

## Load the BINANA module

This notebook was tested in Jupyter Notebook 5.7.8. It did not work when tested in Jupyter Lab. We have confirmed that similar usage works in HTML/JavaScript web pages.

```
In [2]: %%html
<script type="module">
  window.binana = undefined
  import * as bnana from './binana.js';
  window.binana = bnana;
</script>
```

## Define a JavaScript function to output formatted results

```
In [3]: %%javascript

window.output = function(element, txt) {
  element.html("<pre style='font-size:80%;'>" + txt + "</pre>");
};
```

## Define ligand PDBQT text

In [4]: %%javascript

```
window.ligPDBTxt = `REMARK 8 active torsions:
REMARK status: ('A' for Active; 'I' for Inactive)
REMARK 1 A between atoms: C4_1 and C5_2
REMARK 2 A between atoms: C4_1 and N1_7
REMARK 3 A between atoms: C4_1 and O6_5
REMARK 4 A between atoms: C5_2 and N1_6
REMARK 5 A between atoms: C7_4 and N1_6
REMARK 6 A between atoms: C7_4 and C1_8
REMARK 7 A between atoms: N1_6 and C6_14
REMARK 8 A between atoms: N1_7 and C2_9
ROOT
HETATM 1 C5 CHT A 1 16.376 2.063 7.151 1.00 6.35 0.30
ENDROOT
BRANCH 1 2
HETATM 2 N1 CHT A 1 15.723 3.326 7.619 1.00 6.17 -0.00
HETATM 3 C6 CHT A 1 15.386 3.121 9.043 1.00 5.88 0.28
BRANCH 2 4
HETATM 4 C6 CHT A 1 14.451 3.555 6.881 1.00 0.00 0.24
HETATM 5 C7 CHT A 1 14.179 3.052 5.671 1.00 0.00 0.06
HETATM 6 C8 CHT A 1 12.835 3.506 5.294 1.00 0.00 0.02
HETATM 7 C9 CHT A 1 12.365 4.258 6.295 1.00 0.00 0.14
HETATM 8 O2 CHT A 1 13.332 4.389 7.437 1.00 0.00 -0.30
ENDBRANCH 2 4
BRANCH 2 9
HETATM 9 C7 CHT A 1 16.663 4.518 7.461 1.00 4.71 0.35
BRANCH 9 10
HETATM 10 C1 CHT A 1 17.243 5.230 8.677 1.00 0.00 0.20
HETATM 11 O4 CHT A 1 16.818 5.027 9.728 1.00 0.00 -0.64
HETATM 12 O3 CHT A 1 18.046 6.106 8.908 1.00 0.00 -0.64
ENDBRANCH 9 10
ENDBRANCH 2 9
ENDBRANCH 1 2
BRANCH 1 13
HETATM 13 C4 CHT A 1 17.023 2.039 5.749 1.00 7.51 0.35
BRANCH 13 14
HETATM 14 N1 CHT A 1 17.117 0.715 5.182 1.00 0.00 0.00
HETATM 15 H2 CHT A 1 16.240 0.227 5.182 1.00 0.00 0.28
HETATM 16 H1 CHT A 1 17.432 0.801 4.195 1.00 0.00 0.28
BRANCH 14 17
HETATM 17 C2 CHT A 1 18.204 -0.049 5.920 1.00 0.00 0.24
HETATM 18 O1 CHT A 1 19.656 0.045 5.545 1.00 0.00 -0.30
HETATM 19 C5 CHT A 1 20.217 -0.885 6.582 1.00 0.00 0.14
HETATM 20 C4 CHT A 1 19.280 -1.403 7.384 1.00 0.00 0.02
HETATM 21 C3 CHT A 1 17.983 -0.864 6.957 1.00 0.00 0.06
ENDBRANCH 14 17
ENDBRANCH 13 14
BRANCH 13 22
HETATM 22 O6 CHT A 1 18.398 2.270 5.897 1.00 8.52 -0.36
HETATM 23 HO6 CHT A 1 18.813 2.276 5.007 1.00 0.00 0.21
ENDBRANCH 13 22
ENDBRANCH 1 13
TORSDOF 8`;
```

**Define protein PDBQT text**

In [5]: %%javascript

```
window.recepPDBTxt = `ATOM      1  N   ASP A  40      23.366  -3.399  14.66
ATOM      2  CA   ASP A  40      22.530  -2.226  14.843  1.00  15.81    0.20
ATOM      3  C    ASP A  40      23.197  -1.095  14.078  1.00  15.68    0.24
ATOM      4  O    ASP A  40      24.256  -0.613  14.476  1.00  15.64   -0.27
ATOM      5  CB   ASP A  40      22.432  -1.893  16.332  1.00  15.92    0.14
ATOM      6  CG   ASP A  40      21.603  -0.652  16.619  1.00  16.79    0.17
ATOM      7  OD1  ASP A  40      21.101    0.007  15.681  1.00  17.82   -0.64
ATOM      8  OD2  ASP A  40      21.413  -0.255  17.786  1.00  19.39   -0.64
ATOM      9  H    ASP A  40      24.353  -3.311  14.877  1.00    0.00    0.18
ATOM     10  N    VAL A  41      22.581  -0.683  12.973  1.00  15.78   -0.34
ATOM     11  CA   VAL A  41      23.169    0.349  12.110  1.00  15.92    0.18
ATOM     12  C    VAL A  41      23.137    1.720  12.785  1.00  16.19    0.24
ATOM     13  O    VAL A  41      23.963    2.596  12.486  1.00  16.57   -0.27
ATOM     14  CB   VAL A  41      22.514    0.374  10.712  1.00  15.84    0.00
ATOM     15  CG1  VAL A  41      23.234    1.342    9.761  1.00  15.67    0.01
ATOM     16  CG2  VAL A  41      22.531  -1.022  10.096  1.00  16.11    0.01
ATOM     17  H    VAL A  41      21.709  -1.109  12.695  1.00    0.00    0.16
ATOM     18  N    GLY A  42      22.202    1.885  13.713  1.00  15.88   -0.35
ATOM     19  CA   GLY A  42      22.136    3.082  14.535  1.00  15.70    0.22
ATOM     20  C    GLY A  42      20.886    3.924  14.379  1.00  15.32    0.23
ATOM     21  O    GLY A  42      20.671    4.848  15.172  1.00  15.23   -0.27
ATOM     22  H    GLY A  42      21.603    1.109  13.966  1.00    0.00    0.16
ATOM     23  N    TRP A  43      20.067    3.630  13.366  1.00  14.72   -0.34
ATOM     24  CA   TRP A  43      18.778    4.311  13.226  1.00  14.44    0.18
ATOM     25  C    TRP A  43      17.932    3.984  14.459  1.00  14.06    0.24
ATOM     26  O    TRP A  43      18.069    2.906  15.035  1.00  14.14   -0.27
ATOM     27  CB   TRP A  43      18.028    3.887  11.955  1.00  14.50    0.07
ATOM     28  CG   TRP A  43      18.852    3.543  10.764  1.00  14.78   -0.02
ATOM     29  CD1  TRP A  43      19.772    4.326  10.159  1.00  14.91    0.09
ATOM     30  CD2  TRP A  43      18.860    2.280  10.050  1.00  14.20   -0.00
ATOM     31  NE1  TRP A  43      20.356    3.632    9.123  1.00  14.90   -0.36
ATOM     32  CE2  TRP A  43      19.833    2.360    9.011  1.00  14.43    0.04
ATOM     33  CE3  TRP A  43      18.124    1.077  10.178  1.00  14.13    0.01
ATOM     34  CZ2  TRP A  43      20.063    1.286    8.142  1.00  14.63    0.03
ATOM     35  CZ3  TRP A  43      18.350   -0.008    9.313  1.00  14.56    0.00
ATOM     36  CH2  TRP A  43      19.316    0.106    8.298  1.00  14.58    0.00
ATOM     37  H    TRP A  43      20.294    2.873  12.738  1.00    0.00    0.16
ATOM     38  HE1  TRP A  43      21.179    4.024    8.621  1.00    0.00    0.16
ATOM     39  N    THR A  44      17.062    4.907  14.857  1.00  13.58   -0.34
ATOM     40  CA   THR A  44      16.229    4.697  16.050  1.00  13.07    0.20
ATOM     41  C    THR A  44      15.366    3.431  15.946  1.00  12.89    0.24
ATOM     42  O    THR A  44      15.203    2.719  16.929  1.00  12.25   -0.27
ATOM     43  CB   THR A  44      15.358    5.934  16.326  1.00  13.11    0.14
ATOM     44  OG1  THR A  44      16.191    7.100  16.371  1.00  12.54   -0.39
ATOM     45  CG2  THR A  44      14.740    5.865  17.735  1.00  13.56    0.04
ATOM     46  H    THR A  44      16.968    5.767  14.327  1.00    0.00    0.16
ATOM     47  HG1  THR A  44      16.365    7.406  15.487  1.00    0.00    0.21
ATOM     48  N    ASP A  45      14.834    3.144  14.756  1.00  12.67   -0.34
ATOM     49  CA   ASP A  45      13.958    1.979  14.592  1.00  12.87    0.18
ATOM     50  C    ASP A  45      14.693    0.650  14.775  1.00  13.06    0.24
ATOM     51  O    ASP A  45      14.203   -0.233  15.477  1.00  13.06   -0.27
ATOM     52  CB   ASP A  45      13.196    2.016  13.235  1.00  13.01    0.14
ATOM     53  CG   ASP A  45      14.042    1.759  11.988  1.00  13.25    0.17
ATOM     54  OD1  ASP A  45      15.013    2.526  11.815  1.00  14.05   -0.64`
```

ATOM	55	OD2	ASP	A	45	13.740	0.837	11.196	1.00	13.00	-0.64
ATOM	56	H	ASP	A	45	15.036	3.719	13.950	1.00	0.00	0.16
ATOM	57	N	ILE	A	46	15.868	0.512	14.158	1.00	13.12	-0.34
ATOM	58	CA	ILE	A	46	16.648	-0.722	14.301	1.00	13.55	0.18
ATOM	59	C	ILE	A	46	17.199	-0.860	15.723	1.00	13.70	0.24
ATOM	60	O	ILE	A	46	17.346	-1.969	16.223	1.00	13.30	-0.27
ATOM	61	CB	ILE	A	46	17.763	-0.847	13.206	1.00	13.63	0.01
ATOM	62	CG1	ILE	A	46	18.452	-2.215	13.258	1.00	13.94	0.00
ATOM	63	CG2	ILE	A	46	18.797	0.261	13.335	1.00	14.03	0.01
ATOM	64	CD1	ILE	A	46	17.523	-3.407	13.070	1.00	13.44	0.00
ATOM	65	H	ILE	A	46	16.218	1.256	13.569	1.00	0.00	0.16
ATOM	66	N	THR	A	47	17.474	0.267	16.384	1.00	14.15	-0.34
ATOM	67	CA	THR	A	47	17.887	0.227	17.788	1.00	14.72	0.20
ATOM	68	C	THR	A	47	16.727	-0.263	18.660	1.00	14.48	0.24
ATOM	69	O	THR	A	47	16.931	-1.016	19.615	1.00	14.70	-0.27
ATOM	70	CB	THR	A	47	18.408	1.604	18.247	1.00	14.88	0.14
ATOM	71	OG1	THR	A	47	19.530	1.978	17.436	1.00	15.66	-0.39
ATOM	72	CG2	THR	A	47	19.022	1.523	19.646	1.00	16.13	0.04
ATOM	73	H	THR	A	47	17.394	1.166	15.925	1.00	0.00	0.16
ATOM	74	HG1	THR	A	47	20.171	1.276	17.456	1.00	0.00	0.21
ATOM	75	N	ALA	A	48	15.515	0.167	18.315	1.00	14.28	-0.34
ATOM	76	CA	ALA	A	48	14.303	-0.202	19.046	1.00	14.12	0.17
ATOM	77	C	ALA	A	48	13.950	-1.678	18.886	1.00	13.83	0.24
ATOM	78	O	ALA	A	48	13.683	-2.357	19.877	1.00	13.54	-0.27
ATOM	79	CB	ALA	A	48	13.129	0.678	18.618	1.00	14.05	0.04
ATOM	80	H	ALA	A	48	15.423	0.801	17.531	1.00	0.00	0.16
ATOM	81	N	THR	A	49	13.951	-2.172	17.648	1.00	13.66	-0.34
ATOM	82	CA	THR	A	49	13.629	-3.581	17.402	1.00	13.40	0.19
ATOM	83	C	THR	A	49	14.694	-4.504	17.988	1.00	13.28	0.22
ATOM	84	O	THR	A	49	14.371	-5.555	18.535	1.00	13.49	-0.28
ATOM	85	CB	THR	A	49	13.441	-3.883	15.900	1.00	13.46	0.14
ATOM	86	OG1	THR	A	49	14.556	-3.379	15.153	1.00	13.38	-0.39
ATOM	87	CG2	THR	A	49	12.238	-3.145	15.346	1.00	13.62	0.04
ATOM	88	H	THR	A	49	14.157	-1.564	16.866	1.00	0.00	0.16
ATOM	89	HG1	THR	A	49	14.546	-2.434	15.199	1.00	0.00	0.21
ATOM	90	N	GLY	A	88	17.040	-5.422	10.405	1.00	12.46	-0.33
ATOM	91	CA	GLY	A	88	16.804	-4.172	9.687	1.00	12.42	0.22
ATOM	92	C	GLY	A	88	16.909	-4.259	8.184	1.00	12.27	0.21
ATOM	93	O	GLY	A	88	17.363	-3.303	7.556	1.00	12.16	-0.28
ATOM	94	H	GLY	A	88	17.987	-5.765	10.479	1.00	0.00	0.18
ATOM	95	N	TRP	A	90	15.564	-3.624	5.029	1.00	12.20	-0.32
ATOM	96	CA	TRP	A	90	14.502	-2.864	4.372	1.00	12.40	0.19
ATOM	97	C	TRP	A	90	14.476	-3.199	2.875	1.00	12.75	0.24
ATOM	98	O	TRP	A	90	15.493	-3.151	2.174	1.00	13.02	-0.27
ATOM	99	CB	TRP	A	90	14.718	-1.367	4.573	1.00	12.16	0.07
ATOM	100	CG	TRP	A	90	14.277	-0.849	5.935	1.00	11.70	-0.02
ATOM	101	CD1	TRP	A	90	15.070	-0.651	7.015	1.00	11.86	0.09
ATOM	102	CD2	TRP	A	90	12.935	-0.486	6.377	1.00	12.11	-0.00
ATOM	103	NE1	TRP	A	90	14.322	-0.196	8.083	1.00	11.22	-0.36
ATOM	104	CE2	TRP	A	90	12.995	-0.100	7.753	1.00	11.58	0.04
ATOM	105	CE3	TRP	A	90	11.664	-0.452	5.762	1.00	12.22	0.01
ATOM	106	CZ2	TRP	A	90	11.867	0.303	8.478	1.00	11.72	0.03
ATOM	107	CZ3	TRP	A	90	10.522	-0.035	6.478	1.00	11.86	0.00
ATOM	108	CH2	TRP	A	90	10.627	0.353	7.827	1.00	11.69	0.00
ATOM	109	H	TRP	A	90	16.500	-3.228	5.095	1.00	0.00	0.18
ATOM	110	HE1	TRP	A	90	14.655	-0.008	9.037	1.00	0.00	0.16
ATOM	111	N	MET	A	91	13.288	-3.554	2.389	1.00	13.09	-0.34

ATOM	112	CA	MET	A	91	13.056	-3.901	0.997	1.00	13.24	0.17
ATOM	113	C	MET	A	91	11.899	-3.053	0.465	1.00	13.24	0.24
ATOM	114	O	MET	A	91	10.902	-2.887	1.164	1.00	13.54	-0.27
ATOM	115	CB	MET	A	91	12.752	-5.398	0.858	1.00	13.31	0.04
ATOM	116	CG	MET	A	91	13.889	-6.315	1.325	1.00	14.49	0.07
ATOM	117	SD	MET	A	91	15.369	-6.218	0.294	1.00	15.59	-0.17
ATOM	118	CE	MET	A	91	14.916	-7.321	-1.041	1.00	16.54	0.08
ATOM	119	H	MET	A	91	12.484	-3.598	3.016	1.00	0.00	0.16
ATOM	120	N	PRO	A	92	11.985	-2.553	-0.771	1.00	13.31	-0.33
ATOM	121	CA	PRO	A	92	12.964	-2.988	-1.772	1.00	13.27	0.17
ATOM	122	C	PRO	A	92	14.346	-2.294	-1.822	1.00	13.10	0.24
ATOM	123	O	PRO	A	92	15.187	-2.715	-2.602	1.00	12.78	-0.27
ATOM	124	CB	PRO	A	92	12.229	-2.707	-3.080	1.00	13.32	0.03
ATOM	125	CG	PRO	A	92	11.445	-1.452	-2.784	1.00	13.37	0.02
ATOM	126	CD	PRO	A	92	11.080	-1.519	-1.310	1.00	13.30	0.12
ATOM	127	N	THR	A	93	14.665	-1.240	-1.077	1.00	13.14	-0.34
ATOM	128	CA	THR	A	93	15.904	-0.503	-1.373	1.00	13.15	0.20
ATOM	129	C	THR	A	93	17.214	-1.240	-1.093	1.00	13.41	0.24
ATOM	130	O	THR	A	93	18.231	-0.857	-1.689	1.00	13.68	-0.27
ATOM	131	CB	THR	A	93	15.853	0.835	-0.661	1.00	12.81	0.14
ATOM	132	OG1	THR	A	93	15.589	0.602	0.721	1.00	12.43	-0.39
ATOM	133	CG2	THR	A	93	14.783	1.692	-1.378	1.00	12.91	0.04
ATOM	134	H	THR	A	93	14.063	-0.836	-0.375	1.00	0.00	0.16
ATOM	135	HG1	THR	A	93	16.413	0.539	1.229	1.00	0.00	0.21
ATOM	136	N	LYS	A	94	17.186	-2.333	-0.311	1.00	13.91	-0.34
ATOM	137	CA	LYS	A	94	18.430	-3.076	-0.092	1.00	14.19	0.16
ATOM	138	C	LYS	A	94	18.718	-4.139	-1.030	1.00	14.32	0.21
ATOM	139	O	LYS	A	94	19.695	-4.858	-0.825	1.00	14.35	-0.28
ATOM	140	CB	LYS	A	94	18.294	-3.889	1.138	1.00	0.00	0.03
ATOM	141	CG	LYS	A	94	18.731	-2.873	2.065	1.00	0.00	0.00
ATOM	142	CD	LYS	A	94	18.597	-3.520	3.332	1.00	0.00	0.02
ATOM	143	CE	LYS	A	94	18.768	-2.336	4.134	1.00	0.00	0.22
ATOM	144	NZ	LYS	A	94	18.930	-2.951	5.358	1.00	0.00	-0.07
ATOM	145	H	LYS	A	94	16.341	-2.663	0.188	1.00	0.00	0.16
ATOM	146	HZ1	LYS	A	94	18.102	-3.274	5.843	1.00	0.00	0.27
ATOM	147	HZ2	LYS	A	94	19.613	-3.692	5.269	1.00	0.00	0.27
ATOM	148	HZ3	LYS	A	94	19.331	-2.252	5.977	1.00	0.00	0.27
ATOM	149	N	LEU	A	114	8.111	-6.486	9.691	1.00	12.35	-0.32
ATOM	150	CA	LEU	A	114	7.316	-5.252	9.629	1.00	11.61	0.17
ATOM	151	C	LEU	A	114	6.731	-5.002	8.242	1.00	11.30	0.22
ATOM	152	O	LEU	A	114	7.458	-4.994	7.244	1.00	10.95	-0.28
ATOM	153	CB	LEU	A	114	8.136	-4.028	10.079	1.00	11.79	0.03
ATOM	154	CG	LEU	A	114	7.343	-2.710	10.162	1.00	11.19	-0.02
ATOM	155	CD1	LEU	A	114	6.399	-2.729	11.361	1.00	11.81	0.00
ATOM	156	CD2	LEU	A	114	8.291	-1.514	10.220	1.00	11.64	0.00
ATOM	157	H	LEU	A	114	8.559	-6.809	8.844	1.00	0.00	0.18
ATOM	158	N	GLY	A	116	3.931	-2.315	5.960	1.00	9.85	-0.33
ATOM	159	CA	GLY	A	116	3.287	-0.999	5.932	1.00	9.60	0.24
ATOM	160	C	GLY	A	116	4.183	0.158	6.288	1.00	9.85	0.23
ATOM	161	O	GLY	A	116	3.757	1.287	6.463	1.00	9.67	-0.27
ATOM	162	H	GLY	A	116	4.157	-2.755	5.076	1.00	0.00	0.18
ATOM	163	N	ALA	A	117	5.465	-0.095	6.369	1.00	9.43	-0.34
ATOM	164	CA	ALA	A	117	6.400	0.972	6.488	1.00	9.61	0.17
ATOM	165	C	ALA	A	117	6.764	1.450	5.080	1.00	9.59	0.24
ATOM	166	O	ALA	A	117	6.680	0.701	4.106	1.00	9.45	-0.27
ATOM	167	CB	ALA	A	117	7.545	0.353	7.198	1.00	9.53	0.04
ATOM	168	H	ALA	A	117	5.800	-1.018	6.144	1.00	0.00	0.16

ATOM	169	N	LYS	A	118	7.055	2.741	4.970	1.00	9.92	-0.34
ATOM	170	CA	LYS	A	118	7.014	3.486	3.722	1.00	9.68	0.17
ATOM	171	C	LYS	A	118	7.838	4.751	3.874	1.00	9.08	0.24
ATOM	172	O	LYS	A	118	7.817	5.367	4.944	1.00	8.87	-0.27
ATOM	173	CB	LYS	A	118	5.544	3.795	3.317	1.00	10.07	0.03
ATOM	174	CG	LYS	A	118	4.652	4.446	4.405	1.00	11.88	0.00
ATOM	175	CD	LYS	A	118	4.097	5.851	4.088	1.00	15.78	0.02
ATOM	176	CE	LYS	A	118	5.113	7.010	4.110	1.00	17.52	0.22
ATOM	177	NZ	LYS	A	118	5.813	7.122	5.402	1.00	19.32	-0.07
ATOM	178	H	LYS	A	118	7.240	3.259	5.820	1.00	0.00	0.16
ATOM	179	HZ1	LYS	A	118	6.491	6.364	5.479	1.00	0.00	0.27
ATOM	180	HZ2	LYS	A	118	6.350	7.980	5.469	1.00	0.00	0.27
ATOM	181	HZ3	LYS	A	118	5.185	7.084	6.193	1.00	0.00	0.27
ATOM	182	N	GLY	A	119	8.457	5.215	2.797	1.00	8.22	-0.35
ATOM	183	CA	GLY	A	119	9.061	6.528	2.736	1.00	7.98	0.22
ATOM	184	C	GLY	A	119	9.867	6.728	1.468	1.00	8.26	0.23
ATOM	185	O	GLY	A	119	9.973	5.818	0.662	1.00	8.10	-0.27
ATOM	186	H	GLY	A	119	8.483	4.677	1.931	1.00	0.00	0.16
ATOM	187	N	THR	A	120	10.466	7.880	1.245	1.00	8.66	-0.34
ATOM	188	CA	THR	A	120	11.225	8.115	0.031	1.00	9.18	0.20
ATOM	189	C	THR	A	120	12.042	9.380	0.302	1.00	9.49	0.24
ATOM	190	O	THR	A	120	12.297	9.711	1.470	1.00	9.35	-0.27
ATOM	191	CB	THR	A	120	10.256	8.056	-1.205	1.00	9.02	0.14
ATOM	192	OG1	THR	A	120	10.933	8.229	-2.416	1.00	9.63	-0.39
ATOM	193	CG2	THR	A	120	9.048	9.002	-1.172	1.00	8.63	0.04
ATOM	194	H	THR	A	120	10.595	8.555	1.989	1.00	0.00	0.16
ATOM	195	HG1	THR	A	120	10.295	8.230	-3.115	1.00	0.00	0.21
ATOM	196	N	LEU	A	121	12.404	10.131	-0.741	1.00	10.01	-0.34
ATOM	197	CA	LEU	A	121	12.752	11.533	-0.558	1.00	10.62	0.17
ATOM	198	C	LEU	A	121	11.499	12.279	-0.068	1.00	10.95	0.24
ATOM	199	O	LEU	A	121	10.398	12.075	-0.578	1.00	11.41	-0.27
ATOM	200	CB	LEU	A	121	13.317	12.169	-1.842	1.00	10.89	0.03
ATOM	201	CG	LEU	A	121	14.734	11.686	-2.226	1.00	10.87	-0.02
ATOM	202	CD1	LEU	A	121	15.183	12.340	-3.537	1.00	11.50	0.00
ATOM	203	CD2	LEU	A	121	15.780	11.983	-1.137	1.00	11.42	0.00
ATOM	204	H	LEU	A	121	12.110	9.811	-1.656	1.00	0.00	0.16
ATOM	205	N	ALA	A	122	11.665	13.085	0.971	1.00	11.13	-0.34
ATOM	206	CA	ALA	A	122	10.648	13.926	1.569	1.00	11.41	0.17
ATOM	207	C	ALA	A	122	11.131	15.364	1.571	1.00	11.61	0.24
ATOM	208	O	ALA	A	122	12.323	15.632	1.403	1.00	11.78	-0.27
ATOM	209	CB	ALA	A	122	10.348	13.478	2.998	1.00	10.72	0.04
ATOM	210	H	ALA	A	122	12.621	13.193	1.315	1.00	0.00	0.16
ATOM	211	N	THR	A	123	10.196	16.283	1.776	1.00	11.79	-0.34
ATOM	212	CA	THR	A	123	10.534	17.686	1.953	1.00	11.84	0.19
ATOM	213	C	THR	A	123	9.774	18.241	3.152	1.00	12.05	0.22
ATOM	214	O	THR	A	123	8.868	17.586	3.671	1.00	12.08	-0.28
ATOM	215	CB	THR	A	123	10.273	18.491	0.649	1.00	12.02	0.14
ATOM	216	OG1	THR	A	123	10.808	19.813	0.790	1.00	11.74	-0.39
ATOM	217	CG2	THR	A	123	8.779	18.723	0.409	1.00	11.30	0.04
ATOM	218	H	THR	A	123	9.229	16.002	1.885	1.00	0.00	0.16
ATOM	219	HG1	THR	A	123	11.739	19.741	0.956	1.00	0.00	0.21
ATOM	220	N	ILE	A	149	21.031	17.360	-1.244	1.00	11.50	-0.32
ATOM	221	CA	ILE	A	149	20.030	16.443	-0.695	1.00	11.16	0.19
ATOM	222	C	ILE	A	149	20.669	15.806	0.527	1.00	11.40	0.24
ATOM	223	O	ILE	A	149	21.818	15.372	0.464	1.00	11.23	-0.27
ATOM	224	CB	ILE	A	149	19.635	15.356	-1.721	1.00	11.30	0.01
ATOM	225	CG1	ILE	A	149	18.877	15.979	-2.895	1.00	10.65	0.00

ATOM	226	CG2	ILE	A	149	18.794	14.248	-1.046	1.00	11.03	0.01
ATOM	227	CD1	ILE	A	149	18.826	15.097	-4.137	1.00	12.78	0.00
ATOM	228	H	ILE	A	149	21.989	17.032	-1.278	1.00	0.00	0.18
ATOM	229	N	TYR	A	150	19.930	15.761	1.631	1.00	11.16	-0.34
ATOM	230	CA	TYR	A	150	20.458	15.239	2.889	1.00	11.90	0.18
ATOM	231	C	TYR	A	150	20.104	13.785	3.133	1.00	11.90	0.24
ATOM	232	O	TYR	A	150	18.926	13.422	3.221	1.00	12.35	-0.27
ATOM	233	CB	TYR	A	150	20.001	16.110	4.058	1.00	11.76	0.07
ATOM	234	CG	TYR	A	150	20.682	17.447	4.050	1.00	12.50	-0.05
ATOM	235	CD1	TYR	A	150	20.163	18.512	3.312	1.00	12.40	0.01
ATOM	236	CD2	TYR	A	150	21.872	17.642	4.751	1.00	13.12	0.01
ATOM	237	CE1	TYR	A	150	20.801	19.742	3.289	1.00	13.12	0.03
ATOM	238	CE2	TYR	A	150	22.521	18.865	4.731	1.00	13.87	0.03
ATOM	239	CZ	TYR	A	150	21.980	19.910	4.001	1.00	13.21	0.06
ATOM	240	OH	TYR	A	150	22.616	21.125	3.984	1.00	13.02	-0.36
ATOM	241	H	TYR	A	150	18.982	16.116	1.615	1.00	0.00	0.16
ATOM	242	HH	TYR	A	150	23.394	21.145	4.520	1.00	0.00	0.21
ATOM	243	N	GLY	A	151	21.131	12.941	3.228	1.00	11.78	-0.35
ATOM	244	CA	GLY	A	151	20.991	11.520	3.503	1.00	11.88	0.22
ATOM	245	C	GLY	A	151	21.339	11.195	4.955	1.00	11.73	0.23
ATOM	246	O	GLY	A	151	21.381	12.069	5.820	1.00	11.48	-0.27
ATOM	247	H	GLY	A	151	22.083	13.319	3.195	1.00	0.00	0.16
ATOM	248	N	ILE	A	152	21.627	9.925	5.232	1.00	11.73	-0.34
ATOM	249	CA	ILE	A	152	21.999	9.437	6.555	1.00	11.80	0.18
ATOM	250	C	ILE	A	152	23.412	8.862	6.484	1.00	11.89	0.24
ATOM	251	O	ILE	A	152	24.271	9.503	5.869	1.00	11.83	-0.27
ATOM	252	CB	ILE	A	152	20.904	8.523	7.143	1.00	11.64	0.01
ATOM	253	CG1	ILE	A	152	20.536	7.372	6.203	1.00	11.72	0.00
ATOM	254	CG2	ILE	A	152	19.656	9.335	7.510	1.00	13.03	0.01
ATOM	255	CD1	ILE	A	152	19.482	6.459	6.807	1.00	11.33	0.00
ATOM	256	H	ILE	A	152	21.670	9.250	4.470	1.00	0.00	0.16
ATOM	257	N	GLU	A	153	23.706	7.755	7.177	1.00	12.00	-0.34
ATOM	258	CA	GLU	A	153	25.072	7.301	7.365	1.00	12.14	0.16
ATOM	259	C	GLU	A	153	25.688	6.748	6.073	1.00	12.25	0.21
ATOM	260	O	GLU	A	153	24.985	6.183	5.227	1.00	12.49	-0.28
ATOM	261	CB	GLU	A	153	25.167	6.305	8.535	1.00	12.26	0.04
ATOM	262	CG	GLU	A	153	24.804	4.831	8.230	1.00	12.09	0.11
ATOM	263	CD	GLU	A	153	23.324	4.579	7.940	1.00	11.17	0.17
ATOM	264	OE1	GLU	A	153	22.996	3.503	7.395	1.00	11.67	-0.64
ATOM	265	OE2	GLU	A	153	22.476	5.444	8.253	1.00	12.22	-0.64
ATOM	266	H	GLU	A	153	22.981	7.133	7.544	1.00	0.00	0.16
ATOM	267	N	ASN	A	156	24.620	3.641	3.511	1.00	11.56	-0.32
ATOM	268	CA	ASN	A	156	23.174	3.426	3.553	1.00	11.42	0.19
ATOM	269	C	ASN	A	156	22.553	3.137	2.159	1.00	11.44	0.24
ATOM	270	O	ASN	A	156	22.966	3.688	1.134	1.00	11.29	-0.27
ATOM	271	CB	ASN	A	156	22.493	4.626	4.218	1.00	11.60	0.13
ATOM	272	CG	ASN	A	156	21.085	4.270	4.620	1.00	11.51	0.21
ATOM	273	OD1	ASN	A	156	20.164	4.472	3.840	1.00	10.74	-0.27
ATOM	274	ND2	ASN	A	156	20.916	3.707	5.804	1.00	11.00	-0.37
ATOM	275	H	ASN	A	156	25.016	4.493	3.924	1.00	0.00	0.18
ATOM	276	2HD2	ASN	A	156	19.999	3.479	6.150	1.00	0.00	0.15
ATOM	277	1HD2	ASN	A	156	21.740	3.622	6.443	1.00	0.00	0.15
ATOM	278	N	ASP	A	157	21.519	2.288	2.150	1.00	11.51	-0.34
ATOM	279	CA	ASP	A	157	20.731	1.845	0.999	1.00	11.62	0.18
ATOM	280	C	ASP	A	157	19.943	3.001	0.369	1.00	12.02	0.24
ATOM	281	O	ASP	A	157	19.759	3.023	-0.847	1.00	11.71	-0.27
ATOM	282	CB	ASP	A	157	19.723	0.735	1.415	1.00	11.55	0.14



ATOM	283	CG	ASP	A	157	18.765	1.054	2.564	1.00	11.89	0.17
ATOM	284	OD1	ASP	A	157	19.182	1.675	3.557	1.00	10.60	-0.64
ATOM	285	OD2	ASP	A	157	17.582	0.644	2.574	1.00	12.39	-0.64
ATOM	286	H	ASP	A	157	21.161	1.985	3.048	1.00	0.00	0.16
ATOM	287	N	GLY	A	158	19.492	3.973	1.169	1.00	11.98	-0.35
ATOM	288	CA	GLY	A	158	18.846	5.178	0.677	1.00	12.21	0.22
ATOM	289	C	GLY	A	158	19.858	6.139	0.087	1.00	12.14	0.23
ATOM	290	O	GLY	A	158	19.643	6.612	-1.023	1.00	12.46	-0.27
ATOM	291	H	GLY	A	158	19.709	3.906	2.166	1.00	0.00	0.16
ATOM	292	N	ASN	A	159	20.985	6.349	0.784	1.00	11.91	-0.34
ATOM	293	CA	ASN	A	159	22.128	7.158	0.336	1.00	11.69	0.17
ATOM	294	C	ASN	A	159	22.619	6.733	-1.034	1.00	11.98	0.22
ATOM	295	O	ASN	A	159	22.738	7.558	-1.935	1.00	11.83	-0.28
ATOM	296	CB	ASN	A	159	23.309	7.088	1.319	1.00	11.90	0.13
ATOM	297	CG	ASN	A	159	23.088	7.968	2.533	1.00	11.42	0.21
ATOM	298	OD1	ASN	A	159	21.971	8.144	3.023	1.00	14.57	-0.27
ATOM	299	ND2	ASN	A	159	24.150	8.541	3.040	1.00	8.90	-0.37
ATOM	300	H	ASN	A	159	21.061	5.916	1.694	1.00	0.00	0.16
ATOM	301	2HD2	ASN	A	159	24.040	9.116	3.865	1.00	0.00	0.15
ATOM	302	1HD2	ASN	A	159	25.077	8.400	2.642	1.00	0.00	0.15
ATOM	303	N	ILE	A	162	20.190	7.710	-3.901	1.00	12.21	-0.32
ATOM	304	CA	ILE	A	162	20.287	9.128	-4.228	1.00	12.29	0.18
ATOM	305	C	ILE	A	162	21.598	9.426	-4.950	1.00	12.35	0.22
ATOM	306	O	ILE	A	162	21.601	10.142	-5.954	1.00	12.59	-0.28
ATOM	307	CB	ILE	A	162	20.179	10.043	-2.985	1.00	12.46	0.01
ATOM	308	CG1	ILE	A	162	18.987	9.672	-2.097	1.00	12.46	0.00
ATOM	309	CG2	ILE	A	162	20.090	11.519	-3.416	1.00	12.03	0.01
ATOM	310	CD1	ILE	A	162	19.075	10.291	-0.707	1.00	12.48	0.00
ATOM	311	H	ILE	A	162	20.304	7.420	-2.936	1.00	0.00	0.18
ATOM	312	N	VAL	A	179	24.564	14.939	1.077	1.00	12.38	-0.32
ATOM	313	CA	VAL	A	179	25.237	15.236	2.332	1.00	12.08	0.19
ATOM	314	C	VAL	A	179	24.992	14.066	3.276	1.00	11.87	0.24
ATOM	315	O	VAL	A	179	23.853	13.796	3.663	1.00	11.45	-0.27
ATOM	316	CB	VAL	A	179	24.745	16.552	2.969	1.00	12.10	0.01
ATOM	317	CG1	VAL	A	179	25.613	16.914	4.169	1.00	12.06	0.01
ATOM	318	CG2	VAL	A	179	24.731	17.691	1.945	1.00	11.62	0.01
ATOM	319	H	VAL	A	179	23.624	15.286	0.930	1.00	0.00	0.18
ATOM	320	N	GLU	A	180	26.065	13.362	3.618	1.00	11.81	-0.34
ATOM	321	CA	GLU	A	180	25.960	12.170	4.465	1.00	12.14	0.17
ATOM	322	C	GLU	A	180	26.339	12.483	5.900	1.00	12.10	0.24
ATOM	323	O	GLU	A	180	27.287	13.227	6.153	1.00	11.96	-0.27
ATOM	324	CB	GLU	A	180	26.857	11.051	3.937	1.00	12.46	0.04
ATOM	325	CG	GLU	A	180	26.711	10.790	2.450	1.00	12.39	0.11
ATOM	326	CD	GLU	A	180	27.369	9.494	2.039	1.00	13.53	0.17
ATOM	327	OE1	GLU	A	180	28.620	9.469	1.955	1.00	13.91	-0.64
ATOM	328	OE2	GLU	A	180	26.635	8.505	1.809	1.00	12.09	-0.64
ATOM	329	H	GLU	A	180	26.974	13.621	3.263	1.00	0.00	0.16
ATOM	330	N	SER	A	181	25.594	11.907	6.839	1.00	12.07	-0.34
ATOM	331	CA	SER	A	181	25.902	12.055	8.257	1.00	11.98	0.20
ATOM	332	C	SER	A	181	25.385	10.843	9.014	1.00	11.98	0.24
ATOM	333	O	SER	A	181	26.126	9.883	9.248	1.00	11.67	-0.27
ATOM	334	CB	SER	A	181	25.316	13.358	8.823	1.00	12.16	0.19
ATOM	335	OG	SER	A	181	23.935	13.488	8.521	1.00	12.06	-0.39
ATOM	336	H	SER	A	181	24.851	11.275	6.570	1.00	0.00	0.16
ATOM	337	HG	SER	A	181	23.837	13.530	7.581	1.00	0.00	0.20
ATOM	338	N	SER	A	182	24.101	10.901	9.361	1.00	11.98	-0.34
ATOM	339	CA	SER	A	182	23.399	9.874	10.128	1.00	11.77	0.20

ATOM	340	C	SER	A	182	21.911	10.313	10.165	1.00	11.89	0.24
ATOM	341	O	SER	A	182	21.610	11.434	9.858	1.00	11.39	-0.27
ATOM	342	CB	SER	A	182	23.983	9.754	11.538	1.00	12.24	0.19
ATOM	343	OG	SER	A	182	23.845	10.974	12.255	1.00	11.50	-0.39
ATOM	344	H	SER	A	182	23.581	11.740	9.131	1.00	0.00	0.16
ATOM	345	HG	SER	A	182	24.214	10.852	13.117	1.00	0.00	0.20
ATOM	346	N	LYS	A	183	20.859	9.606	10.560	1.00	11.60	-0.34
ATOM	347	CA	LYS	A	183	19.583	10.376	10.752	1.00	11.68	0.17
ATOM	348	C	LYS	A	183	19.576	11.281	11.939	1.00	11.59	0.24
ATOM	349	O	LYS	A	183	18.733	12.171	11.953	1.00	11.49	-0.27
ATOM	350	CB	LYS	A	183	18.309	9.610	10.723	1.00	0.00	0.03
ATOM	351	CG	LYS	A	183	17.455	9.308	11.973	1.00	0.00	0.00
ATOM	352	CD	LYS	A	183	18.177	8.493	13.020	1.00	0.00	0.02
ATOM	353	CE	LYS	A	183	19.161	7.537	12.364	1.00	0.00	0.22
ATOM	354	NZ	LYS	A	183	18.466	6.708	11.341	1.00	0.00	-0.07
ATOM	355	H	LYS	A	183	20.943	8.613	10.692	1.00	0.00	0.16
ATOM	356	HZ1	LYS	A	183	18.878	5.799	11.152	1.00	0.00	0.27
ATOM	357	HZ2	LYS	A	183	17.490	6.496	11.464	1.00	0.00	0.27
ATOM	358	HZ3	LYS	A	183	18.465	7.012	10.355	1.00	0.00	0.27
ATOM	359	N	GLN	A	184	20.465	11.086	12.922	0.70	11.69	-0.34
ATOM	360	CA	GLN	A	184	20.556	12.140	13.886	0.70	11.77	0.17
ATOM	361	C	GLN	A	184	21.042	13.457	13.247	0.70	11.78	0.24
ATOM	362	O	GLN	A	184	20.450	14.518	13.468	0.70	11.77	-0.27
ATOM	363	CB	GLN	A	184	21.433	11.685	15.064	0.70	11.86	0.04
ATOM	364	CG	GLN	A	184	20.881	10.449	15.859	0.70	12.45	0.08
ATOM	365	CD	GLN	A	184	21.005	9.079	15.141	0.70	12.58	0.14
ATOM	366	OE1	GLN	A	184	21.931	8.974	14.196	0.70	13.41	-0.17
ATOM	367	NE2	GLN	A	184	20.269	8.128	15.467	0.70	8.45	-0.38
ATOM	368	H	GLN	A	184	21.090	10.271	13.055	0.70	0.00	0.16
ATOM	369	2HE2	GLN	A	184	20.381	7.228	15.019	0.70	0.00	0.15
ATOM	370	1HE2	GLN	A	184	19.570	8.248	16.186	0.70	0.00	0.15
ATOM	371	N	GLY	A	185	22.087	13.371	12.424	1.00	11.76	-0.35
ATOM	372	CA	GLY	A	185	22.617	14.520	11.671	1.00	11.69	0.22
ATOM	373	C	GLY	A	185	21.616	15.109	10.689	1.00	12.00	0.23
ATOM	374	O	GLY	A	185	21.431	16.328	10.635	1.00	11.70	-0.27
ATOM	375	H	GLY	A	185	22.521	12.468	12.274	1.00	0.00	0.16
ATOM	376	N	MET	A	186	20.961	14.236	9.921	1.00	12.04	-0.34
ATOM	377	CA	MET	A	186	19.958	14.648	8.934	1.00	12.23	0.17
ATOM	378	C	MET	A	186	18.794	15.386	9.603	1.00	12.44	0.24
ATOM	379	O	MET	A	186	18.417	16.470	9.174	1.00	11.89	-0.27
ATOM	380	CB	MET	A	186	19.446	13.428	8.149	1.00	12.10	0.04
ATOM	381	CG	MET	A	186	18.412	13.746	7.082	1.00	11.58	0.07
ATOM	382	SD	MET	A	186	17.457	12.312	6.525	1.00	12.65	-0.17
ATOM	383	CE	MET	A	186	16.449	12.014	7.980	1.00	12.54	0.08
ATOM	384	H	MET	A	186	21.167	13.248	10.008	1.00	0.00	0.16
ATOM	385	N	LEU	A	187	18.255	14.803	10.673	1.00	12.67	-0.34
ATOM	386	CA	LEU	A	187	17.145	15.418	11.407	1.00	13.26	0.17
ATOM	387	C	LEU	A	187	17.502	16.724	12.101	1.00	13.07	0.24
ATOM	388	O	LEU	A	187	16.641	17.590	12.264	1.00	12.98	-0.27
ATOM	389	CB	LEU	A	187	16.536	14.433	12.407	1.00	13.37	0.03
ATOM	390	CG	LEU	A	187	15.819	13.247	11.752	1.00	14.61	-0.02
ATOM	391	CD1	LEU	A	187	15.477	12.202	12.791	1.00	14.72	0.00
ATOM	392	CD2	LEU	A	187	14.568	13.676	10.985	1.00	16.49	0.00
ATOM	393	H	LEU	A	187	18.608	13.909	10.990	1.00	0.00	0.16
ATOM	394	N	ALA	A	188	18.762	16.859	12.512	1.00	13.21	-0.34
ATOM	395	CA	ALA	A	188	19.264	18.111	13.072	1.00	13.31	0.17
ATOM	396	C	ALA	A	188	19.209	19.213	12.011	1.00	13.46	0.24

ATOM	397	O	ALA	A	188	18.840	20.350	12.299	1.00	13.24	-0.27
ATOM	398	CB	ALA	A	188	20.685	17.930	13.583	1.00	13.23	0.04
ATOM	399	H	ALA	A	188	19.411	16.093	12.388	1.00	0.00	0.16
ATOM	400	N	GLN	A	189	19.569	18.851	10.782	1.00	13.81	-0.34
ATOM	401	CA	GLN	A	189	19.539	19.765	9.646	1.00	13.98	0.17
ATOM	402	C	GLN	A	189	18.104	20.136	9.254	1.00	13.85	0.24
ATOM	403	O	GLN	A	189	17.820	21.294	8.937	1.00	13.52	-0.27
ATOM	404	CB	GLN	A	189	20.294	19.145	8.459	1.00	14.41	0.04
ATOM	405	CG	GLN	A	189	20.443	20.049	7.239	1.00	15.38	0.08
ATOM	406	CD	GLN	A	189	21.258	21.307	7.500	1.00	17.22	0.14
ATOM	407	OE1	GLN	A	189	22.257	21.210	8.371	1.00	19.78	-0.17
ATOM	408	NE2	GLN	A	189	20.984	22.354	6.912	1.00	17.35	-0.38
ATOM	409	H	GLN	A	189	19.860	17.896	10.617	1.00	0.00	0.16
ATOM	410	2HE2	GLN	A	189	21.534	23.184	7.080	1.00	0.00	0.15
ATOM	411	1HE2	GLN	A	189	20.219	22.378	6.252	1.00	0.00	0.15
ATOM	412	N	VAL	A	190	17.202	19.156	9.284	1.00	13.86	-0.34
ATOM	413	CA	VAL	A	190	15.775	19.417	9.064	1.00	14.02	0.16
ATOM	414	C	VAL	A	190	15.253	20.421	10.102	1.00	14.30	0.21
ATOM	415	O	VAL	A	190	14.514	21.350	9.762	1.00	14.13	-0.28
ATOM	416	CB	VAL	A	190	14.948	18.102	9.099	1.00	14.45	0.00
ATOM	417	CG1	VAL	A	190	13.451	18.376	9.064	1.00	14.20	0.01
ATOM	418	CG2	VAL	A	190	15.347	17.192	7.939	1.00	13.67	0.01
ATOM	419	H	VAL	A	190	17.494	18.215	9.512	1.00	0.00	0.16
ATOM	420	N	ILE	A	200	14.126	22.005	2.370	1.00	11.66	-0.32
ATOM	421	CA	ILE	A	200	15.143	20.956	2.466	1.00	11.74	0.19
ATOM	422	C	ILE	A	200	14.565	19.673	1.876	1.00	11.78	0.24
ATOM	423	O	ILE	A	200	13.363	19.429	1.988	1.00	11.82	-0.27
ATOM	424	CB	ILE	A	200	15.617	20.759	3.947	1.00	11.89	0.01
ATOM	425	CG1	ILE	A	200	16.806	19.783	4.021	1.00	12.45	0.00
ATOM	426	CG2	ILE	A	200	14.454	20.323	4.850	1.00	11.59	0.01
ATOM	427	CD1	ILE	A	200	17.373	19.578	5.447	1.00	11.83	0.00
ATOM	428	H	ILE	A	200	13.155	21.726	2.409	1.00	0.00	0.18
ATOM	429	N	VAL	A	201	15.414	18.885	1.216	1.00	11.57	-0.34
ATOM	430	CA	VAL	A	201	15.025	17.581	0.684	1.00	11.51	0.18
ATOM	431	C	VAL	A	201	15.910	16.521	1.329	1.00	11.35	0.24
ATOM	432	O	VAL	A	201	17.133	16.668	1.379	1.00	11.16	-0.27
ATOM	433	CB	VAL	A	201	15.104	17.529	-0.869	1.00	11.76	0.00
ATOM	434	CG1	VAL	A	201	14.802	16.125	-1.396	1.00	11.62	0.01
ATOM	435	CG2	VAL	A	201	14.138	18.538	-1.481	1.00	11.93	0.01
ATOM	436	H	VAL	A	201	16.386	19.150	1.143	1.00	0.00	0.16
ATOM	437	N	PHE	A	202	15.276	15.463	1.834	1.00	11.11	-0.34
ATOM	438	CA	PHE	A	202	15.958	14.470	2.661	1.00	11.22	0.18
ATOM	439	C	PHE	A	202	15.260	13.108	2.608	1.00	11.29	0.24
ATOM	440	O	PHE	A	202	14.198	12.967	2.006	1.00	11.42	-0.27
ATOM	441	CB	PHE	A	202	16.048	14.978	4.104	1.00	10.67	0.07
ATOM	442	CG	PHE	A	202	14.707	15.211	4.742	1.00	11.26	-0.05
ATOM	443	CD1	PHE	A	202	14.137	14.244	5.570	1.00	10.85	0.00
ATOM	444	CD2	PHE	A	202	14.007	16.397	4.515	1.00	10.34	0.00
ATOM	445	CE1	PHE	A	202	12.885	14.447	6.150	1.00	11.52	0.00
ATOM	446	CE2	PHE	A	202	12.762	16.608	5.087	1.00	11.79	0.00
ATOM	447	CZ	PHE	A	202	12.200	15.634	5.915	1.00	10.91	0.00
ATOM	448	H	PHE	A	202	14.270	15.390	1.740	1.00	0.00	0.16
ATOM	449	N	LEU	A	203	15.807	12.099	3.287	1.00	11.71	-0.34
ATOM	450	CA	LEU	A	203	15.183	10.789	3.407	1.00	11.70	0.17
ATOM	451	C	LEU	A	203	14.185	10.764	4.578	1.00	12.11	0.24
ATOM	452	O	LEU	A	203	14.587	10.842	5.733	1.00	11.90	-0.27
ATOM	453	CB	LEU	A	203	16.291	9.766	3.700	1.00	11.94	0.03

ATOM	454	CG	LEU	A	203	17.258	9.512	2.526	1.00	11.83	-0.02
ATOM	455	CD1	LEU	A	203	18.461	8.692	3.005	1.00	11.18	0.00
ATOM	456	CD2	LEU	A	203	16.553	8.802	1.372	1.00	12.06	0.00
ATOM	457	H	LEU	A	203	16.661	12.260	3.809	1.00	0.00	0.16
ATOM	458	N	GLY	A	204	12.888	10.612	4.300	1.00	11.84	-0.35
ATOM	459	CA	GLY	A	204	11.849	10.477	5.320	1.00	12.11	0.22
ATOM	460	C	GLY	A	204	11.388	9.026	5.381	1.00	11.88	0.23
ATOM	461	O	GLY	A	204	11.330	8.386	4.331	1.00	12.39	-0.27
ATOM	462	H	GLY	A	204	12.610	10.410	3.346	1.00	0.00	0.16
ATOM	463	N	TRP	A	205	11.021	8.500	6.557	1.00	11.68	-0.34
ATOM	464	CA	TRP	A	205	10.469	7.153	6.724	1.00	11.68	0.18
ATOM	465	C	TRP	A	205	9.365	7.085	7.764	1.00	11.46	0.24
ATOM	466	O	TRP	A	205	9.364	7.863	8.715	1.00	11.65	-0.27
ATOM	467	CB	TRP	A	205	11.527	6.078	7.034	1.00	11.18	0.07
ATOM	468	CG	TRP	A	205	12.368	6.231	8.252	1.00	11.52	-0.02
ATOM	469	CD1	TRP	A	205	12.279	5.486	9.374	1.00	11.31	0.09
ATOM	470	CD2	TRP	A	205	13.567	7.039	8.396	1.00	11.04	-0.00
ATOM	471	NE1	TRP	A	205	13.351	5.771	10.193	1.00	11.88	-0.36
ATOM	472	CE2	TRP	A	205	14.223	6.652	9.595	1.00	12.12	0.04
ATOM	473	CE3	TRP	A	205	14.210	8.013	7.600	1.00	12.40	0.01
ATOM	474	CZ2	TRP	A	205	15.502	7.114	9.918	1.00	11.27	0.03
ATOM	475	CZ3	TRP	A	205	15.512	8.457	7.895	1.00	11.78	0.00
ATOM	476	CH2	TRP	A	205	16.163	8.000	9.051	1.00	11.54	0.00
ATOM	477	H	TRP	A	205	10.990	9.082	7.386	1.00	0.00	0.16
ATOM	478	HE1	TRP	A	205	13.509	5.279	11.068	1.00	0.00	0.16
ATOM	479	N	GLU	A	206	8.490	6.088	7.602	1.00	11.69	-0.34
ATOM	480	CA	GLU	A	206	7.671	5.520	8.669	1.00	12.08	0.17
ATOM	481	C	GLU	A	206	8.153	4.070	8.875	1.00	12.10	0.24
ATOM	482	O	GLU	A	206	8.390	3.397	7.862	1.00	11.88	-0.27
ATOM	483	CB	GLU	A	206	6.196	5.468	8.240	1.00	12.38	0.04
ATOM	484	CG	GLU	A	206	5.479	6.814	8.423	1.00	13.95	0.11
ATOM	485	CD	GLU	A	206	4.975	7.074	9.850	1.00	16.11	0.17
ATOM	486	OE1	GLU	A	206	5.484	6.468	10.816	1.00	16.70	-0.64
ATOM	487	OE2	GLU	A	206	4.058	7.900	9.967	1.00	16.69	-0.64
ATOM	488	H	GLU	A	206	8.642	5.490	6.801	1.00	0.00	0.16
ATOM	489	N	PRO	A	207	8.249	3.566	10.124	1.00	11.89	-0.33
ATOM	490	CA	PRO	A	207	7.910	4.294	11.345	1.00	11.84	0.17
ATOM	491	C	PRO	A	207	9.056	5.215	11.760	1.00	11.79	0.24
ATOM	492	O	PRO	A	207	10.214	4.800	11.728	1.00	11.40	-0.27
ATOM	493	CB	PRO	A	207	7.688	3.228	12.408	1.00	11.84	0.03
ATOM	494	CG	PRO	A	207	8.590	2.088	11.972	1.00	11.93	0.02
ATOM	495	CD	PRO	A	207	8.654	2.197	10.443	1.00	12.02	0.12
ATOM	496	N	HIS	A	208	8.726	6.447	12.151	1.00	12.04	-0.34
ATOM	497	CA	HIS	A	208	9.643	7.356	12.820	1.00	11.94	0.18
ATOM	498	C	HIS	A	208	8.886	8.540	13.444	1.00	12.48	0.24
ATOM	499	O	HIS	A	208	7.987	9.094	12.797	1.00	12.92	-0.27
ATOM	500	CB	HIS	A	208	10.759	7.825	11.868	1.00	11.83	0.09
ATOM	501	CG	HIS	A	208	11.908	8.495	12.555	1.00	10.74	0.05
ATOM	502	ND1	HIS	A	208	11.850	9.779	13.050	1.00	9.65	-0.24
ATOM	503	CD2	HIS	A	208	13.142	8.027	12.872	1.00	10.15	0.11
ATOM	504	CE1	HIS	A	208	13.005	10.088	13.611	1.00	10.80	0.20
ATOM	505	NE2	HIS	A	208	13.804	9.039	13.526	1.00	10.24	-0.35
ATOM	506	H	HIS	A	208	7.737	6.684	12.198	1.00	0.00	0.16
ATOM	507	HE2	HIS	A	208	14.757	8.986	13.877	1.00	0.00	0.16
ATOM	508	N	PRO	A	209	9.273	9.014	14.650	1.00	12.66	-0.33
ATOM	509	CA	PRO	A	209	8.702	10.234	15.252	1.00	12.90	0.17
ATOM	510	C	PRO	A	209	8.732	11.505	14.381	1.00	12.86	0.24

ATOM	511	O	PRO	A	209	7.979	12.443	14.655	1.00	12.39	-0.27
ATOM	512	CB	PRO	A	209	9.555	10.433	16.514	1.00	12.90	0.03
ATOM	513	CG	PRO	A	209	9.994	9.054	16.884	1.00	12.51	0.02
ATOM	514	CD	PRO	A	209	10.225	8.356	15.564	1.00	12.51	0.12
ATOM	515	N	MET	A	210	9.577	11.536	13.351	1.00	13.34	-0.34
ATOM	516	CA	MET	A	210	9.678	12.706	12.465	1.00	13.73	0.17
ATOM	517	C	MET	A	210	8.332	13.063	11.830	1.00	14.03	0.24
ATOM	518	O	MET	A	210	8.060	14.232	11.540	1.00	13.99	-0.27
ATOM	519	CB	MET	A	210	10.755	12.508	11.383	1.00	13.78	0.04
ATOM	520	CG	MET	A	210	10.444	11.440	10.331	1.00	13.35	0.07
ATOM	521	SD	MET	A	210	11.648	11.392	8.987	1.00	13.72	-0.17
ATOM	522	CE	MET	A	210	12.812	10.171	9.605	1.00	10.69	0.08
ATOM	523	H	MET	A	210	10.203	10.757	13.190	1.00	0.00	0.16
ATOM	524	N	ASN	A	211	7.501	12.044	11.628	1.00	14.68	-0.34
ATOM	525	CA	ASN	A	211	6.192	12.192	11.003	1.00	15.25	0.18
ATOM	526	C	ASN	A	211	5.215	12.979	11.868	1.00	15.79	0.24
ATOM	527	O	ASN	A	211	4.373	13.721	11.351	1.00	16.01	-0.27
ATOM	528	CB	ASN	A	211	5.634	10.808	10.646	1.00	15.10	0.13
ATOM	529	CG	ASN	A	211	6.515	10.136	9.590	1.00	15.00	0.21
ATOM	530	OD1	ASN	A	211	6.447	10.437	8.397	1.00	14.34	-0.27
ATOM	531	ND2	ASN	A	211	7.416	9.268	10.031	1.00	14.70	-0.37
ATOM	532	H	ASN	A	211	7.791	11.117	11.908	1.00	0.00	0.16
ATOM	533	2HD2	ASN	A	211	8.056	8.781	9.405	1.00	0.00	0.15
ATOM	534	1HD2	ASN	A	211	7.396	8.986	11.009	1.00	0.00	0.15
ATOM	535	N	ALA	A	212	5.351	12.819	13.183	1.00	16.30	-0.34
ATOM	536	CA	ALA	A	212	4.566	13.559	14.160	1.00	17.03	0.17
ATOM	537	C	ALA	A	212	5.251	14.856	14.600	1.00	17.66	0.24
ATOM	538	O	ALA	A	212	4.579	15.846	14.906	1.00	17.51	-0.27
ATOM	539	CB	ALA	A	212	4.280	12.682	15.367	1.00	16.99	0.04
ATOM	540	H	ALA	A	212	6.074	12.202	13.526	1.00	0.00	0.16
ATOM	541	N	ASN	A	213	6.583	14.838	14.643	1.00	18.15	-0.34
ATOM	542	CA	ASN	A	213	7.367	15.976	15.132	1.00	18.84	0.18
ATOM	543	C	ASN	A	213	7.540	17.082	14.089	1.00	19.09	0.24
ATOM	544	O	ASN	A	213	7.701	18.250	14.440	1.00	19.34	-0.27
ATOM	545	CB	ASN	A	213	8.735	15.512	15.658	1.00	18.73	0.12
ATOM	546	CG	ASN	A	213	8.626	14.642	16.904	1.00	19.14	0.15
ATOM	547	OD1	ASN	A	213	9.693	13.908	17.211	1.00	19.76	-0.17
ATOM	548	ND2	ASN	A	213	7.602	14.634	17.585	1.00	19.07	-0.38
ATOM	549	H	ASN	A	213	7.075	13.984	14.409	1.00	0.00	0.16
ATOM	550	2HD2	ASN	A	213	7.557	14.053	18.409	1.00	0.00	0.15
ATOM	551	1HD2	ASN	A	213	6.808	15.197	17.317	1.00	0.00	0.15
ATOM	552	N	PHE	A	214	7.515	16.707	12.814	1.00	19.61	-0.34
ATOM	553	CA	PHE	A	214	7.601	17.666	11.715	1.00	20.09	0.16
ATOM	554	C	PHE	A	214	6.430	17.453	10.761	1.00	20.31	0.21
ATOM	555	O	PHE	A	214	5.840	16.373	10.722	1.00	20.32	-0.28
ATOM	556	CB	PHE	A	214	8.921	17.504	10.943	1.00	20.30	0.07
ATOM	557	CG	PHE	A	214	10.155	17.721	11.777	1.00	21.29	-0.05
ATOM	558	CD1	PHE	A	214	10.861	16.640	12.294	1.00	21.40	0.00
ATOM	559	CD2	PHE	A	214	10.622	19.012	12.032	1.00	21.88	0.00
ATOM	560	CE1	PHE	A	214	12.010	16.838	13.068	1.00	22.57	0.00
ATOM	561	CE2	PHE	A	214	11.766	19.222	12.799	1.00	22.36	0.00
ATOM	562	CZ	PHE	A	214	12.462	18.130	13.321	1.00	21.63	0.00
ATOM	563	H	PHE	A	214	7.399	15.730	12.576	1.00	0.00	0.16
ATOM	564	N	LEU	A	216	6.041	16.869	7.274	1.00	19.67	-0.32
ATOM	565	CA	LEU	A	216	6.729	16.537	6.027	1.00	19.02	0.19
ATOM	566	C	LEU	A	216	5.797	16.085	4.919	1.00	18.22	0.24
ATOM	567	O	LEU	A	216	4.675	15.632	5.162	1.00	17.79	-0.27

ATOM	568	CB	LEU	A	216	7.871	15.519	6.222	1.00	19.59	0.04
ATOM	569	CG	LEU	A	216	7.897	14.407	7.273	1.00	20.61	-0.02
ATOM	570	CD1	LEU	A	216	8.706	13.221	6.785	1.00	21.08	0.00
ATOM	571	CD2	LEU	A	216	8.500	14.944	8.534	1.00	21.36	0.00
ATOM	572	H	LEU	A	216	5.723	16.117	7.868	1.00	0.00	0.18
ATOM	573	N	THR	A	217	6.292	16.218	3.695	1.00	17.08	-0.34
ATOM	574	CA	THR	A	217	5.601	15.759	2.509	1.00	16.40	0.20
ATOM	575	C	THR	A	217	6.513	14.767	1.824	1.00	15.65	0.24
ATOM	576	O	THR	A	217	7.617	15.126	1.414	1.00	15.57	-0.27
ATOM	577	CB	THR	A	217	5.316	16.946	1.571	1.00	16.32	0.14
ATOM	578	OG1	THR	A	217	4.391	17.841	2.196	1.00	16.48	-0.39
ATOM	579	CG2	THR	A	217	4.583	16.486	0.307	1.00	16.97	0.04
ATOM	580	H	THR	A	217	7.218	16.611	3.580	1.00	0.00	0.16
ATOM	581	HG1	THR	A	217	4.783	18.165	2.993	1.00	0.00	0.21
ATOM	582	N	TYR	A	218	6.064	13.517	1.725	1.00	14.71	-0.34
ATOM	583	CA	TYR	A	218	6.770	12.515	0.931	1.00	14.01	0.18
ATOM	584	C	TYR	A	218	6.542	12.836	-0.540	1.00	13.78	0.24
ATOM	585	O	TYR	A	218	5.423	13.176	-0.938	1.00	13.09	-0.27
ATOM	586	CB	TYR	A	218	6.261	11.105	1.257	1.00	14.04	0.07
ATOM	587	CG	TYR	A	218	6.642	10.605	2.630	1.00	13.76	-0.05
ATOM	588	CD1	TYR	A	218	5.848	10.920	3.752	1.00	14.23	0.01
ATOM	589	CD2	TYR	A	218	7.812	9.841	2.793	1.00	13.15	0.01
ATOM	590	CE1	TYR	A	218	6.228	10.480	5.031	1.00	13.99	0.03
ATOM	591	CE2	TYR	A	218	8.146	9.344	4.061	1.00	13.75	0.03
ATOM	592	CZ	TYR	A	218	7.370	9.681	5.180	1.00	14.52	0.06
ATOM	593	OH	TYR	A	218	7.739	9.248	6.408	1.00	14.08	-0.36
ATOM	594	H	TYR	A	218	5.156	13.281	2.098	1.00	0.00	0.16
ATOM	595	HH	TYR	A	218	7.261	9.670	7.135	1.00	0.00	0.21
ATOM	596	N	LEU	A	219	7.606	12.747	-1.333	1.00	13.49	-0.34
ATOM	597	CA	LEU	A	219	7.539	13.103	-2.750	1.00	13.58	0.16
ATOM	598	C	LEU	A	219	7.068	11.931	-3.600	1.00	13.70	0.21
ATOM	599	O	LEU	A	219	7.506	10.795	-3.399	1.00	14.22	-0.28
ATOM	600	CB	LEU	A	219	8.900	13.591	-3.263	1.00	13.42	0.03
ATOM	601	CG	LEU	A	219	9.700	14.634	-2.477	1.00	13.48	-0.02
ATOM	602	CD1	LEU	A	219	10.969	14.992	-3.250	1.00	12.46	0.00
ATOM	603	CD2	LEU	A	219	8.871	15.885	-2.180	1.00	12.90	0.00
ATOM	604	H	LEU	A	219	8.499	12.455	-0.955	1.00	0.00	0.16
ATOM	605	N	PHE	A	226	12.861	4.334	-5.313	1.00	14.13	-0.32
ATOM	606	CA	PHE	A	226	12.601	3.909	-3.940	1.00	14.03	0.18
ATOM	607	C	PHE	A	226	11.393	2.978	-3.869	1.00	14.36	0.22
ATOM	608	O	PHE	A	226	11.123	2.414	-2.810	1.00	14.92	-0.28
ATOM	609	CB	PHE	A	226	12.357	5.152	-3.075	1.00	13.66	0.07
ATOM	610	CG	PHE	A	226	13.663	5.772	-2.622	1.00	13.26	-0.05
ATOM	611	CD1	PHE	A	226	14.335	6.684	-3.442	1.00	14.02	0.00
ATOM	612	CD2	PHE	A	226	14.256	5.398	-1.408	1.00	13.56	0.00
ATOM	613	CE1	PHE	A	226	15.548	7.255	-3.039	1.00	13.78	0.00
ATOM	614	CE2	PHE	A	226	15.494	5.966	-1.037	1.00	13.49	0.00
ATOM	615	CZ	PHE	A	226	16.124	6.922	-1.819	1.00	13.23	0.00
ATOM	616	H	PHE	A	226	12.280	5.058	-5.717	1.00	0.00	0.18
ATOM	617	N	ASN	A	229	4.060	3.896	-4.348	1.00	15.61	-0.32
ATOM	618	CA	ASN	A	229	3.325	4.282	-3.132	0.50	15.59	0.19
ATOM	619	C	ASN	A	229	4.217	4.992	-2.096	1.00	15.45	0.24
ATOM	620	O	ASN	A	229	4.172	4.715	-0.899	1.00	15.17	-0.27
ATOM	621	CB	ASN	A	229	2.574	3.070	-2.527	0.50	15.73	0.13
ATOM	622	CG	ASN	A	229	1.576	3.420	-1.429	0.50	16.09	0.21
ATOM	623	OD1	ASN	A	229	1.441	2.713	-0.440	0.50	16.12	-0.27
ATOM	624	ND2	ASN	A	229	0.872	4.529	-1.588	0.50	16.05	-0.37



ATOM	625	H	ASN	A	229	3.729	4.255	-5.233	1.00	0.00	0.18
ATOM	626	2HD2	ASN	A	229	0.237	4.765	-0.855	0.50	0.00	0.15
ATOM	627	1HD2	ASN	A	229	0.988	5.101	-2.401	0.50	0.00	0.15
ATOM	628	N	TYR	A	230	5.040	5.932	-2.567	1.00	15.19	-0.34
ATOM	629	CA	TYR	A	230	5.957	6.704	-1.727	1.00	15.12	0.18
ATOM	630	C	TYR	A	230	7.011	5.819	-1.054	1.00	14.50	0.24
ATOM	631	O	TYR	A	230	7.331	6.021	0.119	1.00	14.95	-0.27
ATOM	632	CB	TYR	A	230	5.191	7.609	-0.741	1.00	15.62	0.07
ATOM	633	CG	TYR	A	230	4.178	8.485	-1.451	1.00	15.84	-0.05
ATOM	634	CD1	TYR	A	230	2.846	8.081	-1.591	1.00	16.47	0.01
ATOM	635	CD2	TYR	A	230	4.556	9.704	-2.011	1.00	15.72	0.01
ATOM	636	CE1	TYR	A	230	1.918	8.877	-2.265	1.00	16.79	0.03
ATOM	637	CE2	TYR	A	230	3.637	10.506	-2.680	1.00	16.29	0.03
ATOM	638	CZ	TYR	A	230	2.324	10.088	-2.808	1.00	16.84	0.06
ATOM	639	OH	TYR	A	230	1.414	10.887	-3.477	1.00	17.19	-0.36
ATOM	640	H	TYR	A	230	4.930	6.214	-3.530	1.00	0.00	0.16
ATOM	641	HH	TYR	A	230	1.789	11.695	-3.794	1.00	0.00	0.21
ATOM	642	N	GLY	A	231	7.522	4.842	-1.810	1.00	13.90	-0.35
ATOM	643	CA	GLY	A	231	8.501	3.873	-1.359	1.00	13.24	0.22
ATOM	644	C	GLY	A	231	7.925	2.911	-0.334	1.00	12.81	0.23
ATOM	645	O	GLY	A	231	8.544	2.719	0.704	1.00	13.23	-0.27
ATOM	646	H	GLY	A	231	7.184	4.704	-2.752	1.00	0.00	0.16
ATOM	647	N	GLY	A	232	6.726	2.358	-0.568	1.00	12.46	-0.35
ATOM	648	CA	GLY	A	232	6.094	1.385	0.326	1.00	11.86	0.20
ATOM	649	C	GLY	A	232	7.021	0.184	0.542	1.00	11.80	0.21
ATOM	650	O	GLY	A	232	7.466	-0.424	-0.430	1.00	11.70	-0.28
ATOM	651	H	GLY	A	232	6.295	2.507	-1.473	1.00	0.00	0.16
ATOM	652	N	PHE	A	233	8.707	0.229	2.260	1.00	11.20	-0.33
ATOM	653	CA	PHE	A	233	9.921	-0.550	2.441	1.00	11.33	0.17
ATOM	654	C	PHE	A	233	9.604	-1.911	3.048	1.00	11.26	0.37
ATOM	655	O	PHE	A	233	8.608	-2.080	3.758	1.00	11.40	-0.14
ATOM	656	CB	PHE	A	233	10.913	0.218	3.309	1.00	0.00	0.07
ATOM	657	CG	PHE	A	233	11.526	1.445	2.670	1.00	0.00	-0.05
ATOM	658	CD1	PHE	A	233	10.898	2.695	2.811	1.00	0.00	0.00
ATOM	659	CD2	PHE	A	233	12.719	1.337	1.936	1.00	0.00	0.00
ATOM	660	CE1	PHE	A	233	11.467	3.838	2.224	1.00	0.00	0.00
ATOM	661	CE2	PHE	A	233	13.288	2.481	1.347	1.00	0.00	0.00
ATOM	662	CZ	PHE	A	233	12.662	3.731	1.492	1.00	0.00	0.00
ATOM	663	H	PHE	A	233	8.130	0.337	3.095	1.00	0.00	0.18
ATOM	664	N	THR	A	234	8.824	-3.031	3.305	1.00	11.58	0.10
ATOM	665	CA	THR	A	234	8.732	-4.052	4.330	1.00	11.51	0.34
ATOM	666	C	THR	A	234	10.106	-4.205	4.975	1.00	11.65	0.25
ATOM	667	O	THR	A	234	11.134	-3.940	4.335	1.00	11.46	-0.27
ATOM	668	CB	THR	A	234	8.189	-5.364	3.720	1.00	11.81	0.15
ATOM	669	OG1	THR	A	234	9.060	-5.796	2.686	1.00	11.15	-0.39
ATOM	670	CG2	THR	A	234	6.802	-5.192	3.085	1.00	10.62	0.04
ATOM	671	H	THR	A	234	9.550	-3.189	2.611	1.00	0.00	0.32
ATOM	672	HG1	THR	A	234	9.798	-6.260	3.060	1.00	0.00	0.21
ATOM	673	N	VAL	A	235	10.108	-4.660	6.230	1.00	11.95	-0.34
ATOM	674	CA	VAL	A	235	11.367	-4.886	6.948	1.00	11.76	0.16
ATOM	675	C	VAL	A	235	11.463	-6.360	7.311	1.00	11.88	0.21
ATOM	676	O	VAL	A	235	10.480	-6.965	7.733	1.00	11.90	-0.28
ATOM	677	CB	VAL	A	235	11.531	-3.986	8.187	1.00	12.06	0.00
ATOM	678	CG1	VAL	A	235	12.976	-4.039	8.712	1.00	11.43	0.01
ATOM	679	CG2	VAL	A	235	11.131	-2.537	7.884	1.00	11.50	0.01
ATOM	680	H	VAL	A	235	9.235	-4.847	6.709	1.00	0.00	0.16
ATOM	681	N	LEU	A	261	3.944	-0.771	12.958	1.00	15.84	-0.32

ATOM	682	CA	LEU	A	261	4.265	0.662	12.953	1.00	16.28	0.17
ATOM	683	C	LEU	A	261	3.910	1.328	14.281	1.00	16.27	0.22
ATOM	684	O	LEU	A	261	4.682	2.141	14.791	1.00	16.48	-0.28
ATOM	685	CB	LEU	A	261	3.538	1.374	11.790	1.00	16.36	0.03
ATOM	686	CG	LEU	A	261	4.396	1.901	10.631	1.00	16.91	-0.02
ATOM	687	CD1	LEU	A	261	5.111	0.771	9.892	1.00	17.91	0.00
ATOM	688	CD2	LEU	A	261	3.543	2.737	9.671	1.00	16.66	0.00
ATOM	689	H	LEU	A	261	3.306	-1.122	12.259	1.00	0.00	0.18
ATOM	690	N	GLU	A	264	6.456	0.248	17.052	1.00	15.33	-0.32
ATOM	691	CA	GLU	A	264	7.770	0.832	16.793	1.00	14.94	0.19
ATOM	692	C	GLU	A	264	7.792	2.338	17.071	1.00	15.03	0.24
ATOM	693	O	GLU	A	264	8.703	2.829	17.735	1.00	14.99	-0.27
ATOM	694	CB	GLU	A	264	8.261	0.501	15.383	1.00	14.44	0.04
ATOM	695	CG	GLU	A	264	8.629	-0.971	15.218	1.00	13.96	0.11
ATOM	696	CD	GLU	A	264	9.489	-1.245	14.004	1.00	13.50	0.13
ATOM	697	OE1	GLU	A	264	9.419	-2.371	13.465	1.00	12.57	-0.65
ATOM	698	OE2	GLU	A	264	10.247	-0.346	13.605	1.00	13.37	-0.77
ATOM	699	H	GLU	A	264	5.857	0.013	16.271	1.00	0.00	0.18
ATOM	700	HE2	GLU	A	264	10.753	-0.613	12.853	1.00	0.00	0.16
ATOM	701	N	ASN	A	265	6.773	3.048	16.590	1.00	15.07	-0.34
ATOM	702	CA	ASN	A	265	6.625	4.478	16.858	1.00	15.63	0.17
ATOM	703	C	ASN	A	265	6.558	4.785	18.360	1.00	15.73	0.22
ATOM	704	O	ASN	A	265	7.099	5.797	18.811	1.00	15.76	-0.28
ATOM	705	CB	ASN	A	265	5.410	5.062	16.111	1.00	15.30	0.13
ATOM	706	CG	ASN	A	265	5.764	5.584	14.718	1.00	16.37	0.21
ATOM	707	OD1	ASN	A	265	6.804	6.214	14.522	1.00	16.85	-0.27
ATOM	708	ND2	ASN	A	265	4.883	5.339	13.747	1.00	17.05	-0.37
ATOM	709	H	ASN	A	265	6.053	2.587	16.047	1.00	0.00	0.16
ATOM	710	2HD2	ASN	A	265	5.059	5.688	12.811	1.00	0.00	0.15
ATOM	711	1HD2	ASN	A	265	4.043	4.816	13.944	1.00	0.00	0.15
ATOM	712	N	MET	A	268	10.217	4.159	19.769	1.00	14.93	-0.32
ATOM	713	CA	MET	A	268	11.076	5.197	19.191	1.00	15.12	0.19
ATOM	714	C	MET	A	268	10.774	6.571	19.788	1.00	14.84	0.24
ATOM	715	O	MET	A	268	11.677	7.386	19.971	1.00	14.58	-0.27
ATOM	716	CB	MET	A	268	10.928	5.241	17.673	1.00	15.11	0.04
ATOM	717	CG	MET	A	268	11.388	3.992	16.945	1.00	15.05	0.07
ATOM	718	SD	MET	A	268	10.868	4.027	15.206	1.00	16.23	-0.17
ATOM	719	CE	MET	A	268	12.024	5.261	14.568	1.00	15.55	0.08
ATOM	720	H	MET	A	268	9.566	3.678	19.160	1.00	0.00	0.18
ATOM	721	N	GLY	A	269	9.501	6.817	20.096	1.00	14.94	-0.35
ATOM	722	CA	GLY	A	269	9.095	8.028	20.807	1.00	14.74	0.20
ATOM	723	C	GLY	A	269	9.757	8.159	22.175	1.00	15.10	0.21
ATOM	724	O	GLY	A	269	10.238	9.235	22.534	1.00	14.86	-0.28
ATOM	725	H	GLY	A	269	8.792	6.126	19.888	1.00	0.00	0.16
ATOM	726	N	ILE	A	271	12.583	6.748	23.091	1.00	15.79	-0.32
ATOM	727	CA	ILE	A	271	14.009	6.921	22.831	1.00	16.20	0.19
ATOM	728	C	ILE	A	271	14.317	8.346	22.372	1.00	16.57	0.24
ATOM	729	O	ILE	A	271	15.183	9.015	22.942	1.00	16.13	-0.27
ATOM	730	CB	ILE	A	271	14.500	5.884	21.777	1.00	16.36	0.01
ATOM	731	CG1	ILE	A	271	14.422	4.465	22.350	1.00	16.05	0.00
ATOM	732	CG2	ILE	A	271	15.922	6.229	21.286	1.00	16.38	0.01
ATOM	733	CD1	ILE	A	271	14.458	3.361	21.301	1.00	16.35	0.00
ATOM	734	H	ILE	A	271	12.062	6.121	22.492	1.00	0.00	0.18
ATOM	735	N	LEU	A	272	13.599	8.807	21.350	1.00	16.95	-0.34
ATOM	736	CA	LEU	A	272	13.916	10.080	20.710	1.00	17.45	0.16
ATOM	737	C	LEU	A	272	13.363	11.310	21.411	1.00	17.47	0.21
ATOM	738	O	LEU	A	272	14.100	12.274	21.650	1.00	17.52	-0.28



ATOM	739	CB	LEU A 272	13.486	10.073	19.242	1.00	17.86	0.03
ATOM	740	CG	LEU A 272	14.551	9.701	18.218	1.00	18.82	-0.02
ATOM	741	CD1	LEU A 272	13.991	9.912	16.822	1.00	19.34	0.00
ATOM	742	CD2	LEU A 272	15.808	10.535	18.401	1.00	19.73	0.00
ATOM	743	H	LEU A 272	12.883	8.223	20.933	1.00	0.00	0.16
TER	744		LEU A 272 `						

## Load the PDB texts into models

```
In [6]: %%javascript

let models = binana.load_ligand_receptor.from_texts(
    ligPDBTxt, recepPDBTxt
);
window.ligand = models[0];
window.receptor = models[1];
```

## Get information about the hydrogen bonds (example)

```
In [7]: %%javascript

window.hbondInf = binana.interactions.get_hydrogen_bonds(
    ligand, receptor
);
```

```
In [8]: %%javascript

// Counting/characterizing the acceptors and donors (counts)
output(
    element,
    JSON.stringify(
        hbondInf["counts"],
        null, 2
    )
);

{
  "HDONOR_LIGAND_SIDECHAIN_OTHER": 2,
  "HDONOR_RECEPTOR_SIDECHAIN_OTHER": 1
}
```

In [9]: %%javascript

```
// List the atoms involved in each hydrogen bond
let toShow = "";
for(let hbondLabel of hbondInf["labels"]) {
    toShow += JSON.stringify(
        hbondLabel, null, 2
    ) + "\n";
}
output(element, toShow);
```

```
[
  "A:CHT(1):N1(14)",
  "A:CHT(1):H1(16)",
  "A:ASP(157):OD2(285)",
  "LIGAND"
]
[
  "A:CHT(1):O6(22)",
  "A:ASN(156):2HD2(276)",
  "A:ASN(156):ND2(274)",
  "RECEPTOR"
]
[
  "A:CHT(1):O6(22)",
  "A:CHT(1):HO6(23)",
  "A:ASP(157):OD1(284)",
  "LIGAND"
]
```

## Get information about the cation-pi interactions (example)

In [10]: %%javascript

```
window.cationPiInf = binana.interactions.get_cation_pi(
    ligand,
    receptor
);
```

In [11]: %%javascript

```
// Counting/characterizing the acceptors and donors (counts)
output(
  element,
  JSON.stringify(
    cationPiInf["counts"],
    null, 2
  )
);
```

```
{
  "PI-CATION_LIGAND-CHARGED_OTHER": 2,
  "PI-CATION_LIGAND-CHARGED_BETA": 2,
  "PI-CATION_RECEPTOR-CHARGED_OTHER": 1
}
```

In [12]: %%javascript

```
// List the atoms involved in each cation-pi interaction
let toShow = "";
for(let cationPiLabel of cationPiInf["labels"]) {
    toShow += JSON.stringify(
        cationPiLabel, null, 2
    ) + "\n";
}
output(element, toShow);
```

```
[
  "[A:CHT(1):N1(2) / A:CHT(1):C5(1) / A:CHT(1):C6(3) / A:CHT(1):C6(4) / A:CHT(1):C7(9)]",
  "[A:TRP(43):CG(28) / A:TRP(43):CD1(29) / A:TRP(43):NE1(31) / A:TRP(43):CE2(32) / A:TRP(43):CD2(30)]"
]
[
  "[A:CHT(1):N1(2) / A:CHT(1):C5(1) / A:CHT(1):C6(3) / A:CHT(1):C6(4) / A:CHT(1):C7(9)]",
  "[A:TRP(43):CE2(32) / A:TRP(43):CD2(30) / A:TRP(43):CE3(33) / A:TRP(43):CZ3(35) / A:TRP(43):CH2(36) / A:TRP(43):CZ2(34)]"
]
[
  "[A:CHT(1):N1(2) / A:CHT(1):C5(1) / A:CHT(1):C6(3) / A:CHT(1):C6(4) / A:CHT(1):C7(9)]",
  "[A:TRP(205):CG(468) / A:TRP(205):CD1(469) / A:TRP(205):NE1(471) / A:TRP(205):CE2(472) / A:TRP(205):CD2(470)]"
]
[
  "[A:CHT(1):N1(2) / A:CHT(1):C5(1) / A:CHT(1):C6(3) / A:CHT(1):C6(4) / A:CHT(1):C7(9)]",
  "[A:TRP(205):CE2(472) / A:TRP(205):CD2(470) / A:TRP(205):CE3(473) / A:TRP(205):CZ3(475) / A:TRP(205):CH2(476) / A:TRP(205):CZ2(474)]"
]
[
  "[A:CHT(1):C2(17) / A:CHT(1):O1(18) / A:CHT(1):C5(19) / A:CHT(1):C4(20) / A:CHT(1):C3(21)]",
  "[A:LYS(94):NZ(144) / A:LYS(94):HZ1(146) / A:LYS(94):HZ2(147) / A:LYS(94):HZ3(148)]"
]
```

**Other interactions are also available**

In [13]: %%javascript

```
let toShow = "";
toShow += "Available functions for detecting interactions:\n";
let funcNames = Object.keys(binana.interactions).filter(
  n => n.startsWith("get_")
);
toShow += funcNames.join("\n");
output(element, toShow);
```

Available functions for detecting interactions:

get\_active\_site\_flexibility  
get\_all\_interactions  
get\_cation\_pi  
get\_close  
get\_closest  
get\_electrostatic\_energies  
get\_hydrogen\_bonds  
get\_hydrophobics  
get\_ligand\_atom\_types  
get\_pi\_pi  
get\_salt\_bridges

## Get PDB-formatted text

```

In [14]: %%javascript

window.pdbTxt = binana.output.pdb_file.write(
    ligand,
    receptor,
    null,          // closest
    null,          // close
    null,          // hydrophobics
    hbondInf,      // hydrogen bonds
    null,          // salt_bridges
    null,          // pi_pi
    cationPiInf,   // cat_pi
    null,          // active_site_flexibility
    null,          // log_output
    true,          // as_str
)

let pdbRemarkLines = pdbTxt.split("\n")
    .filter(l => l.startsWith("REMARK") && l !== 'REMARK');
let pdbRemarkTxt = pdbRemarkLines.join(",")
    .replace(/REMARK {0,1}/g, "")
    .replace(".", ".");
output(element, pdbRemarkTxt);

```

The residue named "CCN" contains the closest contacts between the protein and receptor. "CON" indicates close contacts. "ALP", "BET", and "OTH" indicate receptor contacts whose respective protein residues have the alpha-helix, beta-sheet, or "other" secondary structure. "BAC" and "SID" indicate receptor contacts that are part of the protein backbone and sidechain, respectively. "HYD" indicates hydrophobic contacts between the protein and ligand. "HBN" indicates hydrogen bonds. "SAL" indicates salt bridges. "PIS" indicates pi-pi stacking interactions, "PIT" indicates T-stacking interactions, and "PIC" indicates cation-pi interactions. Protein residue names are unchanged, but the ligand residue is now named "LIG".

```
In [15]: %%javascript
```

```
output(element, pdbTxt);
```

REMARK

REMARK The residue named "CCN" contains the closest contacts between the protein and receptor. "CON" indicates close contacts. "ALP", "BET", and "OTH" indicate receptor contacts whose respective protein residues have the alpha-helix, beta-sheet, or "other" secondary structure. "BAC" and "SID" indicate receptor contacts that are part of the protein backbone and sidechain, respectively. "HYD" indicates hydrophobic contacts between the protein and ligand. "HBN" indicates hydrogen bonds. "SAL" indicates salt bridges. "PIS" indicates pi-pi stacking interactions, "PIT" indicates T-stacking interactions, and "PIC" indicates cation-pi interactions. Protein residue names are unchanged, but the ligand residue is now named "LIG".

REMARK

ATOM	1	N	ASP	23.366	-3.399	14.662	N
ATOM	2	CA	ASP	22.530	-2.226	14.843	C
ATOM	3	C	ASP	23.197	-1.095	14.078	C
ATOM	4	O	ASP	24.256	-0.613	14.476	O
ATOM	5	CB	ASP	22.432	-1.893	16.332	C
ATOM	6	CC	ASP	21.602	-0.652	16.610	C

**Get the interactions as a dictionary for easier big-data analysis**

In [16]: %%javascript

```
let data = binana.output.dictionary.collect(
  null,          // closest
  null,          // close
  null,          // hydrophobics
  hbondInf,      // hydrogen bonds
  null,          // salt_bridges
  null,          // pi_pi
  cationPiInf,   // cat_pi
  null,          // active_site_flexibility
  null,          // ligand_atom_types
  true,          // ligand_rotatable_bonds
)

let toShow = "KEYS: ";
toShow += Object.keys(data).join(", ") + ". ";
toShow += "\n\nHYDROGEN-BOND DATA (EXAMPLE):\n\n";
toShow += JSON.stringify(data["hydrogenBonds"], null, 2);

output(element, toShow);
```

KEYS: hydrogenBonds, cationPiInteractions, ligandAtomTypes.

HYDROGEN-BOND DATA (EXAMPLE):

```
[
  {
    "ligandAtoms": [
      {
        "chain": "A",
        "resID": 1,
        "resName": "CHT",
        "atomName": "N1",
        "atomIndex": 14
      },
      {
        "chain": "A",
        "resID": 1,
        "resName": "CHT",
        "atomName": "H1",
        "atomIndex": 16
      }
    ],
    "receptorAtoms": [
      {
        "chain": "A",
        "resID": 157,
        "resName": "ASP",
        "atomName": "OD2",
        "atomIndex": 285
      }
    ]
  }
]
```



```

    }
  ]
},
{
  "ligandAtoms": [
    {
      "chain": "A",
      "resID": 1,
      "resName": "CHT",
      "atomName": "O6",
      "atomIndex": 22
    }
  ],
  "receptorAtoms": [
    {
      "chain": "A",
      "resID": 156,
      "resName": "ASN",
      "atomName": "ND2",
      "atomIndex": 274
    },
    {
      "chain": "A",
      "resID": 156,
      "resName": "ASN",
      "atomName": "2HD2",
      "atomIndex": 276
    }
  ]
},
{
  "ligandAtoms": [
    {
      "chain": "A",
      "resID": 1,
      "resName": "CHT",
      "atomName": "O6",
      "atomIndex": 22
    },
    {
      "chain": "A",
      "resID": 1,
      "resName": "CHT",
      "atomName": "HO6",
      "atomIndex": 23
    }
  ],
  "receptorAtoms": [
    {

```

```

        "chain": "A",
        "resID": 157,
        "resName": "ASP",
        "atomName": "OD1",
        "atomIndex": 284
    }
]
}
]

```

## Get all the interactions at once

```

In [17]: %%javascript

window.allInf = binana.interactions.get_all_interactions(
    ligand, receptor
);

```

```

In [18]: %%javascript

output(
    element,
    JSON.stringify(
        Object.keys(allInf), null, 2
    )
);

```

```

[
  "closest",
  "close",
  "electrostatic_energies",
  "active_site_flexibility",
  "hydrophobics",
  "hydrogen_bonds",
  "ligand_atom_types",
  "pi_pi",
  "cat_pi",
  "salt_bridges",
  "ligand_rotatable_bonds"
]

```

## Get and display PDB-formatted text

In [19]: %%javascript

```
window.pdbTxt = binana.output.pdb_file.write_all(
    ligand, receptor,
    allInf,
    null, // log_output
    true  // as_str
);

output(
    element,
    pdbTxt
);
```

REMARK

REMARK The residue named "CCN" contains the closest contacts between the protein and receptor. "CON" indicates close contacts. "ALP", "BET", and "OTH" indicate receptor contacts whose respective protein residues have the alpha-helix, beta-sheet, or "other" secondary structure. "BAC" and "SID" indicate receptor contacts that are part of the protein backbone and sidechain, respectively. "HYD" indicates hydrophobic contacts between the protein and ligand. "HBN" indicates hydrogen bonds. "SAL" indicates salt bridges. "PIS" indicates pi-pi stacking interactions, "PIT" indicates T-stacking interactions, and "PIC" indicates cation-pi interactions. Protein residue names are unchanged, but the ligand residue is now named "LIG".

REMARK

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ATOM	4	O	ASP	24.256	-0.613	14.476	O
ATOM	5	CB	ASP	22.432	-1.893	16.332	C
ATOM	6	CC	ASP	21.602	-0.652	16.610	C

In [ ]: