Dog POR WT interactions

Intraprotein Hydrophobic Interactions

DOG_POR_snapshot10.pdb

  [help]

Rasmol **Jmol**

Hydrophobic Interactions within 5 Angstroms

Position	Residue	Chain	Position	Residue	Chain
54	PHE	A	57	ILE	A
60	MET	A	64	ALA	A
69	PHE	A	117	TYR	A
69	PHE	A	119	LEU	A
69	PHE	A	122	LEU	A
69	PHE	A	125	LEU	A
69	PHE	A	70	VAL	A
69	PHE	A	73	MET	A
69	PHE	A	81	ILE	A
69	PHE	A	83	PHE	A
70	VAL	A	125	LEU	A
70	VAL	A	128	ILE	A
73	MET	A	110	MET	A
73	MET	A	125	LEU	A
73	MET	A	128	ILE	A
73	MET	A	81	ILE	A
80	ILE	A	102	ALA	A
80	ILE	A	107	MET	A
80	ILE	A	132	LEU	A
80	ILE	A	134	VAL	A
80	ILE	A	224	TRP	A
80	ILE	A	82	VAL	A
81	ILE	A	110	MET	A
81	ILE	A	112	ALA	A
81	ILE	A	125	LEU	A
81	ILE	A	133	ALA	A
81	ILE	A	83	PHE	A
82	VAL	A	111	ALA	A
82	VAL	A	134	VAL	A
82	VAL	A	95	ALA	A
82	VAL	A	98	LEU	A

83	PHE	A	112	ALA	A
83	PHE	A	114	PRO	A
83	PHE	A	117	TYR	A
83	PHE	A	119	LEU	A
83	PHE	A	122	LEU	A
83	PHE	A	133	ALA	A
83	PHE	A	135	PHE	A
83	PHE	A	137	MET	A
84	TYR	A	111	ALA	A
84	TYR	A	91	ALA	A
84	TYR	A	95	ALA	A
91	ALA	A	138	ALA	A
91	ALA	A	173	LEU	A
94	PHE	A	173	LEU	A
94	PHE	A	212	LEU	A
94	PHE	A	216	PHE	A
95	ALA	A	111	ALA	A
98	LEU	A	134	VAL	A
98	LEU	A	171	PHE	A
98	LEU	A	216	PHE	A
98	LEU	A	223	PHE	A
102	ALA	A	107	MET	A
102	ALA	A	224	TRP	A
105	TYR	A	107	MET	A
105	TYR	A	224	TRP	A
105	TYR	A	233	VAL	A
105	TYR	A	235	ALA	A
107	MET	A	224	TRP	A
107	MET	A	227	VAL	A
107	MET	A	231	PHE	A
107	MET	A	233	VAL	A
112	ALA	A	117	TYR	A
114	PRO	A	119	LEU	A
114	PRO	A	137	MET	A
114	PRO	A	152	PHE	A
117	TYR	A	119	LEU	A
119	LEU	A	122	LEU	A
119	LEU	A	135	PHE	A
119	LEU	A	152	PHE	A
119	LEU	A	155	TRP	A
120	ALA	A	155	TRP	A
120	ALA	A	161	VAL	A
122	LEU	A	125	LEU	A
122	LEU	A	133	ALA	A
122	LEU	A	135	PHE	A

122	LEU	A	155	TRP	A
122	LEU	A	163	LEU	A
122	LEU	A	166	VAL	A
122	LEU	A	192	LEU	A
125	LEU	A	126	PRO	A
125	LEU	A	128	ILE	A
125	LEU	A	133	ALA	A
125	LEU	A	166	VAL	A
126	PRO	A	166	VAL	A
132	LEU	A	134	VAL	A
132	LEU	A	169	ALA	A
132	LEU	A	200	ILE	A
132	LEU	A	223	PHE	A
132	LEU	A	227	VAL	A
132	LEU	A	231	PHE	A
133	ALA	A	135	PHE	A
133	ALA	A	168	TYR	A
134	VAL	A	169	ALA	A
134	VAL	A	171	PHE	A
134	VAL	A	223	PHE	A
135	PHE	A	137	MET	A
135	PHE	A	152	PHE	A
135	PHE	A	168	TYR	A
135	PHE	A	170	VAL	A
135	PHE	A	188	VAL	A
135	PHE	A	192	LEU	A
137	MET	A	152	PHE	A
137	MET	A	184	MET	A
137	MET	A	188	VAL	A
138	ALA	A	173	LEU	A
140	TYR	A	455	TYR	A
145	PRO	A	149	ALA	A
145	PRO	A	153	TYR	A
145	PRO	A	184	MET	A
149	ALA	A	184	MET	A
152	PHE	A	155	TRP	A
152	PHE	A	156	LEU	A
152	PHE	A	188	VAL	A
152	PHE	A	192	LEU	A
153	TYR	A	184	MET	A
153	TYR	A	187	TYR	A
155	TRP	A	156	LEU	A
155	TRP	A	161	VAL	A
155	TRP	A	163	LEU	A
156	LEU	A	187	TYR	A

156	LEU	A	188	VAL	A
156	LEU	A	192	LEU	A
156	LEU	A	195	LEU	A
161	VAL	A	163	LEU	A
163	LEU	A	166	VAL	A
163	LEU	A	192	LEU	A
163	LEU	A	195	LEU	A
163	LEU	A	197	ALA	A
166	VAL	A	197	ALA	A
168	TYR	A	170	VAL	A
168	TYR	A	192	LEU	A
168	TYR	A	197	ALA	A
169	ALA	A	201	PHE	A
169	ALA	A	223	PHE	A
170	VAL	A	188	VAL	A
170	VAL	A	192	LEU	A
170	VAL	A	203	LEU	A
171	PHE	A	201	PHE	A
171	PHE	A	216	PHE	A
171	PHE	A	219	TRP	A
171	PHE	A	223	PHE	A
173	LEU	A	212	LEU	A
178	TYR	A	674	LEU	A
178	TYR	A	676	VAL	A
181	PHE	A	205	MET	A
184	MET	A	188	VAL	A
187	TYR	A	188	VAL	A
188	VAL	A	192	LEU	A
192	LEU	A	195	LEU	A
192	LEU	A	197	ALA	A
200	ILE	A	201	PHE	A
200	ILE	A	226	ALA	A
200	ILE	A	227	VAL	A
200	ILE	A	231	PHE	A
201	PHE	A	219	TRP	A
201	PHE	A	223	PHE	A
201	PHE	A	226	ALA	A
203	LEU	A	205	MET	A
205	MET	A	219	TRP	A
216	PHE	A	217	ILE	A
223	PHE	A	224	TRP	A
223	PHE	A	227	VAL	A
224	TRP	A	225	PRO	A
224	TRP	A	227	VAL	A
224	TRP	A	233	VAL	A

227	VAL	A	231	PHE	A
227	VAL	A	233	VAL	A
231	PHE	A	233	VAL	A
245	TYR	A	348	LEU	A
245	TYR	A	360	PRO	A
247	LEU	A	249	VAL	A
247	LEU	A	346	MET	A
247	LEU	A	348	LEU	A
247	LEU	A	367	TYR	A
249	VAL	A	344	VAL	A
249	VAL	A	346	MET	A
253	ILE	A	258	VAL	A
253	ILE	A	345	VAL	A
253	ILE	A	364	PRO	A
255	MET	A	260	VAL	A
258	VAL	A	260	VAL	A
258	VAL	A	345	VAL	A
258	VAL	A	364	PRO	A
259	TYR	A	266	LEU	A
259	TYR	A	362	PRO	A
259	TYR	A	374	TYR	A
263	MET	A	269	TYR	A
263	MET	A	281	PRO	A
263	MET	A	323	TYR	A
263	MET	A	373	TYR	A
263	MET	A	374	TYR	A
263	MET	A	510	PRO	A
269	TYR	A	281	PRO	A
269	TYR	A	283	LEU	A
269	TYR	A	510	PRO	A
274	PRO	A	275	PRO	A
274	PRO	A	276	PHE	A
276	PHE	A	282	PHE	A
276	PHE	A	312	LEU	A
278	ALA	A	323	TYR	A
278	ALA	A	512	PHE	A
281	PRO	A	323	TYR	A
281	PRO	A	510	PRO	A
281	PRO	A	512	PHE	A
282	PHE	A	284	ALA	A
282	PHE	A	307	ILE	A
282	PHE	A	312	LEU	A
282	PHE	A	511	MET	A
283	LEU	A	508	LEU	A
283	LEU	A	510	PRO	A

284	ALA	A	305	LEU	A
284	ALA	A	307	ILE	A
284	ALA	A	511	MET	A
285	ALA	A	500	ALA	A
285	ALA	A	508	LEU	A
286	VAL	A	303	LEU	A
286	VAL	A	305	LEU	A
286	VAL	A	507	ALA	A
286	VAL	A	509	VAL	A
292	LEU	A	300	LEU	A
292	LEU	A	574	LEU	A
292	LEU	A	575	TYR	A
300	LEU	A	474	VAL	A
300	LEU	A	574	LEU	A
301	MET	A	303	LEU	A
301	MET	A	473	ALA	A
301	MET	A	475	ALA	A
301	MET	A	494	LEU	A
303	LEU	A	471	ILE	A
303	LEU	A	494	LEU	A
305	LEU	A	307	ILE	A
305	LEU	A	320	VAL	A
305	LEU	A	322	VAL	A
305	LEU	A	469	VAL	A
305	LEU	A	471	ILE	A
305	LEU	A	509	VAL	A
305	LEU	A	511	MET	A
307	ILE	A	312	LEU	A
307	ILE	A	314	TYR	A
307	ILE	A	469	VAL	A
307	ILE	A	511	MET	A
312	LEU	A	511	MET	A
312	LEU	A	513	VAL	A
314	TYR	A	458	ILE	A
314	TYR	A	469	VAL	A
314	TYR	A	513	VAL	A
320	VAL	A	322	VAL	A
320	VAL	A	456	TYR	A
320	VAL	A	458	ILE	A
320	VAL	A	469	VAL	A
320	VAL	A	471	ILE	A
320	VAL	A	511	MET	A
320	VAL	A	513	VAL	A
321	ALA	A	453	ALA	A
321	ALA	A	455	TYR	A

321	ALA	A	512	PHE	A
322	VAL	A	456	TYR	A
322	VAL	A	471	ILE	A
322	VAL	A	490	ALA	A
322	VAL	A	493	TRP	A
322	VAL	A	494	LEU	A
322	VAL	A	509	VAL	A
322	VAL	A	511	MET	A
323	TYR	A	324	PRO	A
323	TYR	A	453	ALA	A
323	TYR	A	510	PRO	A
323	TYR	A	512	PHE	A
324	PRO	A	451	LEU	A
324	PRO	A	489	VAL	A
324	PRO	A	490	ALA	A
324	PRO	A	493	TRP	A
325	ALA	A	373	TYR	A
325	ALA	A	493	TRP	A
330	LEU	A	377	ILE	A
330	LEU	A	428	LEU	A
331	VAL	A	342	LEU	A
331	VAL	A	371	LEU	A
331	VAL	A	377	ILE	A
334	LEU	A	338	LEU	A
334	LEU	A	371	LEU	A
334	LEU	A	377	ILE	A
334	LEU	A	427	ILE	A
334	LEU	A	428	LEU	A
334	LEU	A	431	LEU	A
334	LEU	A	441	ILE	A
334	LEU	A	444	LEU	A
337	ILE	A	338	LEU	A
337	ILE	A	428	LEU	A
337	ILE	A	431	LEU	A
338	LEU	A	340	ALA	A
338	LEU	A	431	LEU	A
338	LEU	A	439	PRO	A
338	LEU	A	441	ILE	A
338	LEU	A	444	LEU	A
340	ALA	A	342	LEU	A
340	ALA	A	441	ILE	A
342	LEU	A	367	TYR	A
342	LEU	A	371	LEU	A
342	LEU	A	441	ILE	A
344	VAL	A	367	TYR	A

345	VAL	A	364	PRO	A
346	MET	A	361	PHE	A
346	MET	A	367	TYR	A
346	MET	A	370	ALA	A
348	LEU	A	360	PRO	A
348	LEU	A	361	PHE	A
360	PRO	A	361	PHE	A
361	PHE	A	362	PRO	A
361	PHE	A	370	ALA	A
361	PHE	A	374	TYR	A
361	PHE	A	375	LEU	A
362	PRO	A	374	TYR	A
367	TYR	A	441	ILE	A
370	ALA	A	374	TYR	A
370	ALA	A	375	LEU	A
371	LEU	A	375	LEU	A
371	LEU	A	377	ILE	A
371	LEU	A	441	ILE	A
371	LEU	A	448	LEU	A
373	TYR	A	374	TYR	A
374	TYR	A	375	LEU	A
375	LEU	A	377	ILE	A
375	LEU	A	448	LEU	A
377	ILE	A	427	ILE	A
377	ILE	A	448	LEU	A
380	PRO	A	381	PRO	A
380	PRO	A	420	VAL	A
380	PRO	A	421	VAL	A
381	PRO	A	385	VAL	A
381	PRO	A	386	LEU	A
381	PRO	A	420	VAL	A
381	PRO	A	427	ILE	A
381	PRO	A	430	ILE	A
385	VAL	A	386	LEU	A
385	VAL	A	389	LEU	A
385	VAL	A	427	ILE	A
385	VAL	A	444	LEU	A
385	VAL	A	447	LEU	A
385	VAL	A	448	LEU	A
385	VAL	A	449	PRO	A
386	LEU	A	402	LEU	A
386	LEU	A	405	MET	A
386	LEU	A	416	TYR	A
386	LEU	A	420	VAL	A
386	LEU	A	430	ILE	A

387	TYR	A	406	ALA	A
389	LEU	A	392	TYR	A
389	LEU	A	437	LEU	A
389	LEU	A	439	PRO	A
389	LEU	A	444	LEU	A
389	LEU	A	447	LEU	A
390	ALA	A	402	LEU	A
392	TYR	A	437	LEU	A
392	TYR	A	439	PRO	A
392	TYR	A	440	PRO	A
393	ALA	A	402	LEU	A
393	ALA	A	437	LEU	A
402	LEU	A	430	ILE	A
402	LEU	A	434	TYR	A
402	LEU	A	437	LEU	A
405	MET	A	415	LEU	A
405	MET	A	416	TYR	A
405	MET	A	419	TRP	A
405	MET	A	420	VAL	A
405	MET	A	434	TYR	A
415	LEU	A	419	TRP	A
416	TYR	A	420	VAL	A
416	TYR	A	421	VAL	A
417	LEU	A	421	VAL	A
419	TRP	A	420	VAL	A
420	VAL	A	421	VAL	A
420	VAL	A	430	ILE	A
427	ILE	A	430	ILE	A
427	ILE	A	431	LEU	A
427	ILE	A	444	LEU	A
427	ILE	A	448	LEU	A
430	ILE	A	434	TYR	A
430	ILE	A	437	LEU	A
431	LEU	A	437	LEU	A
431	LEU	A	439	PRO	A
431	LEU	A	444	LEU	A
434	TYR	A	435	PRO	A
434	TYR	A	437	LEU	A
437	LEU	A	439	PRO	A
439	PRO	A	440	PRO	A
439	PRO	A	444	LEU	A
441	ILE	A	444	LEU	A
444	LEU	A	448	LEU	A
448	LEU	A	449	PRO	A
451	LEU	A	489	VAL	A

453	ALA	A	455	TYR	A
453	ALA	A	512	PHE	A
455	TYR	A	512	PHE	A
456	TYR	A	471	ILE	A
456	TYR	A	473	ALA	A
456	TYR	A	490	ALA	A
456	TYR	A	494	LEU	A
458	ILE	A	469	VAL	A
458	ILE	A	513	VAL	A
459	ALA	A	538	ALA	A
459	ALA	A	541	ILE	A
464	VAL	A	549	TRP	A
469	VAL	A	471	ILE	A
469	VAL	A	511	MET	A
471	ILE	A	473	ALA	A
471	ILE	A	494	LEU	A
476	VAL	A	478	TYR	A
490	ALA	A	493	TRP	A
490	ALA	A	494	LEU	A
493	TRP	A	494	LEU	A
493	TRP	A	509	VAL	A
493	TRP	A	510	PRO	A
494	LEU	A	509	VAL	A
500	ALA	A	507	ALA	A
509	VAL	A	510	PRO	A
509	VAL	A	511	MET	A
511	MET	A	513	VAL	A
518	PHE	A	539	PRO	A
518	PHE	A	540	PHE	A
518	PHE	A	543	PHE	A
518	PHE	A	628	TYR	A
520	LEU	A	521	PRO	A
520	LEU	A	543	PHE	A
521	PRO	A	528	VAL	A
521	PRO	A	543	PHE	A
521	PRO	A	628	TYR	A
524	ALA	A	550	LEU	A
524	ALA	A	557	VAL	A
527	PRO	A	619	LEU	A
527	PRO	A	625	ALA	A
528	VAL	A	530	MET	A
528	VAL	A	543	PHE	A
528	VAL	A	628	TYR	A
529	ILE	A	531	VAL	A
529	ILE	A	561	LEU	A

529	ILE	A	563	TYR	A
529	ILE	A	609	LEU	A
529	ILE	A	616	LEU	A
529	ILE	A	619	LEU	A
529	ILE	A	620	ILE	A
529	ILE	A	627	ILE	A
529	ILE	A	644	PHE	A
530	MET	A	540	PHE	A
530	MET	A	543	PHE	A
530	MET	A	544	ILE	A
530	MET	A	562	LEU	A
530	MET	A	628	TYR	A
531	VAL	A	533	PRO	A
531	VAL	A	563	TYR	A
531	VAL	A	605	VAL	A
531	VAL	A	609	LEU	A
531	VAL	A	629	VAL	A
531	VAL	A	640	VAL	A
531	VAL	A	644	PHE	A
533	PRO	A	605	VAL	A
533	PRO	A	636	MET	A
537	VAL	A	540	PHE	A
537	VAL	A	541	ILE	A
537	VAL	A	562	LEU	A
537	VAL	A	564	TYR	A
537	VAL	A	574	LEU	A
537	VAL	A	575	TYR	A
537	VAL	A	579	LEU	A
538	ALA	A	539	PRO	A
539	PRO	A	540	PHE	A
539	PRO	A	543	PHE	A
540	PHE	A	543	PHE	A
540	PHE	A	562	LEU	A
540	PHE	A	628	TYR	A
541	ILE	A	575	TYR	A
541	ILE	A	579	LEU	A
543	PHE	A	544	ILE	A
543	PHE	A	628	TYR	A
544	ILE	A	562	LEU	A
544	ILE	A	579	LEU	A
544	ILE	A	582	PHE	A
544	ILE	A	588	LEU	A
548	ALA	A	582	PHE	A
549	TRP	A	550	LEU	A
550	LEU	A	557	VAL	A

561	LEU	A	563	TYR	A
561	LEU	A	616	LEU	A
561	LEU	A	619	LEU	A
562	LEU	A	564	TYR	A
562	LEU	A	579	LEU	A
562	LEU	A	588	LEU	A
563	TYR	A	605	VAL	A
563	TYR	A	608	LEU	A
563	TYR	A	609	LEU	A
563	TYR	A	616	LEU	A
564	TYR	A	573	TYR	A
564	TYR	A	574	LEU	A
564	TYR	A	579	LEU	A
564	TYR	A	593	VAL	A
573	TYR	A	579	LEU	A
573	TYR	A	593	VAL	A
573	TYR	A	595	PHE	A
574	LEU	A	575	TYR	A
575	TYR	A	579	LEU	A
579	LEU	A	582	PHE	A
579	LEU	A	588	LEU	A
579	LEU	A	591	LEU	A
582	PHE	A	588	LEU	A
588	LEU	A	591	LEU	A
591	LEU	A	593	VAL	A
593	VAL	A	595	PHE	A
594	ALA	A	603	VAL	A
594	ALA	A	605	VAL	A
594	ALA	A	608	LEU	A
603	VAL	A	608	LEU	A
604	TYR	A	605	VAL	A
605	VAL	A	636	MET	A
605	VAL	A	640	VAL	A
609	LEU	A	616	LEU	A
609	LEU	A	640	VAL	A
609	LEU	A	644	PHE	A
609	LEU	A	647	ILE	A
616	LEU	A	619	LEU	A
616	LEU	A	620	ILE	A
616	LEU	A	644	PHE	A
616	LEU	A	647	ILE	A
617	TRP	A	620	ILE	A
617	TRP	A	647	ILE	A
617	TRP	A	648	VAL	A
617	TRP	A	651	VAL	A

617	TRP	A	654	MET	A
617	TRP	A	662	TYR	A
620	ILE	A	627	ILE	A
620	ILE	A	644	PHE	A
620	ILE	A	647	ILE	A
620	ILE	A	648	VAL	A
620	ILE	A	662	TYR	A
620	ILE	A	666	LEU	A
627	ILE	A	629	VAL	A
627	ILE	A	644	PHE	A
627	ILE	A	663	ILE	A
627	ILE	A	666	LEU	A
627	ILE	A	672	TYR	A
629	VAL	A	636	MET	A
629	VAL	A	637	ALA	A
629	VAL	A	640	VAL	A
629	VAL	A	644	PHE	A
629	VAL	A	672	TYR	A
629	VAL	A	674	LEU	A
629	VAL	A	676	VAL	A
633	ALA	A	676	VAL	A
636	MET	A	637	ALA	A
636	MET	A	640	VAL	A
637	ALA	A	676	VAL	A
640	VAL	A	644	PHE	A
644	PHE	A	647	ILE	A
644	PHE	A	663	ILE	A
644	PHE	A	672	TYR	A
645	TYR	A	659	ALA	A
645	TYR	A	660	VAL	A
645	TYR	A	663	ILE	A
647	ILE	A	648	VAL	A
647	ILE	A	651	VAL	A
648	VAL	A	654	MET	A
648	VAL	A	659	ALA	A
648	VAL	A	662	TYR	A
648	VAL	A	663	ILE	A
649	ALA	A	654	MET	A
649	ALA	A	659	ALA	A
654	MET	A	659	ALA	A
654	MET	A	662	TYR	A
662	TYR	A	663	ILE	A
662	TYR	A	666	LEU	A
663	ILE	A	666	LEU	A
663	ILE	A	667	MET	A

663	ILE	A	672	TYR	A
666	LEU	A	672	TYR	A
667	MET	A	672	TYR	A
667	MET	A	674	LEU	A
672	TYR	A	674	LEU	A
674	LEU	A	676	VAL	A

NO INTRAPROTEIN DISULPHIDE BRIDGES FOUND

Intraprotein Main Chain-Main Chain Hydrogen Bonds

  [help]

Rasmol **Jmol**

[View the original hbond output]

DOG_POR_snapshot10.pdb

DONOR PARAMETERS						ACCEPTOR					
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**Dd-a**	**Dh-a**	**A(d-H-N)**	**A(a-O=C)**
63	A	S	N	61	A	T	O	3.27	3.17	87.13	71.86
64	A	A	N	61	A	T	O	3.18	2.26	154.39	110.58
64	A	A	N	62	A	S	O	3.49	3.24	96.70	70.35
66	A	D	N	116	A	E	O	2.87	1.87	176.74	172.12
69	A	F	N	67	A	S	O	3.22	3.36	73.28	106.00
70	A	V	N	68	A	S	O	3.39	3.39	81.94	71.74
71	A	E	N	68	A	S	O	3.21	2.62	119.54	106.93
71	A	E	N	69	A	F	O	3.44	3.54	76.41	71.07
72	A	K	N	68	A	S	O	3.02	2.11	155.45	154.22
72	A	K	N	69	A	F	O	3.27	2.78	111.59	102.13
72	A	K	N	70	A	V	O	3.43	3.55	75.20	73.96
73	A	M	N	69	A	F	O	2.89	2.00	150.40	153.34
73	A	M	N	70	A	V	O	3.14	2.61	113.89	106.93
73	A	M	N	71	A	E	O	3.44	3.53	76.66	72.54
74	A	K	N	70	A	V	O	2.84	1.94	151.73	160.25

74	A	K	N	71	A	E	O	3.29	2.75	114.91	103.91
74	A	K	N	72	A	K	O	3.48	3.56	77.33	72.44
75	A	K	N	71	A	E	O	3.04	2.15	150.45	155.04
75	A	K	N	72	A	K	O	3.31	2.71	120.33	106.21
75	A	K	N	73	A	M	O	3.41	3.47	78.67	74.27
76	A	T	N	72	A	K	O	3.30	2.69	120.04	150.18
76	A	T	N	73	A	M	O	3.12	2.26	145.39	112.31
76	A	T	N	74	A	K	O	3.23	3.00	94.89	75.44
77	A	G	N	73	A	M	O	2.90	2.54	102.06	164.56
78	A	R	N	73	A	M	O	2.97	2.01	164.61	138.52
78	A	R	N	76	A	T	O	3.31	3.32	81.06	75.14
79	A	N	N	108	A	R	O	2.98	2.05	156.29	149.35
80	A	I	N	108	A	R	O	3.00	2.08	154.79	156.00
81	A	I	N	132	A	L	O	3.36	2.43	159.43	161.63
82	A	V	N	110	A	M	O	3.00	2.07	156.68	157.16
83	A	F	N	134	A	V	O	2.83	1.84	172.31	161.52
85	A	G	N	136	A	C	O	2.88	1.92	162.07	140.99
90	A	T	N	88	A	T	O	3.26	2.86	105.41	84.22
92	A	E	N	89	A	G	O	3.31	2.76	116.46	101.55
92	A	E	N	90	A	T	O	3.46	3.46	81.72	71.25
93	A	E	N	89	A	G	O	2.97	2.07	153.95	154.44
93	A	E	N	90	A	T	O	3.37	2.78	119.50	105.98
94	A	F	N	90	A	T	O	3.09	2.24	145.75	151.39
94	A	F	N	91	A	A	O	3.28	2.71	118.77	101.75
94	A	F	N	92	A	E	O	3.38	3.41	79.69	73.24
95	A	A	N	91	A	A	O	2.93	2.08	144.27	152.25
95	A	A	N	92	A	E	O	3.11	2.52	118.53	107.54
96	A	N	N	92	A	E	O	2.94	2.02	154.89	158.76
96	A	N	N	94	A	F	O	3.46	3.55	76.71	71.67
97	A	R	N	93	A	E	O	3.00	2.16	141.99	144.39
97	A	R	N	94	A	F	O	3.19	2.63	115.84	102.06
97	A	R	N	95	A	A	O	3.39	3.44	79.07	71.18
98	A	L	N	94	A	F	O	2.95	2.02	157.49	156.34
98	A	L	N	95	A	A	O	3.39	2.86	114.90	104.54
99	A	S	N	95	A	A	O	3.07	2.18	150.25	153.44
99	A	S	N	96	A	N	O	3.35	2.77	118.58	103.76
99	A	S	N	97	A	R	O	3.38	3.40	80.90	74.00
100	A	K	N	96	A	N	O	3.15	2.29	145.46	152.04
100	A	K	N	97	A	R	O	3.20	2.54	124.26	111.54
100	A	K	N	98	A	L	O	3.34	3.37	79.77	73.78
101	A	D	N	97	A	R	O	2.88	2.01	143.91	158.77
101	A	D	N	98	A	L	O	3.25	2.67	116.77	102.44
102	A	A	N	98	A	L	O	3.09	2.30	135.97	153.28
102	A	A	N	100	A	K	O	3.23	3.12	87.10	75.13
103	A	H	N	100	A	K	O	3.22	2.31	153.56	124.02

103	A	H	N	101	A	D	O	3.12	3.10	82.29	80.63
103	A	H	N	107	A	M	O	3.40	4.11	38.47	132.40
104	A	R	N	101	A	D	O	2.94	2.05	148.43	127.95
104	A	R	N	102	A	A	O	3.13	3.00	88.00	78.03
105	A	Y	N	102	A	A	O	3.02	2.08	156.24	122.93
105	A	Y	N	103	A	H	O	3.17	2.78	104.40	76.14
106	A	G	N	102	A	A	O	3.34	3.05	98.68	155.65
106	A	G	N	103	A	H	O	3.14	2.21	159.89	109.46
107	A	M	N	102	A	A	O	3.04	2.17	144.30	137.22
107	A	M	N	105	A	Y	O	3.39	3.08	99.63	72.35
110	A	M	N	80	A	I	O	3.36	2.49	145.42	140.91
112	A	A	N	82	A	V	O	2.85	1.92	155.82	164.60
115	A	E	N	113	A	D	O	3.09	2.91	91.21	81.92
116	A	E	N	113	A	D	O	3.05	2.10	163.32	131.11
116	A	E	N	114	A	P	O	3.38	3.18	93.17	70.85
119	A	L	N	117	A	Y	O	3.29	3.08	93.51	93.87
120	A	A	N	118	A	D	O	3.33	3.03	99.02	73.05
121	A	D	N	118	A	D	O	3.37	2.42	156.56	118.18
121	A	D	N	119	A	L	O	3.15	2.99	89.48	73.12
122	A	L	N	119	A	L	O	3.13	2.17	164.63	120.34
122	A	L	N	120	A	A	O	3.07	2.80	96.22	77.51
123	A	G	N	120	A	A	O	3.10	2.14	168.32	129.93
123	A	G	N	121	A	D	O	3.07	3.00	84.32	77.16
124	A	S	N	121	A	D	O	2.93	1.97	162.13	126.88
124	A	S	N	122	A	L	O	3.13	2.93	92.75	78.08
125	A	L	N	122	A	L	O	3.07	2.13	162.01	119.81
127	A	E	N	124	A	S	O	3.18	2.24	160.00	129.79
127	A	E	N	125	A	L	O	2.97	2.72	95.08	82.29
128	A	I	N	125	A	L	O	2.96	2.00	160.04	132.87
128	A	I	N	126	A	P	O	3.36	3.18	91.50	68.26
131	A	S	N	129	A	E	O	3.17	3.22	78.80	77.86
132	A	L	N	79	A	N	O	2.88	1.93	159.11	166.19
133	A	A	N	167	A	K	O	2.96	1.98	177.64	150.64
134	A	V	N	81	A	I	O	2.95	2.10	144.68	161.44
135	A	F	N	169	A	A	O	3.02	2.15	146.57	148.82
136	A	C	N	83	A	F	O	2.86	1.96	147.85	151.79
137	A	M	N	171	A	F	O	3.05	2.10	161.64	125.02
138	A	A	N	85	A	G	O	2.90	1.94	165.94	137.86
139	A	T	N	173	A	L	O	2.97	2.18	135.55	147.58
140	A	Y	N	144	A	D	O	2.99	2.12	144.33	162.10
142	A	E	N	140	A	Y	O	3.07	3.18	74.16	107.13
143	A	G	N	140	A	Y	O	2.97	2.09	147.55	152.71
143	A	G	N	141	A	G	O	3.11	3.05	84.72	80.46
144	A	D	N	140	A	Y	O	3.24	2.60	122.66	112.44
144	A	D	N	141	A	G	O	3.11	2.23	148.31	112.95

148	A	N	N	146	A	T	O	3.22	3.25	79.63	80.52
149	A	A	N	146	A	T	O	2.94	2.03	152.12	122.11
149	A	A	N	147	A	D	O	3.20	2.86	100.92	75.42
150	A	Q	N	146	A	T	O	3.24	2.85	105.20	165.58
150	A	Q	N	147	A	D	O	3.34	2.38	165.58	110.10
151	A	D	N	149	A	A	O	3.31	3.33	80.53	75.04
152	A	F	N	149	A	A	O	3.25	2.69	116.49	109.45
153	A	Y	N	149	A	A	O	2.87	1.95	153.90	161.12
153	A	Y	N	150	A	Q	O	3.42	2.90	114.11	98.98
154	A	D	N	150	A	Q	O	2.98	2.08	151.85	149.34
154	A	D	N	151	A	D	O	3.38	2.84	115.17	101.34
154	A	D	N	152	A	F	O	3.44	3.55	75.87	72.50
155	A	W	N	151	A	D	O	2.86	2.00	143.24	149.89
155	A	W	N	152	A	F	O	3.20	2.68	113.20	102.15
156	A	L	N	152	A	F	O	2.82	1.92	152.45	157.35
156	A	L	N	154	A	D	O	3.50	3.56	78.05	72.34
157	A	Q	N	153	A	Y	O	3.39	2.52	147.85	145.45
157	A	Q	N	154	A	D	O	3.30	2.65	124.28	107.72
157	A	Q	N	155	A	W	O	3.25	3.29	79.23	76.54
158	A	E	N	154	A	D	O	3.14	2.30	143.04	153.86
158	A	E	N	155	A	W	O	3.12	2.46	124.29	112.78
159	A	T	N	155	A	W	O	2.82	1.96	143.99	169.46
162	A	D	N	160	A	D	O	3.39	3.39	81.65	99.87
163	A	L	N	161	A	V	O	3.25	2.96	98.25	95.95
163	A	L	N	195	A	L	O	3.00	2.08	156.02	148.79
164	A	S	N	162	A	D	O	3.44	2.95	112.69	69.67
165	A	G	N	163	A	L	O	3.26	3.47	69.51	105.72
166	A	V	N	163	A	L	O	2.93	1.99	157.37	136.61
166	A	V	N	164	A	S	O	3.40	2.91	111.93	71.57
168	A	Y	N	198	A	Q	O	2.83	1.87	167.36	151.25
169	A	A	N	133	A	A	O	2.94	2.15	134.66	159.19
171	A	F	N	135	A	F	O	2.78	1.85	153.01	170.40
172	A	G	N	204	A	G	O	3.12	2.19	158.83	130.76
173	A	L	N	137	A	M	O	3.04	2.13	155.20	111.67
174	A	G	N	206	A	G	O	3.03	2.32	128.21	146.70
177	A	T	N	175	A	N	O	3.09	2.81	97.35	79.59
178	A	Y	N	175	A	N	O	3.02	2.08	160.24	131.07
178	A	Y	N	176	A	K	O	3.30	3.24	85.20	70.24
180	A	H	N	178	A	Y	O	3.33	3.32	81.98	67.93
181	A	F	N	178	A	Y	O	3.36	2.98	104.68	111.86
181	A	F	N	179	A	E	O	2.97	2.10	146.37	84.86
182	A	N	N	180	A	H	O	3.09	3.02	84.75	107.41
183	A	A	N	180	A	H	O	3.35	2.49	146.40	124.62
183	A	A	N	181	A	F	O	3.16	3.20	78.79	78.94
184	A	M	N	182	A	N	O	3.17	3.13	83.51	81.02

185	A	G	N	182	A	N	O	3.10	2.51	119.23	122.78
186	A	K	N	182	A	N	O	3.06	2.13	156.64	163.35
186	A	K	N	183	A	A	O	3.37	2.86	113.65	100.50
186	A	K	N	184	A	M	O	3.34	3.41	77.60	73.66
187	A	Y	N	183	A	A	O	2.97	2.09	149.65	152.79
187	A	Y	N	184	A	M	O	3.25	2.66	119.35	108.19
187	A	Y	N	185	A	G	O	3.50	3.57	77.89	73.82
188	A	V	N	184	A	M	O	3.09	2.14	163.06	158.82
188	A	V	N	185	A	G	O	3.37	2.88	112.41	106.77
189	A	D	N	185	A	G	O	2.92	1.98	158.11	157.99
189	A	D	N	187	A	Y	O	3.41	3.53	75.15	73.88
190	A	K	N	186	A	K	O	3.04	2.13	156.77	151.33
190	A	K	N	187	A	Y	O	3.30	2.77	115.43	108.28
190	A	K	N	188	A	V	O	3.45	3.54	76.75	75.73
191	A	R	N	187	A	Y	O	2.88	1.94	159.66	161.20
191	A	R	N	188	A	V	O	3.44	2.95	112.47	105.70
192	A	L	N	188	A	V	O	2.91	1.99	158.43	158.25
193	A	E	N	189	A	D	O	3.25	2.32	159.38	150.49
193	A	E	N	190	A	K	O	3.43	2.88	117.10	108.10
193	A	E	N	191	A	R	O	3.39	3.49	76.08	74.61
194	A	Q	N	190	A	K	O	3.11	2.21	151.57	155.06
194	A	Q	N	191	A	R	O	3.22	2.67	116.27	108.01
194	A	Q	N	192	A	L	O	3.40	3.47	77.75	73.98
195	A	L	N	191	A	R	O	2.93	2.15	134.34	158.80
195	A	L	N	192	A	L	O	3.20	2.48	129.82	107.11
195	A	L	N	193	A	E	O	3.38	3.28	87.29	73.50
196	A	G	N	192	A	L	O	3.28	2.79	111.01	149.37
196	A	G	N	193	A	E	O	2.95	2.09	144.09	112.84
196	A	G	N	194	A	Q	O	3.47	3.15	100.59	64.64
197	A	A	N	192	A	L	O	3.04	2.15	149.97	147.44
198	A	Q	N	166	A	V	O	2.85	1.86	169.78	157.73
200	A	I	N	168	A	Y	O	2.83	1.84	174.58	173.71
200	A	I	N	198	A	Q	O	3.32	3.02	98.89	99.96
204	A	G	N	170	A	V	O	2.89	1.90	171.16	136.79
204	A	G	N	202	A	E	O	3.05	3.00	83.00	109.03
205	A	M	N	203	A	L	O	3.04	2.43	119.24	93.71
206	A	G	N	172	A	G	O	2.79	1.83	163.60	162.93
206	A	G	N	204	A	G	O	3.10	2.67	107.14	100.84
208	A	D	N	174	A	G	O	2.87	1.91	160.81	152.47
209	A	D	N	207	A	D	O	3.38	3.07	100.19	72.19
210	A	G	N	207	A	D	O	3.39	2.53	145.41	115.10
210	A	G	N	208	A	D	O	3.46	3.42	84.19	66.91
212	A	L	N	210	A	G	O	3.17	2.83	100.97	94.79
213	A	E	N	211	A	N	O	3.46	3.49	80.60	74.92
214	A	E	N	211	A	N	O	3.41	2.85	116.77	108.93

215	A	D	N	211	A	N	O	3.02	2.14	147.03	154.91
215	A	D	N	212	A	L	O	3.37	2.83	115.02	99.92
215	A	D	N	213	A	E	O	3.33	3.39	78.53	72.04
216	A	F	N	212	A	L	O	2.89	2.11	136.09	150.24
216	A	F	N	213	A	E	O	3.14	2.49	123.63	104.87
217	A	I	N	213	A	E	O	3.08	2.16	155.69	155.36
217	A	I	N	214	A	E	O	3.37	2.81	117.39	104.67
217	A	I	N	215	A	D	O	3.44	3.53	76.73	71.73
218	A	T	N	214	A	E	O	3.01	2.15	146.28	149.11
218	A	T	N	215	A	D	O	3.16	2.64	112.77	102.07
218	A	T	N	216	A	F	O	3.39	3.47	77.08	71.04
219	A	W	N	215	A	D	O	2.91	2.01	152.00	154.47
219	A	W	N	216	A	F	O	3.15	2.63	113.36	105.71
219	A	W	N	217	A	I	O	3.41	3.56	73.36	74.50
220	A	R	N	216	A	F	O	2.79	1.99	136.59	157.22
220	A	R	N	217	A	I	O	3.15	2.51	122.81	105.12
221	A	E	N	217	A	I	O	3.20	2.30	151.82	155.46
221	A	E	N	219	A	W	O	3.30	3.36	78.21	73.66
222	A	Q	N	219	A	W	O	2.95	2.03	151.84	109.48
222	A	Q	N	220	A	R	O	3.29	2.82	109.63	73.08
223	A	F	N	219	A	W	O	2.81	1.89	152.64	163.56
223	A	F	N	220	A	R	O	3.34	2.79	115.84	103.62
224	A	W	N	220	A	R	O	3.00	2.05	171.43	158.02
226	A	A	N	223	A	F	O	3.17	2.53	122.97	121.85
226	A	A	N	224	A	W	O	3.23	3.28	78.32	79.92
227	A	V	N	223	A	F	O	3.16	2.22	158.84	163.99
227	A	V	N	224	A	W	O	3.18	2.63	115.33	115.96
227	A	V	N	225	A	P	O	3.42	3.51	76.98	73.45
228	A	C	N	224	A	W	O	2.79	1.86	154.66	169.01
228	A	C	N	225	A	P	O	3.29	2.77	112.92	101.37
229	A	E	N	225	A	P	O	2.90	1.98	158.11	155.61
229	A	E	N	227	A	V	O	3.47	3.58	75.66	74.02
230	A	H	N	226	A	A	O	3.05	2.17	150.49	149.10
230	A	H	N	227	A	V	O	3.33	2.79	115.66	105.13
231	A	F	N	227	A	V	O	2.90	1.94	165.80	159.89
232	A	G	N	228	A	C	O	3.04	2.43	119.62	138.21
233	A	V	N	231	A	F	O	3.20	2.88	99.88	76.34
236	A	T	N	104	A	R	O	2.91	1.97	157.46	147.66
239	A	E	N	237	A	G	O	3.32	2.82	111.47	91.24
241	A	S	N	239	A	E	O	3.17	2.80	102.46	75.46
242	A	I	N	240	A	S	O	3.42	3.58	72.33	78.31
246	A	E	N	349	A	N	O	2.93	1.98	159.94	156.69
248	A	V	N	347	A	S	O	2.82	1.85	163.79	168.39
250	A	H	N	345	A	V	O	2.94	1.98	162.01	142.66
256	A	A	N	254	A	D	O	3.08	2.98	86.57	79.12

257	A	K	N	254	A	D	O	2.93	1.98	161.12	129.90
257	A	K	N	255	A	M	O	3.13	2.91	93.47	77.47
258	A	V	N	255	A	M	O	3.13	2.21	155.30	117.45
259	A	Y	N	364	A	P	O	2.83	1.86	167.89	161.56
265	A	R	N	279	A	K	O	2.87	1.92	158.96	154.79
267	A	K	N	265	A	R	O	3.24	3.40	72.44	103.32
268	A	S	N	265	A	R	O	3.08	2.35	129.76	127.09
268	A	S	N	266	A	L	O	3.38	3.44	78.22	74.56
269	A	Y	N	267	A	K	O	3.25	3.11	89.24	75.36
270	A	E	N	267	A	K	O	3.14	2.27	146.94	116.87
270	A	E	N	268	A	S	O	3.39	3.24	89.99	71.55
271	A	N	N	268	A	S	O	3.02	2.13	149.16	106.88
273	A	K	N	271	A	N	O	2.94	2.17	132.88	97.91
277	A	D	N	280	A	N	O	3.14	2.19	161.89	118.81
279	A	K	N	277	A	D	O	3.19	3.14	83.61	80.60
280	A	N	N	277	A	D	O	3.00	2.21	137.08	120.09
282	A	F	N	511	A	M	O	2.89	1.93	161.34	156.12
284	A	A	N	282	A	F	O	3.31	2.94	103.22	92.83
284	A	A	N	509	A	V	O	2.90	1.92	167.42	143.34
286	A	V	N	507	A	A	O	2.97	2.00	168.47	142.99
287	A	T	N	285	A	A	O	3.08	2.54	114.19	92.55
287	A	T	N	304	A	E	O	3.11	2.43	125.57	144.11
288	A	T	N	286	A	V	O	3.38	3.27	87.57	75.51
290	A	R	N	302	A	H	O	2.92	1.96	163.54	167.70
292	A	L	N	300	A	L	O	2.79	1.81	174.13	132.68
294	A	Q	N	571	A	E	O	2.89	1.89	175.22	136.39
301	A	M	N	473	A	A	O	2.82	1.88	158.92	152.73
302	A	H	N	290	A	R	O	2.86	1.88	165.84	168.70
303	A	L	N	471	A	I	O	2.94	1.96	166.31	153.52
304	A	E	N	288	A	T	O	2.93	2.01	155.60	137.93
305	A	L	N	469	A	V	O	2.85	1.90	159.80	164.41
306	A	D	N	285	A	A	O	2.88	1.90	170.68	157.09
307	A	I	N	467	A	N	O	2.87	1.90	165.01	135.26
308	A	S	N	467	A	N	O	3.43	3.14	98.75	125.86
309	A	D	N	307	A	I	O	3.35	3.61	67.17	105.25
310	A	S	N	307	A	I	O	3.05	2.13	157.58	139.66
310	A	S	N	308	A	S	O	3.23	2.84	105.01	76.02
312	A	L	N	310	A	S	O	3.16	2.98	91.20	74.56
317	A	G	N	315	A	E	O	3.43	3.72	65.59	103.25
318	A	D	N	315	A	E	O	3.18	2.26	157.82	146.21
319	A	H	N	514	A	R	O	3.22	2.26	165.91	161.15
320	A	V	N	456	A	Y	O	2.88	1.91	163.48	171.52
321	A	A	N	512	A	F	O	2.89	1.90	174.01	163.50
322	A	V	N	454	A	R	O	2.93	1.97	163.81	156.47
323	A	Y	N	510	A	P	O	3.18	2.24	159.70	151.27

326	A	N	N	372	A	T	O	2.80	1.81	177.94	154.36
328	A	S	N	326	A	N	O	3.28	3.34	77.98	102.07
329	A	A	N	327	A	D	O	3.15	2.98	90.60	79.23
330	A	L	N	327	A	D	O	3.10	2.32	136.08	124.95
330	A	L	N	328	A	S	O	3.49	3.53	80.07	70.38
331	A	V	N	327	A	D	O	3.43	2.51	155.29	153.21
331	A	V	N	328	A	S	O	3.37	2.83	115.32	100.16
331	A	V	N	329	A	A	O	3.41	3.46	78.85	71.07
332	A	N	N	328	A	S	O	2.93	2.04	150.99	150.87
332	A	N	N	329	A	A	O	3.27	2.74	114.69	102.73
333	A	Q	N	329	A	A	O	2.94	2.02	155.68	154.84
333	A	Q	N	330	A	L	O	3.37	2.85	113.85	102.71
333	A	Q	N	331	A	V	O	3.43	3.52	76.84	74.08
334	A	L	N	330	A	L	O	2.99	2.11	147.79	152.68
334	A	L	N	331	A	V	O	3.27	2.67	118.90	107.48
334	A	L	N	332	A	N	O	3.36	3.40	79.49	74.82
335	A	G	N	331	A	V	O	3.04	2.16	151.23	156.11
335	A	G	N	332	A	N	O	3.14	2.57	117.65	110.14
335	A	G	N	333	A	Q	O	3.48	3.56	77.24	70.86
336	A	E	N	332	A	N	O	2.89	1.97	154.27	160.75
336	A	E	N	333	A	Q	O	3.32	2.81	112.52	101.63
337	A	I	N	333	A	Q	O	2.96	2.09	148.11	155.43
337	A	I	N	335	A	G	O	3.44	3.43	82.41	76.19
338	A	L	N	334	A	L	O	3.49	2.62	147.93	144.50
338	A	L	N	335	A	G	O	3.32	2.64	126.80	112.64
338	A	L	N	336	A	E	O	3.37	3.37	82.02	73.02
339	A	G	N	335	A	G	O	2.90	2.38	113.10	155.99
339	A	G	N	336	A	E	O	3.13	2.31	140.05	101.98
340	A	A	N	335	A	G	O	2.92	1.97	159.43	148.70
340	A	A	N	338	A	L	O	3.47	3.53	78.64	65.76
342	A	L	N	340	A	A	O	3.14	2.86	97.49	95.19
343	A	D	N	341	A	D	O	3.48	3.09	104.99	71.49
344	A	V	N	342	A	L	O	3.35	2.92	107.19	71.91
345	A	V	N	343	A	D	O	3.37	3.34	83.52	99.47
346	A	M	N	365	A	T	O	2.93	1.97	160.59	145.64
347	A	S	N	248	A	V	O	2.85	1.90	160.40	154.02
349	A	N	N	246	A	E	O	2.97	2.00	168.79	144.27
350	A	N	N	358	A	K	O	2.95	2.21	131.16	145.83
351	A	L	N	244	A	Q	O	3.24	2.26	170.87	154.45
352	A	D	N	350	A	N	O	3.37	3.31	84.90	68.70
353	A	E	N	351	A	L	O	3.47	3.29	91.53	98.58
358	A	K	N	356	A	N	O	3.04	2.23	138.39	85.43
359	A	H	N	357	A	K	O	3.26	3.14	87.98	76.11
363	A	C	N	361	A	F	O	3.35	3.58	69.05	106.89
365	A	T	N	346	A	M	O	2.94	1.98	164.12	170.68

367	A	Y	N	342	A	L	O	3.07	2.55	113.78	152.82
368	A	R	N	342	A	L	O	2.91	2.06	144.40	132.23
368	A	R	N	366	A	S	O	3.27	3.30	80.17	74.16
369	A	T	N	366	A	S	O	3.20	2.64	116.69	110.90
369	A	T	N	367	A	Y	O	3.43	3.56	74.51	73.49
370	A	A	N	366	A	S	O	2.97	2.05	157.69	160.02
370	A	A	N	367	A	Y	O	3.27	2.77	111.73	103.42
370	A	A	N	368	A	R	O	3.44	3.52	77.22	73.34
371	A	L	N	367	A	Y	O	2.99	2.03	164.08	157.66
371	A	L	N	368	A	R	O	3.37	2.86	113.30	108.96
371	A	L	N	369	A	T	O	3.43	3.58	73.55	75.84
372	A	T	N	368	A	R	O	2.92	2.08	142.36	157.80
372	A	T	N	369	A	T	O	3.25	2.64	121.06	105.71
372	A	T	N	370	A	A	O	3.42	3.38	84.22	73.17
373	A	Y	N	369	A	T	O	2.86	1.95	153.62	160.83
374	A	Y	N	370	A	A	O	2.94	2.07	147.78	139.32
375	A	L	N	370	A	A	O	3.03	2.50	113.66	163.02
376	A	D	N	449	A	P	O	2.81	1.82	173.13	144.98
377	A	I	N	375	A	L	O	3.05	2.31	130.44	89.24
378	A	T	N	376	A	D	O	3.14	2.92	93.67	73.80
379	A	N	N	376	A	D	O	3.15	2.21	162.56	115.52
384	A	N	N	382	A	R	O	3.13	3.09	83.24	79.36
385	A	V	N	382	A	R	O	2.93	2.09	143.41	124.89
385	A	V	N	383	A	T	O	3.37	3.30	85.63	73.71
386	A	L	N	382	A	R	O	3.46	2.57	151.95	155.98
386	A	L	N	383	A	T	O	3.20	2.58	121.21	109.45
386	A	L	N	384	A	N	O	3.40	3.45	78.82	69.80
387	A	Y	N	383	A	T	O	2.87	1.95	153.28	159.24
387	A	Y	N	384	A	N	O	3.45	2.96	112.12	95.93
388	A	E	N	384	A	N	O	2.92	1.97	160.98	147.92
389	A	L	N	385	A	V	O	3.41	2.60	140.02	138.28
389	A	L	N	387	A	Y	O	3.31	3.22	86.45	73.39
390	A	A	N	386	A	L	O	3.10	2.84	95.74	146.80
390	A	A	N	387	A	Y	O	3.22	2.27	161.59	104.95
391	A	Q	N	389	A	L	O	3.19	3.23	78.69	76.60
392	A	Y	N	389	A	L	O	2.95	2.01	157.71	123.96
392	A	Y	N	390	A	A	O	3.00	2.59	105.13	81.32
393	A	A	N	390	A	A	O	3.05	2.09	164.74	128.35
394	A	S	N	436	A	S	O	3.49	2.74	133.97	106.22
397	A	T	N	395	A	E	O	3.27	3.27	81.03	80.62
398	A	E	N	395	A	E	O	3.17	2.50	125.12	119.78
398	A	E	N	396	A	P	O	3.40	3.42	80.62	72.97
399	A	Q	N	395	A	E	O	3.02	2.06	163.14	163.52
399	A	Q	N	396	A	P	O	3.25	2.81	107.35	103.04
400	A	E	N	396	A	P	O	2.85	1.96	150.31	157.26

400	A	E	N	398	A	E	O	3.35	3.42	77.66	76.68
401	A	H	N	397	A	T	O	3.17	2.28	153.17	145.48
401	A	H	N	398	A	E	O	3.22	2.63	119.44	113.48
401	A	H	N	399	A	Q	O	3.46	3.54	77.45	73.99
402	A	L	N	398	A	E	O	3.10	2.15	161.22	161.84
402	A	L	N	399	A	Q	O	3.35	2.84	113.46	107.20
402	A	L	N	400	A	E	O	3.41	3.51	75.88	74.10
403	A	R	N	399	A	Q	O	2.93	2.07	145.93	158.17
403	A	R	N	400	A	E	O	3.35	2.73	121.13	104.64
403	A	R	N	401	A	H	O	3.38	3.37	82.19	75.06
404	A	K	N	400	A	E	O	2.98	2.08	151.85	157.43
404	A	K	N	401	A	H	O	3.43	2.79	123.16	107.84
405	A	M	N	401	A	H	O	3.36	2.59	135.73	155.05
405	A	M	N	403	A	R	O	3.34	3.19	89.80	74.22
406	A	A	N	404	A	K	O	3.05	2.87	90.75	81.96
407	A	S	N	404	A	K	O	2.97	2.09	148.19	132.74
407	A	S	N	405	A	M	O	3.38	2.86	113.49	72.68
409	A	S	N	407	A	S	O	3.50	3.07	107.59	70.13
412	A	G	N	410	A	G	O	3.26	3.22	83.86	76.72
413	A	K	N	410	A	G	O	3.27	2.51	134.73	117.73
413	A	K	N	411	A	E	O	3.41	3.39	83.07	75.67
414	A	E	N	411	A	E	O	3.26	2.62	123.51	112.83
414	A	E	N	412	A	G	O	3.40	3.45	78.76	72.01
415	A	L	N	411	A	E	O	3.02	2.16	146.58	156.91
415	A	L	N	412	A	G	O	3.27	2.71	116.84	101.72
415	A	L	N	413	A	K	O	3.49	3.52	80.46	70.42
416	A	Y	N	412	A	G	O	3.08	2.21	150.50	153.15
416	A	Y	N	413	A	K	O	3.36	2.74	122.77	104.81
416	A	Y	N	414	A	E	O	3.43	3.52	76.71	73.00
417	A	L	N	413	A	K	O	3.20	2.26	163.85	153.52
417	A	L	N	414	A	E	O	3.47	3.01	111.23	104.48
418	A	S	N	414	A	E	O	2.92	1.97	165.47	157.30
419	A	W	N	415	A	L	O	2.90	2.02	149.19	144.87
420	A	V	N	416	A	Y	O	3.29	2.51	136.99	127.53
421	A	V	N	416	A	Y	O	3.07	2.14	158.82	168.76
421	A	V	N	417	A	L	O	3.35	2.75	120.98	121.40
422	A	E	N	417	A	L	O	2.82	1.87	165.44	177.03
423	A	A	N	418	A	S	O	3.43	2.82	120.86	142.05
423	A	A	N	421	A	V	O	3.35	3.34	82.02	72.29
424	A	R	N	420	A	V	O	3.03	2.66	101.89	140.53
424	A	R	N	421	A	V	O	2.99	2.12	143.82	108.46
424	A	R	N	422	A	E	O	3.32	3.01	99.46	69.84
425	A	R	N	420	A	V	O	2.95	1.98	166.33	155.45
425	A	R	N	423	A	A	O	3.32	3.47	73.15	74.42
426	A	H	N	424	A	R	O	3.09	2.42	124.47	93.04

427	A	I	N	377	A	I	O	3.24	2.31	160.10	168.42
428	A	L	N	426	A	H	O	3.17	3.17	81.48	83.05
429	A	A	N	426	A	H	O	2.99	2.42	116.89	125.31
429	A	A	N	427	A	I	O	3.43	3.55	74.86	72.98
430	A	I	N	426	A	H	O	2.98	2.08	151.63	162.38
430	A	I	N	427	A	I	O	3.21	2.66	115.27	103.30
430	A	I	N	428	A	L	O	3.36	3.42	78.03	74.25
431	A	L	N	427	A	I	O	2.94	2.02	156.30	157.22
431	A	L	N	428	A	L	O	3.19	2.65	114.97	109.97
432	A	Q	N	428	A	L	O	2.95	2.06	149.10	159.58
432	A	Q	N	429	A	A	O	3.37	2.79	118.00	101.81
432	A	Q	N	430	A	I	O	3.30	3.31	80.76	75.92
433	A	D	N	429	A	A	O	2.89	2.03	145.08	154.09
433	A	D	N	430	A	I	O	3.20	2.58	121.05	109.74
434	A	Y	N	430	A	I	O	2.81	2.01	135.24	164.36
436	A	S	N	434	A	Y	O	3.20	3.04	90.88	81.07
437	A	L	N	434	A	Y	O	3.11	2.20	152.79	121.48
438	A	R	N	392	A	Y	O	3.14	2.17	169.62	139.28
438	A	R	N	436	A	S	O	3.18	2.81	102.91	98.33
441	A	I	N	439	A	P	O	3.43	3.70	66.93	102.70
442	A	D	N	440	A	P	O	3.35	3.36	80.92	74.81
443	A	H	N	440	A	P	O	3.20	2.53	126.29	111.08
443	A	H	N	441	A	I	O	3.42	3.41	82.29	73.67
444	A	L	N	440	A	P	O	3.03	2.11	155.75	158.45
444	A	L	N	441	A	I	O	3.32	2.80	113.50	104.45
445	A	C	N	441	A	I	O	2.89	1.99	152.46	155.85
445	A	C	N	442	A	D	O	3.39	2.88	113.35	98.24
445	A	C	N	443	A	H	O	3.46	3.56	75.96	72.31
446	A	E	N	442	A	D	O	2.97	2.11	144.95	149.07
446	A	E	N	443	A	H	O	3.29	2.69	119.98	104.54
446	A	E	N	444	A	L	O	3.39	3.42	80.54	74.48
447	A	L	N	443	A	H	O	3.21	2.41	138.38	152.24
447	A	L	N	444	A	L	O	3.21	2.46	132.59	111.98
447	A	L	N	445	A	C	O	3.34	3.30	83.92	73.37
448	A	L	N	444	A	L	O	2.98	2.14	141.99	167.65
451	A	L	N	374	A	Y	O	2.89	1.92	165.51	105.10
454	A	R	N	322	A	V	O	2.94	1.98	163.62	162.08
456	A	Y	N	320	A	V	O	2.86	1.90	158.97	173.03
458	A	I	N	318	A	D	O	2.91	1.96	162.20	161.69
459	A	A	N	457	A	S	O	3.22	3.19	82.93	101.70
459	A	A	N	470	A	H	O	2.94	1.96	169.59	140.08
460	A	S	N	458	A	I	O	3.41	2.73	126.69	73.38
464	A	V	N	461	A	S	O	3.42	2.58	142.60	102.18
465	A	H	N	461	A	S	O	2.81	1.92	146.84	151.27
467	A	N	N	465	A	H	O	3.20	3.01	92.24	77.54

468	A	S	N	465	A	H	O	3.39	2.43	167.20	106.63
469	A	V	N	305	A	L	O	2.94	1.99	157.31	155.47
471	A	I	N	303	A	L	O	2.89	1.90	167.79	152.02
473	A	A	N	301	A	M	O	2.93	1.97	164.07	159.05
475	A	A	N	299	A	H	O	2.90	1.93	167.98	158.77
478	A	Y	N	486	A	N	O	2.94	1.98	164.39	172.50
480	A	T	N	484	A	R	O	2.86	1.89	168.15	160.04
482	A	S	N	480	A	T	O	3.22	3.05	91.04	74.88
483	A	G	N	480	A	T	O	2.98	2.07	151.36	117.78
483	A	G	N	481	A	R	O	3.35	2.95	105.21	69.09
484	A	R	N	482	A	S	O	3.40	2.85	116.48	71.00
486	A	N	N	478	A	Y	O	2.86	1.87	166.56	173.95
488	A	G	N	476	A	V	O	2.85	1.87	175.60	130.80
492	A	S	N	488	A	G	O	3.17	2.27	154.14	144.61
492	A	S	N	490	A	A	O	3.37	3.44	77.70	75.28
493	A	W	N	489	A	V	O	3.19	2.29	150.21	148.41
493	A	W	N	490	A	A	O	3.25	2.77	110.56	105.85
494	A	L	N	490	A	A	O	2.79	1.86	156.51	160.81
494	A	L	N	492	A	S	O	3.47	3.57	76.37	72.78
495	A	R	N	491	A	T	O	2.95	2.07	149.34	147.95
495	A	R	N	492	A	S	O	3.30	2.79	113.21	103.06
496	A	A	N	492	A	S	O	3.03	2.17	144.41	153.99
496	A	A	N	494	A	L	O	3.27	3.26	81.61	75.71
497	A	K	N	494	A	L	O	3.10	2.18	158.22	116.81
497	A	K	N	495	A	R	O	3.33	3.06	97.92	74.92
498	A	E	N	496	A	A	O	3.45	3.54	76.84	102.49
500	A	A	N	286	A	V	O	2.76	1.76	172.96	149.03
500	A	A	N	498	A	E	O	3.03	2.90	87.55	105.12
501	A	G	N	287	A	T	O	3.34	3.05	98.13	122.02
501	A	G	N	499	A	P	O	3.15	2.36	136.47	78.62
502	A	E	N	500	A	A	O	3.36	2.94	106.20	70.63
505	A	R	N	503	A	N	O	3.45	2.86	118.74	68.82
508	A	L	N	506	A	R	O	3.45	3.58	74.21	98.01
509	A	V	N	284	A	A	O	2.88	1.96	151.56	156.19
511	A	M	N	282	A	F	O	2.89	1.96	153.98	152.62
511	A	M	N	509	A	V	O	3.41	3.40	82.12	98.81
512	A	F	N	321	A	A	O	3.01	2.06	158.59	163.20
514	A	R	N	319	A	H	O	2.87	1.89	171.61	159.19
516	A	S	N	514	A	R	O	3.42	3.53	75.70	100.42
519	A	R	N	517	A	Q	O	3.24	2.71	114.10	73.40
520	A	L	N	316	A	S	O	3.02	2.21	138.17	165.96
524	A	A	N	522	A	F	O	3.31	2.96	102.02	96.61
525	A	A	N	523	A	K	O	3.22	3.13	86.31	76.63
526	A	T	N	523	A	K	O	3.13	2.18	165.58	124.41
526	A	T	N	524	A	A	O	3.15	2.87	97.59	77.75

528	A	V	N	559	A	E	O	2.91	1.97	159.05	170.27
529	A	I	N	626	A	H	O	2.88	1.90	166.73	154.73
530	A	M	N	561	A	L	O	2.86	1.91	159.53	152.97
531	A	V	N	628	A	Y	O	2.84	1.95	149.57	167.50
532	A	G	N	563	A	Y	O	2.86	1.88	175.75	173.06
534	A	G	N	565	A	G	O	3.10	2.14	171.83	158.07
536	A	G	N	533	A	P	O	3.18	2.32	145.44	126.35
536	A	G	N	534	A	G	O	3.16	2.84	99.99	74.99
537	A	V	N	532	A	G	O	3.07	3.18	74.54	118.17
537	A	V	N	534	A	G	O	3.34	2.39	162.56	122.71
537	A	V	N	535	A	T	O	3.05	2.79	95.70	75.56
538	A	A	N	535	A	T	O	3.02	2.08	157.48	126.22
538	A	A	N	536	A	G	O	3.26	2.92	101.59	72.07
540	A	F	N	537	A	V	O	2.96	2.28	125.47	129.53
540	A	F	N	538	A	A	O	3.18	3.07	87.42	76.95
541	A	I	N	537	A	V	O	3.07	2.28	137.10	169.70
541	A	I	N	538	A	A	O	3.27	2.47	139.74	115.18
541	A	I	N	539	A	P	O	3.38	3.33	84.37	72.87
542	A	G	N	459	A	A	O	3.44	3.43	82.36	94.62
542	A	G	N	539	A	P	O	3.05	2.46	118.28	113.63
542	A	G	N	540	A	F	O	3.39	3.55	72.43	70.23
543	A	F	N	539	A	P	O	2.93	2.10	141.07	151.07
543	A	F	N	540	A	F	O	3.20	2.66	114.68	97.50
544	A	I	N	540	A	F	O	2.96	2.04	156.87	151.28
544	A	I	N	541	A	I	O	3.43	2.82	121.24	108.39
544	A	I	N	542	A	G	O	3.37	3.46	76.81	74.21
545	A	Q	N	541	A	I	O	3.03	2.11	157.63	154.78
545	A	Q	N	542	A	G	O	3.28	2.83	109.35	103.99
546	A	E	N	542	A	G	O	2.91	2.02	150.40	157.38
546	A	E	N	543	A	F	O	3.41	2.80	120.63	102.92
546	A	E	N	544	A	I	O	3.31	3.34	79.40	76.56
547	A	R	N	543	A	F	O	2.93	2.00	157.51	154.14
547	A	R	N	544	A	I	O	3.40	2.92	111.77	106.22
548	A	A	N	544	A	I	O	2.83	1.92	153.09	158.41
548	A	A	N	546	A	E	O	3.45	3.52	78.10	71.74
549	A	W	N	545	A	Q	O	3.11	2.26	144.34	144.64
549	A	W	N	546	A	E	O	3.16	2.57	118.80	106.58
549	A	W	N	547	A	R	O	3.37	3.45	77.08	73.18
550	A	L	N	546	A	E	O	3.07	2.18	151.39	153.88
550	A	L	N	547	A	R	O	3.19	2.65	115.37	107.55
550	A	L	N	548	A	A	O	3.41	3.51	76.39	73.36
551	A	R	N	547	A	R	O	2.90	1.99	153.00	158.65
551	A	R	N	548	A	A	O	3.23	2.70	114.27	105.03
551	A	R	N	549	A	W	O	3.44	3.52	77.61	73.12
552	A	Q	N	548	A	A	O	2.87	1.98	149.90	157.24

552	A	Q	N	549	A	W	O	3.21	2.65	116.19	105.79
553	A	Q	N	549	A	W	O	3.03	2.17	145.35	154.02
553	A	Q	N	550	A	L	O	3.24	2.64	119.42	104.03
553	A	Q	N	551	A	R	O	3.30	3.36	78.37	74.29
554	A	G	N	550	A	L	O	3.16	2.70	108.77	147.05
554	A	G	N	551	A	R	O	2.91	2.03	147.50	112.27
554	A	G	N	552	A	Q	O	3.36	3.05	99.59	71.17
555	A	K	N	550	A	L	O	3.07	2.13	160.05	152.60
557	A	V	N	555	A	K	O	3.37	3.34	83.17	99.44
558	A	G	N	524	A	A	O	2.87	1.92	162.16	133.81
560	A	T	N	558	A	G	O	3.27	3.52	67.51	104.14
561	A	L	N	528	A	V	O	2.98	2.00	170.83	173.03
563	A	Y	N	530	A	M	O	2.82	1.90	153.00	158.89
564	A	Y	N	592	A	N	O	3.05	2.06	172.34	169.49
566	A	C	N	594	A	A	O	2.96	2.02	154.93	148.20
570	A	D	N	568	A	R	O	3.26	3.17	86.45	73.60
571	A	E	N	568	A	R	O	3.12	2.19	156.01	114.19
571	A	E	N	569	A	S	O	3.44	3.17	97.72	70.67
572	A	D	N	568	A	R	O	3.09	2.18	153.36	161.48
574	A	L	N	572	A	D	O	3.16	3.02	88.40	96.61
576	A	R	N	574	A	L	O	3.18	3.40	69.08	77.79
577	A	E	N	575	A	Y	O	3.26	3.23	83.05	80.89
578	A	E	N	575	A	Y	O	3.15	2.50	123.01	115.18
579	A	L	N	575	A	Y	O	2.88	1.94	161.91	170.23
580	A	A	N	576	A	R	O	3.49	2.63	146.87	133.15
580	A	A	N	577	A	E	O	3.45	2.89	117.70	99.94
580	A	A	N	578	A	E	O	3.40	3.46	78.42	71.18
581	A	Q	N	577	A	E	O	3.06	2.16	151.90	147.97
581	A	Q	N	578	A	E	O	3.21	2.71	111.78	104.45
582	A	F	N	578	A	E	O	2.90	1.99	153.90	156.58
582	A	F	N	579	A	L	O	3.35	2.83	114.42	102.07
582	A	F	N	580	A	A	O	3.41	3.50	76.55	74.58
583	A	H	N	579	A	L	O	2.93	2.09	143.58	151.80
583	A	H	N	580	A	A	O	3.11	2.52	119.55	108.55
583	A	H	N	581	A	Q	O	3.44	3.47	80.10	71.09
584	A	Q	N	580	A	A	O	2.89	1.97	154.89	159.66
584	A	Q	N	581	A	Q	O	3.28	2.78	112.37	102.78
585	A	D	N	581	A	Q	O	2.92	2.07	143.74	152.92
585	A	D	N	582	A	F	O	3.36	2.77	119.03	98.14
585	A	D	N	583	A	H	O	3.37	3.40	79.83	73.81
586	A	G	N	582	A	F	O	3.04	2.50	114.29	145.27
586	A	G	N	583	A	H	O	3.02	2.19	141.72	109.34
586	A	G	N	584	A	Q	O	3.41	3.16	95.87	69.96
587	A	S	N	582	A	F	O	2.92	2.14	134.90	161.14
588	A	L	N	582	A	F	O	3.23	2.35	145.93	117.91

588	A	L	N	586	A	G	O	3.40	3.28	88.03	66.29
589	A	T	N	560	A	T	O	2.86	1.89	171.30	160.06
590	A	Q	N	588	A	L	O	3.47	3.63	72.62	75.56
594	A	A	N	564	A	Y	O	2.96	2.01	161.26	144.90
596	A	S	N	566	A	C	O	2.94	1.97	167.99	152.55
597	A	R	N	567	A	R	O	2.92	2.02	150.74	133.87
597	A	R	N	595	A	F	O	3.16	2.95	93.33	86.87
598	A	E	N	595	A	F	O	3.29	2.35	161.64	127.48
599	A	Q	N	597	A	R	O	3.44	3.12	100.08	67.27
601	A	H	N	599	A	Q	O	3.45	3.50	79.07	78.45
602	A	K	N	600	A	P	O	3.35	3.19	90.89	96.12
603	A	V	N	601	A	H	O	3.27	2.89	103.68	100.19
606	A	Q	N	604	A	Y	O	3.11	3.04	84.88	80.61
607	A	H	N	604	A	Y	O	2.93	2.10	142.79	128.86
607	A	H	N	605	A	V	O	3.29	3.26	83.03	75.39
608	A	L	N	604	A	Y	O	3.34	2.46	150.03	153.76
608	A	L	N	605	A	V	O	3.14	2.55	119.16	108.42
609	A	L	N	605	A	V	O	2.96	2.05	153.59	159.72
609	A	L	N	606	A	Q	O	3.46	2.90	117.14	99.05
609	A	L	N	607	A	H	O	3.40	3.49	76.69	72.63
610	A	K	N	606	A	Q	O	3.21	2.36	144.45	143.85
610	A	K	N	607	A	H	O	3.06	2.47	118.11	107.52
610	A	K	N	608	A	L	O	3.37	3.46	76.62	73.30
611	A	R	N	607	A	H	O	2.93	2.13	138.88	156.34
611	A	R	N	608	A	L	O	3.11	2.46	122.95	107.09
611	A	R	N	609	A	L	O	3.48	3.46	82.81	71.75
612	A	D	N	608	A	L	O	2.98	2.19	136.17	158.69
612	A	D	N	609	A	L	O	3.39	2.65	132.47	103.82
613	A	K	N	609	A	L	O	3.04	2.85	90.70	150.50
614	A	E	N	612	A	D	O	3.24	3.17	85.26	87.11
615	A	H	N	612	A	D	O	3.18	2.55	121.99	133.03
615	A	H	N	613	A	K	O	3.46	3.57	76.05	73.00
616	A	L	N	612	A	D	O	2.90	2.00	151.98	156.55
616	A	L	N	613	A	K	O	3.31	2.82	112.31	98.99
617	A	W	N	613	A	K	O	2.94	2.03	155.71	151.64
617	A	W	N	614	A	E	O	3.43	2.88	117.01	101.31
617	A	W	N	615	A	H	O	3.35	3.51	72.49	73.56
618	A	Q	N	614	A	E	O	3.21	2.34	148.13	144.84
618	A	Q	N	615	A	H	O	3.05	2.52	114.03	108.08
618	A	Q	N	616	A	L	O	3.42	3.51	76.61	74.63
619	A	L	N	615	A	H	O	3.05	2.14	152.94	158.53
619	A	L	N	616	A	L	O	3.19	2.59	119.46	111.52
619	A	L	N	617	A	W	O	3.21	3.31	75.86	77.00
620	A	I	N	616	A	L	O	2.88	1.95	156.98	161.29
620	A	I	N	617	A	W	O	3.13	2.66	109.82	108.88

621	A	H	N	617	A	W	O	2.84	1.91	155.72	163.96
621	A	H	N	619	A	L	O	3.31	3.32	81.13	75.62
622	A	E	N	618	A	Q	O	3.50	2.90	119.96	137.42
622	A	E	N	619	A	L	O	3.06	2.19	146.08	114.85
622	A	E	N	620	A	I	O	3.26	3.06	92.27	74.41
624	A	G	N	622	A	E	O	3.33	3.48	73.44	103.63
625	A	A	N	622	A	E	O	3.39	2.44	166.81	133.89
626	A	H	N	527	A	P	O	2.96	2.01	160.00	162.78
627	A	I	N	671	A	R	O	2.92	2.10	138.56	135.56
628	A	Y	N	529	A	I	O	2.87	1.91	165.23	158.71
629	A	V	N	673	A	S	O	3.00	2.10	150.50	150.00
630	A	C	N	531	A	V	O	2.92	1.97	157.57	173.29
631	A	G	N	675	A	D	O	3.34	2.45	149.90	142.00
633	A	A	N	631	A	G	O	3.12	3.01	87.22	105.98
633	A	A	N	677	A	W	O	2.95	1.98	168.15	134.22
635	A	N	N	633	A	A	O	3.49	3.47	83.14	76.85
637	A	A	N	632	A	D	O	2.95	2.07	149.81	173.24
638	A	R	N	635	A	N	O	3.48	2.93	116.76	106.30
638	A	R	N	636	A	M	O	3.25	3.29	78.96	78.54
639	A	D	N	635	A	N	O	3.06	2.22	142.42	155.17
639	A	D	N	636	A	M	O	3.05	2.38	125.81	117.10
639	A	D	N	637	A	A	O	3.49	3.49	81.74	71.74
640	A	V	N	636	A	M	O	2.96	2.02	158.57	165.38
640	A	V	N	637	A	A	O	3.38	2.88	112.82	101.78
641	A	Q	N	637	A	A	O	2.90	2.02	146.94	151.28
641	A	Q	N	638	A	R	O	3.34	2.81	114.15	97.73
641	A	Q	N	639	A	D	O	3.42	3.52	76.62	72.06
642	A	N	N	638	A	R	O	3.02	2.16	145.17	146.83
642	A	N	N	639	A	D	O	3.17	2.60	117.45	105.39
642	A	N	N	640	A	V	O	3.36	3.44	77.40	74.33
643	A	T	N	639	A	D	O	2.87	2.09	135.46	154.55
643	A	T	N	640	A	V	O	3.06	2.41	123.55	107.42
643	A	T	N	641	A	Q	O	3.42	3.37	84.56	71.75
644	A	F	N	640	A	V	O	2.98	2.07	155.82	159.53
644	A	F	N	641	A	Q	O	3.33	2.79	116.48	106.08
645	A	Y	N	641	A	Q	O	3.03	2.16	148.53	152.15
645	A	Y	N	642	A	N	O	3.34	2.81	114.93	97.36
645	A	Y	N	643	A	T	O	3.39	3.46	78.03	73.45
646	A	D	N	642	A	N	O	3.04	2.15	152.29	148.16
646	A	D	N	643	A	T	O	3.16	2.60	116.72	110.17
646	A	D	N	644	A	F	O	3.43	3.55	75.08	72.95
647	A	I	N	643	A	T	O	2.98	2.08	151.69	160.38
647	A	I	N	644	A	F	O	3.38	2.81	117.64	103.50
647	A	I	N	645	A	Y	O	3.47	3.50	80.12	74.50
648	A	V	N	644	A	F	O	3.12	2.19	159.29	153.92

648	A	V	N	645	A	Y	O	3.40	2.84	117.58	108.37
648	A	V	N	646	A	D	O	3.43	3.53	76.16	72.87
649	A	A	N	645	A	Y	O	2.91	2.04	148.80	157.63
649	A	A	N	646	A	D	O	3.31	2.78	115.17	101.63
650	A	E	N	646	A	D	O	2.95	2.02	156.90	155.24
650	A	E	N	648	A	V	O	3.48	3.56	77.91	74.02
651	A	V	N	647	A	I	O	2.98	2.03	164.79	157.43
652	A	G	N	648	A	V	O	3.00	2.33	124.49	127.34
653	A	A	N	649	A	A	O	3.39	3.04	101.95	118.48
653	A	A	N	650	A	E	O	3.30	2.43	144.69	100.45
653	A	A	N	651	A	V	O	3.38	3.01	102.83	68.74
654	A	M	N	649	A	A	O	3.10	2.14	163.61	134.44
657	A	A	N	655	A	E	O	3.35	3.47	74.75	78.11
658	A	Q	N	655	A	E	O	2.99	2.25	130.58	116.28
658	A	Q	N	656	A	H	O	3.19	3.12	85.09	77.37
659	A	A	N	655	A	E	O	2.98	2.11	147.17	161.96
659	A	A	N	656	A	H	O	3.02	2.41	119.11	113.33
660	A	V	N	656	A	H	O	2.89	1.99	150.92	163.07
660	A	V	N	657	A	A	O	3.45	2.91	116.19	94.51
661	A	D	N	657	A	A	O	3.08	2.19	149.65	141.80
661	A	D	N	658	A	Q	O	3.29	2.78	113.07	101.17
661	A	D	N	659	A	A	O	3.43	3.56	74.66	70.87
662	A	Y	N	658	A	Q	O	2.88	2.04	140.46	150.41
662	A	Y	N	659	A	A	O	3.22	2.66	116.28	100.79
662	A	Y	N	660	A	V	O	3.38	3.39	81.16	74.17
663	A	I	N	659	A	A	O	2.97	2.04	159.48	155.61
663	A	I	N	660	A	V	O	3.41	2.85	117.43	108.79
664	A	K	N	660	A	V	O	3.05	2.14	156.35	155.90
664	A	K	N	661	A	D	O	3.34	2.86	111.75	102.15
664	A	K	N	662	A	Y	O	3.42	3.52	76.59	71.89
665	A	K	N	661	A	D	O	2.90	2.07	141.15	152.16
665	A	K	N	662	A	Y	O	3.13	2.53	120.13	106.75
665	A	K	N	663	A	I	O	3.34	3.40	78.41	74.83
666	A	L	N	662	A	Y	O	2.96	2.12	143.85	154.04
666	A	L	N	663	A	I	O	3.03	2.45	118.53	108.96
667	A	M	N	663	A	I	O	2.97	2.11	146.39	157.10
667	A	M	N	664	A	K	O	3.23	2.65	117.92	101.85
667	A	M	N	665	A	K	O	3.39	3.48	77.01	71.49
668	A	T	N	664	A	K	O	3.14	2.29	146.26	150.17
668	A	T	N	665	A	K	O	3.31	2.71	120.00	104.89
668	A	T	N	666	A	L	O	3.43	3.52	77.09	74.92
669	A	K	N	665	A	K	O	3.05	2.13	155.45	154.41
669	A	K	N	666	A	L	O	3.26	2.74	113.88	106.92
669	A	K	N	667	A	M	O	3.45	3.51	78.40	72.30
670	A	G	N	666	A	L	O	3.03	2.65	103.59	155.12

670	A	G	N	667	A	M	O	3.14	2.23	153.72	107.38
670	A	G	N	668	A	T	O	3.25	2.87	104.30	75.17
671	A	R	N	666	A	L	O	2.80	1.88	150.09	150.10
671	A	R	N	669	A	K	O	3.40	3.25	89.90	69.55
672	A	Y	N	666	A	L	O	3.29	2.67	120.79	103.55
673	A	S	N	627	A	I	O	2.84	2.10	129.32	158.74
675	A	D	N	629	A	V	O	2.92	1.98	156.81	165.06
677	A	W	N	631	A	G	O	2.96	2.00	161.78	163.36

Dd-a = Distance Between Donor and Acceptor
Dh-a = Distance Between Hydrogen and Acceptor
A(d-H-N) = Angle Between Donor-H-N
A(a-O=C) = Angle Between Acceptor-O=C
MO = Multiple Occupancy
Note that angles that are undefined are written as 999.99

Intraprotein Main Chain-Side Chain Hydrogen Bonds

Rasmol **Jmol** **[help]**

[View the original hbond output]

DOG_POR_snapshot10.pdb

DONOR				ACCEPTOR					PARAMETERS			
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**MO**	**Dd-a**	**Dh-a**	**A(d-H-N)**	**A(a-O=C)**
64	A	ALA	N	61	A	THR	OG1	-	3.10	2.54	116.12	999.99
65	A	LYS	NZ	115	A	GLU	O	-	2.88	9.99	999.99	117.74
65	A	LYS	NZ	117	A	TYR	O	-	2.98	9.99	999.99	121.09
69	A	PHE	N	121	A	ASP	OD2	-	3.05	2.55	112.69	168.49
70	A	VAL	N	68	A	SER	OG	-	3.33	2.71	121.59	999.99
70	A	VAL	N	121	A	ASP	OD2	-	3.00	2.04	169.79	136.31
71	A	GLU	N	68	A	SER	OG	-	3.09	2.18	155.96	999.99
72	A	LYS	NZ	354	A	GLU	O	-	2.97	9.99	999.99	154.95
76	A	THR	OG1	72	A	LYS	O	-	2.81	9.99	999.99	133.45
76	A	THR	OG1	73	A	MET	O	-	3.19	9.99	999.99	102.51
79	A	ASN	OD1	108	A	ARG	O	1	3.09	3.23	72.62	120.97
79	A	ASN	OD1	108	A	ARG	O	2	3.09	2.52	112.05	120.97
79	A	ASN	ND2	130	A	ASN	O	1	2.91	3.55	45.38	143.28

79	A	ASN	ND2	130	A	ASN	O	2	2.91	1.87	169.01	143.28
85	A	GLY	N	137	A	MET	SD	-	3.41	3.48	77.53	999.99
86	A	SER	N	146	A	THR	OG1	-	3.07	2.70	103.09	999.99
86	A	SER	N	148	A	ASN	OD1	-	2.89	1.91	170.83	133.26
89	A	GLY	N	86	A	SER	OG	-	3.02	2.51	112.09	999.99
90	A	THR	N	86	A	SER	OG	-	3.44	3.31	89.58	999.99
91	A	ALA	N	86	A	SER	OG	-	3.40	2.76	123.95	999.99
92	A	GLU	N	86	A	SER	OG	-	3.23	2.38	145.31	999.99
96	A	ASN	OD1	92	A	GLU	O	1	3.44	3.71	67.23	141.30
96	A	ASN	OD1	92	A	GLU	O	2	3.44	3.86	58.89	141.30
96	A	ASN	ND2	92	A	GLU	O	1	3.42	3.69	67.23	112.94
96	A	ASN	ND2	92	A	GLU	O	2	3.42	3.79	61.41	112.94
99	A	SER	OG	95	A	ALA	O	-	2.85	9.99	999.99	144.66
99	A	SER	OG	110	A	MET	O	-	3.17	9.99	999.99	78.95
104	A	ARG	NH1	242	A	ILE	O	1	3.20	2.50	123.76	132.74
104	A	ARG	NH1	242	A	ILE	O	2	3.20	3.19	80.99	132.74
108	A	ARG	N	79	A	ASN	OD1	-	2.93	1.95	175.80	172.87
111	A	ALA	N	99	A	SER	OG	-	3.44	3.99	49.70	999.99
113	A	ASP	OD1	148	A	ASN	O	1	3.43	2.56	138.98	120.03
113	A	ASP	OD1	148	A	ASN	O	2	3.43	3.49	78.41	120.03
115	A	GLU	N	113	A	ASP	OD1	-	3.31	2.35	173.43	126.04
120	A	ALA	N	118	A	ASP	OD1	-	3.25	2.31	160.46	106.50
131	A	SER	OG	125	A	LEU	O	-	2.79	9.99	999.99	112.02
131	A	SER	OG	128	A	ILE	O	-	3.02	9.99	999.99	141.43
139	A	THR	OG1	173	A	LEU	O	-	3.05	9.99	999.99	156.99
147	A	ASP	N	87	A	GLN	OE1	-	2.97	2.05	155.50	139.19
148	A	ASN	ND2	84	A	TYR	O	1	3.03	2.05	152.72	133.41
148	A	ASN	ND2	84	A	TYR	O	2	3.03	3.42	59.86	133.41
148	A	ASN	OD1	86	A	SER	O	1	3.08	3.23	72.39	116.17
148	A	ASN	OD1	86	A	SER	O	2	3.08	2.74	98.90	116.17
157	A	GLN	NE2	153	A	TYR	O	1	3.09	3.84	39.59	112.86
157	A	GLN	NE2	153	A	TYR	O	2	3.09	2.11	155.55	112.86
161	A	VAL	N	159	A	THR	OG1	-	3.24	2.27	165.81	999.99
164	A	SER	N	162	A	ASP	OD1	-	3.04	2.12	156.64	111.82
168	A	TYR	OH	189	A	ASP	O	-	2.99	9.99	999.99	130.52
174	A	GLY	N	182	A	ASN	ND2	-	3.47	3.66	71.16	111.44
176	A	LYS	N	207	A	ASP	OD1	-	2.84	1.92	154.77	140.66
177	A	THR	N	175	A	ASN	OD1	-	3.01	2.06	165.49	146.03
178	A	TYR	OH	676	A	VAL	O	-	3.20	9.99	999.99	131.97
182	A	ASN	ND2	172	A	GLY	O	1	3.02	1.97	171.52	91.24
182	A	ASN	ND2	172	A	GLY	O	2	3.02	3.65	45.82	91.24
182	A	ASN	ND2	206	A	GLY	O	1	3.24	3.15	85.53	129.15
182	A	ASN	ND2	206	A	GLY	O	2	3.24	2.56	121.67	129.15
183	A	ALA	N	139	A	THR	OG1	-	3.41	3.27	89.66	999.99
184	A	MET	N	139	A	THR	OG1	-	3.18	2.26	157.33	999.99

186	A	LYS	NZ	181	A	PHE	O	-	2.96	9.99	999.99	158.50
191	A	ARG	NE	156	A	LEU	O	-	2.84	1.97	140.27	138.32
191	A	ARG	NH1	156	A	LEU	O	1	2.96	2.09	139.41	155.90
191	A	ARG	NH1	156	A	LEU	O	2	2.96	3.85	27.87	155.90
191	A	ARG	NH1	157	A	GLN	O	1	3.37	2.93	106.31	105.41
191	A	ARG	NH1	157	A	GLN	O	2	3.37	3.36	81.57	105.41
206	A	GLY	N	182	A	ASN	ND2	-	3.49	3.14	102.43	151.46
207	A	ASP	N	215	A	ASP	OD2	-	3.20	2.33	147.45	141.68
209	A	ASP	N	207	A	ASP	OD1	-	2.99	2.04	161.55	108.44
213	A	GLU	N	211	A	ASN	OD1	-	3.41	2.77	122.94	145.69
214	A	GLU	N	211	A	ASN	OD1	-	3.22	2.27	160.92	109.33
218	A	THR	OG1	214	A	GLU	O	-	2.77	9.99	999.99	135.89
219	A	TRP	NE1	205	A	MET	O	-	3.10	2.46	127.59	96.33
222	A	GLN	NE2	218	A	THR	O	1	3.45	4.25	35.92	106.67
222	A	GLN	NE2	218	A	THR	O	2	3.45	2.50	150.77	106.67
228	A	CYS	SG	224	A	TRP	O	-	3.09	9.99	999.99	121.65
228	A	CYS	SG	233	A	VAL	O	-	3.54	9.99	999.99	112.97
236	A	THR	OG1	104	A	ARG	O	-	3.02	9.99	999.99	102.94
238	A	GLU	OE1	103	A	HIS	O	1	3.23	2.62	116.36	92.04
238	A	GLU	OE1	103	A	HIS	O	2	3.23	3.10	87.31	92.04
241	A	SER	OG	239	A	GLU	O	-	3.18	9.99	999.99	119.57
241	A	SER	OG	388	A	GLU	O	-	3.47	9.99	999.99	102.44
244	A	GLN	N	446	A	GLU	OE2	-	2.89	1.91	167.35	155.88
245	A	TYR	OH	357	A	LYS	O	-	2.74	9.99	999.99	142.28
245	A	TYR	N	446	A	GLU	OE2	-	3.11	2.29	139.05	110.77
256	A	ALA	N	254	A	ASP	OD1	-	3.01	2.04	169.73	130.57
259	A	TYR	OH	264	A	GLY	O	-	2.83	9.99	999.99	144.49
260	A	VAL	N	262	A	GLU	OE1	-	2.78	1.79	169.67	140.78
261	A	GLY	N	374	A	TYR	OH	-	3.24	2.60	122.72	999.99
262	A	GLU	N	374	A	TYR	OH	-	3.30	3.20	87.51	999.99
263	A	MET	N	269	A	TYR	OH	-	3.46	2.84	121.91	999.99
266	A	LEU	N	259	A	TYR	OH	-	3.10	3.09	81.72	999.99
267	A	LYS	NZ	255	A	MET	O	-	3.06	9.99	999.99	140.95
267	A	LYS	NZ	258	A	VAL	O	-	2.90	9.99	999.99	167.48
267	A	LYS	N	262	A	GLU	OE2	-	2.81	1.85	157.58	122.36
268	A	SER	OG	263	A	MET	O	-	2.75	9.99	999.99	144.13
268	A	SER	OG	265	A	ARG	O	-	3.35	9.99	999.99	147.77
272	A	GLN	NE2	269	A	TYR	O	1	3.05	3.75	42.65	122.42
272	A	GLN	NE2	269	A	TYR	O	2	3.05	2.05	160.65	122.42
279	A	LYS	N	277	A	ASP	OD2	-	2.90	1.93	169.78	99.71
280	A	ASN	ND2	268	A	SER	O	1	3.44	2.53	143.95	122.17
280	A	ASN	ND2	268	A	SER	O	2	3.44	4.19	38.55	122.17
280	A	ASN	N	277	A	ASP	OD1	-	3.19	2.55	122.81	114.00
283	A	LEU	N	272	A	GLN	OE1	-	2.99	2.02	171.99	144.31
287	A	THR	OG1	304	A	GLU	O	-	3.26	9.99	999.99	97.74

289	A	ASN	ND2	494	A	LEU	O	1	3.04	2.48	111.91	143.73
289	A	ASN	ND2	494	A	LEU	O	2	3.04	3.13	75.05	143.73
289	A	ASN	ND2	495	A	ARG	O	1	3.24	2.49	127.33	105.84
289	A	ASN	ND2	495	A	ARG	O	2	3.24	3.37	74.01	105.84
289	A	ASN	ND2	497	A	LYS	O	1	2.89	3.39	53.95	135.39
289	A	ASN	ND2	497	A	LYS	O	2	2.89	1.92	152.05	135.39
291	A	LYS	NZ	295	A	GLY	O	-	2.97	9.99	999.99	164.04
293	A	ASN	OD1	298	A	ARG	O	1	3.32	2.54	129.04	121.06
293	A	ASN	OD1	298	A	ARG	O	2	3.32	4.20	30.07	121.06
293	A	ASN	ND2	298	A	ARG	O	1	3.00	2.08	143.56	145.44
293	A	ASN	ND2	298	A	ARG	O	2	3.00	3.73	39.60	145.44
293	A	ASN	OD1	300	A	LEU	O	1	3.37	3.46	76.25	110.31
293	A	ASN	OD1	300	A	LEU	O	2	3.37	2.47	142.15	110.31
300	A	LEU	N	293	A	ASN	OD1	-	2.89	1.94	160.78	143.00
306	A	ASP	OD1	467	A	ASN	O	1	3.14	3.32	70.88	161.82
306	A	ASP	OD1	467	A	ASN	O	2	3.14	2.21	142.83	161.82
308	A	SER	N	306	A	ASP	OD1	-	3.02	2.10	156.86	114.44
310	A	SER	OG	307	A	ILE	O	-	2.66	9.99	999.99	136.10
312	A	LEU	N	310	A	SER	OG	-	3.15	2.22	157.20	999.99
313	A	ARG	NH2	311	A	LYS	O	1	3.18	2.91	94.97	142.41
313	A	ARG	NH2	311	A	LYS	O	2	3.18	3.31	73.97	142.41
314	A	TYR	OH	461	A	SER	O	-	3.36	9.99	999.99	91.40
314	A	TYR	OH	465	A	HIS	O	-	2.99	9.99	999.99	137.19
314	A	TYR	OH	468	A	SER	O	-	2.78	9.99	999.99	160.13
315	A	GLU	N	318	A	ASP	OD2	-	3.09	2.18	150.48	127.36
316	A	SER	OG	460	A	SER	O	-	2.80	9.99	999.99	117.17
316	A	SER	OG	542	A	GLY	O	-	3.12	9.99	999.99	87.17
318	A	ASP	OD2	315	A	GLU	O	1	3.48	4.15	44.73	121.47
318	A	ASP	OD2	315	A	GLU	O	2	3.48	3.20	95.76	121.47
323	A	TYR	OH	278	A	ALA	O	-	2.72	9.99	999.99	119.39
326	A	ASN	ND2	371	A	LEU	O	1	2.93	3.40	55.13	160.36
326	A	ASN	ND2	371	A	LEU	O	2	2.93	1.95	153.78	160.36
326	A	ASN	ND2	372	A	THR	O	1	3.47	4.17	43.02	108.63
326	A	ASN	ND2	372	A	THR	O	2	3.47	2.92	113.25	108.63
326	A	ASN	ND2	375	A	LEU	O	1	2.91	2.11	130.93	168.67
326	A	ASN	ND2	375	A	LEU	O	2	2.91	2.96	77.31	168.67
329	A	ALA	N	327	A	ASP	OD1	-	2.96	2.00	164.79	143.29
333	A	GLN	NE2	329	A	ALA	O	1	3.45	4.23	36.79	101.36
333	A	GLN	NE2	329	A	ALA	O	2	3.45	2.83	117.76	101.36
343	A	ASP	N	341	A	ASP	OD1	-	3.30	2.38	158.06	144.71
348	A	LEU	N	363	A	CYS	SG	-	3.73	2.75	175.60	999.99
350	A	ASN	OD1	244	A	GLN	O	1	3.35	3.38	78.81	147.39
350	A	ASN	OD1	244	A	GLN	O	2	3.35	3.10	93.84	147.39
350	A	ASN	ND2	357	A	LYS	O	1	2.93	3.53	47.77	138.69
350	A	ASN	ND2	357	A	LYS	O	2	2.93	1.88	173.85	138.69

352	A	ASP	N	350	A	ASN	OD1	-	2.89	1.92	165.45	122.70
354	A	GLU	N	352	A	ASP	OD1	-	3.07	2.12	161.92	97.95
355	A	SER	N	352	A	ASP	OD2	-	3.13	3.16	79.42	100.43
355	A	SER	OG	352	A	ASP	O	-	2.80	9.99	999.99	148.22
359	A	HIS	ND1	348	A	LEU	O	-	2.88	1.98	170.18	141.91
363	A	CYS	SG	361	A	PHE	O	-	3.45	9.99	999.99	132.34
365	A	THR	OG1	259	A	TYR	O	-	2.92	9.99	999.99	126.64
368	A	ARG	N	366	A	SER	OG	-	3.46	2.89	117.90	999.99
369	A	THR	N	366	A	SER	OG	-	3.16	2.23	158.83	999.99
372	A	THR	OG1	368	A	ARG	O	-	2.68	9.99	999.99	138.16
374	A	TYR	OH	262	A	GLU	O	-	2.71	9.99	999.99	136.75
379	A	ASN	N	376	A	ASP	OD1	-	3.09	2.60	111.16	124.11
383	A	THR	N	213	A	GLU	OE2	-	2.83	1.89	159.58	124.69
391	A	GLN	NE2	240	A	SER	O	1	3.28	2.32	151.26	127.98
391	A	GLN	NE2	240	A	SER	O	2	3.28	4.01	39.86	127.98
394	A	SER	N	436	A	SER	OG	-	3.09	2.31	135.42	999.99
395	A	GLU	N	436	A	SER	OG	-	3.20	2.26	157.95	999.99
397	A	THR	N	395	A	GLU	OE1	-	2.95	2.01	166.42	119.66
401	A	HIS	ND1	397	A	THR	O	-	3.10	3.01	87.13	131.89
403	A	ARG	NH2	239	A	GLU	O	1	3.15	3.49	62.86	142.89
403	A	ARG	NH2	239	A	GLU	O	2	3.15	2.28	142.82	142.89
407	A	SER	OG	409	A	SER	O	-	3.03	9.99	999.99	131.40
408	A	SER	N	221	A	GLU	OE2	-	3.13	2.33	136.61	125.15
409	A	SER	N	407	A	SER	OG	-	3.42	2.45	168.97	999.99
413	A	LYS	NZ	408	A	SER	O	-	3.08	9.99	999.99	130.33
416	A	TYR	OH	381	A	PRO	O	-	2.70	9.99	999.99	138.90
418	A	SER	OG	414	A	GLU	O	-	2.73	9.99	999.99	139.17
424	A	ARG	NH2	421	A	VAL	O	1	2.85	1.87	151.70	122.80
424	A	ARG	NH2	421	A	VAL	O	2	2.85	3.27	56.86	122.80
425	A	ARG	NH2	419	A	TRP	O	1	2.90	1.87	162.07	129.56
425	A	ARG	NH2	419	A	TRP	O	2	2.90	3.35	55.86	129.56
428	A	LEU	N	426	A	HIS	ND1	-	3.49	2.86	123.83	999.99
429	A	ALA	N	426	A	HIS	ND1	-	3.26	2.38	149.61	999.99
433	A	ASP	OD2	429	A	ALA	O	1	3.48	4.09	48.69	127.11
433	A	ASP	OD2	429	A	ALA	O	2	3.48	3.42	84.15	127.11
436	A	SER	N	398	A	GLU	OE2	-	2.96	2.06	154.28	123.55
438	A	ARG	NE	337	A	ILE	O	-	3.40	3.05	101.56	135.94
438	A	ARG	NH2	431	A	LEU	O	1	3.00	3.60	48.31	130.58
438	A	ARG	NH2	431	A	LEU	O	2	3.00	2.08	152.22	130.58
438	A	ARG	NH2	434	A	TYR	O	1	3.46	3.59	74.49	132.91
438	A	ARG	NH2	434	A	TYR	O	2	3.46	2.85	119.33	132.91
438	A	ARG	NH1	435	A	PRO	O	1	3.33	3.78	56.98	116.45
438	A	ARG	NH1	435	A	PRO	O	2	3.33	3.54	69.85	116.45
438	A	ARG	NH2	435	A	PRO	O	1	3.31	3.74	58.02	100.04
438	A	ARG	NH2	435	A	PRO	O	2	3.31	3.50	70.79	100.04

445	A	CYS	SG	441	A	ILE	O	-	3.14	9.99	999.99	136.82
450	A	ARG	N	93	A	GLU	OE2	-	2.91	1.94	175.58	114.88
454	A	ARG	NH2	452	A	GLN	O	1	3.00	2.30	122.06	140.45
454	A	ARG	NH2	452	A	GLN	O	2	3.00	3.05	77.24	140.45
461	A	SER	N	545	A	GLN	OE1	-	2.92	1.97	159.24	146.28
462	A	SER	OG	314	A	TYR	O	-	2.74	9.99	999.99	132.36
462	A	SER	N	546	A	GLU	OE1	-	2.91	2.21	127.30	156.65
463	A	LYS	N	461	A	SER	OG	-	3.05	2.32	131.57	999.99
463	A	LYS	N	546	A	GLU	OE1	-	3.15	2.24	155.26	149.24
464	A	VAL	N	461	A	SER	OG	-	3.17	2.42	132.33	999.99
470	A	HIS	N	460	A	SER	OG	-	3.18	2.35	141.85	999.99
476	A	VAL	N	491	A	THR	OG1	-	3.10	2.25	143.81	999.99
480	A	THR	OG1	484	A	ARG	O	-	2.74	9.99	999.99	123.46
481	A	ARG	NE	422	A	GLU	O	-	3.09	2.17	147.48	108.00
482	A	SER	N	480	A	THR	OG1	-	3.37	2.63	132.31	999.99
483	A	GLY	N	480	A	THR	OG1	-	3.41	3.00	106.35	999.99
484	A	ARG	N	480	A	THR	OG1	-	3.14	2.63	112.57	999.99
492	A	SER	OG	488	A	GLY	O	-	2.79	9.99	999.99	151.09
497	A	LYS	NZ	508	A	LEU	O	-	3.21	9.99	999.99	165.22
505	A	ARG	NH2	499	A	PRO	O	1	3.04	1.99	171.27	131.36
505	A	ARG	NH2	499	A	PRO	O	2	3.04	3.57	51.57	131.36
514	A	ARG	NH1	145	A	PRO	O	1	3.08	3.38	64.60	140.31
514	A	ARG	NH1	145	A	PRO	O	2	3.08	2.11	152.40	140.31
516	A	SER	OG	317	A	GLY	O	-	2.64	9.99	999.99	113.66
516	A	SER	N	318	A	ASP	OD1	-	3.21	2.25	164.53	144.10
518	A	PHE	N	516	A	SER	OG	-	3.33	2.80	113.59	999.99
519	A	ARG	N	516	A	SER	OG	-	3.00	2.70	97.85	999.99
519	A	ARG	NH2	516	A	SER	O	1	2.91	1.88	160.74	137.67
519	A	ARG	NH2	516	A	SER	O	2	2.91	3.34	56.74	137.67
526	A	THR	OG1	523	A	LYS	O	-	2.76	9.99	999.99	169.78
547	A	ARG	NH1	524	A	ALA	O	1	3.07	3.55	55.14	108.36
547	A	ARG	NH1	524	A	ALA	O	2	3.07	2.95	86.89	108.36
547	A	ARG	NH2	524	A	ALA	O	1	3.38	4.05	44.88	148.11
547	A	ARG	NH2	524	A	ALA	O	2	3.38	3.27	87.67	148.11
547	A	ARG	NH1	526	A	THR	O	1	3.10	3.97	29.69	150.17
547	A	ARG	NH1	526	A	THR	O	2	3.10	2.20	143.81	150.17
547	A	ARG	NH2	526	A	THR	O	1	2.98	3.86	29.51	166.35
547	A	ARG	NH2	526	A	THR	O	2	2.98	2.09	147.60	166.35
560	A	THR	OG1	558	A	GLY	O	-	2.98	9.99	999.99	140.54
560	A	THR	N	589	A	THR	OG1	-	2.89	1.92	164.48	999.99
564	A	TYR	OH	572	A	ASP	O	-	3.07	9.99	999.99	135.18
566	A	CYS	SG	568	A	ARG	O	-	3.92	9.99	999.99	80.83
566	A	CYS	SG	594	A	ALA	O	-	3.42	9.99	999.99	144.36
567	A	ARG	N	572	A	ASP	OD1	-	2.86	2.04	139.48	103.26
567	A	ARG	N	572	A	ASP	OD2	-	3.08	2.16	154.83	92.40

568	A	ARG	N	572	A	ASP	OD1	-	2.84	1.85	169.25	155.81
568	A	ARG	NH2	597	A	ARG	O	1	3.02	2.00	158.26	124.58
568	A	ARG	NH2	597	A	ARG	O	2	3.02	3.41	59.28	124.58
569	A	SER	N	598	A	GLU	OE2	-	2.96	1.99	169.34	148.96
572	A	ASP	OD1	568	A	ARG	O	1	3.11	3.24	73.30	115.13
572	A	ASP	OD1	568	A	ARG	O	2	3.11	2.23	137.21	115.13
574	A	LEU	N	564	A	TYR	OH	-	2.97	2.03	157.54	999.99
576	A	ARG	NH2	569	A	SER	O	1	3.01	2.11	141.37	156.40
576	A	ARG	NH2	569	A	SER	O	2	3.01	3.24	68.20	156.40
581	A	GLN	NE2	577	A	GLU	O	1	3.35	4.12	37.76	104.84
581	A	GLN	NE2	577	A	GLU	O	2	3.35	2.62	126.55	104.84
583	A	HIS	ND1	588	A	LEU	O	-	2.93	2.02	176.03	147.06
583	A	HIS	ND1	589	A	THR	O	-	3.47	3.18	100.87	97.51
589	A	THR	OG1	560	A	THR	O	-	3.26	9.99	999.99	107.89
592	A	ASN	ND2	590	A	GLN	O	1	3.26	3.41	72.72	95.98
592	A	ASN	ND2	590	A	GLN	O	2	3.26	2.37	141.82	95.98
596	A	SER	OG	566	A	CYS	O	-	3.16	9.99	999.99	120.72
599	A	GLN	NE2	601	A	HIS	O	1	3.08	3.85	37.25	143.48
599	A	GLN	NE2	601	A	HIS	O	2	3.08	2.11	153.46	143.48
612	A	ASP	OD2	608	A	LEU	O	1	3.28	3.65	61.37	123.42
612	A	ASP	OD2	608	A	LEU	O	2	3.28	3.38	75.40	123.42
626	A	HIS	ND1	624	A	GLY	O	-	3.11	3.21	75.81	159.63
628	A	TYR	OH	519	A	ARG	O	-	2.76	9.99	999.99	153.62
630	A	CYS	SG	536	A	GLY	O	-	3.53	9.99	999.99	112.15
630	A	CYS	SG	675	A	ASP	O	-	3.20	9.99	999.99	147.77
634	A	ARG	NH2	209	A	ASP	O	1	3.03	3.46	57.81	134.38
634	A	ARG	NH2	209	A	ASP	O	2	3.03	2.10	153.03	134.38
634	A	ARG	N	632	A	ASP	OD1	-	3.08	2.17	153.65	100.02
634	A	ARG	NE	678	A	SER	OXT	-	2.87	2.04	135.44	119.64
634	A	ARG	NH1	678	A	SER	OXT	1	2.97	2.11	137.23	104.76
634	A	ARG	NH1	678	A	SER	OXT	2	2.97	3.85	28.84	104.76
635	A	ASN	N	632	A	ASP	OD2	-	2.99	2.11	148.74	123.73
636	A	MET	N	632	A	ASP	OD2	-	2.87	1.90	171.76	143.63
638	A	ARG	NH1	176	A	LYS	O	1	2.94	2.07	138.52	158.86
638	A	ARG	NH1	176	A	LYS	O	2	2.94	3.23	65.08	158.86
638	A	ARG	NE	177	A	THR	O	-	3.39	3.33	84.74	117.78
643	A	THR	OG1	639	A	ASP	O	-	2.75	9.99	999.99	133.80
646	A	ASP	OD1	642	A	ASN	O	1	3.21	3.79	49.45	151.08
646	A	ASP	OD1	642	A	ASN	O	2	3.21	2.47	125.14	151.08
655	A	GLU	N	658	A	GLN	OE1	-	2.94	1.99	166.03	124.52
659	A	ALA	N	654	A	MET	SD	-	3.76	4.22	56.29	999.99
668	A	THR	OG1	665	A	LYS	O	-	2.90	9.99	999.99	114.15
671	A	ARG	NH1	620	A	ILE	O	1	3.00	3.31	63.75	144.33
671	A	ARG	NH1	620	A	ILE	O	2	3.00	2.06	146.34	144.33
671	A	ARG	NH1	622	A	GLU	O	1	3.15	3.42	66.01	160.36

671	A	ARG	NH1	622	A	GLU	O	2	3.15	2.64	108.66	160.36
671	A	ARG	NE	625	A	ALA	O	-	2.88	1.93	152.53	145.82
671	A	ARG	NH1	625	A	ALA	O	1	3.24	2.41	135.72	113.60
671	A	ARG	NH1	625	A	ALA	O	2	3.24	4.17	25.31	113.60
674	A	LEU	N	142	A	GLU	OE2	-	2.90	1.92	166.25	117.38

Dd-a = Distance Between Donor and Acceptor
Dh-a = Distance Between Hydrogen and Acceptor
A(d-H-N) = Angle Between Donor-H-N
A(a-O=C) = Angle Between Acceptor-O=C
MO = Multiple Occupancy
Note that angles that are undefined are written as 999.99

Intraprotein Side Chain-Side Chain Hydrogen Bonds


[help]

Rasmol **Jmol**

[View the original hbond output]

DOG_POR_snapshot10.pdb

	DONOR PARAMETERS				ACCEPTOR							
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**MO**	**Dd-a**	**Dh-a**	**A(d-H-N)**	**A(a-O=C)**
65	A	LYS	NZ	151	A	ASP	OD2	-	2.87	9.99	999.99	999.99
66	A	ASP	OD2	356	A	ASN	OD1	1	3.05	2.83	91.56	999.99
66	A	ASP	OD2	356	A	ASN	OD1	2	3.05	2.42	116.46	999.99
68	A	SER	OG	121	A	ASP	OD1	-	3.10	9.99	999.99	999.99
68	A	SER	OG	121	A	ASP	OD2	-	2.65	9.99	999.99	999.99
72	A	LYS	NZ	66	A	ASP	OD2	-	2.91	9.99	999.99	999.99
72	A	LYS	NZ	117	A	TYR	OH	-	2.98	9.99	999.99	999.99
72	A	LYS	NZ	356	A	ASN	OD1	-	3.06	9.99	999.99	999.99
74	A	LYS	NZ	127	A	GLU	OE1	-	2.93	9.99	999.99	999.99
78	A	ARG	NH2	110	A	MET	SD	1	3.37	2.44	145.28	999.99
78	A	ARG	NH2	110	A	MET	SD	2	3.37	3.74	61.21	999.99
78	A	ARG	NH1	352	A	ASP	OD1	1	3.01	3.78	37.34	999.99
78	A	ARG	NH1	352	A	ASP	OD1	2	3.01	2.01	158.01	999.99
78	A	ARG	NH1	352	A	ASP	OD2	1	3.41	4.28	29.73	999.99
78	A	ARG	NH1	352	A	ASP	OD2	2	3.41	2.82	116.36	999.99
78	A	ARG	NH2	352	A	ASP	OD1	1	3.29	4.23	23.68	999.99

78	A	ARG	NH2	352	A	ASP	OD1	2	3.29	2.47	137.18	999.99
78	A	ARG	NH2	352	A	ASP	OD2	1	2.92	3.61	42.65	999.99
78	A	ARG	NH2	352	A	ASP	OD2	2	2.92	2.19	127.03	999.99
79	A	ASN	ND2	107	A	MET	SD	1	3.60	2.56	165.15	999.99
79	A	ASN	ND2	107	A	MET	SD	2	3.60	4.00	60.48	999.99
87	A	GLN	NE2	147	A	ASP	OD2	1	2.95	1.95	158.02	999.99
87	A	GLN	NE2	147	A	ASP	OD2	2	2.95	3.61	44.33	999.99
87	A	GLN	NE2	455	A	TYR	OH	1	3.21	3.92	41.34	999.99
87	A	GLN	NE2	455	A	TYR	OH	2	3.21	2.51	123.20	999.99
97	A	ARG	NH1	213	A	GLU	OE1	1	2.88	3.61	39.49	999.99
97	A	ARG	NH1	213	A	GLU	OE1	2	2.88	1.89	155.96	999.99
97	A	ARG	NH1	213	A	GLU	OE2	1	3.50	4.43	24.24	999.99
97	A	ARG	NH1	213	A	GLU	OE2	2	3.50	2.80	124.22	999.99
97	A	ARG	NH2	213	A	GLU	OE1	1	3.29	4.26	21.82	999.99
97	A	ARG	NH2	213	A	GLU	OE1	2	3.29	2.55	130.51	999.99
97	A	ARG	NH2	213	A	GLU	OE2	1	2.86	3.55	42.67	999.99
97	A	ARG	NH2	213	A	GLU	OE2	2	2.86	1.95	147.34	999.99
97	A	ARG	NH2	384	A	ASN	OD1	1	3.26	2.70	112.67	999.99
97	A	ARG	NH2	384	A	ASN	OD1	2	3.26	3.78	51.96	999.99
100	A	LYS	NZ	388	A	GLU	OE1	-	3.25	9.99	999.99	999.99
103	A	HIS	ND1	238	A	GLU	OE1	-	2.77	1.92	154.19	999.99
103	A	HIS	ND1	238	A	GLU	OE2	-	3.39	2.97	110.03	999.99
104	A	ARG	NH1	388	A	GLU	OE1	1	2.88	3.35	54.92	999.99
104	A	ARG	NH1	388	A	GLU	OE1	2	2.88	1.84	166.91	999.99
104	A	ARG	NH1	388	A	GLU	OE2	1	3.32	4.23	25.45	999.99
104	A	ARG	NH1	388	A	GLU	OE2	2	3.32	2.50	133.91	999.99
104	A	ARG	NH2	388	A	GLU	OE2	1	2.88	3.67	36.03	999.99
104	A	ARG	NH2	388	A	GLU	OE2	2	2.88	1.95	152.99	999.99
113	A	ASP	OD1	148	A	ASN	ND2	1	2.97	2.52	104.07	999.99
113	A	ASP	OD1	148	A	ASN	ND2	2	2.97	3.31	62.13	999.99
116	A	GLU	OE1	356	A	ASN	ND2	1	3.01	2.74	93.96	999.99
116	A	GLU	OE1	356	A	ASN	ND2	2	3.01	3.36	61.98	999.99
117	A	TYR	OH	356	A	ASN	OD1	-	3.28	9.99	999.99	999.99
117	A	TYR	OH	356	A	ASN	ND2	-	3.40	9.99	999.99	999.99
146	A	THR	OG1	148	A	ASN	OD1	-	2.91	9.99	999.99	999.99
147	A	ASP	OD2	87	A	GLN	NE2	1	2.95	3.37	58.30	999.99
147	A	ASP	OD2	87	A	GLN	NE2	2	2.95	2.09	136.01	999.99
147	A	ASP	OD1	150	A	GLN	NE2	1	3.25	3.48	68.47	999.99
147	A	ASP	OD1	150	A	GLN	NE2	2	3.25	2.33	142.48	999.99
148	A	ASN	ND2	113	A	ASP	OD1	1	2.97	3.65	42.94	999.99
148	A	ASN	ND2	113	A	ASP	OD1	2	2.97	1.95	163.19	999.99
148	A	ASN	OD1	146	A	THR	OG1	1	2.91	2.60	95.67	999.99
148	A	ASN	OD1	146	A	THR	OG1	2	2.91	2.47	103.30	999.99
150	A	GLN	NE2	147	A	ASP	OD1	1	3.25	3.01	93.49	999.99
150	A	GLN	NE2	147	A	ASP	OD1	2	3.25	3.49	67.96	999.99

164	A	SER	OG	162	A	ASP	OD1	-	2.69	9.99	999.99	999.99
167	A	LYS	NZ	230	A	HIS	NE2	-	3.07	9.99	999.99	999.99
168	A	TYR	OH	189	A	ASP	OD1	-	2.83	9.99	999.99	999.99
175	A	ASN	OD1	177	A	THR	OG1	1	2.69	2.63	81.77	999.99
175	A	ASN	OD1	177	A	THR	OG1	2	2.69	2.72	76.90	999.99
175	A	ASN	ND2	678	A	SER	OG	1	3.27	2.49	129.66	999.99
175	A	ASN	ND2	678	A	SER	OG	2	3.27	3.86	48.90	999.99
177	A	THR	OG1	175	A	ASN	OD1	-	2.69	9.99	999.99	999.99
177	A	THR	OG1	678	A	SER	OG	-	3.38	9.99	999.99	999.99
179	A	GLU	OE1	641	A	GLN	NE2	1	3.09	3.51	58.49	999.99
179	A	GLU	OE1	641	A	GLN	NE2	2	3.09	2.08	155.73	999.99
180	A	HIS	NE2	667	A	MET	SD	-	3.91	3.79	91.21	999.99
199	A	ARG	NH2	189	A	ASP	OD1	1	2.93	1.94	154.07	999.99
199	A	ARG	NH2	189	A	ASP	OD1	2	2.93	3.44	51.89	999.99
199	A	ARG	NH2	189	A	ASP	OD2	1	3.28	2.85	104.06	999.99
199	A	ARG	NH2	189	A	ASP	OD2	2	3.28	3.44	72.49	999.99
199	A	ARG	NE	202	A	GLU	OE1	-	3.40	2.90	110.46	999.99
199	A	ARG	NE	202	A	GLU	OE2	-	2.88	1.95	150.22	999.99
199	A	ARG	NH1	202	A	GLU	OE1	1	3.01	2.51	108.63	999.99
199	A	ARG	NH1	202	A	GLU	OE1	2	3.01	3.60	48.70	999.99
199	A	ARG	NH1	202	A	GLU	OE2	1	3.16	2.33	135.30	999.99
199	A	ARG	NH1	202	A	GLU	OE2	2	3.16	4.06	26.87	999.99
211	A	ASN	ND2	214	A	GLU	OE2	1	3.08	3.72	45.83	999.99
211	A	ASN	ND2	214	A	GLU	OE2	2	3.08	2.58	108.80	999.99
214	A	GLU	OE2	211	A	ASN	ND2	1	3.08	3.42	62.60	999.99
214	A	GLU	OE2	211	A	ASN	ND2	2	3.08	2.21	136.35	999.99
219	A	TRP	NE1	215	A	ASP	OD1	-	3.35	3.07	100.41	999.99
219	A	TRP	NE1	215	A	ASP	OD2	-	3.03	2.32	135.12	999.99
220	A	ARG	NH2	101	A	ASP	OD2	1	2.93	1.95	151.82	999.99
220	A	ARG	NH2	101	A	ASP	OD2	2	2.93	3.34	57.59	999.99
220	A	ARG	NH2	105	A	TYR	OH	1	2.94	3.59	45.57	999.99
220	A	ARG	NH2	105	A	TYR	OH	2	2.94	2.07	143.76	999.99
224	A	TRP	NE1	101	A	ASP	OD2	-	2.83	1.99	154.22	999.99
238	A	GLU	OE1	103	A	HIS	ND1	1	2.77	1.80	149.83	999.99
238	A	GLU	OE1	103	A	HIS	ND1	2	2.77	3.42	45.13	999.99
238	A	GLU	OE2	103	A	HIS	ND1	1	3.39	2.70	122.84	999.99
238	A	GLU	OE2	103	A	HIS	ND1	2	3.39	4.34	23.90	999.99
243	A	ARG	NH1	442	A	ASP	OD1	1	3.10	3.57	55.43	999.99
243	A	ARG	NH1	442	A	ASP	OD1	2	3.10	2.06	167.98	999.99
243	A	ARG	NH1	442	A	ASP	OD2	1	3.00	3.83	32.53	999.99
243	A	ARG	NH1	442	A	ASP	OD2	2	3.00	2.26	126.09	999.99
243	A	ARG	NH2	442	A	ASP	OD2	1	2.86	3.68	33.90	999.99
243	A	ARG	NH2	442	A	ASP	OD2	2	2.86	2.14	126.73	999.99
243	A	ARG	NH2	446	A	GLU	OE1	1	2.94	1.97	149.00	999.99
243	A	ARG	NH2	446	A	GLU	OE1	2	2.94	3.40	54.80	999.99

245	A	TYR	OH	350	A	ASN	ND2	-	3.38	9.99	999.99	999.99
265	A	ARG	NH1	271	A	ASN	ND2	1	3.20	3.41	69.36	999.99
265	A	ARG	NH1	271	A	ASN	ND2	2	3.20	3.18	81.48	999.99
265	A	ARG	NE	280	A	ASN	OD1	-	3.22	2.47	130.13	999.99
265	A	ARG	NH1	280	A	ASN	OD1	1	2.84	1.83	158.96	999.99
265	A	ARG	NH1	280	A	ASN	OD1	2	2.84	3.60	37.38	999.99
288	A	THR	OG1	304	A	GLU	OE1	-	3.04	9.99	999.99	999.99
302	A	HIS	NE2	304	A	GLU	OE2	-	2.88	1.98	166.44	999.99
302	A	HIS	ND1	575	A	TYR	OH	-	2.95	2.05	167.38	999.99
304	A	GLU	OE2	302	A	HIS	NE2	1	2.88	3.58	42.39	999.99
304	A	GLU	OE2	302	A	HIS	NE2	2	2.88	1.85	160.15	999.99
308	A	SER	OG	306	A	ASP	OD1	-	2.65	9.99	999.99	999.99
319	A	HIS	NE2	457	A	SER	OG	-	3.29	2.74	121.59	999.99
319	A	HIS	NE2	675	A	ASP	OD1	-	3.13	2.60	120.23	999.99
319	A	HIS	NE2	675	A	ASP	OD2	-	2.87	2.01	166.19	999.99
326	A	ASN	OD1	378	A	THR	OG1	1	3.32	2.63	121.59	999.99
326	A	ASN	OD1	378	A	THR	OG1	2	3.32	3.40	76.20	999.99
347	A	SER	OG	349	A	ASN	OD1	-	2.70	9.99	999.99	999.99
347	A	SER	OG	359	A	HIS	ND1	-	3.34	9.99	999.99	999.99
349	A	ASN	OD1	347	A	SER	OG	1	2.70	1.99	121.03	999.99
349	A	ASN	OD1	347	A	SER	OG	2	2.70	2.68	79.56	999.99
349	A	ASN	OD1	359	A	HIS	ND1	1	3.28	3.37	75.66	999.99
349	A	ASN	OD1	359	A	HIS	ND1	2	3.28	2.54	125.44	999.99
350	A	ASN	ND2	245	A	TYR	OH	1	3.38	3.53	73.23	999.99
350	A	ASN	ND2	245	A	TYR	OH	2	3.38	2.88	109.42	999.99
356	A	ASN	OD1	66	A	ASP	OD2	1	3.05	2.05	154.83	999.99
356	A	ASN	OD1	66	A	ASP	OD2	2	3.05	3.71	45.47	999.99
356	A	ASN	ND2	116	A	GLU	OE1	1	3.01	3.55	51.26	999.99
356	A	ASN	ND2	116	A	GLU	OE1	2	3.01	1.96	176.23	999.99
356	A	ASN	OD1	117	A	TYR	OH	1	3.28	3.05	92.34	999.99
356	A	ASN	OD1	117	A	TYR	OH	2	3.28	3.85	50.56	999.99
356	A	ASN	ND2	117	A	TYR	OH	1	3.40	3.20	92.11	999.99
356	A	ASN	ND2	117	A	TYR	OH	2	3.40	4.03	47.41	999.99
357	A	LYS	NZ	84	A	TYR	OH	-	2.89	9.99	999.99	999.99
357	A	LYS	NZ	92	A	GLU	OE2	-	2.89	9.99	999.99	999.99
359	A	HIS	ND1	347	A	SER	OG	-	3.34	3.32	83.27	999.99
359	A	HIS	ND1	349	A	ASN	OD1	-	3.28	2.99	100.38	999.99
368	A	ARG	NE	343	A	ASP	OD1	-	2.89	1.87	170.51	999.99
368	A	ARG	NH1	343	A	ASP	OD2	1	2.90	1.85	176.50	999.99
368	A	ARG	NH1	343	A	ASP	OD2	2	2.90	3.49	48.28	999.99
369	A	THR	OG1	366	A	SER	OG	-	2.93	9.99	999.99	999.99
378	A	THR	OG1	326	A	ASN	OD1	-	3.32	9.99	999.99	999.99
378	A	THR	OG1	376	A	ASP	OD1	-	2.74	9.99	999.99	999.99
382	A	ARG	NH2	379	A	ASN	ND2	1	3.48	3.41	84.68	999.99
382	A	ARG	NH2	379	A	ASN	ND2	2	3.48	3.52	79.25	999.99

383	A	THR	OG1	213	A	GLU	OE2	-	2.75	9.99	999.99	999.99
392	A	TYR	OH	443	A	HIS	ND1	-	3.44	9.99	999.99	999.99
397	A	THR	OG1	395	A	GLU	OE1	-	2.72	9.99	999.99	999.99
403	A	ARG	NE	399	A	GLN	OE1	-	2.95	2.00	155.06	999.99
403	A	ARG	NH1	399	A	GLN	OE1	1	3.33	2.49	136.73	999.99
403	A	ARG	NH1	399	A	GLN	OE1	2	3.33	4.25	25.25	999.99
404	A	LYS	NZ	411	A	GLU	OE1	-	2.96	9.99	999.99	999.99
408	A	SER	OG	221	A	GLU	OE1	-	3.15	9.99	999.99	999.99
408	A	SER	OG	221	A	GLU	OE2	-	3.24	9.99	999.99	999.99
425	A	ARG	NE	433	A	ASP	OD2	-	2.81	1.81	164.89	999.99
436	A	SER	OG	398	A	GLU	OE1	-	3.42	9.99	999.99	999.99
436	A	SER	OG	398	A	GLU	OE2	-	2.69	9.99	999.99	999.99
443	A	HIS	ND1	392	A	TYR	OH	-	3.44	2.88	122.67	999.99
450	A	ARG	NH1	92	A	GLU	OE1	1	2.87	3.54	43.46	999.99
450	A	ARG	NH1	92	A	GLU	OE1	2	2.87	1.86	157.65	999.99
450	A	ARG	NH2	92	A	GLU	OE1	1	3.41	4.40	19.11	999.99
450	A	ARG	NH2	92	A	GLU	OE1	2	3.41	2.71	127.54	999.99
454	A	ARG	NH1	376	A	ASP	OD2	1	3.44	4.03	49.64	999.99
454	A	ARG	NH1	376	A	ASP	OD2	2	3.44	2.47	153.91	999.99
455	A	TYR	OH	87	A	GLN	NE2	-	3.21	9.99	999.99	999.99
457	A	SER	OG	319	A	HIS	NE2	-	3.29	9.99	999.99	999.99
457	A	SER	OG	675	A	ASP	OD2	-	2.79	9.99	999.99	999.99
460	A	SER	OG	314	A	TYR	OH	-	2.81	9.99	999.99	999.99
461	A	SER	OG	546	A	GLU	OE1	-	2.66	9.99	999.99	999.99
462	A	SER	OG	546	A	GLU	OE1	-	3.50	9.99	999.99	999.99
472	A	CYS	SG	575	A	TYR	OH	-	3.35	9.99	999.99	999.99
478	A	TYR	OH	486	A	ASN	ND2	-	3.14	9.99	999.99	999.99
480	A	THR	OG1	482	A	SER	OG	-	2.85	9.99	999.99	999.99
484	A	ARG	NE	432	A	GLN	OE1	-	3.08	2.53	112.80	999.99
484	A	ARG	NH1	432	A	GLN	OE1	1	3.35	2.78	114.35	999.99
484	A	ARG	NH1	432	A	GLN	OE1	2	3.35	4.16	34.43	999.99
484	A	ARG	NH1	433	A	ASP	OD1	1	2.95	3.46	52.82	999.99
484	A	ARG	NH1	433	A	ASP	OD1	2	2.95	1.92	168.65	999.99
484	A	ARG	NH1	433	A	ASP	OD2	1	3.38	4.29	25.93	999.99
484	A	ARG	NH1	433	A	ASP	OD2	2	3.38	2.56	134.75	999.99
484	A	ARG	NH2	433	A	ASP	OD2	1	2.95	3.73	36.83	999.99
484	A	ARG	NH2	433	A	ASP	OD2	2	2.95	2.00	156.30	999.99
486	A	ASN	ND2	478	A	TYR	OH	1	3.14	3.41	66.18	999.99
486	A	ASN	ND2	478	A	TYR	OH	2	3.14	2.91	92.43	999.99
487	A	LYS	NZ	477	A	GLU	OE1	-	3.10	9.99	999.99	999.99
495	A	ARG	NH1	477	A	GLU	OE1	1	2.89	3.54	44.63	999.99
495	A	ARG	NH1	477	A	GLU	OE1	2	2.89	1.85	173.46	999.99
514	A	ARG	NE	87	A	GLN	OE1	-	3.37	2.61	131.12	999.99
514	A	ARG	NH1	87	A	GLN	OE1	1	2.99	1.99	158.73	999.99
514	A	ARG	NH1	87	A	GLN	OE1	2	2.99	3.73	39.19	999.99

514	A	ARG	NH2	144	A	ASP	OD2	1	2.94	3.57	46.26	999.99
514	A	ARG	NH2	144	A	ASP	OD2	2	2.94	1.98	158.56	999.99
514	A	ARG	NE	147	A	ASP	OD2	-	3.16	2.55	118.08	999.99
515	A	LYS	NZ	315	A	GLU	OE2	-	3.01	9.99	999.99	999.99
515	A	LYS	NZ	318	A	ASP	OD2	-	2.88	9.99	999.99	999.99
519	A	ARG	NH2	517	A	GLN	OE1	1	3.47	3.94	56.93	999.99
519	A	ARG	NH2	517	A	GLN	OE1	2	3.47	2.57	150.10	999.99
526	A	THR	OG1	626	A	HIS	ND1	-	3.15	9.99	999.99	999.99
559	A	GLU	OE1	615	A	HIS	NE2	1	2.79	1.85	145.60	999.99
559	A	GLU	OE1	615	A	HIS	NE2	2	2.79	3.41	46.96	999.99
559	A	GLU	OE2	615	A	HIS	NE2	1	3.44	2.77	121.39	999.99
559	A	GLU	OE2	615	A	HIS	NE2	2	3.44	4.40	23.45	999.99
563	A	TYR	OH	592	A	ASN	OD1	-	3.17	9.99	999.99	999.99
563	A	TYR	OH	612	A	ASP	OD2	-	2.72	9.99	999.99	999.99
567	A	ARG	NH2	297	A	GLU	OE1	1	2.88	1.93	146.35	999.99
567	A	ARG	NH2	297	A	GLU	OE1	2	2.88	3.21	62.37	999.99
568	A	ARG	NE	571	A	GLU	OE2	-	2.86	1.94	146.31	999.99
568	A	ARG	NH1	571	A	GLU	OE2	1	3.04	2.17	139.08	999.99
568	A	ARG	NH1	571	A	GLU	OE2	2	3.04	3.94	27.22	999.99
569	A	SER	OG	598	A	GLU	OE2	-	2.76	9.99	999.99	999.99
575	A	TYR	OH	302	A	HIS	ND1	-	2.95	9.99	999.99	999.99
592	A	ASN	OD1	563	A	TYR	OH	1	3.17	2.82	98.68	999.99
592	A	ASN	OD1	563	A	TYR	OH	2	3.17	3.56	60.28	999.99
592	A	ASN	OD1	612	A	ASP	OD2	1	1.82	1.28	101.26	999.99
592	A	ASN	OD1	612	A	ASP	OD2	2	1.82	1.79	74.63	999.99
606	A	GLN	NE2	639	A	ASP	OD1	1	3.09	3.43	62.68	999.99
606	A	GLN	NE2	639	A	ASP	OD1	2	3.09	2.24	136.67	999.99
606	A	GLN	NE2	639	A	ASP	OD2	1	3.03	3.64	47.96	999.99
606	A	GLN	NE2	639	A	ASP	OD2	2	3.03	2.02	161.97	999.99
610	A	LYS	NZ	606	A	GLN	OE1	-	3.32	9.99	999.99	999.99
611	A	ARG	NE	607	A	HIS	NE2	-	3.07	2.28	132.54	999.99
611	A	ARG	NH1	607	A	HIS	NE2	1	3.35	2.67	122.44	999.99
611	A	ARG	NH1	607	A	HIS	NE2	2	3.35	4.19	32.54	999.99
612	A	ASP	OD2	592	A	ASN	OD1	1	1.82	1.24	103.69	999.99
612	A	ASP	OD2	592	A	ASN	OD1	2	1.82	1.88	70.75	999.99
613	A	LYS	NZ	650	A	GLU	OE2	-	2.93	9.99	999.99	999.99
615	A	HIS	NE2	559	A	GLU	OE1	-	2.79	1.89	167.81	999.99
615	A	HIS	NE2	559	A	GLU	OE2	-	3.44	2.89	119.76	999.99
615	A	HIS	ND1	618	A	GLN	OE1	-	2.85	1.95	166.40	999.99
618	A	GLN	OE1	615	A	HIS	ND1	1	2.85	2.92	75.60	999.99
618	A	GLN	OE1	615	A	HIS	ND1	2	2.85	2.12	123.66	999.99
626	A	HIS	ND1	526	A	THR	OG1	-	3.15	2.58	122.08	999.99
630	A	CYS	SG	675	A	ASP	OD2	-	3.75	9.99	999.99	999.99
634	A	ARG	NH2	209	A	ASP	OD1	1	3.07	2.68	100.98	999.99
634	A	ARG	NH2	209	A	ASP	OD1	2	3.07	3.06	80.91	999.99

638	A	ARG	NH2	179	A	GLU	OE1	1	3.07	3.41	62.69	999.99
638	A	ARG	NH2	179	A	GLU	OE1	2	3.07	2.14	151.82	999.99
638	A	ARG	NH2	641	A	GLN	OE1	1	3.06	2.18	139.15	999.99
638	A	ARG	NH2	641	A	GLN	OE1	2	3.06	3.50	56.73	999.99
639	A	ASP	OD1	606	A	GLN	NE2	1	3.09	2.46	116.94	999.99
639	A	ASP	OD1	606	A	GLN	NE2	2	3.09	3.88	37.42	999.99
639	A	ASP	OD2	606	A	GLN	NE2	1	3.03	2.38	118.63	999.99
639	A	ASP	OD2	606	A	GLN	NE2	2	3.03	3.80	38.50	999.99
641	A	GLN	NE2	179	A	GLU	OE1	1	3.09	2.18	143.70	999.99
641	A	GLN	NE2	179	A	GLU	OE1	2	3.09	3.33	67.77	999.99
641	A	GLN	NE2	645	A	TYR	OH	1	2.89	3.40	52.91	999.99
641	A	GLN	NE2	645	A	TYR	OH	2	2.89	2.09	131.62	999.99
645	A	TYR	OH	641	A	GLN	NE2	-	2.89	9.99	999.99	999.99
646	A	ASP	OD1	656	A	HIS	NE2	1	2.87	2.78	83.91	999.99
646	A	ASP	OD1	656	A	HIS	NE2	2	2.87	2.52	97.35	999.99
656	A	HIS	NE2	646	A	ASP	OD1	-	2.87	2.00	167.86	999.99
665	A	LYS	NZ	661	A	ASP	OD2	-	3.11	9.99	999.99	999.99
675	A	ASP	OD1	319	A	HIS	NE2	1	3.13	2.53	114.77	999.99
675	A	ASP	OD1	319	A	HIS	NE2	2	3.13	3.98	32.71	999.99
675	A	ASP	OD2	319	A	HIS	NE2	1	2.87	2.20	119.36	999.99
675	A	ASP	OD2	319	A	HIS	NE2	2	2.87	3.57	42.10	999.99
678	A	SER	OG	175	A	ASN	ND2	-	3.27	9.99	999.99	999.99

Dd-a = Distance Between Donor and Acceptor
Dh-a = Distance Between Hydrogen and Acceptor
A(d-H-N) = Angle Between Donor-H-N
A(a-O=C) = Angle Between Acceptor-O=C
MO = Multiple Occupancy
Note that angles that are undefined are written as 999.99

Intraprotein Ionic Interactions


[help]

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Ionic Interactions within 6 Angstroms

Position	Residue	Chain	Position	Residue	Chain

65	LYS	A	151	ASP	A
66	ASP	A	72	LYS	A
71	GLU	A	74	LYS	A
72	LYS	A	354	GLU	A
74	LYS	A	127	GLU	A
75	LYS	A	354	GLU	A
78	ARG	A	352	ASP	A
92	GLU	A	357	LYS	A
92	GLU	A	450	ARG	A
93	GLU	A	382	ARG	A
93	GLU	A	450	ARG	A
97	ARG	A	213	GLU	A
100	LYS	A	388	GLU	A
100	LYS	A	446	GLU	A
101	ASP	A	104	ARG	A
101	ASP	A	220	ARG	A
103	HIS	A	238	GLU	A
104	ARG	A	388	GLU	A
108	ARG	A	238	GLU	A
115	GLU	A	279	LYS	A
142	GLU	A	180	HIS	A
144	ASP	A	514	ARG	A
147	ASP	A	514	ARG	A
176	LYS	A	207	ASP	A
179	GLU	A	638	ARG	A
179	GLU	A	664	LYS	A
189	ASP	A	199	ARG	A
190	LYS	A	193	GLU	A
193	GLU	A	199	ARG	A
199	ARG	A	202	GLU	A
209	ASP	A	634	ARG	A
213	GLU	A	382	ARG	A
214	GLU	A	413	LYS	A
220	ARG	A	221	GLU	A
239	GLU	A	403	ARG	A
243	ARG	A	442	ASP	A
243	ARG	A	446	GLU	A
262	GLU	A	267	LYS	A
297	GLU	A	567	ARG	A
297	GLU	A	568	ARG	A
297	GLU	A	597	ARG	A
298	ARG	A	572	ASP	A
302	HIS	A	304	GLU	A
304	GLU	A	470	HIS	A
306	ASP	A	506	ARG	A

309	ASP	A	311	LYS	A
315	GLU	A	463	LYS	A
315	GLU	A	515	LYS	A
318	ASP	A	515	LYS	A
319	HIS	A	675	ASP	A
343	ASP	A	368	ARG	A
376	ASP	A	454	ARG	A
388	GLU	A	443	HIS	A
400	GLU	A	404	LYS	A
401	HIS	A	411	GLU	A
404	LYS	A	411	GLU	A
422	GLU	A	424	ARG	A
422	GLU	A	481	ARG	A
425	ARG	A	433	ASP	A
433	ASP	A	484	ARG	A
443	HIS	A	446	GLU	A
463	LYS	A	546	GLU	A
477	GLU	A	487	LYS	A
477	GLU	A	495	ARG	A
498	GLU	A	505	ARG	A
502	GLU	A	505	ARG	A
559	GLU	A	615	HIS	A
567	ARG	A	572	ASP	A
568	ARG	A	571	GLU	A
570	ASP	A	576	ARG	A
576	ARG	A	577	GLU	A
610	LYS	A	639	ASP	A
613	LYS	A	650	GLU	A
646	ASP	A	656	HIS	A
661	ASP	A	665	LYS	A

Intraprotein Aromatic-Aromatic Interactions


[help]

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Aromatic-Aromatic Interactions within 4.5 and 7 Angstroms

Position Residue Chain Position Residue Chain D(centroid-centroid) Dihedral Angle

69	PHE	A	117	TYR	A	6.10	84.66
69	PHE	A	83	PHE	A	5.00	105.92
83	PHE	A	117	TYR	A	6.94	106.08
83	PHE	A	135	PHE	A	5.65	20.74
83	PHE	A	152	PHE	A	6.99	165.17
135	PHE	A	152	PHE	A	5.45	169.61
135	PHE	A	168	TYR	A	6.72	66.12
140	TYR	A	455	TYR	A	6.40	112.76
152	PHE	A	155	TRP	A	5.87	166.65
153	TYR	A	187	TYR	A	4.85	51.28
171	PHE	A	201	PHE	A	4.98	47.58
171	PHE	A	216	PHE	A	5.69	33.33
171	PHE	A	223	PHE	A	5.43	40.96
201	PHE	A	219	TRP	A	6.51	74.09
201	PHE	A	223	PHE	A	5.54	87.62
223	PHE	A	224	TRP	A	4.96	79.90
259	TYR	A	374	TYR	A	5.76	101.74
276	PHE	A	282	PHE	A	5.08	107.82
323	TYR	A	512	PHE	A	5.47	41.35
373	TYR	A	374	TYR	A	6.28	47.91
455	TYR	A	512	PHE	A	6.08	89.96
518	PHE	A	540	PHE	A	5.72	133.42
518	PHE	A	543	PHE	A	6.23	138.20
518	PHE	A	628	TYR	A	4.77	117.61
540	PHE	A	543	PHE	A	5.35	86.30
540	PHE	A	628	TYR	A	6.97	80.18
543	PHE	A	628	TYR	A	5.27	76.13
564	TYR	A	573	TYR	A	5.86	39.99
573	TYR	A	595	PHE	A	5.87	54.95
617	TRP	A	662	TYR	A	5.77	48.12
644	PHE	A	672	TYR	A	5.82	88.21

Intraprotein Aromatic-Sulphur Interactions


[help]

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Aromatic-Sulphur Interactions within 5.3 Angstroms

Position Residue Chain Position Residue Chain D(Centroid-Sulphur) Angle

105	TYR	A	228	CYS	A	5.13	113.45
153	TYR	A	184	MET	A	4.84	123.80
171	PHE	A	136	CYS	A	4.78	133.23
181	PHE	A	205	MET	A	4.72	54.22
323	TYR	A	263	MET	A	4.83	144.27
361	PHE	A	363	CYS	A	4.19	34.54
367	TYR	A	346	MET	A	4.61	34.85
540	PHE	A	530	MET	A	4.32	130.92
543	PHE	A	530	MET	A	4.59	60.02
573	TYR	A	566	CYS	A	4.95	38.99
575	TYR	A	472	CYS	A	5.03	85.92
595	PHE	A	566	CYS	A	4.84	65.46
662	TYR	A	654	MET	A	5.20	133.83
677	TRP	A	630	CYS	A	4.36	121.49

Intraprotein Cation-Pi Interactions

  [help]

Rasmol Jmol

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Cation-Pi Interactions within 6 Angstroms

Position	Residue	Chain	Position	Residue	Chain	D(cation-Pi)	Angle
84	TYR	A	357	LYS	A	4.66	111.65
94	PHE	A	97	ARG	A	5.10	95.24
117	TYR	A	72	LYS	A	5.02	79.25
140	TYR	A	514	ARG	A	3.76	152.57
181	PHE	A	176	LYS	A	5.85	144.50
181	PHE	A	186	LYS	A	5.69	62.84
216	PHE	A	97	ARG	A	5.18	126.39
231	PHE	A	167	LYS	A	4.81	56.30
387	TYR	A	403	ARG	A	5.05	15.84
493	TRP	A	497	LYS	A	4.80	133.05

Intraprotein Hydrophobic Interactions

DOG_POR_E315Q_snapshot10.pdb

  [help]

Rasmol **Jmol**

Hydrophobic Interactions within 5 Angstroms

Position	Residue	Chain	Position	Residue	Chain
60	MET	A	64	ALA	A
69	PHE	A	117	TYR	A
69	PHE	A	119	LEU	A
69	PHE	A	122	LEU	A
69	PHE	A	125	LEU	A
69	PHE	A	70	VAL	A
69	PHE	A	81	ILE	A
69	PHE	A	83	PHE	A
70	VAL	A	125	LEU	A
70	VAL	A	128	ILE	A
73	MET	A	110	MET	A
73	MET	A	125	LEU	A
73	MET	A	128	ILE	A
73	MET	A	81	ILE	A
80	ILE	A	102	ALA	A
80	ILE	A	107	MET	A
80	ILE	A	132	LEU	A
80	ILE	A	134	VAL	A
80	ILE	A	224	TRP	A
80	ILE	A	82	VAL	A
81	ILE	A	110	MET	A
81	ILE	A	112	ALA	A
81	ILE	A	125	LEU	A
81	ILE	A	133	ALA	A
81	ILE	A	83	PHE	A
82	VAL	A	111	ALA	A
82	VAL	A	134	VAL	A
82	VAL	A	95	ALA	A
82	VAL	A	98	LEU	A
83	PHE	A	112	ALA	A
83	PHE	A	114	PRO	A

83	PHE	A	117	TYR	A
83	PHE	A	119	LEU	A
83	PHE	A	122	LEU	A
83	PHE	A	135	PHE	A
83	PHE	A	137	MET	A
84	TYR	A	111	ALA	A
84	TYR	A	114	PRO	A
84	TYR	A	91	ALA	A
84	TYR	A	95	ALA	A
91	ALA	A	138	ALA	A
91	ALA	A	173	LEU	A
94	PHE	A	173	LEU	A
94	PHE	A	212	LEU	A
94	PHE	A	216	PHE	A
95	ALA	A	111	ALA	A
98	LEU	A	134	VAL	A
98	LEU	A	171	PHE	A
98	LEU	A	216	PHE	A
98	LEU	A	223	PHE	A
98	LEU	A	224	TRP	A
102	ALA	A	107	MET	A
102	ALA	A	224	TRP	A
105	TYR	A	107	MET	A
105	TYR	A	224	TRP	A
105	TYR	A	233	VAL	A
105	TYR	A	235	ALA	A
107	MET	A	227	VAL	A
107	MET	A	231	PHE	A
107	MET	A	233	VAL	A
112	ALA	A	117	TYR	A
114	PRO	A	119	LEU	A
114	PRO	A	149	ALA	A
114	PRO	A	152	PHE	A
117	TYR	A	119	LEU	A
119	LEU	A	122	LEU	A
119	LEU	A	152	PHE	A
119	LEU	A	155	TRP	A
120	ALA	A	155	TRP	A
120	ALA	A	161	VAL	A
122	LEU	A	125	LEU	A
122	LEU	A	133	ALA	A
122	LEU	A	135	PHE	A
122	LEU	A	152	PHE	A
122	LEU	A	155	TRP	A
122	LEU	A	163	LEU	A

125	LEU	A	126	PRO	A
125	LEU	A	128	ILE	A
125	LEU	A	133	ALA	A
125	LEU	A	166	VAL	A
126	PRO	A	166	VAL	A
132	LEU	A	134	VAL	A
132	LEU	A	200	ILE	A
132	LEU	A	223	PHE	A
132	LEU	A	227	VAL	A
132	LEU	A	231	PHE	A
133	ALA	A	135	PHE	A
133	ALA	A	166	VAL	A
133	ALA	A	168	TYR	A
134	VAL	A	169	ALA	A
134	VAL	A	171	PHE	A
134	VAL	A	223	PHE	A
135	PHE	A	137	MET	A
135	PHE	A	152	PHE	A
135	PHE	A	168	TYR	A
135	PHE	A	170	VAL	A
135	PHE	A	188	VAL	A
135	PHE	A	192	LEU	A
137	MET	A	152	PHE	A
137	MET	A	170	VAL	A
137	MET	A	184	MET	A
137	MET	A	188	VAL	A
138	ALA	A	173	LEU	A
140	TYR	A	455	TYR	A
145	PRO	A	149	ALA	A
145	PRO	A	153	TYR	A
145	PRO	A	184	MET	A
149	ALA	A	152	PHE	A
149	ALA	A	184	MET	A
152	PHE	A	155	TRP	A
152	PHE	A	156	LEU	A
152	PHE	A	184	MET	A
152	PHE	A	188	VAL	A
153	TYR	A	184	MET	A
153	TYR	A	187	TYR	A
155	TRP	A	156	LEU	A
155	TRP	A	161	VAL	A
155	TRP	A	163	LEU	A
155	TRP	A	195	LEU	A
156	LEU	A	187	TYR	A
156	LEU	A	188	VAL	A

156	LEU	A	192	LEU	A
156	LEU	A	195	LEU	A
161	VAL	A	163	LEU	A
163	LEU	A	166	VAL	A
163	LEU	A	192	LEU	A
163	LEU	A	195	LEU	A
163	LEU	A	197	ALA	A
166	VAL	A	197	ALA	A
168	TYR	A	170	VAL	A
168	TYR	A	192	LEU	A
168	TYR	A	197	ALA	A
169	ALA	A	171	PHE	A
169	ALA	A	201	PHE	A
169	ALA	A	223	PHE	A
170	VAL	A	188	VAL	A
170	VAL	A	192	LEU	A
170	VAL	A	203	LEU	A
171	PHE	A	201	PHE	A
171	PHE	A	219	TRP	A
171	PHE	A	223	PHE	A
173	LEU	A	212	LEU	A
178	TYR	A	674	LEU	A
178	TYR	A	676	VAL	A
181	PHE	A	205	MET	A
184	MET	A	187	TYR	A
184	MET	A	188	VAL	A
187	TYR	A	188	VAL	A
188	VAL	A	192	LEU	A
192	LEU	A	195	LEU	A
192	LEU	A	197	ALA	A
200	ILE	A	201	PHE	A
200	ILE	A	231	PHE	A
201	PHE	A	219	TRP	A
201	PHE	A	223	PHE	A
201	PHE	A	226	ALA	A
203	LEU	A	205	MET	A
216	PHE	A	217	ILE	A
217	ILE	A	406	ALA	A
223	PHE	A	224	TRP	A
223	PHE	A	227	VAL	A
224	TRP	A	225	PRO	A
224	TRP	A	227	VAL	A
227	VAL	A	231	PHE	A
227	VAL	A	233	VAL	A
231	PHE	A	233	VAL	A

245	TYR	A	348	LEU	A
245	TYR	A	360	PRO	A
247	LEU	A	249	VAL	A
247	LEU	A	346	MET	A
247	LEU	A	348	LEU	A
247	LEU	A	367	TYR	A
249	VAL	A	344	VAL	A
253	ILE	A	258	VAL	A
253	ILE	A	345	VAL	A
253	ILE	A	364	PRO	A
255	MET	A	258	VAL	A
255	MET	A	260	VAL	A
255	MET	A	345	VAL	A
258	VAL	A	260	VAL	A
258	VAL	A	345	VAL	A
258	VAL	A	364	PRO	A
259	TYR	A	266	LEU	A
259	TYR	A	362	PRO	A
259	TYR	A	364	PRO	A
259	TYR	A	374	TYR	A
263	MET	A	269	TYR	A
263	MET	A	281	PRO	A
263	MET	A	323	TYR	A
263	MET	A	373	TYR	A
263	MET	A	374	TYR	A
269	TYR	A	281	PRO	A
269	TYR	A	283	LEU	A
269	TYR	A	510	PRO	A
274	PRO	A	275	PRO	A
274	PRO	A	276	PHE	A
276	PHE	A	282	PHE	A
276	PHE	A	312	LEU	A
278	ALA	A	323	TYR	A
278	ALA	A	512	PHE	A
281	PRO	A	323	TYR	A
281	PRO	A	510	PRO	A
282	PHE	A	284	ALA	A
282	PHE	A	307	ILE	A
282	PHE	A	312	LEU	A
282	PHE	A	511	MET	A
283	LEU	A	508	LEU	A
283	LEU	A	510	PRO	A
284	ALA	A	305	LEU	A
284	ALA	A	307	ILE	A
284	ALA	A	511	MET	A

285	ALA	A	500	ALA	A
285	ALA	A	508	LEU	A
286	VAL	A	303	LEU	A
286	VAL	A	305	LEU	A
286	VAL	A	507	ALA	A
286	VAL	A	509	VAL	A
292	LEU	A	300	LEU	A
292	LEU	A	574	LEU	A
292	LEU	A	575	TYR	A
300	LEU	A	474	VAL	A
300	LEU	A	574	LEU	A
301	MET	A	303	LEU	A
301	MET	A	473	ALA	A
301	MET	A	475	ALA	A
301	MET	A	494	LEU	A
303	LEU	A	305	LEU	A
303	LEU	A	471	ILE	A
303	LEU	A	494	LEU	A
305	LEU	A	322	VAL	A
305	LEU	A	469	VAL	A
305	LEU	A	471	ILE	A
305	LEU	A	509	VAL	A
305	LEU	A	511	MET	A
307	ILE	A	312	LEU	A
307	ILE	A	314	TYR	A
307	ILE	A	469	VAL	A
307	ILE	A	511	MET	A
312	LEU	A	511	MET	A
312	LEU	A	513	VAL	A
314	TYR	A	458	ILE	A
314	TYR	A	469	VAL	A
314	TYR	A	513	VAL	A
320	VAL	A	322	VAL	A
320	VAL	A	456	TYR	A
320	VAL	A	458	ILE	A
320	VAL	A	469	VAL	A
320	VAL	A	471	ILE	A
320	VAL	A	511	MET	A
320	VAL	A	513	VAL	A
321	ALA	A	453	ALA	A
321	ALA	A	455	TYR	A
321	ALA	A	512	PHE	A
322	VAL	A	456	TYR	A
322	VAL	A	490	ALA	A
322	VAL	A	493	TRP	A

322	VAL	A	494	LEU	A
322	VAL	A	509	VAL	A
322	VAL	A	511	MET	A
323	TYR	A	324	PRO	A
323	TYR	A	453	ALA	A
323	TYR	A	510	PRO	A
323	TYR	A	512	PHE	A
324	PRO	A	451	LEU	A
324	PRO	A	489	VAL	A
324	PRO	A	490	ALA	A
324	PRO	A	493	TRP	A
325	ALA	A	373	TYR	A
325	ALA	A	493	TRP	A
330	LEU	A	334	LEU	A
330	LEU	A	377	ILE	A
330	LEU	A	428	LEU	A
331	VAL	A	342	LEU	A
331	VAL	A	371	LEU	A
331	VAL	A	377	ILE	A
334	LEU	A	338	LEU	A
334	LEU	A	371	LEU	A
334	LEU	A	377	ILE	A
334	LEU	A	427	ILE	A
334	LEU	A	428	LEU	A
334	LEU	A	431	LEU	A
334	LEU	A	441	ILE	A
334	LEU	A	444	LEU	A
337	ILE	A	338	LEU	A
337	ILE	A	428	LEU	A
337	ILE	A	431	LEU	A
338	LEU	A	340	ALA	A
338	LEU	A	431	LEU	A
338	LEU	A	439	PRO	A
338	LEU	A	441	ILE	A
338	LEU	A	444	LEU	A
340	ALA	A	342	LEU	A
340	ALA	A	441	ILE	A
342	LEU	A	367	TYR	A
342	LEU	A	371	LEU	A
342	LEU	A	441	ILE	A
344	VAL	A	346	MET	A
344	VAL	A	367	TYR	A
345	VAL	A	364	PRO	A
346	MET	A	361	PHE	A
346	MET	A	367	TYR	A

346	MET	A	370	ALA	A
348	LEU	A	360	PRO	A
348	LEU	A	361	PHE	A
360	PRO	A	361	PHE	A
361	PHE	A	362	PRO	A
361	PHE	A	370	ALA	A
361	PHE	A	374	TYR	A
361	PHE	A	375	LEU	A
362	PRO	A	374	TYR	A
367	TYR	A	441	ILE	A
370	ALA	A	374	TYR	A
370	ALA	A	375	LEU	A
371	LEU	A	375	LEU	A
371	LEU	A	377	ILE	A
371	LEU	A	441	ILE	A
371	LEU	A	448	LEU	A
373	TYR	A	374	TYR	A
374	TYR	A	375	LEU	A
375	LEU	A	377	ILE	A
375	LEU	A	448	LEU	A
377	ILE	A	427	ILE	A
377	ILE	A	448	LEU	A
380	PRO	A	381	PRO	A
380	PRO	A	420	VAL	A
381	PRO	A	385	VAL	A
381	PRO	A	386	LEU	A
381	PRO	A	420	VAL	A
381	PRO	A	427	ILE	A
381	PRO	A	430	ILE	A
385	VAL	A	386	LEU	A
385	VAL	A	389	LEU	A
385	VAL	A	427	ILE	A
385	VAL	A	444	LEU	A
385	VAL	A	447	LEU	A
385	VAL	A	448	LEU	A
385	VAL	A	449	PRO	A
386	LEU	A	402	LEU	A
386	LEU	A	405	MET	A
386	LEU	A	416	TYR	A
386	LEU	A	420	VAL	A
386	LEU	A	427	ILE	A
386	LEU	A	430	ILE	A
387	TYR	A	406	ALA	A
389	LEU	A	392	TYR	A
389	LEU	A	437	LEU	A

389	LEU	A	439	PRO	A
389	LEU	A	444	LEU	A
389	LEU	A	447	LEU	A
390	ALA	A	402	LEU	A
392	TYR	A	437	LEU	A
392	TYR	A	439	PRO	A
392	TYR	A	440	PRO	A
393	ALA	A	402	LEU	A
393	ALA	A	437	LEU	A
402	LEU	A	405	MET	A
402	LEU	A	430	ILE	A
402	LEU	A	434	TYR	A
402	LEU	A	437	LEU	A
405	MET	A	415	LEU	A
405	MET	A	416	TYR	A
405	MET	A	419	TRP	A
405	MET	A	420	VAL	A
405	MET	A	434	TYR	A
415	LEU	A	419	TRP	A
416	TYR	A	420	VAL	A
416	TYR	A	421	VAL	A
417	LEU	A	421	VAL	A
419	TRP	A	420	VAL	A
419	TRP	A	434	TYR	A
420	VAL	A	421	VAL	A
420	VAL	A	430	ILE	A
427	ILE	A	430	ILE	A
427	ILE	A	431	LEU	A
427	ILE	A	444	LEU	A
427	ILE	A	448	LEU	A
430	ILE	A	434	TYR	A
430	ILE	A	437	LEU	A
431	LEU	A	437	LEU	A
431	LEU	A	439	PRO	A
431	LEU	A	444	LEU	A
434	TYR	A	435	PRO	A
434	TYR	A	437	LEU	A
437	LEU	A	439	PRO	A
439	PRO	A	440	PRO	A
439	PRO	A	444	LEU	A
441	ILE	A	444	LEU	A
444	LEU	A	448	LEU	A
448	LEU	A	449	PRO	A
451	LEU	A	489	VAL	A
453	ALA	A	455	TYR	A

453	ALA	A	512	PHE	A
455	TYR	A	512	PHE	A
456	TYR	A	471	ILE	A
456	TYR	A	473	ALA	A
456	TYR	A	490	ALA	A
456	TYR	A	494	LEU	A
458	ILE	A	469	VAL	A
458	ILE	A	513	VAL	A
459	ALA	A	538	ALA	A
464	VAL	A	549	TRP	A
469	VAL	A	471	ILE	A
469	VAL	A	511	MET	A
471	ILE	A	494	LEU	A
473	ALA	A	494	LEU	A
474	VAL	A	476	VAL	A
476	VAL	A	478	TYR	A
490	ALA	A	493	TRP	A
493	TRP	A	494	LEU	A
493	TRP	A	509	VAL	A
493	TRP	A	510	PRO	A
494	LEU	A	509	VAL	A
500	ALA	A	507	ALA	A
509	VAL	A	510	PRO	A
509	VAL	A	511	MET	A
511	MET	A	513	VAL	A
518	PHE	A	539	PRO	A
518	PHE	A	540	PHE	A
518	PHE	A	543	PHE	A
518	PHE	A	628	TYR	A
520	LEU	A	521	PRO	A
520	LEU	A	528	VAL	A
520	LEU	A	543	PHE	A
520	LEU	A	628	TYR	A
521	PRO	A	528	VAL	A
521	PRO	A	628	TYR	A
524	ALA	A	550	LEU	A
524	ALA	A	557	VAL	A
527	PRO	A	619	LEU	A
527	PRO	A	625	ALA	A
528	VAL	A	530	MET	A
528	VAL	A	543	PHE	A
528	VAL	A	628	TYR	A
529	ILE	A	531	VAL	A
529	ILE	A	561	LEU	A
529	ILE	A	563	TYR	A

529	ILE	A	609	LEU	A
529	ILE	A	616	LEU	A
529	ILE	A	619	LEU	A
529	ILE	A	620	ILE	A
529	ILE	A	627	ILE	A
529	ILE	A	644	PHE	A
530	MET	A	540	PHE	A
530	MET	A	543	PHE	A
530	MET	A	544	ILE	A
530	MET	A	562	LEU	A
530	MET	A	628	TYR	A
531	VAL	A	533	PRO	A
531	VAL	A	563	TYR	A
531	VAL	A	605	VAL	A
531	VAL	A	609	LEU	A
531	VAL	A	629	VAL	A
531	VAL	A	640	VAL	A
531	VAL	A	644	PHE	A
533	PRO	A	564	TYR	A
533	PRO	A	605	VAL	A
533	PRO	A	636	MET	A
537	VAL	A	541	ILE	A
537	VAL	A	562	LEU	A
537	VAL	A	564	TYR	A
537	VAL	A	574	LEU	A
537	VAL	A	575	TYR	A
537	VAL	A	579	LEU	A
538	ALA	A	539	PRO	A
539	PRO	A	540	PHE	A
539	PRO	A	543	PHE	A
540	PHE	A	543	PHE	A
540	PHE	A	562	LEU	A
540	PHE	A	628	TYR	A
541	ILE	A	575	TYR	A
541	ILE	A	579	LEU	A
541	ILE	A	582	PHE	A
543	PHE	A	544	ILE	A
543	PHE	A	628	TYR	A
544	ILE	A	562	LEU	A
544	ILE	A	579	LEU	A
544	ILE	A	582	PHE	A
544	ILE	A	588	LEU	A
548	ALA	A	582	PHE	A
549	TRP	A	550	LEU	A
550	LEU	A	557	VAL	A

561	LEU	A	563	TYR	A
561	LEU	A	616	LEU	A
561	LEU	A	619	LEU	A
562	LEU	A	564	TYR	A
562	LEU	A	579	LEU	A
562	LEU	A	588	LEU	A
563	TYR	A	605	VAL	A
563	TYR	A	608	LEU	A
563	TYR	A	609	LEU	A
563	TYR	A	616	LEU	A
564	TYR	A	573	TYR	A
564	TYR	A	574	LEU	A
564	TYR	A	579	LEU	A
564	TYR	A	593	VAL	A
573	TYR	A	579	LEU	A
573	TYR	A	593	VAL	A
573	TYR	A	595	PHE	A
574	LEU	A	575	TYR	A
575	TYR	A	579	LEU	A
579	LEU	A	582	PHE	A
579	LEU	A	588	LEU	A
579	LEU	A	591	LEU	A
582	PHE	A	588	LEU	A
588	LEU	A	591	LEU	A
591	LEU	A	593	VAL	A
593	VAL	A	595	PHE	A
594	ALA	A	603	VAL	A
594	ALA	A	608	LEU	A
603	VAL	A	608	LEU	A
605	VAL	A	608	LEU	A
605	VAL	A	636	MET	A
605	VAL	A	640	VAL	A
609	LEU	A	616	LEU	A
609	LEU	A	640	VAL	A
609	LEU	A	644	PHE	A
609	LEU	A	647	ILE	A
616	LEU	A	619	LEU	A
616	LEU	A	620	ILE	A
616	LEU	A	644	PHE	A
616	LEU	A	647	ILE	A
617	TRP	A	620	ILE	A
617	TRP	A	647	ILE	A
617	TRP	A	648	VAL	A
617	TRP	A	651	VAL	A
617	TRP	A	654	MET	A

617	TRP	A	662	TYR	A
620	ILE	A	627	ILE	A
620	ILE	A	644	PHE	A
620	ILE	A	647	ILE	A
620	ILE	A	648	VAL	A
620	ILE	A	662	TYR	A
620	ILE	A	666	LEU	A
627	ILE	A	629	VAL	A
627	ILE	A	644	PHE	A
627	ILE	A	666	LEU	A
627	ILE	A	672	TYR	A
629	VAL	A	636	MET	A
629	VAL	A	637	ALA	A
629	VAL	A	640	VAL	A
629	VAL	A	644	PHE	A
629	VAL	A	672	TYR	A
629	VAL	A	674	LEU	A
629	VAL	A	676	VAL	A
633	ALA	A	676	VAL	A
636	MET	A	637	ALA	A
636	MET	A	640	VAL	A
637	ALA	A	676	VAL	A
640	VAL	A	644	PHE	A
644	PHE	A	647	ILE	A
644	PHE	A	663	ILE	A
644	PHE	A	672	TYR	A
645	TYR	A	659	ALA	A
645	TYR	A	660	VAL	A
645	TYR	A	663	ILE	A
647	ILE	A	648	VAL	A
647	ILE	A	651	VAL	A
648	VAL	A	654	MET	A
648	VAL	A	659	ALA	A
648	VAL	A	662	TYR	A
648	VAL	A	663	ILE	A
649	ALA	A	654	MET	A
649	ALA	A	659	ALA	A
654	MET	A	659	ALA	A
654	MET	A	662	TYR	A
662	TYR	A	663	ILE	A
662	TYR	A	666	LEU	A
663	ILE	A	666	LEU	A
663	ILE	A	667	MET	A
663	ILE	A	672	TYR	A
666	LEU	A	672	TYR	A

667	MET	A	672	TYR	A
667	MET	A	674	LEU	A
672	TYR	A	674	LEU	A
674	LEU	A	676	VAL	A

NO INTRAPROTEIN DISULPHIDE BRIDGES FOUND

Intraprotein Main Chain-Main Chain Hydrogen Bonds

  [help]

Rasmol **Jmol**

[View the original hbond output]

DOG_POR_E315Q_snapshot10.pdb

DONOR PARAMETERS						ACCEPTOR					
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**Dd-a**	**Dh-a**	**A(d-H-N)**	**A(a-O=C)**
61	A	T	N	59	A	P	O	3.41	3.33	86.65	103.31
63	A	S	N	61	A	T	O	3.24	3.17	85.01	74.40
64	A	A	N	61	A	T	O	3.19	2.26	157.06	108.96
66	A	D	N	116	A	E	O	2.81	1.84	163.63	169.11
69	A	F	N	67	A	S	O	3.19	3.21	80.44	102.23
72	A	K	N	68	A	S	O	3.09	2.24	145.53	144.45
72	A	K	N	69	A	F	O	3.25	2.75	111.88	97.34
72	A	K	N	70	A	V	O	3.37	3.46	76.51	72.85
73	A	M	N	69	A	F	O	2.84	1.95	149.60	150.42
73	A	M	N	70	A	V	O	3.16	2.63	113.43	106.24
73	A	M	N	71	A	E	O	3.45	3.57	75.27	72.82
74	A	K	N	70	A	V	O	2.92	2.02	152.53	158.15
74	A	K	N	71	A	E	O	3.25	2.70	115.53	104.97
74	A	K	N	72	A	K	O	3.40	3.49	76.91	74.19
75	A	K	N	71	A	E	O	2.93	1.99	157.71	157.15
75	A	K	N	72	A	K	O	3.24	2.74	111.98	107.60
76	A	T	N	72	A	K	O	2.90	2.04	144.52	160.31

76	A	T	N	73	A	M	O	3.43	2.78	123.60	102.44
76	A	T	N	74	A	K	O	3.40	3.38	83.10	74.70
77	A	G	N	73	A	M	O	2.93	2.57	102.15	152.21
77	A	G	N	74	A	K	O	3.36	2.42	158.50	104.88
78	A	R	N	73	A	M	O	2.89	1.90	174.86	144.92
79	A	N	N	108	A	R	O	2.85	1.87	166.56	152.89
80	A	I	N	108	A	R	O	3.07	2.12	164.17	150.03
81	A	I	N	132	A	L	O	3.15	2.20	163.24	168.57
82	A	V	N	110	A	M	O	2.93	2.04	149.04	152.91
83	A	F	N	134	A	V	O	2.93	1.98	162.01	160.79
85	A	G	N	136	A	C	O	2.81	1.84	164.69	155.21
90	A	T	N	88	A	T	O	3.24	2.84	105.70	86.22
92	A	E	N	89	A	G	O	3.29	2.75	115.42	101.67
92	A	E	N	90	A	T	O	3.38	3.41	79.98	72.23
93	A	E	N	89	A	G	O	2.92	2.04	149.86	154.71
93	A	E	N	90	A	T	O	3.23	2.64	119.32	107.37
94	A	F	N	90	A	T	O	2.96	2.07	152.34	157.19
94	A	F	N	91	A	A	O	3.41	2.87	116.17	100.26
94	A	F	N	92	A	E	O	3.47	3.52	78.59	72.21
95	A	A	N	91	A	A	O	2.93	2.04	150.75	150.41
95	A	A	N	92	A	E	O	3.22	2.71	112.96	104.35
96	A	N	N	92	A	E	O	2.87	1.99	148.55	155.27
96	A	N	N	93	A	E	O	3.34	2.81	114.51	99.02
96	A	N	N	94	A	F	O	3.41	3.49	77.42	73.38
97	A	R	N	93	A	E	O	3.01	2.19	141.07	148.23
97	A	R	N	94	A	F	O	3.12	2.49	122.52	107.91
97	A	R	N	95	A	A	O	3.37	3.40	79.97	72.38
98	A	L	N	94	A	F	O	2.94	2.02	156.78	160.16
98	A	L	N	95	A	A	O	3.34	2.83	113.56	104.43
99	A	S	N	95	A	A	O	2.97	2.08	151.26	155.34
99	A	S	N	97	A	R	O	3.38	3.42	79.34	73.96
100	A	K	N	96	A	N	O	3.11	2.27	142.44	145.64
100	A	K	N	97	A	R	O	3.18	2.56	120.96	108.70
100	A	K	N	98	A	L	O	3.42	3.45	80.18	72.24
101	A	D	N	97	A	R	O	2.82	1.93	147.88	159.33
101	A	D	N	98	A	L	O	3.28	2.75	113.96	101.02
102	A	A	N	98	A	L	O	3.06	2.32	131.84	152.55
102	A	A	N	100	A	K	O	3.30	3.19	87.92	75.22
103	A	H	N	100	A	K	O	3.29	2.43	145.36	122.03
103	A	H	N	101	A	D	O	3.10	3.12	79.67	79.16
103	A	H	N	107	A	M	O	3.41	4.14	37.88	133.41
104	A	R	N	101	A	D	O	2.87	2.03	141.07	124.37
104	A	R	N	102	A	A	O	3.18	3.09	85.91	77.26
105	A	Y	N	102	A	A	O	3.05	2.10	157.95	122.80
105	A	Y	N	103	A	H	O	3.08	2.70	103.22	78.79

106	A	G	N	102	A	A	O	3.39	3.04	102.63	154.28
106	A	G	N	103	A	H	O	3.07	2.12	162.07	114.17
107	A	M	N	102	A	A	O	3.06	2.21	143.44	138.21
107	A	M	N	105	A	Y	O	3.49	3.19	99.14	69.10
110	A	M	N	80	A	I	O	3.08	2.24	140.80	148.29
112	A	A	N	82	A	V	O	2.88	1.93	158.64	170.05
115	A	E	N	113	A	D	O	3.11	2.88	94.67	81.76
115	A	E	N	148	A	N	O	3.24	3.26	80.23	151.36
116	A	E	N	113	A	D	O	2.99	2.07	155.36	129.85
119	A	L	N	117	A	Y	O	3.33	3.07	96.66	95.81
120	A	A	N	118	A	D	O	3.17	2.83	101.78	77.91
121	A	D	N	118	A	D	O	3.30	2.34	163.72	126.77
121	A	D	N	119	A	L	O	3.12	3.06	84.32	73.51
122	A	L	N	119	A	L	O	2.94	1.99	163.04	119.73
122	A	L	N	120	A	A	O	3.17	2.88	98.57	76.42
123	A	G	N	120	A	A	O	3.24	2.29	164.33	125.51
123	A	G	N	121	A	D	O	3.10	3.04	84.82	75.26
124	A	S	N	121	A	D	O	2.93	1.99	159.11	122.73
124	A	S	N	122	A	L	O	3.15	2.94	93.06	76.55
125	A	L	N	122	A	L	O	3.15	2.20	163.15	118.70
127	A	E	N	124	A	S	O	3.07	2.12	162.94	135.82
127	A	E	N	125	A	L	O	2.99	2.74	95.55	81.24
128	A	I	N	125	A	L	O	3.02	2.06	164.10	131.70
128	A	I	N	126	A	P	O	3.33	3.08	95.94	69.33
131	A	S	N	129	A	E	O	3.23	3.12	87.37	76.27
132	A	L	N	79	A	N	O	2.94	2.00	157.62	153.70
133	A	A	N	167	A	K	O	2.94	1.96	173.86	155.07
134	A	V	N	81	A	I	O	2.93	2.02	151.09	160.54
135	A	F	N	169	A	A	O	3.00	2.16	142.57	154.61
136	A	C	N	83	A	F	O	2.90	1.94	161.90	159.88
137	A	M	N	171	A	F	O	2.87	1.94	156.63	135.61
138	A	A	N	85	A	G	O	2.94	2.02	155.98	144.81
139	A	T	N	173	A	L	O	3.17	2.67	112.05	145.60
140	A	Y	N	144	A	D	O	2.90	1.96	156.71	160.94
143	A	G	N	140	A	Y	O	3.12	2.46	124.36	143.40
143	A	G	N	141	A	G	O	3.18	3.09	86.69	75.88
144	A	D	N	140	A	Y	O	3.35	2.73	121.05	112.88
144	A	D	N	141	A	G	O	3.18	2.24	155.63	120.37
144	A	D	N	142	A	E	O	3.41	3.20	93.94	71.43
148	A	N	N	146	A	T	O	3.19	3.21	80.09	78.89
149	A	A	N	146	A	T	O	2.91	1.98	156.69	121.11
149	A	A	N	147	A	D	O	3.28	2.82	109.06	74.82
150	A	Q	N	146	A	T	O	3.33	2.97	103.19	166.36
151	A	D	N	149	A	A	O	3.42	3.45	80.12	73.09
152	A	F	N	149	A	A	O	3.31	2.80	113.29	102.88

153	A	Y	N	149	A	A	O	2.87	1.96	151.57	154.57
153	A	Y	N	150	A	Q	O	3.40	2.88	114.08	97.95
153	A	Y	N	151	A	D	O	3.48	3.57	76.48	70.33
154	A	D	N	150	A	Q	O	2.99	2.08	154.00	147.66
154	A	D	N	151	A	D	O	3.31	2.83	111.13	101.65
154	A	D	N	152	A	F	O	3.49	3.62	74.09	72.90
155	A	W	N	151	A	D	O	2.88	1.99	149.17	153.00
155	A	W	N	152	A	F	O	3.27	2.73	114.91	104.38
155	A	W	N	153	A	Y	O	3.38	3.43	78.90	74.26
156	A	L	N	152	A	F	O	2.90	1.96	160.21	158.00
156	A	L	N	153	A	Y	O	3.37	2.86	113.14	106.92
157	A	Q	N	153	A	Y	O	3.06	2.16	150.74	157.22
157	A	Q	N	154	A	D	O	3.40	2.81	119.27	103.15
157	A	Q	N	155	A	W	O	3.32	3.33	80.70	77.14
158	A	E	N	154	A	D	O	3.18	2.47	128.78	152.35
158	A	E	N	155	A	W	O	3.21	2.37	143.44	114.74
158	A	E	N	156	A	L	O	3.44	3.29	90.32	73.14
159	A	T	N	155	A	W	O	2.83	1.97	145.02	163.97
162	A	D	N	160	A	D	O	3.35	3.38	79.88	100.72
163	A	L	N	161	A	V	O	3.50	3.27	95.25	93.59
163	A	L	N	195	A	L	O	3.10	2.25	143.21	158.04
164	A	S	N	195	A	L	O	3.48	3.22	97.37	144.30
165	A	G	N	163	A	L	O	3.23	3.48	67.30	104.25
166	A	V	N	163	A	L	O	2.97	2.02	161.54	142.91
168	A	Y	N	198	A	Q	O	2.85	1.92	156.90	154.61
169	A	A	N	133	A	A	O	3.08	2.23	142.97	160.02
171	A	F	N	135	A	F	O	2.79	1.81	165.80	161.99
172	A	G	N	204	A	G	O	3.08	2.14	160.22	139.09
173	A	L	N	137	A	M	O	3.04	2.11	157.23	112.32
174	A	G	N	206	A	G	O	3.19	2.55	122.30	138.63
177	A	T	N	175	A	N	O	3.12	2.86	96.40	78.08
178	A	Y	N	175	A	N	O	3.15	2.21	161.92	127.82
178	A	Y	N	176	A	K	O	3.30	3.23	85.96	71.73
180	A	H	N	178	A	Y	O	3.32	3.31	82.01	69.91
181	A	F	N	178	A	Y	O	3.46	3.09	103.85	113.83
181	A	F	N	179	A	E	O	2.85	1.95	149.56	88.11
182	A	N	N	180	A	H	O	3.14	3.03	86.80	107.05
183	A	A	N	180	A	H	O	3.48	2.64	143.57	124.47
183	A	A	N	181	A	F	O	3.11	3.19	76.15	80.01
184	A	M	N	182	A	N	O	3.15	3.14	81.78	81.20
185	A	G	N	182	A	N	O	3.10	2.51	119.01	121.56
186	A	K	N	182	A	N	O	3.03	2.07	164.10	167.70
186	A	K	N	183	A	A	O	3.46	2.98	111.40	101.11
186	A	K	N	184	A	M	O	3.38	3.49	75.68	73.37
187	A	Y	N	183	A	A	O	2.96	2.10	146.34	150.76

187	A	Y	N	184	A	M	O	3.22	2.66	116.99	105.59
187	A	Y	N	185	A	G	O	3.40	3.47	77.99	74.12
188	A	V	N	184	A	M	O	2.99	2.04	163.85	160.45
188	A	V	N	185	A	G	O	3.44	2.92	113.99	107.27
189	A	D	N	185	A	G	O	3.05	2.11	162.28	158.12
189	A	D	N	187	A	Y	O	3.40	3.50	76.31	74.92
190	A	K	N	186	A	K	O	3.18	2.30	150.18	149.13
190	A	K	N	187	A	Y	O	3.25	2.65	120.51	110.58
190	A	K	N	188	A	V	O	3.33	3.39	78.33	76.89
191	A	R	N	187	A	Y	O	2.82	1.92	154.73	164.08
191	A	R	N	188	A	V	O	3.35	2.81	115.74	106.40
192	A	L	N	188	A	V	O	2.99	2.07	157.92	158.00
192	A	L	N	190	A	K	O	3.40	3.45	78.91	74.41
193	A	E	N	189	A	D	O	3.48	2.61	149.28	138.65
193	A	E	N	190	A	K	O	3.18	2.60	118.73	109.76
193	A	E	N	191	A	R	O	3.40	3.48	77.37	72.78
194	A	Q	N	190	A	K	O	3.05	2.14	153.33	156.25
194	A	Q	N	191	A	R	O	3.15	2.64	112.95	106.25
194	A	Q	N	192	A	L	O	3.49	3.60	75.75	71.42
195	A	L	N	191	A	R	O	2.89	2.02	144.58	157.02
195	A	L	N	192	A	L	O	3.27	2.68	118.42	102.71
195	A	L	N	193	A	E	O	3.35	3.37	80.53	73.79
196	A	G	N	192	A	L	O	3.19	2.80	104.15	147.78
196	A	G	N	193	A	E	O	2.98	2.08	149.95	112.50
196	A	G	N	194	A	Q	O	3.23	2.85	103.63	72.80
197	A	A	N	192	A	L	O	3.06	2.16	151.25	155.49
198	A	Q	N	166	A	V	O	2.81	1.83	168.63	164.56
200	A	I	N	168	A	Y	O	2.87	1.93	156.93	168.99
204	A	G	N	170	A	V	O	3.12	2.16	163.92	148.76
204	A	G	N	202	A	E	O	3.26	3.42	72.43	106.69
206	A	G	N	172	A	G	O	2.84	1.85	176.31	162.02
206	A	G	N	204	A	G	O	3.50	3.18	100.39	96.73
208	A	D	N	174	A	G	O	2.87	1.92	160.43	151.44
209	A	D	N	207	A	D	O	3.21	2.91	99.26	75.58
210	A	G	N	207	A	D	O	3.09	2.20	148.50	122.61
210	A	G	N	208	A	D	O	3.45	3.37	86.31	64.91
212	A	L	N	210	A	G	O	3.34	3.23	87.82	97.26
215	A	D	N	211	A	N	O	3.14	2.28	145.24	144.17
215	A	D	N	212	A	L	O	3.41	2.92	112.12	95.44
215	A	D	N	213	A	E	O	3.33	3.40	77.46	72.53
216	A	F	N	212	A	L	O	2.93	2.09	142.88	146.09
216	A	F	N	213	A	E	O	3.13	2.54	118.77	107.18
216	A	F	N	214	A	E	O	3.46	3.53	77.75	72.41
217	A	I	N	213	A	E	O	3.00	2.08	156.64	158.14
217	A	I	N	214	A	E	O	3.30	2.77	114.14	104.87

217	A	I	N	215	A	D	O	3.49	3.59	76.50	72.06
218	A	T	N	214	A	E	O	2.91	2.01	151.72	154.45
218	A	T	N	215	A	D	O	3.28	2.77	112.51	103.34
218	A	T	N	216	A	F	O	3.35	3.44	76.73	73.14
219	A	W	N	215	A	D	O	2.97	2.08	151.54	154.20
219	A	W	N	216	A	F	O	3.15	2.59	115.99	108.89
219	A	W	N	217	A	I	O	3.41	3.54	74.45	74.93
220	A	R	N	216	A	F	O	2.80	1.95	141.63	161.10
220	A	R	N	217	A	I	O	3.22	2.60	120.60	105.20
221	A	E	N	217	A	I	O	3.24	2.32	156.49	156.15
221	A	E	N	219	A	W	O	3.31	3.37	77.78	76.00
222	A	Q	N	219	A	W	O	2.99	2.07	154.18	112.81
222	A	Q	N	220	A	R	O	3.30	2.85	108.39	74.28
223	A	F	N	219	A	W	O	2.86	1.93	155.71	166.23
223	A	F	N	220	A	R	O	3.39	2.83	116.13	105.69
224	A	W	N	220	A	R	O	3.07	2.11	176.68	159.99
226	A	A	N	222	A	Q	O	3.30	2.44	146.97	146.63
226	A	A	N	223	A	F	O	3.04	2.43	119.88	117.27
226	A	A	N	224	A	W	O	3.33	3.40	77.54	75.87
227	A	V	N	223	A	F	O	2.98	2.07	152.95	163.60
227	A	V	N	224	A	W	O	3.22	2.67	115.65	108.88
227	A	V	N	225	A	P	O	3.44	3.51	77.82	72.31
228	A	C	N	224	A	W	O	2.89	1.98	153.69	160.05
228	A	C	N	225	A	P	O	3.17	2.66	112.87	103.90
229	A	E	N	225	A	P	O	2.87	1.97	152.11	156.53
229	A	E	N	226	A	A	O	3.36	2.83	114.18	100.07
229	A	E	N	227	A	V	O	3.42	3.52	76.04	74.17
230	A	H	N	226	A	A	O	2.91	2.00	154.45	153.29
230	A	H	N	227	A	V	O	3.37	2.84	114.99	105.34
231	A	F	N	227	A	V	O	2.91	1.97	160.49	158.45
232	A	G	N	228	A	C	O	3.00	2.32	125.35	137.51
233	A	V	N	231	A	F	O	3.41	3.29	88.74	71.75
236	A	T	N	104	A	R	O	2.84	1.92	153.00	139.93
240	A	S	N	238	A	E	O	3.43	2.78	122.18	61.90
241	A	S	N	239	A	E	O	3.00	2.11	148.43	86.87
242	A	I	N	240	A	S	O	3.45	3.63	72.16	78.45
246	A	E	N	349	A	N	O	2.86	1.87	166.32	150.04
248	A	V	N	347	A	S	O	2.84	1.87	162.42	164.93
250	A	H	N	345	A	V	O	2.93	1.97	163.51	150.82
254	A	D	N	252	A	D	O	3.40	3.42	80.54	101.90
255	A	M	N	253	A	I	O	3.46	3.56	76.30	97.84
256	A	A	N	254	A	D	O	3.04	2.89	89.06	78.91
257	A	K	N	254	A	D	O	2.90	1.94	162.57	131.94
257	A	K	N	255	A	M	O	3.15	2.94	92.61	76.34
258	A	V	N	255	A	M	O	3.08	2.15	156.56	113.12

259	A	Y	N	364	A	P	O	2.83	1.86	167.57	162.77
265	A	R	N	263	A	M	O	3.19	2.83	102.67	102.25
265	A	R	N	279	A	K	O	2.92	2.06	146.95	163.47
267	A	K	N	265	A	R	O	3.24	3.37	74.20	102.33
268	A	S	N	265	A	R	O	3.08	2.34	131.31	122.62
268	A	S	N	266	A	L	O	3.39	3.45	78.34	73.46
269	A	Y	N	267	A	K	O	3.15	3.02	88.74	78.67
270	A	E	N	267	A	K	O	3.16	2.46	127.68	118.14
271	A	N	N	267	A	K	O	2.99	2.11	144.72	158.08
271	A	N	N	268	A	S	O	3.30	2.77	114.21	94.67
272	A	Q	N	268	A	S	O	3.38	3.62	68.41	144.45
272	A	Q	N	270	A	E	O	3.07	2.24	140.80	84.30
273	A	K	N	271	A	N	O	2.91	2.16	130.46	100.13
277	A	D	N	280	A	N	O	3.16	2.19	163.47	121.34
279	A	K	N	277	A	D	O	3.17	3.08	86.10	80.69
280	A	N	N	277	A	D	O	3.05	2.26	136.88	120.13
282	A	F	N	511	A	M	O	2.91	1.93	169.61	159.38
284	A	A	N	282	A	F	O	3.49	3.05	108.12	89.00
284	A	A	N	509	A	V	O	2.93	1.96	164.89	143.73
286	A	V	N	507	A	A	O	3.02	2.04	174.65	144.75
287	A	T	N	285	A	A	O	3.06	2.56	112.08	93.34
287	A	T	N	304	A	E	O	2.97	2.18	136.63	151.55
288	A	T	N	286	A	V	O	3.39	3.28	88.09	74.05
290	A	R	N	302	A	H	O	2.81	1.93	145.03	170.52
292	A	L	N	300	A	L	O	2.82	1.84	173.41	132.94
294	A	Q	N	571	A	E	O	2.92	1.93	175.46	131.12
301	A	M	N	473	A	A	O	2.85	1.91	159.45	155.98
302	A	H	N	290	A	R	O	2.83	1.92	149.17	161.90
303	A	L	N	471	A	I	O	3.00	2.05	162.38	142.67
304	A	E	N	288	A	T	O	3.15	2.23	154.28	135.90
305	A	L	N	469	A	V	O	2.82	1.90	151.60	167.33
306	A	D	N	285	A	A	O	2.92	1.95	167.72	149.85
307	A	I	N	305	A	L	O	3.49	3.45	84.42	98.31
307	A	I	N	467	A	N	O	2.94	1.95	170.52	125.72
309	A	D	N	307	A	I	O	3.33	3.58	67.68	105.91
310	A	S	N	307	A	I	O	3.08	2.16	155.82	137.61
310	A	S	N	308	A	S	O	3.19	2.88	99.71	77.79
311	A	K	N	309	A	D	O	3.38	3.06	99.34	69.41
312	A	L	N	310	A	S	O	3.17	2.93	94.48	74.12
317	A	G	N	315	A	Q	O	3.36	3.60	67.77	104.09
318	A	D	N	315	A	Q	O	3.15	2.22	158.32	146.76
319	A	H	N	514	A	R	O	2.94	2.01	157.62	169.88
320	A	V	N	456	A	Y	O	2.93	1.94	172.67	175.95
321	A	A	N	512	A	F	O	2.98	2.00	170.67	166.29
322	A	V	N	454	A	R	O	2.94	1.99	161.95	159.29

323	A	Y	N	510	A	P	O	3.19	2.26	157.29	144.42
326	A	N	N	372	A	T	O	2.82	1.83	171.00	157.36
328	A	S	N	326	A	N	O	3.35	3.50	72.79	102.66
329	A	A	N	327	A	D	O	3.19	3.08	87.84	79.28
330	A	L	N	327	A	D	O	3.11	2.39	130.05	121.56
331	A	V	N	327	A	D	O	3.27	2.33	160.07	158.23
331	A	V	N	328	A	S	O	3.46	2.97	112.03	97.96
331	A	V	N	329	A	A	O	3.40	3.51	75.31	71.08
332	A	N	N	328	A	S	O	2.98	2.14	144.08	146.11
332	A	N	N	329	A	A	O	3.14	2.59	115.09	103.14
332	A	N	N	330	A	L	O	3.42	3.49	77.47	73.22
333	A	Q	N	329	A	A	O	2.93	1.99	159.58	157.23
333	A	Q	N	330	A	L	O	3.35	2.84	113.39	106.51
333	A	Q	N	331	A	V	O	3.43	3.54	75.36	74.80
334	A	L	N	330	A	L	O	2.96	2.09	146.68	156.69
334	A	L	N	331	A	V	O	3.24	2.64	119.79	107.06
334	A	L	N	332	A	N	O	3.39	3.40	81.28	74.28
335	A	G	N	331	A	V	O	3.10	2.21	151.26	156.02
335	A	G	N	332	A	N	O	3.14	2.53	120.32	112.17
335	A	G	N	333	A	Q	O	3.43	3.52	76.57	71.30
336	A	E	N	332	A	N	O	2.96	2.06	150.71	156.64
336	A	E	N	333	A	Q	O	3.24	2.74	112.47	101.67
337	A	I	N	333	A	Q	O	2.94	2.09	145.73	156.70
337	A	I	N	335	A	G	O	3.43	3.39	83.80	76.28
338	A	L	N	335	A	G	O	3.26	2.56	128.01	114.58
338	A	L	N	336	A	E	O	3.44	3.44	82.11	71.12
339	A	G	N	335	A	G	O	2.92	2.46	107.94	155.38
339	A	G	N	336	A	E	O	3.24	2.39	143.25	97.53
340	A	A	N	335	A	G	O	2.96	2.05	151.93	148.03
340	A	A	N	338	A	L	O	3.30	3.29	81.88	70.08
342	A	L	N	340	A	A	O	3.21	2.82	104.62	91.85
343	A	D	N	341	A	D	O	3.26	2.83	107.08	73.74
344	A	V	N	342	A	L	O	3.43	3.00	107.07	70.12
346	A	M	N	365	A	T	O	2.93	1.95	165.81	147.49
347	A	S	N	248	A	V	O	2.91	1.98	155.28	149.02
349	A	N	N	246	A	E	O	2.83	1.87	163.27	154.64
350	A	N	N	358	A	K	O	3.00	2.21	137.08	152.54
351	A	L	N	244	A	Q	O	2.96	1.98	169.32	156.75
352	A	D	N	350	A	N	O	3.46	3.45	82.35	65.46
353	A	E	N	351	A	L	O	3.14	2.50	121.73	90.63
354	A	E	N	352	A	D	O	3.30	3.13	90.90	74.90
355	A	S	N	352	A	D	O	3.17	2.26	154.81	117.42
355	A	S	N	353	A	E	O	3.39	3.19	92.96	70.05
357	A	K	N	355	A	S	O	3.31	2.86	108.21	68.56
358	A	K	N	356	A	N	O	2.99	2.16	140.66	86.20

359	A	H	N	357	A	K	O	3.16	3.15	81.38	80.28
361	A	F	N	359	A	H	O	3.41	3.23	91.78	71.65
363	A	C	N	361	A	F	O	3.32	3.55	68.43	107.51
365	A	T	N	346	A	M	O	2.97	2.01	165.32	170.03
367	A	Y	N	342	A	L	O	3.15	2.64	113.33	147.86
367	A	Y	N	344	A	V	O	3.42	2.59	144.53	164.17
368	A	R	N	342	A	L	O	2.91	2.07	143.10	134.15
368	A	R	N	366	A	S	O	3.25	3.27	80.26	73.69
369	A	T	N	366	A	S	O	3.21	2.65	115.96	110.54
369	A	T	N	367	A	Y	O	3.45	3.59	73.95	73.47
370	A	A	N	366	A	S	O	2.98	2.05	157.60	159.55
370	A	A	N	367	A	Y	O	3.26	2.77	111.71	103.26
370	A	A	N	368	A	R	O	3.43	3.51	77.46	73.55
371	A	L	N	367	A	Y	O	2.98	2.03	163.36	157.58
371	A	L	N	368	A	R	O	3.38	2.86	113.96	109.17
371	A	L	N	369	A	T	O	3.42	3.56	73.78	76.20
372	A	T	N	368	A	R	O	2.94	2.11	141.89	156.98
372	A	T	N	369	A	T	O	3.19	2.58	120.62	106.57
372	A	T	N	370	A	A	O	3.42	3.39	83.79	72.38
373	A	Y	N	369	A	T	O	2.86	1.94	155.46	163.16
374	A	Y	N	370	A	A	O	2.94	2.06	149.08	139.40
375	A	L	N	370	A	A	O	3.07	2.49	116.64	162.91
376	A	D	N	449	A	P	O	2.86	1.89	169.98	147.25
377	A	I	N	375	A	L	O	3.02	2.30	129.18	92.02
378	A	T	N	376	A	D	O	3.32	2.91	105.87	71.58
384	A	N	N	382	A	R	O	3.16	3.11	84.13	76.24
385	A	V	N	382	A	R	O	3.14	2.27	147.48	122.01
385	A	V	N	383	A	T	O	3.23	3.17	84.69	78.19
386	A	L	N	383	A	T	O	3.04	2.32	129.29	116.60
386	A	L	N	384	A	N	O	3.45	3.39	85.00	70.02
387	A	Y	N	383	A	T	O	2.85	1.97	146.24	167.34
388	A	E	N	384	A	N	O	3.36	2.42	161.66	146.18
390	A	A	N	386	A	L	O	3.20	2.88	99.53	146.70
391	A	Q	N	389	A	L	O	3.18	3.17	81.32	75.52
392	A	Y	N	389	A	L	O	2.95	2.01	159.52	124.44
392	A	Y	N	390	A	A	O	3.01	2.67	100.47	80.56
393	A	A	N	390	A	A	O	2.98	2.02	162.05	125.53
394	A	S	N	436	A	S	O	3.39	2.44	162.56	110.33
395	A	E	N	393	A	A	O	3.42	3.22	93.45	71.88
397	A	T	N	395	A	E	O	3.22	3.21	82.11	82.36
398	A	E	N	395	A	E	O	3.11	2.41	127.85	121.84
399	A	Q	N	395	A	E	O	3.05	2.10	161.98	166.05
399	A	Q	N	396	A	P	O	3.41	2.94	110.78	99.42
400	A	E	N	396	A	P	O	2.99	2.11	149.06	149.40
400	A	E	N	397	A	T	O	3.42	2.88	115.87	96.76

400	A	E	N	398	A	E	O	3.37	3.46	76.53	75.01
401	A	H	N	397	A	T	O	3.11	2.22	153.84	147.27
401	A	H	N	398	A	E	O	3.28	2.71	118.49	110.63
401	A	H	N	399	A	Q	O	3.44	3.53	76.97	74.89
402	A	L	N	398	A	E	O	3.12	2.18	161.11	159.64
402	A	L	N	399	A	Q	O	3.31	2.78	114.31	109.44
402	A	L	N	400	A	E	O	3.40	3.51	75.78	74.48
403	A	R	N	399	A	Q	O	2.91	2.00	151.97	161.55
403	A	R	N	400	A	E	O	3.42	2.85	117.78	104.45
403	A	R	N	401	A	H	O	3.45	3.47	80.87	74.45
404	A	K	N	400	A	E	O	3.03	2.15	148.58	154.99
404	A	K	N	401	A	H	O	3.38	2.72	124.58	107.52
404	A	K	N	402	A	L	O	3.47	3.47	81.95	71.85
405	A	M	N	401	A	H	O	3.40	2.75	124.73	153.52
405	A	M	N	402	A	L	O	3.40	2.52	149.69	107.54
405	A	M	N	403	A	R	O	3.36	3.16	93.50	74.80
406	A	A	N	404	A	K	O	3.05	2.89	89.88	82.70
407	A	S	N	404	A	K	O	3.00	2.14	145.44	132.58
407	A	S	N	405	A	M	O	3.37	2.82	116.53	73.00
409	A	S	N	407	A	S	O	3.47	3.10	103.57	70.88
412	A	G	N	410	A	G	O	3.25	3.18	85.26	78.30
413	A	K	N	410	A	G	O	3.24	2.49	133.60	121.32
413	A	K	N	411	A	E	O	3.37	3.38	81.13	75.45
414	A	E	N	410	A	G	O	3.41	2.54	148.45	153.21
414	A	E	N	411	A	E	O	3.13	2.50	121.21	109.95
414	A	E	N	412	A	G	O	3.39	3.40	81.06	70.86
415	A	L	N	411	A	E	O	2.92	2.11	137.89	157.98
415	A	L	N	412	A	G	O	3.19	2.54	123.33	102.71
416	A	Y	N	412	A	G	O	3.13	2.26	149.98	152.05
416	A	Y	N	413	A	K	O	3.38	2.78	120.30	102.34
417	A	L	N	413	A	K	O	3.14	2.23	156.41	148.73
417	A	L	N	414	A	E	O	3.40	2.93	110.73	99.35
417	A	L	N	415	A	L	O	3.46	3.57	75.61	72.40
418	A	S	N	414	A	E	O	2.90	1.96	159.01	152.07
418	A	S	N	415	A	L	O	3.42	2.95	111.11	103.02
418	A	S	N	416	A	Y	O	3.48	3.62	74.14	74.47
419	A	W	N	415	A	L	O	2.85	1.91	162.15	156.94
420	A	V	N	416	A	Y	O	2.99	2.16	143.33	144.31
421	A	V	N	416	A	Y	O	3.21	2.30	154.68	156.45
421	A	V	N	417	A	L	O	3.27	2.62	124.52	123.14
422	A	E	N	417	A	L	O	2.82	1.83	173.24	166.62
423	A	A	N	421	A	V	O	3.36	3.35	82.54	71.71
424	A	R	N	420	A	V	O	3.00	2.63	102.10	134.89
424	A	R	N	421	A	V	O	3.12	2.24	145.99	105.75
424	A	R	N	422	A	E	O	3.39	3.07	100.03	70.23

425	A	R	N	420	A	V	O	3.03	2.15	148.68	143.69
425	A	R	N	423	A	A	O	3.26	3.41	73.10	74.69
426	A	H	N	424	A	R	O	3.21	2.80	105.31	100.09
428	A	L	N	426	A	H	O	3.21	3.22	80.85	82.19
429	A	A	N	426	A	H	O	2.98	2.39	117.58	124.78
429	A	A	N	427	A	I	O	3.41	3.52	75.61	73.27
430	A	I	N	426	A	H	O	2.96	2.06	150.83	161.01
430	A	I	N	427	A	I	O	3.21	2.66	115.29	103.78
430	A	I	N	428	A	L	O	3.39	3.45	78.17	73.73
431	A	L	N	427	A	I	O	2.91	1.99	155.52	156.94
431	A	L	N	428	A	L	O	3.17	2.65	113.39	108.16
432	A	Q	N	428	A	L	O	2.92	2.05	147.21	159.28
432	A	Q	N	429	A	A	O	3.41	2.82	120.27	100.23
432	A	Q	N	430	A	I	O	3.29	3.31	80.79	76.72
433	A	D	N	429	A	A	O	3.02	2.13	149.77	151.43
433	A	D	N	430	A	I	O	3.21	2.59	120.50	112.53
434	A	Y	N	430	A	I	O	2.84	2.11	128.21	164.98
434	A	Y	N	432	A	Q	O	3.48	3.22	96.40	70.39
436	A	S	N	434	A	Y	O	3.13	2.88	95.34	83.04
437	A	L	N	434	A	Y	O	3.06	2.13	157.27	124.47
438	A	R	N	392	A	Y	O	3.18	2.22	167.03	135.64
438	A	R	N	436	A	S	O	3.26	2.88	103.99	97.56
442	A	D	N	440	A	P	O	3.35	3.36	81.16	76.60
443	A	H	N	440	A	P	O	3.23	2.53	128.76	112.95
443	A	H	N	441	A	I	O	3.44	3.38	85.19	73.41
444	A	L	N	440	A	P	O	3.06	2.13	156.67	159.87
444	A	L	N	441	A	I	O	3.39	2.88	113.88	103.54
445	A	C	N	441	A	I	O	2.92	2.03	150.74	153.34
445	A	C	N	442	A	D	O	3.32	2.82	111.93	96.70
446	A	E	N	442	A	D	O	2.96	2.10	144.95	149.61
446	A	E	N	443	A	H	O	3.40	2.77	123.52	103.83
446	A	E	N	444	A	L	O	3.38	3.39	81.37	76.35
447	A	L	N	443	A	H	O	3.31	2.48	142.87	150.57
447	A	L	N	444	A	L	O	3.27	2.54	131.06	113.82
447	A	L	N	445	A	C	O	3.41	3.37	83.89	72.73
448	A	L	N	444	A	L	O	2.93	2.10	141.56	167.61
451	A	L	N	374	A	Y	O	2.88	1.91	165.77	106.83
454	A	R	N	322	A	V	O	2.94	1.97	163.29	162.14
456	A	Y	N	320	A	V	O	2.96	2.00	162.41	175.51
458	A	I	N	318	A	D	O	2.93	1.99	161.46	161.95
459	A	A	N	457	A	S	O	3.36	3.38	80.53	100.64
459	A	A	N	470	A	H	O	2.86	1.88	167.91	140.35
460	A	S	N	458	A	I	O	3.46	2.69	134.59	73.31
463	A	K	N	461	A	S	O	3.26	3.07	92.35	73.15
464	A	V	N	461	A	S	O	3.16	2.30	145.13	115.23

464	A	V	N	462	A	S	O	3.46	3.36	87.18	68.96
465	A	H	N	461	A	S	O	2.81	1.90	147.79	159.85
467	A	N	N	465	A	H	O	3.23	3.03	92.79	79.50
468	A	S	N	465	A	H	O	3.44	2.51	156.03	108.80
469	A	V	N	305	A	L	O	2.89	1.95	156.37	151.36
471	A	I	N	303	A	L	O	2.94	1.96	167.76	158.73
473	A	A	N	301	A	M	O	2.87	1.94	155.10	154.30
475	A	A	N	299	A	H	O	2.94	1.99	163.06	160.19
478	A	Y	N	486	A	N	O	3.01	2.07	161.16	166.88
480	A	T	N	484	A	R	O	2.84	1.94	148.84	172.30
482	A	S	N	480	A	T	O	3.24	3.12	87.92	72.66
483	A	G	N	480	A	T	O	3.01	2.09	155.35	116.06
483	A	G	N	481	A	R	O	3.34	2.92	107.01	71.27
486	A	N	N	478	A	Y	O	2.90	1.94	163.12	174.64
488	A	G	N	476	A	V	O	2.85	1.88	170.56	136.58
492	A	S	N	488	A	G	O	3.29	2.38	154.94	138.38
492	A	S	N	490	A	A	O	3.38	3.46	77.46	75.69
493	A	W	N	489	A	V	O	3.31	2.46	143.82	145.76
493	A	W	N	490	A	A	O	3.18	2.62	115.43	106.80
493	A	W	N	491	A	T	O	3.49	3.48	82.20	70.23
494	A	L	N	490	A	A	O	2.83	1.91	154.18	161.80
494	A	L	N	491	A	T	O	3.49	2.92	117.80	100.55
495	A	R	N	491	A	T	O	3.02	2.13	149.30	149.87
495	A	R	N	492	A	S	O	3.35	2.82	114.40	100.67
496	A	A	N	492	A	S	O	3.14	2.33	138.63	150.16
496	A	A	N	494	A	L	O	3.25	3.20	84.23	76.23
497	A	K	N	494	A	L	O	3.22	2.29	159.16	117.27
497	A	K	N	495	A	R	O	3.45	3.19	96.68	73.95
498	A	E	N	496	A	A	O	3.38	3.47	77.02	103.96
500	A	A	N	286	A	V	O	2.75	1.75	172.55	156.58
500	A	A	N	498	A	E	O	3.11	3.15	78.53	107.67
501	A	G	N	287	A	T	O	3.42	2.88	115.57	112.60
501	A	G	N	499	A	P	O	3.47	2.83	123.56	70.67
502	A	E	N	500	A	A	O	3.09	2.31	134.19	76.13
508	A	L	N	506	A	R	O	3.44	3.46	80.72	96.31
509	A	V	N	284	A	A	O	2.88	1.95	153.71	155.76
511	A	M	N	282	A	F	O	2.89	2.00	148.26	157.66
511	A	M	N	509	A	V	O	3.47	3.48	81.21	97.95
512	A	F	N	321	A	A	O	3.08	2.15	155.86	162.75
514	A	R	N	319	A	H	O	2.90	1.90	179.12	142.03
519	A	R	N	517	A	Q	O	3.22	2.84	102.98	73.61
523	A	K	N	521	A	P	O	3.49	3.59	75.85	72.85
524	A	A	N	522	A	F	O	3.12	2.86	95.95	99.54
525	A	A	N	523	A	K	O	3.17	3.01	89.72	76.88
526	A	T	N	523	A	K	O	3.20	2.25	163.96	126.96

526	A	T	N	524	A	A	O	3.14	2.82	99.97	77.94
528	A	V	N	559	A	E	O	2.84	1.89	160.99	164.94
529	A	I	N	626	A	H	O	2.84	1.89	157.85	161.16
530	A	M	N	561	A	L	O	2.83	2.04	135.41	156.63
531	A	V	N	628	A	Y	O	2.84	1.98	144.61	162.30
532	A	G	N	563	A	Y	O	2.87	1.88	177.28	172.05
534	A	G	N	565	A	G	O	3.03	2.08	167.11	158.64
535	A	T	N	533	A	P	O	3.39	3.43	79.38	103.65
536	A	G	N	533	A	P	O	3.19	2.31	149.14	129.70
536	A	G	N	534	A	G	O	3.18	2.92	96.15	76.81
537	A	V	N	532	A	G	O	3.09	3.29	69.69	119.31
537	A	V	N	534	A	G	O	3.32	2.40	155.95	124.83
537	A	V	N	535	A	T	O	3.12	2.71	105.14	77.49
538	A	A	N	535	A	T	O	3.39	2.46	157.15	125.35
538	A	A	N	536	A	G	O	3.23	2.87	101.91	72.34
540	A	F	N	537	A	V	O	3.07	2.37	127.93	128.09
540	A	F	N	538	A	A	O	3.17	3.03	89.03	76.83
541	A	I	N	537	A	V	O	3.23	2.44	137.10	169.55
541	A	I	N	538	A	A	O	3.35	2.52	142.67	116.05
541	A	I	N	539	A	P	O	3.36	3.31	84.08	74.25
542	A	G	N	539	A	P	O	2.98	2.40	117.91	115.71
542	A	G	N	540	A	F	O	3.40	3.56	73.12	69.80
543	A	F	N	539	A	P	O	2.97	2.21	133.73	150.37
543	A	F	N	540	A	F	O	3.15	2.53	121.09	98.40
543	A	F	N	541	A	I	O	3.42	3.40	83.40	73.91
544	A	I	N	540	A	F	O	3.01	2.09	156.77	151.84
544	A	I	N	541	A	I	O	3.40	2.79	120.47	109.41
544	A	I	N	542	A	G	O	3.48	3.56	77.40	71.48
545	A	Q	N	541	A	I	O	3.00	2.08	157.44	155.32
545	A	Q	N	542	A	G	O	3.36	2.93	107.87	98.47
545	A	Q	N	543	A	F	O	3.49	3.62	74.79	69.96
546	A	E	N	542	A	G	O	2.95	2.08	146.93	152.23
546	A	E	N	543	A	F	O	3.36	2.72	122.77	103.76
546	A	E	N	544	A	I	O	3.36	3.40	79.80	77.64
547	A	R	N	543	A	F	O	3.20	2.27	159.22	151.65
547	A	R	N	544	A	I	O	3.32	2.78	115.48	112.11
547	A	R	N	545	A	Q	O	3.41	3.51	76.54	72.92
548	A	A	N	544	A	I	O	2.80	1.89	151.67	164.77
548	A	A	N	545	A	Q	O	3.37	2.84	114.15	100.62
549	A	W	N	545	A	Q	O	3.05	2.16	150.82	151.44
549	A	W	N	546	A	E	O	3.45	2.83	122.41	103.87
549	A	W	N	547	A	R	O	3.34	3.39	78.39	73.89
550	A	L	N	546	A	E	O	3.33	2.44	150.94	146.95
550	A	L	N	547	A	R	O	3.13	2.57	116.36	110.33
550	A	L	N	548	A	A	O	3.43	3.53	75.81	72.71

551	A	R	N	547	A	R	O	2.87	2.00	147.02	160.97
551	A	R	N	548	A	A	O	3.30	2.71	118.70	102.57
551	A	R	N	549	A	W	O	3.48	3.48	81.93	72.76
552	A	Q	N	548	A	A	O	3.11	2.21	152.41	153.15
552	A	Q	N	549	A	W	O	3.30	2.68	121.60	108.95
552	A	Q	N	550	A	L	O	3.46	3.55	76.78	71.64
553	A	Q	N	549	A	W	O	3.22	2.41	139.00	149.55
553	A	Q	N	550	A	L	O	3.14	2.51	122.26	104.39
553	A	Q	N	551	A	R	O	3.35	3.34	82.13	73.06
554	A	G	N	550	A	L	O	3.18	2.72	108.65	148.59
554	A	G	N	551	A	R	O	2.94	2.06	148.58	112.36
554	A	G	N	552	A	Q	O	3.35	3.05	99.23	70.51
555	A	K	N	550	A	L	O	3.13	2.18	164.04	153.30
557	A	V	N	555	A	K	O	3.36	3.34	82.48	99.39
558	A	G	N	524	A	A	O	2.81	1.85	160.33	132.27
560	A	T	N	558	A	G	O	3.42	3.65	68.59	101.03
561	A	L	N	528	A	V	O	2.90	1.92	169.56	164.76
563	A	Y	N	530	A	M	O	2.83	1.90	153.08	155.62
564	A	Y	N	592	A	N	O	2.98	2.05	154.23	167.58
566	A	C	N	594	A	A	O	2.99	2.08	149.82	148.16
570	A	D	N	568	A	R	O	3.17	3.00	90.75	78.30
571	A	E	N	568	A	R	O	3.10	2.14	162.83	122.55
571	A	E	N	569	A	S	O	3.45	3.11	101.76	70.49
572	A	D	N	568	A	R	O	3.24	2.40	142.86	164.59
574	A	L	N	572	A	D	O	3.05	2.92	87.93	99.62
576	A	R	N	574	A	L	O	3.18	3.39	69.50	77.47
577	A	E	N	575	A	Y	O	3.34	3.36	80.59	79.89
578	A	E	N	575	A	Y	O	3.19	2.63	115.79	110.99
579	A	L	N	575	A	Y	O	2.90	1.95	159.79	166.44
580	A	A	N	576	A	R	O	3.39	2.51	150.38	137.90
580	A	A	N	577	A	E	O	3.43	2.89	116.04	102.55
580	A	A	N	578	A	E	O	3.45	3.50	79.04	72.44
581	A	Q	N	577	A	E	O	3.03	2.12	153.88	152.04
581	A	Q	N	578	A	E	O	3.23	2.71	114.09	106.82
581	A	Q	N	579	A	L	O	3.46	3.58	75.15	71.94
582	A	F	N	578	A	E	O	2.88	2.00	149.95	157.08
582	A	F	N	579	A	L	O	3.31	2.77	114.93	102.16
582	A	F	N	580	A	A	O	3.45	3.53	77.74	73.17
583	A	H	N	579	A	L	O	3.01	2.15	146.79	152.50
583	A	H	N	580	A	A	O	3.19	2.57	121.55	108.20
583	A	H	N	581	A	Q	O	3.36	3.42	78.74	73.22
584	A	Q	N	580	A	A	O	2.98	2.06	155.28	156.72
584	A	Q	N	581	A	Q	O	3.21	2.72	111.43	105.89
585	A	D	N	581	A	Q	O	2.86	2.00	145.13	158.27
585	A	D	N	582	A	F	O	3.43	2.82	120.77	98.23

585	A	D	N	583	A	H	O	3.38	3.40	80.62	73.89
586	A	G	N	582	A	F	O	3.08	2.45	121.29	143.42
586	A	G	N	583	A	H	O	2.98	2.23	131.88	109.12
586	A	G	N	584	A	Q	O	3.38	3.21	91.06	68.96
587	A	S	N	582	A	F	O	3.00	2.39	119.32	164.40
588	A	L	N	582	A	F	O	3.06	2.09	164.63	115.91
588	A	L	N	586	A	G	O	3.39	3.44	79.30	70.75
589	A	T	N	560	A	T	O	2.94	1.96	175.45	154.76
590	A	Q	N	588	A	L	O	3.37	3.50	74.38	77.91
594	A	A	N	564	A	Y	O	3.05	2.12	153.26	141.23
596	A	S	N	566	A	C	O	2.86	1.93	157.18	154.50
596	A	S	N	567	A	R	O	3.45	3.39	85.34	107.83
597	A	R	N	567	A	R	O	2.88	1.95	157.66	138.04
597	A	R	N	595	A	F	O	3.13	2.99	89.23	90.86
598	A	E	N	595	A	F	O	3.18	2.22	165.07	133.76
599	A	Q	N	597	A	R	O	3.24	2.98	96.12	74.01
601	A	H	N	599	A	Q	O	3.34	3.38	79.62	80.01
602	A	K	N	600	A	P	O	3.46	3.30	91.08	94.09
606	A	Q	N	604	A	Y	O	3.17	3.13	83.46	77.95
607	A	H	N	604	A	Y	O	2.97	2.10	148.18	126.96
607	A	H	N	605	A	V	O	3.26	3.23	83.46	76.47
608	A	L	N	605	A	V	O	3.13	2.50	121.87	111.96
608	A	L	N	606	A	Q	O	3.49	3.51	81.08	70.24
609	A	L	N	605	A	V	O	2.99	2.07	156.04	160.05
609	A	L	N	606	A	Q	O	3.34	2.83	112.93	100.45
609	A	L	N	607	A	H	O	3.44	3.55	75.56	70.81
610	A	K	N	606	A	Q	O	2.93	2.06	146.06	150.21
610	A	K	N	607	A	H	O	3.19	2.65	115.03	101.71
610	A	K	N	608	A	L	O	3.44	3.52	77.03	72.82
611	A	R	N	607	A	H	O	2.99	2.14	145.23	153.35
611	A	R	N	608	A	L	O	3.19	2.56	122.27	108.41
611	A	R	N	609	A	L	O	3.43	3.46	80.22	73.23
612	A	D	N	608	A	L	O	3.17	2.42	132.45	154.93
612	A	D	N	609	A	L	O	3.31	2.53	135.93	107.25
612	A	D	N	610	A	K	O	3.40	3.28	88.27	72.14
613	A	K	N	609	A	L	O	3.03	2.84	91.46	155.00
613	A	K	N	610	A	K	O	3.46	2.52	157.44	99.84
614	A	E	N	612	A	D	O	3.24	3.22	82.67	86.84
615	A	H	N	612	A	D	O	3.15	2.52	121.95	132.34
615	A	H	N	613	A	K	O	3.44	3.53	76.28	74.32
616	A	L	N	612	A	D	O	2.91	2.02	151.55	158.12
616	A	L	N	613	A	K	O	3.25	2.74	113.82	102.34
617	A	W	N	613	A	K	O	3.07	2.16	154.98	155.28
617	A	W	N	615	A	H	O	3.30	3.42	74.69	76.42
618	A	Q	N	615	A	H	O	3.03	2.39	122.64	115.42

618	A	Q	N	616	A	L	O	3.35	3.39	79.21	76.04
619	A	L	N	615	A	H	O	3.21	2.32	151.51	159.55
619	A	L	N	616	A	L	O	3.15	2.52	121.45	113.54
619	A	L	N	617	A	W	O	3.26	3.34	76.95	75.48
620	A	I	N	616	A	L	O	2.93	2.00	156.03	161.66
620	A	I	N	617	A	W	O	3.15	2.66	110.85	107.21
621	A	H	N	617	A	W	O	2.86	1.94	153.88	161.99
621	A	H	N	619	A	L	O	3.33	3.34	80.57	75.00
622	A	E	N	618	A	Q	O	3.45	2.82	122.97	139.08
622	A	E	N	619	A	L	O	3.04	2.20	143.24	114.21
622	A	E	N	620	A	I	O	3.32	3.17	90.43	73.12
623	A	A	N	621	A	H	O	3.47	3.60	74.84	101.38
624	A	G	N	622	A	E	O	3.50	3.74	68.27	101.43
625	A	A	N	622	A	E	O	3.32	2.39	159.24	132.15
625	A	A	N	623	A	A	O	3.26	2.86	105.24	77.11
626	A	H	N	527	A	P	O	2.94	2.00	158.64	155.01
627	A	I	N	671	A	R	O	2.90	1.96	154.12	149.01
628	A	Y	N	529	A	I	O	2.87	1.95	154.50	159.89
629	A	V	N	673	A	S	O	3.03	2.16	145.70	157.11
630	A	C	N	531	A	V	O	2.91	1.97	157.72	169.98
633	A	A	N	631	A	G	O	3.20	3.03	90.41	105.01
633	A	A	N	677	A	W	O	2.96	1.98	168.94	135.35
637	A	A	N	632	A	D	O	2.96	2.05	153.10	175.80
638	A	R	N	635	A	N	O	3.28	2.67	120.90	103.29
638	A	R	N	636	A	M	O	3.22	3.19	82.76	77.91
639	A	D	N	635	A	N	O	3.01	2.12	151.15	156.46
639	A	D	N	636	A	M	O	3.18	2.52	124.24	117.17
640	A	V	N	636	A	M	O	3.05	2.10	160.17	162.07
640	A	V	N	637	A	A	O	3.42	2.94	110.75	99.75
640	A	V	N	638	A	R	O	3.49	3.58	76.63	68.68
641	A	Q	N	637	A	A	O	2.87	2.00	146.63	150.56
641	A	Q	N	638	A	R	O	3.30	2.77	114.18	99.62
641	A	Q	N	639	A	D	O	3.44	3.53	76.37	74.45
642	A	N	N	638	A	R	O	2.96	2.09	146.95	149.37
642	A	N	N	639	A	D	O	3.19	2.62	117.10	107.30
642	A	N	N	640	A	V	O	3.36	3.42	78.47	73.74
643	A	T	N	639	A	D	O	2.85	2.03	138.55	157.23
643	A	T	N	640	A	V	O	3.09	2.47	121.27	106.81
643	A	T	N	641	A	Q	O	3.42	3.41	82.50	71.65
644	A	F	N	640	A	V	O	2.95	2.05	153.03	158.49
644	A	F	N	641	A	Q	O	3.29	2.74	116.73	105.12
645	A	Y	N	641	A	Q	O	3.04	2.19	146.07	152.46
645	A	Y	N	642	A	N	O	3.30	2.72	118.60	100.17
645	A	Y	N	643	A	T	O	3.42	3.47	78.84	73.11
646	A	D	N	642	A	N	O	3.15	2.28	148.97	147.78

646	A	D	N	643	A	T	O	3.12	2.53	118.90	110.42
646	A	D	N	644	A	F	O	3.39	3.48	76.32	72.36
647	A	I	N	643	A	T	O	2.96	2.09	146.85	158.36
647	A	I	N	644	A	F	O	3.33	2.74	118.82	102.66
647	A	I	N	645	A	Y	O	3.45	3.47	80.70	73.84
648	A	V	N	644	A	F	O	3.14	2.20	160.55	153.48
648	A	V	N	645	A	Y	O	3.37	2.81	117.23	108.69
648	A	V	N	646	A	D	O	3.43	3.54	75.35	73.45
649	A	A	N	645	A	Y	O	2.88	1.98	151.34	158.28
649	A	A	N	646	A	D	O	3.35	2.85	112.54	100.69
650	A	E	N	646	A	D	O	2.90	1.96	160.18	153.85
651	A	V	N	647	A	I	O	3.15	2.21	160.10	149.67
652	A	G	N	648	A	V	O	3.04	2.30	130.73	134.18
653	A	A	N	649	A	A	O	3.24	2.93	98.65	126.16
653	A	A	N	650	A	E	O	3.25	2.39	143.71	98.78
653	A	A	N	651	A	V	O	3.42	3.02	105.02	67.54
654	A	M	N	649	A	A	O	2.95	2.00	158.86	141.26
654	A	M	N	652	A	G	O	3.40	3.62	69.53	76.91
657	A	A	N	655	A	E	O	3.32	3.40	76.69	73.84
658	A	Q	N	655	A	E	O	3.02	2.36	124.23	113.15
658	A	Q	N	656	A	H	O	3.29	3.34	78.77	76.55
659	A	A	N	655	A	E	O	2.93	2.05	146.11	158.09
659	A	A	N	656	A	H	O	3.05	2.48	116.60	109.08
660	A	V	N	656	A	H	O	2.89	2.00	150.91	164.65
660	A	V	N	657	A	A	O	3.49	2.88	121.92	100.18
661	A	D	N	657	A	A	O	3.27	2.37	152.04	144.07
661	A	D	N	658	A	Q	O	3.27	2.74	114.34	103.80
661	A	D	N	659	A	A	O	3.42	3.52	76.33	70.46
662	A	Y	N	658	A	Q	O	2.85	2.07	134.22	151.40
662	A	Y	N	659	A	A	O	3.20	2.58	120.17	100.23
662	A	Y	N	660	A	V	O	3.29	3.27	82.25	74.36
663	A	I	N	659	A	A	O	3.07	2.19	149.88	152.03
663	A	I	N	660	A	V	O	3.13	2.51	121.55	112.58
664	A	K	N	660	A	V	O	3.04	2.14	154.24	156.03
664	A	K	N	661	A	D	O	3.24	2.75	111.97	101.04
664	A	K	N	662	A	Y	O	3.43	3.53	76.18	71.50
665	A	K	N	661	A	D	O	2.93	2.08	143.44	150.75
665	A	K	N	662	A	Y	O	3.14	2.56	118.02	106.02
665	A	K	N	663	A	I	O	3.33	3.41	76.98	75.27
666	A	L	N	662	A	Y	O	2.91	2.04	148.08	155.45
666	A	L	N	663	A	I	O	3.10	2.56	115.57	108.01
667	A	M	N	663	A	I	O	2.92	2.03	151.66	159.18
667	A	M	N	664	A	K	O	3.23	2.68	115.89	103.47
667	A	M	N	665	A	K	O	3.37	3.48	75.62	72.74
668	A	T	N	664	A	K	O	3.01	2.15	147.65	153.38

668	A	T	N	665	A	K	O	3.28	2.71	118.23	105.41
668	A	T	N	666	A	L	O	3.50	3.58	77.47	74.34
669	A	K	N	665	A	K	O	2.98	2.09	150.26	156.05
669	A	K	N	666	A	L	O	3.30	2.72	118.21	105.93
669	A	K	N	667	A	M	O	3.41	3.42	80.71	72.34
670	A	G	N	666	A	L	O	3.08	2.72	101.86	151.52
670	A	G	N	667	A	M	O	3.05	2.15	151.71	107.91
670	A	G	N	668	A	T	O	3.34	2.97	103.68	70.62
671	A	R	N	666	A	L	O	2.79	1.82	161.34	152.65
671	A	R	N	669	A	K	O	3.48	3.50	80.64	68.59
672	A	Y	N	666	A	L	O	3.30	2.65	123.15	102.89
673	A	S	N	627	A	I	O	2.91	2.05	143.82	165.44
675	A	D	N	629	A	V	O	2.87	1.93	159.09	168.60
677	A	W	N	631	A	G	O	2.96	2.01	162.96	165.09

Dd-a = Distance Between Donor and Acceptor
Dh-a = Distance Between Hydrogen and Acceptor
A(d-H-N) = Angle Between Donor-H-N
A(a-O=C) = Angle Between Acceptor-O=C
MO = Multiple Occupancy
Note that angles that are undefined are written as 999.99

Intraprotein Main Chain-Side Chain Hydrogen Bonds


Rasmol **Jmol** [help]

[View the original hbond output]

DOG_POR_E315Q_snapshot10.pdb

DONOR PARAMETERS						ACCEPTOR						
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**MO**	**Dd-a**	**Dh-a**	**A(d-H-N)**	**A(a-O=C)**
64	A	ALA	N	61	A	THR	OG1	-	3.20	2.71	111.54	999.99
65	A	LYS	NZ	115	A	GLU	O	-	2.89	9.99	999.99	135.12
69	A	PHE	N	121	A	ASP	OD2	-	3.12	2.63	111.87	154.95
70	A	VAL	N	121	A	ASP	OD2	-	2.96	2.00	168.56	149.13
71	A	GLU	N	68	A	SER	OG	-	3.31	2.37	161.86	999.99
72	A	LYS	NZ	354	A	GLU	O	-	2.93	9.99	999.99	148.48
76	A	THR	OG1	72	A	LYS	O	-	2.70	9.99	999.99	129.50

78	A	ARG	NE	76	A	THR	O	-	3.18	2.28	145.22	125.88
78	A	ARG	NH2	109	A	GLY	O	1	3.02	2.09	144.29	128.23
78	A	ARG	NH2	109	A	GLY	O	2	3.02	3.36	61.58	128.23
79	A	ASN	OD1	108	A	ARG	O	1	2.91	3.11	69.70	123.06
79	A	ASN	OD1	108	A	ARG	O	2	2.91	2.24	119.52	123.06
79	A	ASN	ND2	130	A	ASN	O	1	2.93	3.53	47.56	143.19
79	A	ASN	ND2	130	A	ASN	O	2	2.93	1.88	174.92	143.19
86	A	SER	N	146	A	THR	OG1	-	3.16	2.80	101.98	999.99
86	A	SER	N	148	A	ASN	OD1	-	3.02	2.05	168.85	124.79
89	A	GLY	N	86	A	SER	OG	-	3.06	2.53	114.08	999.99
92	A	GLU	N	86	A	SER	OG	-	3.37	2.54	143.38	999.99
96	A	ASN	ND2	92	A	GLU	O	1	3.44	3.82	61.38	112.61
96	A	ASN	ND2	92	A	GLU	O	2	3.44	3.72	67.03	112.61
99	A	SER	OG	95	A	ALA	O	-	2.85	9.99	999.99	144.98
99	A	SER	OG	110	A	MET	O	-	3.29	9.99	999.99	77.55
100	A	LYS	NZ	242	A	ILE	O	-	3.01	9.99	999.99	138.26
104	A	ARG	NH2	238	A	GLU	O	1	2.93	1.91	158.14	149.60
104	A	ARG	NH2	238	A	GLU	O	2	2.93	3.36	56.55	149.60
108	A	ARG	N	79	A	ASN	OD1	-	3.01	2.04	172.31	170.25
111	A	ALA	N	99	A	SER	OG	-	3.43	3.91	54.91	999.99
113	A	ASP	N	84	A	TYR	OH	-	3.47	3.63	72.86	999.99
115	A	GLU	N	113	A	ASP	OD1	-	2.99	2.03	173.03	137.59
120	A	ALA	N	118	A	ASP	OD1	-	3.13	2.18	166.21	108.24
124	A	SER	OG	121	A	ASP	O	-	3.33	9.99	999.99	118.70
131	A	SER	OG	125	A	LEU	O	-	2.77	9.99	999.99	117.54
131	A	SER	OG	128	A	ILE	O	-	3.13	9.99	999.99	137.59
139	A	THR	OG1	173	A	LEU	O	-	3.10	9.99	999.99	161.57
147	A	ASP	N	87	A	GLN	OE1	-	2.98	2.06	154.99	135.67
148	A	ASN	ND2	84	A	TYR	O	1	2.91	1.90	157.95	155.71
148	A	ASN	ND2	84	A	TYR	O	2	2.91	3.35	56.82	155.71
148	A	ASN	OD1	86	A	SER	O	1	3.03	3.02	80.70	122.21
148	A	ASN	OD1	86	A	SER	O	2	3.03	3.02	80.64	122.21
150	A	GLN	NE2	147	A	ASP	O	1	3.05	3.77	40.65	116.67
150	A	GLN	NE2	147	A	ASP	O	2	3.05	2.09	151.46	116.67
154	A	ASP	OD2	150	A	GLN	O	1	3.35	3.87	53.67	126.28
154	A	ASP	OD2	150	A	GLN	O	2	3.35	3.12	93.01	126.28
157	A	GLN	NE2	153	A	TYR	O	1	2.98	3.76	36.58	97.85
157	A	GLN	NE2	153	A	TYR	O	2	2.98	2.02	150.20	97.85
157	A	GLN	N	187	A	TYR	OH	-	3.49	3.95	55.48	999.99
161	A	VAL	N	159	A	THR	OG1	-	3.17	2.23	160.76	999.99
164	A	SER	N	162	A	ASP	OD1	-	3.08	2.15	159.91	121.52
168	A	TYR	OH	189	A	ASP	O	-	2.90	9.99	999.99	147.55
176	A	LYS	N	207	A	ASP	OD1	-	2.84	1.89	160.31	128.91
177	A	THR	N	175	A	ASN	OD1	-	3.00	2.04	166.77	144.19
178	A	TYR	OH	676	A	VAL	O	-	2.74	9.99	999.99	158.44

182	A	ASN	ND2	172	A	GLY	O	1	3.03	1.98	173.99	89.34
182	A	ASN	ND2	172	A	GLY	O	2	3.03	3.66	46.41	89.34
182	A	ASN	ND2	206	A	GLY	O	1	3.26	3.20	83.76	134.68
182	A	ASN	ND2	206	A	GLY	O	2	3.26	2.53	126.14	134.68
184	A	MET	N	139	A	THR	OG1	-	3.47	2.54	160.92	999.99
191	A	ARG	NE	156	A	LEU	O	-	3.02	2.06	155.49	134.17
191	A	ARG	NH1	157	A	GLN	O	1	3.09	2.42	121.24	116.42
191	A	ARG	NH1	157	A	GLN	O	2	3.09	3.28	70.72	116.42
193	A	GLU	N	168	A	TYR	OH	-	3.41	3.24	91.15	999.99
209	A	ASP	N	175	A	ASN	ND2	-	3.49	3.71	69.28	86.21
209	A	ASP	N	207	A	ASP	OD1	-	3.00	2.06	162.77	108.18
213	A	GLU	N	211	A	ASN	OD1	-	3.20	2.61	118.47	134.97
214	A	GLU	N	211	A	ASN	OD1	-	2.89	1.96	157.88	148.96
218	A	THR	OG1	214	A	GLU	O	-	2.70	9.99	999.99	139.69
222	A	GLN	NE2	218	A	THR	O	1	3.03	3.73	41.77	111.21
222	A	GLN	NE2	218	A	THR	O	2	3.03	2.09	147.25	111.21
228	A	CYS	SG	224	A	TRP	O	-	3.16	9.99	999.99	131.61
228	A	CYS	SG	233	A	VAL	O	-	3.57	9.99	999.99	114.28
236	A	THR	OG1	103	A	HIS	O	-	3.43	9.99	999.99	122.71
236	A	THR	OG1	104	A	ARG	O	-	2.97	9.99	999.99	88.81
238	A	GLU	OE1	103	A	HIS	O	1	2.91	2.61	95.27	108.35
238	A	GLU	OE1	103	A	HIS	O	2	2.91	2.43	105.53	108.35
241	A	SER	OG	388	A	GLU	O	-	2.68	9.99	999.99	120.81
244	A	GLN	N	446	A	GLU	OE2	-	2.80	1.82	171.46	152.30
245	A	TYR	OH	357	A	LYS	O	-	2.93	9.99	999.99	137.11
245	A	TYR	N	446	A	GLU	OE2	-	3.13	2.38	132.14	103.32
256	A	ALA	N	254	A	ASP	OD1	-	3.12	2.14	171.68	111.86
259	A	TYR	OH	264	A	GLY	O	-	2.73	9.99	999.99	156.57
260	A	VAL	N	262	A	GLU	OE1	-	2.84	1.86	170.62	132.35
261	A	GLY	N	374	A	TYR	OH	-	3.26	2.63	122.35	999.99
262	A	GLU	N	374	A	TYR	OH	-	3.34	3.33	81.67	999.99
266	A	LEU	N	259	A	TYR	OH	-	3.28	3.34	78.44	999.99
267	A	LYS	NZ	255	A	MET	O	-	2.99	9.99	999.99	143.07
267	A	LYS	NZ	258	A	VAL	O	-	2.89	9.99	999.99	168.05
267	A	LYS	N	262	A	GLU	OE2	-	2.86	1.90	156.79	119.06
268	A	SER	OG	263	A	MET	O	-	2.78	9.99	999.99	143.22
268	A	SER	OG	265	A	ARG	O	-	3.33	9.99	999.99	144.26
272	A	GLN	NE2	269	A	TYR	O	1	2.92	3.64	40.63	129.06
272	A	GLN	NE2	269	A	TYR	O	2	2.92	1.90	163.57	129.06
279	A	LYS	N	277	A	ASP	OD1	-	3.40	2.72	126.77	73.88
279	A	LYS	N	277	A	ASP	OD2	-	2.94	1.98	165.28	94.45
280	A	ASN	ND2	268	A	SER	O	1	3.27	2.36	142.98	120.99
280	A	ASN	ND2	268	A	SER	O	2	3.27	3.96	42.61	120.99
280	A	ASN	N	277	A	ASP	OD1	-	3.06	2.38	125.30	121.20
283	A	LEU	N	272	A	GLN	OE1	-	2.86	1.88	174.44	125.41

287	A	THR	OG1	304	A	GLU	O	-	3.38	9.99	999.99	100.36
289	A	ASN	ND2	494	A	LEU	O	1	2.97	2.13	134.32	150.47
289	A	ASN	ND2	494	A	LEU	O	2	2.97	3.16	70.20	150.47
289	A	ASN	ND2	497	A	LYS	O	1	2.91	3.44	51.85	135.64
289	A	ASN	ND2	497	A	LYS	O	2	2.91	1.97	147.05	135.64
293	A	ASN	OD1	298	A	ARG	O	1	3.29	2.67	116.26	126.07
293	A	ASN	OD1	298	A	ARG	O	2	3.29	4.12	33.66	126.07
293	A	ASN	ND2	298	A	ARG	O	1	2.97	2.25	123.80	156.63
293	A	ASN	ND2	298	A	ARG	O	2	2.97	3.66	42.26	156.63
293	A	ASN	OD1	300	A	LEU	O	1	3.42	3.58	73.09	110.80
293	A	ASN	OD1	300	A	LEU	O	2	3.42	2.48	147.04	110.80
300	A	LEU	N	293	A	ASN	OD1	-	2.94	1.97	165.79	140.28
308	A	SER	N	306	A	ASP	OD1	-	2.91	1.95	164.09	137.45
310	A	SER	OG	307	A	ILE	O	-	2.69	9.99	999.99	136.49
312	A	LEU	N	310	A	SER	OG	-	3.18	2.23	160.24	999.99
314	A	TYR	OH	461	A	SER	O	-	3.41	9.99	999.99	79.00
314	A	TYR	OH	465	A	HIS	O	-	3.01	9.99	999.99	138.29
314	A	TYR	OH	468	A	SER	O	-	2.78	9.99	999.99	158.98
315	A	GLN	N	318	A	ASP	OD2	-	3.08	2.19	149.13	120.76
316	A	SER	OG	460	A	SER	O	-	3.40	9.99	999.99	106.40
316	A	SER	OG	542	A	GLY	O	-	2.76	9.99	999.99	100.24
316	A	SER	N	546	A	GLU	OE1	-	3.13	2.20	158.07	177.39
323	A	TYR	OH	278	A	ALA	O	-	2.97	9.99	999.99	115.13
326	A	ASN	ND2	371	A	LEU	O	1	2.89	3.34	56.65	156.90
326	A	ASN	ND2	371	A	LEU	O	2	2.89	2.00	140.65	156.90
326	A	ASN	ND2	372	A	THR	O	1	3.30	3.96	45.01	109.20
326	A	ASN	ND2	372	A	THR	O	2	3.30	2.65	120.12	109.20
326	A	ASN	ND2	375	A	LEU	O	1	2.84	1.96	138.56	167.57
326	A	ASN	ND2	375	A	LEU	O	2	2.84	3.04	69.06	167.57
329	A	ALA	N	327	A	ASP	OD2	-	3.13	2.23	151.48	140.05
343	A	ASP	N	341	A	ASP	OD1	-	3.24	2.31	157.54	125.48
348	A	LEU	N	363	A	CYS	SG	-	3.82	2.88	159.39	999.99
350	A	ASN	OD1	244	A	GLN	O	1	3.04	3.26	68.94	146.49
350	A	ASN	OD1	244	A	GLN	O	2	3.04	2.49	111.39	146.49
350	A	ASN	ND2	357	A	LYS	O	1	2.92	3.60	42.94	134.41
350	A	ASN	ND2	357	A	LYS	O	2	2.92	1.94	153.98	134.41
352	A	ASP	N	350	A	ASN	OD1	-	2.88	1.91	163.02	111.04
355	A	SER	OG	352	A	ASP	O	-	2.71	9.99	999.99	158.86
357	A	LYS	N	355	A	SER	OG	-	3.37	2.56	138.01	999.99
358	A	LYS	NZ	353	A	GLU	O	-	3.01	9.99	999.99	161.82
358	A	LYS	NZ	355	A	SER	O	-	3.14	9.99	999.99	143.38
359	A	HIS	ND1	348	A	LEU	O	-	2.82	1.93	162.18	134.76
363	A	CYS	SG	361	A	PHE	O	-	3.35	9.99	999.99	135.12
365	A	THR	OG1	259	A	TYR	O	-	2.91	9.99	999.99	129.00
368	A	ARG	N	366	A	SER	OG	-	3.41	2.85	117.18	999.99

369	A	THR	N	366	A	SER	OG	-	3.11	2.17	159.61	999.99
372	A	THR	OG1	368	A	ARG	O	-	2.68	9.99	999.99	137.95
374	A	TYR	OH	262	A	GLU	O	-	2.67	9.99	999.99	138.46
378	A	THR	N	376	A	ASP	OD1	-	3.33	2.51	141.55	148.53
379	A	ASN	N	376	A	ASP	OD1	-	2.94	2.03	154.25	139.52
383	A	THR	N	213	A	GLU	OE2	-	2.88	2.04	143.24	113.85
394	A	SER	N	436	A	SER	OG	-	3.17	2.71	109.51	999.99
395	A	GLU	N	436	A	SER	OG	-	3.06	2.14	154.66	999.99
397	A	THR	N	395	A	GLU	OE2	-	2.93	1.97	168.77	123.38
401	A	HIS	ND1	397	A	THR	O	-	3.41	3.31	88.68	131.44
403	A	ARG	NH1	239	A	GLU	O	1	3.00	3.81	33.87	116.03
403	A	ARG	NH1	239	A	GLU	O	2	3.00	2.06	147.42	116.03
403	A	ARG	NH2	239	A	GLU	O	1	3.09	4.00	27.01	158.31
403	A	ARG	NH2	239	A	GLU	O	2	3.09	2.26	138.44	158.31
403	A	ARG	NH2	387	A	TYR	O	1	3.07	2.08	154.96	131.11
403	A	ARG	NH2	387	A	TYR	O	2	3.07	3.43	61.25	131.11
407	A	SER	OG	409	A	SER	O	-	3.03	9.99	999.99	151.56
413	A	LYS	NZ	408	A	SER	O	-	3.22	9.99	999.99	138.59
416	A	TYR	OH	381	A	PRO	O	-	2.71	9.99	999.99	143.52
418	A	SER	OG	414	A	GLU	O	-	2.91	9.99	999.99	132.06
418	A	SER	OG	415	A	LEU	O	-	3.18	9.99	999.99	103.07
424	A	ARG	NH2	421	A	VAL	O	1	2.90	1.90	154.75	133.42
424	A	ARG	NH2	421	A	VAL	O	2	2.90	3.26	60.09	133.42
425	A	ARG	NH2	419	A	TRP	O	1	2.90	1.86	165.42	119.44
425	A	ARG	NH2	419	A	TRP	O	2	2.90	3.37	54.60	119.44
428	A	LEU	N	426	A	HIS	ND1	-	3.40	2.78	122.70	999.99
429	A	ALA	N	426	A	HIS	ND1	-	3.19	2.31	149.42	999.99
436	A	SER	N	398	A	GLU	OE2	-	2.90	1.98	156.01	117.13
438	A	ARG	NH2	431	A	LEU	O	1	2.89	3.53	46.14	130.06
438	A	ARG	NH2	431	A	LEU	O	2	2.89	1.99	148.52	130.06
438	A	ARG	NH2	434	A	TYR	O	1	3.28	3.53	68.20	137.51
438	A	ARG	NH2	434	A	TYR	O	2	3.28	2.61	124.63	137.51
438	A	ARG	NH1	435	A	PRO	O	1	3.40	3.74	63.13	107.78
438	A	ARG	NH1	435	A	PRO	O	2	3.40	3.55	73.09	107.78
445	A	CYS	SG	441	A	ILE	O	-	3.14	9.99	999.99	138.18
446	A	GLU	OE1	245	A	TYR	O	1	3.43	2.69	125.93	108.20
446	A	GLU	OE1	245	A	TYR	O	2	3.43	3.75	64.48	108.20
450	A	ARG	N	93	A	GLU	OE2	-	2.93	1.95	177.74	128.69
454	A	ARG	NH2	452	A	GLN	O	1	3.21	2.83	101.27	132.17
454	A	ARG	NH2	452	A	GLN	O	2	3.21	3.23	80.20	132.17
461	A	SER	N	545	A	GLN	OE1	-	2.96	2.07	148.24	155.68
462	A	SER	N	314	A	TYR	OH	-	3.50	4.05	50.08	999.99
462	A	SER	OG	314	A	TYR	O	-	2.75	9.99	999.99	155.01
463	A	LYS	N	461	A	SER	OG	-	3.06	2.16	152.58	999.99
470	A	HIS	N	460	A	SER	OG	-	3.11	2.27	143.92	999.99

472	A	CYS	SG	301	A	MET	O	-	3.86	9.99	999.99	144.17
476	A	VAL	N	491	A	THR	OG1	-	3.18	2.39	137.17	999.99
480	A	THR	OG1	484	A	ARG	O	-	3.04	9.99	999.99	113.40
482	A	SER	OG	423	A	ALA	O	-	2.77	9.99	999.99	153.65
482	A	SER	N	480	A	THR	OG1	-	3.32	2.67	123.56	999.99
483	A	GLY	N	480	A	THR	OG1	-	3.27	2.94	100.62	999.99
484	A	ARG	N	480	A	THR	OG1	-	3.06	2.15	151.20	999.99
486	A	ASN	ND2	424	A	ARG	O	1	3.04	2.17	138.28	144.06
486	A	ASN	ND2	424	A	ARG	O	2	3.04	3.56	52.32	144.06
492	A	SER	OG	488	A	GLY	O	-	2.83	9.99	999.99	150.72
497	A	LYS	NZ	508	A	LEU	O	-	3.09	9.99	999.99	163.75
505	A	ARG	NH2	499	A	PRO	O	1	3.04	1.98	172.26	138.34
505	A	ARG	NH2	499	A	PRO	O	2	3.04	3.56	51.25	138.34
514	A	ARG	NH1	145	A	PRO	O	1	3.06	3.31	67.19	139.18
514	A	ARG	NH1	145	A	PRO	O	2	3.06	2.13	145.41	139.18
516	A	SER	OG	317	A	GLY	O	-	2.64	9.99	999.99	117.69
516	A	SER	N	318	A	ASP	OD1	-	3.24	2.28	166.46	130.66
518	A	PHE	N	142	A	GLU	OE2	-	3.21	3.65	56.19	159.83
518	A	PHE	N	516	A	SER	OG	-	3.13	2.34	134.98	999.99
519	A	ARG	NH2	516	A	SER	O	1	2.87	1.87	153.97	136.70
519	A	ARG	NH2	516	A	SER	O	2	2.87	3.26	58.76	136.70
526	A	THR	OG1	523	A	LYS	O	-	2.79	9.99	999.99	172.91
547	A	ARG	NH1	524	A	ALA	O	1	3.05	3.41	61.29	111.07
547	A	ARG	NH1	524	A	ALA	O	2	3.05	3.07	79.16	111.07
547	A	ARG	NH1	526	A	THR	O	1	3.00	3.86	29.78	138.51
547	A	ARG	NH1	526	A	THR	O	2	3.00	2.09	142.15	138.51
547	A	ARG	NH2	526	A	THR	O	1	2.91	3.80	28.03	176.99
547	A	ARG	NH2	526	A	THR	O	2	2.91	2.03	143.81	176.99
549	A	TRP	NE1	463	A	LYS	O	-	3.28	3.25	83.91	130.26
551	A	ARG	NH1	585	A	ASP	O	1	3.24	2.54	124.24	127.68
551	A	ARG	NH1	585	A	ASP	O	2	3.24	3.40	72.61	127.68
551	A	ARG	NH2	586	A	GLY	O	1	3.33	3.78	57.50	106.94
551	A	ARG	NH2	586	A	GLY	O	2	3.33	3.29	83.69	106.94
552	A	GLN	NE2	548	A	ALA	O	1	3.25	4.01	38.49	107.28
552	A	GLN	NE2	548	A	ALA	O	2	3.25	2.37	141.09	107.28
560	A	THR	OG1	558	A	GLY	O	-	3.05	9.99	999.99	132.99
560	A	THR	N	589	A	THR	OG1	-	2.81	1.82	175.12	999.99
564	A	TYR	OH	572	A	ASP	O	-	3.17	9.99	999.99	135.81
566	A	CYS	SG	594	A	ALA	O	-	3.60	9.99	999.99	144.22
567	A	ARG	N	572	A	ASP	OD1	-	2.99	2.26	130.31	95.16
567	A	ARG	N	572	A	ASP	OD2	-	2.90	1.94	166.95	99.62
568	A	ARG	N	572	A	ASP	OD1	-	2.84	1.91	157.25	152.51
569	A	SER	N	598	A	GLU	OE2	-	2.85	1.87	169.98	146.07
572	A	ASP	OD1	568	A	ARG	O	1	3.17	3.21	78.19	114.77
572	A	ASP	OD1	568	A	ARG	O	2	3.17	2.55	116.69	114.77

574	A	LEU	N	564	A	TYR	OH	-	2.95	1.99	163.28	999.99
576	A	ARG	NH2	569	A	SER	O	1	2.97	1.99	151.69	136.91
576	A	ARG	NH2	569	A	SER	O	2	2.97	3.36	58.63	136.91
581	A	GLN	NE2	577	A	GLU	O	1	3.04	3.81	37.42	104.19
581	A	GLN	NE2	577	A	GLU	O	2	3.04	2.09	149.90	104.19
583	A	HIS	ND1	588	A	LEU	O	-	2.97	2.08	165.05	148.21
584	A	GLN	NE2	580	A	ALA	O	1	3.43	4.11	44.37	96.12
584	A	GLN	NE2	580	A	ALA	O	2	3.43	3.11	99.19	96.12
585	A	ASP	OD2	581	A	GLN	O	1	3.12	3.50	60.42	113.11
585	A	ASP	OD2	581	A	GLN	O	2	3.12	3.16	78.20	113.11
589	A	THR	OG1	560	A	THR	O	-	3.15	9.99	999.99	102.09
592	A	ASN	ND2	590	A	GLN	O	1	3.20	3.34	73.39	99.34
592	A	ASN	ND2	590	A	GLN	O	2	3.20	2.38	133.98	99.34
599	A	GLN	NE2	601	A	HIS	O	1	3.00	3.75	38.96	143.13
599	A	GLN	NE2	601	A	HIS	O	2	3.00	2.00	160.55	143.13
612	A	ASP	OD2	608	A	LEU	O	1	3.16	3.42	66.98	126.73
612	A	ASP	OD2	608	A	LEU	O	2	3.16	3.34	71.38	126.73
626	A	HIS	ND1	624	A	GLY	O	-	2.83	2.09	136.98	136.18
626	A	HIS	NE2	670	A	GLY	O	-	3.06	2.65	108.88	142.79
628	A	TYR	OH	519	A	ARG	O	-	2.88	9.99	999.99	122.95
630	A	CYS	SG	536	A	GLY	O	-	3.51	9.99	999.99	107.67
630	A	CYS	SG	675	A	ASP	O	-	3.12	9.99	999.99	157.86
634	A	ARG	N	632	A	ASP	OD1	-	2.99	2.07	155.98	100.43
634	A	ARG	NE	678	A	SER	OXT	-	3.00	2.19	134.89	112.11
634	A	ARG	NH1	678	A	SER	OXT	1	2.91	1.99	144.17	107.44
634	A	ARG	NH1	678	A	SER	OXT	2	2.91	3.74	32.11	107.44
635	A	ASN	N	632	A	ASP	OD2	-	2.90	1.99	151.80	127.70
636	A	MET	N	632	A	ASP	OD2	-	2.92	1.96	170.34	139.04
638	A	ARG	NH1	176	A	LYS	O	1	3.08	2.47	116.58	151.19
638	A	ARG	NH1	176	A	LYS	O	2	3.08	2.97	86.10	151.19
642	A	ASN	ND2	638	A	ARG	O	1	3.27	3.67	59.89	123.52
642	A	ASN	ND2	638	A	ARG	O	2	3.27	3.36	76.27	123.52
643	A	THR	OG1	639	A	ASP	O	-	2.71	9.99	999.99	133.21
655	A	GLU	N	658	A	GLN	OE1	-	3.02	2.05	168.13	141.41
668	A	THR	OG1	664	A	LYS	O	-	3.49	9.99	999.99	124.36
668	A	THR	OG1	665	A	LYS	O	-	2.89	9.99	999.99	109.81
671	A	ARG	NH1	620	A	ILE	O	1	2.99	3.20	68.54	143.82
671	A	ARG	NH1	620	A	ILE	O	2	2.99	2.12	136.89	143.82
671	A	ARG	NH1	622	A	GLU	O	1	2.99	3.43	57.05	155.54
671	A	ARG	NH1	622	A	GLU	O	2	2.99	2.46	110.11	155.54
671	A	ARG	NE	625	A	ALA	O	-	2.82	1.85	154.73	144.33
671	A	ARG	NH1	625	A	ALA	O	1	3.21	2.46	128.81	115.83
671	A	ARG	NH1	625	A	ALA	O	2	3.21	4.13	26.02	115.83

Dd-a = Distance Between Donor and Acceptor
Dh-a = Distance Between Hydrogen and Acceptor
A(d-H-N) = Angle Between Donor-H-N
A(a-O=C) = Angle Between Acceptor-O=C
MO = Multiple Occupancy
Note that angles that are undefined are written as 999.99

Intraprotein Side Chain-Side Chain Hydrogen Bonds


[help]
Rasmol **Jmol**

[View the original hbond output]

DOG_POR_E315Q_snapshot10.pdb

DONOR PARAMETERS						ACCEPTOR						
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**MO**	**Dd-a**	**Dh-a**	**A(d-H-N)**	**A(a-O=C)**
61	A	THR	OG1	63	A	SER	OG	-	3.27	9.99	999.99	999.99
65	A	LYS	NZ	151	A	ASP	OD2	-	2.88	9.99	999.99	999.99
66	A	ASP	OD2	356	A	ASN	ND2	1	3.17	2.90	94.86	999.99
66	A	ASP	OD2	356	A	ASN	ND2	2	3.17	2.57	114.58	999.99
68	A	SER	OG	121	A	ASP	OD1	-	3.40	9.99	999.99	999.99
68	A	SER	OG	121	A	ASP	OD2	-	2.65	9.99	999.99	999.99
72	A	LYS	NZ	117	A	TYR	OH	-	2.96	9.99	999.99	999.99
74	A	LYS	NZ	127	A	GLU	OE2	-	2.95	9.99	999.99	999.99
78	A	ARG	NH1	352	A	ASP	OD1	1	3.10	3.61	53.56	999.99
78	A	ARG	NH1	352	A	ASP	OD1	2	3.10	2.12	155.09	999.99
78	A	ARG	NH1	352	A	ASP	OD2	1	3.47	4.40	24.16	999.99
78	A	ARG	NH1	352	A	ASP	OD2	2	3.47	2.67	132.94	999.99
78	A	ARG	NH2	352	A	ASP	OD2	1	2.92	3.67	39.04	999.99
78	A	ARG	NH2	352	A	ASP	OD2	2	2.92	1.96	158.89	999.99
79	A	ASN	ND2	107	A	MET	SD	1	3.80	2.77	165.78	999.99
79	A	ASN	ND2	107	A	MET	SD	2	3.80	4.27	56.82	999.99
87	A	GLN	NE2	455	A	TYR	OH	1	3.06	3.66	48.16	999.99
87	A	GLN	NE2	455	A	TYR	OH	2	3.06	2.54	110.14	999.99
97	A	ARG	NH1	213	A	GLU	OE1	1	2.86	3.51	43.97	999.99
97	A	ARG	NH1	213	A	GLU	OE1	2	2.86	1.82	168.30	999.99
97	A	ARG	NH2	213	A	GLU	OE1	1	3.46	4.46	17.89	999.99

97	A	ARG	NH2	213	A	GLU	OE1	2	3.46	2.76	127.71	999.99
97	A	ARG	NH2	213	A	GLU	OE2	1	2.93	3.63	42.19	999.99
97	A	ARG	NH2	213	A	GLU	OE2	2	2.93	2.02	149.75	999.99
100	A	LYS	NZ	388	A	GLU	OE1	-	2.96	9.99	999.99	999.99
103	A	HIS	ND1	238	A	GLU	OE1	-	2.85	1.98	158.63	999.99
103	A	HIS	ND1	238	A	GLU	OE2	-	3.31	2.82	114.61	999.99
104	A	ARG	NE	101	A	ASP	OD1	-	2.84	1.90	149.00	999.99
104	A	ARG	NH1	101	A	ASP	OD1	1	3.02	2.16	138.75	999.99
104	A	ARG	NH1	101	A	ASP	OD1	2	3.02	3.93	27.17	999.99
104	A	ARG	NH2	388	A	GLU	OE2	1	2.90	3.61	41.54	999.99
104	A	ARG	NH2	388	A	GLU	OE2	2	2.90	1.92	165.46	999.99
113	A	ASP	OD1	148	A	ASN	ND2	1	2.89	2.32	112.15	999.99
113	A	ASP	OD1	148	A	ASN	ND2	2	2.89	3.25	61.18	999.99
116	A	GLU	OE2	356	A	ASN	ND2	1	2.99	2.50	107.67	999.99
116	A	GLU	OE2	356	A	ASN	ND2	2	2.99	3.41	58.37	999.99
124	A	SER	OG	121	A	ASP	OD1	-	2.84	9.99	999.99	999.99
140	A	TYR	OH	319	A	HIS	ND1	-	2.90	9.99	999.99	999.99
146	A	THR	OG1	148	A	ASN	OD1	-	2.77	9.99	999.99	999.99
147	A	ASP	OD1	150	A	GLN	NE2	1	3.13	3.30	71.86	999.99
147	A	ASP	OD1	150	A	GLN	NE2	2	3.13	3.05	84.35	999.99
148	A	ASN	ND2	113	A	ASP	OD1	1	2.89	3.55	44.35	999.99
148	A	ASN	ND2	113	A	ASP	OD1	2	2.89	1.86	168.98	999.99
148	A	ASN	OD1	146	A	THR	OG1	1	2.77	2.45	95.41	999.99
148	A	ASN	OD1	146	A	THR	OG1	2	2.77	2.30	104.64	999.99
150	A	GLN	NE2	147	A	ASP	OD1	1	3.13	2.73	102.67	999.99
150	A	GLN	NE2	147	A	ASP	OD1	2	3.13	3.10	82.24	999.99
155	A	TRP	NE1	159	A	THR	OG1	-	3.36	3.28	87.30	999.99
164	A	SER	OG	162	A	ASP	OD1	-	2.72	9.99	999.99	999.99
167	A	LYS	NZ	230	A	HIS	NE2	-	3.12	9.99	999.99	999.99
175	A	ASN	OD1	177	A	THR	OG1	1	2.71	2.59	84.93	999.99
175	A	ASN	OD1	177	A	THR	OG1	2	2.71	2.83	72.88	999.99
177	A	THR	OG1	175	A	ASN	OD1	-	2.71	9.99	999.99	999.99
177	A	THR	OG1	678	A	SER	OG	-	3.28	9.99	999.99	999.99
179	A	GLU	OE1	641	A	GLN	NE2	1	3.09	3.43	62.48	999.99
179	A	GLU	OE1	641	A	GLN	NE2	2	3.09	2.28	130.89	999.99
190	A	LYS	NZ	193	A	GLU	OE1	-	2.90	9.99	999.99	999.99
191	A	ARG	NE	187	A	TYR	OH	-	3.47	3.53	78.12	999.99
191	A	ARG	NH2	194	A	GLN	OE1	1	3.37	2.36	158.07	999.99
191	A	ARG	NH2	194	A	GLN	OE1	2	3.37	3.89	51.95	999.99
199	A	ARG	NH2	168	A	TYR	OH	1	3.38	2.35	164.61	999.99
199	A	ARG	NH2	168	A	TYR	OH	2	3.38	3.83	56.82	999.99
199	A	ARG	NH2	193	A	GLU	OE2	1	2.92	3.60	43.31	999.99
199	A	ARG	NH2	193	A	GLU	OE2	2	2.92	2.01	148.28	999.99
199	A	ARG	NE	202	A	GLU	OE1	-	3.12	2.35	130.54	999.99
199	A	ARG	NE	202	A	GLU	OE2	-	2.89	1.90	162.70	999.99

219	A	TRP	NE1	215	A	ASP	OD1	-	3.30	2.72	123.37	999.99
219	A	TRP	NE1	215	A	ASP	OD2	-	3.11	2.56	119.20	999.99
220	A	ARG	NH2	101	A	ASP	OD2	1	2.97	1.95	159.13	999.99
220	A	ARG	NH2	101	A	ASP	OD2	2	2.97	3.42	55.36	999.99
224	A	TRP	NE1	101	A	ASP	OD2	-	3.26	2.49	142.55	999.99
236	A	THR	OG1	238	A	GLU	OE1	-	2.94	9.99	999.99	999.99
238	A	GLU	OE1	103	A	HIS	ND1	1	2.85	1.90	147.38	999.99
238	A	GLU	OE1	103	A	HIS	ND1	2	2.85	3.56	41.94	999.99
238	A	GLU	OE2	103	A	HIS	ND1	1	3.31	2.56	126.76	999.99
238	A	GLU	OE2	103	A	HIS	ND1	2	3.31	4.23	26.54	999.99
243	A	ARG	NH1	442	A	ASP	OD1	1	3.41	3.79	60.82	999.99
243	A	ARG	NH1	442	A	ASP	OD1	2	3.41	2.40	159.79	999.99
243	A	ARG	NH1	442	A	ASP	OD2	1	2.96	3.74	35.97	999.99
243	A	ARG	NH1	442	A	ASP	OD2	2	2.96	2.19	128.58	999.99
243	A	ARG	NH2	442	A	ASP	OD2	1	2.96	3.80	32.67	999.99
243	A	ARG	NH2	442	A	ASP	OD2	2	2.96	2.27	124.83	999.99
243	A	ARG	NH2	446	A	GLU	OE1	1	2.82	1.84	150.25	999.99
243	A	ARG	NH2	446	A	GLU	OE1	2	2.82	3.23	57.36	999.99
245	A	TYR	OH	350	A	ASN	ND2	-	3.34	9.99	999.99	999.99
265	A	ARG	NH1	271	A	ASN	ND2	1	3.32	3.63	64.38	999.99
265	A	ARG	NH1	271	A	ASN	ND2	2	3.32	3.27	83.54	999.99
265	A	ARG	NE	280	A	ASN	OD1	-	2.87	2.02	139.51	999.99
265	A	ARG	NH1	280	A	ASN	OD1	1	2.94	2.05	141.39	999.99
265	A	ARG	NH1	280	A	ASN	OD1	2	2.94	3.82	28.61	999.99
279	A	LYS	NZ	115	A	GLU	OE2	-	3.02	9.99	999.99	999.99
290	A	ARG	NH1	578	A	GLU	OE2	1	2.94	3.80	30.35	999.99
290	A	ARG	NH1	578	A	GLU	OE2	2	2.94	2.03	144.36	999.99
290	A	ARG	NH2	578	A	GLU	OE2	1	2.93	3.83	27.46	999.99
290	A	ARG	NH2	578	A	GLU	OE2	2	2.93	2.07	141.72	999.99
299	A	HIS	NE2	301	A	MET	SD	-	3.85	3.31	121.76	999.99
302	A	HIS	NE2	304	A	GLU	OE2	-	2.98	2.10	160.20	999.99
302	A	HIS	NE2	470	A	HIS	ND1	-	3.47	3.17	101.61	999.99
302	A	HIS	ND1	575	A	TYR	OH	-	3.08	2.23	154.51	999.99
304	A	GLU	OE2	302	A	HIS	NE2	1	2.98	3.65	43.76	999.99
304	A	GLU	OE2	302	A	HIS	NE2	2	2.98	2.10	138.18	999.99
304	A	GLU	OE1	470	A	HIS	NE2	1	3.49	3.95	57.41	999.99
304	A	GLU	OE1	470	A	HIS	NE2	2	3.49	3.43	84.39	999.99
308	A	SER	OG	306	A	ASP	OD1	-	2.75	9.99	999.99	999.99
308	A	SER	OG	306	A	ASP	OD2	-	3.27	9.99	999.99	999.99
311	A	LYS	NZ	309	A	ASP	OD1	-	3.47	9.99	999.99	999.99
316	A	SER	OG	546	A	GLU	OE1	-	3.17	9.99	999.99	999.99
319	A	HIS	ND1	140	A	TYR	OH	-	2.90	2.51	107.76	999.99
319	A	HIS	NE2	675	A	ASP	OD1	-	2.96	2.31	131.03	999.99
319	A	HIS	NE2	675	A	ASP	OD2	-	2.92	2.06	164.04	999.99
326	A	ASN	OD1	378	A	THR	OG1	1	2.78	3.09	63.32	999.99

326	A	ASN	OD1	378	A	THR	OG1	2	2.78	2.21	111.17	999.99
347	A	SER	OG	349	A	ASN	OD1	-	2.68	9.99	999.99	999.99
347	A	SER	OG	359	A	HIS	ND1	-	3.44	9.99	999.99	999.99
349	A	ASN	OD1	347	A	SER	OG	1	2.68	1.91	126.61	999.99
349	A	ASN	OD1	347	A	SER	OG	2	2.68	2.68	78.61	999.99
349	A	ASN	OD1	359	A	HIS	ND1	1	3.23	3.36	73.71	999.99
349	A	ASN	OD1	359	A	HIS	ND1	2	3.23	2.69	110.78	999.99
350	A	ASN	ND2	245	A	TYR	OH	1	3.34	3.53	70.91	999.99
350	A	ASN	ND2	245	A	TYR	OH	2	3.34	3.10	94.18	999.99
350	A	ASN	ND2	355	A	SER	OG	1	3.12	3.25	73.83	999.99
350	A	ASN	ND2	355	A	SER	OG	2	3.12	2.81	97.01	999.99
355	A	SER	OG	350	A	ASN	ND2	-	3.12	9.99	999.99	999.99
356	A	ASN	ND2	66	A	ASP	OD2	1	3.17	2.12	174.96	999.99
356	A	ASN	ND2	66	A	ASP	OD2	2	3.17	3.79	47.13	999.99
356	A	ASN	ND2	116	A	GLU	OE2	1	2.99	3.50	53.32	999.99
356	A	ASN	ND2	116	A	GLU	OE2	2	2.99	1.96	171.11	999.99
357	A	LYS	NZ	84	A	TYR	OH	-	2.95	9.99	999.99	999.99
357	A	LYS	NZ	92	A	GLU	OE2	-	3.15	9.99	999.99	999.99
357	A	LYS	NZ	96	A	ASN	OD1	-	3.17	9.99	999.99	999.99
359	A	HIS	ND1	347	A	SER	OG	-	3.44	3.53	76.92	999.99
359	A	HIS	ND1	349	A	ASN	OD1	-	3.23	2.95	99.23	999.99
368	A	ARG	NH2	332	A	ASN	OD1	1	3.03	3.57	52.05	999.99
368	A	ARG	NH2	332	A	ASN	OD1	2	3.03	2.04	169.11	999.99
368	A	ARG	NE	343	A	ASP	OD2	-	2.87	1.85	168.67	999.99
368	A	ARG	NH1	343	A	ASP	OD1	1	2.97	1.95	166.99	999.99
368	A	ARG	NH1	343	A	ASP	OD1	2	2.97	3.57	48.06	999.99
369	A	THR	OG1	366	A	SER	OG	-	2.94	9.99	999.99	999.99
376	A	ASP	OD1	379	A	ASN	ND2	1	3.10	2.26	134.14	999.99
376	A	ASP	OD1	379	A	ASN	ND2	2	3.10	3.91	34.72	999.99
376	A	ASP	OD2	379	A	ASN	ND2	1	3.09	2.25	134.76	999.99
376	A	ASP	OD2	379	A	ASN	ND2	2	3.09	3.91	34.32	999.99
378	A	THR	OG1	326	A	ASN	OD1	-	2.78	9.99	999.99	999.99
379	A	ASN	ND2	376	A	ASP	OD1	1	3.10	3.86	38.08	999.99
379	A	ASN	ND2	376	A	ASP	OD1	2	3.10	2.11	156.73	999.99
379	A	ASN	ND2	376	A	ASP	OD2	1	3.09	3.63	51.79	999.99
379	A	ASN	ND2	376	A	ASP	OD2	2	3.09	2.30	130.98	999.99
383	A	THR	OG1	213	A	GLU	OE2	-	2.75	9.99	999.99	999.99
387	A	TYR	OH	239	A	GLU	OE1	-	3.12	9.99	999.99	999.99
387	A	TYR	OH	239	A	GLU	OE2	-	3.33	9.99	999.99	999.99
392	A	TYR	OH	443	A	HIS	ND1	-	3.33	9.99	999.99	999.99
397	A	THR	OG1	395	A	GLU	OE2	-	2.75	9.99	999.99	999.99
403	A	ARG	NH1	387	A	TYR	OH	1	3.33	3.34	80.70	999.99
403	A	ARG	NH1	387	A	TYR	OH	2	3.33	3.77	57.67	999.99
404	A	LYS	NZ	411	A	GLU	OE2	-	3.07	9.99	999.99	999.99
408	A	SER	OG	221	A	GLU	OE1	-	2.65	9.99	999.99	999.99

425	A	ARG	NE	433	A	ASP	OD2	-	2.79	1.86	147.38	999.99
425	A	ARG	NH1	433	A	ASP	OD2	1	3.06	2.22	135.90	999.99
425	A	ARG	NH1	433	A	ASP	OD2	2	3.06	3.97	25.57	999.99
436	A	SER	OG	398	A	GLU	OE1	-	3.38	9.99	999.99	999.99
436	A	SER	OG	398	A	GLU	OE2	-	2.68	9.99	999.99	999.99
443	A	HIS	ND1	392	A	TYR	OH	-	3.33	2.64	135.51	999.99
450	A	ARG	NH1	92	A	GLU	OE1	1	2.91	3.66	37.93	999.99
450	A	ARG	NH1	92	A	GLU	OE1	2	2.91	1.90	157.52	999.99
450	A	ARG	NH2	92	A	GLU	OE1	1	3.23	4.19	22.14	999.99
450	A	ARG	NH2	92	A	GLU	OE1	2	3.23	2.44	134.25	999.99
450	A	ARG	NH2	92	A	GLU	OE2	1	3.01	3.58	49.58	999.99
450	A	ARG	NH2	92	A	GLU	OE2	2	3.01	2.21	134.74	999.99
454	A	ARG	NH1	376	A	ASP	OD2	1	3.20	3.71	53.61	999.99
454	A	ARG	NH1	376	A	ASP	OD2	2	3.20	2.17	168.53	999.99
454	A	ARG	NH1	379	A	ASN	ND2	1	3.42	3.06	101.62	999.99
454	A	ARG	NH1	379	A	ASN	ND2	2	3.42	3.09	99.58	999.99
455	A	TYR	OH	87	A	GLN	NE2	-	3.06	9.99	999.99	999.99
457	A	SER	OG	675	A	ASP	OD2	-	2.71	9.99	999.99	999.99
460	A	SER	OG	314	A	TYR	OH	-	2.88	9.99	999.99	999.99
468	A	SER	OG	470	A	HIS	NE2	-	3.38	9.99	999.99	999.99
470	A	HIS	ND1	302	A	HIS	NE2	-	3.47	2.99	115.61	999.99
470	A	HIS	NE2	304	A	GLU	OE1	-	3.49	3.46	84.92	999.99
470	A	HIS	NE2	468	A	SER	OG	-	3.38	2.88	118.09	999.99
472	A	CYS	SG	575	A	TYR	OH	-	3.32	9.99	999.99	999.99
480	A	THR	OG1	482	A	SER	OG	-	2.84	9.99	999.99	999.99
481	A	ARG	NH2	422	A	GLU	OE1	1	2.96	1.97	151.92	999.99
481	A	ARG	NH2	422	A	GLU	OE1	2	2.96	3.29	62.34	999.99
484	A	ARG	NE	432	A	GLN	OE1	-	3.26	2.55	126.05	999.99
484	A	ARG	NH1	432	A	GLN	OE1	1	2.96	2.00	151.22	999.99
484	A	ARG	NH1	432	A	GLN	OE1	2	2.96	3.73	37.17	999.99
484	A	ARG	NH1	433	A	ASP	OD1	1	3.43	3.92	55.12	999.99
484	A	ARG	NH1	433	A	ASP	OD1	2	3.43	2.40	168.35	999.99
484	A	ARG	NH1	433	A	ASP	OD2	1	3.15	4.02	29.72	999.99
484	A	ARG	NH1	433	A	ASP	OD2	2	3.15	2.31	136.46	999.99
484	A	ARG	NH2	433	A	ASP	OD2	1	2.95	3.79	32.57	999.99
484	A	ARG	NH2	433	A	ASP	OD2	2	2.95	2.07	144.48	999.99
495	A	ARG	NH1	477	A	GLU	OE1	1	2.97	3.79	33.69	999.99
495	A	ARG	NH1	477	A	GLU	OE1	2	2.97	2.01	152.49	999.99
495	A	ARG	NH2	477	A	GLU	OE1	1	3.11	4.03	25.87	999.99
495	A	ARG	NH2	477	A	GLU	OE1	2	3.11	2.26	141.14	999.99
505	A	ARG	NH2	502	A	GLU	OE1	1	3.46	3.78	64.51	999.99
505	A	ARG	NH2	502	A	GLU	OE1	2	3.46	3.60	74.01	999.99
514	A	ARG	NE	87	A	GLN	OE1	-	3.28	2.45	137.45	999.99
514	A	ARG	NH1	87	A	GLN	OE1	1	3.04	2.05	155.39	999.99
514	A	ARG	NH1	87	A	GLN	OE1	2	3.04	3.82	36.16	999.99

514	A	ARG	NH1	144	A	ASP	OD2	1	3.49	4.43	22.53	999.99
514	A	ARG	NH1	144	A	ASP	OD2	2	3.49	2.69	132.07	999.99
514	A	ARG	NH2	144	A	ASP	OD2	1	2.89	3.63	39.33	999.99
514	A	ARG	NH2	144	A	ASP	OD2	2	2.89	1.90	165.71	999.99
515	A	LYS	NZ	315	A	GLN	OE1	-	3.01	9.99	999.99	999.99
515	A	LYS	NZ	318	A	ASP	OD2	-	3.00	9.99	999.99	999.99
559	A	GLU	OE1	615	A	HIS	NE2	1	2.82	1.84	151.43	999.99
559	A	GLU	OE1	615	A	HIS	NE2	2	2.82	3.48	44.95	999.99
559	A	GLU	OE2	615	A	HIS	NE2	1	3.41	2.68	124.99	999.99
559	A	GLU	OE2	615	A	HIS	NE2	2	3.41	4.36	23.84	999.99
563	A	TYR	OH	592	A	ASN	OD1	-	3.37	9.99	999.99	999.99
563	A	TYR	OH	612	A	ASP	OD2	-	2.71	9.99	999.99	999.99
567	A	ARG	NH2	297	A	GLU	OE2	1	2.87	1.85	158.73	999.99
567	A	ARG	NH2	297	A	GLU	OE2	2	2.87	3.30	56.40	999.99
568	A	ARG	NE	571	A	GLU	OE1	-	3.03	2.22	134.63	999.99
568	A	ARG	NH1	571	A	GLU	OE1	1	2.87	1.94	145.91	999.99
568	A	ARG	NH1	571	A	GLU	OE1	2	2.87	3.68	33.42	999.99
569	A	SER	OG	598	A	GLU	OE2	-	2.73	9.99	999.99	999.99
575	A	TYR	OH	302	A	HIS	ND1	-	3.08	9.99	999.99	999.99
592	A	ASN	OD1	563	A	TYR	OH	1	3.37	3.03	99.10	999.99
592	A	ASN	OD1	563	A	TYR	OH	2	3.37	3.77	60.46	999.99
592	A	ASN	OD1	612	A	ASP	OD2	1	2.12	1.57	105.11	999.99
592	A	ASN	OD1	612	A	ASP	OD2	2	2.12	2.05	78.65	999.99
606	A	GLN	NE2	639	A	ASP	OD1	1	2.97	3.57	48.10	999.99
606	A	GLN	NE2	639	A	ASP	OD1	2	2.97	1.96	162.77	999.99
606	A	GLN	NE2	639	A	ASP	OD2	1	3.46	4.14	43.96	999.99
606	A	GLN	NE2	639	A	ASP	OD2	2	3.46	2.59	140.17	999.99
611	A	ARG	NE	607	A	HIS	NE2	-	3.24	2.59	121.17	999.99
612	A	ASP	OD2	592	A	ASN	OD1	1	2.12	1.42	115.66	999.99
612	A	ASP	OD2	592	A	ASN	OD1	2	2.12	2.22	70.59	999.99
613	A	LYS	NZ	650	A	GLU	OE1	-	3.12	9.99	999.99	999.99
613	A	LYS	NZ	650	A	GLU	OE2	-	2.97	9.99	999.99	999.99
615	A	HIS	NE2	559	A	GLU	OE1	-	2.82	1.93	162.40	999.99
615	A	HIS	NE2	559	A	GLU	OE2	-	3.41	2.89	116.70	999.99
615	A	HIS	ND1	618	A	GLN	OE1	-	2.88	2.01	157.12	999.99
618	A	GLN	OE1	615	A	HIS	ND1	1	2.88	2.91	77.49	999.99
618	A	GLN	OE1	615	A	HIS	ND1	2	2.88	2.06	131.05	999.99
638	A	ARG	NH2	179	A	GLU	OE1	1	2.85	3.23	59.86	999.99
638	A	ARG	NH2	179	A	GLU	OE1	2	2.85	1.91	153.37	999.99
638	A	ARG	NH2	641	A	GLN	OE1	1	2.91	1.95	148.39	999.99
638	A	ARG	NH2	641	A	GLN	OE1	2	2.91	3.29	59.43	999.99
639	A	ASP	OD1	606	A	GLN	NE2	1	2.97	2.12	135.07	999.99
639	A	ASP	OD1	606	A	GLN	NE2	2	2.97	3.62	46.10	999.99
639	A	ASP	OD2	606	A	GLN	NE2	1	3.46	2.79	121.16	999.99
639	A	ASP	OD2	606	A	GLN	NE2	2	3.46	4.36	28.24	999.99

641	A	GLN	NE2	179	A	GLU	OE1	1	3.09	2.06	165.06	999.99
641	A	GLN	NE2	179	A	GLU	OE1	2	3.09	3.58	54.40	999.99
641	A	GLN	NE2	645	A	TYR	OH	1	3.29	3.80	53.73	999.99
641	A	GLN	NE2	645	A	TYR	OH	2	3.29	2.97	98.87	999.99
645	A	TYR	OH	641	A	GLN	NE2	-	3.29	9.99	999.99	999.99
673	A	SER	OG	142	A	GLU	OE1	-	3.22	9.99	999.99	999.99
675	A	ASP	OD1	319	A	HIS	NE2	1	2.96	2.13	133.71	999.99
675	A	ASP	OD1	319	A	HIS	NE2	2	2.96	3.81	31.77	999.99
675	A	ASP	OD2	319	A	HIS	NE2	1	2.92	2.06	135.31	999.99
675	A	ASP	OD2	319	A	HIS	NE2	2	2.92	3.74	34.02	999.99

Dd-a = Distance Between Donor and Acceptor
Dh-a = Distance Between Hydrogen and Acceptor
A(d-H-N) = Angle Between Donor-H-N
A(a-O=C) = Angle Between Acceptor-O=C
MO = Multiple Occupancy
Note that angles that are undefined are written as 999.99

Intraprotein Ionic Interactions


[help]

Rasmol **Jmol**

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Ionic Interactions within 6 Angstroms

Position	Residue	Chain	Position	Residue	Chain
65	LYS	A	151	ASP	A
66	ASP	A	72	LYS	A
71	GLU	A	75	LYS	A
72	LYS	A	354	GLU	A
74	LYS	A	127	GLU	A
78	ARG	A	352	ASP	A
92	GLU	A	357	LYS	A
92	GLU	A	450	ARG	A
93	GLU	A	382	ARG	A
93	GLU	A	450	ARG	A
97	ARG	A	213	GLU	A
100	LYS	A	388	GLU	A

100	LYS	A	446	GLU	A
101	ASP	A	104	ARG	A
101	ASP	A	220	ARG	A
103	HIS	A	238	GLU	A
104	ARG	A	388	GLU	A
108	ARG	A	238	GLU	A
115	GLU	A	279	LYS	A
116	GLU	A	279	LYS	A
142	GLU	A	180	HIS	A
144	ASP	A	514	ARG	A
147	ASP	A	514	ARG	A
176	LYS	A	207	ASP	A
179	GLU	A	638	ARG	A
179	GLU	A	664	LYS	A
189	ASP	A	199	ARG	A
190	LYS	A	193	GLU	A
193	GLU	A	199	ARG	A
199	ARG	A	202	GLU	A
209	ASP	A	634	ARG	A
213	GLU	A	382	ARG	A
214	GLU	A	413	LYS	A
220	ARG	A	221	GLU	A
220	ARG	A	239	GLU	A
239	GLU	A	403	ARG	A
243	ARG	A	442	ASP	A
243	ARG	A	446	GLU	A
254	ASP	A	257	LYS	A
262	GLU	A	267	LYS	A
277	ASP	A	279	LYS	A
290	ARG	A	304	GLU	A
290	ARG	A	577	GLU	A
290	ARG	A	578	GLU	A
297	GLU	A	567	ARG	A
297	GLU	A	597	ARG	A
298	ARG	A	572	ASP	A
302	HIS	A	304	GLU	A
304	GLU	A	470	HIS	A
309	ASP	A	311	LYS	A
318	ASP	A	515	LYS	A
318	ASP	A	519	ARG	A
319	HIS	A	675	ASP	A
327	ASP	A	487	LYS	A
341	ASP	A	368	ARG	A
343	ASP	A	368	ARG	A
376	ASP	A	454	ARG	A

388	GLU	A	443	HIS	A
400	GLU	A	404	LYS	A
404	LYS	A	411	GLU	A
422	GLU	A	424	ARG	A
422	GLU	A	481	ARG	A
425	ARG	A	433	ASP	A
433	ASP	A	484	ARG	A
443	HIS	A	446	GLU	A
463	LYS	A	546	GLU	A
477	GLU	A	487	LYS	A
477	GLU	A	495	ARG	A
498	GLU	A	505	ARG	A
502	GLU	A	505	ARG	A
523	LYS	A	556	GLU	A
559	GLU	A	615	HIS	A
568	ARG	A	571	GLU	A
570	ASP	A	576	ARG	A
576	ARG	A	577	GLU	A
613	LYS	A	646	ASP	A
613	LYS	A	650	GLU	A
646	ASP	A	656	HIS	A
661	ASP	A	664	LYS	A

Intraprotein Aromatic-Aromatic Interactions

  [help]

Rasmol **Jmol**

DOG_POR_E315Q_snapshot10.pdb

Aromatic-Aromatic Interactions within 4.5 and 7 Angstroms

Position	Residue	Chain	Position	Residue	Chain	D(centroid-centroid)	Dihedral Angle
69	PHE	A	117	TYR	A	6.06	82.95
69	PHE	A	83	PHE	A	5.02	108.29
83	PHE	A	117	TYR	A	6.73	111.51
83	PHE	A	135	PHE	A	6.19	18.50
105	TYR	A	224	TRP	A	4.87	15.73
135	PHE	A	152	PHE	A	5.40	168.19
140	TYR	A	455	TYR	A	5.81	110.78

152	PHE	A	155	TRP	A	6.46	167.61
153	TYR	A	187	TYR	A	4.89	80.98
171	PHE	A	201	PHE	A	5.50	27.38
171	PHE	A	219	TRP	A	6.43	63.51
171	PHE	A	223	PHE	A	5.37	84.83
201	PHE	A	219	TRP	A	6.21	86.61
201	PHE	A	223	PHE	A	5.92	92.13
223	PHE	A	224	TRP	A	4.82	67.12
259	TYR	A	374	TYR	A	6.38	89.55
276	PHE	A	282	PHE	A	4.98	115.49
323	TYR	A	512	PHE	A	5.59	39.63
361	PHE	A	374	TYR	A	6.50	160.54
373	TYR	A	374	TYR	A	6.18	42.76
419	TRP	A	434	TYR	A	4.80	133.51
455	TYR	A	512	PHE	A	6.33	88.77
518	PHE	A	540	PHE	A	5.92	142.80
518	PHE	A	543	PHE	A	5.85	126.26
518	PHE	A	628	TYR	A	4.98	76.95
540	PHE	A	543	PHE	A	5.10	86.65
540	PHE	A	628	TYR	A	6.80	121.59
543	PHE	A	628	TYR	A	5.02	95.58
564	TYR	A	573	TYR	A	5.57	34.76
573	TYR	A	595	PHE	A	5.96	54.75
617	TRP	A	662	TYR	A	5.63	54.86
644	PHE	A	672	TYR	A	5.75	88.69

Intraprotein Aromatic-Sulphur Interactions

  [help]

Rasmol **Jmol**

DOG_POR_E315Q_snapshot10.pdb

Aromatic-Sulphur Interactions within 5.3 Angstroms

Position	Residue	Chain	Position	Residue	Chain	D(Centroid-Sulphur)	Angle
105	TYR	A	228	CYS	A	4.89	130.20
153	TYR	A	184	MET	A	4.92	144.25
181	PHE	A	205	MET	A	4.67	53.75
231	PHE	A	107	MET	A	5.29	154.78

323	TYR	A	263	MET	A	4.57	149.53
361	PHE	A	363	CYS	A	4.28	40.30
367	TYR	A	346	MET	A	4.52	28.79
374	TYR	A	263	MET	A	4.97	90.27
540	PHE	A	530	MET	A	4.33	131.44
543	PHE	A	530	MET	A	4.48	57.54
573	TYR	A	566	CYS	A	4.73	39.37
575	TYR	A	472	CYS	A	5.24	84.91
595	PHE	A	566	CYS	A	4.84	67.46
677	TRP	A	630	CYS	A	4.72	108.24

Intraprotein Cation-Pi Interactions

  [help]

Rasmol **Jmol**

DOG_POR_E315Q_snapshot10.pdb

Cation-Pi Interactions within 6 Angstroms

Position	Residue	Chain	Position	Residue	Chain	D(cation-Pi)	Angle
84	TYR	A	357	LYS	A	4.50	121.76
94	PHE	A	97	ARG	A	5.66	79.10
117	TYR	A	72	LYS	A	5.27	92.53
140	TYR	A	514	ARG	A	3.48	164.47
216	PHE	A	97	ARG	A	4.55	133.29
231	PHE	A	167	LYS	A	4.80	50.54
387	TYR	A	403	ARG	A	3.81	29.24
419	TRP	A	425	ARG	A	5.10	119.39
493	TRP	A	497	LYS	A	4.62	133.61
575	TYR	A	290	ARG	A	5.30	53.48

D570E

Intraprotein Hydrophobic Interactions

DOG_POR_D570E_snapshot10.pdb

  [help]

Rasmol **Jmol**

Hydrophobic Interactions within 5 Angstroms

Position	Residue	Chain	Position	Residue	Chain
60	MET	A	64	ALA	A
69	PHE	A	117	TYR	A
69	PHE	A	119	LEU	A
69	PHE	A	122	LEU	A
69	PHE	A	125	LEU	A
69	PHE	A	70	VAL	A
69	PHE	A	73	MET	A
69	PHE	A	81	ILE	A
69	PHE	A	83	PHE	A
70	VAL	A	125	LEU	A
70	VAL	A	128	ILE	A
73	MET	A	110	MET	A
73	MET	A	125	LEU	A
73	MET	A	128	ILE	A
73	MET	A	81	ILE	A
80	ILE	A	102	ALA	A
80	ILE	A	107	MET	A
80	ILE	A	132	LEU	A
80	ILE	A	134	VAL	A
80	ILE	A	224	TRP	A
80	ILE	A	82	VAL	A
81	ILE	A	110	MET	A
81	ILE	A	112	ALA	A
81	ILE	A	125	LEU	A
81	ILE	A	133	ALA	A
81	ILE	A	83	PHE	A
82	VAL	A	111	ALA	A
82	VAL	A	134	VAL	A

82	VAL	A	95	ALA	A
82	VAL	A	98	LEU	A
83	PHE	A	112	ALA	A
83	PHE	A	114	PRO	A
83	PHE	A	117	TYR	A
83	PHE	A	119	LEU	A
83	PHE	A	122	LEU	A
83	PHE	A	135	PHE	A
83	PHE	A	137	MET	A
84	TYR	A	111	ALA	A
84	TYR	A	114	PRO	A
84	TYR	A	91	ALA	A
84	TYR	A	95	ALA	A
91	ALA	A	138	ALA	A
91	ALA	A	173	LEU	A
91	ALA	A	94	PHE	A
94	PHE	A	173	LEU	A
94	PHE	A	212	LEU	A
94	PHE	A	216	PHE	A
95	ALA	A	111	ALA	A
98	LEU	A	134	VAL	A
98	LEU	A	171	PHE	A
98	LEU	A	216	PHE	A
98	LEU	A	223	PHE	A
98	LEU	A	224	TRP	A
102	ALA	A	107	MET	A
102	ALA	A	224	TRP	A
105	TYR	A	107	MET	A
105	TYR	A	224	TRP	A
105	TYR	A	233	VAL	A
105	TYR	A	235	ALA	A
107	MET	A	227	VAL	A
107	MET	A	231	PHE	A
107	MET	A	233	VAL	A
112	ALA	A	117	TYR	A
114	PRO	A	119	LEU	A
114	PRO	A	137	MET	A
114	PRO	A	152	PHE	A
117	TYR	A	119	LEU	A
119	LEU	A	122	LEU	A
119	LEU	A	135	PHE	A
119	LEU	A	152	PHE	A
119	LEU	A	155	TRP	A
120	ALA	A	155	TRP	A
120	ALA	A	161	VAL	A

122	LEU	A	125	LEU	A
122	LEU	A	133	ALA	A
122	LEU	A	135	PHE	A
122	LEU	A	155	TRP	A
122	LEU	A	163	LEU	A
122	LEU	A	166	VAL	A
122	LEU	A	192	LEU	A
125	LEU	A	126	PRO	A
125	LEU	A	128	ILE	A
125	LEU	A	133	ALA	A
125	LEU	A	166	VAL	A
126	PRO	A	166	VAL	A
132	LEU	A	134	VAL	A
132	LEU	A	169	ALA	A
132	LEU	A	200	ILE	A
132	LEU	A	223	PHE	A
132	LEU	A	227	VAL	A
132	LEU	A	231	PHE	A
133	ALA	A	135	PHE	A
133	ALA	A	166	VAL	A
133	ALA	A	168	TYR	A
134	VAL	A	169	ALA	A
134	VAL	A	171	PHE	A
134	VAL	A	223	PHE	A
135	PHE	A	137	MET	A
135	PHE	A	152	PHE	A
135	PHE	A	168	TYR	A
135	PHE	A	170	VAL	A
135	PHE	A	188	VAL	A
135	PHE	A	192	LEU	A
137	MET	A	152	PHE	A
137	MET	A	184	MET	A
137	MET	A	188	VAL	A
138	ALA	A	173	LEU	A
140	TYR	A	455	TYR	A
145	PRO	A	149	ALA	A
145	PRO	A	153	TYR	A
145	PRO	A	184	MET	A
149	ALA	A	152	PHE	A
149	ALA	A	184	MET	A
152	PHE	A	155	TRP	A
152	PHE	A	156	LEU	A
152	PHE	A	184	MET	A
152	PHE	A	188	VAL	A
153	TYR	A	184	MET	A

153	TYR	A	187	TYR	A
155	TRP	A	156	LEU	A
155	TRP	A	161	VAL	A
155	TRP	A	163	LEU	A
155	TRP	A	195	LEU	A
156	LEU	A	187	TYR	A
156	LEU	A	188	VAL	A
156	LEU	A	192	LEU	A
156	LEU	A	195	LEU	A
161	VAL	A	163	LEU	A
163	LEU	A	166	VAL	A
163	LEU	A	192	LEU	A
163	LEU	A	195	LEU	A
163	LEU	A	197	ALA	A
166	VAL	A	197	ALA	A
168	TYR	A	170	VAL	A
168	TYR	A	192	LEU	A
168	TYR	A	197	ALA	A
169	ALA	A	201	PHE	A
169	ALA	A	223	PHE	A
170	VAL	A	188	VAL	A
170	VAL	A	192	LEU	A
170	VAL	A	203	LEU	A
171	PHE	A	201	PHE	A
171	PHE	A	216	PHE	A
171	PHE	A	219	TRP	A
171	PHE	A	223	PHE	A
173	LEU	A	212	LEU	A
178	TYR	A	633	ALA	A
178	TYR	A	674	LEU	A
178	TYR	A	676	VAL	A
181	PHE	A	205	MET	A
184	MET	A	188	VAL	A
187	TYR	A	188	VAL	A
188	VAL	A	192	LEU	A
192	LEU	A	195	LEU	A
192	LEU	A	197	ALA	A
200	ILE	A	201	PHE	A
200	ILE	A	231	PHE	A
201	PHE	A	219	TRP	A
201	PHE	A	223	PHE	A
201	PHE	A	226	ALA	A
203	LEU	A	205	MET	A
205	MET	A	219	TRP	A
216	PHE	A	217	ILE	A

223	PHE	A	224	TRP	A
223	PHE	A	227	VAL	A
224	TRP	A	225	PRO	A
224	TRP	A	227	VAL	A
227	VAL	A	231	PHE	A
227	VAL	A	233	VAL	A
231	PHE	A	233	VAL	A
245	TYR	A	348	LEU	A
245	TYR	A	360	PRO	A
247	LEU	A	249	VAL	A
247	LEU	A	346	MET	A
247	LEU	A	348	LEU	A
247	LEU	A	367	TYR	A
249	VAL	A	344	VAL	A
253	ILE	A	258	VAL	A
253	ILE	A	345	VAL	A
253	ILE	A	364	PRO	A
255	MET	A	258	VAL	A
255	MET	A	260	VAL	A
255	MET	A	345	VAL	A
258	VAL	A	260	VAL	A
258	VAL	A	345	VAL	A
258	VAL	A	364	PRO	A
259	TYR	A	266	LEU	A
259	TYR	A	362	PRO	A
259	TYR	A	364	PRO	A
259	TYR	A	374	TYR	A
263	MET	A	269	TYR	A
263	MET	A	281	PRO	A
263	MET	A	323	TYR	A
263	MET	A	373	TYR	A
263	MET	A	374	TYR	A
269	TYR	A	281	PRO	A
269	TYR	A	283	LEU	A
269	TYR	A	510	PRO	A
274	PRO	A	275	PRO	A
274	PRO	A	276	PHE	A
276	PHE	A	282	PHE	A
276	PHE	A	312	LEU	A
278	ALA	A	323	TYR	A
278	ALA	A	512	PHE	A
281	PRO	A	323	TYR	A
281	PRO	A	510	PRO	A
281	PRO	A	512	PHE	A
282	PHE	A	284	ALA	A

282	PHE	A	307	ILE	A
282	PHE	A	312	LEU	A
282	PHE	A	511	MET	A
283	LEU	A	508	LEU	A
283	LEU	A	510	PRO	A
284	ALA	A	305	LEU	A
284	ALA	A	307	ILE	A
284	ALA	A	511	MET	A
285	ALA	A	500	ALA	A
285	ALA	A	508	LEU	A
286	VAL	A	303	LEU	A
286	VAL	A	305	LEU	A
286	VAL	A	499	PRO	A
286	VAL	A	507	ALA	A
286	VAL	A	509	VAL	A
292	LEU	A	300	LEU	A
292	LEU	A	574	LEU	A
292	LEU	A	575	TYR	A
300	LEU	A	474	VAL	A
300	LEU	A	574	LEU	A
301	MET	A	303	LEU	A
301	MET	A	473	ALA	A
301	MET	A	475	ALA	A
301	MET	A	494	LEU	A
303	LEU	A	471	ILE	A
303	LEU	A	473	ALA	A
303	LEU	A	494	LEU	A
305	LEU	A	322	VAL	A
305	LEU	A	469	VAL	A
305	LEU	A	509	VAL	A
305	LEU	A	511	MET	A
307	ILE	A	312	LEU	A
307	ILE	A	314	TYR	A
307	ILE	A	469	VAL	A
307	ILE	A	511	MET	A
312	LEU	A	511	MET	A
312	LEU	A	513	VAL	A
314	TYR	A	458	ILE	A
314	TYR	A	469	VAL	A
314	TYR	A	513	VAL	A
320	VAL	A	322	VAL	A
320	VAL	A	456	TYR	A
320	VAL	A	458	ILE	A
320	VAL	A	469	VAL	A
320	VAL	A	471	ILE	A

320	VAL	A	511	MET	A
320	VAL	A	513	VAL	A
321	ALA	A	453	ALA	A
321	ALA	A	455	TYR	A
321	ALA	A	512	PHE	A
322	VAL	A	324	PRO	A
322	VAL	A	456	TYR	A
322	VAL	A	490	ALA	A
322	VAL	A	493	TRP	A
322	VAL	A	494	LEU	A
322	VAL	A	509	VAL	A
322	VAL	A	511	MET	A
323	TYR	A	324	PRO	A
323	TYR	A	453	ALA	A
323	TYR	A	510	PRO	A
323	TYR	A	512	PHE	A
324	PRO	A	451	LEU	A
324	PRO	A	489	VAL	A
324	PRO	A	490	ALA	A
324	PRO	A	493	TRP	A
325	ALA	A	373	TYR	A
325	ALA	A	493	TRP	A
330	LEU	A	377	ILE	A
330	LEU	A	428	LEU	A
331	VAL	A	342	LEU	A
331	VAL	A	371	LEU	A
331	VAL	A	377	ILE	A
334	LEU	A	338	LEU	A
334	LEU	A	371	LEU	A
334	LEU	A	377	ILE	A
334	LEU	A	427	ILE	A
334	LEU	A	428	LEU	A
334	LEU	A	431	LEU	A
334	LEU	A	441	ILE	A
334	LEU	A	444	LEU	A
337	ILE	A	338	LEU	A
337	ILE	A	428	LEU	A
337	ILE	A	431	LEU	A
338	LEU	A	340	ALA	A
338	LEU	A	431	LEU	A
338	LEU	A	439	PRO	A
338	LEU	A	441	ILE	A
338	LEU	A	444	LEU	A
340	ALA	A	342	LEU	A
340	ALA	A	441	ILE	A

342	LEU	A	367	TYR	A
342	LEU	A	371	LEU	A
342	LEU	A	441	ILE	A
344	VAL	A	346	MET	A
344	VAL	A	367	TYR	A
345	VAL	A	364	PRO	A
346	MET	A	361	PHE	A
346	MET	A	367	TYR	A
346	MET	A	370	ALA	A
348	LEU	A	360	PRO	A
348	LEU	A	361	PHE	A
360	PRO	A	361	PHE	A
361	PHE	A	362	PRO	A
361	PHE	A	370	ALA	A
361	PHE	A	374	TYR	A
361	PHE	A	375	LEU	A
362	PRO	A	374	TYR	A
367	TYR	A	441	ILE	A
370	ALA	A	374	TYR	A
370	ALA	A	375	LEU	A
371	LEU	A	375	LEU	A
371	LEU	A	377	ILE	A
371	LEU	A	441	ILE	A
371	LEU	A	448	LEU	A
373	TYR	A	374	TYR	A
374	TYR	A	375	LEU	A
375	LEU	A	377	ILE	A
375	LEU	A	448	LEU	A
377	ILE	A	427	ILE	A
377	ILE	A	448	LEU	A
380	PRO	A	381	PRO	A
380	PRO	A	420	VAL	A
381	PRO	A	385	VAL	A
381	PRO	A	386	LEU	A
381	PRO	A	420	VAL	A
381	PRO	A	427	ILE	A
381	PRO	A	430	ILE	A
381	PRO	A	448	LEU	A
385	VAL	A	386	LEU	A
385	VAL	A	389	LEU	A
385	VAL	A	427	ILE	A
385	VAL	A	444	LEU	A
385	VAL	A	447	LEU	A
385	VAL	A	448	LEU	A
385	VAL	A	449	PRO	A

386	LEU	A	402	LEU	A
386	LEU	A	405	MET	A
386	LEU	A	416	TYR	A
386	LEU	A	420	VAL	A
386	LEU	A	430	ILE	A
387	TYR	A	406	ALA	A
389	LEU	A	392	TYR	A
389	LEU	A	437	LEU	A
389	LEU	A	439	PRO	A
389	LEU	A	440	PRO	A
389	LEU	A	444	LEU	A
389	LEU	A	447	LEU	A
390	ALA	A	402	LEU	A
392	TYR	A	437	LEU	A
392	TYR	A	439	PRO	A
392	TYR	A	440	PRO	A
393	ALA	A	402	LEU	A
393	ALA	A	437	LEU	A
402	LEU	A	405	MET	A
402	LEU	A	430	ILE	A
402	LEU	A	434	TYR	A
402	LEU	A	437	LEU	A
405	MET	A	415	LEU	A
405	MET	A	416	TYR	A
405	MET	A	419	TRP	A
405	MET	A	420	VAL	A
405	MET	A	434	TYR	A
415	LEU	A	419	TRP	A
416	TYR	A	420	VAL	A
416	TYR	A	421	VAL	A
417	LEU	A	421	VAL	A
419	TRP	A	420	VAL	A
419	TRP	A	434	TYR	A
420	VAL	A	421	VAL	A
420	VAL	A	430	ILE	A
427	ILE	A	430	ILE	A
427	ILE	A	431	LEU	A
427	ILE	A	444	LEU	A
427	ILE	A	448	LEU	A
430	ILE	A	434	TYR	A
430	ILE	A	437	LEU	A
431	LEU	A	437	LEU	A
431	LEU	A	439	PRO	A
431	LEU	A	444	LEU	A
434	TYR	A	435	PRO	A

434	TYR	A	437	LEU	A
437	LEU	A	439	PRO	A
439	PRO	A	440	PRO	A
439	PRO	A	444	LEU	A
441	ILE	A	444	LEU	A
444	LEU	A	448	LEU	A
448	LEU	A	449	PRO	A
451	LEU	A	489	VAL	A
453	ALA	A	455	TYR	A
453	ALA	A	512	PHE	A
455	TYR	A	512	PHE	A
456	TYR	A	471	ILE	A
456	TYR	A	473	ALA	A
456	TYR	A	490	ALA	A
456	TYR	A	494	LEU	A
458	ILE	A	469	VAL	A
458	ILE	A	513	VAL	A
459	ALA	A	538	ALA	A
459	ALA	A	541	ILE	A
464	VAL	A	549	TRP	A
469	VAL	A	471	ILE	A
469	VAL	A	511	MET	A
471	ILE	A	494	LEU	A
473	ALA	A	494	LEU	A
474	VAL	A	476	VAL	A
476	VAL	A	478	TYR	A
490	ALA	A	493	TRP	A
490	ALA	A	494	LEU	A
493	TRP	A	494	LEU	A
493	TRP	A	509	VAL	A
493	TRP	A	510	PRO	A
494	LEU	A	509	VAL	A
509	VAL	A	510	PRO	A
509	VAL	A	511	MET	A
511	MET	A	513	VAL	A
518	PHE	A	539	PRO	A
518	PHE	A	540	PHE	A
518	PHE	A	543	PHE	A
518	PHE	A	628	TYR	A
520	LEU	A	521	PRO	A
520	LEU	A	543	PHE	A
521	PRO	A	528	VAL	A
521	PRO	A	543	PHE	A
521	PRO	A	628	TYR	A
524	ALA	A	550	LEU	A

524	ALA	A	557	VAL	A
527	PRO	A	619	LEU	A
527	PRO	A	625	ALA	A
528	VAL	A	530	MET	A
528	VAL	A	543	PHE	A
528	VAL	A	628	TYR	A
529	ILE	A	531	VAL	A
529	ILE	A	561	LEU	A
529	ILE	A	563	TYR	A
529	ILE	A	616	LEU	A
529	ILE	A	619	LEU	A
529	ILE	A	620	ILE	A
529	ILE	A	627	ILE	A
529	ILE	A	644	PHE	A
530	MET	A	540	PHE	A
530	MET	A	543	PHE	A
530	MET	A	544	ILE	A
530	MET	A	562	LEU	A
530	MET	A	588	LEU	A
530	MET	A	628	TYR	A
531	VAL	A	533	PRO	A
531	VAL	A	563	TYR	A
531	VAL	A	605	VAL	A
531	VAL	A	609	LEU	A
531	VAL	A	629	VAL	A
531	VAL	A	640	VAL	A
531	VAL	A	644	PHE	A
533	PRO	A	605	VAL	A
533	PRO	A	636	MET	A
537	VAL	A	540	PHE	A
537	VAL	A	541	ILE	A
537	VAL	A	562	LEU	A
537	VAL	A	564	TYR	A
537	VAL	A	574	LEU	A
537	VAL	A	575	TYR	A
537	VAL	A	579	LEU	A
538	ALA	A	539	PRO	A
539	PRO	A	540	PHE	A
539	PRO	A	543	PHE	A
540	PHE	A	543	PHE	A
540	PHE	A	562	LEU	A
540	PHE	A	628	TYR	A
541	ILE	A	575	TYR	A
541	ILE	A	579	LEU	A
543	PHE	A	544	ILE	A

543	PHE	A	628	TYR	A
544	ILE	A	562	LEU	A
544	ILE	A	579	LEU	A
544	ILE	A	582	PHE	A
544	ILE	A	588	LEU	A
548	ALA	A	582	PHE	A
549	TRP	A	550	LEU	A
550	LEU	A	557	VAL	A
561	LEU	A	563	TYR	A
561	LEU	A	616	LEU	A
561	LEU	A	619	LEU	A
562	LEU	A	564	TYR	A
562	LEU	A	579	LEU	A
562	LEU	A	588	LEU	A
562	LEU	A	591	LEU	A
563	TYR	A	605	VAL	A
563	TYR	A	608	LEU	A
563	TYR	A	609	LEU	A
563	TYR	A	616	LEU	A
564	TYR	A	573	TYR	A
564	TYR	A	574	LEU	A
564	TYR	A	579	LEU	A
564	TYR	A	593	VAL	A
573	TYR	A	579	LEU	A
573	TYR	A	591	LEU	A
573	TYR	A	593	VAL	A
573	TYR	A	595	PHE	A
574	LEU	A	575	TYR	A
575	TYR	A	579	LEU	A
579	LEU	A	582	PHE	A
579	LEU	A	588	LEU	A
579	LEU	A	591	LEU	A
582	PHE	A	588	LEU	A
588	LEU	A	591	LEU	A
591	LEU	A	593	VAL	A
593	VAL	A	595	PHE	A
594	ALA	A	603	VAL	A
594	ALA	A	608	LEU	A
603	VAL	A	608	LEU	A
605	VAL	A	608	LEU	A
605	VAL	A	636	MET	A
605	VAL	A	640	VAL	A
609	LEU	A	616	LEU	A
609	LEU	A	640	VAL	A
609	LEU	A	644	PHE	A

609	LEU	A	647	ILE	A
616	LEU	A	620	ILE	A
616	LEU	A	644	PHE	A
616	LEU	A	647	ILE	A
617	TRP	A	620	ILE	A
617	TRP	A	647	ILE	A
617	TRP	A	648	VAL	A
617	TRP	A	651	VAL	A
617	TRP	A	662	TYR	A
620	ILE	A	627	ILE	A
620	ILE	A	644	PHE	A
620	ILE	A	647	ILE	A
620	ILE	A	648	VAL	A
620	ILE	A	662	TYR	A
620	ILE	A	666	LEU	A
627	ILE	A	629	VAL	A
627	ILE	A	644	PHE	A
627	ILE	A	666	LEU	A
627	ILE	A	672	TYR	A
629	VAL	A	636	MET	A
629	VAL	A	637	ALA	A
629	VAL	A	640	VAL	A
629	VAL	A	644	PHE	A
629	VAL	A	672	TYR	A
629	VAL	A	674	LEU	A
629	VAL	A	676	VAL	A
633	ALA	A	676	VAL	A
636	MET	A	637	ALA	A
636	MET	A	640	VAL	A
637	ALA	A	674	LEU	A
637	ALA	A	676	VAL	A
640	VAL	A	644	PHE	A
644	PHE	A	647	ILE	A
644	PHE	A	663	ILE	A
644	PHE	A	672	TYR	A
645	TYR	A	659	ALA	A
645	TYR	A	660	VAL	A
645	TYR	A	663	ILE	A
647	ILE	A	648	VAL	A
647	ILE	A	651	VAL	A
648	VAL	A	654	MET	A
648	VAL	A	659	ALA	A
648	VAL	A	662	TYR	A
648	VAL	A	663	ILE	A
649	ALA	A	654	MET	A

649	ALA	A	659	ALA	A
654	MET	A	659	ALA	A
654	MET	A	662	TYR	A
662	TYR	A	663	ILE	A
662	TYR	A	666	LEU	A
663	ILE	A	666	LEU	A
663	ILE	A	667	MET	A
663	ILE	A	672	TYR	A
666	LEU	A	672	TYR	A
667	MET	A	672	TYR	A
667	MET	A	674	LEU	A
672	TYR	A	674	LEU	A
674	LEU	A	676	VAL	A

NO INTRAPROTEIN DISULPHIDE BRIDGES FOUND

Intraprotein Main Chain-Main Chain Hydrogen Bonds


Rasmol **Jmol** **[help]**

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DOG_POR_D570E_snapshot10.pdb

DONOR PARAMETERS				ACCEPTOR							
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**Dd-a**	**Dh-a**	**A(d-H-N)**	**A(a-O=C)**
63	A	S	N	61	A	T	O	3.29	3.19	86.86	73.52
64	A	A	N	61	A	T	O	3.13	2.21	155.70	109.19
66	A	D	N	116	A	E	O	2.86	1.86	175.41	171.76
69	A	F	N	67	A	S	O	3.19	3.44	67.09	106.70
71	A	E	N	68	A	S	O	3.47	2.94	115.84	101.52
72	A	K	N	68	A	S	O	3.00	2.13	148.07	146.97
72	A	K	N	69	A	F	O	3.25	2.77	111.14	97.64
72	A	K	N	70	A	V	O	3.41	3.52	75.40	72.55

73	A	M	N	69	A	F	O	2.88	2.00	148.68	149.13
73	A	M	N	70	A	V	O	3.15	2.62	113.97	105.98
73	A	M	N	71	A	E	O	3.34	3.46	75.22	74.70
74	A	K	N	70	A	V	O	2.89	2.01	150.52	158.23
74	A	K	N	71	A	E	O	3.14	2.59	115.84	108.36
74	A	K	N	72	A	K	O	3.50	3.58	77.11	73.47
75	A	K	N	71	A	E	O	2.89	1.95	158.20	162.26
75	A	K	N	72	A	K	O	3.38	2.86	113.59	104.89
75	A	K	N	73	A	M	O	3.48	3.55	77.91	72.60
76	A	T	N	72	A	K	O	3.05	2.31	131.67	153.24
76	A	T	N	73	A	M	O	3.29	2.55	132.62	104.99
76	A	T	N	74	A	K	O	3.28	3.19	86.88	74.44
77	A	G	N	73	A	M	O	2.89	2.42	108.87	154.81
77	A	G	N	74	A	K	O	3.17	2.28	149.69	105.52
78	A	R	N	73	A	M	O	2.90	1.91	178.40	146.80
79	A	N	N	108	A	R	O	2.92	1.95	163.91	151.85
80	A	I	N	108	A	R	O	3.11	2.21	151.21	150.75
81	A	I	N	132	A	L	O	3.23	2.28	163.35	164.65
82	A	V	N	110	A	M	O	2.87	1.94	155.62	152.68
83	A	F	N	134	A	V	O	2.85	1.96	150.53	159.87
84	A	Y	N	112	A	A	O	3.27	2.42	145.15	169.42
85	A	G	N	136	A	C	O	2.88	1.92	164.05	150.96
90	A	T	N	88	A	T	O	3.17	2.78	104.95	85.03
92	A	E	N	89	A	G	O	3.37	2.80	118.03	103.39
92	A	E	N	90	A	T	O	3.41	3.40	82.59	72.07
93	A	E	N	89	A	G	O	3.10	2.26	144.67	153.27
93	A	E	N	90	A	T	O	3.28	2.60	126.51	108.95
93	A	E	N	91	A	A	O	3.41	3.45	79.04	72.74
94	A	F	N	90	A	T	O	2.88	2.01	148.05	156.46
94	A	F	N	91	A	A	O	3.35	2.83	114.16	98.70
95	A	A	N	91	A	A	O	2.95	2.12	141.67	149.43
95	A	A	N	92	A	E	O	3.41	2.77	124.08	98.39
95	A	A	N	93	A	E	O	3.38	3.42	79.77	70.55
96	A	N	N	92	A	E	O	3.41	2.56	145.40	140.01
96	A	N	N	93	A	E	O	3.18	2.60	118.44	105.85
96	A	N	N	94	A	F	O	3.38	3.49	75.54	73.03
97	A	R	N	93	A	E	O	3.01	2.16	146.19	152.17
97	A	R	N	94	A	F	O	3.08	2.52	116.40	105.82
97	A	R	N	95	A	A	O	3.49	3.54	78.78	71.33
98	A	L	N	94	A	F	O	2.95	2.02	156.39	159.45
98	A	L	N	95	A	A	O	3.38	2.84	115.91	104.41
98	A	L	N	96	A	N	O	3.46	3.56	76.01	72.91
99	A	S	N	95	A	A	O	2.96	2.12	142.79	151.91
99	A	S	N	96	A	N	O	3.23	2.65	118.38	102.85
99	A	S	N	97	A	R	O	3.38	3.39	81.25	71.93

100	A	K	N	96	A	N	O	3.00	2.10	153.85	154.24
100	A	K	N	97	A	R	O	3.14	2.59	116.02	109.30
101	A	D	N	97	A	R	O	2.86	2.00	144.83	153.80
101	A	D	N	98	A	L	O	3.18	2.67	112.96	99.44
102	A	A	N	98	A	L	O	2.97	2.10	145.52	152.99
102	A	A	N	99	A	S	O	3.48	2.81	126.01	103.27
102	A	A	N	100	A	K	O	3.29	3.34	78.47	76.02
103	A	H	N	100	A	K	O	3.08	2.32	132.61	119.68
103	A	H	N	101	A	D	O	3.13	3.15	79.89	79.88
103	A	H	N	107	A	M	O	3.49	4.26	34.77	129.26
104	A	R	N	101	A	D	O	2.88	2.08	136.93	124.16
104	A	R	N	102	A	A	O	3.20	3.13	84.69	76.21
105	A	Y	N	102	A	A	O	2.99	2.06	156.40	118.51
105	A	Y	N	103	A	H	O	3.27	2.92	102.32	74.50
106	A	G	N	102	A	A	O	3.42	3.12	99.40	157.98
106	A	G	N	103	A	H	O	3.33	2.39	162.36	110.11
107	A	M	N	102	A	A	O	3.08	2.21	145.19	142.02
110	A	M	N	80	A	I	O	3.08	2.20	146.16	147.76
112	A	A	N	82	A	V	O	2.91	2.03	147.26	132.41
115	A	E	N	113	A	D	O	3.19	3.07	88.60	80.30
116	A	E	N	113	A	D	O	3.05	2.15	152.17	125.61
116	A	E	N	114	A	P	O	3.42	3.26	90.74	69.36
119	A	L	N	117	A	Y	O	3.30	3.04	96.12	95.69
120	A	A	N	118	A	D	O	3.25	2.95	98.92	75.26
121	A	D	N	118	A	D	O	3.31	2.36	161.83	122.82
121	A	D	N	119	A	L	O	3.11	2.96	88.94	74.90
122	A	L	N	119	A	L	O	3.02	2.08	159.01	122.51
122	A	L	N	120	A	A	O	3.19	2.81	104.02	75.20
123	A	G	N	121	A	D	O	3.11	3.07	83.44	77.85
124	A	S	N	121	A	D	O	2.95	2.00	159.52	126.08
124	A	S	N	122	A	L	O	3.06	2.82	94.03	78.85
125	A	L	N	122	A	L	O	3.02	2.07	164.80	123.30
127	A	E	N	124	A	S	O	3.07	2.12	160.16	133.01
127	A	E	N	125	A	L	O	2.95	2.68	95.50	83.98
128	A	I	N	125	A	L	O	2.97	2.00	161.40	136.13
128	A	I	N	126	A	P	O	3.30	3.16	89.23	69.56
131	A	S	N	129	A	E	O	3.15	3.19	79.01	77.88
132	A	L	N	79	A	N	O	3.07	2.12	159.52	161.03
133	A	A	N	167	A	K	O	2.98	2.00	176.51	155.21
134	A	V	N	81	A	I	O	2.85	1.96	148.37	168.08
135	A	F	N	169	A	A	O	3.06	2.22	143.30	146.98
136	A	C	N	83	A	F	O	2.84	1.91	155.91	166.15
137	A	M	N	171	A	F	O	3.04	2.13	153.19	128.66
138	A	A	N	85	A	G	O	2.91	1.94	169.04	141.93
139	A	T	N	173	A	L	O	2.98	2.26	128.55	148.58

140	A	Y	N	144	A	D	O	3.01	2.10	152.54	157.84
143	A	G	N	140	A	Y	O	3.02	2.39	121.67	143.13
143	A	G	N	141	A	G	O	3.15	3.09	84.32	75.26
144	A	D	N	140	A	Y	O	3.33	2.68	123.16	107.77
144	A	D	N	141	A	G	O	3.07	2.15	152.75	121.27
144	A	D	N	142	A	E	O	3.39	3.25	89.64	72.31
148	A	N	N	146	A	T	O	3.22	3.27	78.88	81.07
149	A	A	N	146	A	T	O	2.88	1.97	151.43	124.09
149	A	A	N	147	A	D	O	3.15	2.75	104.17	76.31
150	A	Q	N	146	A	T	O	3.17	2.78	104.88	164.45
150	A	Q	N	147	A	D	O	3.25	2.29	166.12	111.06
151	A	D	N	149	A	A	O	3.42	3.54	75.16	71.84
152	A	F	N	149	A	A	O	3.13	2.51	120.91	102.75
152	A	F	N	150	A	Q	O	3.39	3.37	82.91	72.03
153	A	Y	N	149	A	A	O	2.84	1.91	156.05	158.04
153	A	Y	N	150	A	Q	O	3.41	2.87	115.58	103.67
154	A	D	N	150	A	Q	O	3.03	2.12	155.18	152.12
154	A	D	N	151	A	D	O	3.42	2.92	112.89	99.00
154	A	D	N	152	A	F	O	3.42	3.52	75.70	71.72
155	A	W	N	151	A	D	O	2.83	1.96	146.85	149.24
155	A	W	N	152	A	F	O	3.21	2.72	111.84	102.56
156	A	L	N	152	A	F	O	2.87	1.94	155.82	156.45
156	A	L	N	153	A	Y	O	3.46	2.92	115.20	102.48
156	A	L	N	154	A	D	O	3.38	3.46	76.98	74.68
157	A	Q	N	153	A	Y	O	3.17	2.27	151.91	150.81
157	A	Q	N	154	A	D	O	3.22	2.63	119.23	110.05
157	A	Q	N	155	A	W	O	3.33	3.42	76.76	75.95
158	A	E	N	154	A	D	O	2.89	2.01	146.23	161.94
158	A	E	N	155	A	W	O	3.21	2.60	120.62	108.08
159	A	T	N	155	A	W	O	2.86	2.05	139.58	159.35
162	A	D	N	160	A	D	O	3.42	3.41	82.05	99.46
163	A	L	N	161	A	V	O	3.33	3.07	96.17	96.08
163	A	L	N	195	A	L	O	3.09	2.16	155.42	154.06
164	A	S	N	162	A	D	O	3.49	2.95	115.75	69.92
165	A	G	N	163	A	L	O	3.24	3.44	69.83	106.63
166	A	V	N	163	A	L	O	2.97	2.03	160.34	140.29
166	A	V	N	164	A	S	O	3.45	2.94	113.30	71.58
167	A	K	N	165	A	G	O	3.45	3.44	82.69	96.01
168	A	Y	N	198	A	Q	O	2.87	1.93	160.25	157.03
169	A	A	N	133	A	A	O	2.91	2.06	141.65	160.92
171	A	F	N	135	A	F	O	2.79	1.86	152.65	171.08
172	A	G	N	204	A	G	O	2.97	2.03	161.35	138.47
173	A	L	N	137	A	M	O	3.01	2.08	157.59	118.40
174	A	G	N	206	A	G	O	3.00	2.26	131.57	155.51
177	A	T	N	175	A	N	O	3.18	2.87	98.94	78.61

178	A	Y	N	175	A	N	O	3.20	2.24	161.38	126.86
178	A	Y	N	176	A	K	O	3.26	3.01	95.50	71.23
180	A	H	N	178	A	Y	O	3.21	3.06	89.21	71.80
181	A	F	N	178	A	Y	O	3.31	3.00	99.85	119.68
181	A	F	N	179	A	E	O	3.02	2.18	142.54	81.20
182	A	N	N	180	A	H	O	3.05	2.99	83.55	108.76
183	A	A	N	180	A	H	O	3.16	2.30	146.15	126.60
183	A	A	N	181	A	F	O	3.09	3.16	76.53	78.29
184	A	M	N	182	A	N	O	3.17	3.14	82.57	80.70
185	A	G	N	182	A	N	O	3.09	2.52	117.08	120.53
186	A	K	N	182	A	N	O	2.93	1.98	161.55	167.02
186	A	K	N	183	A	A	O	3.48	3.01	110.61	97.89
186	A	K	N	184	A	M	O	3.38	3.49	75.87	72.67
187	A	Y	N	183	A	A	O	2.89	2.06	141.32	147.76
187	A	Y	N	184	A	M	O	3.19	2.61	118.15	104.40
187	A	Y	N	185	A	G	O	3.42	3.47	79.08	73.04
188	A	V	N	184	A	M	O	3.01	2.08	160.81	158.15
188	A	V	N	185	A	G	O	3.37	2.84	114.80	107.28
189	A	D	N	185	A	G	O	3.00	2.06	162.48	157.03
189	A	D	N	186	A	K	O	3.49	3.04	109.36	101.01
189	A	D	N	187	A	Y	O	3.38	3.52	73.92	73.79
190	A	K	N	186	A	K	O	2.92	2.01	154.28	152.40
190	A	K	N	187	A	Y	O	3.22	2.72	112.24	107.42
190	A	K	N	188	A	V	O	3.44	3.55	75.83	75.41
191	A	R	N	187	A	Y	O	2.82	1.88	160.77	162.95
191	A	R	N	188	A	V	O	3.48	2.96	114.91	105.41
191	A	R	N	189	A	D	O	3.49	3.56	77.74	74.62
192	A	L	N	188	A	V	O	2.97	2.05	158.83	156.31
192	A	L	N	190	A	K	O	3.48	3.56	77.54	73.33
193	A	E	N	189	A	D	O	3.19	2.27	156.22	152.07
193	A	E	N	190	A	K	O	3.26	2.71	115.52	108.40
193	A	E	N	191	A	R	O	3.34	3.45	75.21	74.27
194	A	Q	N	190	A	K	O	2.98	2.07	153.80	155.80
194	A	Q	N	191	A	R	O	3.14	2.64	111.38	107.37
195	A	L	N	191	A	R	O	2.87	1.96	151.10	161.16
195	A	L	N	192	A	L	O	3.31	2.74	117.35	104.36
195	A	L	N	193	A	E	O	3.39	3.43	79.22	74.22
196	A	G	N	192	A	L	O	3.11	2.61	111.36	149.48
196	A	G	N	193	A	E	O	3.02	2.16	144.18	110.67
196	A	G	N	194	A	Q	O	3.23	2.93	98.34	73.38
197	A	A	N	192	A	L	O	2.97	2.06	154.04	150.45
198	A	Q	N	166	A	V	O	2.81	1.84	166.11	164.38
200	A	I	N	168	A	Y	O	2.83	1.87	161.45	168.80
204	A	G	N	170	A	V	O	2.88	1.92	166.04	135.93
204	A	G	N	202	A	E	O	3.14	3.09	83.70	107.80

205	A	M	N	203	A	L	O	3.02	2.46	115.64	93.27
206	A	G	N	172	A	G	O	2.87	1.94	159.33	162.94
206	A	G	N	204	A	G	O	3.07	2.52	115.26	98.17
207	A	D	N	205	A	M	O	3.44	3.46	80.45	100.60
208	A	D	N	174	A	G	O	2.82	1.88	154.16	151.40
210	A	G	N	207	A	D	O	3.43	2.78	123.56	108.57
212	A	L	N	210	A	G	O	3.27	2.93	101.74	94.88
213	A	E	N	211	A	N	O	3.36	3.31	84.41	74.64
214	A	E	N	211	A	N	O	3.35	2.76	119.11	110.99
215	A	D	N	211	A	N	O	3.02	2.15	146.42	155.16
215	A	D	N	212	A	L	O	3.28	2.76	114.44	98.76
215	A	D	N	213	A	E	O	3.44	3.45	81.23	70.54
216	A	F	N	212	A	L	O	2.94	2.14	138.15	149.74
216	A	F	N	213	A	E	O	3.35	2.66	127.60	104.09
216	A	F	N	214	A	E	O	3.27	3.27	81.44	74.56
217	A	I	N	213	A	E	O	3.50	2.68	141.72	146.34
217	A	I	N	214	A	E	O	3.04	2.31	130.35	114.75
217	A	I	N	215	A	D	O	3.38	3.41	80.03	73.05
218	A	T	N	214	A	E	O	3.28	2.36	157.50	158.11
218	A	T	N	215	A	D	O	3.34	2.81	115.08	106.76
218	A	T	N	216	A	F	O	3.47	3.59	75.69	73.15
219	A	W	N	215	A	D	O	3.00	2.09	156.25	157.13
219	A	W	N	216	A	F	O	3.34	2.81	115.09	104.34
219	A	W	N	217	A	I	O	3.40	3.49	76.61	75.08
220	A	R	N	216	A	F	O	2.85	1.97	146.18	156.04
220	A	R	N	217	A	I	O	3.17	2.60	116.44	107.53
221	A	E	N	217	A	I	O	2.93	2.04	149.76	159.93
221	A	E	N	218	A	T	O	3.47	2.86	120.50	101.82
221	A	E	N	219	A	W	O	3.39	3.43	79.28	72.94
222	A	Q	N	218	A	T	O	3.27	2.65	121.36	146.13
222	A	Q	N	219	A	W	O	3.08	2.25	141.84	108.37
222	A	Q	N	220	A	R	O	3.36	3.18	92.00	72.51
223	A	F	N	219	A	W	O	2.89	2.01	146.46	157.88
223	A	F	N	220	A	R	O	3.21	2.65	116.04	104.23
224	A	W	N	220	A	R	O	3.06	2.10	172.23	160.45
226	A	A	N	222	A	Q	O	3.37	2.52	145.34	147.77
226	A	A	N	223	A	F	O	3.01	2.39	120.88	116.91
226	A	A	N	224	A	W	O	3.30	3.36	78.11	75.26
227	A	V	N	223	A	F	O	3.08	2.17	152.05	161.83
227	A	V	N	224	A	W	O	3.19	2.62	116.69	110.59
227	A	V	N	225	A	P	O	3.38	3.47	76.53	73.83
228	A	C	N	224	A	W	O	2.92	2.00	154.86	160.84
228	A	C	N	225	A	P	O	3.18	2.67	112.61	104.48
229	A	E	N	225	A	P	O	2.85	1.92	157.76	159.67
229	A	E	N	226	A	A	O	3.47	2.95	114.21	100.30

229	A	E	N	227	A	V	O	3.44	3.54	76.45	74.36
230	A	H	N	226	A	A	O	3.00	2.15	144.68	150.05
230	A	H	N	227	A	V	O	3.29	2.68	121.13	106.29
230	A	H	N	228	A	C	O	3.47	3.48	81.51	72.81
231	A	F	N	227	A	V	O	2.89	1.95	159.32	161.66
232	A	G	N	228	A	C	O	2.96	2.22	131.57	140.12
233	A	V	N	231	A	F	O	3.35	2.96	104.59	73.68
236	A	T	N	104	A	R	O	2.89	1.92	167.54	158.02
236	A	T	N	234	A	E	O	3.46	3.60	73.95	100.74
239	A	E	N	237	A	G	O	3.28	2.97	99.07	98.74
241	A	S	N	239	A	E	O	2.85	1.93	151.71	96.70
242	A	I	N	240	A	S	O	3.29	3.57	66.07	79.25
246	A	E	N	349	A	N	O	3.09	2.13	162.39	148.12
248	A	V	N	347	A	S	O	2.82	1.85	161.71	157.68
250	A	H	N	345	A	V	O	2.91	1.97	159.79	143.88
256	A	A	N	254	A	D	O	3.09	2.94	89.15	78.47
257	A	K	N	254	A	D	O	2.98	2.02	162.93	129.97
257	A	K	N	255	A	M	O	3.12	2.92	92.42	76.94
258	A	V	N	255	A	M	O	3.16	2.22	156.52	115.82
259	A	Y	N	364	A	P	O	2.82	1.86	163.65	162.36
265	A	R	N	263	A	M	O	3.09	2.67	106.53	104.35
265	A	R	N	279	A	K	O	2.92	2.04	148.00	161.45
267	A	K	N	265	A	R	O	3.23	3.35	74.35	103.17
268	A	S	N	265	A	R	O	3.10	2.32	135.76	124.80
268	A	S	N	266	A	L	O	3.31	3.36	78.57	76.05
269	A	Y	N	267	A	K	O	3.14	3.09	83.62	79.49
270	A	E	N	267	A	K	O	2.91	2.03	147.36	123.17
270	A	E	N	268	A	S	O	3.29	3.08	93.42	73.92
271	A	N	N	267	A	K	O	3.14	2.91	94.11	157.96
271	A	N	N	268	A	S	O	3.10	2.19	150.60	106.26
272	A	Q	N	268	A	S	O	3.35	3.68	63.26	156.77
273	A	K	N	271	A	N	O	2.86	2.03	139.99	95.50
277	A	D	N	280	A	N	O	3.09	2.14	157.66	120.68
279	A	K	N	277	A	D	O	3.14	3.07	84.94	82.79
280	A	N	N	277	A	D	O	2.96	2.06	149.57	122.60
282	A	F	N	511	A	M	O	2.90	1.94	161.08	158.32
284	A	A	N	282	A	F	O	3.42	3.01	106.16	90.28
284	A	A	N	509	A	V	O	2.93	1.96	167.33	140.51
286	A	V	N	507	A	A	O	3.18	2.23	161.46	148.13
287	A	T	N	304	A	E	O	2.89	1.91	174.31	137.70
288	A	T	N	304	A	E	O	3.49	2.58	152.41	122.15
290	A	R	N	302	A	H	O	2.84	1.86	166.53	171.53
292	A	L	N	300	A	L	O	2.81	1.82	175.15	132.48
294	A	Q	N	571	A	E	O	2.84	1.85	173.45	141.44
298	A	R	N	296	A	T	O	3.47	3.61	74.06	74.93

301	A	M	N	473	A	A	O	2.84	1.91	158.49	150.49
302	A	H	N	290	A	R	O	2.83	1.91	151.23	163.77
303	A	L	N	471	A	I	O	3.19	2.25	160.31	133.89
304	A	E	N	288	A	T	O	3.06	2.15	152.87	133.46
305	A	L	N	469	A	V	O	2.87	1.93	155.76	163.83
306	A	D	N	285	A	A	O	2.89	1.91	168.12	162.28
307	A	I	N	467	A	N	O	2.86	1.88	171.83	130.75
309	A	D	N	307	A	I	O	3.34	3.57	68.78	104.98
310	A	S	N	307	A	I	O	3.15	2.25	151.18	133.70
310	A	S	N	308	A	S	O	3.16	2.90	96.14	78.92
312	A	L	N	310	A	S	O	3.19	3.02	90.74	74.71
317	A	G	N	315	A	E	O	3.46	3.76	65.15	102.90
317	A	G	N	458	A	I	O	3.49	2.51	178.23	145.30
318	A	D	N	315	A	E	O	3.21	2.28	157.79	144.82
319	A	H	N	514	A	R	O	2.95	2.02	157.29	167.49
320	A	V	N	456	A	Y	O	2.94	1.95	174.26	173.09
321	A	A	N	512	A	F	O	2.90	1.93	167.96	163.61
322	A	V	N	454	A	R	O	2.88	1.92	162.21	155.13
323	A	Y	N	510	A	P	O	3.08	2.16	155.33	146.79
326	A	N	N	372	A	T	O	2.86	1.88	171.36	158.00
328	A	S	N	326	A	N	O	3.28	3.28	81.50	102.54
329	A	A	N	327	A	D	O	3.15	3.03	87.78	77.90
330	A	L	N	327	A	D	O	3.01	2.26	133.34	124.40
331	A	V	N	327	A	D	O	3.26	2.34	154.64	154.27
331	A	V	N	328	A	S	O	3.37	2.85	113.70	98.87
331	A	V	N	329	A	A	O	3.46	3.50	79.39	69.81
332	A	N	N	328	A	S	O	2.97	2.09	150.70	150.07
332	A	N	N	329	A	A	O	3.32	2.76	117.33	102.42
332	A	N	N	330	A	L	O	3.44	3.55	75.71	72.49
333	A	Q	N	329	A	A	O	3.05	2.14	152.83	151.80
333	A	Q	N	330	A	L	O	3.29	2.76	114.83	104.55
333	A	Q	N	331	A	V	O	3.42	3.49	77.75	74.14
334	A	L	N	330	A	L	O	2.95	2.06	149.52	155.78
334	A	L	N	331	A	V	O	3.26	2.67	118.63	107.77
334	A	L	N	332	A	N	O	3.42	3.47	79.22	72.90
335	A	G	N	331	A	V	O	3.02	2.12	152.82	155.65
335	A	G	N	332	A	N	O	3.19	2.66	114.55	106.19
335	A	G	N	333	A	Q	O	3.44	3.54	76.03	70.53
336	A	E	N	332	A	N	O	2.87	1.96	153.39	157.29
336	A	E	N	333	A	Q	O	3.24	2.75	111.22	102.11
337	A	I	N	333	A	Q	O	2.90	2.04	146.86	156.65
337	A	I	N	335	A	G	O	3.42	3.41	82.73	75.78
338	A	L	N	334	A	L	O	3.28	2.38	153.77	149.82
338	A	L	N	335	A	G	O	3.37	2.75	122.15	110.76
339	A	G	N	335	A	G	O	2.88	2.29	117.66	156.21

339	A	G	N	336	A	E	O	3.27	2.50	134.21	97.85
340	A	A	N	335	A	G	O	3.10	2.32	134.51	150.87
340	A	A	N	338	A	L	O	3.36	3.21	90.32	69.04
343	A	D	N	341	A	D	O	3.38	2.98	105.81	72.76
344	A	V	N	342	A	L	O	3.39	2.94	108.74	70.24
345	A	V	N	343	A	D	O	3.42	3.31	87.83	97.07
346	A	M	N	365	A	T	O	2.91	1.95	162.77	146.38
347	A	S	N	248	A	V	O	2.87	1.95	153.97	142.05
349	A	N	N	246	A	E	O	3.03	2.09	157.73	159.41
350	A	N	N	358	A	K	O	3.03	2.16	146.82	148.96
351	A	L	N	244	A	Q	O	2.87	1.88	177.48	163.24
351	A	L	N	349	A	N	O	3.48	3.51	80.18	99.58
352	A	D	N	350	A	N	O	3.36	3.32	83.75	68.10
353	A	E	N	351	A	L	O	3.04	2.40	121.00	86.88
354	A	E	N	352	A	D	O	3.30	3.16	89.63	76.26
355	A	S	N	352	A	D	O	3.21	2.32	152.06	115.40
357	A	K	N	355	A	S	O	3.48	3.22	97.00	68.94
358	A	K	N	356	A	N	O	2.95	2.18	134.04	88.67
359	A	H	N	357	A	K	O	3.24	3.19	83.53	77.22
361	A	F	N	359	A	H	O	3.45	3.26	91.61	70.97
363	A	C	N	361	A	F	O	3.43	3.72	65.70	106.21
365	A	T	N	346	A	M	O	2.92	1.96	163.04	170.29
367	A	Y	N	342	A	L	O	3.11	2.60	113.59	146.86
367	A	Y	N	344	A	V	O	3.48	2.66	141.91	155.39
368	A	R	N	342	A	L	O	2.92	2.06	145.47	133.76
368	A	R	N	366	A	S	O	3.27	3.29	80.32	73.85
369	A	T	N	366	A	S	O	3.19	2.63	116.67	110.64
369	A	T	N	367	A	Y	O	3.41	3.54	74.31	73.48
370	A	A	N	366	A	S	O	3.01	2.09	156.61	158.89
370	A	A	N	367	A	Y	O	3.22	2.71	112.41	104.41
370	A	A	N	368	A	R	O	3.44	3.52	77.08	73.64
371	A	L	N	367	A	Y	O	2.99	2.03	163.50	159.06
371	A	L	N	368	A	R	O	3.39	2.87	114.22	108.95
371	A	L	N	369	A	T	O	3.43	3.56	74.43	76.24
372	A	T	N	368	A	R	O	2.96	2.12	143.18	157.50
372	A	T	N	369	A	T	O	3.24	2.62	121.45	107.08
372	A	T	N	370	A	A	O	3.43	3.39	83.69	72.80
373	A	Y	N	369	A	T	O	2.88	1.98	152.00	162.60
374	A	Y	N	370	A	A	O	2.94	2.06	149.84	139.87
375	A	L	N	370	A	A	O	2.99	2.25	130.94	160.02
376	A	D	N	449	A	P	O	2.89	1.92	167.08	156.96
377	A	I	N	375	A	L	O	3.04	2.35	126.71	94.41
378	A	T	N	376	A	D	O	3.43	2.89	115.19	67.71
384	A	N	N	382	A	R	O	3.21	3.15	84.39	80.18
385	A	V	N	382	A	R	O	3.09	2.23	145.14	124.98

385	A	V	N	383	A	T	O	3.25	3.15	87.23	76.17
386	A	L	N	383	A	T	O	3.19	2.51	126.08	113.03
387	A	Y	N	383	A	T	O	2.94	2.04	148.68	162.06
388	A	E	N	384	A	N	O	3.04	2.09	165.17	146.23
389	A	L	N	385	A	V	O	3.43	2.72	129.49	138.22
389	A	L	N	387	A	Y	O	3.35	3.11	95.77	72.92
390	A	A	N	386	A	L	O	3.21	2.92	97.79	143.10
390	A	A	N	387	A	Y	O	3.36	2.41	161.75	104.81
391	A	Q	N	389	A	L	O	3.16	3.15	80.98	76.34
392	A	Y	N	389	A	L	O	2.99	2.04	160.90	125.46
392	A	Y	N	390	A	A	O	2.98	2.62	101.15	82.08
393	A	A	N	390	A	A	O	3.01	2.06	162.29	129.87
394	A	S	N	436	A	S	O	3.21	2.28	157.43	115.33
397	A	T	N	395	A	E	O	3.20	3.20	81.60	79.60
398	A	E	N	395	A	E	O	3.08	2.44	121.87	121.08
398	A	E	N	396	A	P	O	3.42	3.51	76.45	72.95
399	A	Q	N	395	A	E	O	2.95	2.02	157.39	162.70
399	A	Q	N	396	A	P	O	3.26	2.79	109.68	100.59
400	A	E	N	396	A	P	O	2.93	2.02	155.76	155.90
400	A	E	N	397	A	T	O	3.49	2.90	119.95	103.14
400	A	E	N	398	A	E	O	3.44	3.53	76.60	75.87
401	A	H	N	397	A	T	O	3.13	2.23	152.72	150.53
401	A	H	N	398	A	E	O	3.27	2.73	115.94	108.06
401	A	H	N	399	A	Q	O	3.47	3.52	78.97	72.03
402	A	L	N	398	A	E	O	3.06	2.14	156.07	158.21
402	A	L	N	399	A	Q	O	3.29	2.73	116.25	107.32
402	A	L	N	400	A	E	O	3.38	3.51	74.72	74.19
403	A	R	N	399	A	Q	O	2.96	2.07	150.11	156.27
403	A	R	N	400	A	E	O	3.30	2.76	115.59	104.02
403	A	R	N	401	A	H	O	3.45	3.49	79.85	73.77
404	A	K	N	400	A	E	O	2.99	2.10	149.23	156.01
404	A	K	N	401	A	H	O	3.30	2.66	122.49	108.37
404	A	K	N	402	A	L	O	3.42	3.44	80.39	72.78
405	A	M	N	401	A	H	O	3.38	2.78	120.31	152.45
405	A	M	N	402	A	L	O	3.27	2.38	151.00	109.48
405	A	M	N	403	A	R	O	3.29	3.06	94.51	75.52
406	A	A	N	404	A	K	O	3.08	2.91	90.29	81.58
407	A	S	N	404	A	K	O	2.98	2.07	155.00	129.06
412	A	G	N	410	A	G	O	3.28	3.19	86.31	73.09
413	A	K	N	410	A	G	O	3.47	2.66	140.34	113.49
413	A	K	N	411	A	E	O	3.35	3.32	83.36	78.21
414	A	E	N	411	A	E	O	3.23	2.58	124.20	115.78
414	A	E	N	412	A	G	O	3.46	3.48	80.40	71.06
415	A	L	N	411	A	E	O	2.86	2.06	136.40	160.55
415	A	L	N	412	A	G	O	3.31	2.69	120.00	97.76

416	A	Y	N	412	A	G	O	2.97	2.08	149.69	149.58
416	A	Y	N	413	A	K	O	3.44	2.84	120.30	99.88
417	A	L	N	413	A	K	O	3.24	2.35	151.53	144.23
417	A	L	N	414	A	E	O	3.34	2.82	113.66	98.83
417	A	L	N	415	A	L	O	3.43	3.52	76.22	72.89
418	A	S	N	414	A	E	O	2.92	2.02	151.40	150.86
418	A	S	N	415	A	L	O	3.37	2.83	115.30	104.57
418	A	S	N	416	A	Y	O	3.49	3.56	77.46	74.23
419	A	W	N	415	A	L	O	2.88	1.93	165.29	158.27
420	A	V	N	416	A	Y	O	3.06	2.24	141.76	142.14
421	A	V	N	416	A	Y	O	3.21	2.30	153.99	155.90
421	A	V	N	417	A	L	O	3.28	2.65	122.38	118.82
422	A	E	N	417	A	L	O	2.84	1.87	175.59	162.44
423	A	A	N	421	A	V	O	3.45	3.35	87.95	69.51
424	A	R	N	420	A	V	O	3.10	2.74	101.24	137.51
424	A	R	N	421	A	V	O	3.07	2.22	142.18	105.65
424	A	R	N	422	A	E	O	3.46	3.14	99.67	65.33
425	A	R	N	420	A	V	O	2.93	2.00	158.39	152.90
425	A	R	N	423	A	A	O	3.36	3.49	74.65	72.93
426	A	H	N	424	A	R	O	3.25	2.65	119.35	93.59
428	A	L	N	426	A	H	O	3.18	3.19	80.70	83.62
429	A	A	N	426	A	H	O	3.00	2.43	116.62	126.29
429	A	A	N	427	A	I	O	3.40	3.53	74.86	73.74
430	A	I	N	426	A	H	O	2.95	2.07	149.60	162.70
430	A	I	N	427	A	I	O	3.21	2.64	117.46	104.17
430	A	I	N	428	A	L	O	3.36	3.40	79.53	74.65
431	A	L	N	427	A	I	O	2.96	2.04	156.84	157.22
431	A	L	N	428	A	L	O	3.15	2.61	114.67	110.97
432	A	Q	N	428	A	L	O	2.93	2.07	145.29	159.60
432	A	Q	N	429	A	A	O	3.42	2.82	119.68	98.67
432	A	Q	N	430	A	I	O	3.27	3.26	81.92	76.01
433	A	D	N	429	A	A	O	3.03	2.22	139.57	150.34
433	A	D	N	430	A	I	O	3.19	2.47	130.29	112.80
434	A	Y	N	430	A	I	O	2.83	2.02	135.44	166.08
436	A	S	N	434	A	Y	O	3.11	2.89	93.97	82.17
437	A	L	N	434	A	Y	O	3.05	2.10	160.13	126.15
438	A	R	N	392	A	Y	O	3.03	2.05	170.71	138.22
438	A	R	N	436	A	S	O	3.33	2.99	101.49	97.18
442	A	D	N	440	A	P	O	3.39	3.42	79.64	75.53
443	A	H	N	440	A	P	O	3.26	2.57	127.65	111.01
443	A	H	N	441	A	I	O	3.40	3.36	84.42	74.49
444	A	L	N	440	A	P	O	3.05	2.13	154.98	158.35
444	A	L	N	441	A	I	O	3.33	2.81	114.22	105.30
445	A	C	N	441	A	I	O	2.92	2.04	147.68	154.99
445	A	C	N	442	A	D	O	3.29	2.76	114.45	97.58

445	A	C	N	443	A	H	O	3.47	3.56	77.10	71.37
446	A	E	N	442	A	D	O	3.01	2.19	141.66	148.57
446	A	E	N	443	A	H	O	3.28	2.63	124.46	105.32
446	A	E	N	444	A	L	O	3.39	3.40	81.31	74.43
447	A	L	N	443	A	H	O	3.15	2.31	143.27	152.71
447	A	L	N	444	A	L	O	3.24	2.57	125.52	109.39
448	A	L	N	444	A	L	O	2.89	1.99	151.02	165.41
451	A	L	N	374	A	Y	O	2.84	1.86	167.70	123.19
454	A	R	N	322	A	V	O	2.87	1.90	165.43	164.71
456	A	Y	N	320	A	V	O	2.89	1.92	162.90	173.39
458	A	I	N	318	A	D	O	2.85	1.90	161.29	169.95
459	A	A	N	457	A	S	O	3.23	3.17	84.66	99.86
459	A	A	N	470	A	H	O	2.89	1.89	172.72	139.99
460	A	S	N	458	A	I	O	3.41	2.70	128.56	72.96
465	A	H	N	461	A	S	O	2.86	1.99	144.21	147.42
467	A	N	N	465	A	H	O	3.23	3.01	93.89	79.48
468	A	S	N	465	A	H	O	3.38	2.43	161.65	109.63
469	A	V	N	305	A	L	O	2.92	1.98	154.39	157.80
471	A	I	N	303	A	L	O	2.90	1.92	166.46	162.40
473	A	A	N	301	A	M	O	2.91	1.99	153.25	149.90
475	A	A	N	299	A	H	O	2.90	1.94	169.28	160.81
476	A	V	N	474	A	V	O	3.39	3.46	78.10	101.13
478	A	Y	N	486	A	N	O	2.97	2.01	168.58	161.29
480	A	T	N	484	A	R	O	2.82	1.85	167.58	173.54
482	A	S	N	480	A	T	O	3.24	3.15	86.44	73.69
483	A	G	N	480	A	T	O	2.93	2.04	149.85	114.50
483	A	G	N	481	A	R	O	3.44	3.18	97.30	69.13
486	A	N	N	478	A	Y	O	2.84	1.86	167.91	171.63
488	A	G	N	476	A	V	O	2.85	1.87	175.91	133.47
489	A	V	N	487	A	K	O	3.50	3.77	66.87	97.95
492	A	S	N	488	A	G	O	3.18	2.24	163.98	147.82
492	A	S	N	490	A	A	O	3.41	3.51	75.59	76.35
493	A	W	N	489	A	V	O	3.41	2.56	143.98	140.80
493	A	W	N	490	A	A	O	3.21	2.70	112.65	106.20
494	A	L	N	490	A	A	O	2.78	1.85	156.81	162.36
495	A	R	N	491	A	T	O	2.96	2.09	145.61	150.01
495	A	R	N	492	A	S	O	3.38	2.85	114.62	98.91
496	A	A	N	492	A	S	O	3.21	2.44	135.06	147.04
496	A	A	N	493	A	W	O	3.41	2.64	135.08	105.58
496	A	A	N	494	A	L	O	3.18	3.14	83.17	76.36
497	A	K	N	494	A	L	O	3.08	2.12	164.52	119.27
497	A	K	N	495	A	R	O	3.46	3.14	100.82	73.75
498	A	E	N	496	A	A	O	3.33	3.06	97.64	102.50
500	A	A	N	286	A	V	O	2.81	1.81	173.73	155.75
501	A	G	N	499	A	P	O	3.00	2.15	143.82	83.73

502	A	E	N	500	A	A	O	3.28	2.69	118.52	80.28
504	A	G	N	502	A	E	O	3.43	3.65	69.31	102.47
505	A	R	N	502	A	E	O	3.13	2.23	149.99	139.77
505	A	R	N	503	A	N	O	3.47	3.05	107.17	69.27
509	A	V	N	284	A	A	O	2.86	1.96	147.86	154.45
511	A	M	N	282	A	F	O	2.88	1.99	148.73	156.48
511	A	M	N	509	A	V	O	3.38	3.40	80.21	100.25
512	A	F	N	321	A	A	O	2.98	2.03	159.39	163.53
514	A	R	N	319	A	H	O	2.92	1.94	171.74	141.98
516	A	S	N	514	A	R	O	3.46	3.58	74.66	99.67
519	A	R	N	517	A	Q	O	3.37	2.79	118.02	70.17
520	A	L	N	316	A	S	O	3.15	2.40	131.85	169.74
524	A	A	N	522	A	F	O	3.31	2.87	108.08	95.68
525	A	A	N	523	A	K	O	3.19	3.05	88.93	77.38
526	A	T	N	523	A	K	O	3.18	2.22	166.26	126.36
526	A	T	N	524	A	A	O	3.15	2.86	98.08	77.61
528	A	V	N	559	A	E	O	2.86	1.90	163.60	162.49
529	A	I	N	626	A	H	O	2.85	1.87	161.45	151.87
530	A	M	N	561	A	L	O	2.89	2.08	138.62	153.87
531	A	V	N	628	A	Y	O	2.86	2.01	142.40	163.84
532	A	G	N	563	A	Y	O	2.92	1.96	167.41	175.69
534	A	G	N	565	A	G	O	3.01	2.05	170.57	157.99
535	A	T	N	533	A	P	O	3.38	3.48	76.31	104.10
536	A	G	N	533	A	P	O	3.07	2.22	144.00	133.41
536	A	G	N	534	A	G	O	3.14	2.90	94.75	77.08
537	A	V	N	532	A	G	O	3.21	3.41	70.30	116.63
537	A	V	N	534	A	G	O	3.26	2.31	161.68	126.13
537	A	V	N	535	A	T	O	3.10	2.76	100.41	78.01
538	A	A	N	535	A	T	O	3.21	2.29	155.55	127.56
538	A	A	N	536	A	G	O	3.26	2.88	103.21	72.20
540	A	F	N	537	A	V	O	3.03	2.28	131.60	132.35
540	A	F	N	538	A	A	O	3.18	3.06	88.07	76.77
541	A	I	N	537	A	V	O	3.34	2.59	134.39	164.58
541	A	I	N	538	A	A	O	3.28	2.44	144.19	115.84
541	A	I	N	539	A	P	O	3.30	3.23	85.67	74.13
542	A	G	N	459	A	A	O	3.42	3.31	88.04	98.13
542	A	G	N	539	A	P	O	3.04	2.43	120.04	116.45
542	A	G	N	540	A	F	O	3.38	3.54	72.54	71.12
543	A	F	N	539	A	P	O	3.01	2.19	139.92	150.70
543	A	F	N	540	A	F	O	3.15	2.58	117.32	99.22
543	A	F	N	541	A	I	O	3.45	3.43	82.60	73.59
544	A	I	N	540	A	F	O	2.99	2.09	152.03	152.70
544	A	I	N	541	A	I	O	3.38	2.73	124.65	109.61
544	A	I	N	542	A	G	O	3.37	3.43	78.52	73.57
545	A	Q	N	541	A	I	O	3.01	2.09	157.60	155.77

545	A	Q	N	542	A	G	O	3.30	2.86	108.27	101.95
546	A	E	N	542	A	G	O	2.93	2.05	148.89	155.70
546	A	E	N	543	A	F	O	3.43	2.80	122.68	101.49
546	A	E	N	544	A	I	O	3.32	3.36	79.13	76.94
547	A	R	N	543	A	F	O	3.03	2.11	156.56	150.77
547	A	R	N	544	A	I	O	3.32	2.83	112.15	108.17
548	A	A	N	544	A	I	O	2.83	1.94	149.65	160.69
548	A	A	N	545	A	Q	O	3.40	2.84	116.69	99.02
548	A	A	N	546	A	E	O	3.42	3.47	78.81	72.37
549	A	W	N	545	A	Q	O	3.05	2.20	144.71	147.32
549	A	W	N	546	A	E	O	3.18	2.59	118.07	106.33
549	A	W	N	547	A	R	O	3.45	3.52	78.05	71.71
550	A	L	N	546	A	E	O	3.05	2.16	150.78	155.02
550	A	L	N	547	A	R	O	3.28	2.71	116.77	104.65
550	A	L	N	548	A	A	O	3.44	3.52	77.47	72.20
551	A	R	N	547	A	R	O	2.94	2.07	147.65	154.62
551	A	R	N	548	A	A	O	3.26	2.69	117.20	103.68
551	A	R	N	549	A	W	O	3.47	3.51	79.37	72.26
552	A	Q	N	548	A	A	O	3.05	2.18	147.06	153.37
552	A	Q	N	549	A	W	O	3.20	2.59	120.99	107.71
552	A	Q	N	550	A	L	O	3.47	3.54	78.03	71.71
553	A	Q	N	549	A	W	O	3.14	2.35	136.95	150.71
553	A	Q	N	550	A	L	O	3.14	2.48	124.37	105.48
553	A	Q	N	551	A	R	O	3.37	3.34	83.04	72.26
554	A	G	N	550	A	L	O	3.17	2.76	105.24	148.53
554	A	G	N	551	A	R	O	3.00	2.11	148.64	109.32
554	A	G	N	552	A	Q	O	3.42	3.06	102.51	67.97
555	A	K	N	550	A	L	O	3.05	2.09	164.81	151.64
557	A	V	N	555	A	K	O	3.37	3.32	84.40	97.85
558	A	G	N	524	A	A	O	2.88	1.92	161.57	139.40
561	A	L	N	528	A	V	O	2.97	2.00	171.27	166.27
562	A	L	N	590	A	Q	O	3.33	2.39	161.03	157.35
563	A	Y	N	530	A	M	O	2.83	1.90	151.88	161.11
564	A	Y	N	592	A	N	O	2.94	1.99	157.33	169.76
566	A	C	N	594	A	A	O	2.98	2.05	154.09	150.94
570	A	E	N	568	A	R	O	3.24	3.18	84.72	75.43
571	A	E	N	568	A	R	O	3.13	2.24	151.69	117.24
572	A	D	N	568	A	R	O	3.17	2.25	155.12	162.51
574	A	L	N	572	A	D	O	2.98	2.69	97.22	97.98
576	A	R	N	574	A	L	O	3.15	3.29	73.67	77.22
577	A	E	N	575	A	Y	O	3.26	3.26	81.03	80.90
578	A	E	N	575	A	Y	O	3.19	2.60	119.27	115.49
579	A	L	N	575	A	Y	O	2.93	1.98	160.99	168.73
580	A	A	N	576	A	R	O	3.04	2.19	145.27	144.99
580	A	A	N	577	A	E	O	3.38	2.83	116.25	100.11

580	A	A	N	578	A	E	O	3.48	3.53	79.36	71.65
581	A	Q	N	577	A	E	O	2.99	2.07	156.05	150.73
581	A	Q	N	578	A	E	O	3.29	2.79	112.54	105.17
581	A	Q	N	579	A	L	O	3.47	3.59	74.84	71.35
582	A	F	N	578	A	E	O	2.98	2.10	149.96	154.48
582	A	F	N	579	A	L	O	3.32	2.77	116.59	102.94
582	A	F	N	580	A	A	O	3.35	3.43	77.05	75.80
583	A	H	N	579	A	L	O	3.01	2.13	147.93	153.42
583	A	H	N	580	A	A	O	3.13	2.53	120.27	111.54
583	A	H	N	581	A	Q	O	3.48	3.51	80.24	72.01
584	A	Q	N	580	A	A	O	2.92	1.97	160.39	163.79
584	A	Q	N	581	A	Q	O	3.46	2.96	112.31	102.35
585	A	D	N	581	A	Q	O	2.95	2.12	142.12	152.21
585	A	D	N	582	A	F	O	3.37	2.75	121.71	99.27
585	A	D	N	583	A	H	O	3.45	3.46	81.45	72.58
586	A	G	N	582	A	F	O	3.05	2.42	121.04	146.98
586	A	G	N	583	A	H	O	3.17	2.38	137.39	106.79
586	A	G	N	584	A	Q	O	3.44	3.23	93.80	69.37
587	A	S	N	582	A	F	O	2.91	2.22	125.41	158.75
588	A	L	N	582	A	F	O	3.14	2.27	145.03	115.25
588	A	L	N	586	A	G	O	3.33	3.21	88.05	70.64
589	A	T	N	560	A	T	O	2.89	1.98	152.66	157.38
592	A	N	N	562	A	L	O	3.03	2.12	153.14	169.74
593	A	V	N	591	A	L	O	3.45	3.18	97.58	92.90
594	A	A	N	564	A	Y	O	2.98	2.04	155.66	141.09
596	A	S	N	566	A	C	O	2.92	1.98	159.55	152.66
596	A	S	N	567	A	R	O	3.41	3.28	89.21	110.28
597	A	R	N	567	A	R	O	2.93	1.99	160.10	135.32
597	A	R	N	595	A	F	O	3.11	2.90	93.08	88.33
598	A	E	N	595	A	F	O	3.28	2.32	166.05	126.75
599	A	Q	N	597	A	R	O	3.26	2.94	99.74	73.95
601	A	H	N	599	A	Q	O	3.25	3.15	86.93	82.35
606	A	Q	N	604	A	Y	O	3.15	3.13	82.56	80.00
607	A	H	N	604	A	Y	O	2.93	2.06	145.74	130.01
607	A	H	N	605	A	V	O	3.22	3.19	82.81	77.15
608	A	L	N	605	A	V	O	3.07	2.40	125.64	113.25
608	A	L	N	606	A	Q	O	3.42	3.41	82.56	71.88
609	A	L	N	605	A	V	O	3.11	2.23	149.14	160.79
609	A	L	N	606	A	Q	O	3.28	2.66	122.09	105.42
609	A	L	N	607	A	H	O	3.43	3.47	79.37	71.33
610	A	K	N	606	A	Q	O	3.25	2.39	145.09	149.14
610	A	K	N	607	A	H	O	3.15	2.54	120.62	105.68
610	A	K	N	608	A	L	O	3.33	3.40	77.86	72.43
611	A	R	N	607	A	H	O	2.94	2.12	139.95	154.68
611	A	R	N	608	A	L	O	3.15	2.53	121.39	104.73

612	A	D	N	608	A	L	O	2.92	2.09	141.17	159.00
613	A	K	N	609	A	L	O	3.19	3.25	77.39	143.04
613	A	K	N	611	A	R	O	3.46	2.72	130.81	67.80
614	A	E	N	612	A	D	O	3.36	3.25	88.41	82.51
616	A	L	N	612	A	D	O	3.13	2.27	147.12	156.01
616	A	L	N	613	A	K	O	3.29	2.82	109.75	99.37
616	A	L	N	614	A	E	O	3.46	3.45	81.89	70.48
617	A	W	N	613	A	K	O	2.88	1.95	158.06	154.27
617	A	W	N	614	A	E	O	3.42	2.84	119.48	106.57
617	A	W	N	615	A	H	O	3.43	3.59	72.83	74.68
618	A	Q	N	614	A	E	O	3.24	2.34	152.73	149.69
618	A	Q	N	615	A	H	O	3.17	2.65	113.72	106.43
618	A	Q	N	616	A	L	O	3.41	3.47	78.30	74.08
619	A	L	N	615	A	H	O	3.07	2.18	151.93	157.51
619	A	L	N	616	A	L	O	3.21	2.59	121.64	112.01
619	A	L	N	617	A	W	O	3.24	3.35	75.30	76.95
620	A	I	N	616	A	L	O	3.03	2.13	152.78	157.73
620	A	I	N	617	A	W	O	3.10	2.58	113.49	110.08
621	A	H	N	617	A	W	O	2.87	1.92	159.30	165.49
621	A	H	N	619	A	L	O	3.39	3.44	78.89	73.56
622	A	E	N	618	A	Q	O	3.18	2.48	127.65	144.26
622	A	E	N	619	A	L	O	3.20	2.44	133.68	106.49
622	A	E	N	620	A	I	O	3.35	3.24	88.13	72.87
623	A	A	N	621	A	H	O	3.43	3.58	73.16	102.56
624	A	G	N	622	A	E	O	3.48	3.69	70.21	101.88
625	A	A	N	622	A	E	O	3.49	2.52	167.50	131.26
625	A	A	N	623	A	A	O	3.35	2.86	111.57	77.27
626	A	H	N	527	A	P	O	2.93	2.02	152.81	150.66
627	A	I	N	671	A	R	O	2.84	1.93	150.12	149.53
628	A	Y	N	529	A	I	O	2.82	1.95	144.39	164.08
629	A	V	N	673	A	S	O	3.06	2.19	146.83	148.03
630	A	C	N	531	A	V	O	2.93	1.97	160.19	172.38
633	A	A	N	631	A	G	O	3.44	3.29	90.54	100.97
633	A	A	N	677	A	W	O	2.85	1.86	173.46	128.28
635	A	N	N	633	A	A	O	3.43	3.40	83.23	78.06
637	A	A	N	632	A	D	O	2.89	1.99	152.07	176.27
638	A	R	N	636	A	M	O	3.28	3.29	80.77	76.46
639	A	D	N	635	A	N	O	3.03	2.20	143.52	151.80
639	A	D	N	636	A	M	O	3.08	2.42	125.52	115.44
640	A	V	N	636	A	M	O	3.03	2.08	159.77	160.48
640	A	V	N	637	A	A	O	3.35	2.88	110.07	100.87
640	A	V	N	638	A	R	O	3.48	3.59	75.75	69.92
641	A	Q	N	637	A	A	O	2.86	1.98	146.91	151.61
641	A	Q	N	638	A	R	O	3.27	2.74	114.24	100.56
641	A	Q	N	639	A	D	O	3.40	3.49	76.72	74.20

642	A	N	N	638	A	R	O	2.93	2.04	150.39	152.07
642	A	N	N	639	A	D	O	3.22	2.67	115.87	107.01
642	A	N	N	640	A	V	O	3.41	3.47	77.84	74.00
643	A	T	N	639	A	D	O	2.80	1.97	141.14	158.67
643	A	T	N	640	A	V	O	3.19	2.58	120.39	105.38
643	A	T	N	641	A	Q	O	3.46	3.44	83.08	71.33
644	A	F	N	640	A	V	O	2.92	2.02	154.47	157.10
644	A	F	N	641	A	Q	O	3.30	2.76	115.38	104.37
645	A	Y	N	641	A	Q	O	3.07	2.22	145.81	150.28
645	A	Y	N	642	A	N	O	3.27	2.71	117.22	99.27
645	A	Y	N	643	A	T	O	3.33	3.41	76.98	74.67
646	A	D	N	642	A	N	O	3.11	2.23	149.18	147.75
646	A	D	N	643	A	T	O	3.07	2.49	117.97	112.61
646	A	D	N	644	A	F	O	3.40	3.49	76.30	73.84
647	A	I	N	643	A	T	O	2.93	2.04	149.94	162.37
647	A	I	N	644	A	F	O	3.32	2.74	118.49	104.54
647	A	I	N	645	A	Y	O	3.45	3.46	81.08	73.45
648	A	V	N	644	A	F	O	2.99	2.05	161.31	157.08
648	A	V	N	645	A	Y	O	3.41	2.89	114.31	105.64
649	A	A	N	645	A	Y	O	2.87	1.99	149.34	156.29
649	A	A	N	647	A	I	O	3.42	3.46	79.62	73.21
650	A	E	N	646	A	D	O	3.05	2.12	160.70	147.78
650	A	E	N	647	A	I	O	3.50	2.95	116.71	107.08
651	A	V	N	647	A	I	O	2.93	1.99	160.13	158.18
652	A	G	N	648	A	V	O	3.04	2.38	123.75	123.75
653	A	A	N	649	A	A	O	3.34	3.02	99.73	123.33
653	A	A	N	651	A	V	O	3.47	3.01	109.12	68.77
654	A	M	N	649	A	A	O	3.03	2.06	168.16	135.34
657	A	A	N	655	A	E	O	3.30	3.39	76.08	76.07
658	A	Q	N	655	A	E	O	3.01	2.28	130.28	115.19
658	A	Q	N	656	A	H	O	3.23	3.18	83.96	77.68
659	A	A	N	655	A	E	O	2.94	2.07	145.80	161.89
659	A	A	N	656	A	H	O	3.08	2.47	120.16	111.20
660	A	V	N	656	A	H	O	3.02	2.15	148.17	161.68
660	A	V	N	657	A	A	O	3.49	2.86	122.58	97.13
660	A	V	N	658	A	Q	O	3.48	3.53	79.00	69.68
661	A	D	N	657	A	A	O	3.37	2.49	149.48	139.39
661	A	D	N	658	A	Q	O	3.20	2.66	115.24	103.91
661	A	D	N	659	A	A	O	3.43	3.56	74.75	71.41
662	A	Y	N	658	A	Q	O	2.89	2.04	142.71	151.75
662	A	Y	N	659	A	A	O	3.20	2.64	115.94	101.66
662	A	Y	N	660	A	V	O	3.38	3.41	80.04	73.59
663	A	I	N	659	A	A	O	3.05	2.13	156.86	155.17
663	A	I	N	660	A	V	O	3.37	2.78	119.53	109.44
663	A	I	N	661	A	D	O	3.42	3.53	75.69	75.38

664	A	K	N	660	A	V	O	3.06	2.14	156.64	156.17
664	A	K	N	661	A	D	O	3.22	2.73	111.60	105.91
665	A	K	N	661	A	D	O	2.90	1.99	154.94	159.35
665	A	K	N	662	A	Y	O	3.30	2.76	115.59	104.87
665	A	K	N	663	A	I	O	3.38	3.50	74.84	74.97
666	A	L	N	662	A	Y	O	3.11	2.25	146.91	150.51
666	A	L	N	663	A	I	O	3.05	2.48	117.90	110.39
666	A	L	N	664	A	K	O	3.36	3.44	77.08	74.28
667	A	M	N	663	A	I	O	2.93	2.04	150.18	159.88
667	A	M	N	664	A	K	O	3.11	2.55	115.76	108.94
667	A	M	N	665	A	K	O	3.44	3.51	77.53	72.27
668	A	T	N	664	A	K	O	2.94	2.03	155.16	162.85
668	A	T	N	665	A	K	O	3.44	2.87	117.84	103.59
669	A	K	N	665	A	K	O	3.14	2.39	132.42	151.25
669	A	K	N	666	A	L	O	3.32	2.56	133.33	105.70
669	A	K	N	667	A	M	O	3.27	3.13	89.58	74.81
670	A	G	N	666	A	L	O	3.14	2.86	97.48	152.71
670	A	G	N	667	A	M	O	3.11	2.18	159.57	111.09
671	A	R	N	666	A	L	O	2.81	1.89	151.74	152.69
671	A	R	N	669	A	K	O	3.30	3.19	87.44	74.07
672	A	Y	N	666	A	L	O	3.17	2.47	127.61	106.37
673	A	S	N	627	A	I	O	2.82	1.86	161.52	158.14
675	A	D	N	629	A	V	O	2.97	1.99	174.06	172.09
677	A	W	N	631	A	G	O	2.94	1.97	164.68	170.54

Dd-a = Distance Between Donor and Acceptor
Dh-a = Distance Between Hydrogen and Acceptor
A(d-H-N) = Angle Between Donor-H-N
A(a-O=C) = Angle Between Acceptor-O=C
MO = Multiple Occupancy
Note that angles that are undefined are written as 999.99

Intraprotein Main Chain-Side Chain Hydrogen Bonds


Rasmol **Jmol** **[help]**

[View the original hbond output]

DOG_POR_D570E_snapshot10.pdb

DONOR PARAMETERS				ACCEPTOR								
POS	**CHAIN**	**RES**	**ATOM**	**POS**	**CHAIN**	**RES**	**ATOM**	**MO**	**Dd-a**	**Dh-a**	**A(d-H-N)**	**A(a-O=C)**
64	A	ALA	N	61	A	THR	OG1	-	3.18	2.72	109.15	999.99
65	A	LYS	NZ	114	A	PRO	O	-	3.27	9.99	999.99	143.51
65	A	LYS	NZ	115	A	GLU	O	-	2.94	9.99	999.99	103.09
65	A	LYS	NZ	117	A	TYR	O	-	2.89	9.99	999.99	120.03
69	A	PHE	N	121	A	ASP	OD2	-	3.21	2.71	111.99	149.88
70	A	VAL	N	121	A	ASP	OD2	-	2.97	2.02	165.93	149.09
71	A	GLU	N	68	A	SER	OG	-	3.19	2.26	160.29	999.99
72	A	LYS	NZ	354	A	GLU	O	-	2.91	9.99	999.99	160.39
76	A	THR	OG1	72	A	LYS	O	-	2.83	9.99	999.99	131.53
76	A	THR	OG1	73	A	MET	O	-	3.11	9.99	999.99	101.80
78	A	ARG	NE	109	A	GLY	O	-	3.40	2.80	117.14	110.52
79	A	ASN	OD1	108	A	ARG	O	1	2.95	3.10	72.08	124.23
79	A	ASN	OD1	108	A	ARG	O	2	2.95	2.39	110.86	124.23
79	A	ASN	ND2	130	A	ASN	O	1	2.95	3.43	54.43	131.78
79	A	ASN	ND2	130	A	ASN	O	2	2.95	1.91	169.57	131.78
85	A	GLY	N	137	A	MET	SD	-	3.53	3.49	84.57	999.99
86	A	SER	N	146	A	THR	OG1	-	3.01	2.66	101.38	999.99
86	A	SER	N	148	A	ASN	OD1	-	3.00	2.03	169.85	136.54
89	A	GLY	N	86	A	SER	OG	-	2.97	2.44	112.94	999.99
90	A	THR	N	86	A	SER	OG	-	3.40	3.21	93.09	999.99
92	A	GLU	N	86	A	SER	OG	-	3.48	2.61	148.17	999.99
99	A	SER	OG	95	A	ALA	O	-	2.85	9.99	999.99	141.89
100	A	LYS	NZ	242	A	ILE	O	-	3.15	9.99	999.99	162.84
101	A	ASP	OD2	97	A	ARG	O	1	3.09	3.47	60.60	105.83
101	A	ASP	OD2	97	A	ARG	O	2	3.09	3.05	82.22	105.83
104	A	ARG	NH2	238	A	GLU	O	1	3.13	2.08	168.72	125.45
104	A	ARG	NH2	238	A	GLU	O	2	3.13	3.61	53.77	125.45
108	A	ARG	N	79	A	ASN	OD1	-	2.97	1.99	177.06	171.83
111	A	ALA	N	99	A	SER	OG	-	3.28	3.32	79.19	999.99
115	A	GLU	N	113	A	ASP	OD1	-	3.18	2.24	166.73	131.76
120	A	ALA	N	118	A	ASP	OD2	-	3.02	2.07	163.11	127.61
124	A	SER	OG	121	A	ASP	O	-	3.41	9.99	999.99	121.89
131	A	SER	OG	125	A	LEU	O	-	2.70	9.99	999.99	106.05
131	A	SER	OG	128	A	ILE	O	-	3.15	9.99	999.99	136.33
139	A	THR	OG1	173	A	LEU	O	-	3.06	9.99	999.99	156.15
147	A	ASP	N	87	A	GLN	OE1	-	2.97	2.08	151.45	144.49
148	A	ASN	ND2	84	A	TYR	O	1	2.93	1.94	155.88	142.93
148	A	ASN	ND2	84	A	TYR	O	2	2.93	3.32	59.79	142.93
148	A	ASN	OD1	86	A	SER	O	1	3.18	3.21	78.85	120.35
148	A	ASN	OD1	86	A	SER	O	2	3.18	2.80	101.51	120.35
161	A	VAL	N	159	A	THR	OG1	-	3.23	2.28	161.91	999.99

164	A	SER	N	162	A	ASP	OD1	-	2.98	2.08	154.65	121.82
168	A	TYR	OH	189	A	ASP	O	-	3.03	9.99	999.99	130.65
174	A	GLY	N	182	A	ASN	ND2	-	3.46	3.65	71.07	110.35
176	A	LYS	N	207	A	ASP	OD1	-	2.88	1.96	153.66	138.35
177	A	THR	N	175	A	ASN	OD1	-	2.95	1.99	164.13	152.30
178	A	TYR	OH	676	A	VAL	O	-	2.71	9.99	999.99	125.46
182	A	ASN	ND2	172	A	GLY	O	1	3.07	2.01	175.61	90.65
182	A	ASN	ND2	172	A	GLY	O	2	3.07	3.68	47.27	90.65
182	A	ASN	ND2	206	A	GLY	O	1	3.32	3.21	86.64	126.85
182	A	ASN	ND2	206	A	GLY	O	2	3.32	2.67	120.46	126.85
183	A	ALA	N	139	A	THR	OG1	-	3.44	3.31	88.90	999.99
184	A	MET	N	139	A	THR	OG1	-	3.14	2.23	153.91	999.99
186	A	LYS	NZ	181	A	PHE	O	-	3.45	9.99	999.99	154.80
191	A	ARG	NE	156	A	LEU	O	-	2.85	1.87	161.36	133.21
191	A	ARG	NH1	157	A	GLN	O	1	3.12	2.43	122.86	117.89
191	A	ARG	NH1	157	A	GLN	O	2	3.12	3.32	70.21	117.89
207	A	ASP	N	215	A	ASP	OD2	-	2.94	2.03	153.01	149.84
209	A	ASP	N	207	A	ASP	OD1	-	2.95	2.01	162.99	109.38
210	A	GLY	N	207	A	ASP	OD2	-	3.43	2.65	135.95	95.55
213	A	GLU	N	211	A	ASN	OD1	-	3.19	2.57	120.96	151.95
214	A	GLU	N	211	A	ASN	OD1	-	3.02	2.09	157.95	127.50
215	A	ASP	OD2	205	A	MET	O	1	3.45	2.70	127.65	120.45
215	A	ASP	OD2	205	A	MET	O	2	3.45	3.49	78.90	120.45
218	A	THR	OG1	214	A	GLU	O	-	3.19	9.99	999.99	125.39
218	A	THR	OG1	215	A	ASP	O	-	2.96	9.99	999.99	102.16
219	A	TRP	NE1	205	A	MET	O	-	3.08	2.48	124.46	91.98
228	A	CYS	SG	224	A	TRP	O	-	3.16	9.99	999.99	130.34
228	A	CYS	SG	233	A	VAL	O	-	3.60	9.99	999.99	115.19
236	A	THR	OG1	104	A	ARG	O	-	2.98	9.99	999.99	108.84
238	A	GLU	OE1	103	A	HIS	O	1	3.43	2.97	106.23	88.62
238	A	GLU	OE1	103	A	HIS	O	2	3.43	3.08	99.71	88.62
238	A	GLU	N	236	A	THR	OG1	-	3.47	2.72	133.11	999.99
241	A	SER	N	388	A	GLU	OE2	-	3.49	3.15	101.91	111.69
241	A	SER	OG	388	A	GLU	O	-	2.65	9.99	999.99	132.24
242	A	ILE	N	388	A	GLU	OE2	-	3.37	2.60	135.94	113.70
243	A	ARG	NH2	245	A	TYR	O	1	3.06	2.09	151.13	144.96
243	A	ARG	NH2	245	A	TYR	O	2	3.06	3.43	60.42	144.96
244	A	GLN	NE2	96	A	ASN	O	1	3.24	2.50	126.83	122.25
244	A	GLN	NE2	96	A	ASN	O	2	3.24	3.90	44.62	122.25
244	A	GLN	N	446	A	GLU	OE2	-	2.77	1.78	169.65	141.55
245	A	TYR	OH	357	A	LYS	O	-	3.48	9.99	999.99	125.00
245	A	TYR	N	446	A	GLU	OE2	-	2.91	1.97	159.79	141.97
256	A	ALA	N	254	A	ASP	OD1	-	3.12	2.15	167.27	129.68
259	A	TYR	OH	264	A	GLY	O	-	2.73	9.99	999.99	154.20
260	A	VAL	N	262	A	GLU	OE1	-	2.85	1.88	167.57	129.49

265	A	ARG	NH1	271	A	ASN	O	1	3.30	2.80	109.75	154.12
265	A	ARG	NH1	271	A	ASN	O	2	3.30	3.05	94.71	154.12
266	A	LEU	N	259	A	TYR	OH	-	3.21	3.21	81.28	999.99
267	A	LYS	NZ	255	A	MET	O	-	2.96	9.99	999.99	144.76
267	A	LYS	NZ	258	A	VAL	O	-	2.84	9.99	999.99	164.21
267	A	LYS	N	262	A	GLU	OE2	-	2.82	1.90	152.01	118.64
268	A	SER	OG	263	A	MET	O	-	2.84	9.99	999.99	143.36
268	A	SER	OG	265	A	ARG	O	-	3.37	9.99	999.99	143.56
272	A	GLN	NE2	269	A	TYR	O	1	2.94	3.64	42.07	125.14
272	A	GLN	NE2	269	A	TYR	O	2	2.94	1.92	162.61	125.14
279	A	LYS	N	277	A	ASP	OD2	-	2.95	1.98	167.53	102.48
280	A	ASN	ND2	275	A	PRO	O	1	3.40	3.81	59.48	139.46
280	A	ASN	ND2	275	A	PRO	O	2	3.40	2.42	155.91	139.46
280	A	ASN	N	277	A	ASP	OD1	-	3.28	2.84	107.40	108.40
283	A	LEU	N	272	A	GLN	OE1	-	2.93	1.96	169.83	132.67
287	A	THR	OG1	304	A	GLU	O	-	3.16	9.99	999.99	84.65
289	A	ASN	ND2	494	A	LEU	O	1	3.11	2.41	122.41	145.95
289	A	ASN	ND2	494	A	LEU	O	2	3.11	3.23	73.75	145.95
289	A	ASN	ND2	497	A	LYS	O	1	2.86	3.49	46.14	138.33
289	A	ASN	ND2	497	A	LYS	O	2	2.86	1.81	174.73	138.33
291	A	LYS	NZ	295	A	GLY	O	-	2.91	9.99	999.99	169.93
293	A	ASN	OD1	298	A	ARG	O	1	3.37	2.69	121.20	124.03
293	A	ASN	OD1	298	A	ARG	O	2	3.37	4.25	30.00	124.03
293	A	ASN	ND2	298	A	ARG	O	1	2.94	2.09	134.86	155.10
293	A	ASN	ND2	298	A	ARG	O	2	2.94	3.62	42.80	155.10
293	A	ASN	OD1	300	A	LEU	O	1	3.36	3.47	75.31	110.56
293	A	ASN	OD1	300	A	LEU	O	2	3.36	2.44	143.32	110.56
300	A	LEU	N	293	A	ASN	OD1	-	2.87	1.92	160.99	141.29
302	A	HIS	ND1	471	A	ILE	O	-	3.12	2.87	97.31	143.75
308	A	SER	N	306	A	ASP	OD1	-	2.84	1.89	162.02	138.57
310	A	SER	OG	307	A	ILE	O	-	2.67	9.99	999.99	134.21
312	A	LEU	N	310	A	SER	OG	-	3.29	2.38	153.42	999.99
314	A	TYR	OH	461	A	SER	O	-	3.41	9.99	999.99	94.72
314	A	TYR	OH	465	A	HIS	O	-	3.04	9.99	999.99	137.91
314	A	TYR	OH	468	A	SER	O	-	2.75	9.99	999.99	155.83
315	A	GLU	N	318	A	ASP	OD2	-	3.05	2.14	150.38	126.93
315	A	GLU	OE1	520	A	LEU	O	1	3.43	3.13	97.13	114.81
315	A	GLU	OE1	520	A	LEU	O	2	3.43	3.74	64.97	114.81
316	A	SER	OG	460	A	SER	O	-	2.73	9.99	999.99	112.19
316	A	SER	OG	542	A	GLY	O	-	3.08	9.99	999.99	84.67
318	A	ASP	OD2	315	A	GLU	O	1	3.49	4.16	44.50	119.14
318	A	ASP	OD2	315	A	GLU	O	2	3.49	3.22	95.56	119.14
323	A	TYR	OH	278	A	ALA	O	-	2.77	9.99	999.99	118.50
326	A	ASN	ND2	371	A	LEU	O	1	2.93	3.42	54.13	158.06
326	A	ASN	ND2	371	A	LEU	O	2	2.93	1.94	155.57	158.06

326	A	ASN	ND2	372	A	THR	O	1	3.43	4.09	45.30	107.82
326	A	ASN	ND2	372	A	THR	O	2	3.43	2.91	111.29	107.82
326	A	ASN	ND2	375	A	LEU	O	1	2.92	2.07	134.92	171.37
326	A	ASN	ND2	375	A	LEU	O	2	2.92	3.06	72.42	171.37
329	A	ALA	N	327	A	ASP	OD2	-	3.05	2.08	168.67	111.15
333	A	GLN	NE2	329	A	ALA	O	1	3.13	3.90	37.84	102.06
333	A	GLN	NE2	329	A	ALA	O	2	3.13	2.22	145.49	102.06
343	A	ASP	N	341	A	ASP	OD1	-	3.08	2.17	155.57	150.66
348	A	LEU	N	363	A	CYS	SG	-	3.71	2.82	149.93	999.99
350	A	ASN	OD1	244	A	GLN	O	1	2.94	3.18	67.46	135.78
350	A	ASN	OD1	244	A	GLN	O	2	2.94	2.37	111.68	135.78
350	A	ASN	ND2	357	A	LYS	O	1	2.94	3.69	38.79	143.74
350	A	ASN	ND2	357	A	LYS	O	2	2.94	1.94	157.65	143.74
352	A	ASP	N	350	A	ASN	OD1	-	2.91	1.95	160.42	116.17
355	A	SER	N	352	A	ASP	OD1	-	3.42	2.80	122.38	112.84
355	A	SER	OG	352	A	ASP	O	-	2.73	9.99	999.99	148.75
357	A	LYS	NZ	92	A	GLU	O	-	3.03	9.99	999.99	131.40
358	A	LYS	NZ	353	A	GLU	O	-	3.12	9.99	999.99	155.42
358	A	LYS	NZ	355	A	SER	O	-	3.00	9.99	999.99	138.19
359	A	HIS	ND1	348	A	LEU	O	-	2.88	1.97	170.76	126.84
363	A	CYS	SG	361	A	PHE	O	-	3.39	9.99	999.99	136.17
365	A	THR	OG1	259	A	TYR	O	-	2.89	9.99	999.99	126.35
368	A	ARG	N	366	A	SER	OG	-	3.43	2.86	117.32	999.99
369	A	THR	N	366	A	SER	OG	-	3.13	2.20	158.09	999.99
372	A	THR	OG1	368	A	ARG	O	-	2.69	9.99	999.99	138.93
374	A	TYR	OH	262	A	GLU	O	-	2.67	9.99	999.99	143.81
378	A	THR	N	376	A	ASP	OD1	-	3.27	2.42	144.00	148.71
379	A	ASN	N	376	A	ASP	OD1	-	2.86	2.01	142.36	154.57
383	A	THR	N	213	A	GLU	OE2	-	2.85	1.89	165.12	135.03
394	A	SER	N	436	A	SER	OG	-	3.29	2.80	111.81	999.99
395	A	GLU	N	436	A	SER	OG	-	3.18	2.21	168.44	999.99
397	A	THR	N	395	A	GLU	OE2	-	2.96	2.01	164.64	121.08
399	A	GLN	NE2	390	A	ALA	O	1	3.31	4.11	35.62	117.96
399	A	GLN	NE2	390	A	ALA	O	2	3.31	2.39	145.68	117.96
399	A	GLN	NE2	393	A	ALA	O	1	3.30	3.49	70.64	149.85
399	A	GLN	NE2	393	A	ALA	O	2	3.30	2.86	105.28	149.85
401	A	HIS	ND1	397	A	THR	O	-	2.84	1.93	171.81	134.99
403	A	ARG	NH2	387	A	TYR	O	1	3.37	3.18	91.22	140.59
403	A	ARG	NH2	387	A	TYR	O	2	3.37	3.52	73.09	140.59
407	A	SER	OG	409	A	SER	O	-	2.72	9.99	999.99	140.11
409	A	SER	N	407	A	SER	OG	-	3.49	2.51	170.07	999.99
413	A	LYS	NZ	408	A	SER	O	-	3.06	9.99	999.99	136.70
416	A	TYR	OH	381	A	PRO	O	-	2.84	9.99	999.99	142.34
418	A	SER	OG	414	A	GLU	O	-	2.92	9.99	999.99	129.53
418	A	SER	OG	415	A	LEU	O	-	3.11	9.99	999.99	102.59

424	A	ARG	NH2	421	A	VAL	O	1	2.88	1.88	155.62	127.36
424	A	ARG	NH2	421	A	VAL	O	2	2.88	3.28	58.23	127.36
425	A	ARG	NH2	419	A	TRP	O	1	2.93	1.88	167.39	122.45
425	A	ARG	NH2	419	A	TRP	O	2	2.93	3.42	53.31	122.45
428	A	LEU	N	426	A	HIS	ND1	-	3.44	2.81	123.83	999.99
429	A	ALA	N	426	A	HIS	ND1	-	3.27	2.36	154.06	999.99
436	A	SER	N	398	A	GLU	OE2	-	2.93	2.01	157.40	124.38
438	A	ARG	NE	337	A	ILE	O	-	3.31	3.00	97.97	137.82
438	A	ARG	NH2	431	A	LEU	O	1	2.95	3.54	48.86	128.74
438	A	ARG	NH2	431	A	LEU	O	2	2.95	2.02	153.45	128.74
438	A	ARG	NH1	435	A	PRO	O	1	3.27	3.73	56.45	116.91
438	A	ARG	NH1	435	A	PRO	O	2	3.27	3.41	73.67	116.91
438	A	ARG	NH2	435	A	PRO	O	1	3.35	3.86	54.12	97.43
438	A	ARG	NH2	435	A	PRO	O	2	3.35	3.46	74.96	97.43
445	A	CYS	SG	441	A	ILE	O	-	3.13	9.99	999.99	134.23
446	A	GLU	OE2	245	A	TYR	O	1	3.43	3.78	62.90	113.61
446	A	GLU	OE2	245	A	TYR	O	2	3.43	2.53	141.40	113.61
450	A	ARG	NH1	89	A	GLY	O	1	3.48	2.66	135.36	106.32
450	A	ARG	NH1	89	A	GLY	O	2	3.48	3.52	79.04	106.32
450	A	ARG	N	93	A	GLU	OE2	-	3.05	2.09	169.38	112.47
452	A	GLN	OE1	88	A	THR	O	1	3.11	3.61	54.54	81.78
452	A	GLN	OE1	88	A	THR	O	2	3.11	3.27	72.30	81.78
452	A	GLN	NE2	450	A	ARG	O	1	3.05	3.63	49.24	107.28
452	A	GLN	NE2	450	A	ARG	O	2	3.05	2.05	159.49	107.28
461	A	SER	N	545	A	GLN	OE1	-	2.88	1.91	163.72	148.62
462	A	SER	OG	314	A	TYR	O	-	2.73	9.99	999.99	134.42
462	A	SER	N	546	A	GLU	OE1	-	2.97	2.27	127.82	155.42
463	A	LYS	N	461	A	SER	OG	-	3.10	2.36	132.08	999.99
463	A	LYS	N	546	A	GLU	OE1	-	3.20	2.28	157.24	150.80
464	A	VAL	N	461	A	SER	OG	-	3.09	2.20	149.13	999.99
470	A	HIS	N	460	A	SER	OG	-	3.30	2.54	133.70	999.99
472	A	CYS	SG	301	A	MET	O	-	3.88	9.99	999.99	149.72
476	A	VAL	N	491	A	THR	OG1	-	3.16	2.30	144.05	999.99
480	A	THR	OG1	484	A	ARG	O	-	3.16	9.99	999.99	117.21
481	A	ARG	NH1	418	A	SER	O	1	3.04	2.56	107.31	114.39
481	A	ARG	NH1	418	A	SER	O	2	3.04	2.91	87.14	114.39
482	A	SER	OG	423	A	ALA	O	-	2.91	9.99	999.99	153.52
482	A	SER	N	480	A	THR	OG1	-	3.31	2.66	123.90	999.99
483	A	GLY	N	480	A	THR	OG1	-	3.12	2.59	113.50	999.99
484	A	ARG	N	480	A	THR	OG1	-	3.14	2.43	128.64	999.99
486	A	ASN	ND2	424	A	ARG	O	1	3.31	2.38	147.18	140.89
486	A	ASN	ND2	424	A	ARG	O	2	3.31	3.74	58.36	140.89
492	A	SER	OG	488	A	GLY	O	-	3.39	9.99	999.99	145.84
516	A	SER	OG	317	A	GLY	O	-	2.66	9.99	999.99	111.85
516	A	SER	N	318	A	ASP	OD1	-	3.15	2.19	162.71	138.13

518	A	PHE	N	516	A	SER	OG	-	3.23	2.60	121.74	999.99
519	A	ARG	N	516	A	SER	OG	-	3.07	2.83	94.70	999.99
519	A	ARG	NH2	516	A	SER	O	1	2.97	1.97	155.23	138.35
519	A	ARG	NH2	516	A	SER	O	2	2.97	3.34	60.05	138.35
526	A	THR	OG1	523	A	LYS	O	-	2.78	9.99	999.99	172.43
547	A	ARG	NH1	524	A	ALA	O	1	3.04	3.41	60.77	108.69
547	A	ARG	NH1	524	A	ALA	O	2	3.04	2.95	85.00	108.69
547	A	ARG	NH1	526	A	THR	O	1	3.05	3.90	30.74	147.81
547	A	ARG	NH1	526	A	THR	O	2	3.05	2.12	144.99	147.81
547	A	ARG	NH2	526	A	THR	O	1	2.99	3.88	28.01	168.72
547	A	ARG	NH2	526	A	THR	O	2	2.99	2.11	144.81	168.72
547	A	ARG	NH2	558	A	GLY	O	1	3.43	2.96	106.80	98.90
547	A	ARG	NH2	558	A	GLY	O	2	3.43	3.25	91.59	98.90
551	A	ARG	NH1	585	A	ASP	O	1	3.16	2.57	115.21	128.42
551	A	ARG	NH1	585	A	ASP	O	2	3.16	3.15	81.04	128.42
551	A	ARG	NH2	586	A	GLY	O	1	3.38	3.75	61.55	111.91
551	A	ARG	NH2	586	A	GLY	O	2	3.38	3.52	73.81	111.91
560	A	THR	OG1	558	A	GLY	O	-	3.18	9.99	999.99	139.99
560	A	THR	N	589	A	THR	OG1	-	2.91	1.92	173.56	999.99
564	A	TYR	OH	572	A	ASP	O	-	3.05	9.99	999.99	138.02
566	A	CYS	SG	568	A	ARG	O	-	3.86	9.99	999.99	80.91
566	A	CYS	SG	594	A	ALA	O	-	3.72	9.99	999.99	146.98
567	A	ARG	N	572	A	ASP	OD1	-	2.98	2.25	130.39	95.84
567	A	ARG	N	572	A	ASP	OD2	-	2.92	1.95	167.64	98.93
568	A	ARG	N	572	A	ASP	OD1	-	2.86	1.89	162.37	152.73
569	A	SER	N	598	A	GLU	OE2	-	2.86	1.88	172.81	153.01
572	A	ASP	OD1	568	A	ARG	O	1	3.14	3.21	76.90	114.84
572	A	ASP	OD1	568	A	ARG	O	2	3.14	2.55	114.01	114.84
574	A	LEU	N	564	A	TYR	OH	-	2.94	1.95	176.84	999.99
576	A	ARG	NH2	569	A	SER	O	1	3.16	2.28	138.60	136.91
576	A	ARG	NH2	569	A	SER	O	2	3.16	3.45	64.80	136.91
581	A	GLN	NE2	577	A	GLU	O	1	3.26	4.06	35.62	105.00
581	A	GLN	NE2	577	A	GLU	O	2	3.26	2.45	134.38	105.00
583	A	HIS	ND1	588	A	LEU	O	-	3.08	2.24	153.08	137.67
585	A	ASP	OD2	581	A	GLN	O	1	3.48	3.92	58.36	123.10
585	A	ASP	OD2	581	A	GLN	O	2	3.48	3.76	66.83	123.10
589	A	THR	OG1	560	A	THR	O	-	3.18	9.99	999.99	107.98
592	A	ASN	ND2	562	A	LEU	O	1	3.44	4.15	41.98	123.71
592	A	ASN	ND2	562	A	LEU	O	2	3.44	2.78	120.98	123.71
599	A	GLN	NE2	601	A	HIS	O	1	3.02	3.79	37.46	149.35
599	A	GLN	NE2	601	A	HIS	O	2	3.02	2.06	151.82	149.35
626	A	HIS	ND1	624	A	GLY	O	-	3.28	3.43	72.57	151.10
628	A	TYR	OH	519	A	ARG	O	-	2.69	9.99	999.99	147.50
630	A	CYS	SG	536	A	GLY	O	-	3.71	9.99	999.99	115.85
630	A	CYS	SG	675	A	ASP	O	-	3.19	9.99	999.99	170.61

634	A	ARG	NH2	209	A	ASP	O	1	3.06	3.39	62.95	118.95
634	A	ARG	NH2	209	A	ASP	O	2	3.06	2.14	151.35	118.95
634	A	ARG	N	632	A	ASP	OD1	-	3.00	2.06	159.13	96.52
634	A	ARG	N	632	A	ASP	OD2	-	3.38	2.89	111.56	79.38
634	A	ARG	NE	678	A	SER	OXT	-	2.89	1.98	146.20	123.13
635	A	ASN	N	632	A	ASP	OD2	-	2.84	1.94	152.22	132.52
636	A	MET	N	632	A	ASP	OD2	-	2.95	1.98	173.50	141.92
638	A	ARG	NH1	176	A	LYS	O	1	3.19	2.38	132.90	146.88
638	A	ARG	NH1	176	A	LYS	O	2	3.19	3.48	65.15	146.88
638	A	ARG	NE	177	A	THR	O	-	2.93	2.17	129.77	120.54
638	A	ARG	NH1	177	A	THR	O	1	3.36	2.67	123.05	91.51
638	A	ARG	NH1	177	A	THR	O	2	3.36	4.24	27.93	91.51
642	A	ASN	ND2	638	A	ARG	O	1	3.22	3.66	58.00	123.63
642	A	ASN	ND2	638	A	ARG	O	2	3.22	3.26	78.93	123.63
643	A	THR	OG1	639	A	ASP	O	-	2.68	9.99	999.99	134.16
655	A	GLU	N	658	A	GLN	OE1	-	3.01	2.03	174.07	136.40
659	A	ALA	N	654	A	MET	SD	-	3.71	4.18	55.74	999.99
661	A	ASP	OD2	657	A	ALA	O	1	3.33	3.60	67.10	129.52
661	A	ASP	OD2	657	A	ALA	O	2	3.33	3.27	84.30	129.52
668	A	THR	OG1	664	A	LYS	O	-	3.17	9.99	999.99	127.46
668	A	THR	OG1	665	A	LYS	O	-	3.09	9.99	999.99	104.87
671	A	ARG	NH1	620	A	ILE	O	1	3.24	3.56	63.96	143.74
671	A	ARG	NH1	620	A	ILE	O	2	3.24	2.42	133.24	143.74
671	A	ARG	NH1	622	A	GLU	O	1	2.94	3.29	61.47	159.88
671	A	ARG	NH1	622	A	GLU	O	2	2.94	2.24	122.08	159.88
671	A	ARG	NE	625	A	ALA	O	-	2.86	1.95	145.99	148.89
671	A	ARG	NH1	625	A	ALA	O	1	3.04	2.18	138.87	115.48
671	A	ARG	NH1	625	A	ALA	O	2	3.04	3.94	27.41	115.48
674	A	LEU	N	142	A	GLU	OE2	-	2.98	2.01	165.49	105.88

Dd-a = Distance Between Donor and Acceptor
Dh-a = Distance Between Hydrogen and Acceptor
A(d-H-N) = Angle Between Donor-H-N
A(a-O=C) = Angle Between Acceptor-O=C
MO = Multiple Occupancy
Note that angles that are undefined are written as 999.99

Intraprotein Side Chain-Side Chain Hydrogen Bonds


[help]

Rasmol **Jmol**

[View the original hbond output]

DOG_POR_D570E_snapshot10.pdb

DONOR				ACCEPTOR					PARAMETERS			
POS	CHAIN	RES	ATOM	POS	CHAIN	RES	ATOM	MO	Dd-a	Dh-a	A(d-H-N)	A(a-O=C)
61	A	THR	OG1	63	A	SER	OG	-	3.15	9.99	999.99	999.99
65	A	LYS	NZ	151	A	ASP	OD2	-	2.84	9.99	999.99	999.99
66	A	ASP	OD2	356	A	ASN	OD1	1	3.33	2.75	114.18	999.99
66	A	ASP	OD2	356	A	ASN	OD1	2	3.33	3.10	92.57	999.99
66	A	ASP	OD2	356	A	ASN	ND2	1	3.19	3.33	73.28	999.99
66	A	ASP	OD2	356	A	ASN	ND2	2	3.19	2.37	132.73	999.99
68	A	SER	OG	121	A	ASP	OD2	-	2.60	9.99	999.99	999.99
72	A	LYS	NZ	66	A	ASP	OD2	-	3.01	9.99	999.99	999.99
72	A	LYS	NZ	117	A	TYR	OH	-	2.92	9.99	999.99	999.99
74	A	LYS	NZ	127	A	GLU	OE1	-	2.92	9.99	999.99	999.99
78	A	ARG	NH2	352	A	ASP	OD1	1	3.13	3.07	83.62	999.99
78	A	ARG	NH2	352	A	ASP	OD1	2	3.13	2.89	94.36	999.99
78	A	ARG	NH2	352	A	ASP	OD2	1	3.30	3.27	82.63	999.99
78	A	ARG	NH2	352	A	ASP	OD2	2	3.30	3.61	64.27	999.99
79	A	ASN	ND2	107	A	MET	SD	1	3.83	2.79	166.52	999.99
79	A	ASN	ND2	107	A	MET	SD	2	3.83	4.23	60.58	999.99
87	A	GLN	NE2	147	A	ASP	OD2	1	2.96	1.94	161.81	999.99
87	A	GLN	NE2	147	A	ASP	OD2	2	2.96	3.60	45.42	999.99
87	A	GLN	NE2	455	A	TYR	OH	1	3.19	3.88	43.23	999.99
87	A	GLN	NE2	455	A	TYR	OH	2	3.19	2.22	153.82	999.99
96	A	ASN	ND2	244	A	GLN	OE1	1	3.34	3.90	50.88	999.99
96	A	ASN	ND2	244	A	GLN	OE1	2	3.34	2.96	101.82	999.99
97	A	ARG	NH1	213	A	GLU	OE1	1	2.91	3.63	40.18	999.99
97	A	ARG	NH1	213	A	GLU	OE1	2	2.91	1.93	153.43	999.99
97	A	ARG	NH1	213	A	GLU	OE2	1	3.44	4.35	26.37	999.99
97	A	ARG	NH1	213	A	GLU	OE2	2	3.44	2.71	126.80	999.99
97	A	ARG	NH2	213	A	GLU	OE1	1	3.30	4.25	22.79	999.99
97	A	ARG	NH2	213	A	GLU	OE1	2	3.30	2.56	130.02	999.99
97	A	ARG	NH2	213	A	GLU	OE2	1	2.93	3.67	39.86	999.99
97	A	ARG	NH2	213	A	GLU	OE2	2	2.93	2.05	144.92	999.99
97	A	ARG	NH2	384	A	ASN	OD1	1	2.99	2.45	109.99	999.99
97	A	ARG	NH2	384	A	ASN	OD1	2	2.99	3.44	55.64	999.99
100	A	LYS	NZ	388	A	GLU	OE1	-	3.20	9.99	999.99	999.99
100	A	LYS	NZ	446	A	GLU	OE1	-	2.92	9.99	999.99	999.99
103	A	HIS	ND1	238	A	GLU	OE1	-	2.83	1.97	155.64	999.99
104	A	ARG	NE	101	A	ASP	OD1	-	3.19	2.28	146.31	999.99
104	A	ARG	NH1	388	A	GLU	OE2	1	2.91	3.69	36.13	999.99

104	A	ARG	NH1	388	A	GLU	OE2	2	2.91	1.92	156.35	999.99
104	A	ARG	NH2	388	A	GLU	OE2	1	3.16	4.11	23.14	999.99
104	A	ARG	NH2	388	A	GLU	OE2	2	3.16	2.35	136.62	999.99
113	A	ASP	OD1	148	A	ASN	ND2	1	2.96	2.49	105.51	999.99
113	A	ASP	OD1	148	A	ASN	ND2	2	2.96	3.32	61.16	999.99
116	A	GLU	OE2	356	A	ASN	ND2	1	2.94	2.69	92.86	999.99
116	A	GLU	OE2	356	A	ASN	ND2	2	2.94	3.23	65.07	999.99
117	A	TYR	OH	356	A	ASN	ND2	-	3.29	9.99	999.99	999.99
124	A	SER	OG	121	A	ASP	OD1	-	2.78	9.99	999.99	999.99
140	A	TYR	OH	319	A	HIS	ND1	-	3.43	9.99	999.99	999.99
144	A	ASP	OD1	517	A	GLN	NE2	1	3.35	3.16	90.66	999.99
144	A	ASP	OD1	517	A	GLN	NE2	2	3.35	3.68	63.98	999.99
146	A	THR	OG1	148	A	ASN	OD1	-	2.99	9.99	999.99	999.99
147	A	ASP	OD2	87	A	GLN	NE2	1	2.96	3.00	77.37	999.99
147	A	ASP	OD2	87	A	GLN	NE2	2	2.96	2.90	82.61	999.99
148	A	ASN	ND2	113	A	ASP	OD1	1	2.96	3.61	44.63	999.99
148	A	ASN	ND2	113	A	ASP	OD1	2	2.96	1.92	169.20	999.99
148	A	ASN	OD1	146	A	THR	OG1	1	2.99	2.69	95.59	999.99
148	A	ASN	OD1	146	A	THR	OG1	2	2.99	2.54	104.24	999.99
164	A	SER	OG	162	A	ASP	OD1	-	2.68	9.99	999.99	999.99
167	A	LYS	NZ	230	A	HIS	NE2	-	3.08	9.99	999.99	999.99
168	A	TYR	OH	189	A	ASP	OD1	-	2.76	9.99	999.99	999.99
175	A	ASN	OD1	177	A	THR	OG1	1	2.70	2.33	98.45	999.99
175	A	ASN	OD1	177	A	THR	OG1	2	2.70	2.84	71.70	999.99
175	A	ASN	ND2	678	A	SER	OG	1	3.06	2.47	114.49	999.99
175	A	ASN	ND2	678	A	SER	OG	2	3.06	3.45	60.02	999.99
177	A	THR	OG1	175	A	ASN	OD1	-	2.70	9.99	999.99	999.99
177	A	THR	OG1	678	A	SER	OG	-	3.40	9.99	999.99	999.99
179	A	GLU	OE1	641	A	GLN	NE2	1	3.12	3.61	54.70	999.99
179	A	GLU	OE1	641	A	GLN	NE2	2	3.12	2.09	160.94	999.99
191	A	ARG	NH2	194	A	GLN	OE1	1	3.20	2.14	173.08	999.99
191	A	ARG	NH2	194	A	GLN	OE1	2	3.20	3.73	51.81	999.99
199	A	ARG	NH2	168	A	TYR	OH	1	3.20	2.18	161.37	999.99
199	A	ARG	NH2	168	A	TYR	OH	2	3.20	3.63	57.64	999.99
199	A	ARG	NH2	193	A	GLU	OE1	1	2.89	3.62	39.97	999.99
199	A	ARG	NH2	193	A	GLU	OE1	2	2.89	1.90	165.73	999.99
199	A	ARG	NE	202	A	GLU	OE1	-	3.05	2.28	130.06	999.99
199	A	ARG	NE	202	A	GLU	OE2	-	2.93	2.01	147.59	999.99
199	A	ARG	NH1	202	A	GLU	OE1	1	3.33	2.65	122.80	999.99
199	A	ARG	NH1	202	A	GLU	OE1	2	3.33	4.18	32.06	999.99
199	A	ARG	NH1	202	A	GLU	OE2	1	3.24	2.41	135.14	999.99
199	A	ARG	NH1	202	A	GLU	OE2	2	3.24	4.14	26.68	999.99
219	A	TRP	NE1	215	A	ASP	OD1	-	3.33	3.06	99.67	999.99
219	A	TRP	NE1	215	A	ASP	OD2	-	3.16	2.39	143.27	999.99
238	A	GLU	OE1	103	A	HIS	ND1	1	2.83	1.86	148.39	999.99

238	A	GLU	OE1	103	A	HIS	ND1	2	2.83	3.31	54.37	999.99
241	A	SER	OG	391	A	GLN	OE1	-	3.16	9.99	999.99	999.99
241	A	SER	OG	391	A	GLN	NE2	-	3.30	9.99	999.99	999.99
243	A	ARG	NH1	442	A	ASP	OD2	1	2.89	3.69	34.56	999.99
243	A	ARG	NH1	442	A	ASP	OD2	2	2.89	1.94	148.84	999.99
243	A	ARG	NH2	442	A	ASP	OD2	1	3.05	3.99	24.70	999.99
243	A	ARG	NH2	442	A	ASP	OD2	2	3.05	2.25	136.91	999.99
244	A	GLN	OE1	96	A	ASN	ND2	1	3.34	2.85	107.84	999.99
244	A	GLN	OE1	96	A	ASN	ND2	2	3.34	3.78	57.99	999.99
265	A	ARG	NH1	271	A	ASN	ND2	1	3.42	3.78	62.33	999.99
265	A	ARG	NH1	271	A	ASN	ND2	2	3.42	3.16	95.29	999.99
265	A	ARG	NE	280	A	ASN	OD1	-	3.03	2.27	129.73	999.99
265	A	ARG	NH1	280	A	ASN	OD1	1	3.03	2.18	136.55	999.99
265	A	ARG	NH1	280	A	ASN	OD1	2	3.03	3.86	32.11	999.99
288	A	THR	OG1	304	A	GLU	OE1	-	2.77	9.99	999.99	999.99
290	A	ARG	NH1	578	A	GLU	OE2	1	2.86	3.66	34.15	999.99
290	A	ARG	NH1	578	A	GLU	OE2	2	2.86	1.91	148.72	999.99
290	A	ARG	NH2	578	A	GLU	OE2	1	3.03	3.98	23.97	999.99
290	A	ARG	NH2	578	A	GLU	OE2	2	3.03	2.24	134.83	999.99
299	A	HIS	NE2	301	A	MET	SD	-	3.94	3.42	120.26	999.99
302	A	HIS	NE2	304	A	GLU	OE2	-	2.88	2.01	156.92	999.99
302	A	HIS	ND1	575	A	TYR	OH	-	2.98	2.15	150.43	999.99
304	A	GLU	OE2	302	A	HIS	NE2	1	2.88	3.58	42.26	999.99
304	A	GLU	OE2	302	A	HIS	NE2	2	2.88	1.85	162.66	999.99
308	A	SER	OG	306	A	ASP	OD1	-	2.78	9.99	999.99	999.99
308	A	SER	OG	306	A	ASP	OD2	-	3.19	9.99	999.99	999.99
311	A	LYS	NZ	309	A	ASP	OD1	-	3.15	9.99	999.99	999.99
319	A	HIS	ND1	140	A	TYR	OH	-	3.43	3.01	111.04	999.99
319	A	HIS	NE2	675	A	ASP	OD2	-	2.77	1.92	160.34	999.99
326	A	ASN	OD1	378	A	THR	OG1	1	2.88	2.41	105.45	999.99
326	A	ASN	OD1	378	A	THR	OG1	2	2.88	2.86	80.71	999.99
332	A	ASN	ND2	336	A	GLU	OE2	1	3.33	2.59	126.90	999.99
332	A	ASN	ND2	336	A	GLU	OE2	2	3.33	3.66	63.67	999.99
336	A	GLU	OE2	332	A	ASN	ND2	1	3.33	3.57	68.62	999.99
336	A	GLU	OE2	332	A	ASN	ND2	2	3.33	3.13	91.06	999.99
347	A	SER	OG	349	A	ASN	OD1	-	3.25	9.99	999.99	999.99
349	A	ASN	OD1	347	A	SER	OG	1	3.25	2.91	98.37	999.99
349	A	ASN	OD1	347	A	SER	OG	2	3.25	2.71	110.60	999.99
350	A	ASN	ND2	355	A	SER	OG	1	3.19	3.30	74.72	999.99
350	A	ASN	ND2	355	A	SER	OG	2	3.19	3.01	89.97	999.99
355	A	SER	OG	350	A	ASN	ND2	-	3.19	9.99	999.99	999.99
356	A	ASN	OD1	66	A	ASP	OD2	1	3.33	2.41	143.39	999.99
356	A	ASN	OD1	66	A	ASP	OD2	2	3.33	4.19	32.07	999.99
356	A	ASN	ND2	66	A	ASP	OD2	1	3.19	2.22	153.12	999.99
356	A	ASN	ND2	66	A	ASP	OD2	2	3.19	3.99	35.60	999.99

356	A	ASN	ND2	116	A	GLU	OE2	1	2.94	3.61	43.89	999.99
356	A	ASN	ND2	116	A	GLU	OE2	2	2.94	1.95	155.54	999.99
356	A	ASN	ND2	117	A	TYR	OH	1	3.29	3.09	91.38	999.99
356	A	ASN	ND2	117	A	TYR	OH	2	3.29	3.69	59.97	999.99
357	A	LYS	NZ	96	A	ASN	OD1	-	2.89	9.99	999.99	999.99
368	A	ARG	NH2	332	A	ASN	OD1	1	3.33	3.84	54.49	999.99
368	A	ARG	NH2	332	A	ASN	OD1	2	3.33	2.35	167.83	999.99
368	A	ARG	NE	343	A	ASP	OD1	-	2.86	1.88	158.16	999.99
368	A	ARG	NH1	343	A	ASP	OD1	1	3.27	2.45	134.60	999.99
368	A	ARG	NH1	343	A	ASP	OD1	2	3.27	4.20	24.46	999.99
368	A	ARG	NH1	343	A	ASP	OD2	1	3.12	2.11	161.84	999.99
368	A	ARG	NH1	343	A	ASP	OD2	2	3.12	3.59	55.69	999.99
369	A	THR	OG1	366	A	SER	OG	-	2.90	9.99	999.99	999.99
376	A	ASP	OD1	379	A	ASN	ND2	1	3.03	2.12	142.30	999.99
376	A	ASP	OD1	379	A	ASN	ND2	2	3.03	3.90	31.42	999.99
376	A	ASP	OD2	379	A	ASN	ND2	1	2.98	2.04	145.58	999.99
376	A	ASP	OD2	379	A	ASN	ND2	2	2.98	3.82	33.02	999.99
378	A	THR	OG1	326	A	ASN	OD1	-	2.88	9.99	999.99	999.99
378	A	THR	OG1	376	A	ASP	OD1	-	3.23	9.99	999.99	999.99
379	A	ASN	ND2	376	A	ASP	OD1	1	3.03	3.79	38.21	999.99
379	A	ASN	ND2	376	A	ASP	OD1	2	3.03	2.12	144.99	999.99
379	A	ASN	ND2	376	A	ASP	OD2	1	2.98	3.51	52.14	999.99
379	A	ASN	ND2	376	A	ASP	OD2	2	2.98	2.04	147.84	999.99
382	A	ARG	NH2	213	A	GLU	OE1	1	3.04	2.00	167.28	999.99
382	A	ARG	NH2	213	A	GLU	OE1	2	3.04	3.54	52.78	999.99
383	A	THR	OG1	213	A	GLU	OE2	-	2.80	9.99	999.99	999.99
387	A	TYR	OH	239	A	GLU	OE2	-	2.99	9.99	999.99	999.99
391	A	GLN	OE1	241	A	SER	OG	1	3.16	3.14	81.27	999.99
391	A	GLN	OE1	241	A	SER	OG	2	3.16	3.68	53.46	999.99
391	A	GLN	NE2	241	A	SER	OG	1	3.30	3.28	81.50	999.99
391	A	GLN	NE2	241	A	SER	OG	2	3.30	3.86	50.64	999.99
397	A	THR	OG1	395	A	GLU	OE2	-	2.76	9.99	999.99	999.99
404	A	LYS	NZ	411	A	GLU	OE1	-	2.88	9.99	999.99	999.99
408	A	SER	OG	221	A	GLU	OE1	-	2.72	9.99	999.99	999.99
408	A	SER	OG	221	A	GLU	OE2	-	3.39	9.99	999.99	999.99
424	A	ARG	NH2	422	A	GLU	OE1	1	3.32	3.77	57.58	999.99
424	A	ARG	NH2	422	A	GLU	OE1	2	3.32	2.70	120.36	999.99
425	A	ARG	NE	433	A	ASP	OD2	-	2.76	1.80	152.23	999.99
425	A	ARG	NH1	433	A	ASP	OD2	1	3.19	2.40	131.60	999.99
425	A	ARG	NH1	433	A	ASP	OD2	2	3.19	4.13	23.50	999.99
436	A	SER	OG	398	A	GLU	OE1	-	3.48	9.99	999.99	999.99
436	A	SER	OG	398	A	GLU	OE2	-	2.69	9.99	999.99	999.99
450	A	ARG	NH1	92	A	GLU	OE1	1	2.95	3.71	37.61	999.99
450	A	ARG	NH1	92	A	GLU	OE1	2	2.95	1.95	157.79	999.99
450	A	ARG	NH2	92	A	GLU	OE1	1	3.26	4.21	22.64	999.99

450	A	ARG	NH2	92	A	GLU	OE1	2	3.26	2.46	135.63	999.99
450	A	ARG	NH2	92	A	GLU	OE2	1	3.21	3.85	45.98	999.99
450	A	ARG	NH2	92	A	GLU	OE2	2	3.21	2.49	128.15	999.99
450	A	ARG	NE	93	A	GLU	OE2	-	2.98	2.00	161.03	999.99
455	A	TYR	OH	87	A	GLN	NE2	-	3.19	9.99	999.99	999.99
460	A	SER	OG	314	A	TYR	OH	-	2.85	9.99	999.99	999.99
461	A	SER	OG	546	A	GLU	OE1	-	2.62	9.99	999.99	999.99
465	A	HIS	NE2	545	A	GLN	OE1	-	3.36	2.84	119.12	999.99
472	A	CYS	SG	575	A	TYR	OH	-	3.46	9.99	999.99	999.99
478	A	TYR	OH	486	A	ASN	ND2	-	3.42	9.99	999.99	999.99
480	A	THR	OG1	482	A	SER	OG	-	2.81	9.99	999.99	999.99
484	A	ARG	NE	432	A	GLN	OE1	-	3.01	2.35	121.15	999.99
484	A	ARG	NH1	432	A	GLN	OE1	1	3.04	2.28	128.17	999.99
484	A	ARG	NH1	432	A	GLN	OE1	2	3.04	3.87	33.23	999.99
484	A	ARG	NH1	433	A	ASP	OD2	1	2.89	3.74	31.35	999.99
484	A	ARG	NH1	433	A	ASP	OD2	2	2.89	1.98	143.84	999.99
484	A	ARG	NH2	433	A	ASP	OD2	1	2.91	3.82	26.60	999.99
484	A	ARG	NH2	433	A	ASP	OD2	2	2.91	2.07	140.10	999.99
486	A	ASN	ND2	478	A	TYR	OH	1	3.42	4.14	41.59	999.99
486	A	ASN	ND2	478	A	TYR	OH	2	3.42	2.53	142.68	999.99
495	A	ARG	NH1	477	A	GLU	OE2	1	3.43	4.37	23.22	999.99
495	A	ARG	NH1	477	A	GLU	OE2	2	3.43	2.62	134.58	999.99
495	A	ARG	NH2	477	A	GLU	OE2	1	2.91	3.67	38.75	999.99
495	A	ARG	NH2	477	A	GLU	OE2	2	2.91	1.93	164.69	999.99
505	A	ARG	NE	498	A	GLU	OE2	-	3.39	3.62	69.20	999.99
505	A	ARG	NH1	498	A	GLU	OE2	1	3.34	3.49	73.18	999.99
505	A	ARG	NH1	498	A	GLU	OE2	2	3.34	3.79	57.29	999.99
514	A	ARG	NE	87	A	GLN	OE1	-	3.32	2.50	136.46	999.99
514	A	ARG	NE	87	A	GLN	NE2	-	3.47	2.61	140.66	999.99
514	A	ARG	NH1	87	A	GLN	OE1	1	3.39	2.57	135.44	999.99
514	A	ARG	NH1	87	A	GLN	OE1	2	3.39	4.20	34.75	999.99
514	A	ARG	NH1	144	A	ASP	OD2	1	2.95	3.53	48.69	999.99
514	A	ARG	NH1	144	A	ASP	OD2	2	2.95	1.97	153.26	999.99
514	A	ARG	NE	147	A	ASP	OD1	-	2.99	2.50	108.44	999.99
514	A	ARG	NE	147	A	ASP	OD2	-	3.26	2.49	131.10	999.99
514	A	ARG	NH1	147	A	ASP	OD1	1	3.17	2.69	107.97	999.99
514	A	ARG	NH1	147	A	ASP	OD1	2	3.17	3.95	36.71	999.99
515	A	LYS	NZ	315	A	GLU	OE2	-	3.06	9.99	999.99	999.99
515	A	LYS	NZ	318	A	ASP	OD2	-	2.94	9.99	999.99	999.99
517	A	GLN	NE2	144	A	ASP	OD1	1	3.35	3.63	66.04	999.99
517	A	GLN	NE2	144	A	ASP	OD1	2	3.35	2.88	107.22	999.99
519	A	ARG	NH2	517	A	GLN	OE1	1	3.01	3.50	54.43	999.99
519	A	ARG	NH2	517	A	GLN	OE1	2	3.01	2.05	158.97	999.99
526	A	THR	OG1	626	A	HIS	ND1	-	3.26	9.99	999.99	999.99
545	A	GLN	OE1	465	A	HIS	NE2	1	3.36	2.93	104.00	999.99

545	A	GLN	OE1	465	A	HIS	NE2	2	3.36	3.82	56.94	999.99
559	A	GLU	OE1	615	A	HIS	NE2	1	2.86	1.99	136.96	999.99
559	A	GLU	OE1	615	A	HIS	NE2	2	2.86	3.68	34.42	999.99
559	A	GLU	OE2	615	A	HIS	NE2	1	2.96	2.13	132.58	999.99
559	A	GLU	OE2	615	A	HIS	NE2	2	2.96	3.83	30.56	999.99
567	A	ARG	NH2	297	A	GLU	OE2	1	3.10	2.22	139.01	999.99
567	A	ARG	NH2	297	A	GLU	OE2	2	3.10	3.27	71.27	999.99
568	A	ARG	NH1	570	A	GLU	OE1	1	3.26	2.85	103.65	999.99
568	A	ARG	NH1	570	A	GLU	OE1	2	3.26	3.09	89.66	999.99
568	A	ARG	NE	571	A	GLU	OE2	-	3.41	2.82	117.11	999.99
569	A	SER	OG	598	A	GLU	OE2	-	2.75	9.99	999.99	999.99
575	A	TYR	OH	302	A	HIS	ND1	-	2.98	9.99	999.99	999.99
592	A	ASN	OD1	612	A	ASP	OD2	1	2.51	2.80	63.64	999.99
592	A	ASN	OD1	612	A	ASP	OD2	2	2.51	2.73	66.82	999.99
592	A	ASN	ND2	612	A	ASP	OD2	1	3.26	3.50	68.62	999.99
592	A	ASN	ND2	612	A	ASP	OD2	2	3.26	3.95	43.33	999.99
597	A	ARG	NH2	297	A	GLU	OE2	1	3.35	3.21	88.27	999.99
597	A	ARG	NH2	297	A	GLU	OE2	2	3.35	3.16	91.93	999.99
606	A	GLN	NE2	639	A	ASP	OD1	1	3.07	3.73	44.71	999.99
606	A	GLN	NE2	639	A	ASP	OD1	2	3.07	2.03	169.49	999.99
606	A	GLN	NE2	639	A	ASP	OD2	1	3.23	3.73	54.47	999.99
606	A	GLN	NE2	639	A	ASP	OD2	2	3.23	2.58	119.94	999.99
610	A	LYS	NZ	606	A	GLN	OE1	-	3.27	9.99	999.99	999.99
612	A	ASP	OD2	592	A	ASN	OD1	1	2.51	2.24	91.77	999.99
612	A	ASP	OD2	592	A	ASN	OD1	2	2.51	2.49	79.05	999.99
612	A	ASP	OD2	592	A	ASN	ND2	1	3.26	3.47	70.06	999.99
612	A	ASP	OD2	592	A	ASN	ND2	2	3.26	2.47	131.31	999.99
615	A	HIS	NE2	559	A	GLU	OE1	-	2.86	1.96	162.83	999.99
615	A	HIS	NE2	559	A	GLU	OE2	-	2.96	2.25	132.96	999.99
615	A	HIS	ND1	618	A	GLN	OE1	-	2.88	2.04	151.56	999.99
618	A	GLN	OE1	615	A	HIS	ND1	1	2.88	2.91	77.66	999.99
618	A	GLN	OE1	615	A	HIS	ND1	2	2.88	2.13	125.27	999.99
626	A	HIS	ND1	526	A	THR	OG1	-	3.26	2.80	113.01	999.99
634	A	ARG	NH2	209	A	ASP	OD1	1	2.92	2.23	120.59	999.99
634	A	ARG	NH2	209	A	ASP	OD1	2	2.92	2.94	78.91	999.99
638	A	ARG	NH2	179	A	GLU	OE1	1	2.90	3.55	44.72	999.99
638	A	ARG	NH2	179	A	GLU	OE1	2	2.90	2.03	142.48	999.99
638	A	ARG	NH2	641	A	GLN	NE2	1	3.44	3.33	87.02	999.99
638	A	ARG	NH2	641	A	GLN	NE2	2	3.44	3.38	85.18	999.99
639	A	ASP	OD1	606	A	GLN	NE2	1	3.07	2.37	121.97	999.99
639	A	ASP	OD1	606	A	GLN	NE2	2	3.07	3.80	40.71	999.99
639	A	ASP	OD2	606	A	GLN	NE2	1	3.23	2.60	117.90	999.99
639	A	ASP	OD2	606	A	GLN	NE2	2	3.23	4.04	36.04	999.99
641	A	GLN	NE2	179	A	GLU	OE1	1	3.12	2.31	132.47	999.99
641	A	GLN	NE2	179	A	GLU	OE1	2	3.12	3.21	75.54	999.99

641	A	GLN	NE2	645	A	TYR	OH	1	2.87	3.43	50.58	999.99
641	A	GLN	NE2	645	A	TYR	OH	2	2.87	1.89	155.61	999.99
645	A	TYR	OH	641	A	GLN	NE2	-	2.87	9.99	999.99	999.99
675	A	ASP	OD2	319	A	HIS	NE2	1	2.77	1.89	137.87	999.99
675	A	ASP	OD2	319	A	HIS	NE2	2	2.77	3.05	64.81	999.99
678	A	SER	OG	175	A	ASN	ND2	-	3.06	9.99	999.99	999.99

Dd-a = Distance Between Donor and Acceptor
Dh-a = Distance Between Hydrogen and Acceptor
A(d-H-N) = Angle Between Donor-H-N
A(a-O=C) = Angle Between Acceptor-O=C
MO = Multiple Occupancy
Note that angles that are undefined are written as 999.99

Intraprotein Ionic Interactions

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Ionic Interactions within 6 Angstroms

Position	Residue	Chain	Position	Residue	Chain
65	LYS	A	118	ASP	A
65	LYS	A	151	ASP	A
66	ASP	A	72	LYS	A
71	GLU	A	75	LYS	A
72	LYS	A	354	GLU	A
74	LYS	A	127	GLU	A
78	ARG	A	352	ASP	A
92	GLU	A	357	LYS	A
92	GLU	A	450	ARG	A
93	GLU	A	450	ARG	A
97	ARG	A	213	GLU	A
100	LYS	A	388	GLU	A
100	LYS	A	446	GLU	A
101	ASP	A	104	ARG	A
101	ASP	A	220	ARG	A
103	HIS	A	238	GLU	A

104	ARG	A	238	GLU	A
104	ARG	A	388	GLU	A
108	ARG	A	238	GLU	A
115	GLU	A	279	LYS	A
142	GLU	A	180	HIS	A
144	ASP	A	514	ARG	A
147	ASP	A	514	ARG	A
176	LYS	A	207	ASP	A
179	GLU	A	638	ARG	A
179	GLU	A	664	LYS	A
189	ASP	A	199	ARG	A
190	LYS	A	193	GLU	A
193	GLU	A	199	ARG	A
199	ARG	A	202	GLU	A
209	ASP	A	634	ARG	A
213	GLU	A	382	ARG	A
214	GLU	A	413	LYS	A
220	ARG	A	221	GLU	A
239	GLU	A	403	ARG	A
243	ARG	A	246	GLU	A
243	ARG	A	442	ASP	A
243	ARG	A	446	GLU	A
254	ASP	A	257	LYS	A
262	GLU	A	267	LYS	A
267	LYS	A	270	GLU	A
277	ASP	A	279	LYS	A
290	ARG	A	304	GLU	A
290	ARG	A	577	GLU	A
290	ARG	A	578	GLU	A
297	GLU	A	567	ARG	A
297	GLU	A	597	ARG	A
298	ARG	A	572	ASP	A
302	HIS	A	304	GLU	A
304	GLU	A	470	HIS	A
309	ASP	A	311	LYS	A
315	GLU	A	515	LYS	A
318	ASP	A	515	LYS	A
319	HIS	A	675	ASP	A
327	ASP	A	487	LYS	A
343	ASP	A	368	ARG	A
376	ASP	A	454	ARG	A
388	GLU	A	443	HIS	A
404	LYS	A	411	GLU	A
422	GLU	A	424	ARG	A
422	GLU	A	481	ARG	A

425	ARG	A	433	ASP	A
433	ASP	A	484	ARG	A
443	HIS	A	446	GLU	A
463	LYS	A	546	GLU	A
477	GLU	A	487	LYS	A
477	GLU	A	495	ARG	A
498	GLU	A	505	ARG	A
502	GLU	A	505	ARG	A
559	GLU	A	615	HIS	A
568	ARG	A	570	GLU	A
568	ARG	A	571	GLU	A
568	ARG	A	598	GLU	A
576	ARG	A	577	GLU	A
610	LYS	A	639	ASP	A
613	LYS	A	646	ASP	A
613	LYS	A	650	GLU	A
646	ASP	A	656	HIS	A
661	ASP	A	664	LYS	A

D570E Intraprotein Aromatic-Aromatic Interactions


[help]

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DOG_POR_D570E_snapshot10.pdb

Aromatic-Aromatic Interactions within 4.5 and 7 Angstroms

Position	Residue	Chain	Position	Residue	Chain	D(centroid-centroid)	Dihedral Angle
69	PHE	A	117	TYR	A	6.42	103.23
69	PHE	A	83	PHE	A	5.23	95.17
83	PHE	A	117	TYR	A	6.92	107.70
83	PHE	A	135	PHE	A	5.56	15.12
83	PHE	A	152	PHE	A	6.78	164.76
105	TYR	A	224	TRP	A	4.72	8.16
135	PHE	A	152	PHE	A	5.55	171.20
135	PHE	A	168	TYR	A	6.79	70.43
140	TYR	A	455	TYR	A	6.22	120.96
152	PHE	A	155	TRP	A	6.16	173.90
171	PHE	A	201	PHE	A	5.28	46.75

171	PHE	A	216	PHE	A	6.35	37.81
171	PHE	A	223	PHE	A	5.14	80.76
201	PHE	A	219	TRP	A	6.86	77.07
201	PHE	A	223	PHE	A	5.15	127.38
223	PHE	A	224	TRP	A	4.58	53.28
259	TYR	A	374	TYR	A	6.57	85.96
276	PHE	A	282	PHE	A	5.00	122.05
323	TYR	A	512	PHE	A	5.44	41.01
361	PHE	A	374	TYR	A	6.12	158.80
373	TYR	A	374	TYR	A	6.55	54.14
419	TRP	A	434	TYR	A	5.21	121.10
455	TYR	A	512	PHE	A	6.09	93.13
518	PHE	A	540	PHE	A	5.72	131.19
518	PHE	A	543	PHE	A	6.17	136.72
518	PHE	A	628	TYR	A	4.84	108.09
540	PHE	A	543	PHE	A	5.37	88.66
540	PHE	A	628	TYR	A	6.88	89.62
543	PHE	A	628	TYR	A	5.00	85.35
564	TYR	A	573	TYR	A	5.51	43.42
573	TYR	A	595	PHE	A	6.28	47.74
617	TRP	A	662	TYR	A	5.97	50.97
644	PHE	A	672	TYR	A	5.65	81.99

Intraprotein Aromatic-Sulphur Interactions

  [help]

Rasmol **Jmol**

DOG_POR_D570E_snapshot10.pdb

Aromatic-Sulphur Interactions within 5.3 Angstroms

Position	Residue	Chain	Position	Residue	Chain	D(Centroid-Sulphur)	Angle
105	TYR	A	228	CYS	A	4.63	122.12
153	TYR	A	184	MET	A	5.18	108.83
171	PHE	A	136	CYS	A	4.95	132.94
181	PHE	A	205	MET	A	4.85	58.31
323	TYR	A	263	MET	A	4.07	159.83
361	PHE	A	363	CYS	A	4.40	40.73
367	TYR	A	346	MET	A	4.52	31.86

518	PHE	A	630	CYS	A	5.21	139.85
540	PHE	A	530	MET	A	4.43	128.41
543	PHE	A	530	MET	A	4.70	59.52
573	TYR	A	566	CYS	A	4.92	42.37
595	PHE	A	566	CYS	A	4.71	65.95
677	TRP	A	630	CYS	A	4.55	125.38

Intraprotein Cation-Pi Interactions

  [help]

Rasmol **Jmol**

DOG_POR_D570E_snapshot10.pdb

Cation-Pi Interactions within 6 Angstroms

Position	Residue	Chain	Position	Residue	Chain	D(cation-Pi)	Angle
84	TYR	A	357	LYS	A	4.64	137.60
94	PHE	A	97	ARG	A	4.70	104.55
117	TYR	A	72	LYS	A	4.95	84.94
140	TYR	A	514	ARG	A	4.33	132.96
181	PHE	A	176	LYS	A	5.63	141.16
181	PHE	A	186	LYS	A	5.72	63.86
216	PHE	A	97	ARG	A	5.17	140.23
231	PHE	A	167	LYS	A	5.22	55.07
387	TYR	A	403	ARG	A	5.02	6.48
419	TRP	A	425	ARG	A	5.76	117.69
493	TRP	A	497	LYS	A	4.80	135.34
549	TRP	A	463	LYS	A	5.73	33.48
575	TYR	A	290	ARG	A	5.65	52.42