Supporting Information

Mechanism of Intramolecular Electron Transfer in the photo-excited Zn-Substituted Cytochrome *c*: Theoretical and Experimental Perspective

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Table S1 Cartesian coordinate of Zn-cyt *c* (Å) used by the all-electron DFT calculation.

Atom No.	Residue ^a	Residue No.	x	y	z	Charge	Atom
1	GLY	1	-14.167	-5.342	-5.509	1	N
2	GLY	1	-14.213	-4.356	-4.437		C
3	GLY	1	-14.788	-3.04	-4.962		C
4	GLY	1	-14.941	-2.863	-6.171		O
5	GLY	1	-13.587	-5.002	-6.25		H
6	GLY	1	-15.091	-5.502	-5.856		H
7	GLY	1	-14.792	-4.698	-3.697		H
8	GLY	1	-13.288	-4.199	-4.092		H
9	ASP	2	-15.121	-2.147	-4.014		N
10	ASP	2	-15.84	-0.908	-4.308		C
11	ASP	2	-15.057	0.238	-3.662		C
12	ASP	2	-14.741	0.187	-2.483		O
13	ASP	2	-17.252	-0.934	-3.678		C
14	ASP	2	-18.104	-2.123	-4.128		C
15	ASP	2	-18.1	-3.153	-3.454		O
16	ASP	2	-18.791	-2.022	-5.145		O
17	ASP	2	-20.61	-3.438	-5.374		X
18	ASP	2	-14.865	-2.338	-3.066		H
19	ASP	2	-15.926	-0.798	-5.298		H
20	ASP	2	-17.153	-0.975	-2.684		H
21	ASP	2	-17.727	-0.091	-3.932		H
22	VAL	3	-14.782	1.276	-4.466	1	N
23	VAL	3	-13.937	2.386	-4.015		C
24	VAL	3	-14.489	3.043	-2.723		C
25	VAL	3	-13.753	3.426	-1.818		O
26	VAL	3	-13.798	3.424	-5.157		C
27	VAL	3	-12.733	4.487	-4.841		C
28	VAL	3	-13.476	2.766	-6.51		C
29	VAL	3	-15.161	1.293	-5.392		H
30	VAL	3	-13.032	2.025	-3.788		H
31	VAL	3	-14.691	3.869	-5.227		H
32	VAL	3	-12.674	5.136	-5.599		H
33	VAL	3	-11.846	4.043	-4.713		H
34	VAL	3	-12.985	4.974	-4.005		H
35	VAL	3	-13.396	3.472	-7.214		H
36	VAL	3	-14.21	2.132	-6.756		H
37	VAL	3	-12.613	2.265	-6.441		H
38	GLU	4	-15.83	3.15	-2.696		N
39	GLU	4	-16.5	3.813	-1.58		C
40	GLU	4	-16.3	3.048	-0.253		C
41	GLU	4	-16.258	3.631	0.826		O
42	GLU	4	-17.998	3.973	-1.895		C
43	GLU	4	-18.255	4.786	-3.18		C
44	GLU	4	-19.749	5.048	-3.38		C
45	GLU	4	-20.306	5.896	-2.688		O
46	GLU	4	-20.366	4.41	-4.23		O
47	GLU	4	-22.512	4.992	-3.632	1	X
48	GLU	4	-16.372	2.772	-3.447		H

49	GLU	4	-16.087	4.717	-1.462	H
50	GLU	4	-18.4	3.064	-2.006	H
51	GLU	4	-18.437	4.441	-1.128	H
52	GLU	4	-17.777	5.662	-3.113	H
53	GLU	4	-17.906	4.274	-3.965	H
54	LYS	5	-16.187	1.719	-0.398	N
55	LYS	5	-15.866	0.874	0.748	C
56	LYS	5	-14.363	0.973	1.042	C
57	LYS	5	-13.932	0.991	2.188	O
58	LYS	5	-16.338	-0.562	0.45	C
59	LYS	5	-17.86	-0.692	0.638	C
60	LYS	5	-18.528	-1.881	-0.071	C
61	LYS	5	-17.892	-3.261	0.181	C
62	LYS	5	-16.987	-3.721	-0.871	N
63	LYS	5	-16.323	1.304	-1.297	H
64	LYS	5	-16.342	1.177	1.573	H
65	LYS	5	-16.104	-0.794	-0.494	H
66	LYS	5	-15.876	-1.194	1.073	H
67	LYS	5	-18.041	-0.779	1.618	H
68	LYS	5	-18.283	0.146	0.294	H
69	LYS	5	-19.48	-1.923	0.233	H
70	LYS	5	-18.499	-1.706	-1.055	H
71	LYS	5	-17.376	-3.214	1.036	H
72	LYS	5	-18.629	-3.931	0.272	H
73	LYS	5	-16.621	-4.619	-0.628	H
74	LYS	5	-17.486	-3.788	-1.735	H
75	GLY	6	-13.608	1.096	-0.057	N
76	GLY	6	-12.159	1.247	-0.025	C
77	GLY	6	-11.697	2.353	0.923	C
78	GLY	6	-10.776	2.171	1.708	O
79	GLY	6	-14.063	1.083	-0.948	H
80	GLY	6	-11.755	0.382	0.273	H
81	GLY	6	-11.841	1.464	-0.948	H
82	LYS	7	-12.422	3.485	0.85	N
83	LYS	7	-12.229	4.577	1.811	C
84	LYS	7	-12.174	4.048	3.258	C
85	LYS	7	-11.27	4.335	4.033	O
86	LYS	7	-13.41	5.567	1.689	C
87	LYS	7	-13.28	6.581	0.54	C
88	LYS	7	-12.564	7.874	0.976	C
89	LYS	7	-12.562	8.961	-0.117	C
90	LYS	7	-12.054	10.27	0.301	N
91	LYS	7	-13.105	3.584	0.126	H
92	LYS	7	-11.362	5.029	1.603	H
93	LYS	7	-14.246	5.038	1.545	H
94	LYS	7	-13.48	6.076	2.547	H
95	LYS	7	-12.759	6.16	-0.202	H
96	LYS	7	-14.196	6.815	0.214	H
97	LYS	7	-13.027	8.237	1.785	H
98	LYS	7	-11.616	7.651	1.205	H
99	LYS	7	-11.994	8.637	-0.874	H

100	LYS	7	-13.503	9.082	-0.434		H
101	LYS	7	-12.091	10.905	-0.471		H
102	LYS	7	-12.615	10.623	1.049		H
103	LYS	8	-13.224	3.278	3.565		N
104	LYS	8	-13.438	2.814	4.925		C
105	LYS	8	-12.31	1.868	5.355		C
106	LYS	8	-11.813	1.922	6.475		O
107	LYS	8	-14.804	2.108	5.022		C
108	LYS	8	-15.96	2.888	4.371		C
109	LYS	8	-16.181	4.281	4.975		C
110	LYS	8	-17.366	5.01	4.315		C
111	LYS	8	-17.66	6.328	4.875		N
112	LYS	8	-18.935	8.343	6.183	-1	X
113	LYS	8	-13.871	3.019	2.848		H
114	LYS	8	-13.435	3.6	5.543		H
115	LYS	8	-14.731	1.219	4.57		H
116	LYS	8	-15.021	1.974	5.989		H
117	LYS	8	-15.76	2.994	3.397		H
118	LYS	8	-16.801	2.358	4.483		H
119	LYS	8	-16.365	4.184	5.953		H
120	LYS	8	-15.353	4.826	4.844		H
121	LYS	8	-17.16	5.123	3.343		H
122	LYS	8	-18.18	4.439	4.419		H
123	LYS	8	-18.438	6.73	4.393		H
124	LYS	8	-16.861	6.921	4.77		H
125	LYS	8	-17.881	6.237	5.846		H
126	ILE	9	-11.942	0.987	4.411		N
127	ILE	9	-10.898	0.022	4.731		C
128	ILE	9	-9.556	0.746	4.924		C
129	ILE	9	-8.77	0.393	5.789		O
130	ILE	9	-10.827	-1.105	3.678		C
131	ILE	9	-12.211	-1.704	3.36		C
132	ILE	9	-9.862	-2.221	4.115		C
133	ILE	9	-12.992	-2.185	4.592		C
134	ILE	9	-12.375	0.992	3.509		H
135	ILE	9	-11.122	-0.427	5.596		H
136	ILE	9	-10.478	-0.682	2.842		H
137	ILE	9	-12.756	-1.004	2.898		H
138	ILE	9	-12.081	-2.484	2.748		H
139	ILE	9	-9.838	-2.934	3.415		H
140	ILE	9	-10.176	-2.614	4.979		H
141	ILE	9	-8.945	-1.841	4.235		H
142	ILE	9	-13.874	-2.558	4.304		H
143	ILE	9	-13.143	-1.416	5.213		H
144	ILE	9	-12.468	-2.895	5.063		H
145	PHE	10	-9.341	1.795	4.118		N
146	PHE	10	-8.09	2.536	4.244		C
147	PHE	10	-8.004	3.19	5.633		C
148	PHE	10	-7.003	3.096	6.334		O
149	PHE	10	-7.982	3.568	3.113		C
150	PHE	10	-6.563	4.052	2.949		C

151	PHE	10	-5.678	3.348	2.137	C
152	PHE	10	-6.114	5.195	3.605	C
153	PHE	10	-4.364	3.776	1.981	C
154	PHE	10	-4.799	5.624	3.456	C
155	PHE	10	-3.923	4.913	2.644	C
156	PHE	10	-10.026	2.065	3.441	H
157	PHE	10	-7.315	1.909	4.159	H
158	PHE	10	-8.284	3.147	2.258	H
159	PHE	10	-8.57	4.348	3.326	H
160	PHE	10	-5.99	2.526	1.661	H
161	PHE	10	-6.741	5.712	4.188	H
162	PHE	10	-3.738	3.265	1.392	H
163	PHE	10	-4.484	6.444	3.933	H
164	PHE	10	-2.977	5.22	2.538	H
165	VAL	11	-9.13	3.822	6.001	N
166	VAL	11	-9.24	4.493	7.295	C
167	VAL	11	-8.945	3.526	8.464	C
168	VAL	11	-8.348	3.9	9.472	O
169	VAL	11	-10.634	5.157	7.389	C
170	VAL	11	-10.991	5.655	8.801	C
171	VAL	11	-10.737	6.331	6.402	C
172	VAL	11	-9.91	3.835	5.376	H
173	VAL	11	-8.546	5.21	7.369	H
174	VAL	11	-11.29	4.44	7.156	H
175	VAL	11	-11.9	6.071	8.788	H
176	VAL	11	-10.319	6.334	9.095	H
177	VAL	11	-10.986	4.884	9.438	H
178	VAL	11	-11.642	6.749	6.474	H
179	VAL	11	-10.598	5.997	5.47	H
180	VAL	11	-10.037	7.012	6.619	H
181	GLN	12	-9.407	2.281	8.292	N
182	GLN	12	-9.247	1.302	9.361	C
183	GLN	12	-7.82	0.725	9.399	C
184	GLN	12	-7.226	0.555	10.461	O
185	GLN	12	-10.299	0.2	9.174	C
186	GLN	12	-11.712	0.724	9.487	C
187	GLN	12	-12.772	-0.333	9.18	C
188	GLN	12	-13.23	-1.07	10.053	O
189	GLN	12	-13.138	-0.357	7.903	N
190	GLN	12	-9.858	2.024	7.437	H
191	GLN	12	-9.387	1.75	10.244	H
192	GLN	12	-10.272	-0.12	8.227	H
193	GLN	12	-10.089	-0.56	9.789	H
194	GLN	12	-11.763	0.966	10.456	H
195	GLN	12	-11.89	1.536	8.931	H
196	GLN	12	-12.724	0.279	7.252	H
197	GLN	12	-13.827	-1.012	7.593	H
198	LYS	13	-7.331	0.393	8.199	N
199	LYS	13	-6.098	-0.373	8.069	C
200	LYS	13	-4.883	0.569	7.997	C
201	LYS	13	-3.967	0.516	8.81	O

202	LYS	13	-6.167	-1.262	6.809	C
203	LYS	13	-7.388	-2.196	6.72	C
204	LYS	13	-7.404	-3.378	7.696	C
205	LYS	13	-8.534	-4.361	7.32	C
206	LYS	13	-8.745	-5.491	8.222	N
207	LYS	13	-7.821	0.677	7.374	H
208	LYS	13	-5.994	-0.957	8.874	H
209	LYS	13	-6.18	-0.662	6.009	H
210	LYS	13	-5.344	-1.829	6.787	H
211	LYS	13	-8.206	-1.647	6.892	H
212	LYS	13	-7.423	-2.566	5.792	H
213	LYS	13	-6.525	-3.853	7.654	H
214	LYS	13	-7.556	-3.038	8.624	H
215	LYS	13	-9.387	-3.841	7.28	H
216	LYS	13	-8.326	-4.731	6.414	H
217	LYS	13	-8.973	-5.152	9.135	H
218	LYS	13	-7.911	-6.041	8.27	H
219	CYS	14	-4.902	1.39	6.936	N
220	CYS	14	-3.682	2.055	6.492	C
221	CYS	14	-3.465	3.389	7.201	C
222	CYS	14	-2.339	3.81	7.437	O
223	CYS	14	-3.742	2.313	4.984	C
224	CYS	14	-4.39	0.925	4.041	S
225	CYS	14	-5.76	1.548	6.446	H
226	CYS	14	-2.921	1.446	6.716	H
227	CYS	14	-4.329	3.106	4.822	H
228	CYS	14	-2.817	2.511	4.66	H
229	ALA	15	-4.591	4.044	7.523	N
230	ALA	15	-4.554	5.434	7.976	C
231	ALA	15	-3.963	5.599	9.391	C
232	ALA	15	-3.915	6.695	9.944	O
233	ALA	15	-5.961	6.031	7.911	C
234	ALA	15	-5.471	3.574	7.452	H
235	ALA	15	-3.94	5.927	7.36	H
236	ALA	15	-5.935	6.981	8.221	H
237	ALA	15	-6.574	5.505	8.501	H
238	ALA	15	-6.295	5.997	6.969	H
239	GLN	16	-3.5	4.47	9.947	N
240	GLN	16	-2.671	4.516	11.138	C
241	GLN	16	-1.337	5.237	10.84	C
242	GLN	16	-0.786	5.939	11.685	O
243	GLN	16	-2.392	3.078	11.607	C
244	GLN	16	-3.674	2.269	11.878	C
245	GLN	16	-3.326	0.889	12.444	C
246	GLN	16	-3.288	0.68	13.656	O
247	GLN	16	-3.058	-0.027	11.518	N
248	GLN	16	-3.728	3.587	9.537	H
249	GLN	16	-3.15	5.023	11.855	H
250	GLN	16	-1.864	2.609	10.898	H
251	GLN	16	-1.857	3.117	12.451	H
252	GLN	16	-4.241	2.762	12.538	H

253	GLN	16	-4.179	2.156	11.022	H
254	GLN	16	-3.094	0.216	10.548	H
255	GLN	16	-2.82	-0.959	11.79	H
256	CYS	17	-0.856	4.981	9.607	N
257	CYS	17	0.504	5.315	9.199	C
258	CYS	17	0.522	6.226	7.956	C
259	CYS	17	1.329	7.143	7.86	O
260	CYS	17	1.229	4.001	8.886	C
261	CYS	17	1.148	2.829	10.261	S
262	CYS	17	-1.459	4.543	8.941	H
263	CYS	17	0.956	5.815	9.938	H
264	CYS	17	0.805	3.583	8.082	H
265	CYS	17	2.189	4.202	8.691	H
266	HIS	18	-0.374	5.907	7.007	N
267	HIS	18	-0.461	6.645	5.746	C
268	HIS	18	-1.61	7.654	5.85	C
269	HIS	18	-2.37	7.667	6.812	O
270	HIS	18	-0.738	5.669	4.586	C
271	HIS	18	0.513	4.907	4.221	C
272	HIS	18	1.299	5.203	3.158	N
273	HIS	18	1.059	3.793	4.876	C
274	HIS	18	2.288	4.296	3.162	C
275	HIS	18	2.174	3.435	4.19	N
276	HIS	18	-1	5.144	7.167	H
277	HIS	18	0.402	7.12	5.571	H
278	HIS	18	-1.447	5.021	4.864	H
279	HIS	18	-1.052	6.186	3.79	H
280	HIS	18	1.169	5.947	2.503	H
281	HIS	18	0.695	3.347	5.694	H
282	HIS	18	3.021	4.264	2.483	H
283	THR	19	-1.707	8.469	4.791	N
284	THR	19	-2.836	9.371	4.607	C
285	THR	19	-2.691	10.013	3.216	C
286	THR	19	-2.692	11.232	3.067	O
287	THR	19	-2.929	10.42	5.749	C
288	THR	19	-3.945	11.384	5.527	O
289	THR	19	-1.599	11.127	6.048	C
290	THR	19	-0.98	8.457	4.104	H
291	THR	19	-3.699	8.867	4.652	H
292	THR	19	-3.171	9.882	6.557	H
293	THR	19	-3.76	11.875	4.676	H
294	THR	19	-1.73	11.785	6.789	H
295	THR	19	-1.284	11.607	5.229	H
296	THR	19	-0.915	10.45	6.321	H
297	VAL	20	-2.541	9.129	2.212	N
298	VAL	20	-2.31	9.597	0.847	C
299	VAL	20	-3.621	10.121	0.221	C
300	VAL	20	-4.305	9.443	-0.539	O
301	VAL	20	-1.6	8.5	0.015	C
302	VAL	20	-2.359	7.164	-0.056	C
303	VAL	20	-1.224	8.989	-1.394	C

304	VAL	20	-2.589	8.148	2.4	H
305	VAL	20	-1.686	10.379	0.857	H
306	VAL	20	-0.758	8.312	0.521	H
307	VAL	20	-1.838	6.513	-0.608	H
308	VAL	20	-3.256	7.311	-0.474	H
309	VAL	20	-2.478	6.798	0.867	H
310	VAL	20	-0.77	8.251	-1.893	H
311	VAL	20	-0.606	9.772	-1.322	H
312	VAL	20	-2.052	9.263	-1.884	H
313	GLU	21	-3.907	11.384	0.564	N
314	GLU	21	-4.992	12.126	-0.059	C
315	GLU	21	-4.47	13.55	-0.297	C
316	GLU	21	-4.492	14.407	0.583	O
317	GLU	21	-6.252	12.086	0.833	C
318	GLU	21	-7.527	12.569	0.107	C
319	GLU	21	-8.778	12.424	0.981	C
320	GLU	21	-9.374	11.275	1.508	O
321	GLU	21	-9.597	13.359	0.705	O
322	GLU	21	-3.358	11.831	1.27	H
323	GLU	21	-5.268	11.724	-0.932	H
324	GLU	21	-6.397	11.144	1.136	H
325	GLU	21	-6.097	12.673	1.628	H
326	GLU	21	-7.414	13.532	-0.137	H
327	GLU	21	-7.65	12.027	-0.724	H
328	GLU	21	-10.269	11.313	1.844	H
329	LYS	22	-3.993	13.738	-1.539	N
330	LYS	22	-3.526	15.039	-2.015	C
331	LYS	22	-2.31	15.554	-1.211	C
332	LYS	22	-2.221	16.729	-0.86	O
333	LYS	22	-4.666	16.079	-2.042	C
334	LYS	22	-5.887	15.625	-2.859	C
335	LYS	22	-6.974	16.708	-2.923	C
336	LYS	22	-8.201	16.263	-3.739	C
337	LYS	22	-9.262	17.265	-3.828	N
338	LYS	22	-12.143	18.188	-4.771	X
339	LYS	22	-3.956	12.957	-2.162	H
340	LYS	22	-3.217	14.906	-2.957	H
341	LYS	22	-4.96	16.251	-1.102	H
342	LYS	22	-4.314	16.925	-2.442	H
343	LYS	22	-5.591	15.41	-3.79	H
344	LYS	22	-6.273	14.806	-2.434	H
345	LYS	22	-7.269	16.922	-1.992	H
346	LYS	22	-6.587	17.527	-3.347	H
347	LYS	22	-7.898	16.046	-4.667	H
348	LYS	22	-8.581	15.443	-3.311	H
349	LYS	22	-10.019	16.902	-4.372	H
350	LYS	22	-8.905	18.091	-4.265	H
351	LYS	22	-9.588	17.488	-2.91	H
352	GLY	23	-1.371	14.623	-0.973	N
353	GLY	23	-0.123	15.001	-0.315	C
354	GLY	23	-0.339	15.25	1.18	C

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355	GLY	23	-0.179	16.359	1.69		O
356	GLY	23	-1.526	13.673	-1.245		H
357	GLY	23	0.543	14.264	-0.43		H
358	GLY	23	0.228	15.837	-0.737		H
359	GLY	24	-0.725	14.156	1.847		N
360	GLY	24	-0.953	14.214	3.283		C
361	GLY	24	0.379	14.171	4.035		C
362	GLY	24	1.457	14.072	3.453		O
363	GLY	24	-0.858	13.295	1.357		H
364	GLY	24	-1.431	15.064	3.507		H
365	GLY	24	-1.513	13.433	3.56		H
366	LYS	25	0.247	14.249	5.368		N
367	LYS	25	1.421	14.139	6.222		C
368	LYS	25	1.961	12.702	6.133		C
369	LYS	25	1.234	11.742	6.361		O
370	LYS	25	1.042	14.463	7.678		C
371	LYS	25	0.507	15.892	7.861		C
372	LYS	25	0.171	16.201	9.326		C
373	LYS	25	-0.372	17.629	9.514		C
374	LYS	25	-0.711	17.97	10.895		N
375	LYS	25	-1.605	18.825	13.903	-1	X
376	LYS	25	-0.657	14.382	5.774		H
377	LYS	25	2.121	14.787	5.92		H
378	LYS	25	0.336	13.819	7.973		H
379	LYS	25	1.855	14.352	8.25		H
380	LYS	25	1.202	16.539	7.547		H
381	LYS	25	-0.321	15.999	7.311		H
382	LYS	25	-0.52	15.551	9.641		H
383	LYS	25	1.001	16.098	9.874		H
384	LYS	25	0.324	18.272	9.195		H
385	LYS	25	-1.197	17.726	8.957		H
386	LYS	25	-1.054	18.908	10.932		H
387	LYS	25	0.106	17.892	11.468		H
388	LYS	25	-1.414	17.344	11.231		H
389	HIS	26	3.255	12.597	5.793		N
390	HIS	26	3.872	11.276	5.699		C
391	HIS	26	4.232	10.835	7.132		C
392	HIS	26	5.37	10.949	7.577		O
393	HIS	26	5.134	11.315	4.813		C
394	HIS	26	4.866	11.793	3.395		C
395	HIS	26	3.872	12.632	3.016		N
396	HIS	26	5.615	11.483	2.246		C
397	HIS	26	4.013	12.825	1.698		C
398	HIS	26	5.062	12.141	1.201		N
399	HIS	26	3.793	13.418	5.604		H
400	HIS	26	3.238	10.628	5.277		H
401	HIS	26	5.798	11.933	5.235		H
402	HIS	26	5.518	10.393	4.769		H
403	HIS	26	3.169	13.029	3.606		H
404	HIS	26	6.414	10.883	2.208		H
405	HIS	26	3.412	13.406	1.149		H

406	LYS	27	3.181	10.39	7.838		N
407	LYS	27	3.251	10.175	9.278		C
408	LYS	27	4.217	9.025	9.617		C
409	LYS	27	5.172	9.175	10.377		O
410	LYS	27	1.823	9.906	9.793		C
411	LYS	27	1.722	9.687	11.312		C
412	LYS	27	0.365	9.1	11.722		C
413	LYS	27	0.343	8.661	13.195		C
414	LYS	27	-0.849	7.908	13.573		N
415	LYS	27	-3.53	7.066	13.676	-1	X
416	LYS	27	2.323	10.199	7.361		H
417	LYS	27	3.615	10.987	9.734		H
418	LYS	27	1.252	10.691	9.552		H
419	LYS	27	1.476	9.087	9.336		H
420	LYS	27	2.445	9.057	11.595		H
421	LYS	27	1.846	10.566	11.773		H
422	LYS	27	-0.341	9.794	11.582		H
423	LYS	27	0.171	8.306	11.146		H
424	LYS	27	1.144	8.087	13.364		H
425	LYS	27	0.392	9.479	13.768		H
426	LYS	27	-0.793	7.658	14.54		H
427	LYS	27	-0.91	7.079	13.018		H
428	LYS	27	-1.661	8.471	13.422		H
429	THR	28	3.902	7.868	9.026		N
430	THR	28	4.722	6.683	9.243		C
431	THR	28	4.653	5.79	7.999		C
432	THR	28	4.701	4.567	8.068		O
433	THR	28	4.271	5.972	10.541		C
434	THR	28	3.98	6.904	11.574		O
435	THR	28	5.301	4.962	11.071		C
436	THR	28	3.1	7.815	8.431		H
437	THR	28	5.683	6.928	9.374		H
438	THR	28	3.444	5.471	10.287		H
439	THR	28	4.798	7.443	11.777		H
440	THR	28	4.953	4.538	11.907		H
441	THR	28	6.16	5.434	11.27		H
442	THR	28	5.461	4.256	10.381		H
443	GLY	29	4.556	6.483	6.859		N
444	GLY	29	4.627	5.793	5.587		C
445	GLY	29	4.641	6.849	4.484		C
446	GLY	29	4.19	7.973	4.689		O
447	GLY	29	4.436	7.475	6.885		H
448	GLY	29	5.462	5.245	5.544		H
449	GLY	29	3.831	5.198	5.478		H
450	PRO	30	5.192	6.468	3.307		N
451	PRO	30	5.223	7.359	2.149		C
452	PRO	30	3.817	7.568	1.56		C
453	PRO	30	3.033	6.634	1.449		O
454	PRO	30	6.122	6.618	1.147		C
455	PRO	30	6.018	5.139	1.534		C
456	PRO	30	5.805	5.159	3.048		C

457	PRO	30	5.556	8.272	2.38	H
458	PRO	30	5.797	6.76	0.212	H
459	PRO	30	7.067	6.935	1.223	H
460	PRO	30	5.243	4.706	1.073	H
461	PRO	30	6.86	4.652	1.301	H
462	PRO	30	5.194	4.419	3.33	H
463	PRO	30	6.677	5.074	3.53	H
464	ASN	31	3.521	8.822	1.163	N
465	ASN	31	2.352	8.992	0.295	C
466	ASN	31	2.606	8.217	-1.006	C
467	ASN	31	3.553	8.489	-1.738	O
468	ASN	31	2.096	10.471	-0.064	C
469	ASN	31	1.062	11.155	0.836	C
470	ASN	31	0.205	11.891	0.357	O
471	ASN	31	1.157	10.878	2.137	N
472	ASN	31	4.076	9.603	1.449	H
473	ASN	31	1.55	8.652	0.786	H
474	ASN	31	2.96	10.968	0.014	H
475	ASN	31	1.77	10.514	-1.008	H
476	ASN	31	1.87	10.259	2.466	H
477	ASN	31	0.515	11.289	2.784	H
478	LEU	32	1.72	7.244	-1.236	N
479	LEU	32	1.839	6.326	-2.359	C
480	LEU	32	1.235	6.97	-3.624	C
481	LEU	32	0.331	6.439	-4.256	O
482	LEU	32	1.085	5.038	-1.981	C
483	LEU	32	1.549	4.38	-0.665	C
484	LEU	32	0.607	3.233	-0.282	C
485	LEU	32	3.004	3.892	-0.736	C
486	LEU	32	0.946	7.142	-0.611	H
487	LEU	32	2.796	6.116	-2.556	H
488	LEU	32	0.114	5.261	-1.892	H
489	LEU	32	1.209	4.376	-2.72	H
490	LEU	32	1.513	5.082	0.047	H
491	LEU	32	0.919	2.816	0.572	H
492	LEU	32	0.606	2.545	-1.008	H
493	LEU	32	-0.32	3.589	-0.16	H
494	LEU	32	3.259	3.475	0.136	H
495	LEU	32	3.607	4.667	-0.923	H
496	LEU	32	3.094	3.216	-1.468	H
497	HIS	33	1.748	8.168	-3.938	N
498	HIS	33	1.12	8.994	-4.961	C
499	HIS	33	1.439	8.443	-6.367	C
500	HIS	33	2.4	8.843	-7.02	O
501	HIS	33	1.608	10.442	-4.792	C
502	HIS	33	0.835	11.369	-5.704	C
503	HIS	33	1.09	11.516	-7.021	N
504	HIS	33	-0.241	12.206	-5.365	C
505	HIS	33	0.202	12.414	-7.478	C
506	HIS	33	-0.617	12.851	-6.498	N
507	HIS	33	2.566	8.498	-3.467	H

508	HIS	33	0.125	8.974	-4.858	H
509	HIS	33	1.473	10.726	-3.843	H
510	HIS	33	2.58	10.491	-5.02	H
511	HIS	33	1.798	11.05	-7.551	H
512	HIS	33	-0.652	12.307	-4.459	H
513	HIS	33	0.153	12.721	-8.428	H
514	GLY	34	0.563	7.524	-6.795	N
515	GLY	34	0.728	6.889	-8.094	C
516	GLY	34	1.564	5.623	-7.931	C
517	GLY	34	2.763	5.618	-8.179	O
518	GLY	34	-0.213	7.272	-6.217	H
519	GLY	34	-0.169	6.652	-8.466	H
520	GLY	34	1.192	7.518	-8.717	H
521	LEU	35	0.873	4.56	-7.492	N
522	LEU	35	1.54	3.266	-7.346	C
523	LEU	35	1.756	2.641	-8.725	C
524	LEU	35	2.844	2.225	-9.103	O
525	LEU	35	0.672	2.323	-6.489	C
526	LEU	35	0.726	2.644	-4.99	C
527	LEU	35	-0.436	1.967	-4.253	C
528	LEU	35	2.07	2.212	-4.379	C
529	LEU	35	-0.097	4.651	-7.266	H
530	LEU	35	2.423	3.403	-6.898	H
531	LEU	35	-0.277	2.399	-6.796	H
532	LEU	35	0.993	1.386	-6.625	H
533	LEU	35	0.64	3.634	-4.883	H
534	LEU	35	-0.386	2.186	-3.279	H
535	LEU	35	-0.377	0.976	-4.375	H
536	LEU	35	-1.304	2.297	-4.624	H
537	LEU	35	2.079	2.432	-3.404	H
538	LEU	35	2.816	2.696	-4.836	H
539	LEU	35	2.19	1.226	-4.499	H
540	PHE	36	0.624	2.577	-9.434	N
541	PHE	36	0.554	1.804	-10.665	C
542	PHE	36	1.551	2.348	-11.705	C
543	PHE	36	1.397	3.449	-12.231	O
544	PHE	36	-0.885	1.841	-11.205	C
545	PHE	36	-1.856	1.221	-10.233	C
546	PHE	36	-2.135	-0.141	-10.284	C
547	PHE	36	-2.482	1.999	-9.264	C
548	PHE	36	-3.019	-0.717	-9.379	C
549	PHE	36	-3.368	1.426	-8.361	C
550	PHE	36	-3.635	0.065	-8.413	C
551	PHE	36	-0.187	3.067	-9.114	H
552	PHE	36	0.806	0.855	-10.476	H
553	PHE	36	-1.148	2.793	-11.364	H
554	PHE	36	-0.921	1.336	-12.067	H
555	PHE	36	-1.695	-0.711	-10.978	H
556	PHE	36	-2.292	2.98	-9.217	H
557	PHE	36	-3.211	-1.697	-9.424	H
558	PHE	36	-3.815	1.996	-7.671	H

559	PHE	36	-4.267	-0.349	-7.758		H
560	GLY	37	2.56	1.512	-11.979		N
561	GLY	37	3.554	1.856	-12.989		C
562	GLY	37	4.754	2.62	-12.408		C
563	GLY	37	5.545	3.199	-13.15		O
564	GLY	37	2.634	0.645	-11.487		H
565	GLY	37	3.886	1.012	-13.41		H
566	GLY	37	3.118	2.427	-13.684		H
567	ARG	38	4.865	2.594	-11.068		N
568	ARG	38	6.007	3.184	-10.376		C
569	ARG	38	6.84	2.032	-9.794		C
570	ARG	38	6.313	0.984	-9.431		O
571	ARG	38	5.519	4.146	-9.275		C
572	ARG	38	6.65	5.032	-8.721		C
573	ARG	38	6.235	5.906	-7.532		C
574	ARG	38	5.256	6.919	-7.906		N
575	ARG	38	5.573	8.11	-8.469		C
576	ARG	38	6.819	8.381	-8.847		N
577	ARG	38	4.622	9.015	-8.637		N
578	ARG	38	6.686	10.654	-10.608	-1	X
579	ARG	38	4.143	2.158	-10.531		H
580	ARG	38	6.571	3.72	-11.003		H
581	ARG	38	4.808	4.736	-9.657		H
582	ARG	38	5.138	3.607	-8.524		H
583	ARG	38	7.399	4.438	-8.428		H
584	ARG	38	6.968	5.632	-9.456		H
585	ARG	38	5.838	5.32	-6.825		H
586	ARG	38	7.047	6.362	-7.169		H
587	ARG	38	4.29	6.723	-7.737		H
588	ARG	38	7.54	7.701	-8.717		H
589	ARG	38	7.034	9.266	-9.26		H
590	ARG	38	3.685	8.815	-8.35		H
591	ARG	38	4.84	9.899	-9.051		H
592	LYS	39	8.159	2.278	-9.756		N
593	LYS	39	9.094	1.351	-9.129		C
594	LYS	39	9.104	1.635	-7.619		C
595	LYS	39	8.582	2.644	-7.152		O
596	LYS	39	10.472	1.523	-9.8		C
597	LYS	39	11.553	0.531	-9.329		C
598	LYS	39	12.794	0.486	-10.237		C
599	LYS	39	12.524	0.039	-11.689		C
600	LYS	39	11.869	-1.259	-11.841		N
601	LYS	39	9.811	-4.25	-12.61	-1	X
602	LYS	39	8.51	3.12	-10.167		H
603	LYS	39	8.829	0.394	-9.25		H
604	LYS	39	10.353	1.408	-10.786		H
605	LYS	39	10.797	2.449	-9.609		H
606	LYS	39	11.845	0.796	-8.41		H
607	LYS	39	11.15	-0.384	-9.301		H
608	LYS	39	13.192	1.403	-10.264		H
609	LYS	39	13.451	-0.151	-9.833		H

610	LYS	39	11.942	0.729	-12.12	H
611	LYS	39	13.402	-0.002	-12.166	H
612	LYS	39	11.74	-1.456	-12.812	H
613	LYS	39	10.98	-1.24	-11.383	H
614	LYS	39	12.44	-1.971	-11.43	H
615	THR	40	9.703	0.689	-6.892	N
616	THR	40	9.742	0.75	-5.442	C
617	THR	40	10.569	1.958	-4.955	C
618	THR	40	11.479	2.437	-5.628	O
619	THR	40	10.317	-0.601	-4.986	C
620	THR	40	11.35	-1.02	-5.869	O
621	THR	40	9.249	-1.693	-5.051	C
622	THR	40	10.137	-0.081	-7.358	H
623	THR	40	8.835	0.891	-5.044	H
624	THR	40	10.654	-0.475	-4.053	H
625	THR	40	10.979	-1.118	-6.793	H
626	THR	40	9.642	-2.562	-4.751	H
627	THR	40	8.92	-1.783	-5.991	H
628	THR	40	8.485	-1.449	-4.453	H
629	GLY	41	10.206	2.414	-3.745	N
630	GLY	41	10.879	3.565	-3.161	C
631	GLY	41	10.249	4.854	-3.696	C
632	GLY	41	9.037	5.038	-3.639	O
633	GLY	41	9.47	1.96	-3.243	H
634	GLY	41	10.784	3.536	-2.166	H
635	GLY	41	11.849	3.542	-3.405	H
636	GLN	42	11.129	5.729	-4.212	N
637	GLN	42	10.719	7.009	-4.793	C
638	GLN	42	9.883	7.863	-3.811	C
639	GLN	42	8.866	8.45	-4.173	O
640	GLN	42	9.958	6.817	-6.118	C
641	GLN	42	10.739	6.007	-7.165	C
642	GLN	42	10.053	6.089	-8.536	C
643	GLN	42	9.134	6.873	-8.756	O
644	GLN	42	10.565	5.267	-9.449	N
645	GLN	42	12.102	5.497	-4.198	H
646	GLN	42	11.563	7.51	-4.985	H
647	GLN	42	9.101	6.339	-5.924	H
648	GLN	42	9.758	7.719	-6.501	H
649	GLN	42	11.666	6.374	-7.239	H
650	GLN	42	10.781	5.051	-6.876	H
651	GLN	42	11.33	4.668	-9.21	H
652	GLN	42	10.184	5.247	-10.374	H
653	ALA	43	10.378	7.904	-2.564	N
654	ALA	43	9.69	8.627	-1.498	C
655	ALA	43	10.601	9.735	-0.931	C
656	ALA	43	11.16	9.593	0.15	O
657	ALA	43	9.313	7.638	-0.386	C
658	ALA	43	11.235	7.43	-2.361	H
659	ALA	43	8.863	9.053	-1.865	H
660	ALA	43	8.841	8.126	0.348	H

661	ALA	43	10.142	7.212	-0.024	H
662	ALA	43	8.71	6.932	-0.758	H
663	PRO	44	10.734	10.876	-1.665	N
664	PRO	44	11.573	11.969	-1.167	C
665	PRO	44	10.989	12.686	0.071	C
666	PRO	44	11.673	13.452	0.749	O
667	PRO	44	11.659	12.929	-2.365	C
668	PRO	44	10.416	12.632	-3.211	C
669	PRO	44	10.12	11.149	-2.965	C
670	PRO	44	12.459	11.629	-0.853	H
671	PRO	44	11.652	13.879	-2.054	H
672	PRO	44	12.491	12.757	-2.893	H
673	PRO	44	9.646	13.198	-2.917	H
674	PRO	44	10.601	12.798	-4.18	H
675	PRO	44	9.134	10.984	-2.934	H
676	PRO	44	10.531	10.582	-3.678	H
677	GLY	45	9.705	12.392	0.344	N
678	GLY	45	9.053	12.949	1.523	C
679	GLY	45	9.249	12.066	2.764	C
680	GLY	45	9.131	12.528	3.896	O
681	GLY	45	9.193	11.788	-0.267	H
682	GLY	45	9.438	13.853	1.707	H
683	GLY	45	8.074	13.034	1.34	H
684	PHE	46	9.528	10.779	2.498	N
685	PHE	46	9.627	9.78	3.555	C
686	PHE	46	10.714	8.792	3.128	C
687	PHE	46	10.447	7.778	2.491	O
688	PHE	46	8.264	9.085	3.725	C
689	PHE	46	8.193	8.21	4.949	C
690	PHE	46	7.769	8.74	6.164	C
691	PHE	46	8.536	6.864	4.883	C
692	PHE	46	7.685	7.937	7.294	C
693	PHE	46	8.451	6.057	6.011	C
694	PHE	46	8.025	6.593	7.218	C
695	PHE	46	9.671	10.499	1.549	H
696	PHE	46	9.867	10.187	4.437	H
697	PHE	46	7.556	9.787	3.795	H
698	PHE	46	8.094	8.518	2.919	H
699	PHE	46	7.523	9.707	6.224	H
700	PHE	46	8.846	6.473	4.016	H
701	PHE	46	7.38	8.327	8.163	H
702	PHE	46	8.697	5.089	5.953	H
703	PHE	46	7.963	6.013	8.03	H
704	THR	47	11.948	9.17	3.492	N
705	THR	47	13.127	8.448	3.043	C
706	THR	47	13.023	6.939	3.361	C
707	THR	47	13.028	6.516	4.515	O
708	THR	47	14.345	9.094	3.733	C
709	THR	47	14.173	10.503	3.836	O
710	THR	47	15.676	8.757	3.043	C
711	THR	47	12.059	9.967	4.086	H

712	THR	47	13.22	8.512	2.049	H
713	THR	47	14.395	8.702	4.652	H
714	THR	47	14.074	10.895	2.921	H
715	THR	47	16.427	9.201	3.532	H
716	THR	47	15.654	9.084	2.098	H
717	THR	47	15.814	7.767	3.05	H
718	TYR	48	12.931	6.176	2.26	N
719	TYR	48	12.856	4.725	2.338	C
720	TYR	48	14.106	4.179	3.051	C
721	TYR	48	15.224	4.635	2.823	O
722	TYR	48	12.689	4.127	0.924	C
723	TYR	48	13.595	4.757	-0.106	C
724	TYR	48	13.117	5.758	-0.947	C
725	TYR	48	14.919	4.357	-0.232	C
726	TYR	48	13.947	6.358	-1.888	C
727	TYR	48	15.752	4.951	-1.17	C
728	TYR	48	15.272	5.953	-2.001	C
729	TYR	48	16.136	6.525	-2.92	O
730	TYR	48	12.913	6.617	1.363	H
731	TYR	48	12.057	4.454	2.875	H
732	TYR	48	12.892	3.149	0.968	H
733	TYR	48	11.741	4.259	0.635	H
734	TYR	48	12.163	6.05	-0.874	H
735	TYR	48	15.276	3.634	0.359	H
736	TYR	48	13.591	7.079	-2.482	H
737	TYR	48	16.704	4.655	-1.247	H
738	TYR	48	15.78	6.387	-3.844	H
739	THR	49	13.865	3.186	3.917	N
740	THR	49	14.942	2.567	4.678	C
741	THR	49	15.627	1.459	3.846	C
742	THR	49	15.65	0.288	4.211	O
743	THR	49	14.328	2.052	5.998	C
744	THR	49	13.446	3.021	6.551	O
745	THR	49	15.374	1.658	7.052	C
746	THR	49	12.927	2.864	4.043	H
747	THR	49	15.668	3.22	4.893	H
748	THR	49	13.826	1.222	5.757	H
749	THR	49	13.951	3.865	6.736	H
750	THR	49	14.911	1.335	7.877	H
751	THR	49	15.938	2.453	7.276	H
752	THR	49	15.955	0.929	6.69	H
753	ASP	50	16.195	1.93	2.722	N
754	ASP	50	16.989	1.163	1.768	C
755	ASP	50	16.226	-0.032	1.162	C
756	ASP	50	15.769	0.024	0.028	O
757	ASP	50	18.37	0.787	2.353	C
758	ASP	50	19.348	0.289	1.28	C
759	ASP	50	20.486	0.615	1.409	O
760	ASP	50	18.949	0.199	0.011	O
761	ASP	50	16.059	2.9	2.52	H
762	ASP	50	17.166	1.764	0.988	H

763	ASP	50	18.762	1.595	2.794	H
764	ASP	50	18.244	0.064	3.032	H
765	ASP	50	19.597	0.142	-0.689	H
766	ALA	51	16.127	-1.112	1.954	N
767	ALA	51	15.617	-2.406	1.496	C
768	ALA	51	14.357	-2.287	0.62	C
769	ALA	51	14.228	-2.936	-0.413	O
770	ALA	51	15.323	-3.296	2.711	C
771	ALA	51	16.416	-1.028	2.908	H
772	ALA	51	16.327	-2.814	0.921	H
773	ALA	51	14.975	-4.18	2.4	H
774	ALA	51	14.639	-2.854	3.291	H
775	ALA	51	16.164	-3.435	3.234	H
776	ASN	52	13.449	-1.417	1.087	N
777	ASN	52	12.161	-1.259	0.414	C
778	ASN	52	12.308	-0.861	-1.063	C
779	ASN	52	11.563	-1.325	-1.917	O
780	ASN	52	11.269	-0.247	1.157	C
781	ASN	52	10.687	-0.854	2.439	C
782	ASN	52	11.269	-0.777	3.517	O
783	ASN	52	9.521	-1.471	2.263	N
784	ASN	52	13.654	-0.873	1.901	H
785	ASN	52	11.72	-2.156	0.433	H
786	ASN	52	11.816	0.555	1.396	H
787	ASN	52	10.518	0.028	0.557	H
788	ASN	52	9.106	-1.507	1.354	H
789	ASN	52	9.059	-1.9	3.04	H
790	LYS	53	13.292	0.011	-1.345	N
791	LYS	53	13.445	0.451	-2.731	C
792	LYS	53	14.029	-0.664	-3.627	C
793	LYS	53	13.878	-0.653	-4.844	O
794	LYS	53	14.299	1.734	-2.822	C
795	LYS	53	15.797	1.566	-2.477	C
796	LYS	53	16.73	2.212	-3.511	C
797	LYS	53	18.188	1.715	-3.435	C
798	LYS	53	18.95	2.076	-2.24	N
799	LYS	53	13.901	0.349	-0.627	H
800	LYS	53	12.53	0.664	-3.073	H
801	LYS	53	14.236	2.08	-3.758	H
802	LYS	53	13.912	2.406	-2.191	H
803	LYS	53	15.968	1.989	-1.587	H
804	LYS	53	16.004	0.589	-2.428	H
805	LYS	53	16.376	2.01	-4.424	H
806	LYS	53	16.727	3.201	-3.363	H
807	LYS	53	18.17	0.717	-3.491	H
808	LYS	53	18.675	2.085	-4.226	H
809	LYS	53	19.874	1.699	-2.306	H
810	LYS	53	19.002	3.072	-2.165	H
811	ASN	54	14.744	-1.592	-2.961	N
812	ASN	54	15.67	-2.482	-3.662	C
813	ASN	54	14.955	-3.61	-4.407	C

814	ASN	54	15.588	-4.336	-5.171		O
815	ASN	54	16.691	-3.112	-2.69		C
816	ASN	54	17.925	-2.233	-2.475		C
817	ASN	54	18.968	-2.428	-3.097		O
818	ASN	54	17.778	-1.301	-1.539		N
819	ASN	54	14.639	-1.675	-1.97		H
820	ASN	54	16.142	-1.904	-4.328		H
821	ASN	54	16.244	-3.257	-1.807		H
822	ASN	54	16.986	-3.992	-3.063		H
823	ASN	54	16.912	-1.221	-1.045		H
824	ASN	54	18.532	-0.679	-1.33		H
825	LYS	55	13.636	-3.757	-4.172		N
826	LYS	55	12.916	-4.8	-4.905		C
827	LYS	55	12.965	-4.507	-6.42		C
828	LYS	55	13.174	-5.387	-7.253		O
829	LYS	55	11.472	-4.961	-4.372		C
830	LYS	55	11.189	-6.382	-3.855		C
831	LYS	55	11.21	-7.441	-4.97		C
832	LYS	55	11.198	-8.881	-4.429		C
833	LYS	55	11.329	-9.922	-5.45		N
834	LYS	55	11.412	-11.313	-8.361	-1	X
835	LYS	55	13.163	-3.17	-3.515		H
836	LYS	55	13.367	-5.68	-4.754		H
837	LYS	55	11.333	-4.314	-3.623		H
838	LYS	55	10.832	-4.756	-5.113		H
839	LYS	55	11.885	-6.619	-3.177		H
840	LYS	55	10.287	-6.391	-3.424		H
841	LYS	55	10.405	-7.311	-5.548		H
842	LYS	55	12.038	-7.312	-5.516		H
843	LYS	55	11.958	-8.978	-3.787		H
844	LYS	55	10.334	-9.025	-3.947		H
845	LYS	55	11.312	-10.822	-5.014		H
846	LYS	55	12.195	-9.805	-5.937		H
847	LYS	55	10.57	-9.852	-6.098		H
848	GLY	56	12.806	-3.21	-6.709		N
849	GLY	56	13.064	-2.693	-8.046		C
850	GLY	56	12.063	-3.213	-9.082		C
851	GLY	56	12.377	-3.34	-10.264		O
852	GLY	56	12.504	-2.582	-5.992		H
853	GLY	56	13.008	-1.695	-8.02		H
854	GLY	56	13.984	-2.968	-8.324		H
855	ILE	57	10.855	-3.502	-8.578		N
856	ILE	57	9.799	-4.054	-9.419		C
857	ILE	57	9.046	-2.887	-10.095		C
858	ILE	57	9.629	-1.859	-10.437		O
859	ILE	57	8.923	-5.004	-8.561		C
860	ILE	57	8.297	-4.306	-7.335		C
861	ILE	57	9.749	-6.225	-8.128		C
862	ILE	57	7.202	-5.136	-6.653		C
863	ILE	57	10.674	-3.337	-7.608		H
864	ILE	57	10.154	-4.617	-10.166		H

865	ILE	57	8.159	-5.3	-9.135	H
866	ILE	57	9.021	-4.128	-6.668	H
867	ILE	57	7.898	-3.439	-7.634	H
868	ILE	57	9.18	-6.834	-7.575	H
869	ILE	57	10.534	-5.922	-7.588	H
870	ILE	57	10.071	-6.715	-8.938	H
871	ILE	57	6.839	-4.631	-5.87	H
872	ILE	57	7.588	-6.004	-6.339	H
873	ILE	57	6.465	-5.315	-7.304	H
874	THR	58	7.734	-3.085	-10.25	N
875	THR	58	6.833	-2.018	-10.632	C
876	THR	58	5.46	-2.435	-10.108	C
877	THR	58	5.008	-3.543	-10.381	O
878	THR	58	6.841	-1.847	-12.168	C
879	THR	58	8.139	-2	-12.727	O
880	THR	58	6.263	-0.494	-12.595	C
881	THR	58	7.361	-4.001	-10.097	H
882	THR	58	7.101	-1.133	-10.252	H
883	THR	58	6.257	-2.578	-12.522	H
884	THR	58	8.753	-1.313	-12.338	H
885	THR	58	6.285	-0.421	-13.592	H
886	THR	58	6.808	0.243	-12.195	H
887	THR	58	5.318	-0.419	-12.277	H
888	TRP	59	4.848	-1.541	-9.318	N
889	TRP	59	3.589	-1.907	-8.685	C
890	TRP	59	2.472	-1.968	-9.735	C
891	TRP	59	2.32	-1.098	-10.59	O
892	TRP	59	3.225	-0.903	-7.582	C
893	TRP	59	4.258	-0.942	-6.476	C
894	TRP	59	5.264	0.004	-6.252	C
895	TRP	59	4.392	-1.94	-5.445	C
896	TRP	59	5.981	-0.363	-5.158	N
897	TRP	59	5.48	-1.55	-4.631	C
898	TRP	59	3.7	-3.086	-5.162	C
899	TRP	59	5.841	-2.319	-3.556	C
900	TRP	59	4.062	-3.875	-4.068	C
901	TRP	59	5.137	-3.489	-3.264	C
902	TRP	59	5.25	-0.637	-9.167	H
903	TRP	59	3.694	-2.81	-8.268	H
904	TRP	59	3.193	0.018	-7.971	H
905	TRP	59	2.329	-1.137	-7.205	H
906	TRP	59	5.429	0.819	-6.808	H
907	TRP	59	6.756	0.147	-4.785	H
908	TRP	59	2.932	-3.36	-5.741	H
909	TRP	59	6.61	-2.042	-2.98	H
910	TRP	59	3.554	-4.712	-3.861	H
911	TRP	59	5.402	-4.05	-2.48	H
912	LYS	60	1.706	-3.046	-9.583	N
913	LYS	60	0.423	-3.255	-10.219	C
914	LYS	60	-0.477	-3.867	-9.14	C
915	LYS	60	-0.026	-4.163	-8.036	O

916	LYS	60	0.582	-4.176	-11.443	C
917	LYS	60	1.121	-5.579	-11.107	C
918	LYS	60	1.338	-6.468	-12.34	C
919	LYS	60	0.064	-6.667	-13.183	C
920	LYS	60	0.161	-7.725	-14.185	N
921	LYS	60	2.043	-3.769	-8.98	H
922	LYS	60	0.023	-2.407	-10.566	H
923	LYS	60	-0.313	-4.279	-11.877	H
924	LYS	60	1.215	-3.741	-12.083	H
925	LYS	60	1.996	-5.476	-10.634	H
926	LYS	60	0.466	-6.032	-10.502	H
927	LYS	60	2.037	-6.045	-12.917	H
928	LYS	60	1.657	-7.364	-12.032	H
929	LYS	60	-0.688	-6.891	-12.564	H
930	LYS	60	-0.136	-5.808	-13.654	H
931	LYS	60	-0.702	-7.79	-14.686	H
932	LYS	60	0.902	-7.514	-14.823	H
933	GLU	61	-1.752	-4.064	-9.519	N
934	GLU	61	-2.748	-4.567	-8.573	C
935	GLU	61	-2.283	-5.865	-7.885	C
936	GLU	61	-2.363	-6.011	-6.672	O
937	GLU	61	-4.115	-4.721	-9.277	C
938	GLU	61	-4.101	-5.587	-10.557	C
939	GLU	61	-5.472	-5.594	-11.24	C
940	GLU	61	-5.269	-6.199	-12.266	O
941	GLU	61	-6.704	-5.216	-10.692	O
942	GLU	61	-2.024	-3.864	-10.46	H
943	GLU	61	-2.858	-3.897	-7.84	H
944	GLU	61	-4.752	-5.138	-8.628	H
945	GLU	61	-4.44	-3.808	-9.524	H
946	GLU	61	-3.423	-5.218	-11.192	H
947	GLU	61	-3.854	-6.525	-10.313	H
948	GLU	61	-6.763	-4.855	-9.811	H
949	GLU	62	-1.78	-6.779	-8.733	N
950	GLU	62	-1.383	-8.105	-8.27	C
951	GLU	62	-0.339	-8.02	-7.14	C
952	GLU	62	-0.5	-8.577	-6.06	O
953	GLU	62	-0.853	-8.936	-9.455	C
954	GLU	62	-1.9	-9.113	-10.573	C
955	GLU	62	-1.419	-10.102	-11.639	C
956	GLU	62	-2	-10.971	-12.327	O
957	GLU	62	-0.081	-9.801	-11.901	O
958	GLU	62	-1.676	-6.546	-9.7	H
959	GLU	62	-2.188	-8.561	-7.891	H
960	GLU	62	-0.052	-8.474	-9.837	H
961	GLU	62	-0.588	-9.84	-9.119	H
962	GLU	62	-2.749	-9.455	-10.172	H
963	GLU	62	-2.068	-8.227	-11.004	H
964	GLU	62	0.393	-10.281	-12.578	H
965	THR	63	0.736	-7.287	-7.456	N
966	THR	63	1.845	-7.175	-6.519	C

967	THR	63	1.39	-6.548	-5.19	C
968	THR	63	1.825	-6.938	-4.115	O
969	THR	63	2.926	-6.326	-7.209	C
970	THR	63	2.326	-5.367	-8.063	O
971	THR	63	3.815	-7.174	-8.119	C
972	THR	63	0.779	-6.817	-8.338	H
973	THR	63	2.207	-8.077	-6.285	H
974	THR	63	3.459	-5.904	-6.475	H
975	THR	63	1.783	-5.835	-8.761	H
976	THR	63	4.504	-6.591	-8.55	H
977	THR	63	3.254	-7.605	-8.826	H
978	THR	63	4.269	-7.881	-7.577	H
979	LEU	64	0.487	-5.559	-5.328	N
980	LEU	64	-0.009	-4.864	-4.147	C
981	LEU	64	-0.773	-5.839	-3.239	C
982	LEU	64	-0.498	-5.971	-2.052	O
983	LEU	64	-0.901	-3.687	-4.588	C
984	LEU	64	-0.117	-2.535	-5.246	C
985	LEU	64	-1.048	-1.614	-6.047	C
986	LEU	64	0.667	-1.727	-4.203	C
987	LEU	64	0.158	-5.303	-6.237	H
988	LEU	64	0.759	-4.5	-3.62	H
989	LEU	64	-1.573	-4.028	-5.245	H
990	LEU	64	-1.373	-3.329	-3.783	H
991	LEU	64	0.538	-2.947	-5.879	H
992	LEU	64	-0.513	-0.878	-6.462	H
993	LEU	64	-1.736	-1.222	-5.436	H
994	LEU	64	-1.502	-2.141	-6.766	H
995	LEU	64	1.164	-0.988	-4.658	H
996	LEU	64	1.316	-2.327	-3.735	H
997	LEU	64	0.032	-1.339	-3.535	H
998	MET	65	-1.745	-6.527	-3.852	N
999	MET	65	-2.614	-7.37	-3.034	C
1000	MET	65	-1.884	-8.603	-2.476	C
1001	MET	65	-2.357	-9.219	-1.53	O
1002	MET	65	-3.887	-7.761	-3.802	C
1003	MET	65	-3.637	-8.617	-5.05	C
1004	MET	65	-5.176	-8.958	-5.926	S
1005	MET	65	-5.28	-7.45	-6.91	C
1006	MET	65	-1.873	-6.465	-4.842	H
1007	MET	65	-2.89	-6.825	-2.242	H
1008	MET	65	-4.48	-8.276	-3.183	H
1009	MET	65	-4.351	-6.922	-4.086	H
1010	MET	65	-3.015	-8.128	-5.662	H
1011	MET	65	-3.221	-9.483	-4.773	H
1012	MET	65	-6.105	-7.476	-7.474	H
1013	MET	65	-4.475	-7.38	-7.5	H
1014	MET	65	-5.317	-6.657	-6.302	H
1015	GLU	66	-0.737	-8.947	-3.081	N
1016	GLU	66	0.081	-10.014	-2.506	C
1017	GLU	66	0.952	-9.454	-1.362	C

1018	GLU	66	1.14	-10.086	-0.327	O
1019	GLU	66	0.92	-10.657	-3.622	C
1020	GLU	66	0.078	-11.413	-4.678	C
1021	GLU	66	-0.396	-12.795	-4.203	C
1022	GLU	66	0.092	-13.92	-4.106	O
1023	GLU	66	-1.746	-12.688	-4.394	O
1024	GLU	66	-0.445	-8.479	-3.915	H
1025	GLU	66	-0.499	-10.725	-2.108	H
1026	GLU	66	1.434	-9.935	-4.086	H
1027	GLU	66	1.557	-11.305	-3.204	H
1028	GLU	66	-0.726	-10.86	-4.898	H
1029	GLU	66	0.635	-11.534	-5.5	H
1030	GLU	66	-2.261	-13.481	-4.367	H
1031	TYR	67	1.458	-8.231	-1.593	N
1032	TYR	67	2.328	-7.555	-0.625	C
1033	TYR	67	1.6	-7.375	0.715	C
1034	TYR	67	2.111	-7.642	1.796	O
1035	TYR	67	2.756	-6.201	-1.232	C
1036	TYR	67	3.738	-5.428	-0.386	C
1037	TYR	67	3.384	-4.224	0.216	C
1038	TYR	67	5.027	-5.91	-0.202	C
1039	TYR	67	4.301	-3.522	0.996	C
1040	TYR	67	5.945	-5.216	0.58	C
1041	TYR	67	5.586	-4.023	1.186	C
1042	TYR	67	6.519	-3.376	1.979	O
1043	TYR	67	1.235	-7.768	-2.45	H
1044	TYR	67	3.143	-8.104	-0.438	H
1045	TYR	67	3.178	-6.375	-2.122	H
1046	TYR	67	1.938	-5.64	-1.355	H
1047	TYR	67	2.462	-3.859	0.087	H
1048	TYR	67	5.299	-6.768	-0.638	H
1049	TYR	67	4.035	-2.656	1.42	H
1050	TYR	67	6.868	-5.58	0.705	H
1051	TYR	67	6.69	-2.46	1.614	H
1052	LEU	68	0.347	-6.938	0.568	N
1053	LEU	68	-0.489	-6.672	1.732	C
1054	LEU	68	-0.927	-7.962	2.458	C
1055	LEU	68	-1.453	-7.905	3.566	O
1056	LEU	68	-1.702	-5.854	1.264	C
1057	LEU	68	-1.344	-4.468	0.691	C
1058	LEU	68	-2.566	-3.834	0.011	C
1059	LEU	68	-0.779	-3.526	1.762	C
1060	LEU	68	-0.021	-6.793	-0.35	H
1061	LEU	68	0.041	-6.156	2.404	H
1062	LEU	68	-2.176	-6.374	0.554	H
1063	LEU	68	-2.312	-5.723	2.045	H
1064	LEU	68	-0.626	-4.608	0.009	H
1065	LEU	68	-2.317	-2.937	-0.354	H
1066	LEU	68	-3.302	-3.728	0.679	H
1067	LEU	68	-2.876	-4.423	-0.735	H
1068	LEU	68	-0.561	-2.642	1.348	H

1069	LEU	68	0.051	-3.924	2.152		H
1070	LEU	68	-1.458	-3.397	2.485		H
1071	GLU	69	-0.69	-9.115	1.801		N
1072	GLU	69	-0.945	-10.407	2.436		C
1073	GLU	69	0.245	-10.727	3.349		C
1074	GLU	69	0.123	-10.866	4.564		O
1075	GLU	69	-1.167	-11.474	1.341		C
1076	GLU	69	-1.971	-12.721	1.789		C
1077	GLU	69	-1.113	-13.82	2.428		C
1078	GLU	69	-1.265	-14.099	3.617		O
1079	GLU	69	-0.307	-14.43	1.728		O
1080	GLU	69	0.598	-15.237	4.05	1	X
1081	GLU	69	-0.336	-9.086	0.866		H
1082	GLU	69	-1.772	-10.391	2.998		H
1083	GLU	69	-1.66	-11.043	0.585		H
1084	GLU	69	-0.27	-11.782	1.023		H
1085	GLU	69	-2.657	-12.43	2.456		H
1086	GLU	69	-2.428	-13.105	0.987		H
1087	ASN	70	1.408	-10.813	2.689		N
1088	ASN	70	2.668	-11.03	3.4		C
1089	ASN	70	3.763	-10.245	2.666		C
1090	ASN	70	4.285	-10.702	1.652		O
1091	ASN	70	3.038	-12.523	3.443		C
1092	ASN	70	4.301	-12.743	4.296		C
1093	ASN	70	5.043	-11.817	4.613		O
1094	ASN	70	4.492	-14.01	4.661		N
1095	ASN	70	1.415	-10.727	1.693		H
1096	ASN	70	2.573	-10.717	4.345		H
1097	ASN	70	2.279	-13.038	3.841		H
1098	ASN	70	3.21	-12.846	2.512		H
1099	ASN	70	3.843	-14.715	4.378		H
1100	ASN	70	5.286	-14.255	5.218		H
1101	PRO	71	4.124	-9.052	3.199		N
1102	PRO	71	5.048	-8.188	2.472		C
1103	PRO	71	6.493	-8.695	2.524		C
1104	PRO	71	7.335	-8.344	1.704		O
1105	PRO	71	4.922	-6.852	3.213		C
1106	PRO	71	4.492	-7.219	4.637		C
1107	PRO	71	3.639	-8.474	4.455		C
1108	PRO	71	4.83	-8.139	1.497		H
1109	PRO	71	5.8	-6.374	3.225		H
1110	PRO	71	4.233	-6.273	2.777		H
1111	PRO	71	5.289	-7.411	5.21		H
1112	PRO	71	3.956	-6.481	5.047		H
1113	PRO	71	3.775	-9.11	5.215		H
1114	PRO	71	2.67	-8.238	4.387		H
1115	LYS	72	6.73	-9.575	3.512		N
1116	LYS	72	8.083	-10.039	3.784		C
1117	LYS	72	8.579	-10.968	2.66		C
1118	LYS	72	9.774	-11.169	2.469		O
1119	LYS	72	8.09	-10.729	5.161		C

1120	LYS	72	9.49	-10.841	5.779		C
1121	LYS	72	9.472	-11.432	7.194		C
1122	LYS	72	10.876	-11.462	7.826		C
1123	LYS	72	10.916	-11.977	9.193		N
1124	LYS	72	11.085	-13.026	11.745	-1	X
1125	LYS	72	5.969	-9.915	4.066		H
1126	LYS	72	8.717	-9.267	3.808		H
1127	LYS	72	7.51	-10.202	5.783		H
1128	LYS	72	7.715	-11.65	5.056		H
1129	LYS	72	10.05	-11.428	5.195		H
1130	LYS	72	9.895	-9.927	5.82		H
1131	LYS	72	8.872	-10.876	7.768		H
1132	LYS	72	9.119	-12.366	7.149		H
1133	LYS	72	11.462	-12.04	7.258		H
1134	LYS	72	11.235	-10.529	7.834		H
1135	LYS	72	11.858	-11.963	9.528		H
1136	LYS	72	10.572	-12.916	9.206		H
1137	LYS	72	10.344	-11.406	9.782		H
1138	LYS	73	7.601	-11.514	1.917		N
1139	LYS	73	7.938	-12.346	0.768		C
1140	LYS	73	8.581	-11.508	-0.355		C
1141	LYS	73	9.425	-11.99	-1.107		O
1142	LYS	73	6.668	-13.051	0.262		C
1143	LYS	73	6.087	-14.054	1.273		C
1144	LYS	73	6.932	-15.331	1.411		C
1145	LYS	73	6.305	-16.349	2.381		C
1146	LYS	73	7.046	-17.604	2.504		N
1147	LYS	73	8.922	-19.313	2.453	-1	X
1148	LYS	73	6.643	-11.351	2.153		H
1149	LYS	73	8.608	-13.032	1.049		H
1150	LYS	73	5.975	-12.357	0.069		H
1151	LYS	73	6.891	-13.542	-0.58		H
1152	LYS	73	6.034	-13.61	2.167		H
1153	LYS	73	5.168	-14.311	0.973		H
1154	LYS	73	7.019	-15.757	0.511		H
1155	LYS	73	7.839	-15.081	1.751		H
1156	LYS	73	6.253	-15.927	3.286		H
1157	LYS	73	5.383	-16.561	2.058		H
1158	LYS	73	6.576	-18.207	3.149		H
1159	LYS	73	7.969	-17.415	2.838		H
1160	LYS	73	7.099	-18.049	1.61		H
1161	TYR	74	8.132	-10.243	-0.432		N
1162	TYR	74	8.674	-9.332	-1.433		C
1163	TYR	74	9.958	-8.698	-0.898		C
1164	TYR	74	11.046	-8.87	-1.439		O
1165	TYR	74	7.641	-8.244	-1.773		C
1166	TYR	74	6.658	-8.717	-2.806		C
1167	TYR	74	5.514	-9.418	-2.443		C
1168	TYR	74	6.896	-8.462	-4.153		C
1169	TYR	74	4.629	-9.876	-3.414		C
1170	TYR	74	6.014	-8.918	-5.124		C

1171	TYR	74	4.886	-9.635	-4.761	C
1172	TYR	74	4.053	-10.1	-5.764	O
1173	TYR	74	7.424	-9.926	0.199	H
1174	TYR	74	8.883	-9.841	-2.269	H
1175	TYR	74	7.144	-7.998	-0.941	H
1176	TYR	74	8.121	-7.44	-2.126	H
1177	TYR	74	5.326	-9.594	-1.477	H
1178	TYR	74	7.709	-7.946	-4.424	H
1179	TYR	74	3.808	-10.379	-3.144	H
1180	TYR	74	6.194	-8.728	-6.089	H
1181	TYR	74	4.006	-11.098	-5.722	H
1182	ILE	75	9.741	-7.928	0.172	N
1183	ILE	75	10.778	-7.113	0.779	C
1184	ILE	75	10.993	-7.676	2.202	C
1185	ILE	75	10.33	-7.269	3.15	O
1186	ILE	75	10.297	-5.642	0.782	C
1187	ILE	75	9.979	-5.13	-0.641	C
1188	ILE	75	11.319	-4.714	1.459	C
1189	ILE	75	9.241	-3.785	-0.666	C
1190	ILE	75	8.825	-7.913	0.572	H
1191	ILE	75	11.647	-7.136	0.284	H
1192	ILE	75	9.449	-5.625	1.313	H
1193	ILE	75	10.84	-5.026	-1.138	H
1194	ILE	75	9.409	-5.811	-1.101	H
1195	ILE	75	10.978	-3.774	1.444	H
1196	ILE	75	12.189	-4.76	0.968	H
1197	ILE	75	11.456	-5.003	2.407	H
1198	ILE	75	9.069	-3.516	-1.614	H
1199	ILE	75	9.802	-3.088	-0.219	H
1200	ILE	75	8.371	-3.873	-0.182	H
1201	PRO	76	11.943	-8.64	2.349	N
1202	PRO	76	12.078	-9.357	3.619	C
1203	PRO	76	12.619	-8.522	4.796	C
1204	PRO	76	12.652	-8.982	5.936	O
1205	PRO	76	13.021	-10.523	3.288	C
1206	PRO	76	13.807	-10.065	2.055	C
1207	PRO	76	12.854	-9.125	1.311	C
1208	PRO	76	11.176	-9.638	3.947	H
1209	PRO	76	13.64	-10.701	4.053	H
1210	PRO	76	12.498	-11.35	3.083	H
1211	PRO	76	14.638	-9.58	2.327	H
1212	PRO	76	14.049	-10.847	1.481	H
1213	PRO	76	13.356	-8.366	0.897	H
1214	PRO	76	12.352	-9.619	0.601	H
1215	GLY	77	13.028	-7.288	4.471	N
1216	GLY	77	13.464	-6.336	5.483	C
1217	GLY	77	12.664	-5.039	5.37	C
1218	GLY	77	13.189	-3.952	5.598	O
1219	GLY	77	13.035	-7.014	3.509	H
1220	GLY	77	13.324	-6.732	6.391	H
1221	GLY	77	14.435	-6.137	5.352	H

1222	THR	78	11.383	-5.205	4.996		N
1223	THR	78	10.507	-4.047	4.862		C
1224	THR	78	10.378	-3.341	6.214		C
1225	THR	78	10.381	-3.965	7.277		O
1226	THR	78	9.134	-4.472	4.298		C
1227	THR	78	8.331	-3.316	4.083		O
1228	THR	78	8.374	-5.466	5.191		C
1229	THR	78	11.031	-6.123	4.81		H
1230	THR	78	10.904	-3.399	4.212		H
1231	THR	78	9.317	-4.948	3.438		H
1232	THR	78	8.201	-2.834	4.95		H
1233	THR	78	7.499	-5.695	4.765		H
1234	THR	78	8.21	-5.052	6.087		H
1235	THR	78	8.918	-6.298	5.303		H
1236	LYS	79	10.269	-2.01	6.112		N
1237	LYS	79	10.022	-1.208	7.3		C
1238	LYS	79	8.509	-1.174	7.612		C
1239	LYS	79	8.083	-0.653	8.639		O
1240	LYS	79	10.659	0.181	7.098		C
1241	LYS	79	11.031	0.899	8.412		C
1242	LYS	79	10.061	2.018	8.821		C
1243	LYS	79	10.178	3.285	7.954		C
1244	LYS	79	11.464	3.972	8.049		N
1245	LYS	79	13.729	5.281	8.566	-1	X
1246	LYS	79	10.358	-1.568	5.22		H
1247	LYS	79	10.451	-1.61	8.108		H
1248	LYS	79	11.491	0.069	6.555		H
1249	LYS	79	10.009	0.755	6.599		H
1250	LYS	79	11.051	0.219	9.145		H
1251	LYS	79	11.941	1.299	8.303		H
1252	LYS	79	9.127	1.669	8.746		H
1253	LYS	79	10.249	2.267	9.771		H
1254	LYS	79	10.034	3.024	7		H
1255	LYS	79	9.462	3.923	8.237		H
1256	LYS	79	11.456	4.779	7.459		H
1257	LYS	79	12.195	3.354	7.759		H
1258	LYS	79	11.623	4.254	8.996		H
1259	MET	80	7.715	-1.774	6.7		N
1260	MET	80	6.278	-1.864	6.934		C
1261	MET	80	5.973	-2.892	8.036		C
1262	MET	80	5.766	-4.076	7.786		O
1263	MET	80	5.555	-2.244	5.63		C
1264	MET	80	4.027	-2.181	5.774		C
1265	MET	80	3.162	-2.25	4.196		S
1266	MET	80	3.072	-4.035	4.028		C
1267	MET	80	8.111	-2.157	5.866		H
1268	MET	80	5.946	-0.971	7.238		H
1269	MET	80	5.837	-1.611	4.909		H
1270	MET	80	5.816	-3.175	5.377		H
1271	MET	80	3.729	-2.954	6.334		H
1272	MET	80	3.786	-1.325	6.231		H

1273	MET	80	2.605	-4.267	3.175	H
1274	MET	80	2.565	-4.418	4.8	H
1275	MET	80	3.996	-4.416	4.015	H
1276	ILE	81	5.913	-2.37	9.267	N
1277	ILE	81	5.5	-3.173	10.414	C
1278	ILE	81	3.955	-3.242	10.474	C
1279	ILE	81	3.313	-2.746	11.395	O
1280	ILE	81	6.171	-2.599	11.688	C
1281	ILE	81	5.877	-3.412	12.966	C
1282	ILE	81	5.872	-1.105	11.913	C
1283	ILE	81	6.283	-4.889	12.864	C
1284	ILE	81	6.156	-1.41	9.403	H
1285	ILE	81	5.805	-4.122	10.333	H
1286	ILE	81	7.151	-2.687	11.506	H
1287	ILE	81	6.379	-2.998	13.726	H
1288	ILE	81	4.895	-3.366	13.15	H
1289	ILE	81	6.33	-0.795	12.746	H
1290	ILE	81	4.885	-0.972	12.007	H
1291	ILE	81	6.206	-0.576	11.133	H
1292	ILE	81	6.066	-5.355	13.722	H
1293	ILE	81	7.266	-4.954	12.689	H
1294	ILE	81	5.782	-5.322	12.114	H
1295	PHE	82	3.4	-3.88	9.431	N
1296	PHE	82	1.957	-4.067	9.31	C
1297	PHE	82	1.668	-5.554	9.557	C
1298	PHE	82	2.543	-6.407	9.421	O
1299	PHE	82	1.512	-3.611	7.907	C
1300	PHE	82	0.022	-3.656	7.672	C
1301	PHE	82	-0.491	-4.261	6.528	C
1302	PHE	82	-0.865	-3.086	8.582	C
1303	PHE	82	-1.86	-4.298	6.297	C
1304	PHE	82	-2.235	-3.119	8.356	C
1305	PHE	82	-2.733	-3.726	7.213	C
1306	PHE	82	3.996	-4.24	8.712	H
1307	PHE	82	1.446	-3.523	9.975	H
1308	PHE	82	1.82	-2.669	7.774	H
1309	PHE	82	1.952	-4.204	7.233	H
1310	PHE	82	0.133	-4.674	5.865	H
1311	PHE	82	-0.511	-2.648	9.408	H
1312	PHE	82	-2.217	-4.736	5.472	H
1313	PHE	82	-2.861	-2.706	9.017	H
1314	PHE	82	-3.719	-3.752	7.049	H
1315	ALA	83	0.411	-5.813	9.951	N
1316	ALA	83	-0.013	-7.176	10.249	C
1317	ALA	83	-0.171	-8.002	8.96	C
1318	ALA	83	0.162	-9.185	8.906	O
1319	ALA	83	-1.341	-7.133	11.018	C
1320	ALA	83	-0.243	-5.062	10.041	H
1321	ALA	83	0.688	-7.617	10.809	H
1322	ALA	83	-1.637	-8.065	11.225	H
1323	ALA	83	-2.036	-6.68	10.459	H

1324	ALA	83	-1.217	-6.626	11.871		H
1325	GLY	84	-0.708	-7.31	7.942		N
1326	GLY	84	-1.095	-7.981	6.706		C
1327	GLY	84	-2.535	-8.478	6.848		C
1328	GLY	84	-2.926	-9.034	7.872		O
1329	GLY	84	-0.843	-6.323	8.032		H
1330	GLY	84	-1.034	-7.339	5.942		H
1331	GLY	84	-0.486	-8.757	6.54		H
1332	ILE	85	-3.315	-8.201	5.798		N
1333	ILE	85	-4.741	-8.51	5.8		C
1334	ILE	85	-4.896	-9.859	5.093		C
1335	ILE	85	-4.597	-9.98	3.915		O
1336	ILE	85	-5.49	-7.381	5.057		C
1337	ILE	85	-5.303	-6.028	5.766		C
1338	ILE	85	-6.987	-7.692	4.858		C
1339	ILE	85	-5.67	-4.837	4.878		C
1340	ILE	85	-2.911	-7.772	4.99		H
1341	ILE	85	-5.123	-8.569	6.723		H
1342	ILE	85	-5.082	-7.322	4.146		H
1343	ILE	85	-5.884	-6.011	6.58		H
1344	ILE	85	-4.345	-5.94	6.038		H
1345	ILE	85	-7.424	-6.934	4.375		H
1346	ILE	85	-7.424	-7.815	5.749		H
1347	ILE	85	-7.085	-8.53	4.321		H
1348	ILE	85	-5.531	-3.987	5.386		H
1349	ILE	85	-6.629	-4.908	4.604		H
1350	ILE	85	-5.09	-4.837	4.063		H
1351	LYS	86	-5.371	-10.862	5.845		N
1352	LYS	86	-5.464	-12.202	5.266		C
1353	LYS	86	-6.498	-12.243	4.12		C
1354	LYS	86	-6.26	-12.776	3.038		O
1355	LYS	86	-5.817	-13.207	6.38		C
1356	LYS	86	-5.756	-14.673	5.925		C
1357	LYS	86	-6.035	-15.654	7.073		C
1358	LYS	86	-5.955	-17.123	6.623		C
1359	LYS	86	-6.193	-18.098	7.685		N
1360	LYS	86	-6.947	-18.758	10.175	-1	X
1361	LYS	86	-5.656	-10.697	6.789		H
1362	LYS	86	-4.582	-12.452	4.869		H
1363	LYS	86	-5.172	-13.083	7.134		H
1364	LYS	86	-6.745	-13.013	6.699		H
1365	LYS	86	-6.438	-14.815	5.208		H
1366	LYS	86	-4.844	-14.858	5.559		H
1367	LYS	86	-5.36	-15.503	7.796		H
1368	LYS	86	-6.952	-15.477	7.43		H
1369	LYS	86	-6.639	-17.268	5.908		H
1370	LYS	86	-5.042	-17.285	6.249		H
1371	LYS	86	-6.123	-19.023	7.312		H
1372	LYS	86	-7.108	-17.961	8.066		H
1373	LYS	86	-5.511	-17.979	8.407		H
1374	LYS	87	-7.667	-11.668	4.435		N

1375	LYS	87	-8.804	-11.796	3.534		C
1376	LYS	87	-8.595	-10.972	2.25		C
1377	LYS	87	-8.688	-9.749	2.257		O
1378	LYS	87	-10.083	-11.32	4.241		C
1379	LYS	87	-10.454	-12.179	5.46		C
1380	LYS	87	-11.785	-11.744	6.086		C
1381	LYS	87	-12.172	-12.603	7.304		C
1382	LYS	87	-13.436	-12.225	7.934		N
1383	LYS	87	-15.949	-11.168	8.941	-1	X
1384	LYS	87	-7.758	-11.153	5.287		H
1385	LYS	87	-8.891	-12.759	3.28		H
1386	LYS	87	-9.946	-10.378	4.546		H
1387	LYS	87	-10.839	-11.353	3.587		H
1388	LYS	87	-10.53	-13.133	5.171		H
1389	LYS	87	-9.732	-12.094	6.146		H
1390	LYS	87	-11.706	-10.791	6.378		H
1391	LYS	87	-12.505	-11.823	5.396		H
1392	LYS	87	-12.244	-13.555	7.005		H
1393	LYS	87	-11.446	-12.522	7.987		H
1394	LYS	87	-13.614	-12.827	8.712		H
1395	LYS	87	-14.178	-12.312	7.269		H
1396	LYS	87	-13.381	-11.278	8.25		H
1397	LYS	88	-8.398	-11.719	1.145		N
1398	LYS	88	-8.444	-11.149	-0.206		C
1399	LYS	88	-9.66	-10.212	-0.365		C
1400	LYS	88	-9.576	-9.119	-0.912		O
1401	LYS	88	-8.557	-12.293	-1.239		C
1402	LYS	88	-7.269	-13.112	-1.446		C
1403	LYS	88	-6.416	-12.59	-2.615		C
1404	LYS	88	-5.169	-13.456	-2.888		C
1405	LYS	88	-4.324	-12.969	-3.977		N
1406	LYS	88	-8.215	-12.696	1.25		H
1407	LYS	88	-7.606	-10.624	-0.358		H
1408	LYS	88	-9.276	-12.917	-0.933		H
1409	LYS	88	-8.815	-11.893	-2.118		H
1410	LYS	88	-6.724	-13.069	-0.608		H
1411	LYS	88	-7.52	-14.062	-1.632		H
1412	LYS	88	-6.981	-12.577	-3.44		H
1413	LYS	88	-6.117	-11.66	-2.4		H
1414	LYS	88	-4.619	-13.484	-2.053		H
1415	LYS	88	-5.474	-14.38	-3.118		H
1416	LYS	88	-3.998	-12.049	-3.761		H
1417	LYS	88	-4.853	-12.945	-4.825		H
1418	THR	89	-10.783	-10.719	0.168		N
1419	THR	89	-12.068	-10.043	0.082		C
1420	THR	89	-12.028	-8.595	0.629		C
1421	THR	89	-12.7	-7.708	0.111		O
1422	THR	89	-13.076	-10.927	0.844		C
1423	THR	89	-12.756	-12.302	0.672		O
1424	THR	89	-14.538	-10.657	0.457		C
1425	THR	89	-10.734	-11.597	0.643		H

1426	THR	89	-12.337	-9.935	-0.875		H
1427	THR	89	-12.995	-10.683	1.811		H
1428	THR	89	-12.79	-12.534	-0.3		H
1429	THR	89	-15.139	-11.259	0.983		H
1430	THR	89	-14.663	-10.833	-0.52		H
1431	THR	89	-14.765	-9.704	0.655		H
1432	GLU	90	-11.225	-8.404	1.692		N
1433	GLU	90	-11.069	-7.058	2.237		C
1434	GLU	90	-10.089	-6.262	1.36		C
1435	GLU	90	-10.28	-5.083	1.075		O
1436	GLU	90	-10.607	-7.12	3.708		C
1437	GLU	90	-11.68	-7.74	4.633		C
1438	GLU	90	-11.395	-7.583	6.137		C
1439	GLU	90	-11.636	-8.386	7.025		O
1440	GLU	90	-10.617	-6.635	6.631		O
1441	GLU	90	-10.741	-9.176	2.104		H
1442	GLU	90	-11.95	-6.586	2.226		H
1443	GLU	90	-9.777	-7.675	3.761		H
1444	GLU	90	-10.409	-6.192	4.022		H
1445	GLU	90	-12.556	-7.3	4.434		H
1446	GLU	90	-11.743	-8.717	4.428		H
1447	GLU	90	-10.471	-6.626	7.563		H
1448	ARG	91	-9.031	-6.966	0.933		N
1449	ARG	91	-7.992	-6.278	0.176		C
1450	ARG	91	-8.493	-5.738	-1.175		C
1451	ARG	91	-7.973	-4.746	-1.671		O
1452	ARG	91	-6.747	-7.165	0.031		C
1453	ARG	91	-6.187	-7.589	1.399		C
1454	ARG	91	-4.686	-7.896	1.362		C
1455	ARG	91	-4.335	-8.874	0.345		N
1456	ARG	91	-4.569	-10.201	0.439		C
1457	ARG	91	-5.183	-10.717	1.492		N
1458	ARG	91	-4.155	-10.99	-0.536		N
1459	ARG	91	-5.058	-13.979	0.887	-1	X
1460	ARG	91	-8.956	-7.944	1.13		H
1461	ARG	91	-7.728	-5.469	0.701		H
1462	ARG	91	-6.992	-7.985	-0.487		H
1463	ARG	91	-6.043	-6.656	-0.464		H
1464	ARG	91	-6.345	-6.848	2.051		H
1465	ARG	91	-6.673	-8.409	1.702		H
1466	ARG	91	-4.191	-7.048	1.173		H
1467	ARG	91	-4.411	-8.251	2.255		H
1468	ARG	91	-3.889	-8.54	-0.486		H
1469	ARG	91	-5.483	-10.121	2.237		H
1470	ARG	91	-5.346	-11.702	1.543		H
1471	ARG	91	-3.679	-10.601	-1.325		H
1472	ARG	91	-4.318	-11.975	-0.485		H
1473	GLU	92	-9.532	-6.379	-1.74		N
1474	GLU	92	-10.091	-5.858	-2.992		C
1475	GLU	92	-10.516	-4.382	-2.871		C
1476	GLU	92	-10.37	-3.598	-3.803		O

1477	GLU	92	-11.328	-6.655	-3.442	C
1478	GLU	92	-11.043	-8.092	-3.92	C
1479	GLU	92	-12.264	-8.716	-4.619	C
1480	GLU	92	-12.703	-8.167	-5.842	O
1481	GLU	92	-13.141	-8.91	-3.824	O
1482	GLU	92	-9.918	-7.196	-1.312	H
1483	GLU	92	-9.355	-5.947	-3.664	H
1484	GLU	92	-11.961	-6.706	-2.67	H
1485	GLU	92	-11.759	-6.158	-4.195	H
1486	GLU	92	-10.277	-8.073	-4.563	H
1487	GLU	92	-10.801	-8.654	-3.129	H
1488	GLU	92	-12.096	-7.668	-6.388	H
1489	ASP	93	-11.085	-4.068	-1.696	N
1490	ASP	93	-11.628	-2.726	-1.483	C
1491	ASP	93	-10.477	-1.72	-1.379	C
1492	ASP	93	-10.572	-0.577	-1.813	O
1493	ASP	93	-12.517	-2.715	-0.215	C
1494	ASP	93	-13.916	-3.317	-0.418	C
1495	ASP	93	-14.383	-3.187	-1.812	O
1496	ASP	93	-14.517	-4.222	0.236	O
1497	ASP	93	-11.137	-4.751	-0.967	H
1498	ASP	93	-12.201	-2.461	-2.259	H
1499	ASP	93	-12.051	-3.239	0.498	H
1500	ASP	93	-12.625	-1.767	0.084	H
1501	ASP	93	-15.17	-3.627	-2.079	H
1502	LEU	94	-9.364	-2.211	-0.812	N
1503	LEU	94	-8.164	-1.38	-0.753	C
1504	LEU	94	-7.623	-1.121	-2.16	C
1505	LEU	94	-7.313	0.004	-2.519	O
1506	LEU	94	-7.103	-2.048	0.133	C
1507	LEU	94	-7.417	-1.904	1.631	C
1508	LEU	94	-6.658	-2.955	2.447	C
1509	LEU	94	-7.084	-0.492	2.14	C
1510	LEU	94	-9.356	-3.137	-0.434	H
1511	LEU	94	-8.4	-0.497	-0.347	H
1512	LEU	94	-7.061	-3.021	-0.094	H
1513	LEU	94	-6.217	-1.623	-0.052	H
1514	LEU	94	-8.399	-2.053	1.748	H
1515	LEU	94	-6.875	-2.845	3.417	H
1516	LEU	94	-5.674	-2.837	2.311	H
1517	LEU	94	-6.928	-3.87	2.147	H
1518	LEU	94	-7.298	-0.429	3.115	H
1519	LEU	94	-7.626	0.181	1.636	H
1520	LEU	94	-6.111	-0.308	2.001	H
1521	ILE	95	-7.545	-2.192	-2.958	N
1522	ILE	95	-7.062	-2.018	-4.33	C
1523	ILE	95	-7.984	-1.05	-5.102	C
1524	ILE	95	-7.542	-0.245	-5.912	O
1525	ILE	95	-6.929	-3.4	-5.009	C
1526	ILE	95	-5.931	-4.315	-4.267	C
1527	ILE	95	-6.566	-3.311	-6.504	C

1528	ILE	95	-4.458	-3.893	-4.406	C
1529	ILE	95	-7.811	-3.096	-2.624	H
1530	ILE	95	-6.153	-1.601	-4.326	H
1531	ILE	95	-7.839	-3.811	-4.952	H
1532	ILE	95	-6.167	-4.312	-3.295	H
1533	ILE	95	-6.026	-5.242	-4.631	H
1534	ILE	95	-6.495	-4.233	-6.886	H
1535	ILE	95	-5.69	-2.839	-6.607	H
1536	ILE	95	-7.277	-2.804	-6.991	H
1537	ILE	95	-3.879	-4.532	-3.9	H
1538	ILE	95	-4.339	-2.971	-4.037	H
1539	ILE	95	-4.198	-3.901	-5.372	H
1540	ALA	96	-9.287	-1.159	-4.789	N
1541	ALA	96	-10.268	-0.265	-5.395	C
1542	ALA	96	-10	1.195	-5.003	C
1543	ALA	96	-10.148	2.11	-5.805	O
1544	ALA	96	-11.681	-0.69	-4.971	C
1545	ALA	96	-9.585	-1.856	-4.138	H
1546	ALA	96	-10.191	-0.331	-6.389	H
1547	ALA	96	-12.353	-0.077	-5.387	H
1548	ALA	96	-11.759	-0.643	-3.975	H
1549	ALA	96	-11.853	-1.627	-5.275	H
1550	TYR	97	-9.596	1.356	-3.73	N
1551	TYR	97	-9.271	2.684	-3.22	C
1552	TYR	97	-8.067	3.259	-3.97	C
1553	TYR	97	-8.104	4.347	-4.527	O
1554	TYR	97	-8.981	2.61	-1.71	C
1555	TYR	97	-8.831	3.979	-1.099	C
1556	TYR	97	-9.887	4.884	-1.124	C
1557	TYR	97	-7.633	4.365	-0.508	C
1558	TYR	97	-9.74	6.155	-0.581	C
1559	TYR	97	-7.489	5.633	0.046	C
1560	TYR	97	-8.542	6.53	0.008	C
1561	TYR	97	-8.387	7.787	0.565	O
1562	TYR	97	-9.517	0.56	-3.13	H
1563	TYR	97	-10.053	3.29	-3.367	H
1564	TYR	97	-9.737	2.136	-1.259	H
1565	TYR	97	-8.134	2.098	-1.568	H
1566	TYR	97	-10.759	4.618	-1.536	H
1567	TYR	97	-6.866	3.724	-0.481	H
1568	TYR	97	-10.502	6.802	-0.615	H
1569	TYR	97	-6.624	5.897	0.472	H
1570	TYR	97	-8.529	8.483	-0.139	H
1571	LEU	98	-7.008	2.445	-3.962	N
1572	LEU	98	-5.732	2.789	-4.578	C
1573	LEU	98	-5.913	3.184	-6.057	C
1574	LEU	98	-5.306	4.129	-6.558	O
1575	LEU	98	-4.779	1.59	-4.387	C
1576	LEU	98	-3.957	1.634	-3.077	C
1577	LEU	98	-4.782	1.971	-1.826	C
1578	LEU	98	-3.193	0.319	-2.872	C

1579	LEU	98	-7.095	1.556	-3.512	H
1580	LEU	98	-5.333	3.594	-4.139	H
1581	LEU	98	-5.325	0.753	-4.386	H
1582	LEU	98	-4.141	1.571	-5.157	H
1583	LEU	98	-3.311	2.388	-3.191	H
1584	LEU	98	-4.184	1.981	-1.024	H
1585	LEU	98	-5.495	1.281	-1.701	H
1586	LEU	98	-5.204	2.871	-1.937	H
1587	LEU	98	-2.669	0.367	-2.022	H
1588	LEU	98	-2.569	0.172	-3.64	H
1589	LEU	98	-3.842	-0.44	-2.821	H
1590	LYS	99	-6.804	2.437	-6.728	N
1591	LYS	99	-7.074	2.709	-8.138	C
1592	LYS	99	-7.689	4.102	-8.385	C
1593	LYS	99	-7.667	4.588	-9.512	O
1594	LYS	99	-7.964	1.603	-8.727	C
1595	LYS	99	-7.17	0.325	-9.038	C
1596	LYS	99	-8.036	-0.755	-9.697	C
1597	LYS	99	-7.202	-1.947	-10.197	C
1598	LYS	99	-7.965	-2.941	-10.951	N
1599	LYS	99	-7.285	1.694	-6.261	H
1600	LYS	99	-6.191	2.711	-8.607	H
1601	LYS	99	-8.683	1.383	-8.068	H
1602	LYS	99	-8.378	1.939	-9.573	H
1603	LYS	99	-6.419	0.556	-9.657	H
1604	LYS	99	-6.799	-0.038	-8.183	H
1605	LYS	99	-8.701	-1.086	-9.028	H
1606	LYS	99	-8.518	-0.351	-10.475	H
1607	LYS	99	-6.476	-1.595	-10.788	H
1608	LYS	99	-6.796	-2.4	-9.403	H
1609	LYS	99	-8.37	-2.509	-11.757	H
1610	LYS	99	-8.69	-3.314	-10.373	H
1611	LYS	100	-8.209	4.732	-7.322	N
1612	LYS	100	-8.618	6.133	-7.411	C
1613	LYS	100	-8.252	6.876	-6.12	C
1614	LYS	100	-9.021	7.672	-5.582	O
1615	LYS	100	-10.112	6.258	-7.768	C
1616	LYS	100	-10.347	5.983	-9.261	C
1617	LYS	100	-11.703	6.48	-9.783	C
1618	LYS	100	-11.654	6.748	-11.298	C
1619	LYS	100	-10.942	7.977	-11.661	N
1620	LYS	100	-8.318	4.239	-6.458	H
1621	LYS	100	-8.116	6.569	-8.158	H
1622	LYS	100	-10.633	5.597	-7.228	H
1623	LYS	100	-10.423	7.184	-7.553	H
1624	LYS	100	-9.624	6.437	-9.782	H
1625	LYS	100	-10.296	4.996	-9.41	H
1626	LYS	100	-12.398	5.785	-9.597	H
1627	LYS	100	-11.943	7.328	-9.31	H
1628	LYS	100	-11.196	5.977	-11.739	H
1629	LYS	100	-12.593	6.816	-11.636	H

1630	LYS	100	-10.95	8.086	-12.655	H
1631	LYS	100	-11.392	8.762	-11.235	H
1632	ALA	101	-7.01	6.608	-5.7	N
1633	ALA	101	-6.394	7.358	-4.612	C
1634	ALA	101	-4.936	7.58	-4.992	C
1635	ALA	101	-4.446	8.699	-5.111	O
1636	ALA	101	-6.522	6.594	-3.284	C
1637	ALA	101	-6.492	5.877	-6.143	H
1638	ALA	101	-6.853	8.236	-4.477	H
1639	ALA	101	-6.094	7.124	-2.552	H
1640	ALA	101	-6.066	5.708	-3.364	H
1641	ALA	101	-7.489	6.453	-3.072	H
1642	THR	102	-4.292	6.436	-5.218	N
1643	THR	102	-2.893	6.378	-5.585	C
1644	THR	102	-2.781	6.164	-7.107	C
1645	THR	102	-1.994	5.348	-7.58	O
1646	THR	102	-2.339	5.171	-4.811	C
1647	THR	102	-3.176	4.051	-5.015	O
1648	THR	102	-2.356	5.401	-3.295	C
1649	THR	102	-4.799	5.578	-5.13	H
1650	THR	102	-2.389	7.214	-5.367	H
1651	THR	102	-1.405	5.034	-5.142	H
1652	THR	102	-4.098	4.259	-4.688	H
1653	THR	102	-1.989	4.595	-2.831	H
1654	THR	102	-3.296	5.56	-2.992	H
1655	THR	102	-1.795	6.198	-3.072	H
1656	ASN	103	-3.635	6.902	-7.842	N
1657	ASN	103	-3.732	6.693	-9.286	C
1658	ASN	103	-4.424	7.903	-9.946	C
1659	ASN	103	-3.77	8.897	-10.26	O
1660	ASN	103	-4.429	5.355	-9.601	C
1661	ASN	103	-4.46	5.086	-11.113	C
1662	ASN	103	-3.5	5.348	-11.833	O
1663	ASN	103	-5.607	4.576	-11.558	N
1664	ASN	103	-4.204	7.594	-7.399	H
1665	ASN	103	-2.814	6.628	-9.677	H
1666	ASN	103	-3.932	4.614	-9.148	H
1667	ASN	103	-5.367	5.387	-9.256	H
1668	ASN	103	-6.356	4.4	-10.92	H
1669	ASN	103	-5.718	4.368	-12.53	H
1670	GLU	104	-5.752	7.77	-10.159	N
1671	GLU	104	-6.53	8.732	-10.937	C
1672	GLU	104	-7.618	9.338	-10.022	C
1673	GLU	104	-7.694	10.558	-9.773	O
1674	GLU	104	-7.115	8.017	-12.178	C
1675	GLU	104	-7.749	8.988	-13.197	C
1676	GLU	104	-8.481	8.243	-14.324	C
1677	GLU	104	-9.589	7.585	-14.321	O
1678	GLU	104	-8.053	8.402	-15.412	O
1679	GLU	104	-8.121	8.404	-9.268	O
1680	GLU	104	-6.223	6.979	-9.769	H

1681	GLU	104	-5.962	9.485	-11.27	H
1682	GLU	104	-6.379	7.516	-12.632	H
1683	GLU	104	-7.817	7.374	-11.873	H
1684	GLU	104	-8.403	9.575	-12.72	H
1685	GLU	104	-7.027	9.551	-13.598	H
1686	GLU	104	-7.958	7.521	-9.539	H
1687	GLU	104	-8.498	8.008	-16.162	H
1688	HES	105	2.267	0.613	4.197	ZN
1689	HES	105	5.244	0.612	2.434	C
1690	HES	105	0.565	0.115	1.22	C
1691	HES	105	-0.547	0.133	6.025	C
1692	HES	105	4.006	1.522	7.058	C
1693	HES	105	2.823	0.4	2.229	N
1694	HES	105	4.227	0.393	1.642	C
1695	HES	105	3.848	0.137	0.411	C
1696	HES	105	2.66	-0.013	-0.082	C
1697	HES	105	1.959	0.186	1.193	C
1698	HES	105	2.064	-0.363	-1.424	C
1699	HES	105	5.016	-0.226	-0.484	C
1700	HES	105	5.607	0.989	-1.218	C
1701	HES	105	6.939	0.701	-1.859	C
1702	HES	105	7.767	-0.027	-1.291	O
1703	HES	105	7.195	1.542	-2.921	O
1704	HES	105	0.313	0.223	3.697	N
1705	HES	105	-0.241	0.093	2.256	C
1706	HES	105	-1.494	-0.027	2.619	C
1707	HES	105	-1.786	-0.055	3.851	C
1708	HES	105	-0.825	0.092	4.738	C
1709	HES	105	-2.5	0.006	1.486	C
1710	HES	105	-3.177	-0.364	4.391	C
1711	HES	105	-3.725	-1.712	3.904	C
1712	HES	105	1.868	0.748	6.189	N
1713	HES	105	0.635	0.49	6.697	C
1714	HES	105	0.588	0.721	8.143	C
1715	HES	105	1.835	1.072	8.255	C
1716	HES	105	2.767	1.191	7.335	C
1717	HES	105	-0.595	0.549	9.064	C
1718	HES	105	2.285	1.582	9.615	C
1719	HES	105	2.559	0.452	10.616	C
1720	HES	105	4.207	1.012	4.645	N
1721	HES	105	4.7	1.382	5.841	C
1722	HES	105	6.118	1.6	5.765	C
1723	HES	105	6.485	1.251	4.487	C
1724	HES	105	5.257	0.941	3.803	C
1725	HES	105	7.036	2.08	6.869	C
1726	HES	105	7.907	1.223	3.96	C
1727	HES	105	8.376	2.647	3.662	C
1728	HES	105	9.837	2.666	3.336	C
1729	HES	105	10.656	2.483	4.246	O
1730	HES	105	10.136	2.659	1.984	O
1731	HES	105	6.144	0.535	2.005	H

1732	HES	105	0.118	0.075	0.326	H
1733	HES	105	-1.302	-0.134	6.623	H
1734	HES	105	4.526	1.927	7.81	H
1735	HES	105	1.066	-0.368	-1.355	H
1736	HES	105	2.383	-1.268	-1.705	H
1737	HES	105	2.348	0.315	-2.102	H
1738	HES	105	4.703	-0.888	-1.164	H
1739	HES	105	5.733	-0.639	0.078	H
1740	HES	105	4.966	1.273	-1.931	H
1741	HES	105	5.725	1.732	-0.559	H
1742	HES	105	-2.427	0.877	1	H
1743	HES	105	-2.314	-0.745	0.853	H
1744	HES	105	-3.424	-0.092	1.857	H
1745	HES	105	-3.044	-0.408	5.381	H
1746	HES	105	-4.636	-1.86	4.288	H
1747	HES	105	-3.115	-2.447	4.2	H
1748	HES	105	-3.782	-1.708	2.906	H
1749	HES	105	-0.327	0.781	9.999	H
1750	HES	105	-1.337	1.153	8.771	H
1751	HES	105	-0.907	-0.401	9.033	H
1752	HES	105	3.167	2.033	9.478	H
1753	HES	105	2.85	0.843	11.489	H
1754	HES	105	1.725	-0.083	10.752	H
1755	HES	105	3.281	-0.142	10.26	H
1756	HES	105	7.973	2.137	6.523	H
1757	HES	105	7.002	1.437	7.634	H
1758	HES	105	6.74	2.983	7.18	H
1759	HES	105	8.507	0.813	4.646	H
1760	HES	105	7.939	0.68	3.121	H
1761	HES	105	7.861	3.006	2.883	H
1762	HES	105	8.211	3.221	4.464	H
1763	HES	105	8.103	1.49	-3.216	H
1764	HES	105	11.127	2.581	1.873	H
1765	HES	105				

^aThree letters notation of amino acid residues. HES means Zn-protoporphyrin part.

Table S2. Cartesian coordinate of CM (Å).

Atom No.	Atom	x	y	z
1	Zn	-1.14	-0.13	-0.012
2	C	-3.042	0.508	-2.831
3	C	-0.337	3.238	0.143
4	C	0.29	-0.732	3.002
5	C	-1.653	-3.528	-0.481
6	N	-1.618	1.526	-1.133
7	C	-2.525	1.609	-2.352
8	C	-2.443	2.913	-2.482
9	C	-1.77	3.78	-1.794
10	C	-1.192	2.797	-0.869
11	N	-0.149	1.059	1.339
12	C	0.148	2.57	1.164
13	C	0.866	2.678	2.254
14	C	1.007	1.673	3.011
15	C	0.47	0.525	2.653
16	N	-0.824	-1.834	1.057
17	C	-0.227	-1.82	2.276
18	C	-0.055	-3.174	2.808
19	C	-0.605	-3.778	1.797
20	C	-1.102	-3.283	0.684
21	N	-2.114	-1.27	-1.381
22	C	-2.183	-2.613	-1.411
23	C	-2.941	-3.062	-2.545
24	C	-3.415	-1.925	-3.156
25	C	-2.833	-0.826	-2.431
26	H	-3.678	0.63	-3.593
27	H	-0.055	4.196	0.082
28	H	0.567	-0.949	3.939
29	H	-1.702	-4.492	-0.744
30	H	-2.985	3.298	-3.229
31	H	-1.676	4.773	-1.868
32	H	1.3	3.549	2.487
33	H	1.518	1.75	3.867
34	H	0.346	-3.516	3.657
35	H	-0.66	-4.773	1.877
36	H	-3.093	-4.008	-2.833
37	H	-4.035	-1.872	-3.939
38	C	1.66	-0.318	-2.612
39	N	1.059	-0.946	-1.585
40	C	2.041	-1.315	-0.725
41	C	3.257	-0.889	-1.281
42	N	2.993	-0.273	-2.458
43	C	4.641	-1.049	-0.702
44	C	5.173	-2.474	-0.949
45	H	1.173	0.068	-3.396
46	H	1.921	-1.8	0.141
47	H	3.657	0.132	-3.087
48	H	4.608	-0.878	0.283

49	H	5.257	-0.391	-1.135
50	H	4.974	-2.735	-1.894
51	C	-5.182	1.169	2.051
52	S	-3.892	0.451	1.029
53	C	-4.441	-1.263	1.085
54	C	-5.483	-1.601	0.008
55	C	-5.697	-3.118	-0.138
56	H	-5.032	2.155	2.132
57	H	-5.159	0.753	2.959
58	H	-6.074	1.002	1.629
59	H	-4.846	-1.437	1.983
60	H	-3.647	-1.856	0.957
61	H	-5.17	-1.234	-0.869
62	H	-6.353	-1.175	0.255
63	H	-4.811	-3.555	-0.294
64	H	4.586	-3.328	-0.113
65	H	6.485	-2.503	-0.731
66	H	-6.485	-3.368	-1.181
67	H	-6.221	-3.623	0.976

The full list of authors of *Gaussian 03*.

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