

Supporting Information

Fluorine Bonding — How Does It Work In Protein–Ligand Interactions?

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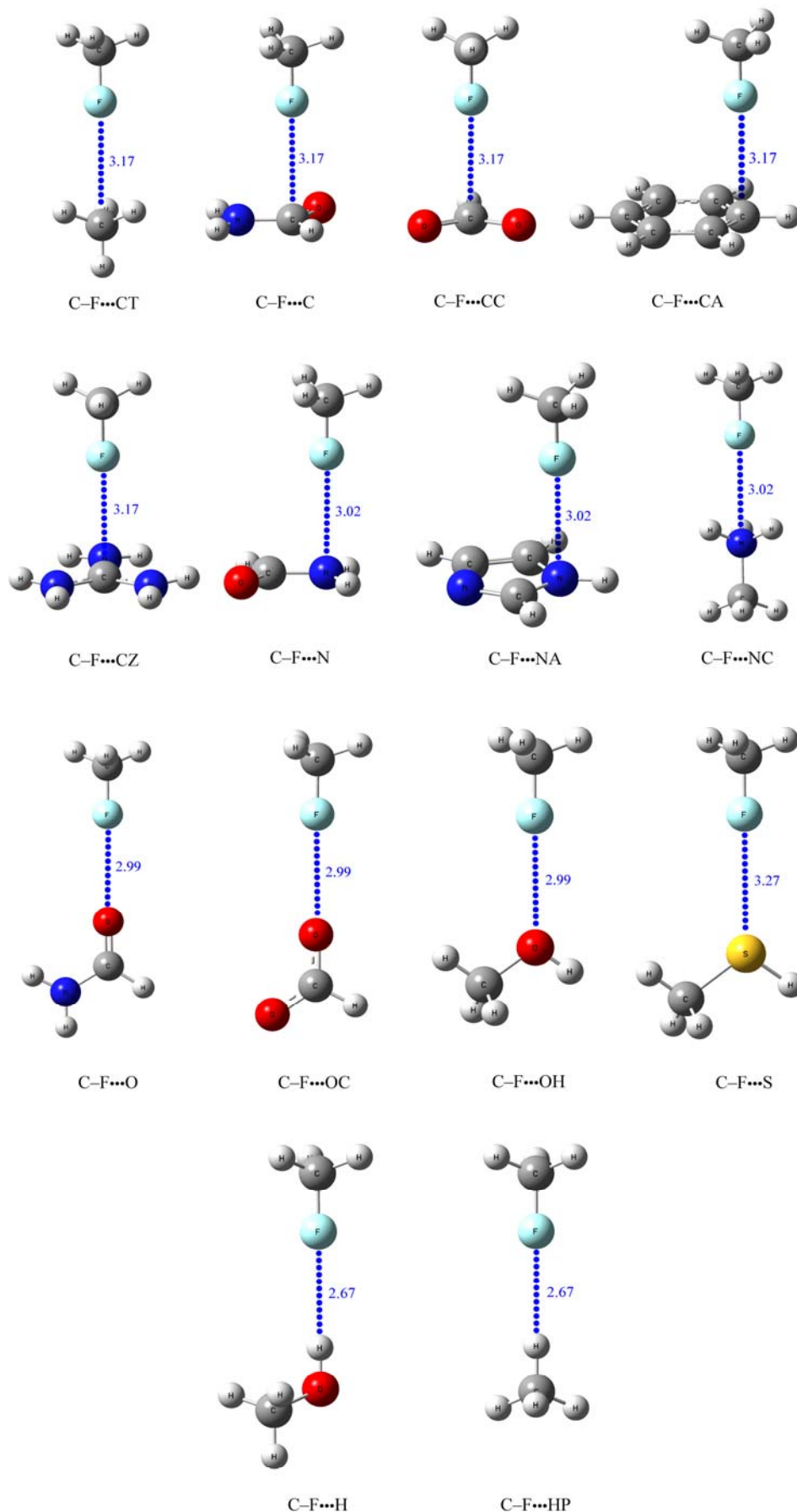


Figure S1. The model dimers used for calculating contact energy (ΔE_{ce}). All model dimers are arranged to low-energy conformations with the donor atom F in van der Waals contact with acceptor atom X.

Table S1. Short contacts involving fluorine atoms extracted from the PDB

No.	PDB	Chain	Residue	Atom	d (Å) <i>a</i>	SR (%) <i>b</i>	θ (°) <i>c</i>
1	1A5S	A	Ile153	CD1	2.918	7.9	161.3
2	1A08	A	Ser180	OG	2.554	14.6	123.9
3	1A08	A	Ser180	HG	1.842	31.0	107.2
4	1A08	A	Ser180	HG	2.326	12.9	85.5
5	1A08	A	Cys188	HB2	2.553	4.4	167.0
6	1A08	B	Ser180	OG	2.605	12.9	116.4
7	1A08	B	Ser180	HA	2.656	0.5	123.8
8	1A08	B	Cys188	HB2	2.371	11.2	152.9
9	1A9U	A	Leu104	HB3	2.510	6.0	99.8
10	1A9U	A	Thr106	HB	2.214	17.1	89.6
11	1A29	A	Leu105	HG	2.425	9.2	142.3
12	1A29	A	Phe141	HE1	2.656	0.5	145.7
13	1A50	A	Ile153	CD1	2.879	9.2	156.0
14	1A71	A	Ser48	OG	2.727	8.8	116.2
15	1A71	A	Ser48	HG	2.058	22.9	102.2
16	1A71	A	Trp93	CZ3	3.023	4.6	117.8
17	1A71	B	Ser48	CB	3.095	2.4	99.6
18	1A71	B	Ser48	HB3	2.577	3.5	103.6
19	1A71	B	Ser48	CB	3.141	0.9	97.5
20	1A71	B	Ser48	OG	2.600	13.0	108.6
21	1A71	B	Ser48	HG	1.901	28.8	94.6
22	1AD8	H	His57	HE2	2.354	11.8	101.1
23	1AD8	H	Ser195	OG	2.818	5.7	63.8
24	1AD8	H	Trp60	HZ3	2.645	0.9	131.4
25	1AD8	H	Cys42	SG	3.042	7.0	130.3
26	1AD8	H	Ser195	CB	2.953	6.8	101.1
27	1AD8	H	Ser195	OG	2.974	0.5	86.1
28	1AD8	H	Ser195	HB2	2.419	9.4	93.0
29	1AD8	H	Ser195	HB2	2.661	0.3	83.2
30	1AFQ	C	Gly216	HA3	2.529	5.3	87.1
31	1AH3	A	Ser302	OG	2.696	9.8	126.5
32	1AH3	A	Ser302	HG	2.307	13.6	125.4
33	1AH3	A	Cys303	HB2	2.519	5.7	149.1
34	1AID	A	Pro81	HD2	2.446	8.4	132.4
35	1AID	B	Thr80	HA	2.631	1.5	144.4
36	1AID	B	Pro81	HD2	2.446	8.4	132.4
37	1AMN	A	Gly119	CA	3.154	0.5	135.9
38	1AMN	A	Gly119	HA2	2.501	6.3	133.3
39	1AMN	A	Phe288	CE1	3.164	0.2	112.6
40	1AMN	A	Phe288	CZ	2.920	7.9	138.1
41	1AMN	A	Phe288	HZ	2.268	15.0	145.2

42	1AMN	A	Trp233	CZ2	3.166	0.1	148.0
43	1AMN	A	Trp233	CH2	2.823	10.9	166.7
44	1APV	I	Val2	C	3.120	1.6	114.5
45	1APV	E	Gly35	HA3	2.483	7.0	127.7
46	1APV	E	Asp213	OD2	2.876	3.8	107.4
47	1APW	E	Gly35	HA3	2.432	8.9	131.3
48	1APW	E	Asp213	OD2	2.957	1.1	104.7
49	1AXE	A	Ser48	CB	3.001	5.3	120.5
50	1AXE	A	Ser48	OG	2.696	9.8	115.3
51	1AXE	A	Ser48	HB3	2.435	8.8	127.2
52	1AXE	A	Ser48	HG	2.119	20.6	96.1
53	1AXE	B	Trp93	CZ3	2.944	7.1	126.6
54	1AXE	B	Ser48	HG	2.647	0.9	65.6
55	1AXE	B	Ser48	OG	2.829	5.4	100.7
56	1AXE	B	Ser48	HG	2.079	22.1	87.6
57	1AXE	B	Val294	CG2	3.118	1.7	160.8
58	1AXG	A	Ser48	HG	2.508	6.1	89.0
59	1AXG	A	Leu116	CD1	3.143	0.8	127.8
60	1AXG	B	Leu116	CD1	3.107	2.0	109.3
61	1AXG	C	Phe93	CD1	2.975	6.1	151.3
62	1AXG	C	Phe93	CE1	3.154	0.5	126.8
63	1AXG	C	Leu141	CD1	2.925	7.7	112.7
64	1AXG	C	Ser48	HB3	2.659	0.4	128.5
65	1AXG	C	Leu116	CD2	3.119	1.6	156.2
66	1AXG	D	Val294	CG2	3.093	2.4	163.2
67	1B0E	A	Cys42	SG	3.260	0.3	156.7
68	1B0E	A	His57	HE2	2.485	6.9	74.6
69	1B0E	A	Ser195	CB	2.880	9.1	86.7
70	1B0E	A	Ser195	OG	2.804	6.2	58.7
71	1B0E	A	Ser195	HB2	2.288	14.3	97.4
72	1B0E	A	His57	CD2	3.154	0.5	110.4
73	1B0E	A	His57	NE2	2.878	4.7	98.8
74	1B0E	A	His57	HE2	2.279	14.6	83.0
75	1B0E	A	Ser195	OG	2.900	3.0	55.0
76	1B0E	A	Gln192	HG3	2.545	4.7	170.3
77	1B0E	A	Gly193	H	2.500	6.4	106.4
78	1B0F	A	Cys42	SG	3.034	7.2	155.5
79	1B0F	A	His57	HE2	2.298	13.9	75.7
80	1B0F	A	Ser195	CB	2.617	17.4	87.4
81	1B0F	A	Ser195	OG	2.758	7.8	56.5
82	1B0F	A	Ser195	HB2	1.924	28.0	101.8
83	1B0F	A	His57	NE2	2.801	7.3	99.0
84	1B0F	A	His57	HE2	2.104	21.2	84.1
85	1B0F	A	Ser195	OG	2.843	4.9	53.2

86	1B0F	A	Phe192	HD1	2.599	2.6	161.4
87	1B0F	A	Gly193	N	2.853	5.5	128.3
88	1B0F	A	Gly193	CA	3.168	0.1	155.3
89	1B0F	A	Gly193	H	2.241	16.1	114.7
90	1B0F	A	Gly193	HA2	2.552	4.4	173.5
91	1B02	A	Tyr108	OH	2.933	1.9	153.2
92	1B02	A	Tyr108	HH	2.597	2.7	140.0
93	1B02	A	Cys161	SG	3.028	7.4	69.1
94	1B99	A	Lys16	NZ	2.698	10.7	135.4
95	1B99	A	Lys16	HZ1	2.637	1.3	114.3
96	1B99	A	Lys16	HZ3	2.094	21.6	151.7
97	1BCD	A	Trp209	CZ2	3.112	1.8	149.1
98	1BCD	A	Trp209	HZ2	2.375	11.0	164.1
99	1BJG	A	Tyr94	HH	2.520	5.6	163.4
100	1BJG	A	Cys146	SG	2.979	8.9	72.0
101	1BJG	A	Cys146	HB2	2.643	1.0	88.7
102	1BL6	A	Leu104	CB	3.168	0.1	122.6
103	1BL6	A	Leu104	HB2	2.666	0.1	103.9
104	1BL7	A	Leu104	C	3.080	2.8	113.8
105	1BL7	A	Leu104	CB	3.143	0.9	102.6
106	1BL7	A	Leu104	HB3	2.513	5.9	114.2
107	1BL7	A	Val105	N	2.957	2.1	134.6
108	1BL7	A	Val105	C	3.076	3.0	127.7
109	1BM7	A	Leu110	HB3	2.573	3.6	136.0
110	1BM7	A	Ser117	CB	2.904	8.4	151.7
111	1BM7	A	Ser117	HB2	2.252	15.7	170.7
112	1BM7	A	Ser117	HB3	2.622	1.8	131.0
113	1BM7	A	Thr119	HB	2.361	11.6	157.6
114	1BM7	B	Leu110	CD2	2.998	5.4	125.6
115	1BM7	B	Ser117	CB	2.929	7.6	150.6
116	1BM7	B	Ser117	HB2	2.204	17.5	167.0
117	1BM7	B	Thr119	HB	2.434	8.9	157.0
118	1BMA	A	Cys199	O	2.911	2.6	134.0
119	1BMA	A	Ser203	H	2.592	2.9	139.9
120	1BMK	A	Leu104	HB3	2.595	2.8	120.0
121	1BVV	A	Glu78	CD	3.106	2.0	81.8
122	1BVV	A	Glu78	OE1	2.783	6.9	97.1
123	1BVV	A	Glu78	OE2	2.865	4.2	59.4
124	1BVV	A	Arg112	HE	2.176	18.5	112.6
125	1BVV	A	Phe125	CZ	3.149	0.7	127.9
126	1BVV	A	Phe125	HZ	2.368	11.3	115.5
127	1BWF	Y	Thr267	OG1	2.696	9.8	96.5
128	1BWF	Y	Thr267	N	2.901	4.0	126.2
129	1BWF	Y	Thr267	CB	3.022	4.7	123.6

130	1BWF	Y	Thr267	OG1	2.674	10.6	95.7
131	1BWF	Y	Thr267	H	1.929	27.8	127.5
132	1BWF	Y	Thr267	HB	2.572	3.7	140.2
133	1BWF	O	Thr267	N	2.994	0.9	145.5
134	1BWF	O	Thr267	H	2.321	13.1	131.8
135	1BWF	O	Thr14	OG1	2.756	7.8	152.5
136	1BWF	O	Thr14	HG1	2.390	10.5	173.2
137	1BZC	A	Asp181	HB2	2.363	11.5	151.7
138	1BZC	A	Arg221	HH21	2.660	0.4	97.5
139	1BZC	A	Gln262	HG3	2.378	10.9	151.0
140	1BZJ	A	Asp181	HB2	2.384	10.7	152.3
141	1BZJ	A	Phe182	H	2.608	2.3	132.0
142	1BZJ	A	Gly220	HA3	2.331	12.7	126.9
143	1BZJ	A	Gln262	CG	3.133	1.2	149.2
144	1BZJ	A	Gln262	HG3	2.176	18.5	138.0
145	1C0L	A	Met1213	HE1	2.597	2.7	92.9
146	1C0L	A	Tyr1223	CD2	2.954	6.8	145.7
147	1C0L	A	Tyr1223	CE2	2.772	12.5	140.2
148	1C0L	A	Tyr1223	CZ	2.932	7.5	145.8
149	1C0L	A	Met1213	CE	3.026	4.5	114.3
150	1C0L	A	Met1213	HE1	2.383	10.8	102.6
151	1C0L	A	Tyr1238	OH	2.454	17.9	125.1
152	1C0L	A	Tyr1238	HH	1.830	31.5	121.3
153	1C5I	A	Glu78	CD	3.071	3.1	81.7
154	1C5I	A	Glu78	OE1	2.661	11.0	98.7
155	1C5I	A	Glu78	OE2	2.885	3.5	58.7
156	1C5I	A	Arg112	NE	3.011	0.3	115.9
157	1C5I	A	Arg112	HE	2.022	24.3	116.6
158	1C5I	A	Phe125	HZ	2.379	10.9	115.0
159	1C8M	1	Tyr144	HB2	2.431	8.9	93.4
160	1C8M	1	Tyr142	O	2.788	6.8	135.7
161	1C8M	1	Val168	CG2	3.008	5.1	153.7
162	1C8M	1	Phe179	CE2	3.025	4.6	118.6
163	1C9D	A	Ile153	CD1	3.098	2.3	169.1
164	1C22	A	Trp221	CZ3	3.115	1.7	136.2
165	1C22	A	Trp221	HZ3	2.541	4.8	134.8
166	1C22	A	Cys70	SG	3.108	5.0	123.1
167	1CSR	A	His320	HD2	2.620	1.9	146.1
168	1CSS	A	His320	CD2	3.060	3.5	159.5
169	1CSS	A	His320	HD2	2.393	10.4	141.7
170	1CT8	B	Tyr97	HE1	2.179	18.4	129.2
171	1CTR	A	Met124	HG2	2.478	7.2	130.3
172	1CX2	A	Arg120	HH11	2.319	13.1	96.2
173	1CX2	A	Arg120	HD2	2.408	9.8	139.8

174	1CX2	A	Arg120	HH11	2.437	8.7	91.1
175	1CX2	A	Tyr355	CE2	3.112	1.8	137.1
176	1CX2	A	Tyr355	HH	2.582	3.3	133.2
177	1CX2	A	Tyr355	HE2	2.104	21.2	139.4
178	1CX2	B	Arg120	CD	2.995	5.5	144.0
179	1CX2	B	Arg120	NH1	2.927	3.1	93.9
180	1CX2	B	Arg120	HH11	1.931	27.7	94.3
181	1CX2	B	Arg120	HD2	2.049	23.3	151.1
182	1CX2	B	Arg120	NH1	2.616	13.4	108.5
183	1CX2	B	Arg120	HH11	2.049	23.2	88.4
184	1CX2	B	Arg120	HH12	2.543	4.7	130.8
185	1CX2	B	Tyr355	HH	2.334	12.6	131.5
186	1CX2	B	Tyr355	HE2	2.241	16.1	127.9
187	1CX2	C	Arg120	HH11	2.624	1.7	90.5
188	1CX2	C	Arg120	HD2	2.380	10.9	132.8
189	1CX2	C	Leu531	CD1	3.053	3.7	147.5
190	1CX2	C	Arg120	HH11	2.497	6.5	96.2
191	1CX2	C	Tyr355	HE2	2.574	3.6	149.5
192	1CX2	D	Arg120	CD	2.949	7.0	137.1
193	1CX2	D	Arg120	NH1	3.020	0.0	89.5
194	1CX2	D	Arg120	HH11	2.026	24.1	88.9
195	1CX2	D	Arg120	HD2	1.989	25.5	143.4
196	1CX2	D	Arg120	NH1	2.555	15.4	111.8
197	1CX2	D	Arg120	HH11	1.977	25.9	91.1
198	1CX2	D	Arg120	HH12	2.495	6.5	134.6
199	1CX2	D	Tyr355	HH	2.457	8.0	134.5
200	1CX2	D	Tyr355	HE2	2.360	11.6	127.5
201	1D3G	A	Val134	CG1	3.168	0.1	142.8
202	1D3H	A	Leu359	HG	2.261	15.3	119.6
203	1D3H	A	Pro364	HD3	2.587	3.1	99.8
204	1D4S	B	Arg8	CZ	3.131	1.2	119.2
205	1D4Y	B	Val82	CG2	3.158	0.4	118.4
206	1DIF	A	Gly27	CA	3.132	1.2	166.3
207	1DIF	A	Gly27	C	3.021	4.7	141.1
208	1DIF	A	Gly27	HA3	2.445	8.4	161.3
209	1DIF	A	Asp25	OD2	2.646	11.5	117.9
210	1DTQ	A	Tyr188	CB	3.126	1.4	91.1
211	1DTQ	A	Tyr188	HB3	2.175	18.5	101.4
212	1DTT	A	Tyr188	CB	3.019	4.8	94.5
213	1DTT	A	Tyr188	HB3	2.024	24.2	105.4
214	1DVR	B	Lys55	NZ	2.977	1.4	115.3
215	1DVR	B	Lys55	HZ2	2.670	0.0	101.3
216	1DVR	A	Lys17	HB2	2.500	6.4	130.1
217	1DVR	A	Lys17	HE2	2.529	5.3	116.5

218	1DVR	A	Gly18	H	2.512	5.9	113.0
219	1DVR	B	Lys17	HB2	2.609	2.3	145.4
220	1DVR	B	Lys17	HE2	2.274	14.8	137.9
221	1DVY	A	Ala108	HB1	2.495	6.6	137.3
222	1DVY	B	Ala108	HB1	2.487	6.9	135.7
223	1DVY	A	Leu110	HB2	2.491	6.7	102.4
224	1DVY	B	Leu110	HB2	2.599	2.6	103.6
225	1DY9	A	Lys136	CE	3.087	2.6	130.2
226	1DY9	A	Lys136	NZ	2.965	1.8	129.7
227	1DY9	A	Lys136	HE2	2.591	3.0	138.8
228	1DY9	A	Lys136	HZ3	2.252	15.7	116.9
229	1DY9	F	Glu402	O	2.675	10.5	138.5
230	1DY9	B	Lys136	CE	2.921	7.8	156.4
231	1DY9	B	Lys136	HE2	2.226	16.6	157.7
232	1DY9	B	Lys136	HZ3	2.498	6.4	132.3
233	1E0V	A	His81	CE1	2.915	8.0	137.6
234	1E0V	A	His81	HE1	2.221	16.8	156.9
235	1E0V	A	Glu236	CD	3.151	0.6	85.6
236	1E0V	A	Glu236	OE1	2.791	6.7	60.9
237	1E0V	A	Glu236	OE2	2.690	10.0	105.7
238	1E0X	A	His81	CE1	2.912	8.1	136.6
239	1E0X	A	His81	HE1	2.283	14.5	156.7
240	1E0X	A	Glu236	OE1	2.957	1.1	57.7
241	1E0X	A	Glu236	OE2	2.686	10.2	101.0
242	1E0X	B	His81	CE1	2.910	8.2	136.9
243	1E0X	B	His81	HE1	2.234	16.3	156.0
244	1E0X	B	Glu236	OE1	2.982	0.3	56.8
245	1E0X	B	Glu236	OE2	2.655	11.2	99.9
246	1E0Y	B	Ser170	HG	2.432	8.9	116.3
247	1E0Y	B	Tyr187	OH	2.813	5.9	135.6
248	1E0Y	B	Glu457	OE2	2.971	0.6	121.4
249	1E0Y	B	Glu457	OE1	2.914	2.5	103.3
250	1E4I	A	His121	CE1	3.146	0.8	118.7
251	1E4I	A	His121	HE2	2.522	5.5	134.3
252	1E4I	A	Asn165	OD1	2.819	5.7	149.4
253	1E4I	A	Glu352	OE2	2.486	16.8	58.0
254	1E7B	A	Arg209	HG2	2.533	5.1	142.8
255	1E7B	A	Phe403	HE2	2.499	6.4	121.5
256	1E7B	A	Phe403	HZ	2.514	5.8	144.8
257	1E7B	A	Leu430	O	2.809	6.1	148.8
258	1E7B	A	Val433	HB	2.217	17.0	148.2
259	1E7B	B	Asp324	OD1	2.771	7.3	124.5
260	1E7B	B	Arg209	O	2.937	1.8	121.6
261	1E7B	B	Arg209	CG	2.560	19.3	163.3

262	1E7B	B	Arg209	HG2	1.979	25.9	168.0
263	1E7B	B	Arg209	HG3	2.227	16.6	139.4
264	1E7B	B	Lys212	HB3	2.267	15.1	142.2
265	1E7B	B	Phe403	CE2	3.169	0.0	131.0
266	1E7B	B	Phe403	CZ	3.040	4.1	147.9
267	1E7B	B	Phe403	HE2	2.629	1.6	112.6
268	1E7B	B	Phe403	HZ	2.341	12.3	144.3
269	1E7B	B	Leu430	O	2.733	8.6	148.3
270	1E7B	B	Val433	HB	2.624	1.7	142.7
271	1E7C	A	Asp324	CB	2.747	13.3	144.8
272	1E7C	A	Asp324	CG	3.125	1.4	120.5
273	1E7C	A	Asp324	HB3	1.916	28.2	140.0
274	1E7C	A	Arg209	CG	2.889	8.9	162.3
275	1E7C	A	Arg209	HG2	2.174	18.6	143.1
276	1E7C	A	Arg209	HG3	2.663	0.3	174.3
277	1E7C	A	Arg209	CZ	3.152	0.6	137.9
278	1E7C	A	Arg209	NH1	2.746	9.1	153.0
279	1E7C	A	Arg209	HH12	2.246	15.9	171.0
280	1E7C	A	Arg209	HH22	2.636	1.3	130.6
281	1E7C	A	Ser232	CA	3.075	3.0	144.1
282	1E7C	A	Ser232	OG	2.834	5.2	108.2
283	1E7C	A	Ser232	HA	2.092	21.7	140.0
284	1E7C	A	Val216	CG2	2.573	18.8	171.8
285	1E7C	A	Phe228	CZ	2.908	8.3	156.4
286	1E7C	A	Phe228	HZ	2.270	15.0	165.2
287	1E7C	A	Ile290	CG2	3.149	0.6	123.4
288	1E7C	A	Phe70	HB2	2.532	5.2	109.1
289	1E7C	A	Leu251	CD1	2.753	13.1	145.5
290	1E7C	A	Phe70	CB	3.120	1.6	104.5
291	1E7C	A	Phe70	CG	2.901	8.5	111.2
292	1E7C	A	Phe70	CD2	2.850	10.1	135.6
293	1E7C	A	Lys136	CE	2.955	6.8	122.1
294	1E7C	A	Lys136	HD3	2.602	2.5	118.5
295	1E7C	A	Lys136	HE2	2.210	17.2	130.8
296	1E8G	A	Asp170	OD2	2.906	2.8	145.7
297	1E8G	B	Asp170	OD2	2.926	2.1	145.7
298	1E+70	M	His141	HE2	2.622	1.8	97.1
299	1E+70	M	Asn186	ND2	2.939	2.7	135.9
300	1E+70	M	Glu409	OE2	2.688	10.1	120.0
301	1E+70	M	Glu409	CD	3.087	2.6	98.7
302	1E+73	M	His141	HE2	2.464	7.7	105.2
303	1E+73	M	Asn186	ND2	2.929	3.0	143.4
304	1E+73	M	Glu409	OE1	2.978	0.4	65.9
305	1E+73	M	Glu409	OE2	2.743	8.3	110.8

306	1EA1	A	Phe255	CD1	2.889	8.9	159.6
307	1EA1	A	Phe255	HD1	2.124	20.5	141.6
308	1EAS	A	His57	NE2	2.828	6.4	113.0
309	1EAS	A	His57	HE2	2.156	19.3	96.3
310	1EAS	A	Ser195	OG	2.803	6.3	59.0
311	1EAS	A	Ser195	CB	2.907	8.3	86.3
312	1EAS	A	Ser195	OG	2.803	6.2	59.0
313	1EAS	A	Ser195	HB2	2.269	15.0	100.6
314	1EAT	A	His57	NE2	2.794	7.5	113.7
315	1EAT	A	His57	HE2	2.123	20.5	96.6
316	1EAT	A	Ser195	OG	2.834	5.2	58.5
317	1EAT	A	Ser195	CB	2.902	8.5	85.9
318	1EAT	A	Ser195	OG	2.835	5.2	58.5
319	1EAT	A	Ser195	HB2	2.241	16.1	100.3
320	1EAT	A	Gln192	HG3	2.625	1.7	137.7
321	1EAU	A	His57	NE2	2.952	2.3	93.0
322	1EAU	A	His57	HE2	2.166	18.9	84.7
323	1EAU	A	Ser195	CB	2.735	13.7	94.2
324	1EAU	A	Ser195	OG	2.645	11.5	67.4
325	1EAU	A	Ser195	HB2	2.248	15.8	101.8
326	1EAU	A	His57	NE2	2.834	6.2	97.9
327	1EAU	A	His57	HE2	2.281	14.6	79.7
328	1EC0	A	Gly49	HA2	2.549	4.5	93.6
329	1EET	B	Glu1138	HG2	2.188	18.1	151.5
330	1ELA	B	Lys257	N	2.820	6.6	63.1
331	1ELA	A	Cys199	O	2.858	4.4	123.4
332	1ELA	A	Ser203	OG	2.857	4.4	91.5
333	1ELA	A	Ser203	H	2.480	7.1	150.1
334	1ELB	A	His60	HE2	2.335	12.6	108.8
335	1ELB	A	Ser203	HG	2.625	1.7	92.5
336	1ELB	B	Lys257	N	2.979	1.4	56.4
337	1ELB	A	Gln200	HA	2.398	10.2	138.5
338	1ELB	A	Gly201	H	2.568	3.8	100.3
339	1ELB	A	Ser203	HG	2.624	1.7	92.3
340	1ELB	B	Lys257	N	2.915	3.5	59.0
341	1ELB	B	Leu258	H	2.593	2.9	98.7
342	1ELB	B	Leu258	HG	2.608	2.3	166.5
343	1ELC	A	His60	HE2	2.630	1.5	88.5
344	1ELC	A	Ser203	HB2	2.513	5.9	124.2
345	1ELC	A	Gln200	HA	2.522	5.6	143.8
346	1ELC	A	Gly201	H	2.560	4.1	109.3
347	1ELC	A	Ser203	OG	2.846	4.8	103.5
348	1ELC	A	Ser203	HG	2.338	12.4	88.1
349	1ELC	B	Lys257	N	2.942	2.6	63.1

350	1ELD	E	Cys199	O	2.620	12.4	112.8
351	1ELD	E	Ser203	OG	2.693	9.9	95.0
352	1ELD	E	Ser203	H	2.524	5.5	154.1
353	1ELD	I	Phe257	N	2.855	5.5	39.5
354	1ELD	E	Ser203	OG	2.784	6.9	91.3
355	1ELD	I	Phe257	N	2.299	23.9	60.3
356	1ELE	E	Ser203	OG	2.792	6.6	92.2
357	1ELE	I	Val257	N	2.794	7.5	63.2
358	1ELE	E	Cys199	O	2.907	2.8	138.9
359	1ELE	E	Ser203	OG	2.898	3.1	87.8
360	1ELE	E	Ser203	H	2.613	2.1	138.8
361	1ELE	E	Ala104	HB2	2.220	16.8	148.6
362	1EXA	A	Ala234	HA	2.585	3.2	101.6
363	1EXP	A	His80	CE1	2.958	6.7	110.8
364	1EXP	A	His80	HE1	2.238	16.2	125.0
365	1EXP	A	Asn126	ND2	2.781	7.9	163.0
366	1EXX	A	Leu271	O	2.370	20.7	158.0
367	1EXX	A	Ile275	H	2.515	5.8	142.9
368	1EXX	A	Ile275	HB	2.282	14.5	83.9
369	1EXX	A	Phe230	CE1	3.106	2.0	133.4
370	1EXX	A	Ala234	HA	2.668	0.1	89.2
371	1EXX	A	Ala234	HB2	2.425	9.2	145.9
372	1FDK	A	Leu19	HA	2.438	8.7	119.7
373	1FDK	A	Asn23	HB2	2.608	2.3	170.7
374	1FDK	A	Pro18	HB3	2.563	4.0	137.2
375	1FDK	A	Phe22	HB2	2.345	12.2	118.7
376	1FJS	A	Gln192	CB	3.104	2.1	136.4
377	1FJS	A	Gln192	CG	2.981	6.0	136.8
378	1FJS	A	Gln192	CD	2.895	8.7	152.8
379	1FJS	A	Gln192	HB2	2.351	12.0	133.4
380	1FJS	A	Gln192	HG3	2.640	1.1	115.7
381	1FK9	A	Val179	CG1	2.937	7.3	128.6
382	1FK9	A	Tyr188	HB3	2.463	7.7	139.8
383	1FK9	A	Gly190	HA3	2.498	6.4	136.9
384	1FKO	A	Tyr188	HB3	2.359	11.6	123.8
385	1FKO	A	Tyr181	HD2	2.378	10.9	148.7
386	1FKO	A	Gly190	CA	3.160	0.3	136.1
387	1FKO	A	Gly190	HA3	2.351	12.0	146.2
388	1FX9	A	Phe5	CD2	2.996	5.5	148.3
389	1FX9	A	Phe5	CE2	2.650	16.4	159.2
390	1FX9	A	Phe5	HE2	2.474	7.3	135.9
391	1FX9	A	Phe22	HB2	2.416	9.5	154.5
392	1FXF	A	Phe5	CD2	2.819	11.1	161.7
393	1FXF	A	Phe5	CE2	2.517	20.6	155.5

394	1FXF	A	Phe5	HE2	2.473	7.4	130.8
395	1G4J	A	Val131	CG1	3.040	4.1	82.7
396	1G4J	A	Val135	CG1	2.887	8.9	138.1
397	1G4J	A	Gln92	HG2	2.295	14.0	168.3
398	1G4P	A	Ser206	OG	2.740	8.4	158.5
399	1G4P	A	Ser206	HG	1.750	34.5	157.7
400	1G4P	A	Gln57	NE2	2.913	3.6	134.2
401	1G4P	A	His107	CE1	3.135	1.1	95.1
402	1G4P	A	Tyr147	HE1	2.501	6.3	124.7
403	1G4P	A	Gly149	HA3	2.526	5.4	128.6
404	1G4P	A	Val184	CG1	3.167	0.1	124.6
405	1G4P	B	Tyr1029	CE2	2.983	5.9	128.3
406	1G4P	B	Tyr1147	HE1	2.401	10.1	133.1
407	1G4P	B	Val1184	CG1	3.143	0.9	122.8
408	1G4P	B	Ser1206	HG	2.325	12.9	162.2
409	1G4T	A	Ser206	HG	2.352	11.9	140.8
410	1G4T	A	Tyr29	CE2	2.984	5.9	118.3
411	1G4T	A	Tyr29	HE2	2.631	1.5	114.1
412	1G4T	A	Gln57	NE2	2.956	2.1	133.7
413	1G4T	A	His107	CE1	3.141	0.9	93.4
414	1G4T	A	His107	HE1	2.650	0.8	112.7
415	1G4T	A	Tyr147	HE1	2.297	14.0	118.4
416	1G4T	A	Gly149	HA3	2.414	9.6	133.6
417	1G4T	B	Tyr1029	CE2	3.017	4.8	117.8
418	1G4T	B	Tyr1029	HE2	2.667	0.1	114.0
419	1G4T	B	Gln1057	NE2	2.951	2.3	133.5
420	1G4T	B	His1107	CE1	3.108	2.0	95.9
421	1G4T	B	Tyr1147	HE1	2.264	15.2	121.9
422	1G4T	B	Gly1149	HA3	2.443	8.5	133.6
423	1G4T	B	Ser1206	HG	2.349	12.0	144.9
424	1G6C	A	Ser206	HG	2.337	12.5	138.4
425	1G6C	A	Tyr29	CE2	2.954	6.8	121.4
426	1G6C	A	Tyr29	HE2	2.652	0.7	115.2
427	1G6C	A	Gln57	NE2	2.959	2.0	134.8
428	1G6C	A	Tyr147	HE1	2.286	14.4	122.6
429	1G6C	A	Gly149	HA3	2.435	8.8	129.2
430	1G6C	B	Tyr1029	CE2	2.948	7.0	124.5
431	1G6C	B	Tyr1029	HE2	2.659	0.4	117.8
432	1G6C	B	Gln1057	NE2	2.965	1.8	133.4
433	1G6C	B	Tyr1147	HE1	2.271	15.0	125.9
434	1G6C	B	Gly1149	HA3	2.419	9.4	129.2
435	1G6C	B	Ser1206	HG	2.418	9.4	137.4
436	1G6U	A	Leu2	HB3	2.274	14.8	106.0
437	1G6U	B	Ser1	HB2	2.506	6.2	82.4

438	1G6U	B	Leu2	N	2.653	12.1	118.5
439	1G6U	B	Leu2	H	1.705	36.1	123.1
440	1G6U	B	Ser1	CB	2.849	10.1	120.3
441	1G6U	B	Ser1	HB2	1.928	27.8	108.5
442	1G6U	B	Ala3	H	2.384	10.7	107.8
443	1G6U	A	Ser1	HB2	2.327	12.9	95.8
444	1G6U	A	Ala3	H	2.223	16.8	136.4
445	1G9R	A	His244	CE1	3.115	1.7	170.2
446	1G9R	A	His244	HE1	2.186	18.1	166.9
447	1G48	A	Val135	CG1	3.143	0.8	136.3
448	1G53	A	Phe131	HE2	2.303	13.7	114.5
449	1G54	A	Val135	CG2	3.130	1.3	122.4
450	1GA8	A	His244	CE1	3.096	2.3	163.4
451	1GA8	A	His244	HE1	2.199	17.6	158.2
452	1GG6	B	Val67	CG1	3.166	0.1	145.9
453	1GG6	B	Glu70	OE2	2.765	7.5	113.0
454	1GG6	B	His57	HE2	2.315	13.3	101.5
455	1GG6	C	Ser195	OG	2.746	8.2	61.4
456	1GG6	C	Ser195	CB	2.903	8.4	83.5
457	1GG6	C	Ser195	OG	2.892	3.3	55.9
458	1GG6	C	Ser195	HB2	2.207	17.4	96.6
459	1GG6	C	Met192	HA	2.668	0.1	112.7
460	1GJ8	B	Val213	CG1	2.938	7.3	126.7
461	1GS4	A	Leu704	HB3	2.374	11.1	125.1
462	1GSZ	A	Trp169	CB	2.958	6.7	130.7
463	1GSZ	A	Trp169	HB2	2.034	23.8	129.9
464	1GSZ	B	Trp169	CB	3.141	0.9	131.1
465	1GSZ	B	Trp169	HB2	2.322	13.0	126.1
466	1GSZ	B	Phe601	HZ	2.481	7.1	108.4
467	1GSZ	C	Trp169	CD1	3.157	0.4	166.0
468	1GSZ	C	Trp169	HB2	2.513	5.9	115.5
469	1GSZ	C	Phe601	CZ	3.096	2.3	105.2
470	1GSZ	C	Phe601	HZ	2.171	18.7	116.0
471	1GVY	A	His143	HE2	2.438	8.7	110.5
472	1GVY	A	His211	CE1	2.976	6.1	143.1
473	1GVY	A	His211	HE1	2.063	22.7	129.2
474	1GW1	A	His143	CE1	3.001	5.3	117.7
475	1GW1	A	His143	HE1	2.270	15.0	115.1
476	1GW1	A	His211	NE2	2.953	2.2	145.5
477	1GW1	A	His211	CE1	2.604	17.8	157.9
478	1GW1	A	His211	HE2	2.238	16.2	131.7
479	1GW1	A	Glu320	OE1	2.935	1.8	90.6
480	1GW1	A	Glu320	OE1	2.697	9.8	100.7
481	1GWX	A	Thr288	CG2	2.762	12.9	144.3

482	1GWX	A	Thr292	HG1	2.660	0.4	52.3
483	1GWX	B	Thr288	CG2	2.627	17.1	136.3
484	1GY Y	B	Cys7	HA	2.354	11.8	119.9
485	1GY Y	B	Phe8	CD1	3.135	1.1	93.2
486	1GY Y	B	Phe8	H	2.660	0.4	91.6
487	1GY Y	B	Trp51	CZ3	2.996	5.5	140.9
488	1GY Y	B	Trp51	CH2	3.051	3.7	121.1
489	1GY Y	A	Cys7	HA	2.249	15.8	121.9
490	1GY Y	A	Phe8	N	3.015	0.1	109.1
491	1GY Y	A	Phe8	CD1	3.098	2.3	90.5
492	1GY Y	A	Phe8	H	2.561	4.1	91.6
493	1GY Y	A	Trp51	CZ3	3.043	4.0	141.5
494	1GY Y	A	Trp51	CH2	3.060	3.5	122.1
495	1GZG	A	Asp131	OD1	2.950	1.3	112.7
496	1GZG	A	Asn139	ND2	2.464	18.4	100.6
497	1GZG	A	Ser175	OG	2.793	6.6	125.3
498	1GZG	A	Ser175	HG	2.595	2.8	149.4
499	1GZG	A	Lys260	NZ	2.774	8.2	58.2
500	1GZG	B	Ser175	O	2.773	7.3	105.1
501	1GZG	B	Ser175	OG	2.614	12.6	110.8
502	1GZG	B	Ser175	HG	2.668	0.1	95.9
503	1GZG	B	Ser175	HB2	2.538	5.0	159.3
504	1GZG	B	Lys260	NZ	2.810	6.9	56.9
505	1GZG	B	Ser175	OG	2.815	5.9	91.0
506	1GZG	B	Ser175	HG	2.146	19.6	105.1
507	1H00	A	Lys33	HD2	2.438	8.7	146.8
508	1H00	A	Asp145	CG	3.025	4.6	94.5
509	1H00	A	Asp145	OD1	1.941	35.1	108.2
510	1H2J	A	Asn138	ND2	2.925	3.1	136.4
511	1H2J	A	Glu228	OE2	2.713	9.2	96.8
512	1H2J	A	Glu228	OE1	2.725	8.9	125.5
513	1H2J	A	Glu228	OE2	2.880	3.7	86.3
514	1H2J	A	Glu228	OE2	2.971	0.6	85.1
515	1H2J	A	His101	CE1	2.957	6.7	139.5
516	1H2J	A	His101	NE2	2.986	1.1	121.2
517	1H2J	A	His101	HE1	2.546	4.6	135.6
518	1H2J	A	His101	HE2	2.639	1.2	102.0
519	1H2J	A	Asn138	ND2	2.904	3.8	141.2
520	1H2J	A	Glu228	CD	2.986	5.8	93.9
521	1H2J	A	Glu228	OE1	2.675	10.5	115.3
522	1H2J	A	Glu228	OE2	2.565	14.2	69.4
523	1H2J	A	Glu228	CD	3.011	5.0	82.8
524	1H2J	A	Glu228	OE1	2.632	12.0	95.8
525	1H2J	A	Glu228	OE2	2.720	9.0	60.4

526	1H2J	A	Glu228	OE2	2.841	5.0	59.0
527	1H3A	A	Ser307	HB3	2.626	1.7	109.6
528	1H3A	B	Ser307	HB3	2.598	2.7	110.0
529	1H3A	C	Ser307	HB3	2.646	0.9	109.7
530	1H4G	A	Glu94	CD	3.051	3.8	85.3
531	1H4G	A	Glu94	OE1	2.800	6.3	99.8
532	1H4G	A	Glu94	OE2	2.801	6.3	61.3
533	1H4G	A	Arg129	NE	2.973	1.5	111.9
534	1H4G	A	Arg129	HE	2.304	13.7	113.0
535	1H4G	B	Glu94	CD	3.137	1.0	83.5
536	1H4G	B	Glu94	OE1	2.840	5.0	99.2
537	1H4G	B	Glu94	OE2	2.832	5.3	60.3
538	1H4G	B	Arg129	NE	2.911	3.6	118.5
539	1H4G	B	Arg129	HE	2.114	20.8	121.5
540	1H4G	B	Phe141	HE2	2.558	4.2	137.0
541	1H4G	B	Phe141	HZ	2.527	5.4	110.7
542	1H11	A	His101	CE1	3.166	0.1	131.1
543	1H11	A	Asn138	ND2	2.904	3.8	147.6
544	1H11	A	Glu228	OE2	2.680	10.4	63.6
545	1H11	A	Glu228	CD	3.007	5.2	86.8
546	1H11	A	Glu228	OE1	2.669	10.7	104.3
547	1H11	A	Glu228	OE2	2.703	9.6	61.9
548	1HBJ	A	Ser200	OG	2.885	3.5	52.5
549	1HBJ	A	Trp233	CZ3	2.983	5.9	173.2
550	1HBJ	A	Trp233	CH2	2.909	8.2	154.2
551	1HBJ	A	Gly119	CA	3.075	3.0	114.1
552	1HBJ	A	Gly119	HA2	2.595	2.8	99.6
553	1HBJ	A	Phe290	CZ	3.163	0.2	128.2
554	1HBJ	A	Ser200	OG	2.702	9.6	59.1
555	1HBJ	A	Phe288	CE1	3.138	1.0	129.3
556	1HBJ	A	Phe288	HE1	2.598	2.7	112.5
557	1HBJ	A	Phe330	CE2	2.882	9.1	93.2
558	1HBJ	A	Phe330	HE2	2.280	14.6	111.5
559	1HL9	A	Trp67	HE1	2.294	14.1	109.7
560	1HL9	A	His129	HE2	2.286	14.4	98.2
561	1HL9	A	Trp67	HE1	2.439	8.7	111.7
562	1HL9	A	His129	CE1	3.146	0.8	83.9
563	1HL9	A	His129	NE2	2.356	22.0	101.1
564	1HL9	A	His129	HE2	1.406	47.3	111.0
565	1HL9	B	Trp67	HE1	2.335	12.5	109.0
566	1HL9	B	His129	HE2	2.370	11.3	94.9
567	1HL9	B	Trp67	HE1	2.446	8.4	105.1
568	1HL9	B	Trp67	HZ2	2.618	2.0	163.0
569	1HL9	B	His129	NE2	2.692	10.9	89.7

570	1HL9	B	His129	HE2	1.701	36.3	92.5
571	1HLD	A	Phe140	HZ	2.663	0.2	140.9
572	1HLD	B	Val294	CG2	3.166	0.1	88.4
573	1HLD	B	Ser48	CB	3.124	1.5	88.2
574	1HLD	B	His67	CE1	3.155	0.5	157.8
575	1HWI	A	Val683	CG1	2.754	13.1	100.2
576	1HWI	A	Val683	CG2	3.067	3.2	140.2
577	1HWI	B	Arg590	HD3	2.649	0.8	135.1
578	1HWI	B	Val683	CG1	2.805	11.5	104.7
579	1HWI	B	Val683	CG2	3.036	4.2	150.8
580	1HWI	C	Val683	CG1	2.991	5.6	140.2
581	1HWI	D	Val683	CG1	2.957	6.7	141.0
582	1HWJ	A	Arg590	NE	2.794	7.5	124.6
583	1HWJ	A	Arg590	CZ	2.948	7.0	101.0
584	1HWJ	B	Arg590	NE	2.859	5.3	123.4
585	1HWJ	B	Arg590	CZ	2.992	5.6	101.0
586	1HWJ	C	Arg590	NE	2.900	4.0	122.2
587	1HWJ	C	Arg590	CZ	3.041	4.1	100.7
588	1HWJ	D	Arg590	NE	2.932	2.9	119.4
589	1HWJ	D	Arg590	CZ	3.076	3.0	97.8
590	1HWJ	D	Val683	CG1	3.135	1.1	94.2
591	1HWK	A	Arg590	NE	2.766	8.4	124.2
592	1HWK	A	Arg590	CZ	3.125	1.4	100.2
593	1HWK	A	Arg590	HE	2.646	0.9	124.2
594	1HWK	B	Arg590	CD	3.152	0.6	143.9
595	1HWK	B	Arg590	NH1	2.957	2.1	88.7
596	1HWK	B	Arg590	HD3	2.192	17.9	151.8
597	1HWK	B	Arg590	HH11	2.629	1.5	94.5
598	1HWK	C	Arg590	NE	2.920	3.3	125.4
599	1HWK	C	Val683	CG1	3.091	2.5	93.9
600	1HWK	D	Arg590	NE	2.908	3.7	125.6
601	1HWK	D	Val683	CG1	3.160	0.3	94.0
602	1HWL	A	Arg590	NE	2.926	3.1	116.1
603	1HWL	A	Arg590	CZ	3.099	2.2	95.2
604	1HWL	A	Ser684	HB2	2.633	1.4	115.6
605	1HWL	B	Arg590	NE	2.974	1.5	116.5
606	1HWL	B	Arg590	CZ	3.151	0.6	95.5
607	1HWL	B	Ser684	HB2	2.662	0.3	112.9
608	1HWL	C	Arg590	NE	2.972	1.6	114.9
609	1HWL	C	Arg590	CZ	3.145	0.8	95.1
610	1HWL	C	Ser684	HB2	2.554	4.3	118.8
611	1HWL	D	Arg590	NE	2.926	3.1	114.4
612	1HWL	D	Arg590	CZ	3.116	1.7	93.9
613	1HWL	D	Ser684	HB2	2.587	3.1	114.7

614	1I9L	A	Gly132	HA2	2.395	10.3	112.8
615	1I9M	A	Pro202	HG3	2.292	14.1	92.2
616	1I9M	A	Leu198	CD1	2.886	8.9	117.9
617	1I9N	A	Leu198	CD1	2.981	5.9	113.6
618	1I9N	A	Leu204	CD1	3.023	4.6	125.1
619	1I9O	A	Pro202	HG3	2.556	4.3	82.4
620	1I9O	A	Val135	CG1	3.084	2.7	130.4
621	1I9O	A	Leu204	CD1	3.015	4.9	124.2
622	1I9O	A	Gln92	HG2	2.476	7.3	159.8
623	1I9P	A	Pro202	HG2	2.603	2.5	134.5
624	1I9P	A	Pro202	HD2	2.644	1.0	148.5
625	1I9P	A	Gly132	HA2	2.408	9.8	171.5
626	1I9Q	A	Val135	CG1	2.780	12.3	152.7
627	1I9Q	A	Ile91	CG2	3.138	1.0	123.4
628	1IEI	A	Cys298	C	3.071	3.1	156.1
629	1IEI	A	Cys298	O	2.473	17.3	142.6
630	1IEI	A	Leu300	CB	3.112	1.8	78.4
631	1IEI	A	Leu300	HB2	2.392	10.4	74.8
632	1IEW	A	Arg158	NH1	2.920	3.3	117.3
633	1IEW	A	Arg158	HH12	2.099	21.4	112.9
634	1IEW	A	Tyr253	HE2	2.586	3.2	117.9
635	1IEW	A	Asp285	CG	3.062	3.4	84.8
636	1IEW	A	Asp285	OD1	2.934	1.9	62.2
637	1IEW	A	Asp285	OD2	2.568	14.1	99.6
638	1IF5	A	Thr200	OG1	2.854	4.5	124.9
639	1IF5	A	His94	HE1	2.494	6.6	85.8
640	1IF5	A	Val121	CG2	2.816	11.2	130.5
641	1IF6	A	Val121	CG1	3.080	2.8	131.0
642	1IF6	A	Thr200	OG1	2.969	0.7	107.1
643	1IF6	A	Thr200	HG1	2.564	4.0	112.8
644	1IKV	A	Tyr188	CB	3.121	1.6	129.2
645	1IKV	A	Tyr188	HB3	2.105	21.2	137.1
646	1IKV	A	Gly190	HA3	2.532	5.2	144.6
647	1IKV	A	Val179	CG2	3.059	3.5	119.5
648	1IKW	A	Tyr188	HB3	2.402	10.0	127.4
649	1IKW	A	Gly190	HA3	2.461	7.8	134.4
650	1IKW	A	Val179	CG2	3.047	3.9	113.1
651	1J4R	A	Phe36	CE1	3.021	4.7	129.2
652	1J4R	A	Phe36	HE1	2.374	11.1	110.3
653	1J4R	B	Phe36	CE1	2.934	7.4	132.1
654	1J4R	B	Phe36	HE1	2.204	17.5	114.1
655	1J4R	D	Phe36	CE1	3.066	3.3	136.5
656	1J4R	D	Phe36	HE1	2.320	13.1	119.3
657	1JKH	A	Tyr188	HB3	2.563	4.0	121.3

658	1JKH	A	Gly190	HA3	2.381	10.8	132.0
659	1JLC	A	Tyr188	CB	3.076	3.0	78.7
660	1JLC	A	Tyr188	HB3	1.988	25.5	78.7
661	1JYY	A	Glu461	OE2	2.816	5.8	112.3
662	1JYY	B	Glu461	OE2	2.817	5.8	112.3
663	1JYY	C	Glu461	OE2	2.816	5.8	112.3
664	1JYY	D	Glu461	OE2	2.816	5.8	112.3
665	1JYY	E	Glu461	OE2	2.816	5.8	112.3
666	1JYY	F	Glu461	OE2	2.816	5.8	112.3
667	1JYY	G	Glu461	OE2	2.816	5.8	112.3
668	1JYY	H	Glu461	OE2	2.816	5.8	112.3
669	1JYZ	I	Glu461	OE2	2.816	5.8	112.3
670	1JYZ	J	Glu461	OE2	2.816	5.8	112.3
671	1JYZ	K	Glu461	OE2	2.816	5.8	112.3
672	1JYZ	L	Glu461	OE2	2.815	5.8	112.3
673	1JYZ	M	Glu461	OE2	2.816	5.8	112.3
674	1JYZ	N	Glu461	OE2	2.815	5.8	112.3
675	1JYZ	O	Glu461	OE2	2.816	5.8	112.3
676	1JYZ	P	Glu461	OE2	2.817	5.8	112.3
677	1JZ0	A	Asn460	ND2	2.928	3.0	132.0
678	1JZ0	A	Glu537	OE1	2.887	3.5	102.4
679	1JZ0	B	Asn460	ND2	2.928	3.0	132.0
680	1JZ0	B	Glu537	OE1	2.887	3.5	102.4
681	1JZ0	C	Asn460	ND2	2.928	3.1	132.0
682	1JZ0	C	Glu537	OE1	2.886	3.5	102.3
683	1JZ0	D	Asn460	ND2	2.928	3.1	132.0
684	1JZ0	D	Glu537	OE1	2.887	3.5	102.3
685	1JZ0	E	Asn460	ND2	2.928	3.1	132.0
686	1JZ0	E	Glu537	OE1	2.887	3.5	102.3
687	1JZ0	F	Asn460	ND2	2.928	3.0	132.0
688	1JZ0	F	Glu537	OE1	2.887	3.4	102.3
689	1JZ0	G	Asn460	ND2	2.928	3.1	132.0
690	1JZ0	G	Glu537	OE1	2.887	3.5	102.3
691	1JZ0	H	Asn460	ND2	2.927	3.1	132.0
692	1JZ0	H	Glu537	OE1	2.886	3.5	102.3
693	1JZ1	I	Asn460	ND2	2.928	3.0	132.0
694	1JZ1	I	Glu537	OE1	2.886	3.5	102.4
695	1JZ1	J	Asn460	ND2	2.927	3.1	132.0
696	1JZ1	J	Glu537	OE1	2.887	3.4	102.3
697	1JZ1	K	Asn460	ND2	2.928	3.1	132.0
698	1JZ1	K	Glu537	OE1	2.886	3.5	102.3
699	1JZ1	L	Asn460	ND2	2.928	3.1	132.0
700	1JZ1	L	Glu537	OE1	2.887	3.5	102.3
701	1JZ1	M	Asn460	ND2	2.928	3.1	132.0

702	1JZ1	M	Glu537	OE1	2.886	3.5	102.3
703	1JZ1	N	Asn460	ND2	2.927	3.1	132.0
704	1JZ1	N	Glu537	OE1	2.886	3.5	102.4
705	1JZ1	O	Asn460	ND2	2.928	3.0	132.0
706	1JZ1	O	Glu537	OE1	2.886	3.5	102.4
707	1JZ1	P	Asn460	ND2	2.928	3.1	132.0
708	1JZ1	P	Glu537	OE1	2.887	3.5	102.3
709	1JZ2	A	Asn460	ND2	3.004	0.5	124.1
710	1JZ2	A	Glu537	CD	3.039	4.1	85.5
711	1JZ2	A	Glu537	OE1	2.672	10.6	101.3
712	1JZ2	A	Glu537	OE2	2.899	3.0	60.9
713	1JZ2	B	Asn460	ND2	2.864	5.2	132.1
714	1JZ2	B	Glu537	OE1	2.921	2.3	89.0
715	1JZ2	C	Asn460	ND2	2.772	8.2	134.0
716	1JZ2	C	Glu537	OE1	2.973	0.6	93.9
717	1JZ2	C	Glu537	OE2	2.945	1.5	58.3
718	1JZ2	D	Asn460	ND2	2.942	2.6	119.6
719	1JZ2	D	Glu537	CD	2.938	7.3	88.4
720	1JZ2	D	Glu537	OE1	2.500	16.4	106.1
721	1JZ2	D	Glu537	OE2	2.904	2.9	62.6
722	1K2O	A	Gly93	C	3.048	3.8	131.4
723	1K2O	A	Glu94	HB2	2.629	1.5	162.2
724	1K2O	A	Gly93	HA2	2.507	6.1	96.4
725	1K2O	A	Thr185	HA	2.301	13.8	98.8
726	1K2O	A	Phe193	HE1	2.580	3.4	140.7
727	1K2O	A	Tyr96	HE2	2.115	20.8	111.2
728	1K2O	A	Gly93	C	2.948	7.0	130.6
729	1K2O	A	Glu94	HB2	2.488	6.8	158.5
730	1K2O	A	Gly93	HA2	2.549	4.5	94.0
731	1K2O	A	Thr185	CA	3.129	1.3	116.5
732	1K2O	A	Thr185	HA	2.187	18.1	104.7
733	1K2O	A	Phe193	HE1	2.410	9.7	140.2
734	1K2O	A	Tyr96	HE2	2.237	16.2	105.4
735	1K2O	B	Gly93	C	3.141	0.9	138.1
736	1K2O	B	Thr185	CA	2.987	5.8	118.8
737	1K2O	B	Thr185	HA	2.063	22.7	105.1
738	1K2O	B	Pro187	HD3	2.591	2.9	143.2
739	1K2O	B	Phe193	HE1	2.609	2.3	137.1
740	1K2O	B	Tyr96	HE2	2.442	8.5	103.5
741	1K2O	B	Gly93	C	2.997	5.5	137.9
742	1K2O	B	Gly93	O	2.922	2.3	137.7
743	1K2O	B	Glu94	HB2	2.489	6.8	159.7
744	1K2O	B	Gly93	HA2	2.560	4.1	106.6
745	1K2O	B	Thr185	CA	2.989	5.7	124.3

746	1K2O	B	Thr185	HA	2.016	24.5	112.4
747	1K2O	B	Pro187	HG3	2.633	1.4	156.8
748	1K2O	B	Pro187	HD3	2.650	0.8	139.8
749	1K2O	B	Phe193	HE1	2.467	7.6	139.2
750	1K2O	B	Tyr96	HE2	2.534	5.1	104.4
751	1K2O	B	Phe87	HE2	2.581	3.3	72.9
752	1K2U	B	Trp678	HZ3	2.618	1.9	156.6
753	1KAK	A	Lys120	NZ	2.933	2.9	137.1
754	1KAK	A	Lys120	HZ1	1.993	25.4	132.9
755	1KAK	A	Phe182	CZ	3.121	1.5	92.5
756	1KAK	A	Ser216	HB3	2.307	13.6	127.8
757	1KAK	A	Ala217	CB	2.970	6.3	117.7
758	1KAK	A	Ala217	H	2.584	3.2	134.4
759	1KAK	A	Ala217	HB2	2.311	13.5	118.4
760	1KAV	A	Gln262	HG3	2.314	13.3	144.5
761	1KJR	A	His158	HE1	2.487	6.9	108.6
762	1KJR	A	Ala146	HB2	2.553	4.4	115.7
763	1KKQ	A	Glu269	O	2.843	4.9	159.9
764	1KKQ	A	Ile272	HB	2.574	3.6	104.8
765	1KKQ	C	Phe351	HB3	2.613	2.1	143.3
766	1KKQ	D	Phe351	CB	3.143	0.9	152.5
767	1KKQ	D	Phe351	HB3	2.180	18.3	150.2
768	1KKQ	D	Phe351	HD1	2.588	3.1	123.6
769	1KKQ	D	Ile272	HB	2.368	11.3	118.3
770	1LGX	A	Val103	CG2	3.011	5.0	135.6
771	1LGX	A	Ile78	CG2	3.133	1.2	161.5
772	1LGX	A	Tyr88	HB2	2.344	12.2	124.7
773	1LGX	A	Val87	HB	2.600	2.6	111.8
774	1LGX	A	Tyr88	N	2.736	9.4	151.3
775	1LGX	A	Tyr88	CA	2.998	5.4	139.6
776	1LGX	A	Tyr88	HA	2.545	4.7	134.6
777	1LGX	A	Val87	CG1	3.138	1.0	119.7
778	1LIN	A	Met109	SD	3.260	0.3	165.3
779	1LIN	A	Met145	HE1	2.487	6.9	159.5
780	1LIN	A	Phe68	HD1	2.653	0.6	157.5
781	1LIN	A	Ile63	CG1	3.076	3.0	121.5
782	1LQF	A	Gly720	HA3	2.497	6.5	134.4
783	1LQF	A	Gln762	HG3	2.545	4.7	129.5
784	1LQF	A	Asp681	HB2	2.514	5.9	175.2
785	1LQF	B	Arg547	HD3	2.462	7.8	81.9
786	1LQF	B	Gly720	HA3	2.647	0.9	122.3
787	1LQF	B	Gln762	HG3	2.246	15.9	149.8
788	1LQF	C	Arg547	CZ	3.063	3.4	135.7
789	1LQF	C	Arg547	NH2	2.937	2.8	158.1

790	1LQF	C	Gly720	HA3	2.207	17.3	127.3
791	1LQF	C	Gln762	HG3	2.298	13.9	134.4
792	1LQF	D	Arg547	NH1	2.689	11.0	144.3
793	1LQF	D	Gly720	HA3	2.322	13.0	129.9
794	1LQF	D	Gln762	HG3	2.205	17.4	140.9
795	1M2Z	A	Phe623	CE2	3.148	0.7	160.2
796	1M2Z	A	Phe623	HE2	2.176	18.5	155.4
797	1M2Z	D	Phe623	HE1	2.209	17.3	164.3
798	1M7Q	A	Leu104	HB3	2.587	3.1	152.1
799	1MFI	A	Tyr36	HB3	2.511	5.9	114.6
800	1MFI	A	Tyr36	HD2	2.565	3.9	167.1
801	1MFI	B	Tyr36	HB3	2.475	7.3	110.3
802	1MFI	C	Tyr36	HB3	2.205	17.4	125.6
803	1MG0	A	Ser48	HB3	2.323	13.0	120.8
804	1MG0	B	Ser48	HB3	2.309	13.5	119.6
805	1MG0	B	Leu57	CD1	3.086	2.7	165.2
806	1MG0	C	Ser48	HB3	2.453	8.1	111.6
807	1MG0	C	Leu57	CD1	3.092	2.5	157.1
808	1MG0	D	Ser48	HB3	2.435	8.8	119.2
809	1MG0	D	Leu57	CD1	3.124	1.5	159.4
810	1MG0	D	Leu116	CD1	2.904	8.4	103.3
811	1MGO	B	Ile137	C	3.142	0.9	162.2
812	1MGO	B	Ser128	HB2	2.461	7.8	118.8
813	1MGO	B	Leu309	CD2	2.487	21.5	135.8
814	1MGO	A	Ser117	HA	2.257	15.5	112.0
815	1MKD	A	Asn418	CB	3.103	2.1	137.5
816	1MKD	A	Asn418	HB2	2.269	15.0	152.5
817	1MKD	A	Thr430	HA	2.632	1.4	96.0
818	1MKD	B	Asn418	CB	3.105	2.1	136.4
819	1MKD	B	Asn418	HB2	2.289	14.3	151.8
820	1MKD	B	Tyr426	HE1	2.666	0.2	79.2
821	1MKD	C	Asn418	CB	3.124	1.5	138.0
822	1MKD	C	Asn418	HB2	2.310	13.5	153.4
823	1MKD	C	Thr430	HA	2.631	1.5	95.0
824	1MKD	D	Asn418	CB	3.139	1.0	137.9
825	1MKD	D	Asn418	HB2	2.344	12.2	153.0
826	1MKD	D	Tyr426	HE1	2.624	1.7	79.9
827	1MKD	D	Thr430	HA	2.589	3.0	96.0
828	1MKD	E	Asn418	CB	3.107	2.0	138.2
829	1MKD	E	Asn418	HB2	2.294	14.1	153.2
830	1MKD	E	Tyr426	HE1	2.612	2.2	80.0
831	1MKD	E	Thr430	HA	2.622	1.8	94.3
832	1MKD	F	Asn418	CB	3.088	2.6	135.7
833	1MKD	F	Asn418	HB2	2.278	14.7	150.9

834	1MKD	F	Tyr426	HE1	2.619	1.9	77.8
835	1MKD	G	Asn418	CB	3.134	1.1	136.6
836	1MKD	G	Asn418	HB2	2.318	13.2	151.7
837	1MKD	G	Tyr426	HE1	2.625	1.7	81.2
838	1MKD	G	Thr430	HA	2.666	0.2	93.1
839	1MKD	H	Asn418	CB	3.114	1.8	137.5
840	1MKD	H	Asn418	HB2	2.313	13.4	152.6
841	1MKD	H	Tyr426	HE1	2.630	1.5	80.1
842	1MKD	H	Thr430	HA	2.636	1.3	93.5
843	1MKD	I	Asn418	CB	3.098	2.3	137.5
844	1MKD	I	Asn418	HB2	2.307	13.6	153.3
845	1MKD	I	Thr430	HA	2.591	3.0	94.7
846	1MKD	J	Asn418	CB	3.050	3.8	138.6
847	1MKD	J	Asn418	HB2	2.258	15.4	154.5
848	1MKD	J	Tyr426	HE1	2.643	1.0	79.0
849	1MKD	J	Thr430	HA	2.624	1.7	95.0
850	1MKD	K	Asn418	CB	3.134	1.1	138.0
851	1MKD	K	Asn418	HB2	2.326	12.9	153.4
852	1MKD	K	Tyr426	HE1	2.635	1.3	80.1
853	1MKD	K	Thr430	HA	2.570	3.7	96.1
854	1MKD	L	Asn418	CB	3.083	2.7	137.2
855	1MKD	L	Asn418	HB2	2.281	14.6	152.3
856	1MKD	L	Tyr426	HE1	2.659	0.4	79.7
857	1MKD	L	Thr430	HA	2.636	1.3	94.2
858	1MMJ	N	Gln185	HB3	2.443	8.5	163.5
859	1MMJ	N	Ser188	HB2	2.665	0.2	93.9
860	1MMJ	N	His45	NE2	2.662	11.9	120.9
861	1MMJ	N	His45	HE2	1.848	30.8	105.9
862	1MQI	A	Met196	CE	3.144	0.8	112.9
863	1MQI	A	Met196	HE2	2.208	17.3	110.0
864	1MU6	B	Glu217	HG2	2.492	6.7	123.3
865	1MU8	B	Glu217	HG2	2.468	7.6	127.0
866	1MU8	B	Val213	CG1	3.099	2.2	112.8
867	1MUE	B	Trp215	CE3	3.119	1.6	140.4
868	1MUE	B	Trp215	HE3	2.587	3.1	140.1
869	1MUE	B	Glu217	CG	3.126	1.4	126.4
870	1MUE	B	Glu217	HG2	2.503	6.3	107.7
871	1N0Q	B	Tyr93	HD1	2.517	5.7	126.5
872	1N0Q	B	His73	HE1	2.200	17.6	120.3
873	1NCQ	A	Val176	CG2	2.656	16.2	137.9
874	1NCQ	A	Ala150	O	2.688	10.1	121.6
875	1NCQ	A	Pro174	O	2.933	1.9	138.7
876	1NCQ	A	Ser175	CA	2.838	10.5	136.8
877	1NCQ	A	Ser175	HA	1.749	34.5	139.3

878	1NCR	A	Met124	HE1	2.606	2.4	154.2
879	1NCR	A	Tyr142	HB3	2.619	1.9	126.7
880	1NCR	A	Val168	CB	3.163	0.2	151.0
881	1NCR	A	Val168	CG2	2.941	7.2	170.9
882	1NCR	A	Val168	HB	2.507	6.1	135.7
883	1NCR	A	Tyr142	C	3.168	0.1	116.2
884	1NCR	A	Tyr142	O	2.652	11.3	117.7
885	1NCR	A	Met143	HA	2.591	3.0	165.1
886	1ND3	A	Val168	CG2	2.633	16.9	170.1
887	1ND3	A	Tyr142	O	2.807	6.1	111.0
888	1ND3	A	Met143	HA	2.563	4.0	157.7
889	1ND3	A	Tyr144	N	2.912	3.6	136.5
890	1ND3	A	Tyr144	H	2.517	5.7	145.8
891	1ND3	A	Ala166	O	2.775	7.2	142.7
892	1NHX	A	Leu293	HB2	2.432	8.9	111.7
893	1NJS	A	Met89	HE1	2.285	14.4	104.0
894	1NJS	A	Ser118	HA	2.630	1.5	114.2
895	1NJS	B	Met89	CE	3.162	0.3	105.9
896	1NJS	B	Met89	HE1	2.246	15.9	96.0
897	1NJS	B	Met89	HE1	2.371	11.2	92.8
898	1NJT	A	Arg165	HG3	2.334	12.6	155.0
899	1NJT	E	Ala264	CA	2.832	10.6	64.3
900	1NJT	E	Ala264	C	2.404	24.2	36.5
901	1NJT	E	Ala264	O	2.948	1.4	53.4
902	1NJT	E	Ala264	HA	2.319	13.1	85.9
903	1NJT	A	Ser132	OG	2.976	0.5	54.9
904	1NJT	A	Cys161	HG	2.526	5.4	141.4
905	1NJT	E	Ala264	C	2.390	24.6	37.2
906	1NJT	E	Ala264	O	2.727	8.8	62.0
907	1NJT	A	His63	CD2	3.041	4.1	140.0
908	1NJT	A	His63	NE2	2.874	4.8	122.8
909	1NJT	A	His63	HE2	2.327	12.8	104.7
910	1NJT	A	Ser132	OG	2.728	8.7	64.5
911	1NJT	E	Ala264	CA	3.011	5.0	57.2
912	1NJT	E	Ala264	C	2.356	25.7	38.2
913	1NJT	B	Arg465	HG3	2.197	17.7	160.3
914	1NJT	B	Arg465	HE	2.670	0.0	139.1
915	1NJT	F	Ala564	CA	2.883	9.0	62.8
916	1NJT	F	Ala564	C	2.398	24.3	36.9
917	1NJT	F	Ala564	O	2.875	3.9	56.0
918	1NJT	F	Ala564	HA	2.386	10.6	83.7
919	1NJT	B	Ser432	OG	2.941	1.6	56.5
920	1NJT	B	Cys461	HG	2.519	5.6	141.1
921	1NJT	F	Ala564	C	2.378	25.0	37.6

922	1NJT	F	Ala564	O	2.728	8.8	61.6
923	1NJT	B	His363	CD2	3.078	2.9	134.7
924	1NJT	B	His363	NE2	2.874	4.8	117.0
925	1NJT	B	His363	HE2	2.315	13.3	98.9
926	1NJT	B	Ser432	OG	2.811	6.0	61.6
927	1NJT	F	Ala564	CA	3.038	4.2	56.7
928	1NJT	F	Ala564	C	2.396	24.4	36.8
929	1NJT	C	Arg1165	CG	3.140	0.9	155.3
930	1NJT	C	Arg1165	HG3	2.148	19.5	160.3
931	1NJT	G	Ala1264	CA	2.971	6.3	60.1
932	1NJT	G	Ala1264	C	2.418	23.7	36.4
933	1NJT	G	Ala1264	O	2.861	4.3	57.1
934	1NJT	G	Ala1264	HA	2.504	6.2	80.1
935	1NJT	C	Ser1132	CB	3.134	1.1	83.2
936	1NJT	C	Ser1132	OG	2.900	3.0	58.2
937	1NJT	C	Cys1161	HG	2.553	4.4	135.5
938	1NJT	G	Ala1264	C	2.412	23.9	36.7
939	1NJT	G	Ala1264	O	2.841	5.0	57.9
940	1NJT	C	His1063	CD2	3.077	2.9	130.8
941	1NJT	C	His1063	NE2	2.786	7.7	116.4
942	1NJT	C	His1063	HE2	2.182	18.3	98.8
943	1NJT	C	Ser1132	OG	2.831	5.3	60.8
944	1NJT	G	Ala1264	N	3.019	0.0	87.8
945	1NJT	G	Ala1264	CA	2.963	6.5	60.4
946	1NJT	G	Ala1264	C	2.376	25.1	37.9
947	1NJT	D	Arg1465	HG3	2.176	18.5	150.7
948	1NJT	H	Ala1564	CA	3.015	4.9	58.2
949	1NJT	H	Ala1564	C	2.483	21.7	33.8
950	1NJT	H	Ala1564	O	2.981	0.3	52.8
951	1NJT	H	Ala1564	HA	2.540	4.9	78.4
952	1NJT	D	Ser1432	CB	3.145	0.8	83.8
953	1NJT	D	Ser1432	OG	2.891	3.3	58.5
954	1NJT	D	Cys1461	HG	2.638	1.2	138.1
955	1NJT	H	Ala1564	C	2.393	24.5	37.6
956	1NJT	H	Ala1564	O	2.809	6.0	59.5
957	1NJT	D	His1363	CD2	3.032	4.3	134.9
958	1NJT	D	His1363	NE2	2.752	8.9	120.0
959	1NJT	D	His1363	HE2	2.173	18.6	101.5
960	1NJT	D	Ser1432	OG	2.760	7.7	63.5
961	1NJT	H	Ala1564	N	3.005	0.5	87.8
962	1NJT	H	Ala1564	CA	2.969	6.3	60.0
963	1NJT	H	Ala1564	C	2.355	25.7	38.9
964	1NKK	A	Arg165	CG	3.000	5.4	162.6
965	1NKK	A	Arg165	H	2.582	3.3	115.1

966	1NKK	A	Arg165	HG3	1.902	28.8	162.1
967	1NKK	E	Ala264	CA	2.916	8.0	62.6
968	1NKK	E	Ala264	C	2.325	26.7	39.4
969	1NKK	E	Ala264	O	2.719	9.1	62.1
970	1NKK	E	Ala264	HA	2.462	7.8	81.6
971	1NKK	A	Ser132	CB	3.039	4.1	84.2
972	1NKK	A	Ser132	OG	2.860	4.3	58.3
973	1NKK	A	Ser132	HB2	2.560	4.1	93.6
974	1NKK	A	Cys161	HG	2.437	8.7	133.2
975	1NKK	E	Ala264	C	2.398	24.3	36.6
976	1NKK	E	Ala264	O	2.825	5.5	58.0
977	1NKK	A	His63	CD2	3.120	1.6	120.6
978	1NKK	A	His63	NE2	2.985	1.1	106.6
979	1NKK	A	His63	HE2	2.402	10.0	91.9
980	1NKK	A	Ser132	OG	2.901	3.0	56.7
981	1NKK	E	Ala264	CA	2.987	5.8	59.8
982	1NKK	E	Ala264	C	2.417	23.8	35.7
983	1NKK	B	Arg465	CG	3.135	1.1	145.7
984	1NKK	B	Arg465	HG3	2.082	22.0	147.7
985	1NKK	F	Ala564	CA	2.891	8.8	63.5
986	1NKK	F	Ala564	C	2.458	22.5	34.3
987	1NKK	F	Ala564	HA	2.343	12.2	84.6
988	1NKK	B	Ser432	CB	3.140	0.9	80.3
989	1NKK	B	Ser432	HB2	2.525	5.4	94.3
990	1NKK	B	Cys461	HG	2.429	9.0	143.5
991	1NKK	B	Gly464	HA2	2.555	4.3	116.0
992	1NKK	F	Ala564	C	2.369	25.3	38.2
993	1NKK	F	Ala564	O	2.646	11.5	65.5
994	1NKK	B	His363	CD2	3.072	3.1	148.1
995	1NKK	B	His363	NE2	2.943	2.6	125.1
996	1NKK	B	His363	HD2	2.605	2.4	158.4
997	1NKK	B	His363	HE2	2.328	12.8	108.2
998	1NKK	B	Ser432	OG	2.650	11.4	67.2
999	1NKK	F	Ala564	CA	3.116	1.7	54.6
1000	1NKK	F	Ala564	C	2.356	25.7	38.6
1001	1NKK	C	Arg1165	CG	3.054	3.6	167.5
1002	1NKK	C	Arg1165	HG3	2.124	20.4	178.5
1003	1NKK	G	Ala1264	CA	2.780	12.3	67.6
1004	1NKK	G	Ala1264	C	2.269	28.4	41.6
1005	1NKK	G	Ala1264	O	2.687	10.1	62.6
1006	1NKK	G	Ala1264	HA	2.283	14.5	87.0
1007	1NKK	C	Ser1132	CB	3.125	1.4	81.3
1008	1NKK	C	Ser1132	OG	2.978	0.4	55.0
1009	1NKK	C	Ser1132	HB2	2.563	4.0	93.0

1010	1NKK	C	Cys1161	HG	2.368	11.3	144.0
1011	1NKK	G	Ala1264	C	2.415	23.8	35.9
1012	1NKK	G	Ala1264	O	2.762	7.6	59.8
1013	1NKK	C	His1063	CD2	3.126	1.4	126.9
1014	1NKK	C	His1063	NE2	2.947	2.4	106.5
1015	1NKK	C	His1063	HE2	2.329	12.8	89.8
1016	1NKK	C	Ser1132	OG	2.959	1.0	55.8
1017	1NKK	G	Ala1264	CA	3.064	3.3	56.5
1018	1NKK	G	Ala1264	C	2.462	22.3	34.0
1019	1NKK	D	Arg1465	CG	3.144	0.8	143.7
1020	1NKK	D	Arg1465	HG3	2.183	18.3	145.9
1021	1NKK	H	Ala1564	CA	3.079	2.9	54.9
1022	1NKK	H	Ala1564	C	2.396	24.4	36.9
1023	1NKK	H	Ala1564	O	2.749	8.1	62.4
1024	1NKK	D	His1363	HE2	2.565	3.9	74.4
1025	1NKK	D	Ser1432	CB	2.996	5.5	89.3
1026	1NKK	D	Ser1432	OG	2.705	9.5	64.6
1027	1NKK	D	Ser1432	HB2	2.658	0.4	94.7
1028	1NKK	D	Cys1461	HG	2.592	2.9	132.1
1029	1NKK	H	Ala1564	C	2.355	25.7	38.4
1030	1NKK	H	Ala1564	O	2.918	2.4	55.9
1031	1NKK	D	His1363	NE2	2.973	1.5	98.0
1032	1NKK	D	His1363	HE2	2.377	11.0	81.7
1033	1NKK	D	Ser1432	OG	2.977	0.4	54.1
1034	1NKK	H	Ala1564	N	2.957	2.1	88.7
1035	1NKK	H	Ala1564	CA	2.873	9.4	63.0
1036	1NKK	H	Ala1564	C	2.420	23.7	36.0
1037	1NMX	A	Tyr151	HD1	2.412	9.7	127.3
1038	1NMY	A	Tyr151	HD1	2.435	8.8	120.2
1039	1NMY	A	Tyr151	HD1	2.410	9.8	125.7
1040	1O2O	A	Ser190	OG	2.850	4.7	109.1
1041	1O2O	A	Ser190	HG	2.325	12.9	107.1
1042	1O2R	A	Ser190	HG	2.532	5.2	91.9
1043	1O3M	A	Gln192	CD	3.035	4.3	117.4
1044	1O3M	A	Gln192	NE2	2.643	12.5	95.0
1045	1O3M	A	Gln192	NE2	2.606	13.7	96.9
1046	1O3N	A	Gln192	CD	3.052	3.7	114.3
1047	1O3N	A	Gln192	NE2	2.483	17.8	92.3
1048	1O3N	A	Gln192	NE2	2.518	16.6	90.7
1049	1O3O	A	Ser195	HG	2.640	1.1	154.4
1050	1O5C	B	Ala190	CB	3.168	0.1	136.8
1051	1O5C	B	Ala190	HB3	2.529	5.3	137.2
1052	1O5C	B	Val213	CG1	2.696	14.9	123.2
1053	1O5D	H	Ser190	OG	2.586	13.5	119.2

1054	1O5D	H	Ser190	HG	1.798	32.6	110.4
1055	1O5F	H	Ala190	CB	2.971	6.3	144.3
1056	1O5F	H	Ala190	HB2	2.336	12.5	145.0
1057	1O5F	H	Val213	CG1	2.924	7.8	116.9
1058	1O5G	H	Ala190	HB1	2.583	3.2	110.4
1059	1O5G	H	Val213	CG1	2.919	7.9	119.6
1060	1O28	A	Arg90	HD3	2.368	11.3	95.9
1061	1O28	A	Tyr91	HE1	2.488	6.8	142.1
1062	1O28	B	Arg90	HD3	2.449	8.3	93.0
1063	1O28	B	Tyr91	HE1	2.328	12.8	138.6
1064	1O28	C	Arg90	HD3	2.240	16.1	106.7
1065	1O28	C	Tyr91	HE1	2.557	4.2	148.1
1066	1O28	D	Arg90	CD	3.079	2.9	107.8
1067	1O28	D	Arg90	HD3	2.225	16.7	98.4
1068	1O28	D	Tyr91	HE1	2.349	12.0	143.7
1069	1O29	A	Arg90	CG	3.116	1.7	134.8
1070	1O29	A	Arg90	CD	2.982	5.9	111.5
1071	1O29	A	Arg90	HD3	2.120	20.6	101.8
1072	1O29	B	Arg90	CD	3.116	1.7	106.5
1073	1O29	B	Arg90	HD3	2.100	21.3	109.6
1074	1O29	C	Arg90	CG	3.141	0.9	135.1
1075	1O29	C	Arg90	CD	3.059	3.5	111.6
1076	1O29	C	Arg90	HD3	2.210	17.2	101.0
1077	1O29	D	Arg90	CD	3.110	1.9	112.8
1078	1O29	D	Arg90	HD3	2.226	16.6	103.0
1079	1O30	A	Gly193	H	2.632	1.4	170.2
1080	1O30	A	Ser195	OG	2.945	1.5	123.3
1081	1O30	A	Ser195	HG	2.298	13.9	111.2
1082	1O46	A	Ser36	OG	2.830	5.3	147.9
1083	1O47	A	Cys44	CB	3.085	2.7	151.7
1084	1O47	A	Cys44	HB2	2.029	24.0	158.5
1085	1O47	A	Ser36	OG	2.816	5.8	129.0
1086	1OD1	A	Gly37	HA3	2.627	1.6	131.8
1087	1OD1	A	Asp219	OD2	2.973	0.6	110.8
1088	1OIN	A	His121	NE2	2.936	2.8	126.9
1089	1OIN	A	His121	HE2	2.313	13.4	109.7
1090	1OIN	A	Asn165	ND2	2.886	4.4	129.8
1091	1OIN	A	Glu351	OE2	2.719	9.1	62.7
1092	1OIN	B	His121	CE1	3.147	0.7	143.6
1093	1OIN	B	His121	NE2	2.917	3.4	125.4
1094	1OIN	B	His121	HE2	2.316	13.2	107.8
1095	1OIN	B	Asn165	ND2	2.999	0.7	134.5
1096	1OIN	B	Glu351	OE2	2.650	11.4	64.3
1097	1OL1	D	Leu214	HB2	2.498	6.4	134.7

1098	1OL1	H	Leu502	CD1	2.959	6.6	109.3
1099	1OUK	A	Lys53	HE2	2.433	8.9	135.6
1100	1OUY	A	Leu104	HB3	2.423	9.3	109.1
1101	1OUY	A	Lys53	HB2	2.589	3.0	82.2
1102	1OVE	A	Leu104	CB	3.112	1.8	136.2
1103	1OVE	A	Leu104	HB3	2.467	7.6	153.0
1104	1OWZ	A	Leu84	HB3	2.621	1.8	115.5
1105	1OWZ	A	Tyr88	HB2	2.503	6.3	121.6
1106	1OYT	H	Asn98	CA	3.155	0.5	147.1
1107	1OYT	H	Asn98	HA	2.104	21.2	153.0
1108	1OZ1	A	Leu104	HB3	2.436	8.8	119.6
1109	1P2A	A	Asp145	CG	2.864	9.6	149.8
1110	1P2A	A	Asp145	OD2	2.794	6.6	150.2
1111	1P2S	A	Arg97	NE	2.843	5.9	87.2
1112	1P2S	A	Arg97	CZ	2.798	11.7	106.9
1113	1P2S	A	Arg97	NH2	2.688	11.0	101.2
1114	1P2S	A	Arg97	HH21	2.577	3.5	80.8
1115	1P2S	A	Lys101	HD3	2.603	2.5	67.5
1116	1P2S	A	Lys101	CD	2.746	13.4	108.6
1117	1P2S	A	Lys101	HD3	1.693	36.6	105.6
1118	1P2S	A	Lys101	HZ3	2.423	9.2	83.8
1119	1P2S	A	Arg97	NE	2.561	15.2	100.2
1120	1P2S	A	Arg97	HE	1.907	28.6	100.6
1121	1P2S	A	Lys101	CE	3.045	3.9	110.6
1122	1P2S	A	Lys101	NZ	2.720	9.9	117.0
1123	1P2S	A	Lys101	HD3	2.633	1.4	66.5
1124	1P2S	A	Lys101	HZ3	1.885	29.4	109.8
1125	1P62	B	Arg128	HH12	2.302	13.8	147.0
1126	1P62	B	Tyr86	OH	2.818	5.8	118.4
1127	1P93	B	Phe623	HE1	2.293	14.1	153.9
1128	1P93	C	Phe623	HE1	2.511	6.0	159.8
1129	1P93	D	Phe623	CE1	3.077	2.9	157.8
1130	1P93	D	Phe623	HE1	2.074	22.3	152.5
1131	1PFV	A	Leu13	HG	2.583	3.3	98.2
1132	1PFV	A	Ala256	C	3.130	1.3	116.9
1133	1PFV	A	Ala256	HB1	2.448	8.3	120.6
1134	1PFV	A	Trp253	HZ3	2.477	7.2	135.4
1135	1PFW	A	Pro257	HA	2.654	0.6	110.5
1136	1PFW	A	Tyr260	CE1	3.155	0.5	152.7
1137	1PFW	A	Ala256	C	3.154	0.5	119.7
1138	1PFW	A	Ala256	HB1	2.500	6.4	106.6
1139	1PHQ	A	Arg168	CB	3.154	0.5	107.9
1140	1PHQ	A	Arg168	CG	2.959	6.7	96.5
1141	1PHQ	A	Arg168	NE	2.511	16.8	124.1

1142	1PHQ	A	Arg168	CZ	2.447	22.8	153.1
1143	1PHQ	A	Arg168	NH1	3.015	0.2	166.1
1144	1PHQ	A	Arg168	NH2	2.800	7.3	142.1
1145	1PHQ	A	Arg168	HG2	2.343	12.3	76.8
1146	1PKE	C	Met180	HG3	2.667	0.1	98.6
1147	1PQ6	A	His435	HE2	2.551	4.5	137.5
1148	1PQ9	A	Leu345	CD2	2.983	5.9	153.1
1149	1PQ9	A	Phe349	HE2	2.624	1.7	126.6
1150	1PQ9	A	Leu442	CD1	3.026	4.5	129.9
1151	1PQ9	A	Thr316	HG1	2.490	6.8	88.8
1152	1PQ9	A	Thr316	HG1	2.641	1.1	82.7
1153	1PQ9	A	Phe349	HZ	2.602	2.6	175.7
1154	1PQ9	B	His435	CD2	3.121	1.6	131.0
1155	1PQ9	B	His435	HD2	2.434	8.8	148.8
1156	1PQ9	B	Leu442	CD1	2.924	7.8	120.7
1157	1PQ9	B	Leu449	CD2	3.086	2.7	136.0
1158	1PQ9	B	Thr316	HG1	2.410	9.7	79.0
1159	1PQ9	B	Thr316	HG1	2.281	14.6	84.0
1160	1PQ9	C	His435	CD2	3.029	4.4	134.6
1161	1PQ9	C	His435	NE2	3.011	0.3	108.4
1162	1PQ9	C	His435	HD2	2.489	6.8	153.5
1163	1PQ9	C	His435	HE2	2.475	7.3	90.8
1164	1PQ9	C	Leu442	CD1	3.106	2.0	129.7
1165	1PQ9	C	Thr316	HG1	2.495	6.6	77.5
1166	1PQ9	C	Ile353	CG2	3.032	4.4	157.8
1167	1PQ9	C	Thr316	HG1	2.336	12.5	83.4
1168	1PQ9	D	Gln438	HG2	2.625	1.7	125.2
1169	1PQ9	D	Leu449	CD2	2.941	7.2	148.5
1170	1PQ9	D	Thr316	HG1	2.536	5.0	73.5
1171	1PQ9	D	Leu313	HA	2.556	4.3	128.5
1172	1PQ9	D	Thr316	HG1	2.287	14.3	83.2
1173	1PQC	A	Thr316	HG1	2.492	6.7	86.9
1174	1PQC	A	Phe349	HZ	2.618	1.9	170.8
1175	1PQC	A	Leu442	CD1	2.928	7.6	138.9
1176	1PQC	A	Phe349	HE2	2.643	1.0	128.8
1177	1PQC	A	His435	HD2	2.650	0.8	141.5
1178	1PQC	A	Gln438	HG2	2.621	1.8	120.0
1179	1PQC	A	Leu345	CD2	3.016	4.8	153.8
1180	1PQC	B	Thr316	HG1	2.354	11.8	80.0
1181	1PQC	B	Leu313	HA	2.655	0.6	126.3
1182	1PQC	B	Thr316	HG1	2.384	10.7	78.6
1183	1PQC	B	Phe349	HZ	2.589	3.0	169.8
1184	1PQC	B	Leu442	CD1	2.994	5.5	119.7
1185	1PQC	B	His435	HD2	2.550	4.5	136.0

1186	1PQC	B	Leu449	CD2	3.037	4.2	127.7
1187	1PQC	C	Thr316	HG1	2.561	4.1	71.1
1188	1PQC	C	Thr316	HG1	2.244	16.0	83.5
1189	1PQC	C	Leu442	CD1	3.129	1.3	131.2
1190	1PQC	C	His435	CD2	3.000	5.4	135.0
1191	1PQC	C	His435	NE2	2.956	2.1	108.4
1192	1PQC	C	His435	HD2	2.501	6.3	153.7
1193	1PQC	C	His435	HE2	2.417	9.5	90.6
1194	1PQC	C	Trp457	HZ3	2.629	1.5	134.2
1195	1PQC	C	Phe268	HE1	2.433	8.9	141.0
1196	1PQC	D	Phe349	HZ	2.602	2.5	166.4
1197	1PQC	D	Thr316	HG1	2.172	18.6	79.5
1198	1PQC	D	Thr316	HG1	2.400	10.1	70.8
1199	1PQC	D	His435	CD2	3.042	4.0	129.5
1200	1PQC	D	His435	HD2	2.579	3.4	148.0
1201	1PQC	D	His435	HE2	2.623	1.7	88.0
1202	1PQC	D	Leu449	CD2	3.132	1.2	149.9
1203	1PWL	A	Ala299	CA	3.042	4.0	163.4
1204	1PWL	A	Ala299	C	2.955	6.8	137.6
1205	1PXH	A	Asp181	HB2	2.611	2.2	169.7
1206	1PXH	A	Gly220	HA3	2.654	0.6	125.0
1207	1PXH	A	Gln262	HG3	2.343	12.2	143.4
1208	1PXH	A	Arg47	HD3	2.446	8.4	110.5
1209	1PXL	A	Lys89	CE	3.056	3.6	121.0
1210	1PXL	A	Lys89	HB2	2.401	10.1	157.5
1211	1PXL	A	Lys89	HE3	2.366	11.4	102.7
1212	1PYE	A	Lys33	CD	3.024	4.6	131.2
1213	1PYE	A	Lys33	HD2	1.977	25.9	129.1
1214	1PYE	A	Ala144	CB	3.140	1.0	120.2
1215	1PYE	A	Ala144	HB3	2.495	6.5	132.2
1216	1Q6J	A	Gln262	HG3	2.440	8.6	141.6
1217	1Q6J	A	Gly259	HA3	2.486	6.9	150.5
1218	1Q6M	A	Gln262	HG3	2.603	2.5	139.8
1219	1Q6M	A	Gly259	HA3	2.503	6.2	156.9
1220	1Q6M	A	Ser118	HB3	2.105	21.2	140.6
1221	1Q6N	A	Gln762	HG3	2.557	4.2	137.6
1222	1Q6N	B	Gln1262	HG3	2.377	11.0	139.0
1223	1Q6P	B	Gln1262	HG3	2.632	1.4	139.0
1224	1Q6S	A	Gly720	HA3	2.669	0.1	118.5
1225	1Q6S	A	Gln762	HG3	2.335	12.6	133.1
1226	1Q6S	B	Gly1220	HA3	2.505	6.2	118.3
1227	1Q6S	B	Gln1262	HG3	2.422	9.3	132.7
1228	1Q6T	A	Asp681	HB2	2.515	5.8	170.5
1229	1Q6T	A	Gln762	HG3	2.610	2.2	137.7

1230	1Q6T	B	Phe1182	H	2.657	0.5	124.4
1231	1Q6T	B	Gln1262	HG3	2.448	8.3	134.3
1232	1QB1	A	Gln180	CG	2.635	16.9	125.4
1233	1QB1	A	Gln180	CD	2.893	8.7	145.3
1234	1QB1	A	Gln180	HG2	2.438	8.7	102.5
1235	1QB1	A	Gln180	HG3	2.316	13.3	126.5
1236	1QB6	A	Gln180	CD	2.905	8.4	148.2
1237	1QB6	A	Gln180	OE1	2.504	16.3	130.8
1238	1QH6	A	Glu94	CD	3.022	4.7	86.4
1239	1QH6	A	Glu94	OE1	2.814	5.9	100.5
1240	1QH6	A	Glu94	OE2	2.742	8.3	63.4
1241	1QH6	A	Arg129	NE	2.949	2.4	107.9
1242	1QH6	A	Arg129	HE	2.281	14.6	110.3
1243	1QH6	A	Phe141	HZ	2.646	0.9	110.8
1244	1QH6	B	Glu94	CD	3.161	0.3	82.0
1245	1QH6	B	Glu94	OE1	2.931	2.0	97.6
1246	1QH6	B	Glu94	OE2	2.870	4.0	59.1
1247	1QH6	B	Arg129	NE	2.685	11.1	123.8
1248	1QH6	B	Arg129	HE	1.861	30.3	128.8
1249	1QH6	B	Phe141	HE2	2.667	0.1	134.9
1250	1QH6	B	Phe141	HZ	2.486	6.9	110.4
1251	1QI2	A	Asn138	ND2	2.861	5.3	145.4
1252	1QI2	A	Glu228	OE2	2.680	10.4	65.8
1253	1QV6	A	Ser48	HB3	2.575	3.6	118.4
1254	1QV6	B	Ser48	HB3	2.505	6.2	120.0
1255	1QWN	A	Phe206	CE1	3.165	0.2	121.3
1256	1QWN	A	Phe206	HE1	2.665	0.2	105.8
1257	1QWU	A	Phe206	CE1	3.150	0.6	119.1
1258	1QWU	A	Phe206	HE1	2.611	2.2	106.1
1259	1R0E	A	Gly63	CA	3.107	2.0	122.7
1260	1R0E	A	Gly63	HA3	2.026	24.1	124.4
1261	1R0E	A	Val70	HB	2.572	3.7	112.6
1262	1R0E	B	Gly63	CA	3.073	3.1	121.9
1263	1R0E	B	Gly63	HA3	1.989	25.5	124.4
1264	1R0E	B	Val70	HB	2.613	2.1	113.0
1265	1RAK	A	Ser314	OG	2.979	0.4	169.9
1266	1RBM	A	Met89	HE1	2.446	8.4	108.6
1267	1RBM	A	His108	HD1	2.567	3.8	97.1
1268	1RBQ	A	Met89	HE1	2.383	10.8	104.6
1269	1RBQ	A	Ser118	HA	2.595	2.8	110.7
1270	1RBQ	A	Pro109	HD2	2.565	3.9	157.6
1271	1RBQ	B	Met89	HE1	2.313	13.4	103.3
1272	1RBQ	B	Ser118	HA	2.665	0.2	106.1
1273	1RBQ	C	Met89	HE1	2.281	14.6	96.4

1274	1RBQ	C	Met89	HE1	2.340	12.4	95.7
1275	1RBQ	D	Met89	HE1	2.377	11.0	97.8
1276	1RBQ	D	Met89	HE1	2.441	8.6	96.5
1277	1RBY	A	Ser118	HA	2.588	3.1	109.9
1278	1RBY	B	Met89	HE1	2.564	4.0	103.1
1279	1RBY	B	His108	HD1	2.650	0.8	96.9
1280	1RBY	C	Met89	HE1	2.285	14.4	99.7
1281	1RBY	C	Met89	HE1	2.552	4.4	89.5
1282	1RBY	D	Met89	HE1	2.250	15.7	99.3
1283	1RBY	D	Met89	HE1	2.445	8.4	92.3
1284	1RBY	D	Pro109	HD3	2.637	1.3	164.1
1285	1RBZ	A	Met89	CE	3.159	0.3	111.6
1286	1RBZ	A	Met89	HE1	2.258	15.4	104.6
1287	1RBZ	A	His108	HD1	2.666	0.2	94.4
1288	1RBZ	A	Pro109	HD2	2.523	5.5	159.2
1289	1RBZ	B	Met89	HE1	2.236	16.2	96.1
1290	1RBZ	B	Met89	HE1	2.253	15.6	98.6
1291	1RBZ	B	Pro109	HD2	2.660	0.4	156.1
1292	1RC0	A	Met89	HE1	2.484	7.0	97.7
1293	1RC0	A	Met89	HE1	2.611	2.2	93.4
1294	1RC0	B	Met89	HE1	2.304	13.7	100.8
1295	1RC0	B	Ser118	HA	2.639	1.2	107.2
1296	1RC0	B	Met89	HE1	2.649	0.8	87.2
1297	1RC1	A	Met89	HE1	2.391	10.4	105.4
1298	1RC1	A	Pro109	HD2	2.665	0.2	157.0
1299	1RF4	A	Arg120	HH22	2.608	2.3	85.0
1300	1RF4	A	Glu340	HG3	2.401	10.1	168.5
1301	1RF4	D	Lys339	CD	3.162	0.3	140.6
1302	1RF4	D	Lys339	HD2	2.074	22.3	136.9
1303	1RHR	A	Met176	HE1	2.383	10.8	92.6
1304	1RJW	B	Pro215	HB2	2.660	0.4	105.6
1305	1RJW	B	Pro242	CB	3.072	3.1	159.5
1306	1RJW	B	Pro242	HB2	2.018	24.4	152.9
1307	1RJW	C	Thr40	OG1	2.978	0.4	101.2
1308	1RJW	C	Thr40	HG1	2.308	13.6	85.1
1309	1RJW	C	Ile285	CD1	3.010	5.0	157.4
1310	1RJW	C	Trp87	NE1	2.994	0.9	146.9
1311	1RJW	C	Trp87	CE2	2.969	6.3	126.7
1312	1RJW	C	Tyr171	HD2	2.612	2.2	125.5
1313	1RJW	C	Pro242	HB2	2.487	6.9	109.9
1314	1RJW	D	Ile285	CD1	2.968	6.4	139.2
1315	1RJW	D	Ser246	HB2	2.314	13.4	129.1
1316	1RJW	D	Ala220	H	2.655	0.6	101.1
1317	1RJW	D	Ala220	HB3	2.503	6.3	137.6

1318	1RJW	D	Ala221	H	2.306	13.7	144.0
1319	1RJW	D	Ser246	OG	2.859	4.4	116.6
1320	1RJW	D	Asp195	HA	2.495	6.6	103.8
1321	1RJW	D	Pro215	HG2	2.360	11.6	134.5
1322	1RJW	D	Pro264	CG	3.027	4.5	140.9
1323	1RJW	D	Pro264	CD	2.915	8.0	113.8
1324	1RJW	D	Pro264	HG3	2.422	9.3	145.9
1325	1RJW	D	Pro264	HD3	2.084	21.9	99.3
1326	1RJW	D	Trp49	HE1	2.497	6.5	146.0
1327	1RJW	D	His43	CE1	2.928	7.6	104.3
1328	1RJW	D	His43	HE1	2.472	7.4	111.5
1329	1RO7	A	His188	NE2	2.840	5.9	120.7
1330	1RO7	A	His188	HE2	1.992	25.4	132.7
1331	1RO7	B	His188	NE2	2.879	4.7	154.2
1332	1RO7	C	His188	CE1	3.134	1.1	114.7
1333	1RO7	C	His188	HE1	2.556	4.3	105.1
1334	1RO7	D	His188	NE2	2.965	1.8	149.6
1335	1RQR	A	Phe156	HA	2.608	2.3	74.6
1336	1RQR	A	Phe156	HD1	2.630	1.5	117.9
1337	1RQR	A	Ser158	N	2.911	3.6	146.2
1338	1RQR	A	Ser158	CB	3.027	4.5	153.9
1339	1RQR	A	Ser158	H	1.953	26.9	139.5
1340	1RQR	A	Ser158	HB2	2.395	10.3	152.2
1341	1RQR	B	Phe156	HD1	2.634	1.3	100.1
1342	1RQR	B	Ser158	N	2.708	10.3	166.7
1343	1RQR	B	Ser158	CB	3.014	4.9	140.7
1344	1RQR	B	Ser158	H	1.764	33.9	158.7
1345	1RQR	B	Ser158	HB2	2.303	13.7	128.0
1346	1RQR	C	Phe156	HA	2.519	5.7	75.0
1347	1RQR	C	Phe156	HD1	2.398	10.2	112.4
1348	1RQR	C	Ser158	N	2.852	5.6	157.3
1349	1RQR	C	Ser158	CB	3.118	1.6	148.8
1350	1RQR	C	Ser158	OG	2.867	4.1	127.9
1351	1RQR	C	Ser158	H	1.878	29.7	151.7
1352	1RQR	C	Ser158	HB2	2.659	0.4	142.6
1353	1RW8	A	His283	N	2.940	2.6	135.9
1354	1RW8	A	His283	H	1.941	27.3	136.1
1355	1RXC	B	Ile220	CG1	3.046	3.9	136.8
1356	1RXC	B	Ile220	CD1	3.165	0.2	122.5
1357	1RXC	C	Pro229	HG3	2.621	1.8	141.7
1358	1RXC	D	Pro229	HG3	2.634	1.3	143.3
1359	1RXC	E	Ile220	CG1	3.125	1.4	128.8
1360	1RXC	E	Pro229	HG3	2.596	2.8	136.6
1361	1RXC	F	Ile220	CG1	3.159	0.3	128.9

1362	1RXC	I	Val221	CG1	3.140	0.9	132.1
1363	1RXC	K	Ile220	CG1	3.168	0.1	132.5
1364	1S2C	A	Tyr216	OH	2.933	1.9	141.5
1365	1S2C	A	Asn167	CG	3.142	0.9	113.0
1366	1S2C	A	Met120	HE1	2.517	5.7	107.1
1367	1S2C	A	Leu261	O	2.878	3.7	138.9
1368	1S2C	A	Gln262	HA	2.345	12.2	137.8
1369	1S2C	A	Gln6	CG	3.082	2.8	136.1
1370	1S2C	A	Gln6	HG2	2.653	0.6	142.5
1371	1S2C	A	Gln6	HG3	2.521	5.6	126.1
1372	1S2C	A	Arg258	CZ	2.786	12.1	146.2
1373	1S2C	A	Arg258	NH2	2.476	18.0	119.9
1374	1S2C	A	Arg258	HH21	2.662	0.3	113.2
1375	1S9J	A	Val211	H	2.650	0.8	118.0
1376	1S9J	A	Ser212	H	2.528	5.3	162.8
1377	1S9J	A	Leu115	CD2	3.053	3.7	148.0
1378	1S9J	A	Lys97	HD2	2.584	3.2	148.8
1379	1SBY	A	Leu188	CD2	3.043	4.0	148.8
1380	1SBY	A	Tyr151	CE2	2.796	11.8	125.6
1381	1SBY	A	Tyr151	HE2	2.554	4.4	109.0
1382	1SBY	B	Tyr151	CE2	3.033	4.3	120.3
1383	1SBY	B	Tyr151	HE2	2.628	1.6	108.0
1384	1SEZ	A	Ala174	O	2.953	1.2	101.8
1385	1SEZ	A	Gly370	C	3.067	3.3	148.7
1386	1SEZ	B	Ala174	O	2.885	3.5	106.9
1387	1SEZ	B	Gly178	N	2.980	1.3	146.6
1388	1SEZ	B	Leu334	CD1	2.995	5.5	118.2
1389	1SEZ	B	Leu369	CD1	3.126	1.4	152.1
1390	1SEZ	B	Gly370	C	2.952	6.9	151.7
1391	1SHL	B	Tyr223	HD2	2.642	1.1	105.0
1392	1SHL	A	Ile183	CD1	3.121	1.5	157.2
1393	1SHL	A	Phe221	CD2	3.000	5.4	98.9
1394	1SHL	A	Phe221	HD2	2.539	4.9	114.4
1395	1SL3	A	Glu217	CG	3.084	2.7	125.4
1396	1SL3	A	Glu217	HG2	2.329	12.8	108.4
1397	1SS9	A	Asn153	ND2	2.805	7.1	111.2
1398	1SS9	A	Cys246	SG	3.166	3.2	137.3
1399	1STD	A	Val108	CG1	3.112	1.8	98.6
1400	1STD	A	His110	HE2	2.599	2.7	149.2
1401	1SVH	A	Ser53	HB2	2.461	7.8	140.7
1402	1T40	A	Tyr309	HD1	2.420	9.4	141.2
1403	1T40	A	Val47	O	2.951	1.3	148.7
1404	1T40	A	Cys80	HG	2.230	16.5	133.7
1405	1T40	A	Tyr309	HE1	2.295	14.1	131.7

1406	1T41	A	Tyr309	HD1	2.483	7.0	142.1
1407	1T41	A	Tyr48	HD1	2.499	6.4	127.1
1408	1T41	A	Cys80	HG	2.227	16.6	133.8
1409	1T41	A	Phe115	HZ	2.653	0.7	83.7
1410	1T41	A	Leu300	H	2.463	7.8	119.1
1411	1T41	A	Tyr309	HE1	2.396	10.2	142.9
1412	1T47	B	Asn363	C	3.139	1.0	148.4
1413	1T47	B	Asn363	CB	3.163	0.2	110.4
1414	1TKX	A	Leu234	HB3	2.482	7.0	113.5
1415	1TLS	A	Tyr94	HH	2.441	8.6	154.3
1416	1TLS	A	Cys146	SG	2.980	8.9	71.3
1417	1TLS	B	Cys146	SG	3.091	5.5	67.5
1418	1TNH	A	Gln192	HA	2.591	2.9	110.7
1419	1TNH	A	Ser195	HG	2.616	2.0	127.7
1420	1TOU	A	Cys117	SG	3.200	2.1	119.2
1421	1TQF	A	Tyr14	HE1	2.495	6.6	141.7
1422	1TQF	A	Ala335	CB	3.075	3.0	114.0
1423	1TQF	A	Ala335	HB2	2.607	2.4	100.6
1424	1TSN	A	Tyr94	HH	2.492	6.7	143.0
1425	1TSN	A	Cys146	SG	3.166	3.2	72.3
1426	1TU6	A	Asp175	OD2	2.967	0.8	168.8
1427	1TV5	A	Gly535	HA2	2.487	6.9	119.7
1428	1TV5	A	Met536	HG3	2.295	14.1	121.8
1429	1TV5	A	Phe171	HE2	2.661	0.3	157.9
1430	1TV5	A	Met536	HE2	2.426	9.2	125.9
1431	1UDA	A	Thr126	CB	2.958	6.7	161.3
1432	1UDA	A	Thr126	HB	2.062	22.8	149.9
1433	1UDB	A	Val86	CG2	2.820	11.0	138.4
1434	1UDB	A	Tyr149	CD2	3.164	0.2	141.7
1435	1UDB	A	Tyr149	CE2	3.103	2.1	124.6
1436	1UDB	A	Tyr149	HD2	2.570	3.7	140.4
1437	1UDB	A	Tyr149	HE2	2.442	8.5	106.8
1438	1UHL	B	Met298	O	2.882	3.6	170.2
1439	1UHL	B	Met298	HG3	2.667	0.1	114.7
1440	1UHL	B	Thr302	OG1	2.431	18.7	120.6
1441	1UHL	B	Thr302	HG1	1.606	39.8	104.2
1442	1UHL	B	Thr302	HG1	2.494	6.6	66.3
1443	1UHL	B	Ile339	CG2	2.983	5.9	131.7
1444	1UHL	B	His421	CD2	2.951	6.9	132.9
1445	1UHL	B	His421	NE2	2.789	7.6	114.5
1446	1UHL	B	His421	HE2	2.339	12.4	94.6
1447	1UHV	A	His54	HE2	2.636	1.3	103.7
1448	1UHV	A	Asn159	ND2	2.935	2.8	146.3
1449	1UHV	A	Glu277	OE1	2.931	2.0	60.8

1450	1UHV	B	Asn159	ND2	2.733	9.5	135.6
1451	1UHV	B	Glu277	OE1	2.914	2.6	61.1
1452	1UHV	C	His54	HE2	2.369	11.3	100.2
1453	1UHV	C	Asn159	ND2	2.878	4.7	141.2
1454	1UHV	C	Glu277	OE1	2.890	3.4	61.2
1455	1UHV	C	Glu277	OE2	2.927	2.1	106.1
1456	1UHV	D	His54	HE2	2.666	0.1	97.9
1457	1UHV	D	Asn159	ND2	2.909	3.7	132.0
1458	1UHV	D	Glu277	OE1	2.908	2.7	61.5
1459	1UK1	A	Ala898	N	2.799	7.3	126.3
1460	1UK1	A	Ala898	H	2.354	11.8	142.8
1461	1UK1	B	Phe897	C	3.100	2.2	104.5
1462	1UK1	B	Ala898	N	2.904	3.8	127.7
1463	1UK1	B	Ser904	HB3	2.624	1.7	133.0
1464	1UPF	D	Ala168	CB	3.038	4.2	119.0
1465	1UPF	D	Ala168	HB2	2.029	24.0	109.2
1466	1UPF	D	Tyr228	HA	2.599	2.6	88.0
1467	1UPF	D	Ile229	N	2.987	1.1	116.9
1468	1UPF	D	Ile229	CD1	2.956	6.7	102.1
1469	1UPF	D	Ile229	H	2.253	15.6	103.9
1470	1UPF	C	Ala168	CB	2.964	6.5	139.5
1471	1UPF	C	Ala168	HB2	1.980	25.8	129.4
1472	1UPF	B	Tyr227	O	2.792	6.6	140.7
1473	1UPF	B	Tyr228	CA	3.154	0.5	117.3
1474	1UPF	B	Tyr228	HA	2.134	20.1	109.9
1475	1UPF	B	Ile229	H	2.563	4.0	102.9
1476	1UPF	A	Ala168	CB	3.110	1.9	126.4
1477	1UPF	A	Ala168	HB2	2.296	14.0	116.1
1478	1UPV	A	Leu313	CD2	3.134	1.1	88.0
1479	1UPV	A	Leu313	CD2	2.959	6.6	95.7
1480	1UPV	A	Ile353	CG2	2.764	12.8	142.7
1481	1UPV	A	Thr316	HG1	2.210	17.2	110.3
1482	1UPV	A	Leu449	CD2	3.149	0.7	145.1
1483	1UPV	A	His435	HD2	2.583	3.3	136.0
1484	1UPW	A	Leu313	CD2	3.091	2.5	90.5
1485	1UPW	A	Leu313	CD2	3.008	5.1	94.2
1486	1UPW	A	Ile353	CG2	2.840	10.4	143.3
1487	1UPW	A	Thr316	HG1	2.301	13.8	111.1
1488	1UPW	A	Leu449	CD2	3.133	1.2	140.3
1489	1UQT	A	Trp85	HH2	2.634	1.3	137.6
1490	1UQT	B	Trp85	HH2	2.595	2.8	131.9
1491	1US0	A	Tyr48	HD1	2.489	6.8	118.1
1492	1US0	A	Ala299	CA	3.059	3.5	161.4
1493	1US0	A	Ala299	C	2.993	5.6	135.0

1494	1US0	A	Ala299	HA	2.604	2.5	153.2
1495	1UUO	A	Val134	CG1	3.086	2.7	150.7
1496	1UWH	A	Gly592	HA2	2.410	9.7	107.3
1497	1UWH	B	Gly592	HA2	2.134	20.1	109.8
1498	1UWR	A	His150	HE2	2.479	7.2	100.3
1499	1UWR	A	Asn205	ND2	2.905	3.8	156.6
1500	1UWR	A	Glu387	OE2	2.824	5.5	58.3
1501	1UWR	B	Glu387	OE2	2.694	9.9	63.5
1502	1UWS	B	His150	HE2	2.503	6.3	99.5
1503	1UWS	B	Asn205	ND2	2.913	3.6	140.8
1504	1UWS	B	Glu387	OE2	2.686	10.2	63.3
1505	1UWS	A	His150	HE2	2.616	2.0	98.1
1506	1UWS	A	Glu387	OE2	2.614	12.6	66.7
1507	1UYI	A	Gly97	H	2.564	4.0	135.5
1508	1UYK	A	Ile96	CG2	2.808	11.4	134.2
1509	1UYK	A	Gly97	N	2.640	12.6	150.3
1510	1UYK	A	Gly97	CA	2.950	6.9	128.7
1511	1UYK	A	Gly97	C	2.916	8.0	120.3
1512	1UYK	A	Gly97	O	2.579	13.7	122.4
1513	1UYK	A	Gly97	H	2.309	13.5	135.5
1514	1UYQ	A	Asn165	OD1	2.885	3.5	147.5
1515	1UYQ	A	Glu352	OE1	2.690	10.0	59.5
1516	1UYS	C	Trp1924	CE3	2.962	6.6	114.5
1517	1UYS	C	Trp1924	CZ3	3.052	3.7	140.9
1518	1UYS	C	Trp1924	CG	3.090	2.5	131.6
1519	1UYS	C	Trp1924	CD2	3.123	1.5	107.2
1520	1UYS	B	Trp1924	CB	3.149	0.7	153.7
1521	1V1J	A	Ala81	HB1	2.645	0.9	91.0
1522	1V1J	B	Ala81	HB1	2.633	1.4	90.0
1523	1V1J	C	Ala81	HB1	2.589	3.0	95.5
1524	1V1J	D	Ala81	HB1	2.466	7.6	95.9
1525	1V1J	F	Ala81	HB1	2.658	0.5	95.5
1526	1V1J	H	Ala81	HB1	2.586	3.2	94.5
1527	1V1J	I	Ala81	HB1	2.622	1.8	98.2
1528	1V1J	J	Ala81	HB1	2.653	0.7	93.4
1529	1V1J	K	Ala81	HB1	2.658	0.4	84.8
1530	1V1J	L	Ala81	HB1	2.556	4.3	91.9
1531	1V1K	A	Leu134	CD2	3.146	0.8	151.7
1532	1V1K	A	Val18	CG2	2.515	20.7	142.3
1533	1V1K	A	Gly11	HA3	2.491	6.7	168.7
1534	1V4S	A	Tyr214	CG	3.011	5.0	141.9
1535	1V4S	A	Tyr214	CD1	3.110	1.9	167.3
1536	1VSN	A	Asn158	HA	2.526	5.4	169.4
1537	1W3C	A	Lys136	HE2	2.578	3.4	94.5

1538	1W4Q	A	His12	CE1	2.688	15.2	119.0
1539	1W4Q	A	His12	NE2	2.801	7.2	126.3
1540	1W4Q	A	His12	HE1	2.064	22.7	110.4
1541	1W4Q	A	His12	HE2	2.364	11.5	127.5
1542	1W4Q	A	Lys41	NZ	2.759	8.6	136.4
1543	1W4Q	A	Lys41	HZ1	1.846	30.9	135.4
1544	1W4Q	B	His12	CE1	2.815	11.2	116.9
1545	1W4Q	B	His12	NE2	2.859	5.3	125.0
1546	1W4Q	B	His12	HE1	2.226	16.6	108.1
1547	1W4Q	B	His12	HE2	2.362	11.5	127.3
1548	1W4Q	B	Lys41	HZ1	2.221	16.8	118.9
1549	1W5V	A	Pro81	CG	2.958	6.7	106.8
1550	1W5V	A	Pro81	HG3	2.291	14.2	122.8
1551	1W5V	A	Gly49	HA2	2.640	1.1	87.2
1552	1W5V	B	Pro81	CG	3.162	0.3	119.1
1553	1W5V	B	Pro81	HG2	2.343	12.3	127.4
1554	1W5W	B	Arg8	NH2	2.970	1.6	113.6
1555	1W5W	B	Arg8	HH22	2.269	15.0	129.2
1556	1W5W	A	Arg8	HH22	2.565	3.9	106.6
1557	1W5W	A	Gly49	HA2	2.514	5.8	92.4
1558	1W5W	A	Ile50	CD1	3.008	5.1	136.0
1559	1W5X	B	Pro81	CB	3.104	2.1	109.5
1560	1W5X	B	Pro81	HB2	2.518	5.7	90.4
1561	1W5X	B	Pro81	HG2	2.650	0.8	122.1
1562	1W5X	A	Pro81	CG	3.045	3.9	107.3
1563	1W5X	A	Pro81	HG3	2.432	8.9	121.7
1564	1W5X	A	Gly49	HA2	2.555	4.3	90.6
1565	1W5X	A	Ile50	CD1	3.033	4.3	138.7
1566	1W5Y	B	Arg8	CZ	2.820	11.0	129.8
1567	1W5Y	A	Arg8	NE	2.859	5.3	153.9
1568	1W5Y	A	Arg8	CZ	2.646	16.5	126.4
1569	1W5Y	A	Arg8	NH1	2.974	1.5	112.0
1570	1W5Y	A	Ile50	CD1	3.128	1.3	137.9
1571	1W70	B	Ile170	CG1	3.076	3.0	101.5
1572	1W70	B	Ile170	CD1	2.987	5.8	129.7
1573	1W83	A	Glu71	HG3	2.221	16.8	104.8
1574	1WBT	A	Glu71	HG3	2.597	2.7	95.2
1575	1WRK	A	Met80	HG2	2.393	10.4	106.1
1576	1WRK	A	Met80	CE	3.148	0.7	149.0
1577	1WRK	A	Met80	HE3	2.174	18.6	154.7
1578	1WRK	A	Phe27	HZ	2.420	9.4	136.8
1579	1WRK	A	Met81	HE1	2.550	4.5	85.8
1580	1WRK	A	Met81	HE1	2.599	2.7	83.8
1581	1WRK	B	Phe27	CZ	3.039	4.1	142.2

1582	1WRK	B	Phe27	HE2	2.600	2.6	97.8
1583	1WRK	B	Phe27	HZ	2.266	15.1	159.1
1584	1WRK	B	Phe27	HE2	2.343	12.2	110.9
1585	1WRK	B	Phe77	HZ	2.519	5.7	124.6
1586	1WRK	B	Met81	CE	3.051	3.7	118.8
1587	1WRK	B	Met81	HE1	2.456	8.0	106.8
1588	1WRK	B	Met80	HG2	2.568	3.8	118.6
1589	1WRL	A	Met80	HG2	2.426	9.1	130.9
1590	1WRL	A	Met80	HE3	2.533	5.1	166.1
1591	1WRL	A	Phe27	CZ	3.108	2.0	137.6
1592	1WRL	A	Phe27	HZ	2.353	11.9	148.4
1593	1WRL	B	Phe27	CE2	3.069	3.2	125.0
1594	1WRL	B	Phe27	CZ	2.985	5.8	139.2
1595	1WRL	B	Phe27	HE2	2.560	4.1	106.0
1596	1WRL	B	Phe27	HZ	2.379	10.9	132.2
1597	1WRL	B	Phe27	HE2	2.644	1.0	101.0
1598	1WRL	B	Phe77	HZ	2.520	5.6	145.3
1599	1WRL	B	Met80	SD	3.065	6.3	158.8
1600	1WRL	B	Met80	HG2	2.587	3.1	114.6
1601	1WRL	C	Met80	CG	3.084	2.7	126.2
1602	1WRL	C	Met80	HG2	2.377	11.0	108.3
1603	1WRL	C	Met80	HE3	2.505	6.2	101.6
1604	1WRL	C	Met80	HG2	2.610	2.2	96.4
1605	1WRL	C	Met80	HE3	2.522	5.6	100.8
1606	1WRL	C	Phe27	CZ	3.084	2.7	124.0
1607	1WRL	C	Phe27	HZ	2.128	20.3	132.3
1608	1WRL	C	Phe27	HE2	2.378	11.0	129.2
1609	1WRL	D	Phe27	HZ	2.601	2.6	140.9
1610	1WRL	D	Phe77	HZ	2.559	4.1	140.1
1611	1WRL	D	Met81	SD	3.237	1.0	121.7
1612	1WRL	D	Ser84	HB2	2.383	10.8	131.7
1613	1WRL	D	Ser84	HG	2.592	2.9	131.3
1614	1WRL	D	Met80	HG2	2.234	16.3	129.7
1615	1WRL	E	Met80	HG2	2.184	18.2	133.9
1616	1WRL	E	Met80	HE3	2.280	14.6	146.1
1617	1WRL	E	Phe27	CZ	3.096	2.3	142.2
1618	1WRL	E	Phe27	HZ	2.364	11.5	144.4
1619	1WRL	E	Met81	HE1	2.667	0.1	91.5
1620	1WRL	F	Phe27	HZ	2.585	3.2	109.8
1621	1WRL	F	Phe77	HZ	2.665	0.2	132.3
1622	1WRL	F	Met80	SD	3.128	4.4	132.3
1623	1WRL	F	Met80	HG2	2.663	0.3	102.8
1624	1WRL	F	Met81	HE1	2.562	4.1	105.6
1625	1WW3	A	His377	HB2	2.445	8.4	118.9

1626	1WW3	A	Thr378	HB	2.467	7.6	118.0
1627	1WW3	A	Asn284	HA	2.505	6.2	171.6
1628	1X7A	C	Arg143	NH2	2.884	4.5	117.3
1629	1X7A	C	Arg143	HH22	2.463	7.7	100.0
1630	1X7A	C	Arg143	HH22	2.481	7.1	100.2
1631	1X7A	C	Gln192	NE2	2.877	4.7	148.4
1632	1X7A	C	Glu217	CA	3.054	3.7	120.2
1633	1X7A	C	Glu217	HA	2.066	22.6	120.5
1634	1X7A	C	Glu219	H	2.407	9.9	138.2
1635	1X7B	A	Leu339	O	2.885	3.5	131.5
1636	1X7B	A	Met340	HA	2.582	3.3	152.7
1637	1X7B	A	Leu343	HB2	2.443	8.5	132.7
1638	1X7B	B	Leu339	C	3.057	3.6	122.6
1639	1X7B	B	Leu339	O	2.799	6.4	133.3
1640	1X7B	B	Met340	HA	2.454	8.1	153.1
1641	1X7B	B	Leu343	CB	3.153	0.5	139.4
1642	1X7B	B	Leu343	HB2	2.358	11.7	127.3
1643	1X70	A	Tyr631	HD2	2.349	12.0	143.1
1644	1X70	A	Arg125	HH22	2.572	3.7	146.8
1645	1X70	A	Arg358	NE	2.978	1.4	114.7
1646	1X70	A	Arg358	HG2	2.624	1.7	102.4
1647	1X70	A	Arg358	HE	2.188	18.1	128.5
1648	1X70	A	Arg358	HG2	2.669	0.1	99.2
1649	1X70	A	Val656	CG2	3.068	3.2	145.8
1650	1X70	B	Tyr631	HD2	2.308	13.6	147.1
1651	1X70	B	Arg125	HH22	2.656	0.5	143.3
1652	1X70	B	Arg358	NE	2.839	6.0	108.0
1653	1X70	B	Arg358	HE	1.889	29.2	114.9
1654	1X70	B	Ser209	OG	2.888	3.4	139.2
1655	1X70	B	Ser209	HG	2.655	0.6	123.4
1656	1X70	B	Arg358	HG2	2.418	9.4	109.0
1657	1X70	B	Val656	CG2	3.081	2.8	149.7
1658	1XE5	A	Tyr77	CD1	3.125	1.4	129.0
1659	1XE5	B	Asn76	HB3	2.480	7.1	158.3
1660	1XE5	B	Gly216	O	2.850	4.7	121.8
1661	1XE5	B	Gly216	HA3	2.668	0.1	168.0
1662	1XE6	A	Tyr77	CD1	3.148	0.7	118.9
1663	1XE6	A	Gly216	O	2.894	3.2	138.8
1664	1XE6	B	Tyr77	C	3.161	0.3	115.5
1665	1XE6	B	Gly216	O	2.718	9.1	125.7
1666	1XH5	A	Ser53	H	2.370	11.2	152.5
1667	1XHA	A	Ser53	H	2.256	15.5	158.6
1668	1XHA	A	Ser53	HB2	2.531	5.2	120.2
1669	1XKK	A	Cys775	HB3	2.668	0.1	115.9

1670	1XKK	A	Arg776	C	3.123	1.5	134.2
1671	1XKK	A	Thr790	HG1	2.361	11.6	141.1
1672	1XL5	A	Asp30	H	2.496	6.5	104.0
1673	1XL5	A	Asp30	HB2	2.307	13.6	158.1
1674	1XMU	A	Asn395	CB	3.126	1.4	127.7
1675	1XMU	A	Asn395	HB2	2.276	14.8	141.3
1676	1XMU	A	Tyr403	HE1	2.439	8.6	80.4
1677	1XMU	A	Trp406	C	3.143	0.9	141.6
1678	1XMU	A	Thr407	HA	2.649	0.8	97.5
1679	1XMU	B	Asn395	HB2	2.502	6.3	139.4
1680	1XMU	B	Tyr403	HE1	2.340	12.4	93.9
1681	1XMU	B	Thr407	HA	2.619	1.9	90.2
1682	1XOQ	A	Trp332	C	3.167	0.1	142.3
1683	1XOQ	A	Trp332	HB3	2.665	0.2	144.8
1684	1XOQ	A	Asn321	HB2	2.337	12.5	135.2
1685	1XOQ	A	Tyr329	HE1	2.569	3.8	82.5
1686	1XOQ	B	Thr333	HA	2.659	0.4	97.2
1687	1XOQ	B	Asn321	HB2	2.318	13.2	136.5
1688	1XOQ	B	Tyr329	HE1	2.437	8.7	85.0
1689	1XOR	A	Phe372	HB2	2.503	6.3	124.5
1690	1XOR	A	Asn321	HB2	2.487	6.8	109.7
1691	1XOR	A	Pro322	HG3	2.558	4.2	168.3
1692	1XOR	A	Tyr329	HE1	2.462	7.8	112.5
1693	1XOR	A	Phe372	HE2	2.458	8.0	111.7
1694	1XOR	A	Met357	SD	3.253	0.5	115.5
1695	1XOR	A	Phe340	HE2	2.497	6.5	111.2
1696	1XOR	A	Met357	SD	3.187	2.5	109.6
1697	1XOR	A	Thr333	HA	2.526	5.4	144.5
1698	1XOR	B	Phe340	HE2	2.444	8.5	150.8
1699	1XOR	B	Met357	SD	2.884	11.8	128.2
1700	1XOR	B	Met357	CE	3.116	1.7	143.8
1701	1XOR	B	Met357	HE1	2.548	4.6	133.4
1702	1XOR	B	Asn321	HB2	2.416	9.5	117.3
1703	1XOR	B	Tyr329	HE1	2.657	0.5	106.1
1704	1XOR	B	Phe372	HE2	2.463	7.8	117.2
1705	1XOR	B	Phe372	HB2	2.341	12.3	102.1
1706	1XOR	B	Thr333	HA	2.512	5.9	142.3
1707	1XSK	A	Cys307	SG	3.097	5.3	159.3
1708	1XSK	A	Cys307	HG	2.639	1.2	152.9
1709	1XSK	B	Cys307	SG	3.188	2.5	158.0
1710	1XSK	B	Trp345	HE1	2.488	6.8	111.4
1711	1XSK	C	Cys307	SG	3.111	4.9	161.6
1712	1XSK	C	Trp345	HE1	2.500	6.4	112.7
1713	1XSK	E	Cys307	SG	3.133	4.2	160.4

1714	1XUD	A	Val219	HA	2.474	7.3	99.3
1715	1XUD	B	Val219	HA	2.591	3.0	96.7
1716	1XUD	B	Phe217	HD2	2.499	6.4	86.8
1717	1XVD	A	Met288	CE	3.153	0.5	145.9
1718	1XVD	A	Met288	HE3	2.069	22.5	142.5
1719	1XVD	B	Met288	HE3	2.321	13.1	134.9
1720	1XZ3	A	Leu24	CD2	3.083	2.8	113.3
1721	1XZ3	A	Tyr28	HB2	2.656	0.5	120.5
1722	1Y0S	A	Ile326	CG2	2.933	7.5	110.2
1723	1Y0S	A	Leu330	HB2	2.391	10.4	106.6
1724	1Y0S	B	Ile326	CG2	3.044	4.0	108.7
1725	1Y0S	B	Leu330	HB2	2.372	11.2	113.2
1726	1Y6O	B	Pro18	HB3	2.443	8.5	126.5
1727	1YL1	X	Ile58	HA	2.180	18.4	124.8
1728	1YL1	X	Asn59	H	2.144	19.7	104.5
1729	1YL1	X	Asn59	H	2.602	2.6	84.3
1730	1YL1	X	Asn59	HB2	2.548	4.6	121.5
1731	1YL1	X	Gly4	HA3	2.259	15.4	98.2
1732	1YL1	X	Cys6	N	2.859	5.3	113.4
1733	1YL1	X	Cys6	CA	2.931	7.6	138.2
1734	1YL1	X	Cys6	C	2.905	8.4	164.2
1735	1YL1	X	Cys6	CB	2.819	11.1	125.9
1736	1YL1	X	Cys6	H	2.509	6.0	94.9
1737	1YL1	X	Cys6	HB2	1.967	26.3	111.9
1738	1YL1	X	Glu7	N	2.326	23.0	149.6
1739	1YL1	X	Glu7	H	1.730	35.2	127.3
1740	1YQY	A	His686	CB	2.943	7.2	123.0
1741	1YQY	A	His686	CG	2.919	7.9	98.4
1742	1YQY	A	His686	ND1	3.012	0.3	95.1
1743	1YQY	A	His686	HB3	2.646	0.9	117.8
1744	1YT7	A	Asp61	HB2	2.607	2.4	75.8
1745	1YT7	A	Asp61	HB2	2.434	8.8	82.5
1746	1YW2	A	Leu1104	C	3.124	1.5	128.6
1747	1YW2	A	Leu1104	CB	3.119	1.6	119.0
1748	1YW2	A	Leu1104	HB3	2.645	0.9	130.1
1749	1YW9	A	Ala230	CB	3.076	3.0	142.9
1750	1YW9	A	Ala230	HB3	2.649	0.8	143.7
1751	1YWN	A	Glu883	CG	3.166	0.1	144.2
1752	1YWN	A	Glu883	HG3	2.312	13.4	133.1
1753	1YWR	A	Leu104	C	3.127	1.3	127.3
1754	1YWR	A	Leu104	HB3	2.535	5.1	126.9
1755	1YYE	A	Leu339	C	3.139	1.0	131.5
1756	1YYE	A	Met340	HA	2.522	5.5	171.9
1757	1YYE	B	Leu339	C	2.991	5.7	131.4

1758	1YYE	B	Leu339	O	2.884	3.6	136.4
1759	1YYE	B	Met340	HA	2.442	8.6	165.9
1760	1YYE	B	Leu343	HB2	2.596	2.8	117.1
1761	1Z3N	A	Cys80	HG	2.407	9.8	129.4
1762	1Z3N	A	Leu300	H	2.605	2.4	118.8
1763	1Z3N	A	Tyr309	HE1	2.449	8.3	136.8
1764	1Z3N	A	Tyr309	HD1	2.545	4.7	141.7
1765	1Z71	A	Glu217	HG2	2.484	7.0	110.0
1766	1ZUA	X	Gln303	HG2	2.364	11.5	96.4
1767	1ZUA	X	Gln303	CG	2.688	15.2	111.2
1768	1ZUA	X	Gln303	CD	2.908	8.3	141.6
1769	1ZUA	X	Gln303	HG2	2.213	17.1	102.7
1770	1ZUA	X	Gln303	HG3	2.594	2.8	96.4
1771	1ZZ2	A	Leu104	CB	3.167	0.1	101.4
1772	1ZZ2	A	Leu104	HB3	2.405	9.9	114.2
1773	1ZZR	A	Ala654	HA	2.424	9.2	137.8
1774	1ZZR	B	Gly417	HA2	2.614	2.1	91.9
1775	2A4Z	A	Ala885	HB3	2.292	14.2	159.6
1776	2A4Z	A	Met953	CE	2.924	7.8	109.0
1777	2A4Z	A	Met953	HE1	2.014	24.6	108.2
1778	2A7Q	A	Arg128	HH12	2.598	2.7	139.9
1779	2A9N	H	Gly57	CA	3.159	0.3	127.2
1780	2A9N	H	Gly57	HA3	2.331	12.7	112.2
1781	2A9N	I	His131	ND1	2.971	1.6	167.9
1782	2A9N	I	His131	HD1	2.644	1.0	148.8
1783	2A9N	I	Gly57	CA	3.072	3.1	134.8
1784	2A9N	I	Gly57	HA3	2.197	17.7	120.1
1785	2A9N	I	His69	HB2	2.585	3.2	131.4
1786	2A75	A	Arg36	NH2	3.005	0.5	110.2
1787	2A75	A	Arg36	HH22	2.312	13.4	112.0
1788	2A75	A	Asp60	OD2	2.939	1.7	153.4
1789	2ABJ	A	Phe47	CZ	3.076	3.0	107.0
1790	2ABJ	A	Phe47	HZ	2.490	6.7	116.5
1791	2ABJ	A	Phe47	CE2	3.160	0.3	121.1
1792	2ABJ	D	Phe47	HZ	2.643	1.0	129.8
1793	2ABJ	G	Phe47	HZ	2.573	3.6	128.2
1794	2ABJ	J	Phe47	CZ	3.117	1.7	105.4
1795	2ABJ	J	Phe47	HZ	2.589	3.0	114.1
1796	2ABJ	J	Phe47	CE2	3.168	0.1	121.7
1797	2AEI	H	Trp215	CB	2.857	9.9	152.6
1798	2AEI	H	Trp215	HB2	2.405	9.9	157.9
1799	2AEI	H	Trp215	HB3	2.430	9.0	142.7
1800	2AGS	A	Arg36	HH22	2.355	11.8	110.9
1801	2AGS	A	Asp60	OD2	2.934	1.9	159.1

1802	2AGT	A	Val47	O	2.904	2.9	146.2
1803	2AH2	A	Arg35	HH22	2.623	1.8	101.6
1804	2AH2	A	Asp59	OD1	2.696	9.8	156.3
1805	2AH2	A	Asp59	OD2	2.959	1.0	112.4
1806	2AID	A	Asp29	H	2.567	3.9	82.0
1807	2AID	A	Leu10	CD1	3.146	0.8	158.1
1808	2AL5	A	Met196	HG2	2.668	0.1	167.8
1809	2AL5	A	Met196	HE2	2.271	14.9	108.7
1810	2AL5	B	Met196	CE	3.164	0.2	112.7
1811	2AL5	B	Met196	HG2	2.634	1.4	168.2
1812	2AL5	B	Met196	HE2	2.246	15.9	108.7
1813	2AM4	A	Tyr184	CE2	2.920	7.9	133.5
1814	2ANO	A	Ser49	CB	3.158	0.4	124.9
1815	2ANO	A	Ser49	HB3	2.234	16.3	137.7
1816	2ANO	A	Leu54	CD2	3.044	4.0	171.6
1817	2AS4	A	Lys179	CA	3.039	4.1	116.9
1818	2AS4	A	Lys179	HA	1.993	25.3	122.8
1819	2AS4	A	Pro190	CA	3.168	0.1	141.5
1820	2AS4	A	Pro190	HA	2.183	18.2	147.4
1821	2AS4	A	Ser104	HA	2.591	3.0	156.6
1822	2ATI	B	Lys191	HB3	2.578	3.4	163.8
1823	2ATI	B	Arg193	HD3	2.661	0.3	88.7
1824	2ATI	A	Lys191	HB3	2.500	6.4	167.0
1825	2AX6	A	Met745	HB3	2.524	5.5	123.1
1826	2AX6	A	Phe764	HE2	2.633	1.4	94.5
1827	2AX7	A	His874	HE2	2.601	2.6	116.5
1828	2AX7	A	Phe764	HE2	2.619	1.9	95.0
1829	2AX9	A	Met745	HB3	2.633	1.4	121.4
1830	2AXA	A	His874	HE2	2.602	2.6	107.1
1831	2AXA	A	Phe764	HE2	2.637	1.2	96.5
1832	2AYL	A	Ala527	HA	2.471	7.5	80.6
1833	2AYL	A	Ser530	CB	3.167	0.1	149.1
1834	2AYL	A	Ser530	HB3	2.390	10.5	141.6
1835	2AYL	A	Ser530	HG	2.642	1.1	140.7
1836	2AYL	B	Ala1527	HA	2.520	5.6	79.2
1837	2AYL	B	Ser1530	HB3	2.376	11.0	142.4
1838	2AZ5	A	Leu57	CD2	3.160	0.3	120.0
1839	2AZ5	A	Gly121	CA	3.155	0.5	113.0
1840	2AZ5	A	Gly121	C	2.597	18.1	136.1
1841	2AZ5	A	Gly121	O	2.743	8.3	159.8
1842	2AZ5	A	Gly121	HA3	2.656	0.5	96.2
1843	2AZ5	A	Gly122	N	2.892	4.2	123.6
1844	2AZ5	C	Gly121	HA3	2.626	1.6	96.5
1845	2AZ5	C	Leu57	CD2	3.091	2.5	121.7

1846	2AZ5	C	Gly121	C	2.822	11.0	123.2
1847	2AZ5	C	Gly121	O	2.924	2.2	144.7
1848	2AZ5	C	Gly122	HA2	2.539	4.9	130.6
1849	2B6A	A	Leu100	CD2	3.069	3.2	133.0
1850	2B6A	A	Tyr188	HB3	2.516	5.8	130.5
1851	2B6A	A	Leu100	CD2	3.088	2.6	93.9
1852	2BAL	A	Leu104	CB	3.153	0.5	145.1
1853	2BAL	A	Leu104	HB2	2.397	10.2	131.9
1854	2BAQ	A	Leu104	CB	3.080	2.8	140.8
1855	2BAQ	A	Leu104	HB2	2.559	4.2	124.6
1856	2BAQ	A	Leu104	HB3	2.664	0.2	145.4
1857	2BU2	A	Phe28	HE2	2.358	11.7	141.5
1858	2BU2	A	Gln163	HB2	2.624	1.7	125.3
1859	2BU5	A	Phe28	HE2	2.145	19.7	133.6
1860	2BU6	A	Phe44	HE2	2.547	4.6	161.6
1861	2BU6	A	Phe28	CE2	2.936	7.4	163.6
1862	2BU6	A	Phe28	HE2	1.980	25.9	160.1
1863	2BU9	A	Tyr189	OH	2.923	2.3	89.4
1864	2BU9	A	Tyr189	OH	2.923	2.2	90.7
1865	2BU9	A	Phe211	CB	2.998	5.4	119.6
1866	2BU9	A	Phe211	CG	3.163	0.2	105.7
1867	2BU9	A	Phe211	HB2	2.381	10.8	108.2
1868	2BU9	A	Phe211	CD1	2.965	6.5	121.3
1869	2BU9	A	Ile187	CD1	3.049	3.8	136.4
1870	2BU9	A	Thr331	HB	2.578	3.5	107.2
1871	2BUB	A	Tyr662	OH	2.950	1.3	73.8
1872	2BUB	A	Asn710	OD1	2.850	4.7	164.6
1873	2BUB	B	Ser630	HG	2.617	2.0	76.4
1874	2BXE	A	Gly434	HA2	2.471	7.5	155.6
1875	2BXE	A	Leu347	HB3	2.656	0.5	129.5
1876	2BXE	A	Ala350	HB1	2.341	12.3	134.1
1877	2BXE	A	Arg222	CD	2.500	21.1	148.6
1878	2BXE	A	Arg222	NH1	2.880	4.6	99.0
1879	2BXE	A	Arg222	HD2	2.657	0.5	162.8
1880	2BXE	A	Arg222	HD3	1.526	42.8	135.7
1881	2BXE	A	Arg222	HH11	1.980	25.9	101.4
1882	2BXE	B	Leu387	CD2	3.073	3.1	153.5
1883	2BXE	B	Gly434	HA2	2.587	3.1	151.0
1884	2BXE	B	Leu347	HB3	2.259	15.4	137.0
1885	2BXE	B	Ala350	CB	3.123	1.5	115.3
1886	2BXE	B	Ala350	HB1	2.261	15.3	130.0
1887	2BXE	B	Arg222	CD	2.498	21.2	145.4
1888	2BXE	B	Arg222	NH1	2.748	9.0	102.7
1889	2BXE	B	Arg222	HD3	1.472	44.9	135.5

1890	2BXE	B	Arg222	HH11	1.893	29.1	108.5
1891	2BXU	H	Trp215	HE3	2.546	4.6	142.4
1892	2BXV	A	Leu42	CD1	3.117	1.7	129.6
1893	2BXV	A	Phe62	HD2	2.500	6.4	152.2
1894	2BXV	A	Leu359	HG	2.512	5.9	108.3
1895	2C1P	B	Trp103	HZ2	2.237	16.2	120.1
1896	2C1P	H	Trp103	HZ2	2.355	11.8	121.1
1897	2C1Z	A	Gln375	NE2	2.958	2.1	118.8
1898	2C4F	H	Trp215	HB2	2.496	6.5	131.1
1899	2C4F	H	Gly216	H	2.392	10.4	164.5
1900	2C5B	A	Thr155	O	2.953	1.2	124.6
1901	2C5B	A	Phe156	CA	2.940	7.3	143.4
1902	2C5B	A	Phe156	C	3.162	0.2	141.9
1903	2C5B	A	Phe156	HA	2.001	25.0	132.7
1904	2C5B	A	Phe156	HD1	2.413	9.6	93.0
1905	2C5B	A	Tyr157	N	3.000	0.6	146.8
1906	2C5B	A	Ser158	H	2.364	11.5	92.2
1907	2C5B	B	Phe156	HA	2.592	2.9	86.3
1908	2C5B	B	Phe156	HD1	2.563	4.0	101.8
1909	2C5B	B	Ser158	N	2.797	7.4	165.4
1910	2C5B	B	Ser158	H	1.803	32.5	167.3
1911	2C5B	B	Ser158	HB2	2.385	10.7	107.7
1912	2C5B	C	Phe156	CA	2.967	6.4	129.4
1913	2C5B	C	Phe156	C	3.066	3.3	155.9
1914	2C5B	C	Phe156	HA	2.062	22.8	114.9
1915	2C5B	C	Phe156	HD1	2.391	10.4	107.7
1916	2C5B	C	Tyr157	N	2.952	2.3	173.0
1917	2C5B	C	Ser158	H	2.055	23.1	129.8
1918	2C5V	A	Gln85	CB	3.119	1.6	116.9
1919	2C5V	A	Asp86	OD2	2.815	5.8	115.7
1920	2C5V	A	Lys89	HZ3	2.387	10.6	129.7
1921	2C5V	C	Gln85	HB3	2.504	6.2	139.4
1922	2C5V	C	Asp86	OD2	2.619	12.4	143.6
1923	2C5V	C	Lys89	NZ	2.734	9.5	117.4
1924	2C5V	C	Lys89	HZ3	1.781	33.3	109.6
1925	2C5V	C	Lys89	HZ3	2.638	1.2	71.3
1926	2C94	A	Gly85	CA	3.029	4.5	139.7
1927	2C94	A	Gly85	HA3	2.200	17.6	127.9
1928	2C94	B	Gly85	N	2.839	6.0	160.7
1929	2C94	B	Gly85	CA	2.884	9.0	143.0
1930	2C94	B	Gly85	HA3	2.094	21.6	127.8
1931	2C94	C	Gly85	CA	3.163	0.2	116.8
1932	2C94	C	Gly85	HA3	2.181	18.3	110.5
1933	2C94	D	Gly85	CA	2.904	8.4	136.8

1934	2C94	D	Gly85	HA3	1.995	25.3	129.9
1935	2C94	E	Gly85	N	2.805	7.1	153.9
1936	2C94	E	Gly85	CA	2.784	12.2	138.3
1937	2C94	E	Gly85	HA3	1.966	26.4	123.4
1938	2CHL	A	Ile173	CG2	2.947	7.0	111.9
1939	2CHL	A	Leu46	HB2	2.444	8.5	151.3
1940	2CIT	A	Phe41	HE1	2.585	3.2	163.4
1941	2CIT	A	His108	HE2	2.240	16.1	117.0
1942	2CIT	A	Tyr115	OH	2.980	0.3	83.9
1943	2CIT	A	Tyr115	HH	2.523	5.5	81.7
1944	2CIT	A	Glu222	CD	3.008	5.1	87.4
1945	2CIT	A	Glu222	OE1	2.749	8.1	63.4
1946	2CIT	A	Glu222	OE2	2.814	5.9	102.3
1947	2CLE	A	Ile153	CD1	2.945	7.1	156.1
1948	2CLE	A	Phe212	HZ	2.653	0.6	87.8
1949	2CLE	A	Ala59	CB	3.054	3.7	103.0
1950	2CLE	A	Ala59	HB1	2.190	18.0	89.6
1951	2CLE	B	Pro18	HB3	2.458	7.9	133.4
1952	2CLE	A	Phe212	HZ	2.329	12.8	102.7
1953	2CLF	B	Pro18	HB3	2.163	19.0	143.8
1954	2CLF	A	Phe212	HZ	2.338	12.4	121.0
1955	2CLF	B	Thr110	CA	3.030	4.4	143.6
1956	2CLF	B	Thr110	C	3.024	4.6	170.3
1957	2CLF	B	Thr110	OG1	2.805	6.2	120.8
1958	2CLF	B	Thr110	HA	2.378	10.9	126.5
1959	2CLF	B	Gly111	N	2.186	27.6	161.4
1960	2CLF	B	Gly111	H	1.208	54.7	154.0
1961	2CLF	B	Lys87	HE2	2.523	5.5	108.9
1962	2CLF	B	His115	N	2.798	7.3	137.1
1963	2CLF	B	His115	H	1.826	31.6	134.3
1964	2CLI	B	Pro18	HB3	2.270	15.0	163.1
1965	2CLI	A	Ala129	HA	2.615	2.1	118.7
1966	2CLL	B	Pro18	HB3	2.467	7.6	166.3
1967	2CLL	A	Ala129	HA	2.455	8.1	130.0
1968	2CLM	A	Ile153	CD1	2.744	13.4	125.2
1969	2CLM	B	Pro18	HB3	2.301	13.8	147.4
1970	2CLM	A	Ala59	CB	3.126	1.4	101.5
1971	2CLM	A	Ala59	HB1	2.031	23.9	102.9
1972	2CLM	A	Phe212	HZ	2.310	13.5	111.7
1973	2CMC	A	Asp181	HB2	2.591	2.9	167.7
1974	2CMC	A	Gln262	HG3	2.306	13.6	135.6
1975	2CN0	H	Asn98	HA	2.550	4.5	156.8
1976	2CN0	H	His57	HB2	2.651	0.7	117.2
1977	2CN0	H	Leu99	CD1	2.972	6.2	133.9

1978	2CNB	A	Ser142	OG	2.657	11.1	125.2
1979	2CNB	A	Ser142	HG	2.163	19.0	134.8
1980	2CNB	A	Tyr173	OH	2.827	5.4	151.1
1981	2CNB	A	Tyr173	HE2	2.658	0.5	137.5
1982	2CNB	A	Tyr173	HH	2.010	24.7	163.6
1983	2CNB	B	Ser142	OG	2.850	4.7	123.1
1984	2CNB	B	Ser142	HG	2.414	9.6	132.2
1985	2CNB	B	Tyr173	OH	2.850	4.7	153.0
1986	2CNB	B	Tyr173	HE2	2.604	2.5	141.3
1987	2CNB	B	Tyr173	HH	2.053	23.1	162.6
1988	2CNB	C	Ser142	OG	2.850	4.7	127.6
1989	2CNB	C	Ser142	HG	2.357	11.7	135.7
1990	2CNB	C	Tyr173	OH	2.961	1.0	155.6
1991	2CNB	C	Tyr173	HH	2.136	20.0	168.4
1992	2CNB	D	Ser142	HG	2.549	4.5	126.3
1993	2CNB	D	Tyr173	OH	2.857	4.5	153.9
1994	2CNB	D	Tyr173	HE2	2.619	1.9	146.0
1995	2CNB	D	Tyr173	HH	2.099	21.4	159.4
1996	2CNE	A	Gln262	HG3	2.417	9.5	138.6
1997	2CNG	A	Arg47	NH1	2.978	1.4	109.4
1998	2CNG	A	Arg47	H	2.635	1.3	169.8
1999	2CNG	A	Arg47	HG2	2.429	9.0	126.5
2000	2D3Z	A	Leu489	CD1	3.103	2.1	134.6
2001	2D3Z	B	Leu489	CD1	3.129	1.3	134.3
2002	2DUX	A	Trp111	HE3	2.553	4.4	118.4
2003	2DUX	A	Cys303	CB	3.092	2.5	118.8
2004	2DUX	A	Cys303	HB3	2.198	17.7	132.7
2005	2DUX	A	Tyr309	HD1	2.580	3.4	98.0
2006	2DUX	A	Tyr309	CD1	2.992	5.6	121.6
2007	2DUX	A	Tyr309	CE1	3.082	2.8	137.4
2008	2DUX	A	Tyr309	HD1	2.504	6.2	100.9
2009	2DUX	A	Pro310	CD	3.137	1.0	113.7
2010	2DUX	A	Pro310	HD2	2.366	11.4	127.1
2011	2DUZ	A	Trp111	HE3	2.603	2.5	118.4
2012	2DUZ	A	Pro310	HD3	2.560	4.1	104.8
2013	2DUZ	A	Cys303	CB	3.159	0.3	114.9
2014	2DUZ	A	Cys303	HB3	2.179	18.4	125.5
2015	2DUZ	A	Tyr309	HD1	2.456	8.0	109.0
2016	2DUZ	A	Tyr309	CD1	3.053	3.7	114.6
2017	2DUZ	A	Tyr309	CE1	3.129	1.3	129.7
2018	2DUZ	A	Pro310	CD	3.023	4.6	115.6
2019	2DUZ	A	Pro310	HD2	2.348	12.1	132.9
2020	2DV0	A	Trp111	HE3	2.590	3.0	117.2
2021	2DV0	A	Cys303	CB	3.148	0.7	122.5

2022	2DV0	A	Cys303	HB3	2.281	14.6	137.0
2023	2DV0	A	Tyr309	HD1	2.640	1.1	103.4
2024	2DV0	A	Tyr309	CD1	2.912	8.1	128.8
2025	2DV0	A	Tyr309	CE1	3.072	3.1	145.4
2026	2DV0	A	Tyr309	HD1	2.558	4.2	107.1
2027	2DV0	A	Pro310	HD2	2.340	12.4	120.1
2028	2E2B	A	His361	CD2	3.164	0.2	161.0
2029	2E2B	A	Ile293	CD1	3.111	1.9	136.4
2030	2E2B	B	His361	CD2	3.169	0.0	157.4
2031	2E+25	A	Asn44	ND2	2.940	2.7	142.1
2032	2EA2	A	Ala230	CB	3.033	4.3	136.2
2033	2EA2	A	Ala230	HB3	2.449	8.3	137.1
2034	2EA4	A	Ala230	CB	3.101	2.2	137.1
2035	2EA4	A	Ala230	HB3	2.544	4.7	140.3
2036	2EST	E	Phe215	C	3.115	1.7	130.7
2037	2EST	E	Phe215	HA	2.510	6.0	91.3
2038	2EST	E	Ser214	C	2.970	6.3	122.2
2039	2EST	E	Ser214	O	2.896	3.2	107.7
2040	2EST	I	Lys2	N	3.012	0.3	53.7
2041	2EST	E	Ala99	HB2	2.464	7.7	127.4
2042	2EST	E	Thr175	CG2	3.114	1.8	132.3
2043	2EU3	A	Leu198	HB3	2.595	2.8	108.2
2044	2EU3	A	Thr200	OG1	2.516	15.9	139.1
2045	2EU3	A	Thr200	H	2.547	4.6	158.6
2046	2EUD	A	Gly247	CA	3.117	1.7	165.9
2047	2EUD	A	Gly247	HA3	2.424	9.2	160.2
2048	2EUD	A	Arg293	HD2	2.588	3.1	155.4
2049	2EVC	A	Phe177	HE2	2.591	3.0	143.6
2050	2EVC	A	Tyr62	HB3	2.642	1.1	128.3
2051	2EVC	A	Tyr65	CB	2.939	7.3	137.0
2052	2EVC	A	Tyr65	HB2	2.336	12.5	131.5
2053	2EWA	A	Leu104	HB3	2.616	2.0	108.6
2054	2EWA	A	Leu104	C	2.976	6.1	138.8
2055	2EWA	A	Leu104	CB	3.086	2.6	125.4
2056	2EWA	A	Leu104	HB2	2.592	2.9	106.9
2057	2FDP	A	Arg128	NE	2.957	2.1	151.9
2058	2FDP	A	Arg128	HE	2.213	17.1	147.9
2059	2FDP	B	Arg128	HG2	2.612	2.2	155.3
2060	2FDP	B	Arg128	HE	2.610	2.3	139.4
2061	2FDP	C	Arg128	HG2	2.460	7.9	155.3
2062	2FDP	C	Arg128	HE	2.613	2.1	143.6
2063	2FHR	A	Arg36	HH22	2.457	8.0	118.6
2064	2FHR	A	Asp60	OD2	2.976	0.5	147.2
2065	2FJ0	A	Tyr99	OH	2.931	2.0	160.8

2066	2FJ0	A	Gly146	H	2.646	0.9	89.8
2067	2FJ0	A	Ser226	OG	2.692	10.0	61.8
2068	2FJ0	A	Ser226	OG	2.747	8.1	59.7
2069	2FJ0	A	His471	HD2	2.592	2.9	143.9
2070	2FJ0	A	Gly147	H	2.654	0.6	105.0
2071	2FJM	A	Gln762	HG3	2.603	2.5	136.7
2072	2FJM	A	Asp681	HB2	2.582	3.3	171.9
2073	2FJM	B	Gln762	HG3	2.581	3.3	138.3
2074	2FJM	B	Asp681	HB2	2.564	4.0	174.7
2075	2FJN	A	Gln762	HG3	2.576	3.5	133.8
2076	2FJN	B	Gln762	HG3	2.518	5.7	137.8
2077	2FJP	A	Tyr631	CB	2.939	7.3	163.4
2078	2FJP	A	Tyr631	HB2	2.106	21.1	159.3
2079	2FJP	A	Tyr631	HD2	2.404	10.0	102.9
2080	2FJP	B	Tyr631	CB	3.097	2.3	166.2
2081	2FJP	B	Tyr631	HB2	2.211	17.2	169.5
2082	2FJP	B	Tyr631	HD2	2.329	12.8	109.7
2083	2FKY	A	Glu116	CB	3.138	1.0	106.8
2084	2FKY	A	Glu116	HB3	2.330	12.7	102.6
2085	2FKY	A	Gly217	HA3	2.556	4.3	141.0
2086	2FKY	B	Glu116	HG2	2.370	11.2	85.3
2087	2FKY	B	Gly217	HA3	2.523	5.5	132.4
2088	2FL2	A	Glu116	HB3	2.572	3.7	96.1
2089	2FL2	A	Ile136	HB	2.533	5.1	138.9
2090	2FL2	B	Ile136	HB	2.633	1.4	143.0
2091	2FL6	A	Glu116	HB3	2.553	4.4	91.4
2092	2FL6	B	Pro137	HD3	2.432	8.9	162.5
2093	2FM0	A	Trp332	C	3.106	2.0	136.6
2094	2FM0	A	Trp332	HB3	2.523	5.5	145.3
2095	2FM0	A	Asn321	HB2	2.434	8.9	135.4
2096	2FM0	A	Tyr329	HE1	2.541	4.8	85.4
2097	2FM0	A	Met357	HE1	2.175	18.5	118.1
2098	2FM0	A	Ile376	CD1	3.004	5.3	154.4
2099	2FM0	B	Trp332	HB3	2.469	7.5	146.8
2100	2FM0	B	Asn321	CB	3.160	0.3	121.0
2101	2FM0	B	Asn321	HB2	2.506	6.1	135.8
2102	2FM0	B	Tyr329	HE1	2.531	5.2	87.3
2103	2FM0	B	Phe372	HE2	2.646	0.9	126.6
2104	2FM0	B	Met357	HE1	2.347	12.1	116.7
2105	2FM0	B	Ile376	CD1	3.150	0.6	153.1
2106	2FM0	B	Met273	HG3	2.633	1.4	104.4
2107	2FM0	C	Trp332	C	3.147	0.7	134.4
2108	2FM0	C	Trp332	HB3	2.425	9.2	148.0
2109	2FM0	C	Asn321	HB2	2.419	9.4	135.0

2110	2FM0	C	Tyr329	HE1	2.338	12.4	93.9
2111	2FM0	C	Met357	HE1	2.266	15.1	115.0
2112	2FM0	C	Ile376	CD1	3.028	4.5	165.5
2113	2FM0	D	Trp332	C	3.067	3.2	140.0
2114	2FM0	D	Trp332	HB3	2.458	7.9	146.5
2115	2FM0	D	Thr333	HA	2.655	0.6	89.6
2116	2FM0	D	Asn321	CB	3.141	0.9	126.2
2117	2FM0	D	Asn321	HB2	2.453	8.1	140.9
2118	2FM0	D	Tyr329	HE1	2.534	5.1	83.4
2119	2FM0	D	Met357	HE1	2.599	2.6	107.2
2120	2FM0	D	Ile376	CD1	2.991	5.6	134.1
2121	2FM5	A	Trp332	HB3	2.630	1.5	140.9
2122	2FM5	A	Asn321	HB2	2.467	7.6	136.7
2123	2FM5	A	Tyr329	HE1	2.536	5.0	85.3
2124	2FM5	A	Met357	CE	3.051	3.7	126.7
2125	2FM5	A	Met357	HE1	1.968	26.3	130.4
2126	2FM5	A	Ile376	CD1	3.010	5.0	175.4
2127	2FM5	A	Met273	HG3	2.659	0.4	99.1
2128	2FM5	B	Asn321	HB2	2.465	7.7	132.4
2129	2FM5	B	Pro322	HG3	2.626	1.6	124.9
2130	2FM5	B	Phe372	HE2	2.603	2.5	122.9
2131	2FM5	B	Met357	HE1	2.444	8.5	119.9
2132	2FM5	B	Ile376	CD1	2.936	7.4	157.6
2133	2FM5	B	Met273	HG3	2.598	2.7	105.4
2134	2FM5	C	Trp332	HB3	2.534	5.1	143.9
2135	2FM5	C	Asn321	CB	3.107	2.0	122.5
2136	2FM5	C	Asn321	HB2	2.333	12.6	138.1
2137	2FM5	C	Tyr329	HE1	2.613	2.1	81.0
2138	2FM5	C	Met357	HE1	2.606	2.4	117.4
2139	2FM5	C	Ile376	CD1	2.686	15.3	153.8
2140	2FM5	C	Met273	CE	3.133	1.2	151.0
2141	2FM5	C	Met273	HG3	2.644	1.0	99.2
2142	2FM5	C	Met273	HE2	2.500	6.4	136.3
2143	2FM5	D	Thr333	HA	2.601	2.6	101.9
2144	2FM5	D	Asn321	CB	3.109	1.9	127.5
2145	2FM5	D	Asn321	HB2	2.315	13.3	143.1
2146	2FM5	D	Met357	HE1	2.580	3.4	115.8
2147	2FM5	D	Ile376	CD1	2.894	8.7	153.0
2148	2FM5	D	Met273	HG3	2.502	6.3	111.0
2149	2FOG	A	Cys199	C	3.103	2.1	124.1
2150	2FOG	A	Ser203	OG	2.638	11.8	109.6
2151	2FOH	A	Ser203	OG	2.984	0.2	106.3
2152	2FOH	A	Cys199	CA	3.152	0.6	140.7
2153	2FOH	A	Cys199	C	3.024	4.6	113.1

2154	2FOH	A	Phe223	HA	2.504	6.2	128.4
2155	2FPT	A	Leu359	HG	2.476	7.3	110.5
2156	2FPT	A	Ala55	HB1	2.266	15.1	162.1
2157	2FPT	A	Ala55	HB1	2.242	16.0	163.4
2158	2FPT	A	Leu359	HG	2.533	5.1	109.8
2159	2FPT	A	Thr360	HA	2.668	0.1	89.4
2160	2FPT	A	Phe62	HD2	2.477	7.2	152.3
2161	2FPT	A	Phe62	HD2	2.423	9.2	145.0
2162	2FPV	A	Leu359	HG	2.423	9.2	106.2
2163	2FPV	A	Phe98	HE1	2.564	4.0	95.3
2164	2FPV	A	Leu359	HG	2.342	12.3	101.4
2165	2FPY	A	Phe62	CD2	3.058	3.5	134.0
2166	2FPY	A	Phe62	HD2	2.185	18.2	144.7
2167	2FPY	A	Leu359	HG	2.322	13.1	110.0
2168	2FPY	A	Thr360	HA	2.650	0.8	88.3
2169	2FPY	A	Ala55	HB1	2.244	16.0	153.7
2170	2FQ9	A	Lys61	CG	3.126	1.4	145.7
2171	2FQ9	A	Lys61	HG3	2.415	9.6	156.4
2172	2FQ9	A	Lys61	HD2	2.633	1.4	114.7
2173	2FQ9	A	Asn158	HA	2.659	0.4	160.2
2174	2FQ9	B	Lys61	CG	3.092	2.5	135.2
2175	2FQ9	B	Lys61	HG3	2.152	19.4	143.4
2176	2FQ9	B	Lys61	HE3	2.425	9.2	129.9
2177	2FQI	A	Ala55	HB1	2.387	10.6	159.6
2178	2FQI	A	Ala55	HB1	2.363	11.5	156.7
2179	2FQI	A	Leu46	CD2	3.025	4.6	141.7
2180	2FQI	A	Leu46	CD2	3.004	5.2	140.1
2181	2FQI	A	Leu359	HG	2.472	7.4	111.7
2182	2FQI	A	Leu359	HG	2.467	7.6	113.9
2183	2FQI	A	Leu359	HG	2.413	9.6	113.5
2184	2FQI	A	Leu359	HG	2.485	6.9	113.4
2185	2FQI	A	Thr360	HA	2.663	0.3	94.0
2186	2FQI	A	Leu42	CD1	3.156	0.4	136.2
2187	2FQI	A	Phe62	CD2	3.049	3.8	136.2
2188	2FQI	A	Phe62	HD2	2.147	19.6	146.4
2189	2FQI	A	Phe62	CD2	3.102	2.1	135.7
2190	2FQI	A	Phe62	HD2	2.197	17.7	145.5
2191	2FRA	B	Asn158	HA	2.527	5.4	171.1
2192	2FT2	A	Gly59	O	2.935	1.9	120.7
2193	2FT2	A	Lys61	HG3	2.486	6.9	134.3
2194	2FT2	B	Gly59	O	2.734	8.5	120.5
2195	2FVD	A	Lys33	HB2	2.645	0.9	121.5
2196	2FVD	A	Lys33	CG	3.030	4.4	157.7
2197	2FVD	A	Lys33	CD	2.866	9.6	138.5

2198	2FVD	A	Lys33	HG3	2.595	2.8	170.6
2199	2FVD	A	Lys33	HD2	2.162	19.0	119.3
2200	2FYU	C	Met124	HB3	2.607	2.3	141.2
2201	2FZ8	A	Trp111	HE3	2.479	7.1	117.9
2202	2FZ8	A	Cys303	HB3	2.279	14.7	127.0
2203	2FZ8	A	Tyr309	HD1	2.537	5.0	98.7
2204	2FZ8	A	Tyr309	CD1	2.984	5.9	119.0
2205	2FZ8	A	Tyr309	CE1	3.134	1.1	134.8
2206	2FZ8	A	Tyr309	HD1	2.525	5.4	98.0
2207	2FZ8	A	Pro310	CD	3.105	2.0	114.0
2208	2FZ8	A	Pro310	HD2	2.277	14.7	126.3
2209	2FZ9	A	Thr113	HG1	2.577	3.5	88.9
2210	2FZ9	A	Pro310	HD3	2.638	1.2	116.6
2211	2FZ9	A	Thr113	HG1	2.557	4.2	90.7
2212	2FZ9	A	Cys303	CB	2.999	5.4	121.4
2213	2FZ9	A	Cys303	HB3	2.073	22.4	134.9
2214	2FZ9	A	Tyr309	CD1	3.081	2.8	129.2
2215	2FZ9	A	Tyr309	HD1	2.612	2.2	109.2
2216	2FZ9	A	Pro310	HD2	2.379	10.9	128.4
2217	2FZB	A	Ser302	OG	2.551	14.7	121.7
2218	2FZB	A	Ser302	HG	2.125	20.4	122.9
2219	2FZB	A	Phe115	HZ	2.653	0.6	122.7
2220	2FZB	A	Trp20	HE1	2.254	15.6	119.8
2221	2FZD	A	Ser302	OG	2.944	1.5	115.1
2222	2FZD	A	Cys303	HB2	2.582	3.3	129.0
2223	2FZD	A	Phe122	HD1	2.553	4.4	128.0
2224	2FZZ	A	Glu146	HG3	2.610	2.3	111.1
2225	2FZZ	A	Gly218	HA2	2.655	0.6	130.1
2226	2G00	A	Glu146	HG3	2.573	3.6	103.1
2227	2G00	A	Gly218	HA2	2.665	0.2	135.6
2228	2G0G	A	Tyr473	HE2	2.339	12.4	121.2
2229	2G0H	A	Tyr473	CE2	2.892	8.8	116.0
2230	2G0H	A	Tyr473	HE2	1.937	27.5	122.5
2231	2G0H	A	Cys285	HG	2.666	0.2	126.5
2232	2G0H	A	Arg288	HB3	2.309	13.5	122.0
2233	2G0H	A	Arg288	HE	2.052	23.1	120.4
2234	2G0H	B	Gln286	HG2	2.644	1.0	74.2
2235	2G0H	B	Met364	HE2	2.436	8.8	126.8
2236	2G0H	B	Arg288	C	2.956	6.7	153.2
2237	2G0H	B	Arg288	CB	3.083	2.8	126.3
2238	2G0H	B	Arg288	HB3	2.180	18.3	125.8
2239	2G0H	B	Ser289	N	2.980	1.3	167.3
2240	2G0H	B	Arg288	HG2	2.285	14.4	121.5
2241	2G1Q	A	Glu116	HB3	2.648	0.8	103.0

2242	2G1Q	A	Gly217	HA3	2.465	7.7	135.5
2243	2G1Q	B	Gly217	C	3.166	0.1	145.4
2244	2G1Q	B	Gly217	HA3	2.583	3.3	127.9
2245	2G1S	A	Leu116	CD1	3.026	4.5	115.6
2246	2G1S	A	Thr80	HB	2.621	1.8	124.7
2247	2G1S	B	Leu116	CD1	3.095	2.4	96.5
2248	2G1S	B	Thr80	CG2	3.151	0.6	126.1
2249	2G1S	B	Thr80	HB	2.380	10.9	116.2
2250	2G6W	A	Asn47	ND2	2.715	10.1	79.9
2251	2G6W	A	Lys236	NZ	2.434	19.4	35.4
2252	2G6W	A	Asn47	ND2	2.480	17.9	88.1
2253	2G6W	A	His207	HE1	2.656	0.5	125.3
2254	2G6W	A	Lys236	CE	3.125	1.4	59.7
2255	2G6W	A	Lys236	NZ	2.523	16.4	32.7
2256	2G7Y	B	Val157	O	2.946	1.5	116.7
2257	2G71	A	Ala186	CB	3.163	0.2	136.8
2258	2G71	A	Ala186	HB2	2.327	12.8	135.6
2259	2G71	A	Gly54	CA	2.994	5.6	102.9
2260	2G71	A	Gly54	HA2	2.637	1.2	83.9
2261	2G71	A	Gly54	HA3	2.462	7.8	123.3
2262	2G71	A	Tyr126	HH	2.479	7.1	84.7
2263	2G71	A	Tyr40	CD2	3.043	4.0	154.5
2264	2G71	A	Tyr40	HD2	2.630	1.5	172.9
2265	2G71	A	Tyr126	CE2	3.095	2.4	119.7
2266	2G71	A	Tyr126	OH	2.859	4.4	119.2
2267	2G71	A	Tyr126	HE2	2.242	16.0	109.6
2268	2G71	A	Tyr126	HH	1.913	28.4	111.6
2269	2G71	A	Gly54	CA	3.015	4.9	101.9
2270	2G71	A	Gly54	HA2	2.025	24.1	112.8
2271	2G71	A	Lys57	CE	3.017	4.8	139.9
2272	2G71	A	Lys57	HE2	2.405	9.9	134.9
2273	2G71	B	Ala186	HB2	2.622	1.8	113.1
2274	2G71	B	Tyr126	HE2	2.637	1.3	96.9
2275	2G71	B	Tyr126	HH	2.181	18.3	104.9
2276	2G71	B	Tyr40	HE2	2.501	6.3	122.4
2277	2G71	B	Lys57	HZ1	2.309	13.5	99.7
2278	2G71	B	Tyr126	HE2	2.420	9.4	107.4
2279	2G71	B	Gly54	CA	2.938	7.3	112.8
2280	2G71	B	Gly54	HA2	2.140	19.8	108.4
2281	2G71	B	Lys57	HE2	2.501	6.3	118.3
2282	2G72	A	Glu219	OE2	2.862	4.3	123.1
2283	2GG0	A	Tyr62	HD2	2.463	7.8	109.9
2284	2GG0	A	Tyr62	HE2	2.667	0.1	146.6
2285	2GG2	A	Trp221	HZ3	2.523	5.5	88.4

2286	2GG2	A	His63	HD2	2.519	5.6	130.7
2287	2GG2	A	Trp221	HZ3	2.367	11.3	95.3
2288	2GG3	A	His63	HB2	2.544	4.7	126.6
2289	2GG3	A	Trp221	CZ3	3.102	2.2	100.8
2290	2GG3	A	Trp221	HZ3	2.212	17.1	89.1
2291	2GG5	A	Cys70	SG	2.943	10.0	155.9
2292	2GG5	A	Cys70	HG	2.273	14.9	170.2
2293	2GG5	A	Tyr65	CB	3.059	3.5	162.4
2294	2GG5	A	Tyr65	CG	3.153	0.5	137.2
2295	2GG5	A	Tyr65	HB2	2.506	6.2	152.8
2296	2GG5	A	Phe177	HE2	2.550	4.5	153.3
2297	2GH6	A	His142	HD2	2.575	3.6	111.0
2298	2GH6	A	His143	CD2	3.151	0.6	121.8
2299	2GH6	A	His143	HD2	2.539	4.9	121.0
2300	2GH6	A	Cys153	SG	3.109	4.9	149.5
2301	2GH6	A	Pro140	CG	2.891	8.8	123.4
2302	2GH6	A	Pro140	HG3	2.180	18.3	141.7
2303	2GH6	A	His142	HE2	2.554	4.3	88.8
2304	2GH6	A	Asp180	OD2	2.899	3.0	129.8
2305	2GH6	B	His142	HD2	2.596	2.8	120.5
2306	2GH6	B	His143	CD2	3.154	0.5	122.0
2307	2GH6	B	His143	HD2	2.591	3.0	123.0
2308	2GH6	B	Cys153	SG	3.183	2.7	153.1
2309	2GH6	B	Pro140	CG	3.091	2.5	120.0
2310	2GH6	B	Pro140	HG3	2.341	12.3	136.8
2311	2GH6	B	Tyr312	OH	2.916	2.5	111.8
2312	2GH6	B	Tyr312	HH	2.667	0.1	91.9
2313	2GH6	B	Asp180	OD2	2.908	2.7	131.4
2314	2GH6	B	Gly310	N	2.943	2.6	142.5
2315	2GH6	C	His142	HD2	2.517	5.7	120.0
2316	2GH6	C	His143	HD2	2.572	3.7	118.2
2317	2GH6	C	Cys153	SG	3.100	5.2	154.8
2318	2GH6	C	Pro140	CG	3.052	3.7	119.6
2319	2GH6	C	Pro140	HG3	2.291	14.2	136.8
2320	2GH6	C	Asp180	OD2	2.938	1.7	137.7
2321	2GH6	C	Gly310	N	2.933	2.9	146.2
2322	2GH6	D	His142	HD2	2.654	0.6	109.9
2323	2GH6	D	His143	HD2	2.549	4.5	121.8
2324	2GH6	D	Cys153	SG	3.077	5.9	156.8
2325	2GH6	D	Pro140	CG	3.034	4.3	116.9
2326	2GH6	D	Pro140	HG3	2.268	15.1	134.2
2327	2GH6	D	Tyr312	OH	2.936	1.8	113.5
2328	2GH6	D	His142	NE2	3.015	0.2	100.9
2329	2GH6	D	His142	HE2	2.441	8.6	89.6

2330	2GH6	D	Asp180	OD2	2.960	1.0	132.2
2331	2GH6	D	Glu309	HB3	2.668	0.1	169.2
2332	2GH6	D	Gly310	N	3.010	0.3	132.1
2333	2GIQ	A	Gly410	CA	3.150	0.6	160.3
2334	2GIQ	A	Gly410	C	2.903	8.4	137.9
2335	2GIQ	A	Gly410	HA3	2.559	4.2	170.2
2336	2GIQ	B	Gly410	CA	3.136	1.1	162.4
2337	2GIQ	B	Gly410	C	2.901	8.5	138.8
2338	2GIQ	B	Gly410	HA3	2.538	5.0	171.8
2339	2GMV	A	Asn533	ND2	2.794	7.5	118.0
2340	2GTM	A	Gly110	HA2	2.468	7.5	112.2
2341	2GTN	A	Ala51	HB1	2.639	1.2	145.3
2342	2GTN	A	Lys53	HB2	2.576	3.5	82.4
2343	2GTN	A	Gly110	CA	3.142	0.9	109.5
2344	2GTN	A	Gly110	C	3.097	2.3	84.5
2345	2GYD	A	Tyr28	HA	2.617	2.0	116.2
2346	2GYD	A	Leu24	O	2.875	3.8	147.3
2347	2GYD	A	Ser27	HB3	2.537	5.0	91.3
2348	2GYD	A	Tyr28	N	2.906	3.8	108.3
2349	2GYD	A	Tyr28	HB2	2.659	0.4	143.6
2350	2GZ7	A	Thr190	H	2.492	6.7	170.9
2351	2GZ7	A	Gln192	NE2	2.705	10.4	102.4
2352	2GZ7	A	Gln192	NE2	2.725	9.8	101.8
2353	2GZ8	A	Gly143	HA2	2.646	0.9	94.7
2354	2GZ8	A	Gly143	CA	2.929	7.6	110.0
2355	2GZ8	A	Gly143	C	2.918	8.0	139.1
2356	2GZ8	A	Gly143	H	2.497	6.5	77.1
2357	2GZ8	A	Gly143	HA2	2.529	5.3	100.7
2358	2GZ8	A	Cys145	N	2.772	8.2	138.9
2359	2GZ8	A	Cys145	CB	3.148	0.7	99.3
2360	2GZ8	A	Cys145	H	1.848	30.8	133.8
2361	2GZ8	A	Cys145	HB2	2.333	12.6	95.2
2362	2GZ8	A	His41	HE1	2.412	9.7	170.5
2363	2GZ8	A	Cys145	CB	3.040	4.1	103.8
2364	2GZ8	A	Cys145	SG	3.014	7.8	107.4
2365	2GZ8	A	Cys145	HB2	2.270	15.0	97.3
2366	2JXR	A	Gly34	HA3	2.532	5.2	125.3
2367	2H1H	A	His266	CD2	3.017	4.8	149.6
2368	2H1H	A	His266	HD2	2.382	10.8	165.5
2369	2H1H	A	His266	HE2	2.623	1.8	107.0
2370	2H1H	B	Thr262	C	2.949	7.0	123.3
2371	2H1H	B	His266	CD2	3.047	3.9	140.0
2372	2H1H	B	His266	HD2	2.390	10.5	155.5
2373	2H9Y	A	Gly122	CA	3.049	3.8	133.6

2374	2H9Y	A	Gly122	HA2	2.353	11.9	129.8
2375	2H9Y	A	Phe297	CE2	3.052	3.7	137.2
2376	2H9Y	A	Phe297	CZ	2.961	6.6	138.9
2377	2H9Y	A	Ser203	OG	2.796	6.5	64.8
2378	2H9Y	A	Ser203	HG	2.628	1.6	67.0
2379	2H9Y	A	Phe338	HZ	2.472	7.4	142.7
2380	2H9Y	A	Ser203	OG	2.607	12.8	72.1
2381	2H9Y	A	Trp236	CH2	3.075	3.0	166.1
2382	2H9Y	B	Gly122	CA	2.919	7.9	143.6
2383	2H9Y	B	Gly122	HA2	2.224	16.7	140.3
2384	2H9Y	B	Phe297	CE2	3.012	5.0	130.7
2385	2H9Y	B	Phe297	CZ	3.014	4.9	127.1
2386	2H9Y	B	Ser203	OG	2.945	1.5	59.9
2387	2H9Y	B	Phe338	HZ	2.551	4.4	142.9
2388	2H9Y	B	Ser203	OG	2.559	14.4	74.9
2389	2H55	A	Gly97	H	2.603	2.5	134.5
2390	2HAI	A	Met423	SD	3.212	1.8	112.7
2391	2HAI	A	Met423	HE1	2.405	9.9	138.3
2392	2HAI	A	Leu497	HB2	2.467	7.6	87.3
2393	2HCY	A	Trp92	CD1	3.098	2.3	123.4
2394	2HCY	A	Trp92	NE1	2.667	11.7	137.9
2395	2HCY	A	Trp92	CE2	3.002	5.3	115.5
2396	2HCY	A	Tyr294	HE1	2.434	8.8	142.7
2397	2HCY	A	Thr45	OG1	2.413	19.3	112.0
2398	2HCY	A	Thr45	CG2	3.019	4.8	125.9
2399	2HCY	A	Thr45	HG1	1.997	25.2	89.8
2400	2HCY	A	Trp54	CH2	2.962	6.6	154.8
2401	2HCY	A	Trp54	HH2	2.058	22.9	162.3
2402	2HCY	B	Thr45	OG1	2.648	11.4	128.9
2403	2HCY	B	Thr45	HG1	1.818	31.9	118.2
2404	2HCY	B	Met270	SD	3.035	7.2	109.1
2405	2HCY	C	Met270	HE1	2.367	11.3	113.4
2406	2HCY	C	Trp92	CD1	3.088	2.6	130.6
2407	2HCY	C	Trp92	NE1	2.891	4.3	132.6
2408	2HCY	C	Trp92	CE2	3.163	0.2	107.3
2409	2HCY	C	Tyr294	HE1	2.569	3.8	128.1
2410	2HCY	C	Thr45	CG2	3.054	3.7	128.0
2411	2HCY	C	Thr45	HG1	2.501	6.3	79.8
2412	2HCY	C	Trp54	CH2	3.157	0.4	141.0
2413	2HCY	C	Trp54	HH2	2.390	10.5	131.2
2414	2HCY	D	Val295	CG1	3.088	2.6	127.3
2415	2HFP	A	Leu469	CD1	3.012	5.0	160.5
2416	2HFP	A	Tyr473	HH	2.412	9.7	88.7
2417	2HFP	A	Gln286	CB	3.051	3.7	124.3

2418	2HFP	A	Gln286	HB2	2.660	0.4	103.6
2419	2HFP	A	Tyr473	HH	2.575	3.6	82.0
2420	2HH5	A	Phe146	HB2	2.592	2.9	171.2
2421	2HH5	B	Arg141	HA	2.395	10.3	114.9
2422	2HH5	A	Pro143	CA	3.110	1.9	169.3
2423	2HH5	A	Pro143	HA	2.339	12.4	155.0
2424	2HH5	B	Trp186	CH2	3.011	5.0	157.0
2425	2HH5	B	Trp186	HH2	2.066	22.6	163.0
2426	2HH5	B	Pro143	HA	2.514	5.9	150.0
2427	2HH5	A	Trp186	CH2	2.976	6.1	151.0
2428	2HH5	A	Trp186	HH2	1.977	25.9	157.4
2429	2HHN	B	Gln19	CG	3.138	1.0	146.4
2430	2HHN	B	Trp186	CD1	3.049	3.8	120.3
2431	2HHN	B	Gly20	O	2.644	11.6	119.2
2432	2HM1	A	Phe108	HA	2.642	1.1	113.3
2433	2HM1	A	Phe108	HD1	2.316	13.3	96.0
2434	2HM1	A	Trp115	CZ2	3.031	4.4	129.1
2435	2HM1	A	Trp115	HZ2	2.256	15.5	145.8
2436	2HNZ	A	Tyr188	HB3	2.406	9.9	98.6
2437	2HOC	A	Val135	CG1	3.154	0.5	107.3
2438	2HOC	A	Leu198	CD1	2.973	6.2	104.9
2439	2HOC	A	Leu204	CD1	3.073	3.1	132.9
2440	2HOC	A	Val135	C	3.168	0.1	149.2
2441	2HOC	A	Val135	O	2.201	26.4	163.4
2442	2HOC	A	Gln136	CA	3.150	0.6	112.7
2443	2HOC	A	Gln136	HA	2.142	19.8	107.0
2444	2HV5	A	Trp111	HE3	2.664	0.2	118.7
2445	2HV5	A	Pro310	HD3	2.566	3.9	122.2
2446	2HV5	A	Thr113	HG1	2.656	0.5	92.3
2447	2HV5	A	Cys303	CB	2.958	6.7	124.4
2448	2HV5	A	Cys303	HB3	2.113	20.9	140.3
2449	2HV5	A	Tyr309	CD1	2.998	5.4	131.9
2450	2HV5	A	Tyr309	CE1	3.134	1.1	151.3
2451	2HV5	A	Tyr309	HD1	2.465	7.7	111.8
2452	2HV5	A	Pro310	HD2	2.541	4.8	123.9
2453	2HVC	A	Val746	HA	2.228	16.6	143.8
2454	2HVC	A	Phe764	HE1	2.519	5.6	98.6
2455	2HVC	A	Asn705	OD1	2.771	7.3	117.8
2456	2HVC	A	Met742	HE1	2.596	2.8	128.4
2457	2HVC	A	Thr877	HG1	2.653	0.6	124.3
2458	2HVC	A	Phe876	HD1	2.310	13.5	146.1
2459	2HVC	A	Thr877	CG2	2.931	7.6	131.9
2460	2HVC	A	Met780	HE1	2.495	6.5	124.3
2461	2HVN	A	Trp111	HE3	2.534	5.1	119.3

2462	2HVN	A	Cys303	HB3	2.257	15.5	126.5
2463	2HVN	A	Tyr309	HD1	2.423	9.2	104.7
2464	2HVN	A	Tyr309	CD1	3.026	4.5	114.3
2465	2HVN	A	Tyr309	CE1	3.075	3.0	129.5
2466	2HVN	A	Tyr309	HD1	2.634	1.3	93.4
2467	2HVN	A	Pro310	CD	3.068	3.2	114.4
2468	2HVN	A	Pro310	HD2	2.308	13.6	126.8
2469	2HVO	A	Trp111	HE3	2.571	3.7	117.6
2470	2HVO	A	Cys303	CB	3.103	2.1	120.4
2471	2HVO	A	Cys303	HB3	2.264	15.2	135.5
2472	2HVO	A	Tyr309	HD1	2.667	0.1	101.4
2473	2HVO	A	Tyr309	CD1	3.060	3.5	124.8
2474	2HVO	A	Tyr309	CE1	3.167	0.1	140.5
2475	2HVO	A	Tyr309	HD1	2.601	2.6	104.4
2476	2HVO	A	Pro310	HD2	2.507	6.1	131.7
2477	2HWI	A	Arg422	HB2	2.511	6.0	127.4
2478	2HWI	A	Met423	N	2.871	4.9	164.4
2479	2HWI	A	Met423	HB2	2.473	7.4	105.3
2480	2HWI	B	Arg422	HB2	2.425	9.2	131.2
2481	2HWI	B	Met423	N	2.899	4.0	166.1
2482	2HWI	B	Met423	HB2	2.365	11.4	106.5
2483	2HZ0	B	Ala380	HA	2.496	6.5	110.8
2484	2HZN	A	Ala380	CA	3.016	4.9	142.4
2485	2HZN	A	Ala380	C	3.030	4.4	144.1
2486	2HZN	A	Ala380	HA	2.355	11.8	124.4
2487	2I0H	A	Leu75	CD1	3.066	3.3	128.3
2488	2I0H	A	Leu104	HB3	2.459	7.9	139.2
2489	2I0H	A	Leu104	HB3	2.427	9.1	142.6
2490	2I0H	A	Thr106	CG2	3.063	3.4	79.0
2491	2I0U	A	Trp20	CZ2	3.137	1.1	114.0
2492	2I0U	A	Trp20	HZ2	2.120	20.6	119.4
2493	2I0U	E	Trp20	CZ2	2.971	6.3	167.1
2494	2I0U	E	Trp20	HE1	2.580	3.4	108.4
2495	2I0U	E	Trp20	HZ2	2.049	23.3	164.5
2496	2I1R	A	Arg422	HB2	2.478	7.2	143.4
2497	2I1R	A	Met423	HB2	2.591	3.0	101.6
2498	2I1R	B	Arg422	HB2	2.614	2.1	137.8
2499	2I1R	B	Met423	HB2	2.455	8.0	107.9
2500	2I4Q	A	Thr80	HB	2.490	6.7	125.3
2501	2I4Q	B	Leu116	CD1	3.156	0.4	102.5
2502	2I4Q	B	Thr80	CB	2.886	9.0	136.7
2503	2I4Q	B	Thr80	CG2	2.955	6.8	144.9
2504	2I4Q	B	Thr80	HB	2.253	15.6	134.3
2505	2I16	A	Tyr49	HD1	2.512	5.9	118.0

2506	2I16	A	Ala300	CA	3.046	3.9	161.5
2507	2I16	A	Ala300	C	2.996	5.5	134.6
2508	2I16	A	Ala300	HA	2.601	2.6	153.5
2509	2I17	A	Tyr49	HD1	2.502	6.3	118.1
2510	2I17	A	Ala300	CA	3.049	3.8	161.5
2511	2I17	A	Ala300	C	2.987	5.8	134.9
2512	2I17	A	Ala300	HA	2.605	2.5	153.4
2513	2I78	B	Arg125	NH2	2.786	7.8	168.8
2514	2I78	B	Arg125	HH21	2.668	0.1	157.8
2515	2I78	B	Arg125	HH22	2.264	15.2	159.1
2516	2I78	B	Tyr631	HD2	2.441	8.6	141.5
2517	2I78	B	Phe357	HE2	2.620	1.9	116.6
2518	2I80	A	Phe92	HD1	2.610	2.2	149.5
2519	2I80	A	Val117	CG1	3.110	1.9	103.1
2520	2I80	A	Pro93	HD2	2.503	6.2	139.5
2521	2I80	A	Gly118	HA3	2.451	8.2	127.1
2522	2I80	A	Gly118	HA3	2.465	7.7	155.2
2523	2I80	B	Gly118	HA3	2.373	11.1	164.7
2524	2IGO	A	Thr169	HB	2.633	1.4	103.6
2525	2IGO	A	Gln448	NE2	2.919	3.3	102.9
2526	2IGO	B	Gln448	NE2	2.923	3.2	102.2
2527	2IGO	D	Thr169	HB	2.654	0.6	107.7
2528	2IGO	D	Gln448	NE2	2.968	1.7	103.6
2529	2IGO	C	Gln448	NE2	2.803	7.2	107.2
2530	2IGO	E	Gln448	NE2	2.834	6.2	112.0
2531	2IGO	F	Thr169	HB	2.586	3.1	115.9
2532	2IGO	H	Gln448	NE2	2.836	6.1	107.0
2533	2IGO	G	Thr169	HB	2.576	3.5	111.6
2534	2IGO	G	Gln448	NE2	2.879	4.7	101.6
2535	2IHJ	A	Asp141	OD2	2.614	12.6	96.8
2536	2IHK	A	Asp141	O	2.720	9.0	162.2
2537	2IHZ	A	Asp141	OD2	2.438	18.5	88.8
2538	2IIT	A	Tyr631	HB2	2.628	1.6	99.0
2539	2IIT	A	Tyr631	HD2	2.303	13.7	144.0
2540	2IIT	A	Val656	CG2	3.068	3.2	140.3
2541	2IIT	B	Tyr631	HD2	2.392	10.4	149.0
2542	2IIT	B	Val656	CG2	3.026	4.5	146.6
2543	2IIV	A	Tyr631	HB2	2.578	3.4	98.4
2544	2IIV	A	Tyr631	HD2	2.223	16.7	149.8
2545	2IIV	A	Arg125	HH22	2.502	6.3	147.0
2546	2IIV	B	Tyr631	HD2	2.155	19.3	148.2
2547	2IIV	B	Arg125	HH22	2.611	2.2	143.2
2548	2IIV	B	Asn710	ND2	3.002	0.6	130.9
2549	2IIV	B	Val656	CG2	2.997	5.5	154.8

2550	2IJ7	A	Thr229	CG2	2.524	20.4	130.3
2551	2IJ7	A	Asn85	HB3	2.502	6.3	101.4
2552	2IJ7	A	Met86	H	2.368	11.3	160.1
2553	2IJ7	A	Phe168	HE2	2.395	10.3	159.7
2554	2IJ7	B	Asn85	HB3	2.599	2.7	107.7
2555	2IJ7	B	Met86	H	2.635	1.3	161.7
2556	2IJ7	C	Asn85	HB3	2.369	11.3	104.2
2557	2IJ7	C	Met86	H	2.463	7.8	169.2
2558	2IJ7	D	Thr229	CB	3.073	3.1	140.3
2559	2IJ7	D	Thr229	HB	2.064	22.7	130.4
2560	2IJ7	D	Asn85	HB3	2.299	13.9	104.7
2561	2IJ7	D	Met86	H	2.551	4.5	154.5
2562	2IJ7	D	Phe168	HE2	2.566	3.9	163.4
2563	2IJ7	F	Thr229	HB	2.653	0.6	118.7
2564	2IJ7	F	Asn85	CB	3.166	0.1	107.4
2565	2IJ7	F	Asn85	HB3	2.203	17.5	110.5
2566	2IJ7	F	Met86	H	2.519	5.7	167.7
2567	2IJ7	F	Phe168	HE2	2.466	7.6	169.4
2568	2IJN	A	Arg386	NH1	2.904	3.8	110.8
2569	2IJN	A	Arg386	HH11	2.077	22.2	118.9
2570	2IJN	A	Tyr415	OH	2.721	9.0	129.4
2571	2IJN	A	Tyr415	HH	1.854	30.5	123.4
2572	2IJN	A	Leu384	CD2	3.114	1.8	107.7
2573	2IJN	A	Tyr448	OH	2.824	5.6	153.0
2574	2IJN	A	Tyr448	HE1	2.472	7.4	106.5
2575	2IJN	A	Met414	HE3	2.531	5.2	137.5
2576	2IJN	B	Ser367	HB2	2.599	2.7	114.4
2577	2IJN	B	Arg386	NH1	2.739	9.3	110.1
2578	2IJN	B	Arg386	HD2	2.652	0.7	165.8
2579	2IJN	B	Arg386	HH11	1.901	28.8	120.9
2580	2IJN	B	Tyr415	OH	2.751	8.0	131.1
2581	2IJN	B	Tyr415	HH	1.896	29.0	126.0
2582	2IJN	B	Leu384	CD2	3.156	0.4	107.4
2583	2IJN	B	Tyr448	OH	2.906	2.8	153.5
2584	2IJN	B	Tyr448	HE1	2.446	8.4	107.8
2585	2IJN	B	Met414	HE3	2.497	6.5	130.5
2586	2IKI	A	Ala299	CA	3.137	1.1	160.0
2587	2IKI	A	Ala299	C	3.124	1.5	132.6
2588	2IKI	A	Ala299	HA	2.660	0.4	157.6
2589	2IKO	A	Thr80	HB	2.595	2.8	117.3
2590	2INX	A	Tyr16	OH	2.919	2.4	109.4
2591	2INX	A	Tyr16	HH	2.364	11.5	96.4
2592	2INX	A	Asn40	ND2	2.748	9.0	92.0
2593	2INX	A	Ala118	CB	2.881	9.1	172.5

2594	2INX	A	Ala118	HB1	2.275	14.8	164.0
2595	2INX	A	Ala118	HB2	2.643	1.0	153.9
2596	2IQG	A	Gly74	N	3.018	0.1	139.1
2597	2IQG	A	Gly74	H	2.381	10.8	131.0
2598	2IQG	A	Phe108	HD1	2.199	17.7	95.7
2599	2IQG	A	Trp115	CZ2	3.139	1.0	129.1
2600	2IQG	A	Trp115	HZ2	2.332	12.7	144.9
2601	2IRZ	A	Tyr14	HE1	2.352	11.9	145.6
2602	2IRZ	A	Ala335	CB	3.049	3.8	111.6
2603	2IRZ	A	Ala335	HB2	2.624	1.7	98.7
2604	2IS0	A	Tyr14	HE1	2.375	11.0	146.4
2605	2IS0	A	Ala335	CB	3.072	3.1	110.8
2606	2IS0	A	Ala335	HB2	2.615	2.1	98.6
2607	2ITZ	A	Lys745	HE2	2.342	12.3	87.0
2608	2IVD	B	Ile168	C	3.124	1.4	133.2
2609	2IVD	B	Ile412	CD1	3.052	3.7	117.7
2610	2IVU	A	Ala756	CB	3.158	0.4	147.6
2611	2IVU	A	Ala756	HB1	2.610	2.3	157.1
2612	2IW1	A	Arg208	HH22	2.567	3.9	145.5
2613	2IY7	A	Asp141	OD2	2.710	9.4	106.0
2614	2IZS	A	Asn53	OD1	2.625	12.2	125.5
2615	2J51	A	Val48	CG1	3.163	0.2	151.2
2616	2JC0	A	Cys366	HB2	2.465	7.7	108.2
2617	2JC0	A	Ser368	HG	2.560	4.1	130.0
2618	2JC0	A	Cys366	HG	2.543	4.7	132.3
2619	2JC0	A	Met423	CG	2.499	21.2	124.0
2620	2JC0	A	Met423	HG2	2.146	19.6	149.6
2621	2JC0	A	Met423	HG3	2.052	23.1	102.9
2622	2JC0	A	Trp528	CD2	2.839	10.4	117.8
2623	2JC0	A	Trp528	CE3	2.993	5.6	127.2
2624	2JC0	A	Leu419	HA	2.288	14.3	162.9
2625	2JC0	A	Arg422	HB2	2.359	11.7	116.4
2626	2JC0	A	Met423	HG3	2.370	11.2	87.6
2627	2JC0	A	Arg422	CZ	2.784	12.2	144.6
2628	2JC0	A	Arg422	NH1	2.712	10.2	124.8
2629	2JC0	A	Trp528	CB	3.144	0.8	124.4
2630	2JC0	A	Trp528	CG	2.952	6.9	113.1
2631	2JC0	B	Cys366	HB2	2.652	0.7	103.8
2632	2JC0	B	Ser368	HG	2.577	3.5	130.8
2633	2JC0	B	Cys366	HG	2.643	1.0	138.7
2634	2JC0	B	Met423	CG	2.184	31.1	138.0
2635	2JC0	B	Met423	SD	2.951	9.8	121.6
2636	2JC0	B	Met423	HG2	1.855	30.5	166.7
2637	2JC0	B	Met423	HG3	1.859	30.4	110.0

2638	2JC0	B	Trp528	CD2	3.129	1.3	101.4
2639	2JC0	B	Trp528	CE3	3.112	1.8	115.1
2640	2JC0	B	Leu419	HA	2.645	0.9	157.0
2641	2JC0	B	Arg422	HB2	2.611	2.2	107.4
2642	2JC0	B	Met423	HG3	2.521	5.6	80.4
2643	2JC0	B	Arg422	CZ	2.935	7.4	127.8
2644	2JC0	B	Trp528	CB	2.910	8.2	134.2
2645	2JC0	B	Trp528	CG	2.737	13.7	126.4
2646	2JFL	A	Val48	CG1	3.136	1.1	157.8
2647	2JFL	A	Val48	CG2	2.969	6.3	128.5
2648	2JIE	A	Glu356	OE1	2.725	8.8	51.3
2649	2JJI	A	Gly37	HA3	2.531	5.2	134.5
2650	2JJI	A	Asp219	OD2	2.942	1.6	108.1
2651	2JJJ	A	Asp219	OD2	2.959	1.0	107.3
2652	2JLD	A	Lys85	HZ2	2.189	18.0	169.4
2653	2JLD	A	Asp200	CG	3.066	3.3	120.5
2654	2JLD	B	Lys85	HD2	2.502	6.3	108.6
2655	2JLD	B	Lys85	HZ2	2.120	20.6	169.7
2656	2NLR	A	Glu120	CD	2.841	10.4	86.8
2657	2NLR	A	Glu120	CD	3.080	2.8	83.2
2658	2NLR	A	Glu120	OE1	1.993	33.3	107.6
2659	2NLR	A	Glu120	OE1	2.945	1.5	91.2
2660	2NLR	A	Glu120	OE1	2.797	6.5	61.1
2661	2NLR	A	Glu120	OE2	2.920	2.3	60.7
2662	2NLR	A	Asn155	ND2	2.740	9.3	123.7
2663	2NLR	A	Glu120	OE1	2.727	8.8	112.7
2664	2NLR	A	Ile134	CD1	3.141	0.9	107.8
2665	2NLR	A	Asn155	ND2	2.930	3.0	122.1
2666	2NO0	A	Arg128	HH12	2.355	11.8	143.9
2667	2NO0	A	Ile30	CD1	3.094	2.4	130.7
2668	2NO0	A	Tyr86	OH	2.783	6.9	122.9
2669	2NO0	B	Arg128	NH1	2.936	2.8	157.7
2670	2NO0	B	Arg128	HH12	2.294	14.1	146.3
2671	2NO0	B	Ile30	CD1	3.122	1.5	130.3
2672	2NO0	B	Tyr86	OH	2.872	3.9	125.5
2673	2NO6	A	Arg104	NH2	2.861	5.3	162.4
2674	2NO6	A	Arg104	HH21	2.436	8.8	148.5
2675	2NO6	A	Arg104	HH22	2.605	2.4	157.5
2676	2NO6	B	Arg104	NH2	2.818	6.7	158.5
2677	2NO6	B	Arg104	HH21	2.431	8.9	146.9
2678	2NO6	B	Arg104	HH22	2.529	5.3	152.4
2679	2NP8	A	Lys143	NZ	2.918	3.4	108.1
2680	2NP8	A	Lys143	HZ3	1.974	26.1	115.5
2681	2NP8	A	Gly142	CA	2.872	9.4	115.3

2682	2NP8	A	Gly142	HA2	2.409	9.8	93.4
2683	2NP8	A	Gly142	HA3	2.582	3.3	131.9
2684	2NP8	A	Gly142	HA2	2.425	9.2	92.6
2685	2NUD	A	Gly267	H	2.452	8.2	81.3
2686	2NUD	A	Gly267	HA2	2.397	10.2	124.1
2687	2NUD	A	Arg266	CD	3.151	0.6	171.5
2688	2NUD	A	Arg266	NE	2.656	12.1	149.2
2689	2NUD	A	Arg266	HG3	2.632	1.4	130.3
2690	2NUD	A	Arg266	HE	1.983	25.7	138.7
2691	2NUD	A	Gly267	H	2.241	16.1	90.2
2692	2NUD	B	Arg266	NE	2.959	2.0	127.2
2693	2NUD	B	Arg266	HE	2.215	17.0	118.8
2694	2NUD	B	Gly267	H	2.158	19.2	101.0
2695	2NW9	B	Tyr27	HD2	2.374	11.1	114.2
2696	2NW9	B	Leu28	HG	2.489	6.8	161.2
2697	2O2U	A	Met146	HG2	2.454	8.1	96.7
2698	2O4L	A	Arg8	CD	3.125	1.4	124.0
2699	2O4L	A	Arg8	HD3	2.355	11.8	130.9
2700	2O4L	B	Arg8	CZ	3.088	2.6	93.0
2701	2O4L	B	Arg8	NH1	2.749	9.0	113.8
2702	2O4L	B	Arg8	HH12	2.663	0.2	133.1
2703	2O4L	A	Arg8	CZ	2.889	8.9	98.0
2704	2O4L	A	Arg8	NH1	2.523	16.5	122.5
2705	2O4L	A	Arg8	HH12	2.641	1.1	140.4
2706	2O4L	B	Val82	CG2	3.159	0.3	126.9
2707	2O4L	A	Val82	CG1	2.887	8.9	139.1
2708	2O4N	B	Leu82	CD2	3.103	2.1	128.0
2709	2O5D	A	Arg422	CB	3.160	0.3	130.6
2710	2O5D	A	Arg422	HB2	2.516	5.8	125.5
2711	2O5D	A	Met423	N	2.806	7.1	168.6
2712	2O5D	A	Met423	H	2.591	3.0	154.2
2713	2O5D	A	Met423	HB2	2.353	11.9	106.0
2714	2O5D	B	Met423	N	2.841	5.9	170.6
2715	2O5D	B	Met423	CA	3.084	2.7	150.8
2716	2O5D	B	Met423	CB	3.049	3.8	125.7
2717	2O5D	B	Met423	HB2	2.212	17.2	110.0
2718	2O9I	A	Leu209	O	2.762	7.6	116.5
2719	2O9I	A	Leu209	CB	3.020	4.7	116.1
2720	2O9I	A	Leu209	HB3	2.039	23.6	124.8
2721	2O9I	A	Leu209	CD2	3.009	5.1	131.9
2722	2O9I	A	Phe420	CE1	3.132	1.2	140.8
2723	2O9I	A	Phe420	HE1	2.277	14.7	130.8
2724	2O9I	A	Met243	HB3	2.408	9.8	147.9
2725	2O9I	B	Met1323	HB3	2.563	4.0	124.0

2726	209I	B	Met1323	HE3	2.488	6.8	160.2
2727	209I	B	Trp1299	HH2	2.530	5.3	102.6
2728	209I	B	Leu1324	CD1	3.055	3.6	133.3
2729	209I	B	Phe1420	CE1	3.068	3.2	161.9
2730	209I	B	Phe1420	HE1	2.181	18.3	159.8
2731	209I	B	Met1243	CB	3.041	4.1	125.5
2732	209I	B	Met1243	HB3	2.405	9.9	111.2
2733	209I	B	Ser1247	HG	2.606	2.4	156.3
2734	209I	B	Ile1414	CD1	3.167	0.1	123.5
2735	2OAG	B	Arg125	NH2	3.016	0.1	162.2
2736	2OAG	B	Arg125	HH22	2.479	7.1	148.5
2737	2OAG	B	Val711	CG2	3.056	3.6	110.3
2738	2OAG	B	Tyr631	HB2	2.534	5.1	102.0
2739	2OAG	B	Tyr631	HD2	2.276	14.7	145.4
2740	2OFV	B	Leu300	CD2	2.953	6.8	126.7
2741	2OGZ	A	Tyr631	HA	2.602	2.6	124.2
2742	2OGZ	B	Tyr631	HA	2.429	9.0	124.5
2743	2OGZ	B	Val656	CG2	3.045	3.9	107.9
2744	2OH4	A	Glu883	HG3	2.299	13.9	140.3
2745	2OH4	A	Cys1043	C	3.130	1.3	145.7
2746	2OH4	A	Cys1043	HA	2.638	1.2	123.9
2747	2OJJ	A	Gly32	CA	3.153	0.5	109.6
2748	2OJJ	A	Gly32	HA3	2.399	10.1	94.0
2749	2OJJ	A	Gly35	C	3.073	3.1	138.3
2750	2OJJ	A	Gly35	O	2.896	3.1	151.9
2751	2OLE	A	Tyr631	HD2	2.234	16.3	155.7
2752	2OLE	B	Tyr631	HD2	2.337	12.5	150.2
2753	2OLE	B	Val711	CG2	3.166	0.1	117.4
2754	2OLE	B	Arg125	NH2	3.018	0.1	154.8
2755	2OLE	B	Arg125	HH22	2.531	5.2	162.0
2756	2ONG	B	Arg315	HH22	2.288	14.3	85.5
2757	2ONG	B	Thr349	HA	2.611	2.2	105.9
2758	2ONH	A	Tyr573	OH	2.766	7.5	118.6
2759	2ONH	B	Tyr573	HH	2.336	12.5	82.2
2760	2OO8	X	Asp982	HB2	2.645	0.9	118.4
2761	2OO8	X	Ala981	HA	2.557	4.2	116.4
2762	2OOW	C	Ile64	CG2	2.934	7.5	84.8
2763	2OP3	A	Trp26	HB3	2.354	11.8	113.3
2764	2OP3	A	Gly165	HA3	2.669	0.0	130.3
2765	2OP3	A	Trp26	HB3	2.615	2.1	103.3
2766	2OP3	A	Gly69	H	2.453	8.1	114.3
2767	2OP3	B	Trp26	HB3	2.251	15.7	114.7
2768	2OP3	B	Gly165	HA3	2.656	0.5	129.5
2769	2OP3	B	Cys25	SG	3.237	1.0	101.0

2770	2OP3	B	Trp26	HB3	2.617	2.0	102.0
2771	2OP3	B	Gly69	H	2.473	7.4	110.0
2772	2OPA	A	Met7	HA	2.629	1.5	132.3
2773	2OPA	B	Pro1	CA	3.022	4.7	110.3
2774	2OPA	B	Pro1	H3	2.371	11.2	71.7
2775	2OPA	B	Pro1	HA	2.163	19.0	125.7
2776	2OPB	A	Glu219	OE2	2.633	11.9	134.7
2777	2OPB	B	Ala186	HB2	2.607	2.4	119.0
2778	2OPB	B	Glu219	OE2	2.850	4.7	119.1
2779	2OPH	A	Tyr631	CB	3.013	4.9	154.3
2780	2OPH	A	Tyr631	HB2	2.067	22.6	157.8
2781	2OPH	A	Tyr631	HD2	2.568	3.8	98.4
2782	2OPH	B	Tyr631	HB2	2.287	14.4	165.0
2783	2OPH	B	Tyr631	HD2	2.433	8.9	105.2
2784	2OPP	A	Phe227	HD2	2.377	11.0	161.5
2785	2OPQ	A	Phe227	HD2	2.511	5.9	154.9
2786	2OPR	A	Phe227	HD2	2.406	9.9	147.7
2787	2OPS	A	Phe227	HD2	2.423	9.2	165.2
2788	2OQI	B	Tyr631	HD2	2.214	17.1	148.1
2789	2OQI	B	Arg125	HH22	2.438	8.7	151.8
2790	2OQV	A	Arg125	HH21	2.608	2.3	149.4
2791	2OQV	A	Tyr631	HB2	2.496	6.5	104.9
2792	2OQV	A	Tyr631	HD2	2.237	16.2	160.8
2793	2OSC	A	Leu879	CD1	3.106	2.0	102.8
2794	2OSC	A	Phe960	CZ	2.993	5.6	136.1
2795	2OW1	A	His411	HE1	2.492	6.6	106.2
2796	2OW1	B	His411	HE1	2.578	3.4	100.5
2797	2OW2	A	Pro421	O	2.936	1.8	121.7
2798	2OW2	B	Leu187	CG	2.854	10.0	132.9
2799	2OW2	B	Leu187	HG	1.811	32.2	138.9
2800	2P4I	A	Ile980	O	2.820	5.7	156.8
2801	2P4I	B	His962	HE2	2.643	1.0	165.3
2802	2P4I	B	Ala981	C	3.092	2.5	127.1
2803	2P4I	B	Ala981	O	2.912	2.6	150.1
2804	2P4Y	A	Tyr327	HE2	2.306	13.6	111.4
2805	2P4Y	B	Met364	CE	2.899	8.5	162.6
2806	2P4Y	B	Met364	HE1	2.065	22.7	171.1
2807	2P4Y	B	Tyr327	HE2	2.271	15.0	122.5
2808	2P5A	A	Leu104	C	3.153	0.5	117.6
2809	2P5A	A	Leu104	CB	3.109	1.9	111.4
2810	2P5A	A	Leu104	HB3	2.416	9.5	123.1
2811	2P5A	A	Pro242	HG2	2.585	3.2	103.6
2812	2P8H	A	Tyr14	CE1	3.106	2.0	135.4
2813	2P8H	A	Tyr14	HE1	2.287	14.3	150.9

2814	2P8H	A	Ala335	CB	3.018	4.8	112.0
2815	2P8H	A	Ala335	HB2	2.563	4.0	99.7
2816	2P8S	A	Tyr631	HD2	2.174	18.6	148.1
2817	2P8S	A	Tyr631	HB2	2.644	1.0	101.8
2818	2P8S	A	Tyr631	HD2	2.373	11.1	151.2
2819	2P8S	A	Arg125	NH2	2.974	1.5	146.9
2820	2P8S	A	Arg125	HH21	2.604	2.5	148.0
2821	2P8S	A	Arg125	HH22	2.640	1.1	138.2
2822	2P8S	A	Asn710	ND2	2.998	0.7	130.9
2823	2P8S	A	Ser209	HG	2.488	6.8	98.0
2824	2P8S	A	Ser209	OG	2.875	3.8	144.3
2825	2P8S	A	Ser209	HG	1.976	26.0	139.9
2826	2P8S	A	Val656	CG2	2.986	5.8	161.2
2827	2P8S	A	Val711	CG2	3.112	1.8	115.0
2828	2P8S	B	Tyr631	HD2	2.207	17.3	145.2
2829	2P8S	B	Tyr631	HD2	2.355	11.8	147.3
2830	2P8S	B	Arg125	NH2	2.909	3.7	145.0
2831	2P8S	B	Arg125	HH21	2.451	8.2	147.6
2832	2P8S	B	Ser209	HG	2.129	20.3	100.3
2833	2P8S	B	Ser209	HG	2.380	10.8	147.9
2834	2P8S	B	Val656	CG2	3.005	5.2	159.6
2835	2P8S	B	Val711	CG2	3.056	3.6	115.4
2836	2P15	A	Phe404	HZ	2.630	1.5	93.2
2837	2P15	A	Phe404	HZ	2.598	2.7	94.3
2838	2P15	B	Phe404	HZ	2.526	5.4	91.3
2839	2P15	B	Phe425	HD1	2.597	2.7	128.3
2840	2P15	B	Phe404	HZ	2.654	0.6	85.9
2841	2P55	A	Leu115	CD2	3.150	0.6	136.4
2842	2P55	A	Val211	CG2	3.166	0.1	129.4
2843	2P55	A	Ser212	N	2.967	1.8	163.4
2844	2P55	A	Ser212	CB	3.156	0.4	148.9
2845	2P55	A	Ser212	H	2.098	21.4	153.3
2846	2P55	A	Ser212	HB3	2.207	17.4	137.2
2847	2P55	A	Lys97	HD2	2.386	10.6	166.0
2848	2P83	A	Trp115	HZ2	2.428	9.1	146.8
2849	2P83	A	Gly74	H	2.659	0.4	129.7
2850	2P83	A	Phe108	HD1	2.154	19.3	98.0
2851	2P83	B	Trp115	CZ2	3.128	1.3	134.7
2852	2P83	B	Trp115	HZ2	2.470	7.5	152.5
2853	2P83	B	Gly74	H	2.354	11.8	128.2
2854	2P83	B	Phe108	HD1	2.249	15.8	98.2
2855	2P83	C	Trp115	CZ2	3.041	4.1	125.2
2856	2P83	C	Trp115	HZ2	2.142	19.8	137.8
2857	2P83	C	Gln73	HG3	2.581	3.3	116.3

2858	2P83	C	Gly74	H	2.613	2.1	137.4
2859	2P83	C	Phe108	HD1	2.450	8.2	102.7
2860	2PB1	A	His135	CE1	3.014	4.9	146.5
2861	2PB1	A	His135	NE2	2.978	1.4	122.0
2862	2PB1	A	His135	HE1	2.544	4.7	157.1
2863	2PB1	A	His135	HE2	2.484	7.0	103.9
2864	2PB1	A	Glu292	CD	3.109	1.9	83.7
2865	2PB1	A	Glu292	OE1	2.696	9.8	103.3
2866	2PB1	A	Glu292	OE2	2.906	2.8	60.6
2867	2PD5	A	Trp111	HE3	2.563	4.0	117.1
2868	2PD5	A	Pro310	HD3	2.622	1.8	116.1
2869	2PD5	A	Cys303	CB	3.096	2.3	118.0
2870	2PD5	A	Cys303	HB3	2.211	17.2	132.2
2871	2PD5	A	Tyr309	HD1	2.585	3.2	106.5
2872	2PD5	A	Pro310	CD	3.122	1.5	113.9
2873	2PD5	A	Pro310	HD2	2.286	14.4	125.0
2874	2PDB	A	Trp111	HE3	2.494	6.6	116.5
2875	2PDB	A	Cys303	CB	3.165	0.2	115.9
2876	2PDB	A	Cys303	HB3	2.257	15.5	129.3
2877	2PDB	A	Tyr309	HD1	2.638	1.2	106.1
2878	2PDB	A	Pro310	HD2	2.485	6.9	120.1
2879	2PDF	A	Trp111	HE3	2.544	4.7	111.1
2880	2PDF	A	Cys303	CB	2.924	7.8	130.2
2881	2PDF	A	Cys303	HB3	2.106	21.1	147.2
2882	2PDF	A	Tyr309	HD1	2.545	4.7	117.3
2883	2PDF	A	Pro310	HD2	2.502	6.3	115.1
2884	2PDI	A	Trp111	HE3	2.514	5.8	115.0
2885	2PDI	A	Thr113	CG2	3.154	0.5	113.0
2886	2PDI	A	Thr113	HG1	2.483	7.0	95.8
2887	2PDI	A	Cys303	HB3	2.215	17.0	122.1
2888	2PDI	A	Tyr309	CD1	3.097	2.3	121.7
2889	2PDI	A	Tyr309	HD1	2.599	2.6	101.8
2890	2PDI	A	Pro310	CD	3.144	0.8	116.0
2891	2PDI	A	Pro310	HD2	2.332	12.6	129.4
2892	2PDL	A	Cys303	HB2	2.649	0.8	129.9
2893	2PDL	A	Phe122	HD1	2.525	5.4	132.4
2894	2PDM	A	Trp111	HE3	2.462	7.8	120.8
2895	2PDM	A	Pro310	CD	3.105	2.0	102.8
2896	2PDM	A	Pro310	HD3	2.304	13.7	110.9
2897	2PDM	A	Thr113	HG1	2.592	2.9	98.7
2898	2PDM	A	Cys303	CB	3.013	5.0	115.8
2899	2PDM	A	Cys303	HB3	2.247	15.8	133.3
2900	2PDM	A	Tyr309	HD1	2.500	6.4	97.6
2901	2PDM	A	Tyr309	CD1	2.840	10.4	119.2

2902	2PDM	A	Tyr309	CE1	2.969	6.4	133.9
2903	2PDM	A	Tyr309	HD1	2.481	7.1	96.6
2904	2PDM	A	Pro310	CD	2.903	8.4	114.8
2905	2PDM	A	Pro310	HD2	2.208	17.3	132.5
2906	2PDX	A	Thr113	HG1	2.508	6.1	99.6
2907	2PDX	A	Leu301	HB2	2.379	10.9	124.2
2908	2PDX	A	Tyr309	HD1	2.322	13.0	114.0
2909	2PEV	A	Val47	O	2.944	1.6	143.9
2910	2PEV	A	Tyr48	HD1	2.586	3.1	117.4
2911	2PEV	A	Trp111	CH2	3.166	0.1	78.9
2912	2PEV	A	Ala299	CA	3.058	3.5	160.7
2913	2PEV	A	Ala299	C	3.001	5.3	135.3
2914	2PEV	A	Ala299	C	2.664	16.0	140.1
2915	2PEV	A	Ala299	HA	2.626	1.6	151.1
2916	2PEV	A	Leu300	N	1.617	46.5	132.9
2917	2PEV	A	Leu300	CA	1.836	42.1	83.0
2918	2PEV	A	Leu300	CB	1.970	37.8	55.4
2919	2PEV	A	Leu300	CG	3.110	1.9	31.7
2920	2PEV	A	Leu300	CD1	3.167	0.1	11.5
2921	2PF8	A	Val47	O	2.965	0.8	143.7
2922	2PF8	A	Tyr48	HD1	2.562	4.1	118.4
2923	2PF8	A	Ala299	CA	3.080	2.8	159.9
2924	2PF8	A	Ala299	C	3.004	5.2	134.0
2925	2PF8	A	Ala299	C	2.660	16.1	139.2
2926	2PF8	A	Leu300	N	1.604	46.9	130.9
2927	2PF8	A	Leu300	CA	1.874	40.9	81.4
2928	2PF8	A	Leu300	CB	2.014	36.5	54.5
2929	2PFH	A	Val47	O	2.900	3.0	143.1
2930	2PFH	A	Tyr48	HD1	2.609	2.3	120.0
2931	2PFH	A	Ala299	CA	2.949	7.0	160.4
2932	2PFH	A	Ala299	C	2.929	7.6	132.8
2933	2PFH	A	Ala299	C	2.611	17.6	138.6
2934	2PFH	A	Ala299	HA	2.492	6.7	152.8
2935	2PFH	A	Leu300	N	1.580	47.7	128.7
2936	2PFH	A	Leu300	CA	1.948	38.5	81.1
2937	2PFH	A	Leu300	CB	2.051	35.3	56.5
2938	2PH6	A	Tyr14	HE1	2.561	4.1	143.9
2939	2PH6	A	Ala335	CB	3.023	4.6	116.7
2940	2PH6	A	Ala335	HB2	2.648	0.8	103.3
2941	2PHB	A	Gly216	O	2.785	6.9	105.8
2942	2PHB	A	Glu217	HA	2.510	6.0	153.1
2943	2PIX	A	Phe673	CB	3.136	1.1	135.9
2944	2PIX	A	Phe673	CD1	3.059	3.5	114.6
2945	2PIX	A	Phe673	HB2	2.199	17.6	134.3

2946	2PIX	A	Phe673	HD1	2.569	3.8	96.1
2947	2PIX	A	Phe673	HD1	2.656	0.5	92.2
2948	2PKK	A	Ser8	CB	3.145	0.8	110.9
2949	2PKK	A	Ser8	HB3	2.365	11.4	123.8
2950	2PKK	A	Ser8	HG	2.659	0.4	74.8
2951	2PNU	A	His874	HD2	2.659	0.4	134.6
2952	2POW	A	Phe131	CZ	3.064	3.4	132.0
2953	2POW	A	Phe131	HZ	2.207	17.3	129.3
2954	2PQ9	A	Lys340	HB3	2.454	8.1	120.3
2955	2PQB	A	Arg128	HH22	2.260	15.4	110.0
2956	2PQB	A	Lys353	HD2	2.626	1.7	76.3
2957	2PQB	A	Glu354	CD	3.109	1.9	157.5
2958	2PQB	A	Glu354	OE1	2.198	26.5	175.6
2959	2PQD	A	Arg128	HH22	2.254	15.6	113.3
2960	2PQD	A	Lys353	HD2	2.625	1.7	74.8
2961	2PR3	A	Gly216	O	2.952	1.3	96.8
2962	2PR3	A	Glu217	HA	2.531	5.2	144.1
2963	2PU1	A	Ser40	OG	2.680	10.4	116.7
2964	2PU1	A	Gln164	CD	2.954	6.8	138.5
2965	2PU1	A	Gln164	OE1	2.721	9.0	113.5
2966	2PU1	A	Ser373	HB3	2.421	9.3	113.0

a d : contact distance of C–F $\cdots$ X, where C–F belongs to ligand and X is protein atom.

b SR: shortening rate. It indicates the percentage of d shorter than the sum of van der Waals radii of interacting atoms, F and X.

c θ : contact angle of $\angle$ C–F $\cdots$ X.