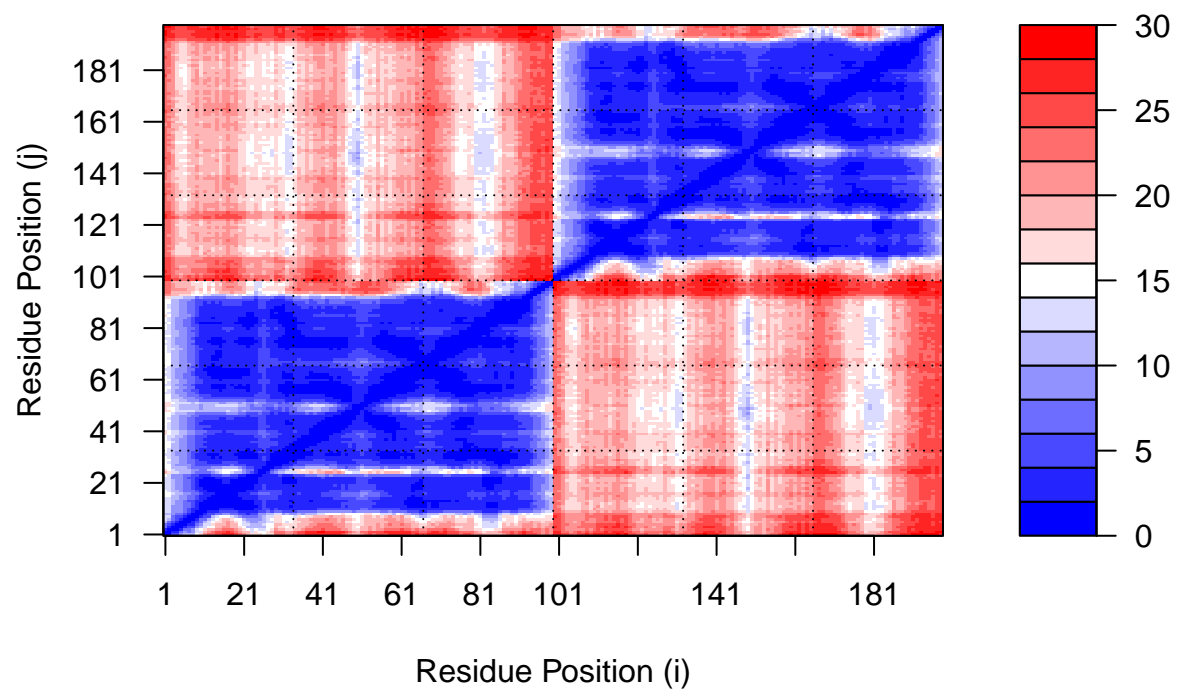
We can now plot the PAE scores using a Bio3d plot function

```
plot.dmat(pae1$pae,
          xlab="Residue Position (i)",
          ylab="Residue Position (j)")
```



This plot is for model 1.

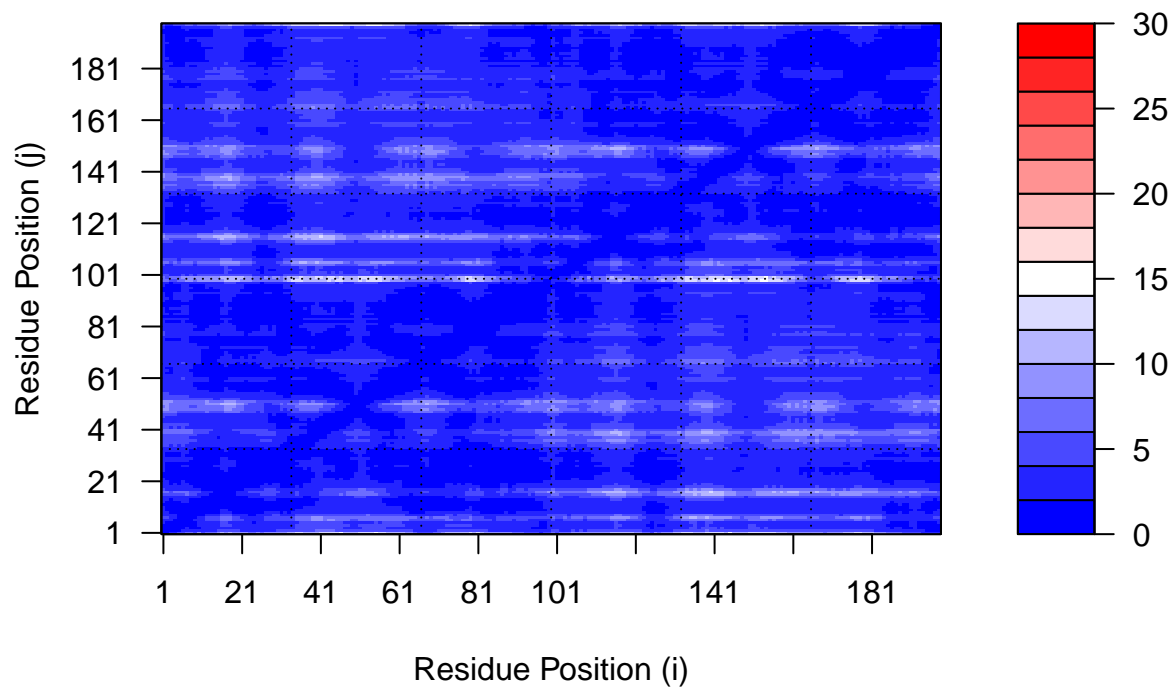
```
plot.dmat(pae5$pae,
          xlab="Residue Position (i)",
          ylab="Residue Position (j)",
          grid.col = "black",
          zlim=c(0,30))
```



This plot is for model 5.

Now, to make model 1 have the same data range as model 5.

```
plot.dmat(pae1$pae,
          xlab="Residue Position (i)",
          ylab="Residue Position (j)",
          grid.col = "black",
          zlim=c(0,30))
```

```
aln_file <- list.files(path=results_dir,
                       pattern=".a3m$",
                       full.names = TRUE)
```

```
aln_file
```

```
## [1] "hivprdimer/hivprdimer_23119.a3m"
```

```
aln <- read.fasta(aln_file[1], to.upper = TRUE)
```

```
## [1] " ** Duplicated sequence id's: 101 **"
```

```
## [2] " ** Duplicated sequence id's: 101 **"
```

To determine how many sequences are in the alignment

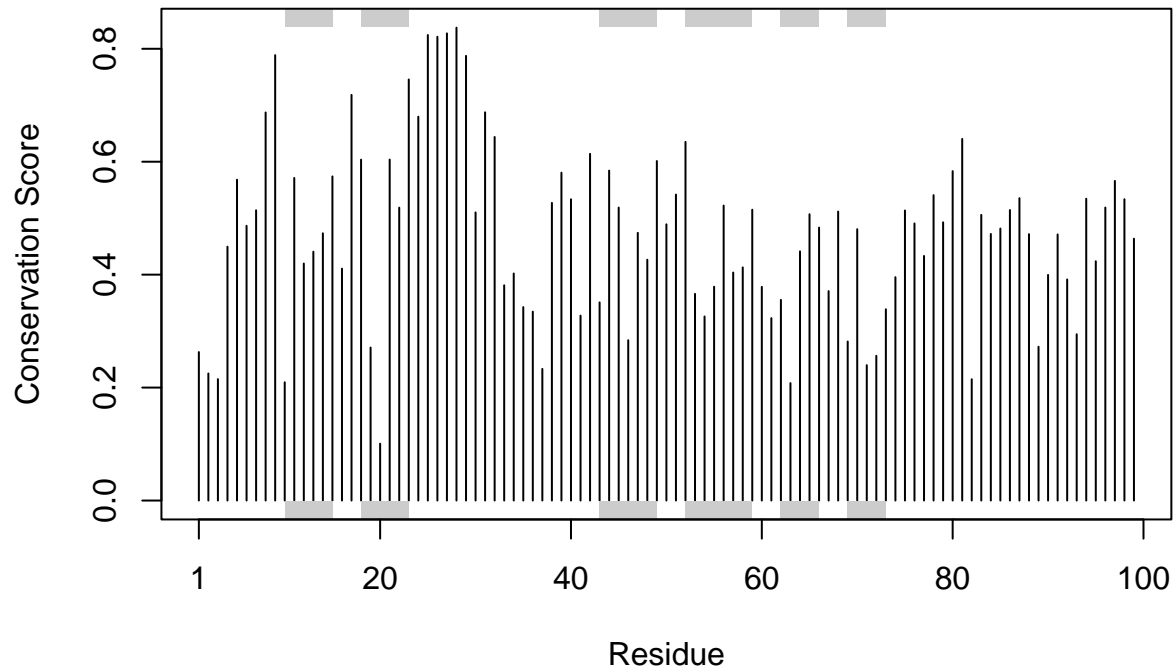
```
dim(aln$ali)
```

```
## [1] 5378 132
```

To score and plot residue conservation in the alignment

```
sim <- conserv(aln)

plotb3(sim[1:99], sse=trim.pdb(pdb, chain="A"),
       ylab="Conservation Score")
```



To make the active site residues stand out

```
con <- consensus(aln, cutoff = 0.9)

con$seq
```

```
## [1] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [19] "-" "-" "-" "-" "-" "-" "D" "T" "G" "A" "-" "-" "-" "-" "-" "-" "-"
## [37] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [55] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [73] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [91] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [109] "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-" "-"
## [127] "-" "-" "-" "-" "-" "-"
```

For the final visualization of the functionally important sites:

```
m1.pdb <- read.pdb(pdb_files[1])  
occ <- vec2resno(c(sim[1:99], sim[1:99]), m1.pdb$atom$resno)  
write.pdb(m1.pdb, o=occ, file="m1_conserv.pdb")
```