



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 09:43 AM JST

PDB ID : 5XTH / pdb_00005xth
EMDB ID : EMD-6775
Title : Cryo-EM structure of human respiratory supercomplex I1III2IV1
Authors : Gu, J.; Wu, M.; Yang, M.
Deposited on : 2017-06-19
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

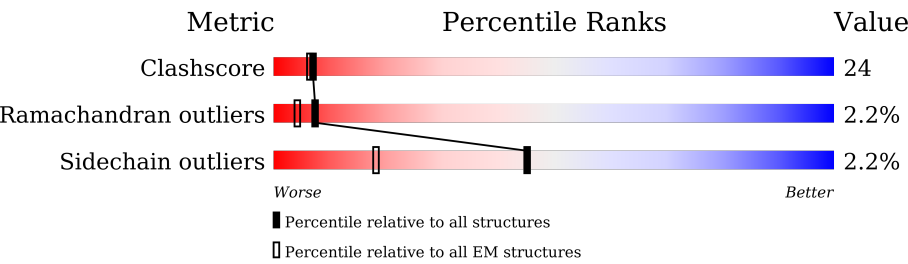
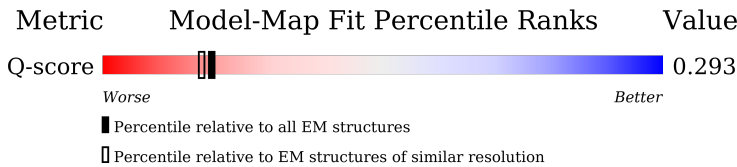
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	<div><div>6%</div><div>47%</div><div>51%</div><div>.</div></div>
2	B	176	<div><div>45%</div><div>53%</div><div>.</div></div>
3	C	156	<div><div>51%</div><div>48%</div><div>.</div></div>
4	E	113	<div><div>12%</div><div>44%</div><div>53%</div><div>.</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	83	
6	G	85	
6	X	85	
7	H	112	
8	I	110	
9	J	337	
10	K	33	
11	L	118	
12	M	687	
13	N	143	
14	O	212	
15	P	208	
16	Q	430	
17	S	70	
18	T	95	
19	U	83	
20	V	140	
21	W	138	
22	Y	59	
23	Z	80	
24	a	138	
25	b	124	
26	c	153	
27	d	171	
28	e	97	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	f	47	
30	g	119	
31	h	104	
32	i	347	
33	j	115	
34	k	97	
35	l	603	
36	m	174	
37	n	56	
38	o	128	
39	p	172	
40	r	459	
41	s	318	
42	u	169	
43	v	122	
44	w	320	
45	x	514	
46	y	227	
47	z	261	
48	0	144	
49	1	109	
50	2	98	
51	3	84	
52	4	75	
53	5	73	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	6	56	
55	7	49	
56	8	47	
57	9	43	
58	AA	81	
58	AN	81	
59	AB	57	
59	AO	57	
60	AC	196	
60	AP	196	
61	AD	62	
61	AQ	62	
62	AE	74	
62	AR	74	
63	AF	106	
63	AS	106	
64	AG	51	
64	AT	51	
65	AH	241	
65	AU	241	
66	AJ	378	
66	AV	378	
67	AK	419	
67	AW	419	
68	AL	446	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
68	AY	446	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
69	SF4	A	501	-	-	X	-
69	SF4	B	302	-	-	X	-
69	SF4	M	801	-	-	X	-
70	FMN	A	502	-	-	X	-
71	PLX	b	201	-	-	X	-
73	NDP	J	401	-	-	X	-
74	FES	AC	301	-	-	X	-
74	FES	AP	301	-	-	X	-
74	FES	O	301	-	-	X	-
75	CDL	AG	101	-	-	X	-
75	CDL	AL	502	-	-	X	-
76	PEE	AH	401	-	-	X	-
76	PEE	AL	503	-	-	X	-
76	PEE	AU	401	-	-	X	-
76	PEE	AV	403	-	-	X	-
76	PEE	AY	502	-	-	X	-
76	PEE	V	202	-	-	X	-
76	PEE	l	701	-	-	X	-

2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 115642 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3322	2096	594	612	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1420	893	243	271	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1249	794	227	214	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	113	Total	C	N	O	S	0	0
			968	623	178	162	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	83	Total	C	N	O	S	0	0
			670	422	124	122	2		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	85	Total	C	N	O	S	0	0
			672	434	99	134	5		
6	X	85	Total	C	N	O	S	0	0
			686	442	101	138	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			922	593	157	169	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	95	Total	C	N	O	S	0	0
			769	483	146	138	2		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	337	Total	C	N	O	S	0	0
			2712	1759	482	463	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	33	Total	C	N	O	S	0	0
			274	173	47	53	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	118	Total	C	N	O	S	0	0
			964	608	173	179	4		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	687	Total	C	N	O	S	0	0
			5274	3310	917	1009	38		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	143	Total	C	N	O	S	0	0
			1195	770	210	212	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	212	Total	C	N	O	S	0	0
			1643	1047	276	310	10		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1730	1117	297	313	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	430	Total	C	N	O	S	0	0
			3460	2214	599	624	23		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			568	367	101	96	4		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	95	Total	C	N	O	S	0	0
			742	459	138	142	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			647	427	105	113	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1038	668	178	187	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	138	Total	C	N	O	S	0	0
			1135	727	202	200	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	59	Total	C	N	O	S	0	0
			533	354	87	91	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	80	Total	C	N	O	S	0	0
			648	426	110	110	2		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1174	771	199	202	2		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	124	Total	C	N	O	S	0	0
			1059	697	181	176	5		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	153	Total	C	N	O	S	0	0
			1236	795	208	222	11		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	171	Total	C	N	O	S	0	0
			1418	885	262	259	12		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	97	Total	C	N	O	S	0	0
			810	522	132	152	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	47	Total	C	N	O	0	0
			405	269	69	67		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	119	Total	C	N	O	S	0	0
			1004	658	173	169	4		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	104	Total	C	N	O	S	0	0
			863	546	161	150	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2735	1819	421	470	25		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	115	Total	C	N	O	S	0	0
			919	626	132	152	9		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	97	Total	C	N	O	S	0	0
			740	487	113	127	13		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4717	3119	742	823	33		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	174	Total	C	N	O	S	0	0
			1313	879	194	229	11		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			473	305	85	80	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	128	Total	C	N	O	S	0	0
			1066	685	192	187	2		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	172	Total	C	N	O	S	0	0
			1495	961	265	261	8		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3629	2411	569	619	30		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	318	Total	C	N	O	S	0	0
			2509	1678	380	435	16		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	169	Total	C	N	O	S	0	0
			1394	886	247	252	9		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	111	Total	C	N	O	S	0	0
			921	569	187	156	9		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2474	1573	429	464	8		

- Molecule 45 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		

- Molecule 46 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	y	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		

- Molecule 47 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		

- Molecule 48 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 49 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

- Molecule 50 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	98	Total	C	N	O	S	0	0
			748	464	134	145	5		

- Molecule 51 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	84	Total	C	N	O	S	0	0
			672	431	129	111	1		

- Molecule 52 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 53 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	5	73	Total	C	N	O	S	0	0
			598	388	107	99	4		

- Molecule 54 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	6	56	Total	C	N	O	S	0	0
			441	285	73	80	3		

- Molecule 55 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	7	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	8	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	9	43	Total	C	N	O	0	0
			335	223	53	59		

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AA	81	Total	C	N	O	S	0	0
			694	450	126	117	1		
58	AN	81	Total	C	N	O	S	0	0
			687	444	126	116	1		

- Molecule 59 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AB	57	Total	C	N	O	S	0	0
			413	261	75	76	1		
59	AO	57	Total	C	N	O	S	0	0
			409	259	74	75	1		

- Molecule 60 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AC	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		
60	AP	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		

- Molecule 61 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AD	62	Total	C	N	O	S	0	0
			509	332	87	89	1		
61	AQ	62	Total	C	N	O	S	0	0
			509	332	87	89	1		

- Molecule 62 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AE	74	Total	C	N	O	S	0	0
			580	351	108	116	5		
62	AR	74	Total	C	N	O	S	0	0
			580	351	108	116	5		

- Molecule 63 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AF	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AS	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

- Molecule 64 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AG	51	Total	C	N	O		0	0
			425	287	72	66			
64	AT	51	Total	C	N	O		0	0
			425	287	72	66			

- Molecule 65 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AH	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		
65	AU	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		

- Molecule 66 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AJ	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		
66	AV	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		

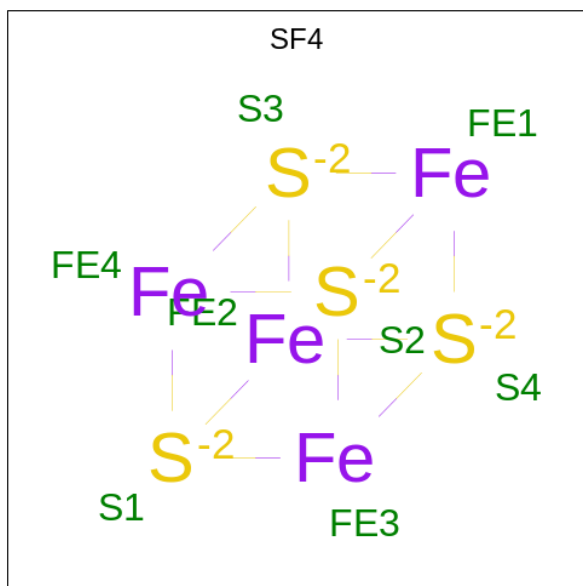
- Molecule 67 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AK	419	Total	C	N	O	S	0	0
			3159	1986	553	610	10		
67	AW	419	Total	C	N	O	S	0	0
			3162	1989	553	610	10		

- Molecule 68 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

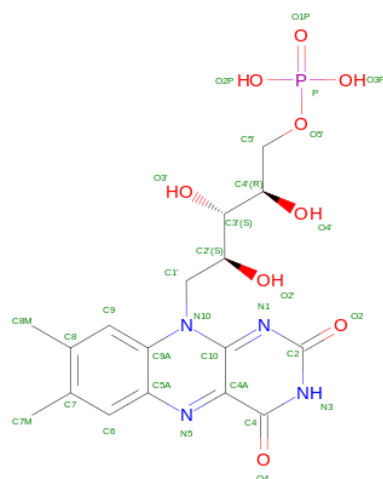
Mol	Chain	Residues	Atoms					AltConf	Trace
68	AL	446	Total	C	N	O	S	0	0
			3453	2169	603	661	20		
68	AY	446	Total	C	N	O	S	0	0
			3453	2169	603	661	20		

- Molecule 69 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



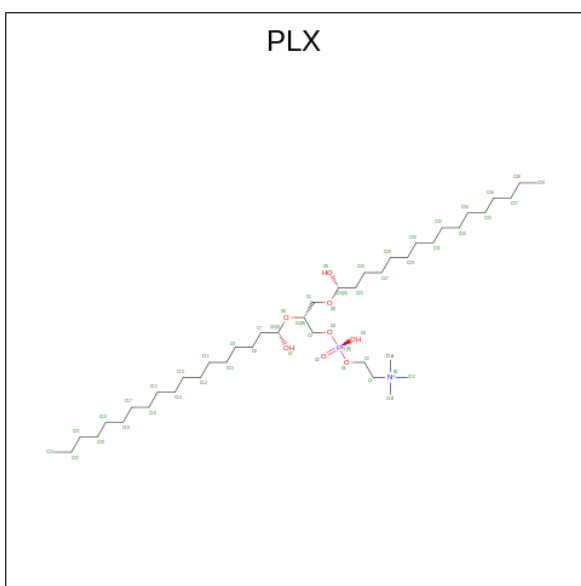
Mol	Chain	Residues	Atoms			AltConf
69	A	1	Total	Fe	S	0
			8	4	4	
69	B	1	Total	Fe	S	0
			8	4	4	
69	B	1	Total	Fe	S	0
			8	4	4	
69	C	1	Total	Fe	S	0
			8	4	4	
69	M	1	Total	Fe	S	0
			8	4	4	
69	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 70 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



Mol	Chain	Residues	Atoms					AltConf
70	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 71 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P).



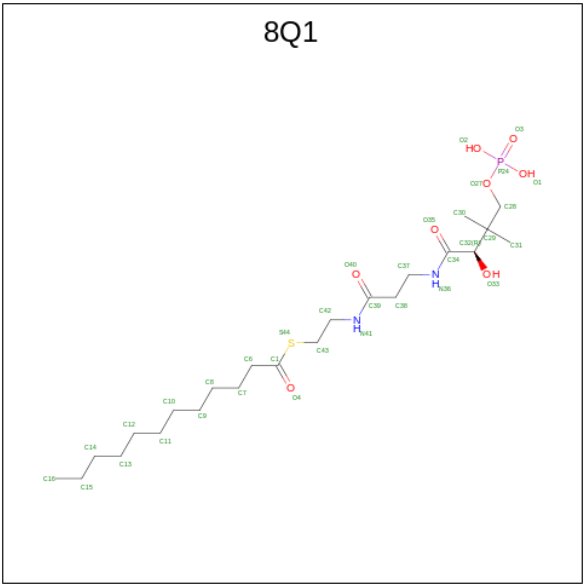
Mol	Chain	Residues	Atoms					AltConf
71	B	1	Total 52	C 42	N 1	O 8	P 1	0
71	U	1	Total 52	C 42	N 1	O 8	P 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
71	V	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	b	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	AL	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	AQ	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	AT	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 72 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



Mol	Chain	Residues	Atoms						AltConf
72	p	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

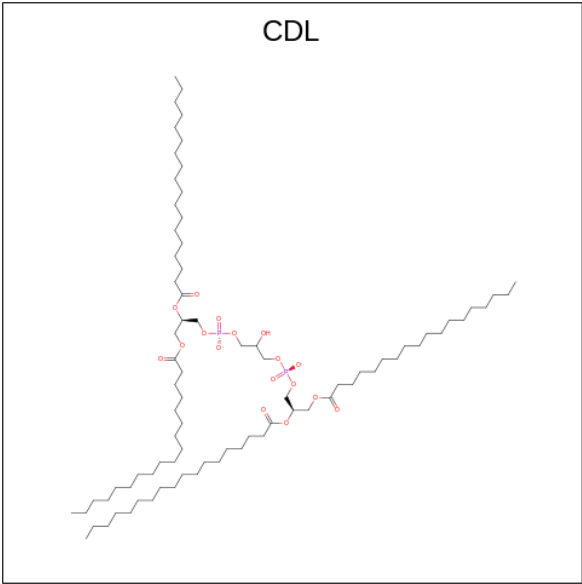
- # NDP

Mol	Chain	Residues	Atoms					AltConf
73	J	1	Total 48	C 21	N 7	O 17	P 3	0

- FES
-
- S1 S⁻² Fe FE2
- Fe S⁻² S2 FE1

Mol	Chain	Residues	Atoms			AltConf
74	M	1	Total	Fe	S	0
			4	2	2	
74	O	1	Total	Fe	S	0
			4	2	2	
74	AC	1	Total	Fe	S	0
			4	2	2	
74	AP	1	Total	Fe	S	0
			4	2	2	

- Molecule 75 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



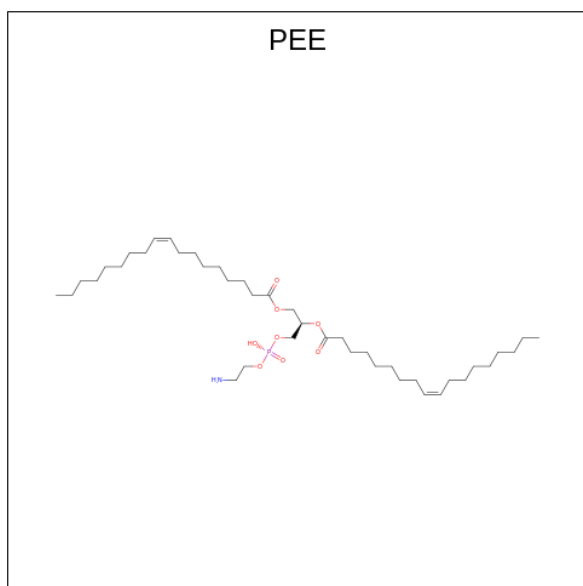
Mol	Chain	Residues	Atoms				AltConf
75	V	1	Total	C	O	P	0
			63	44	17	2	
75	i	1	Total	C	O	P	0
			64	45	17	2	
75	l	1	Total	C	O	P	0
			64	45	17	2	
75	l	1	Total	C	O	P	0
			64	45	17	2	
75	n	1	Total	C	O	P	0
			64	45	17	2	
75	AA	1	Total	C	O	P	0
			64	45	17	2	
75	AG	1	Total	C	O	P	0
			64	45	17	2	
75	AH	1	Total	C	O	P	0
			64	45	17	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
75	AJ	1	Total	C	O	P	0
			64	45	17	2	
75	AJ	1	Total	C	O	P	0
			64	45	17	2	
75	AL	1	Total	C	O	P	0
			64	45	17	2	
75	AN	1	Total	C	O	P	0
			64	45	17	2	
75	AU	1	Total	C	O	P	0
			64	45	17	2	
75	AY	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 76 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
76	V	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	W	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	1	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	1	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	AH	1	Total	C	N	O	P	0
			49	39	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
76	AJ	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	AL	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	AU	1	Total	C	N	O	P	0
			41	31	1	8	1	
76	AV	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	AY	1	Total	C	N	O	P	0
			49	39	1	8	1	

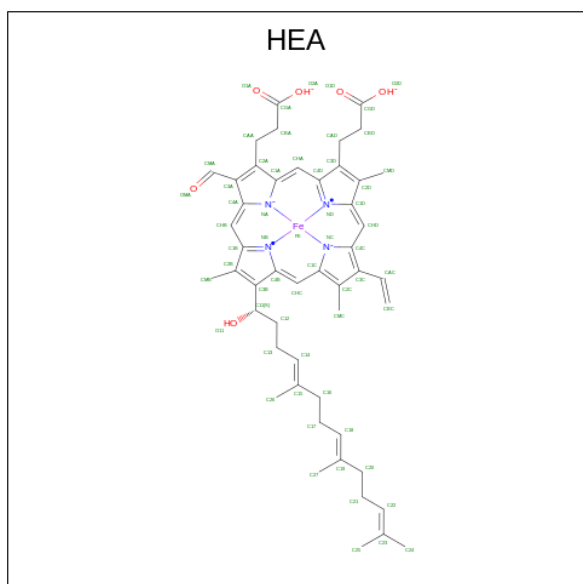
- Molecule 77 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
77	x	1	Total	Cu	0
			1	1	
77	y	2	Total	Cu	0
			2	2	

- Molecule 78 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
78	x	1	Total	Mg	0
			1	1	

- Molecule 79 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).

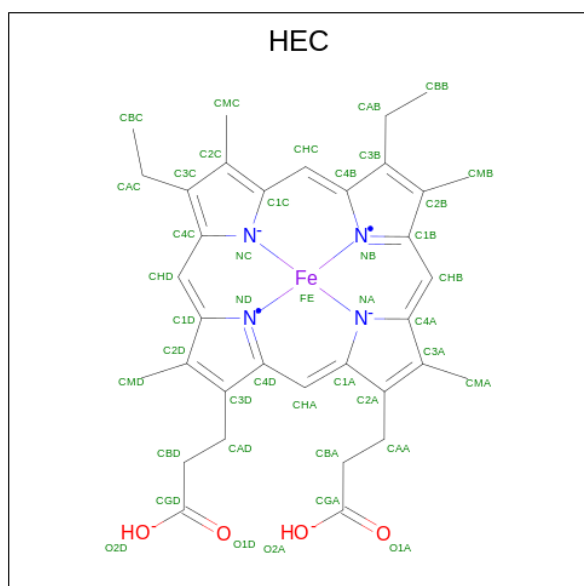


Mol	Chain	Residues	Atoms					AltConf
79	x	1	Total 60	C 49	Fe 1	N 4	O 6	0
79	x	1	Total 60	C 49	Fe 1	N 4	O 6	0

- Molecule 80 is ZINC ION (CCD ID: ZN) (formula: Zn).

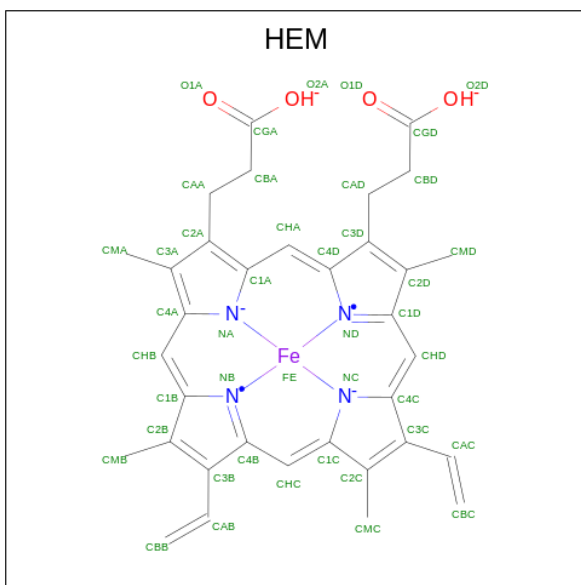
Mol	Chain	Residues	Atoms	AltConf
80	2	1	Total Zn 1 1	0

- Molecule 81 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms					AltConf
81	AH	1	Total 43	C 34	Fe 1	N 4	O 4	0
81	AU	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 82 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

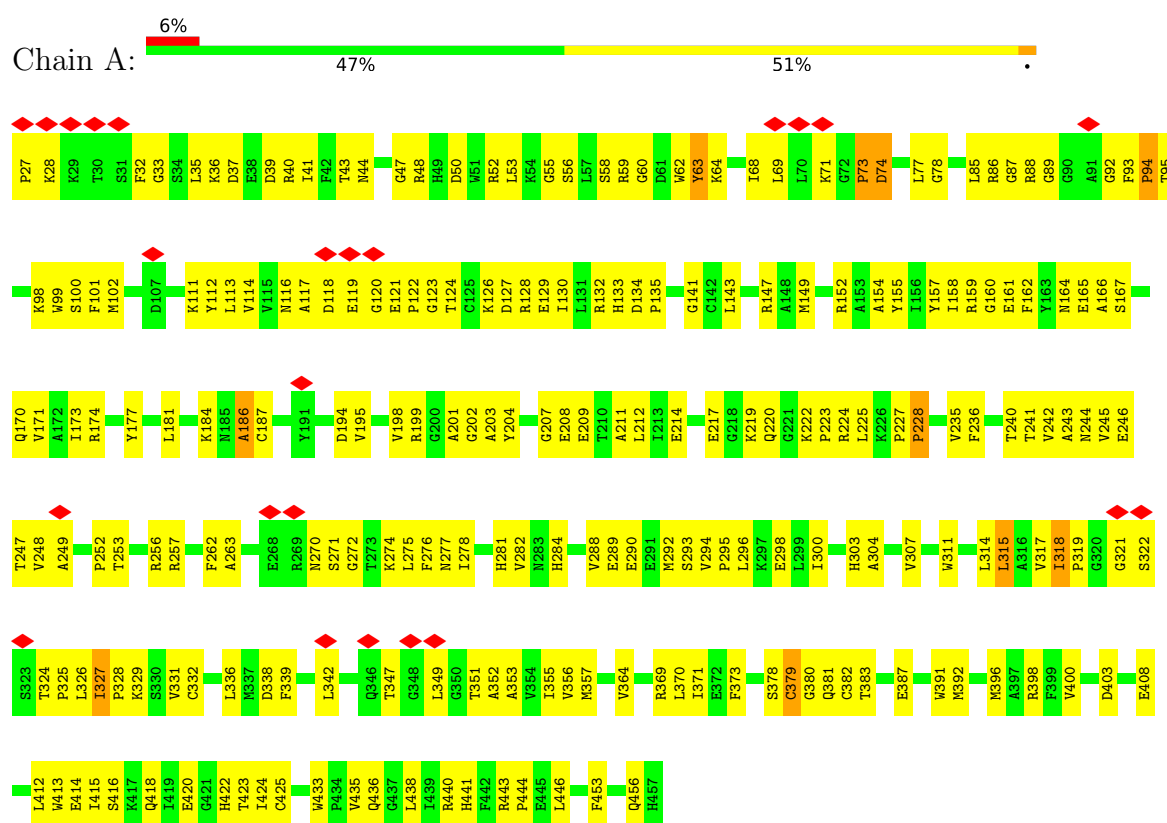


Mol	Chain	Residues	Atoms					AltConf
82	AJ	1	Total 43	C 34	Fe 1	N 4	O 4	0
82	AJ	1	Total 43	C 34	Fe 1	N 4	O 4	0
82	AV	1	Total 43	C 34	Fe 1	N 4	O 4	0
82	AV	1	Total 43	C 34	Fe 1	N 4	O 4	0

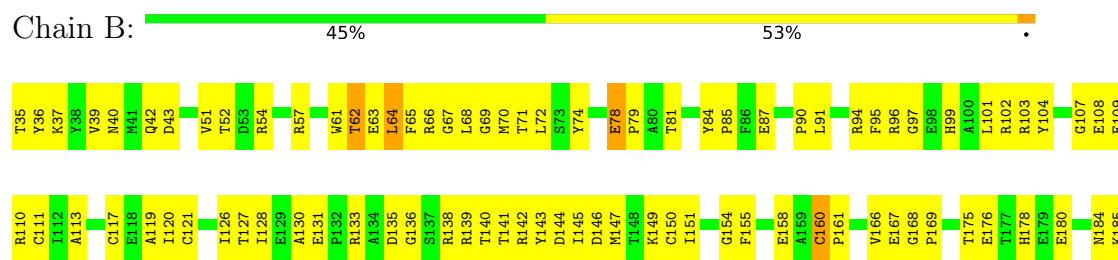
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



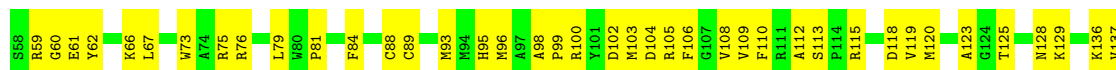
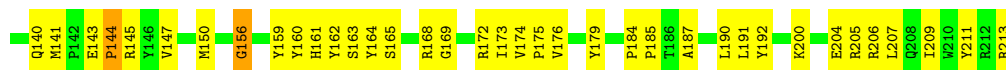
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial





- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain C: 51% 48%



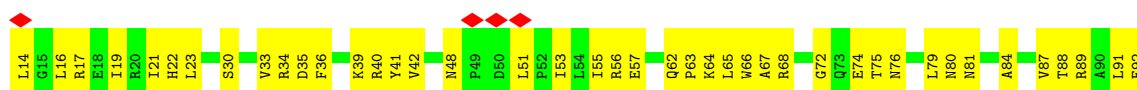
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E: 12% 44% 53%



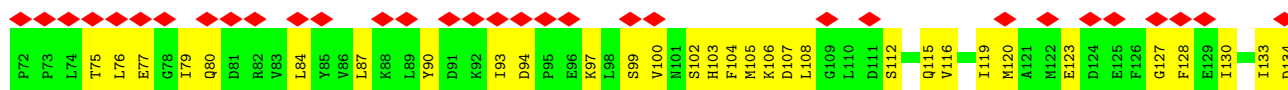
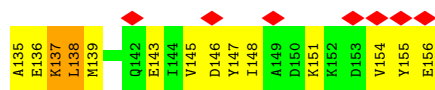
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F: 5% 49% 51%



- Molecule 6: Acyl carrier protein, mitochondrial

Chain G: 46% 47% 51%

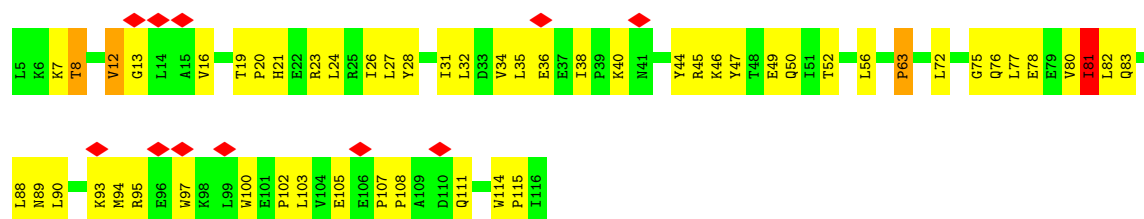


- Molecule 6: Acyl carrier protein, mitochondrial

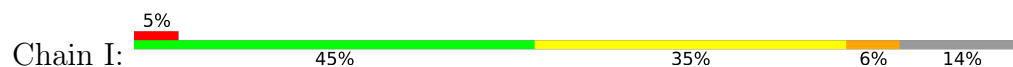
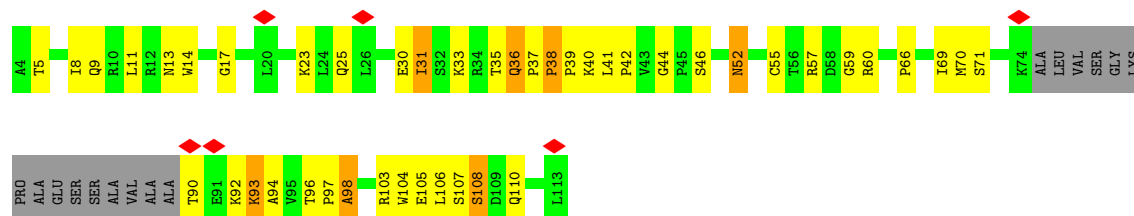
Chain X: 53% 45%



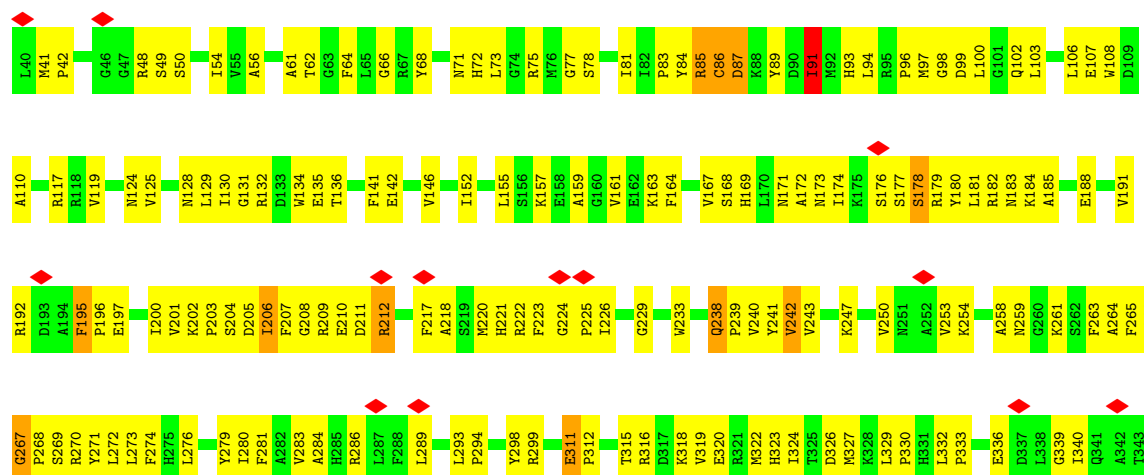
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

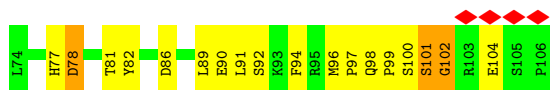


- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

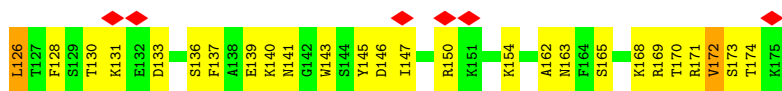




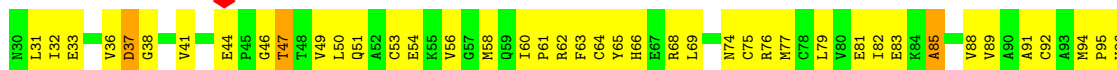
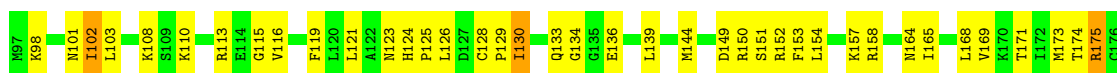
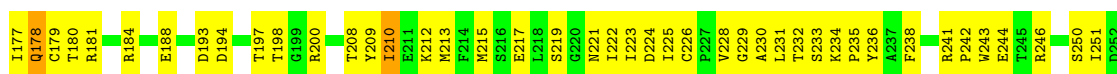
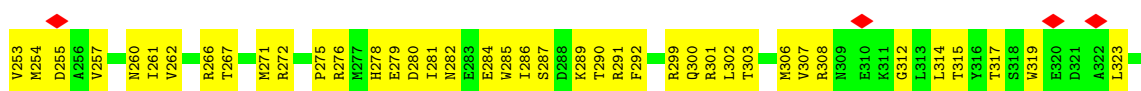
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

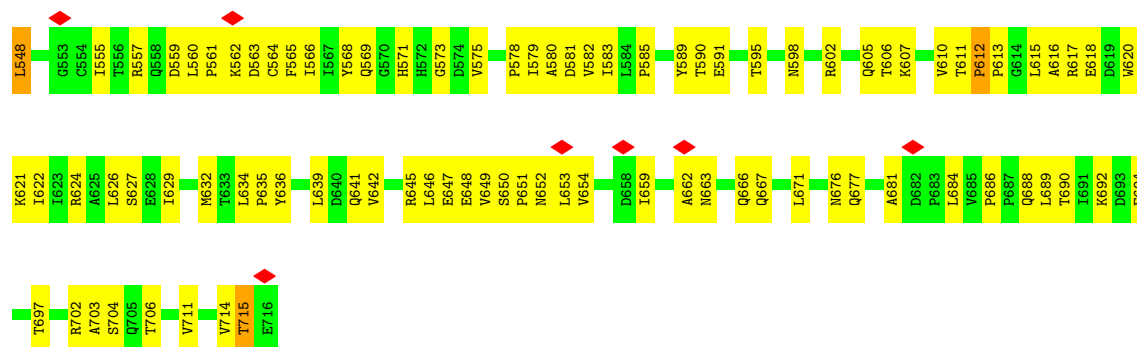


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

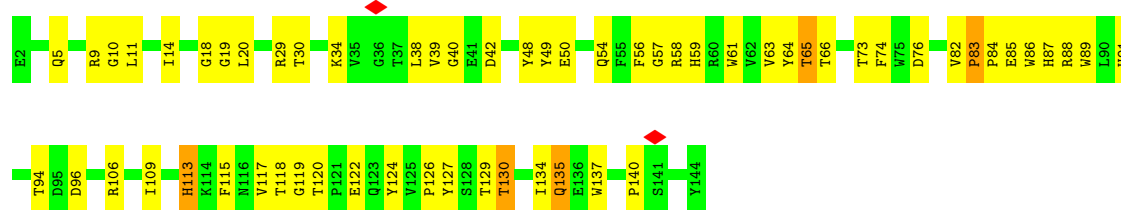


- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

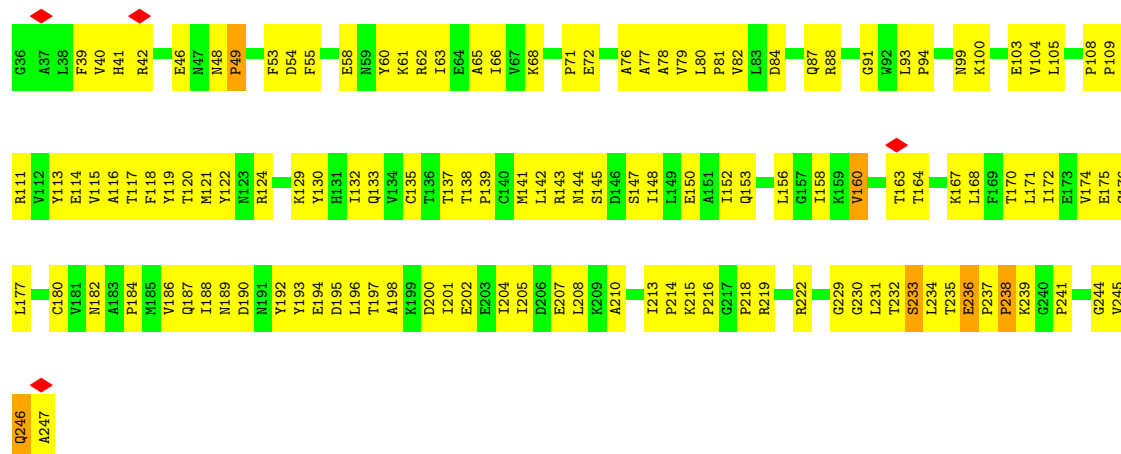




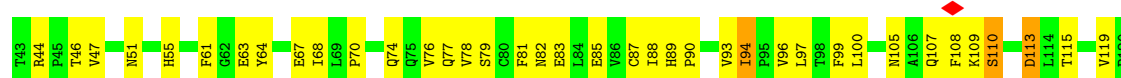
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

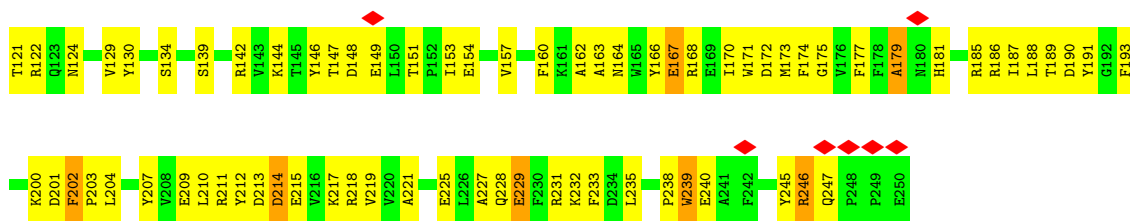


- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

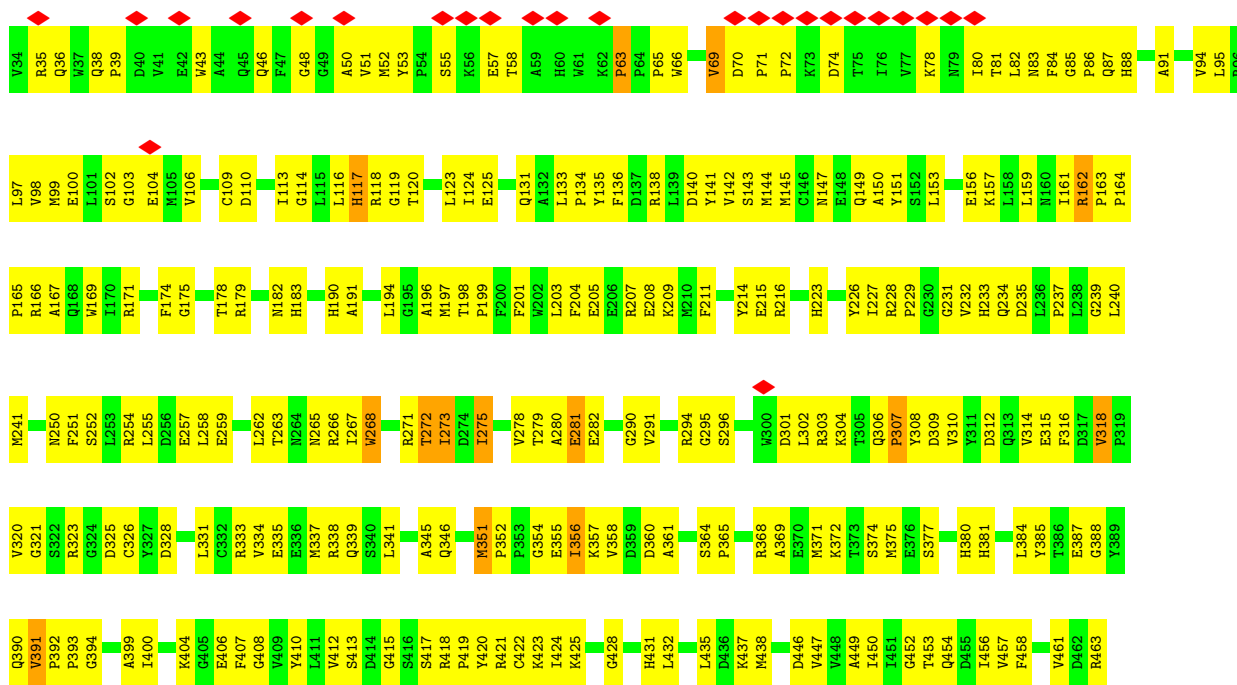


- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial





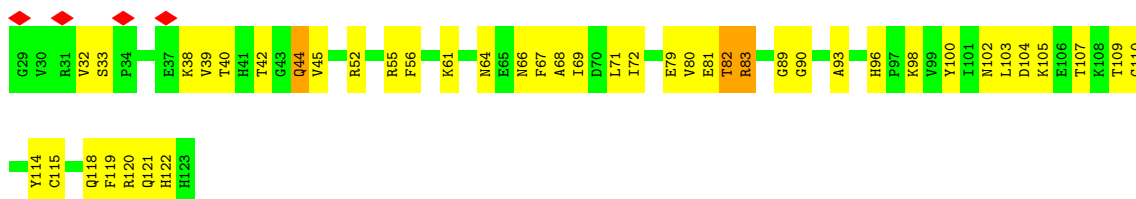
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

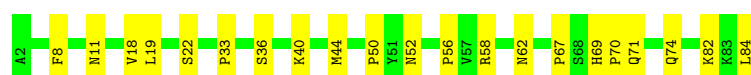


- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



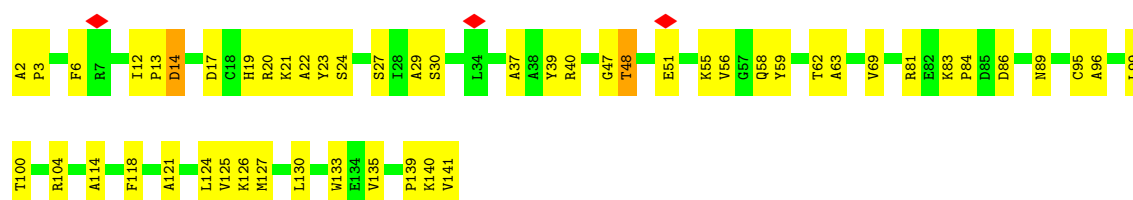
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:  75% 25%



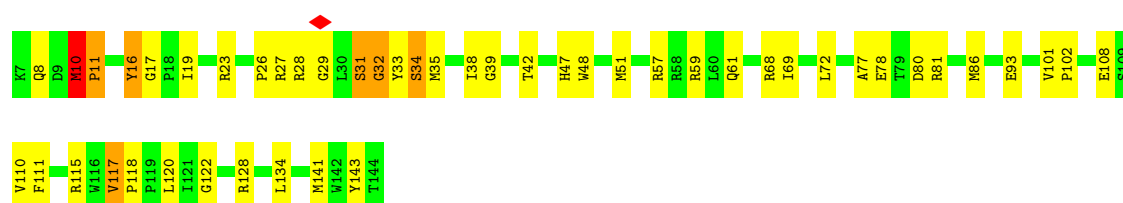
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:  63% 36% .

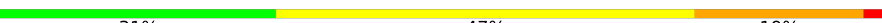


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:  65% 30% . .



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:  31% 47% 19% .



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:  74% 26%



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  59% 37% .

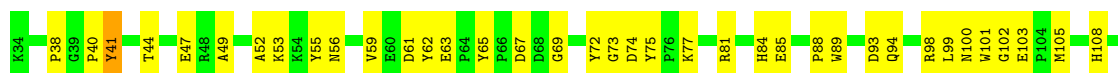
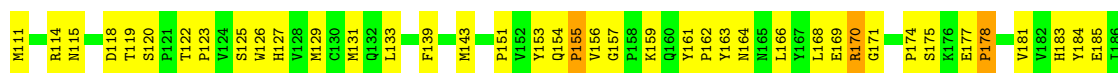




- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



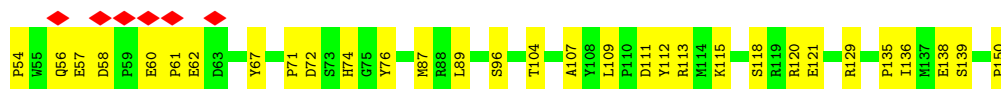
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

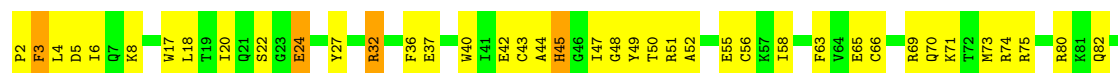
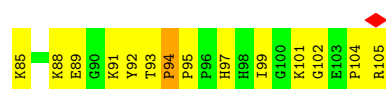




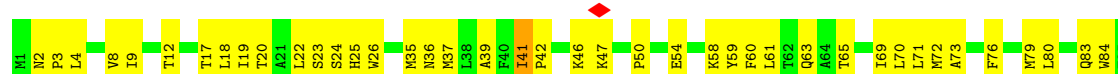
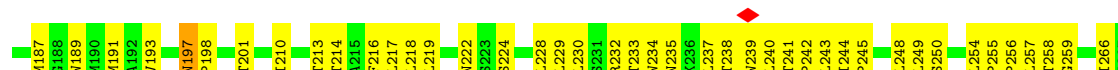
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



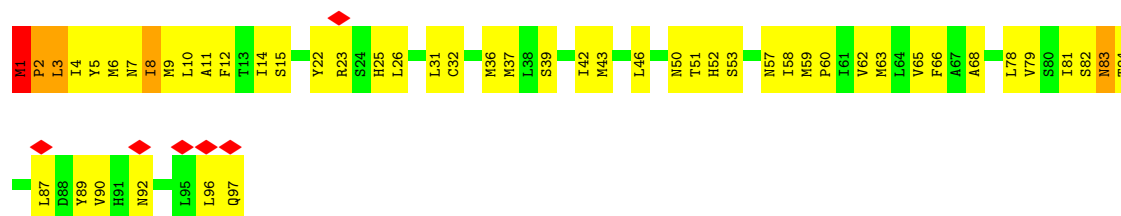
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



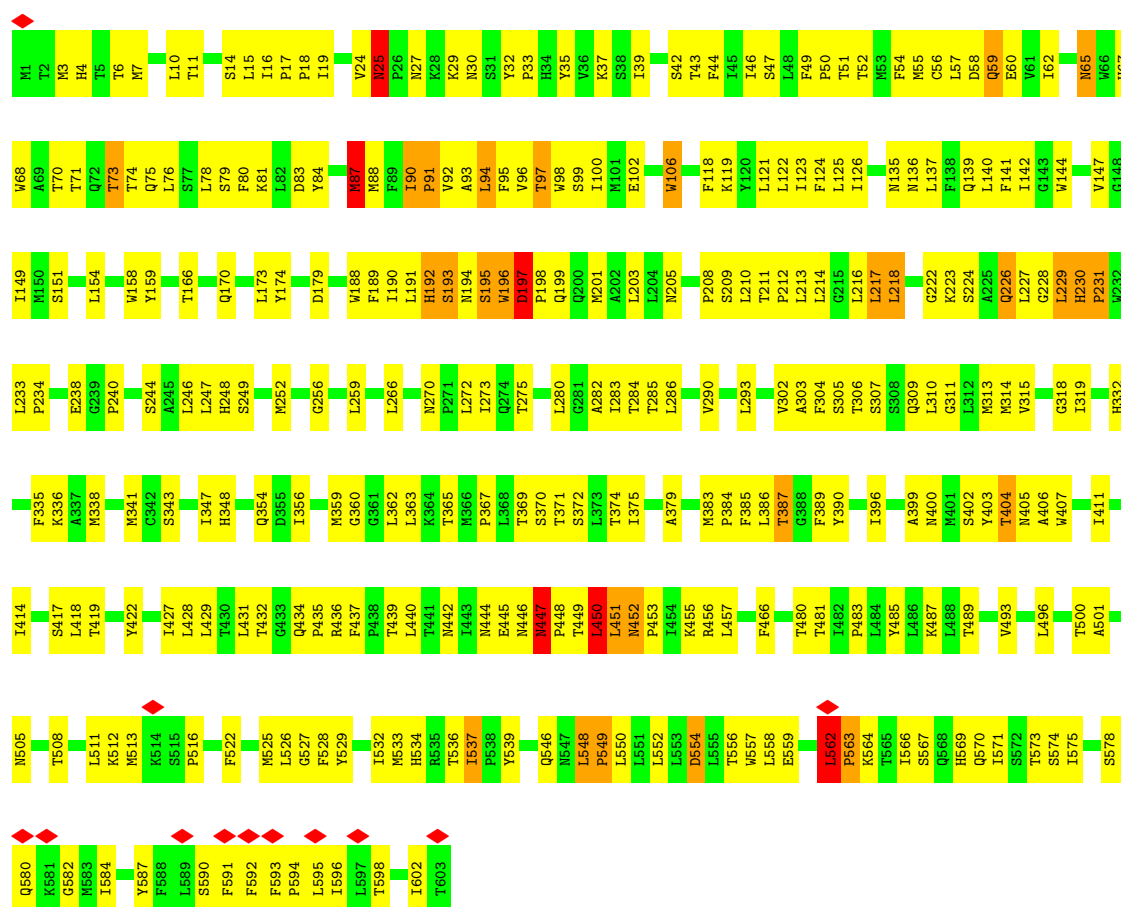
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



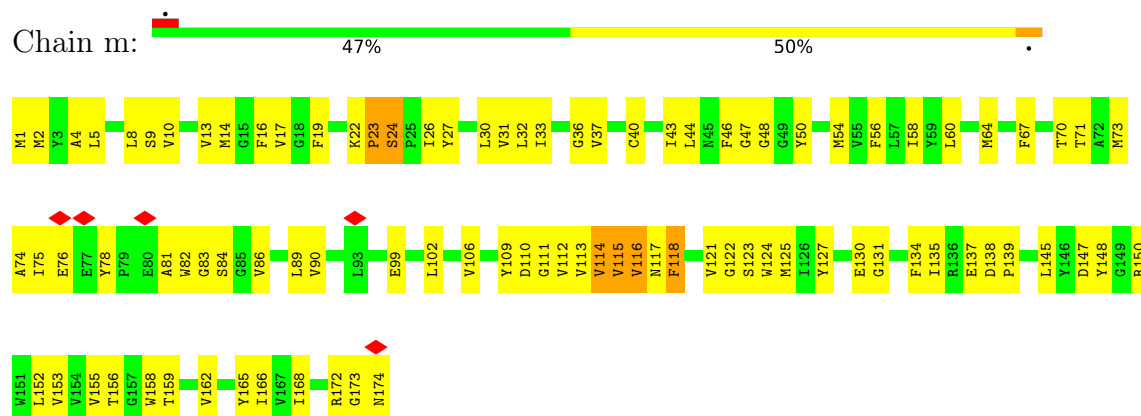
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



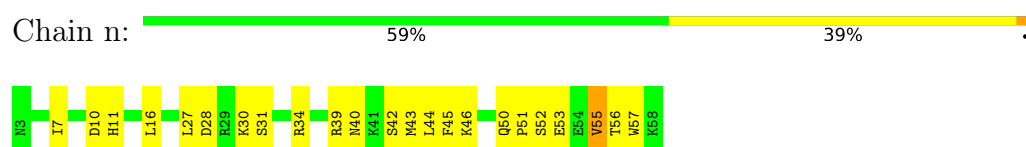
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5



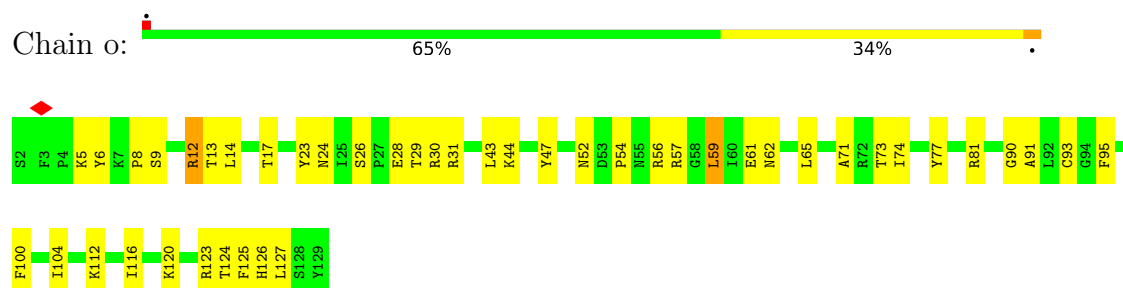
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



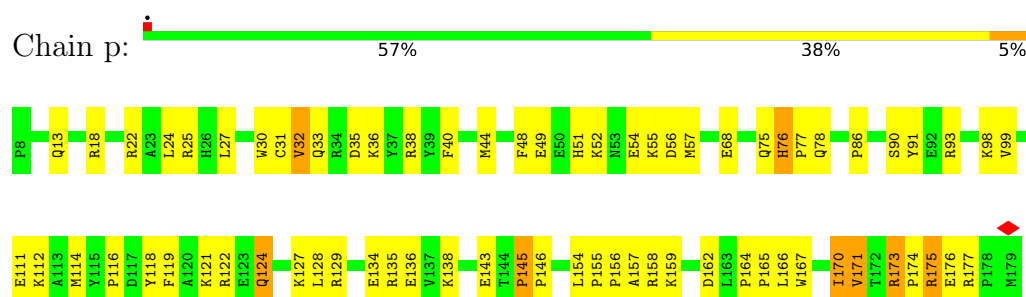
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



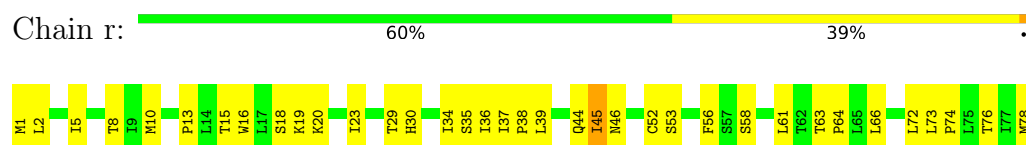
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

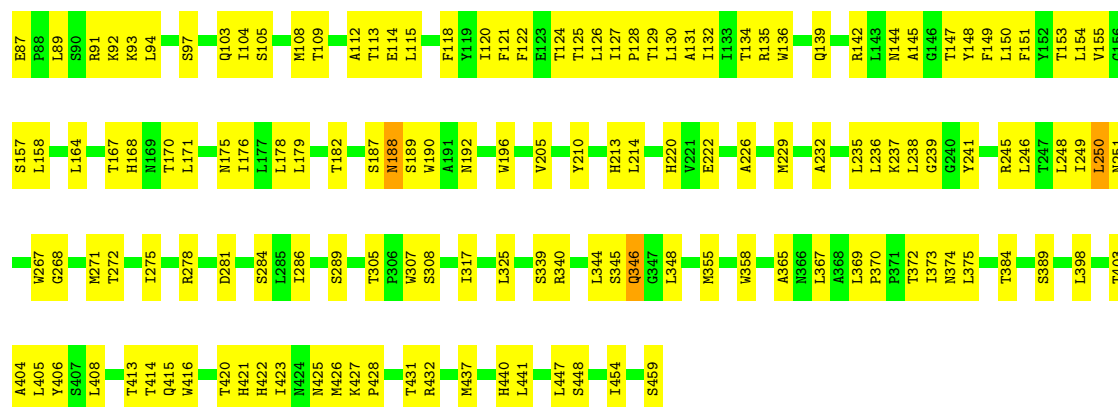


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

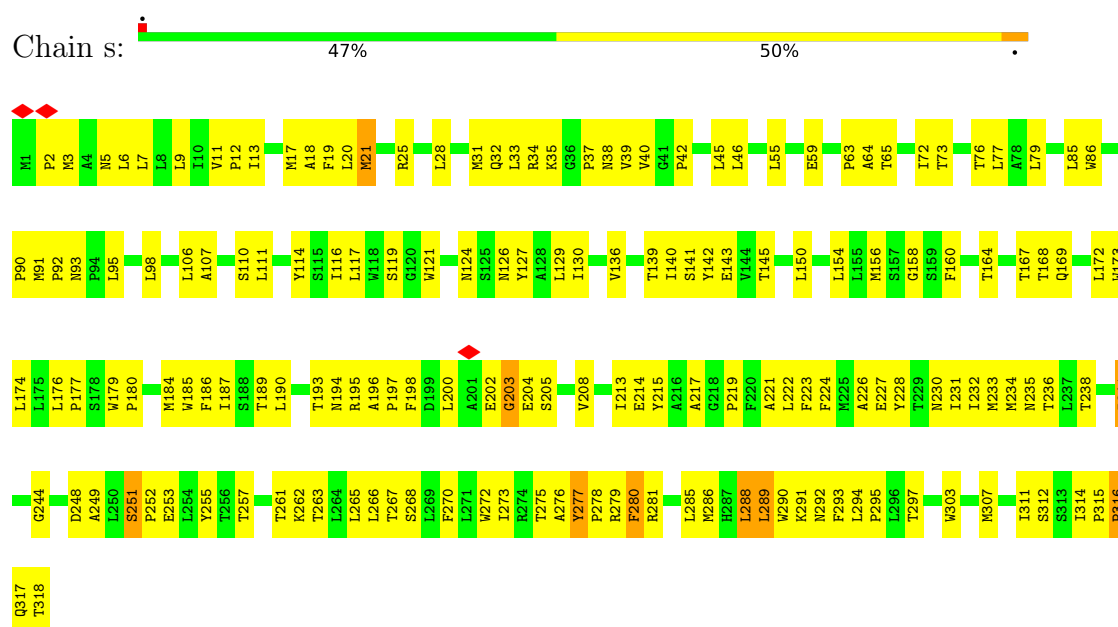


- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

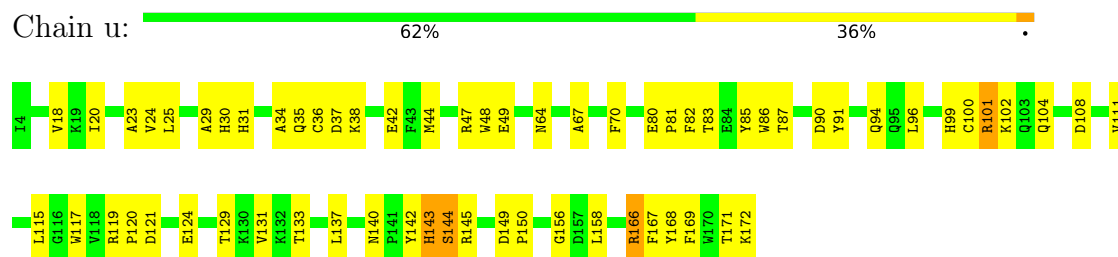




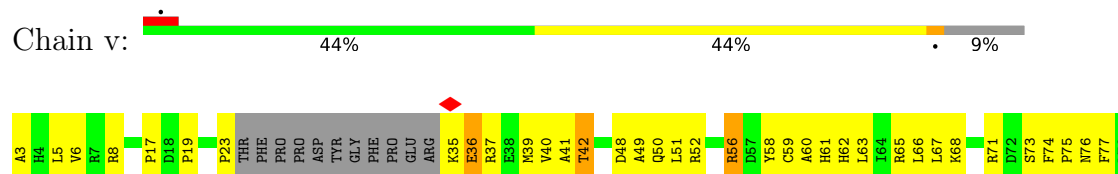
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

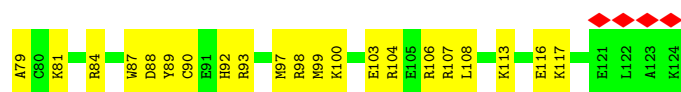


• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

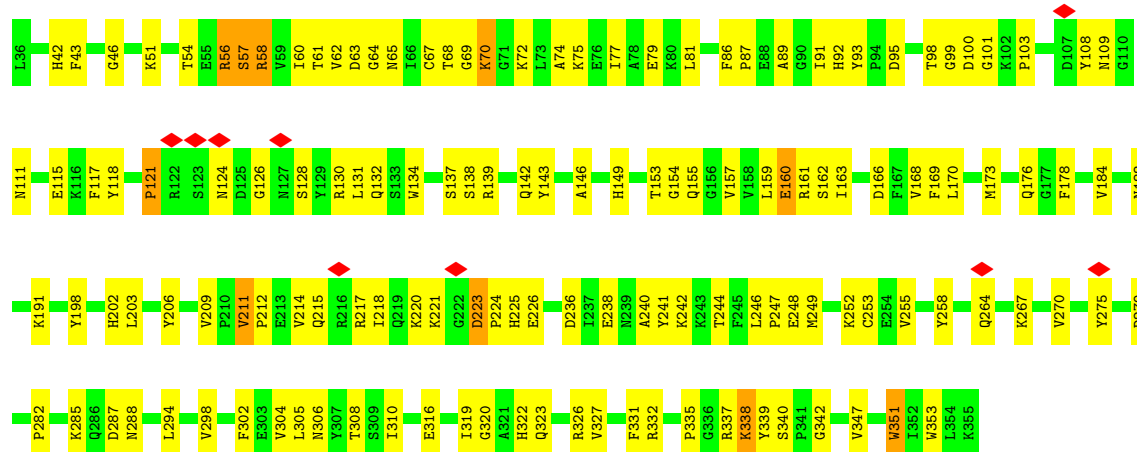


• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

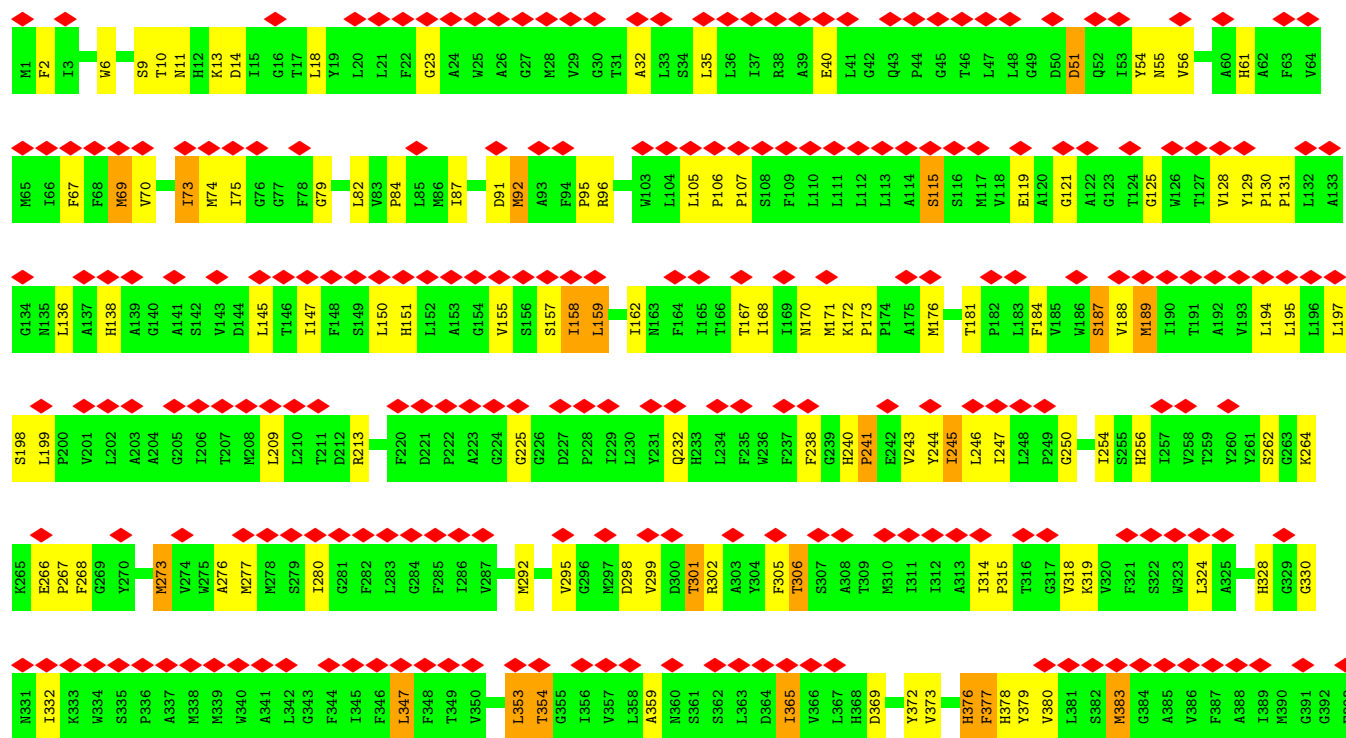




- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

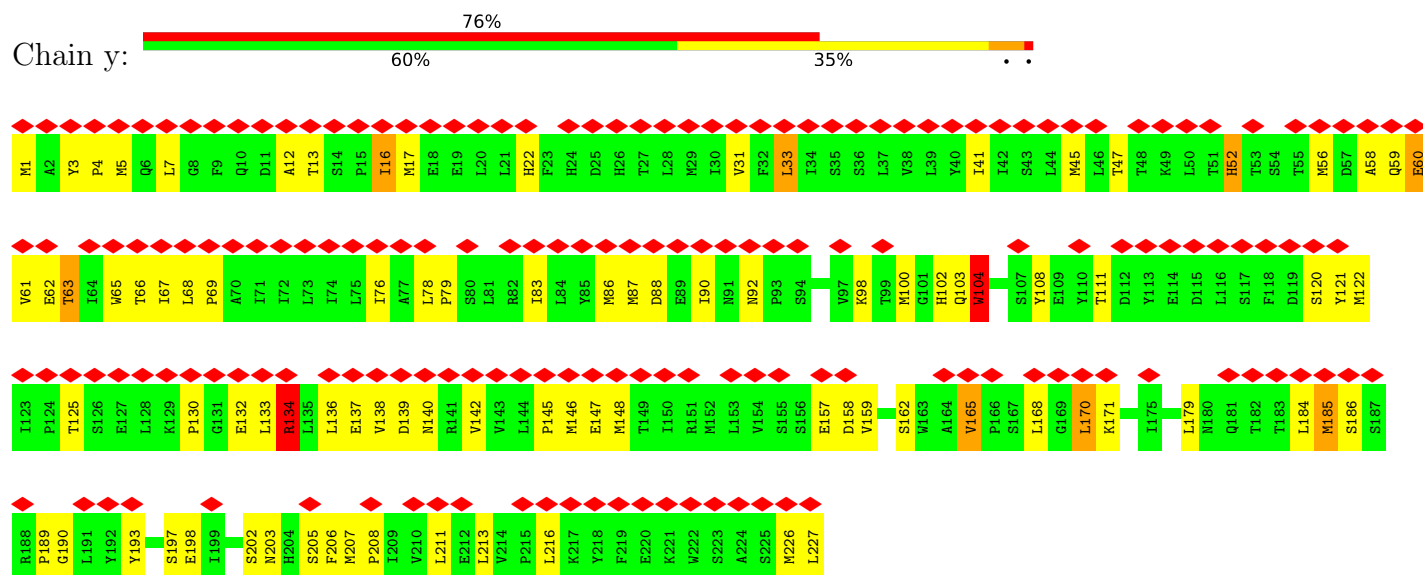


- Molecule 45: Cytochrome c oxidase subunit 1

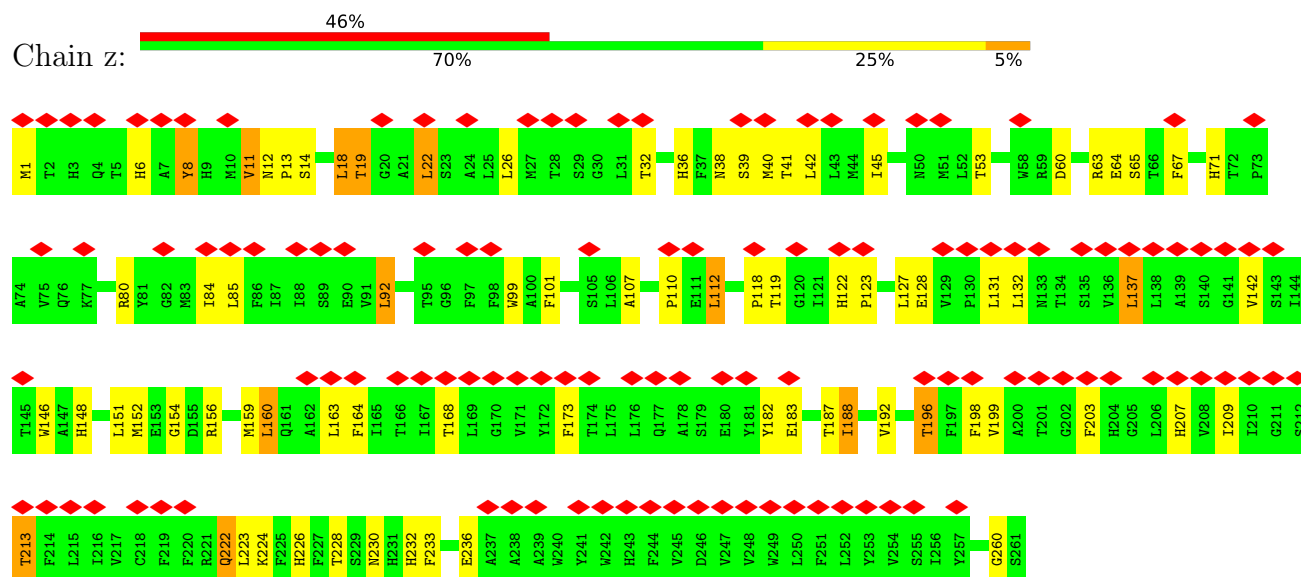




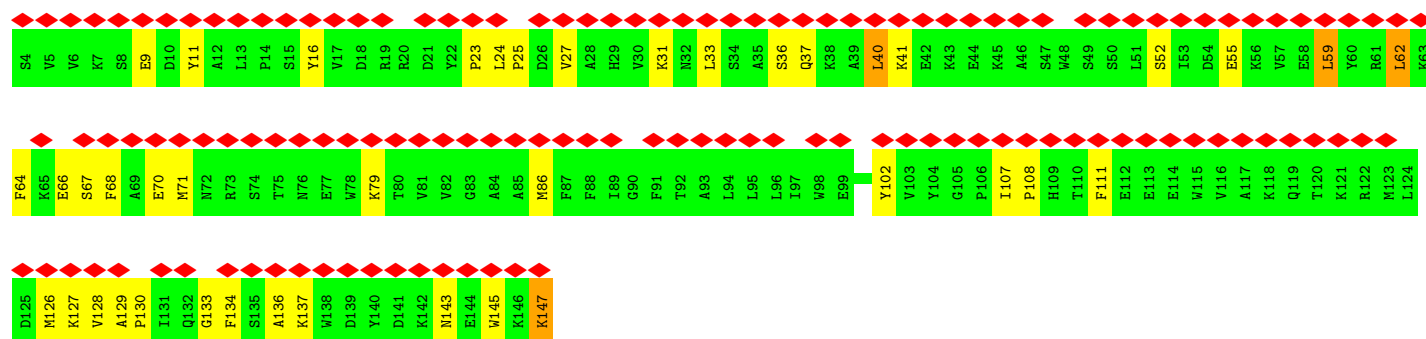
• Molecule 46: Cytochrome c oxidase subunit 2



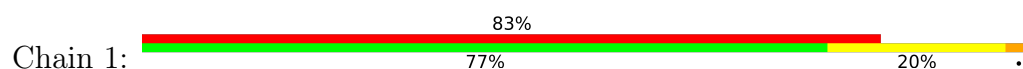
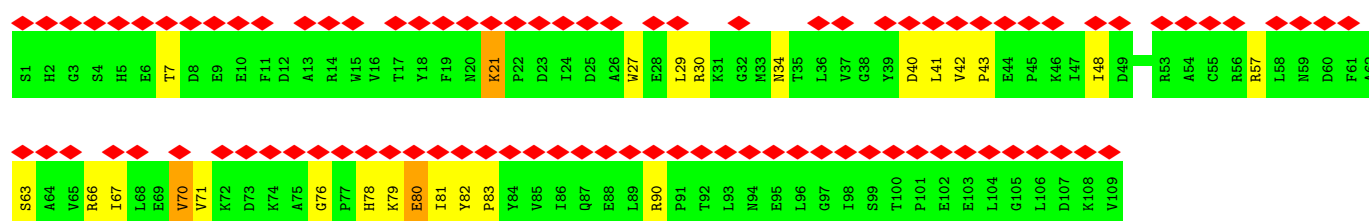
• Molecule 47: Cytochrome c oxidase subunit 3



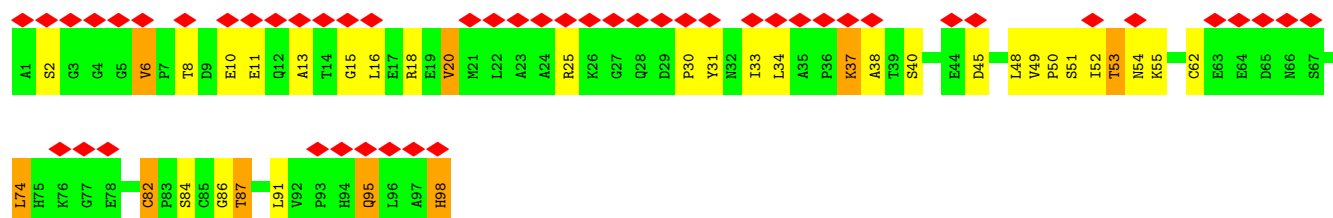
• Molecule 48: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



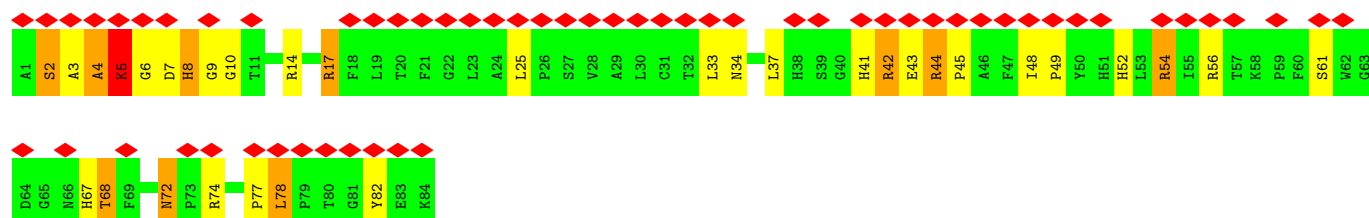
• Molecule 49: Cytochrome c oxidase subunit 5A, mitochondrial



• Molecule 50: Cytochrome c oxidase subunit 5B, mitochondrial



• Molecule 51: Cytochrome c oxidase subunit 6A2, mitochondrial

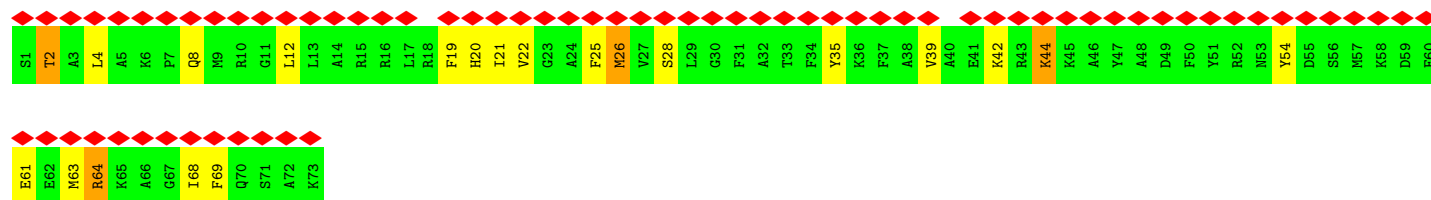


• Molecule 52: Cytochrome c oxidase subunit 6B1

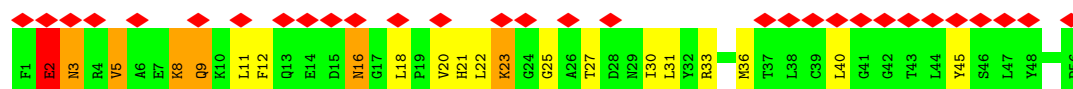




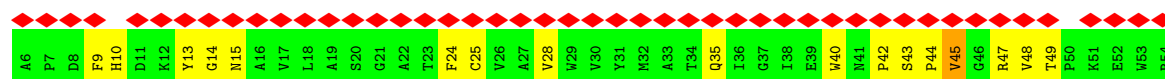
• Molecule 53: Cytochrome c oxidase subunit 6C



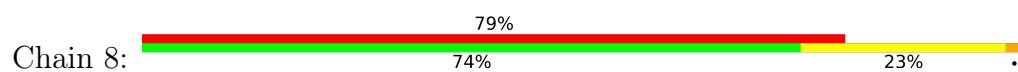
• Molecule 54: Cytochrome c oxidase subunit 7A1, mitochondrial



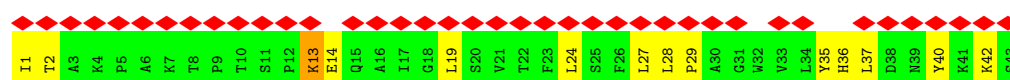
• Molecule 55: Cytochrome c oxidase subunit 7B, mitochondrial



• Molecule 56: Cytochrome c oxidase subunit 7C, mitochondrial



• Molecule 57: Cytochrome c oxidase subunit 8B, mitochondrial

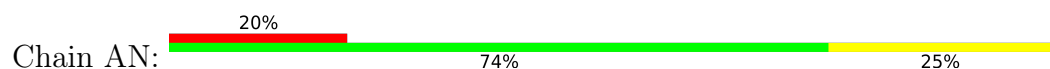


• Molecule 58: Cytochrome b-c1 complex subunit 8

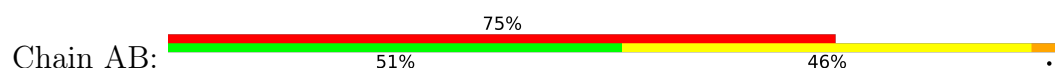
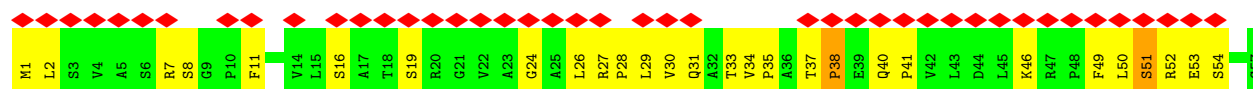




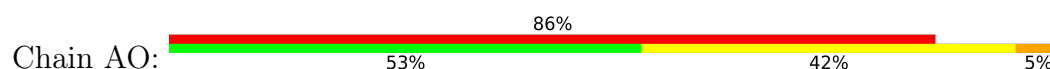
- Molecule 58: Cytochrome b-c1 complex subunit 8



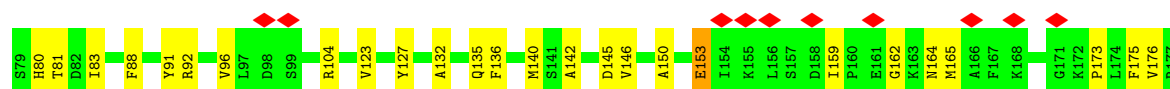
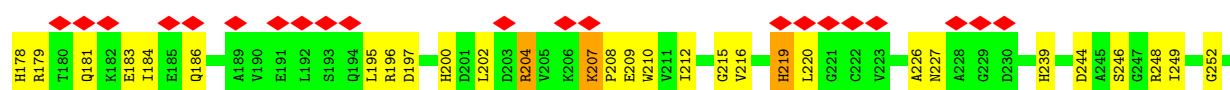
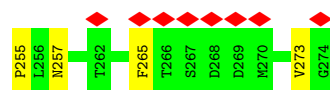
- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial



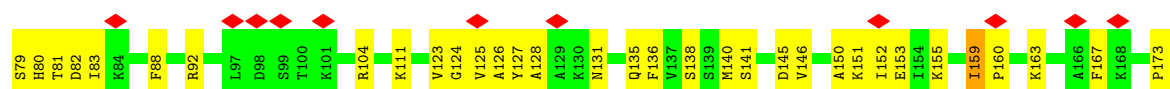
- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial

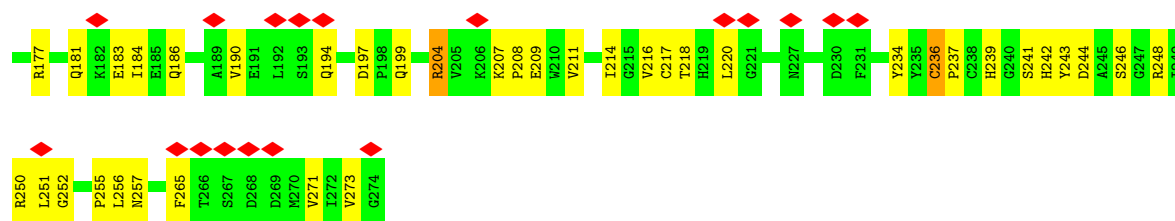


- Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial

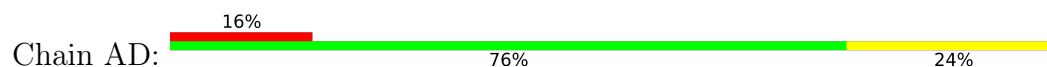


- Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial

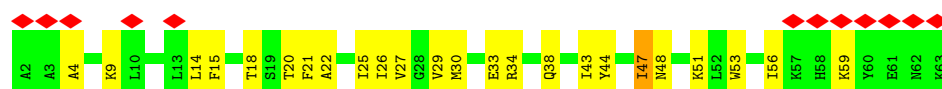




- Molecule 61: Cytochrome b-c1 complex subunit 9



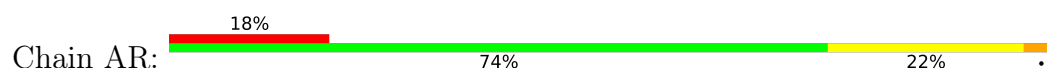
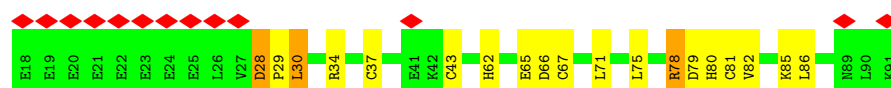
- Molecule 61: Cytochrome b-c1 complex subunit 9



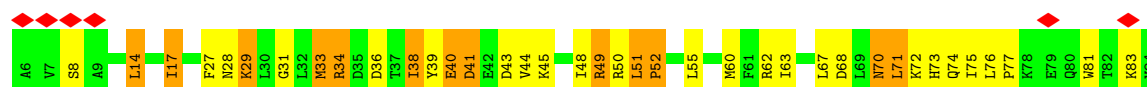
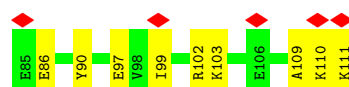
- Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial



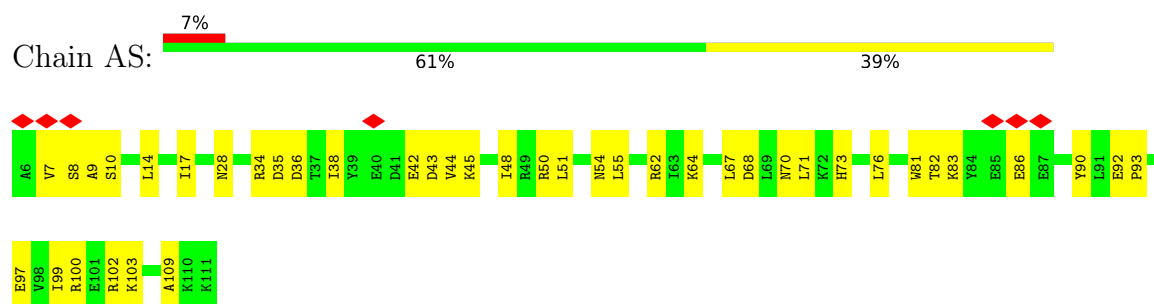
- Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial



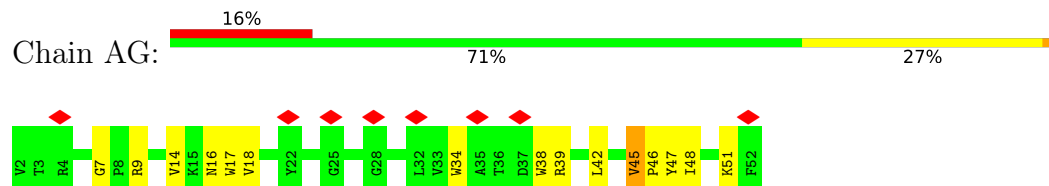
- Molecule 63: Cytochrome b-c1 complex subunit 7



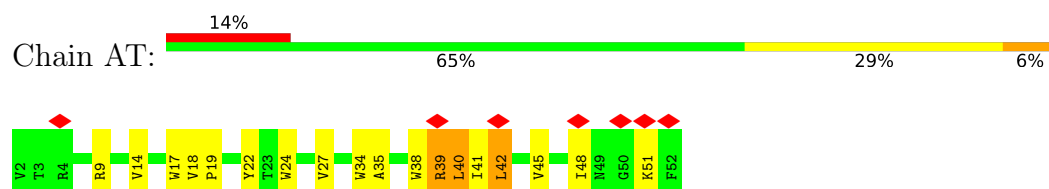
- Molecule 63: Cytochrome b-c1 complex subunit 7



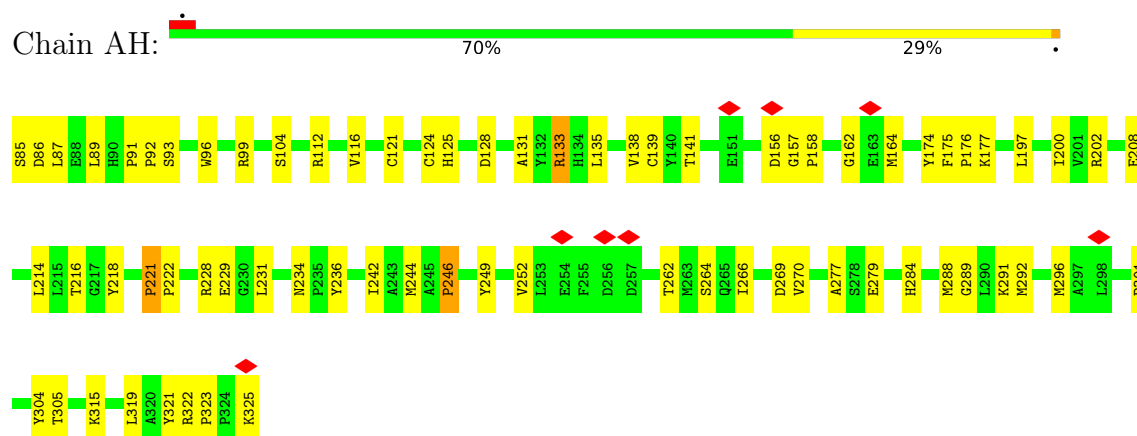
- Molecule 64: Cytochrome b-c1 complex subunit 10



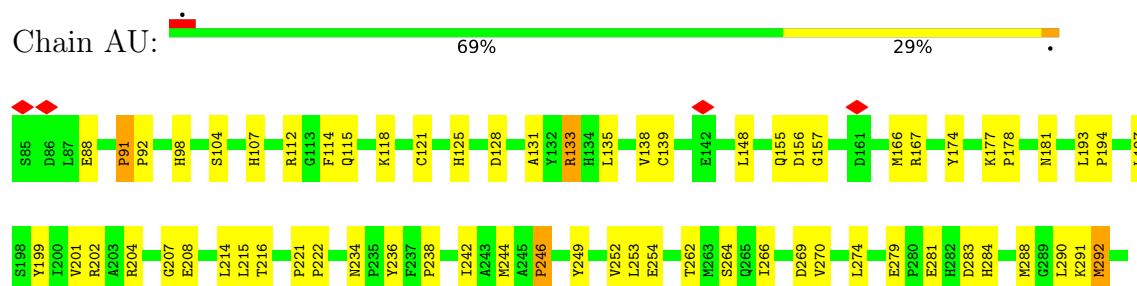
- Molecule 64: Cytochrome b-c1 complex subunit 10



- Molecule 65: Cytochrome c1, heme protein, mitochondrial



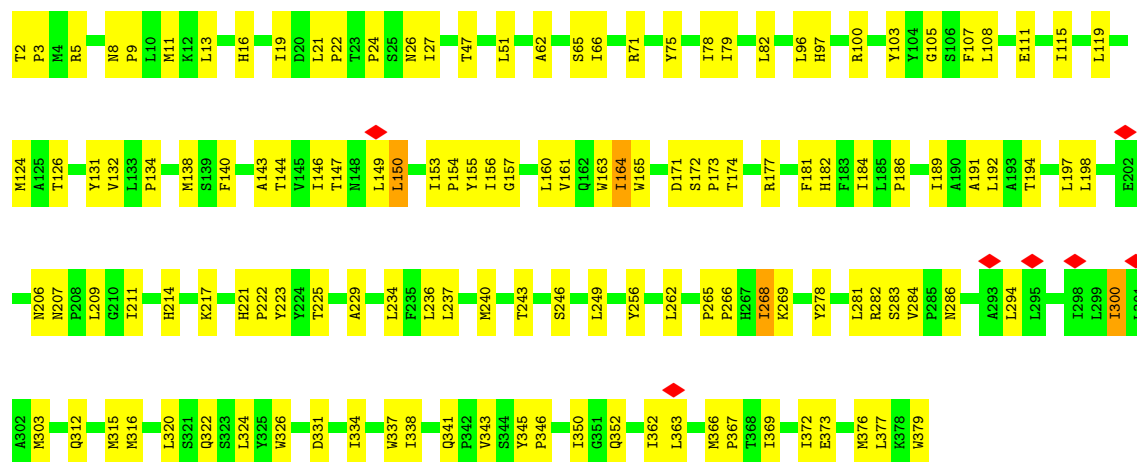
- Molecule 65: Cytochrome c1, heme protein, mitochondrial





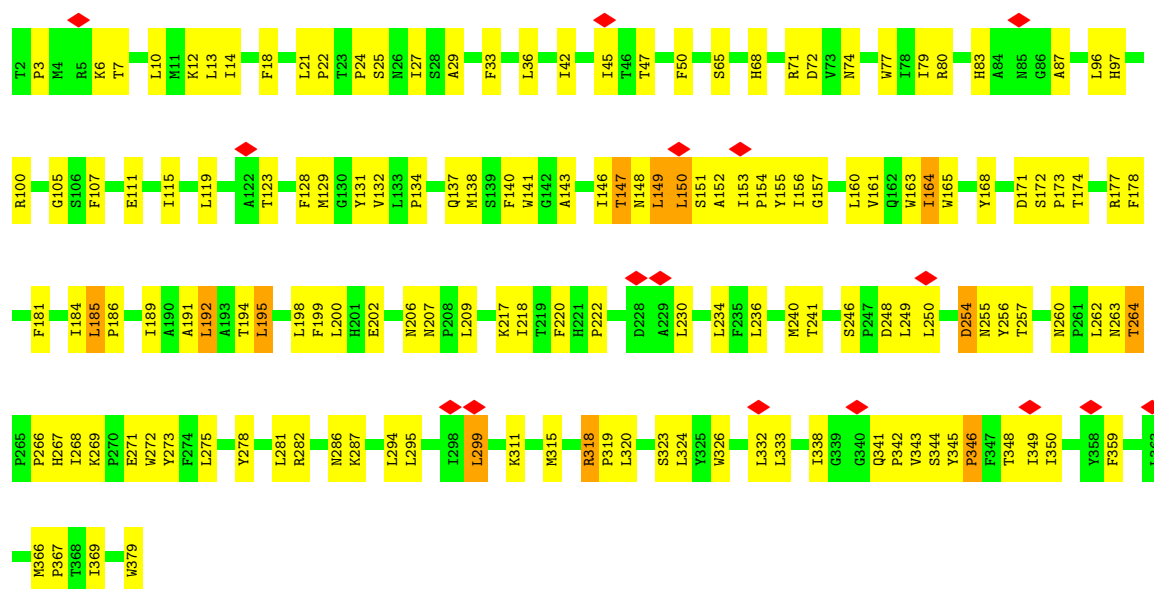
• Molecule 66: Cytochrome b

Chain AJ: 65% 34%



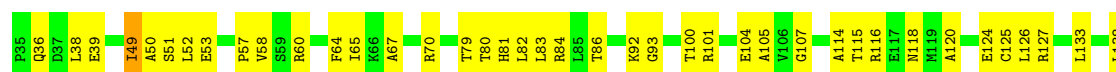
• Molecule 66: Cytochrome b

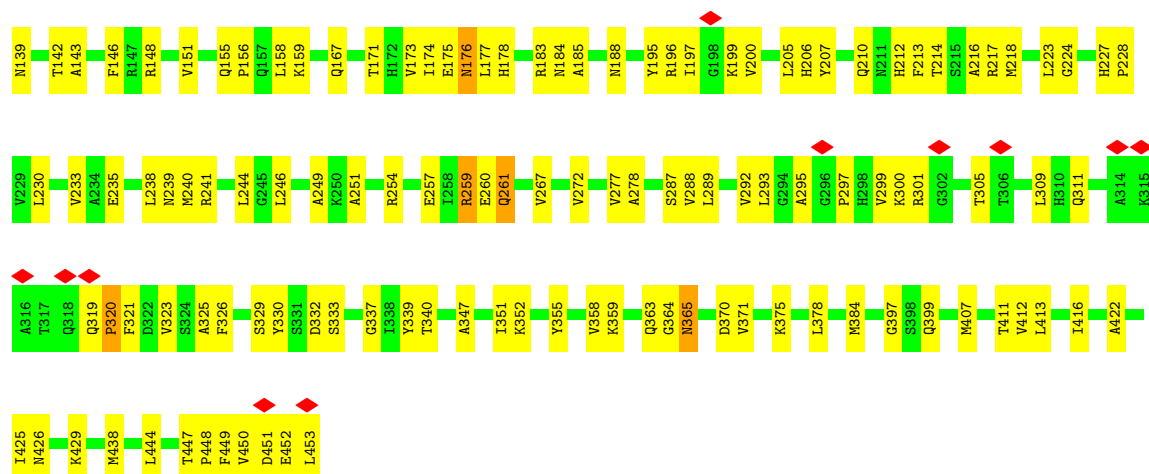
Chain AV: 60% 37%



• Molecule 67: Cytochrome b-c1 complex subunit 2, mitochondrial

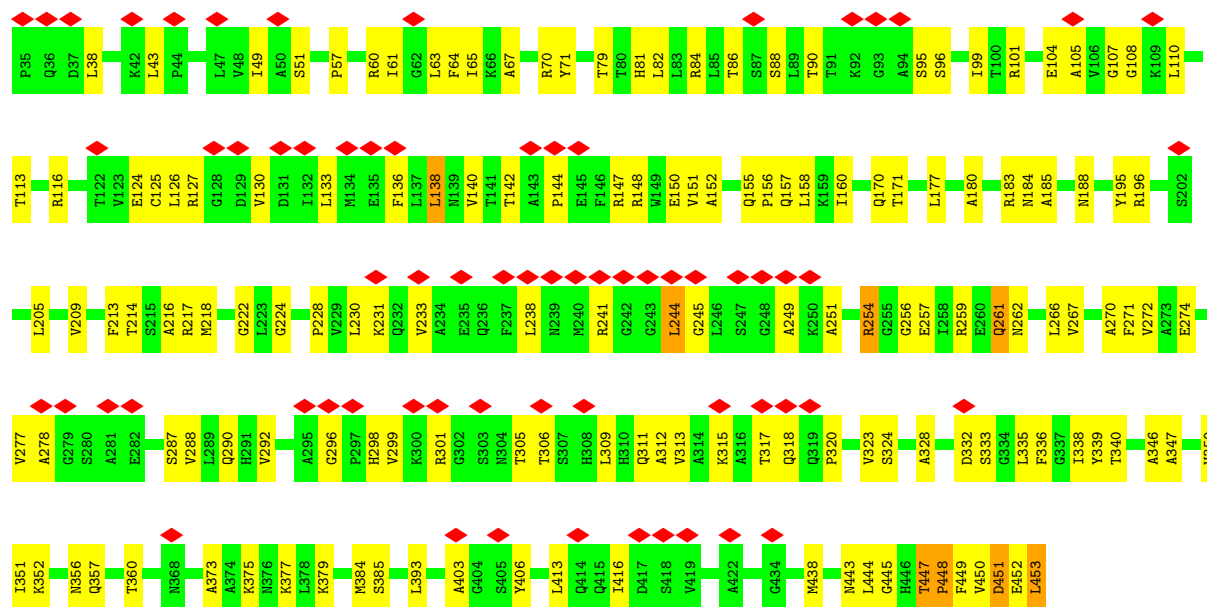
Chain AK: 62% 37%





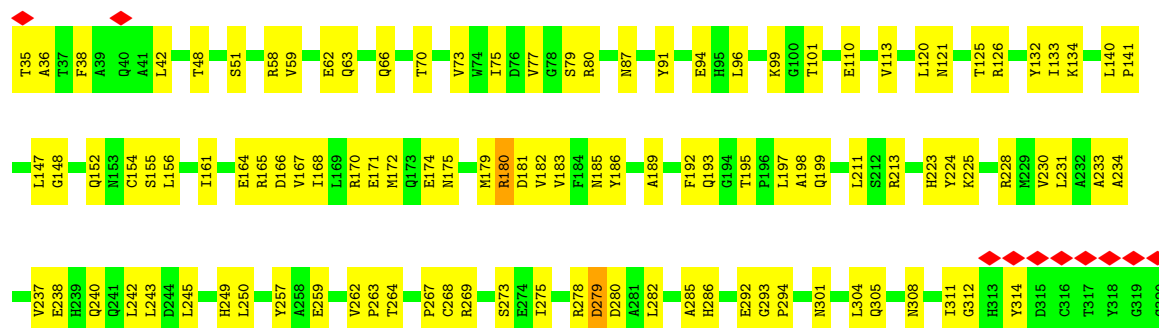
• Molecule 67: Cytochrome b-c1 complex subunit 2, mitochondrial

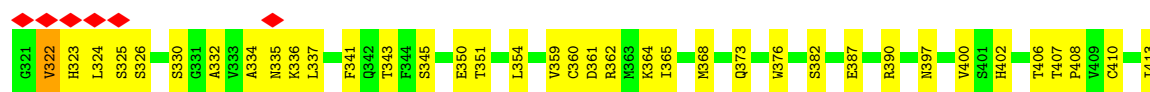
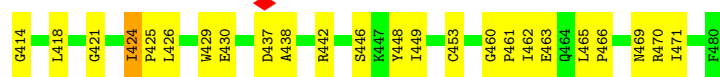
Chain AW: 16% 63% 35%



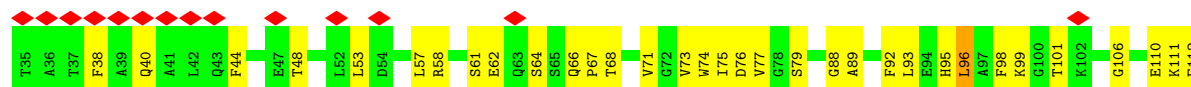
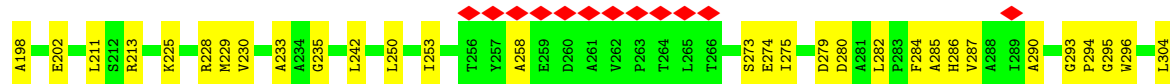
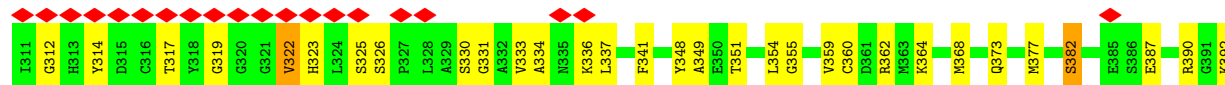
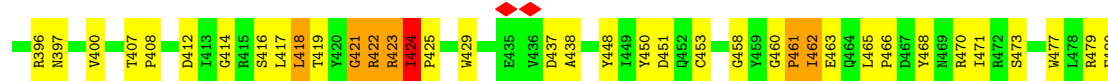
• Molecule 68: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain AL: 62% 37%





- Molecule 68: Cytochrome b-c1 complex subunit 1, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.385	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0354	Depositor
Map size ($\text{\AA}$)	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.083, 1.083, 1.083	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FES, NDP, ZN, 8Q1, HEC, MG, SF4, CDL, CU, FMN, HEM, PEE, HEA, PLX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.39	0/3398	0.87	6/4590 (0.1%)
2	B	0.59	0/1452	0.96	10/1964 (0.5%)
3	C	0.74	0/1280	0.93	3/1732 (0.2%)
4	E	0.44	0/993	0.92	3/1335 (0.2%)
5	F	0.37	0/682	0.87	0/922
6	G	0.40	0/684	0.83	0/926
6	X	0.71	0/698	0.89	0/942
7	H	0.45	0/941	0.87	2/1275 (0.2%)
8	I	0.45	0/788	1.10	7/1066 (0.7%)
9	J	0.44	0/2785	0.91	13/3771 (0.3%)
10	K	0.30	0/282	0.73	0/381
11	L	0.42	0/987	0.83	1/1331 (0.1%)
12	M	0.43	0/5362	0.87	9/7266 (0.1%)
13	N	0.44	0/1236	0.91	6/1681 (0.4%)
14	O	0.40	0/1682	0.87	4/2289 (0.2%)
15	P	0.48	0/1780	0.94	5/2424 (0.2%)
16	Q	0.55	0/3552	1.01	14/4815 (0.3%)
17	S	0.81	0/583	0.94	1/785 (0.1%)
18	T	0.37	0/755	0.79	0/1017
19	U	0.69	0/670	1.05	4/920 (0.4%)
20	V	0.64	0/1065	0.89	4/1450 (0.3%)
21	W	0.74	1/1166 (0.1%)	1.12	8/1579 (0.5%)
22	Y	0.61	0/559	1.16	7/763 (0.9%)
23	Z	0.56	0/669	0.82	0/899
24	a	0.85	0/1209	0.98	6/1639 (0.4%)
25	b	0.71	3/1095 (0.3%)	1.08	6/1480 (0.4%)
26	c	0.69	0/1287	0.99	10/1761 (0.6%)
27	d	0.78	0/1445	0.97	3/1945 (0.2%)
28	e	0.76	0/835	0.95	2/1134 (0.2%)
29	f	0.66	0/418	0.87	1/566 (0.2%)
30	g	0.78	0/1035	0.97	4/1398 (0.3%)
31	h	0.79	0/884	0.98	3/1182 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.92	1/2808 (0.0%)	1.08	11/3843 (0.3%)
33	j	0.76	0/945	1.01	3/1292 (0.2%)
34	k	0.95	1/751 (0.1%)	1.04	3/1019 (0.3%)
35	l	0.84	4/4840 (0.1%)	1.04	29/6611 (0.4%)
36	m	0.82	0/1346	0.99	5/1832 (0.3%)
37	n	0.63	0/484	0.99	0/652
38	o	0.71	0/1093	0.89	0/1479
39	p	0.70	0/1549	1.00	11/2098 (0.5%)
40	r	0.96	1/3723 (0.0%)	1.02	2/5089 (0.0%)
41	s	0.83	0/2580	1.09	15/3539 (0.4%)
42	u	0.70	0/1433	0.96	2/1937 (0.1%)
43	v	0.64	0/934	1.00	4/1241 (0.3%)
44	w	0.54	1/2533 (0.0%)	0.91	8/3440 (0.2%)
45	x	0.86	7/4164 (0.2%)	1.16	36/5688 (0.6%)
46	y	0.78	0/1868	1.12	11/2544 (0.4%)
47	z	0.75	0/2211	1.02	7/3023 (0.2%)
48	0	0.68	0/1229	0.96	3/1658 (0.2%)
49	1	0.64	0/898	1.02	6/1218 (0.5%)
50	2	0.72	0/765	1.13	3/1038 (0.3%)
51	3	0.69	0/699	1.10	6/950 (0.6%)
52	4	0.67	0/648	1.17	5/877 (0.6%)
53	5	0.71	0/611	0.94	2/810 (0.2%)
54	6	0.70	0/451	1.04	3/610 (0.5%)
55	7	0.76	0/398	1.01	1/546 (0.2%)
56	8	0.78	0/399	0.97	2/534 (0.4%)
57	9	0.69	0/345	0.99	1/470 (0.2%)
58	AA	0.44	0/715	0.83	1/964 (0.1%)
58	AN	0.37	0/707	0.86	2/953 (0.2%)
59	AB	0.37	0/421	0.91	0/574
59	AO	0.40	0/417	0.98	0/569
60	AC	0.32	0/1554	0.81	6/2104 (0.3%)
60	AP	0.30	0/1554	0.84	6/2104 (0.3%)
61	AD	0.30	0/521	0.63	0/699
61	AQ	0.31	0/521	0.67	0/699
62	AE	0.48	1/587 (0.2%)	0.84	2/789 (0.3%)
62	AR	0.37	0/587	0.77	2/789 (0.3%)
63	AF	0.61	2/942 (0.2%)	0.85	3/1263 (0.2%)
63	AS	0.33	0/942	0.65	0/1263
64	AG	0.38	0/442	0.82	4/608 (0.7%)
64	AT	0.40	0/442	0.80	1/608 (0.2%)
65	AH	0.35	0/1983	0.84	6/2691 (0.2%)
65	AU	0.35	0/1983	0.79	4/2691 (0.1%)
66	AJ	0.42	2/3108 (0.1%)	0.82	7/4254 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
66	AV	0.46	4/3108 (0.1%)	0.86	11/4254 (0.3%)
67	AK	0.36	0/3217	0.79	0/4361
67	AW	0.39	2/3220 (0.1%)	0.81	4/4365 (0.1%)
68	AL	0.37	0/3527	0.82	8/4788 (0.2%)
68	AY	0.40	2/3527 (0.1%)	0.82	6/4788 (0.1%)
All	All	0.61	32/115987 (0.0%)	0.94	394/157444 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
44	w	0	1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	i	278	ILE	CA-CB	-7.60	1.50	1.54
45	x	61	HIS	CG-CD2	7.48	1.44	1.35
45	x	378	HIS	ND1-CE1	7.38	1.40	1.32
62	AE	28	ASP	C-N	7.28	1.41	1.34
45	x	378	HIS	CE1-NE2	-6.50	1.26	1.32
25	b	117	ILE	C-N	6.49	1.41	1.33
45	x	69	MET	SD-CE	-6.23	1.64	1.79
21	W	117	VAL	CA-CB	-6.05	1.49	1.54
40	r	37	ILE	CA-CB	-5.88	1.51	1.54
25	b	105	PHE	C-N	5.84	1.41	1.33
63	AF	51	LEU	C-N	5.75	1.41	1.33
45	x	61	HIS	ND1-CE1	5.70	1.38	1.32
68	AY	424	ILE	C-N	5.66	1.41	1.33
67	AW	447	THR	C-N	5.64	1.40	1.33
44	w	211	VAL	CA-CB	5.63	1.57	1.54
45	x	376	HIS	ND1-CE1	5.55	1.38	1.32
66	AJ	153	ILE	C-N	5.54	1.40	1.34
67	AW	448	PRO	N-CD	5.41	1.55	1.47
45	x	378	HIS	CG-CD2	5.32	1.41	1.35
66	AJ	154	PRO	N-CD	5.29	1.55	1.47
66	AV	154	PRO	N-CD	5.29	1.55	1.47
34	k	2	PRO	N-CD	5.25	1.55	1.47
25	b	118	PRO	N-CD	5.24	1.55	1.47
66	AV	153	ILE	C-N	5.20	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	l	230	HIS	C-N	5.17	1.41	1.34
68	AY	425	PRO	N-CD	5.15	1.54	1.47
35	l	90	ILE	C-N	5.13	1.41	1.34
35	l	91	PRO	N-CD	5.11	1.54	1.47
35	l	231	PRO	N-CD	5.09	1.54	1.47
63	AF	52	PRO	N-CD	5.09	1.54	1.47
66	AV	345	TYR	C-N	5.08	1.41	1.34
66	AV	346	PRO	N-CD	5.08	1.54	1.47

All (394) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	31	SER	N-CA-C	-16.80	92.09	112.59
21	W	10	MET	CA-C-N	-10.86	109.19	120.38
21	W	10	MET	C-N-CA	-10.86	109.19	120.38
8	I	38	PRO	CA-C-N	10.33	130.64	119.28
8	I	38	PRO	C-N-CA	10.33	130.64	119.28
45	x	376	HIS	ND1-CE1-NE2	10.33	118.73	108.40
16	Q	162	ARG	CA-C-N	10.24	127.04	119.66
16	Q	162	ARG	C-N-CA	10.24	127.04	119.66
16	Q	365	PRO	CA-C-N	9.95	129.90	119.85
16	Q	365	PRO	C-N-CA	9.95	129.90	119.85
41	s	314	ILE	CA-C-N	9.80	126.81	119.66
41	s	314	ILE	C-N-CA	9.80	126.81	119.66
4	E	18	LYS	CA-C-N	9.29	129.23	119.85
4	E	18	LYS	C-N-CA	9.29	129.23	119.85
52	4	52	VAL	N-CA-C	8.97	121.26	108.17
52	4	81	PHE	CA-C-N	8.78	128.43	119.56
52	4	81	PHE	C-N-CA	8.78	128.43	119.56
66	AV	264	THR	CA-C-N	8.58	125.93	119.66
66	AV	264	THR	C-N-CA	8.58	125.93	119.66
3	C	60	GLY	N-CA-C	8.53	122.81	112.49
32	i	323	THR	CA-C-N	8.51	147.42	127.00
32	i	323	THR	C-N-CA	8.51	147.42	127.00
22	Y	86	TYR	C-N-CD	8.45	139.20	120.60
22	Y	92	TRP	N-CA-C	-8.40	92.12	107.75
22	Y	47	PHE	CA-C-N	8.23	128.26	119.78
22	Y	47	PHE	C-N-CA	8.23	128.26	119.78
13	N	82	VAL	CA-C-N	8.13	125.60	119.66
13	N	82	VAL	C-N-CA	8.13	125.60	119.66
45	x	82	LEU	N-CA-C	8.12	122.46	112.23
68	AY	421	GLY	N-CA-C	-8.11	99.64	112.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	8	20	ARG	N-CA-C	-8.06	102.57	111.36
27	d	119	CYS	N-CA-C	8.05	120.06	111.28
45	x	378	HIS	ND1-CE1-NE2	8.01	116.41	108.40
9	J	311	GLU	CA-C-N	7.99	128.00	119.78
9	J	311	GLU	C-N-CA	7.99	128.00	119.78
60	AP	252	GLY	CA-C-N	7.92	127.99	119.28
60	AP	252	GLY	C-N-CA	7.92	127.99	119.28
32	i	255	PRO	N-CA-C	7.84	120.27	110.70
27	d	2	PRO	N-CA-CB	7.79	111.43	103.25
45	x	56	VAL	N-CA-C	-7.78	103.21	110.53
45	x	435	GLY	N-CA-C	7.72	126.16	115.27
60	AP	236	CYS	CA-C-N	7.59	127.62	119.28
60	AP	236	CYS	C-N-CA	7.59	127.62	119.28
16	Q	318	VAL	N-CA-C	7.49	115.32	107.76
43	v	17	PRO	N-CA-CB	7.48	110.40	103.15
43	v	42	THR	CB-CA-C	-7.46	107.98	116.63
57	9	27	LEU	N-CA-C	7.44	119.47	111.36
41	s	89	LEU	CA-C-N	7.43	129.12	119.84
41	s	89	LEU	C-N-CA	7.43	129.12	119.84
32	i	323	THR	C-N-CD	-7.38	104.37	120.60
45	x	330	GLY	N-CA-C	7.36	120.43	112.33
25	b	117	ILE	CA-C-N	-7.30	112.86	120.38
25	b	117	ILE	C-N-CA	-7.30	112.86	120.38
3	C	141	MET	CA-C-N	7.29	127.29	119.78
3	C	141	MET	C-N-CA	7.29	127.29	119.78
60	AP	159	ILE	CA-C-N	7.26	127.26	119.78
60	AP	159	ILE	C-N-CA	7.26	127.26	119.78
19	U	33	PRO	N-CA-C	7.25	119.54	110.70
45	x	9	SER	N-CA-C	7.20	119.86	110.43
49	1	76	GLY	CA-C-N	7.17	128.41	120.45
49	1	76	GLY	C-N-CA	7.17	128.41	120.45
41	s	277	TYR	CA-C-N	7.16	127.08	119.85
41	s	277	TYR	C-N-CA	7.16	127.08	119.85
45	x	376	HIS	CE1-NE2-CD2	-7.14	101.86	109.00
30	g	21	PRO	CA-C-N	7.13	124.80	119.66
30	g	21	PRO	C-N-CA	7.13	124.80	119.66
39	p	173	ARG	CA-C-N	7.12	127.12	119.28
39	p	173	ARG	C-N-CA	7.12	127.12	119.28
45	x	332	ILE	N-CA-C	7.11	118.97	109.37
49	1	42	VAL	N-CA-C	-7.04	99.74	108.05
39	p	171	VAL	N-CA-C	7.04	117.83	110.72
16	Q	351	MET	CA-C-N	7.03	124.79	119.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	351	MET	C-N-CA	7.03	124.79	119.66
14	O	237	PRO	N-CA-C	7.01	119.25	110.70
45	x	130	PRO	N-CA-C	-6.98	102.19	110.70
35	l	537	ILE	CA-C-N	-6.97	111.62	119.28
35	l	537	ILE	C-N-CA	-6.97	111.62	119.28
68	AL	424	ILE	CA-C-N	6.96	126.95	119.78
68	AL	424	ILE	C-N-CA	6.96	126.95	119.78
32	i	197	ASN	CA-C-N	6.95	126.92	119.28
32	i	197	ASN	C-N-CA	6.95	126.92	119.28
22	Y	93	THR	N-CA-C	6.91	120.02	108.20
16	Q	356	ILE	N-CA-C	-6.90	105.80	112.29
1	A	318	ILE	CA-C-N	6.87	126.86	119.78
1	A	318	ILE	C-N-CA	6.87	126.86	119.78
47	z	36	HIS	N-CA-C	6.87	122.08	113.43
45	x	125	GLY	N-CA-C	-6.87	104.17	112.48
31	h	94	PRO	CA-C-N	-6.83	113.34	120.38
31	h	94	PRO	C-N-CA	-6.83	113.34	120.38
9	J	224	GLY	CA-C-N	6.83	126.79	120.03
9	J	224	GLY	C-N-CA	6.83	126.79	120.03
62	AE	28	ASP	CA-C-N	-6.82	113.17	120.47
62	AE	28	ASP	C-N-CA	-6.82	113.17	120.47
35	l	24	VAL	CA-C-N	-6.79	115.39	122.85
35	l	24	VAL	C-N-CA	-6.79	115.39	122.85
60	AC	252	GLY	CA-C-N	6.77	126.73	119.28
60	AC	252	GLY	C-N-CA	6.77	126.73	119.28
35	l	511	LEU	N-CA-C	6.77	118.60	108.31
26	c	157	GLY	CA-C-N	6.75	126.74	119.78
26	c	157	GLY	C-N-CA	6.75	126.74	119.78
48	0	133	GLY	N-CA-C	6.75	129.17	113.18
1	A	327	ILE	CA-C-N	6.74	126.73	119.78
1	A	327	ILE	C-N-CA	6.74	126.73	119.78
51	3	5	LYS	N-CA-C	6.74	125.15	110.80
25	b	105	PHE	CA-C-N	-6.73	112.83	119.76
25	b	105	PHE	C-N-CA	-6.73	112.83	119.76
45	x	507	GLU	N-CA-C	-6.72	97.92	109.15
26	c	72	TYR	N-CA-C	-6.69	100.13	110.10
43	v	23	PRO	N-CA-CB	6.68	110.35	103.00
49	1	81	ILE	N-CA-C	6.63	116.76	110.53
15	P	166	TYR	N-CA-C	-6.62	104.06	111.28
2	B	168	GLY	CA-C-N	6.60	126.54	119.28
2	B	168	GLY	C-N-CA	6.60	126.54	119.28
35	l	562	LEU	CA-C-N	-6.59	111.60	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	l	562	LEU	C-N-CA	-6.59	111.60	119.84
68	AL	293	GLY	CA-C-N	6.59	126.56	119.78
68	AL	293	GLY	C-N-CA	6.59	126.56	119.78
17	S	61	TYR	N-CA-C	-6.58	104.11	111.28
22	Y	87	PRO	CA-N-CD	-6.56	102.31	111.50
45	x	61	HIS	CB-CG-CD2	-6.55	122.69	131.20
67	AW	447	THR	CA-C-N	-6.54	113.24	119.85
67	AW	447	THR	C-N-CA	-6.54	113.24	119.85
45	x	74	MET	N-CA-C	6.53	118.06	111.07
16	Q	63	PRO	CA-C-N	6.51	124.41	119.66
16	Q	63	PRO	C-N-CA	6.51	124.41	119.66
66	AV	269	LYS	CA-C-N	6.51	126.48	119.78
66	AV	269	LYS	C-N-CA	6.51	126.48	119.78
45	x	506	GLU	N-CA-C	-6.50	104.19	111.28
36	m	135	ILE	N-CA-C	6.50	117.47	108.12
35	l	548	LEU	CA-C-N	-6.46	111.76	119.84
35	l	548	LEU	C-N-CA	-6.46	111.76	119.84
29	f	34	PRO	N-CA-C	6.39	118.50	110.70
60	AC	159	ILE	CA-C-N	6.38	126.35	119.78
60	AC	159	ILE	C-N-CA	6.38	126.35	119.78
45	x	61	HIS	ND1-CE1-NE2	6.37	114.77	108.40
9	J	91	ILE	CB-CA-C	-6.35	104.89	112.19
44	w	211	VAL	CA-C-N	-6.34	112.01	119.05
44	w	211	VAL	C-N-CA	-6.34	112.01	119.05
65	AU	91	PRO	CA-C-N	6.32	126.08	119.76
65	AU	91	PRO	C-N-CA	6.32	126.08	119.76
39	p	78	GLN	CA-C-N	6.32	126.29	119.78
39	p	78	GLN	C-N-CA	6.32	126.29	119.78
8	I	98	ALA	CA-C-N	-6.28	113.91	120.38
8	I	98	ALA	C-N-CA	-6.28	113.91	120.38
43	v	19	PRO	N-CA-CB	6.27	110.16	103.39
12	M	505	GLY	N-CA-C	-6.25	107.08	115.21
68	AY	424	ILE	CA-C-N	-6.25	113.33	119.76
68	AY	424	ILE	C-N-CA	-6.25	113.33	119.76
9	J	238	GLN	CA-C-N	6.24	126.21	119.78
9	J	238	GLN	C-N-CA	6.24	126.21	119.78
45	x	10	THR	N-CA-C	-6.24	103.85	112.03
63	AF	51	LEU	CA-C-N	-6.23	113.56	119.85
63	AF	51	LEU	C-N-CA	-6.23	113.56	119.85
20	V	14	ASP	N-CA-C	6.21	117.72	111.07
41	s	179	TRP	CA-C-N	-6.21	112.45	119.28
41	s	179	TRP	C-N-CA	-6.21	112.45	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	w	56	ARG	N-CA-C	-6.21	105.64	112.72
15	P	119	VAL	CA-C-N	6.21	126.11	119.28
15	P	119	VAL	C-N-CA	6.21	126.11	119.28
66	AV	359	PHE	N-CA-C	6.20	118.12	111.36
31	h	94	PRO	N-CA-C	6.19	118.25	110.70
51	3	2	SER	N-CA-C	6.18	119.44	109.79
45	x	157	SER	N-CA-C	6.16	118.96	111.82
26	c	155	PRO	CA-C-N	-6.13	116.89	123.08
26	c	155	PRO	C-N-CA	-6.13	116.89	123.08
45	x	170	ASN	N-CA-C	6.12	120.82	113.23
35	l	447	ASN	N-CA-C	6.12	116.00	108.11
44	w	253	CYS	CB-CA-C	-6.09	109.53	116.54
51	3	44	ARG	CA-C-N	6.09	126.11	119.90
51	3	44	ARG	C-N-CA	6.09	126.11	119.90
49	1	21	LYS	CA-C-N	6.08	126.26	119.32
49	1	21	LYS	C-N-CA	6.08	126.26	119.32
66	AJ	341	GLN	CA-C-N	6.08	126.05	119.78
66	AJ	341	GLN	C-N-CA	6.08	126.05	119.78
41	s	251	SER	CA-C-N	6.07	125.95	119.28
41	s	251	SER	C-N-CA	6.07	125.95	119.28
66	AV	345	TYR	CA-C-N	-6.07	112.32	119.05
66	AV	345	TYR	C-N-CA	-6.07	112.32	119.05
12	M	175	ARG	N-CA-C	6.05	117.88	111.28
9	J	86	CYS	N-CA-C	6.05	117.54	111.07
46	y	47	THR	N-CA-C	6.04	119.96	112.59
52	4	63	LEU	N-CA-C	6.04	119.12	111.69
68	AL	453	CYS	CA-C-N	6.04	125.94	119.85
68	AL	453	CYS	C-N-CA	6.04	125.94	119.85
13	N	64	TYR	N-CA-C	6.03	120.48	113.18
16	Q	391	VAL	CA-C-N	-6.03	115.26	119.66
16	Q	391	VAL	C-N-CA	-6.03	115.26	119.66
2	B	160	CYS	CA-C-N	6.01	125.89	119.28
2	B	160	CYS	C-N-CA	6.01	125.89	119.28
46	y	207	MET	CA-C-N	5.99	127.32	119.84
46	y	207	MET	C-N-CA	5.99	127.32	119.84
35	l	404	THR	N-CA-C	5.98	116.32	108.07
66	AV	153	ILE	CA-C-N	-5.98	112.75	118.97
66	AV	153	ILE	C-N-CA	-5.98	112.75	118.97
24	a	106	VAL	CA-C-N	5.98	125.89	119.85
24	a	106	VAL	C-N-CA	5.98	125.89	119.85
47	z	8	TYR	N-CA-C	5.96	118.22	110.53
45	x	171	MET	N-CA-C	5.95	120.26	111.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	s	158	GLY	N-CA-C	5.92	121.73	114.69
39	p	155	PRO	CA-C-N	5.91	125.82	119.85
39	p	155	PRO	C-N-CA	5.91	125.82	119.85
46	y	134	ARG	N-CA-C	5.91	123.39	110.80
35	l	106	TRP	N-CA-C	5.91	117.80	111.36
45	x	67	PHE	N-CA-C	5.90	119.67	112.23
58	AN	50	VAL	N-CA-C	5.90	119.43	112.35
64	AT	42	LEU	N-CA-C	5.90	117.71	111.28
65	AH	322	ARG	CA-C-N	5.89	123.96	119.66
65	AH	322	ARG	C-N-CA	5.89	123.96	119.66
47	z	198	PHE	N-CA-C	5.88	117.69	111.28
21	W	118	PRO	CA-C-N	5.86	125.82	119.78
21	W	118	PRO	C-N-CA	5.86	125.82	119.78
41	s	315	PRO	CA-C-N	5.86	127.17	119.84
41	s	315	PRO	C-N-CA	5.86	127.17	119.84
44	w	340	SER	N-CA-C	5.85	117.07	109.64
35	l	90	ILE	O-C-N	5.85	124.22	120.07
65	AU	246	PRO	CA-C-N	5.84	125.70	119.28
65	AU	246	PRO	C-N-CA	5.84	125.70	119.28
45	x	119	GLU	CB-CA-C	-5.83	109.83	116.54
65	AH	221	PRO	CA-C-N	5.83	125.79	119.78
65	AH	221	PRO	C-N-CA	5.83	125.79	119.78
46	y	202	SER	N-CA-C	5.83	118.11	111.11
21	W	27	ARG	N-CA-C	-5.81	105.03	111.36
15	P	113	ASP	N-CA-C	5.78	117.89	108.76
46	y	190	GLY	N-CA-C	5.78	117.77	110.38
8	I	36	GLN	CA-C-N	5.77	123.87	119.66
8	I	36	GLN	C-N-CA	5.77	123.87	119.66
13	N	65	THR	CB-CA-C	-5.77	108.92	115.79
20	V	22	ALA	N-CA-C	-5.76	105.08	111.36
22	Y	85	PRO	N-CA-C	5.76	124.34	112.47
35	l	87	MET	N-CA-C	5.76	117.36	111.14
25	b	37	PRO	CA-N-CD	-5.75	103.95	112.00
45	x	129	TYR	CB-CA-C	-5.74	100.41	109.42
2	B	64	LEU	N-CA-C	-5.74	104.93	111.07
1	A	318	ILE	N-CA-C	5.73	114.19	107.77
42	u	166	ARG	N-CA-C	-5.72	106.53	112.93
7	H	81	ILE	N-CA-C	-5.71	104.96	110.72
54	6	25	GLY	N-CA-C	5.70	118.93	110.60
33	j	45	SER	CA-C-N	5.70	125.61	119.85
33	j	45	SER	C-N-CA	5.70	125.61	119.85
41	s	280	PHE	N-CA-C	5.70	118.43	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	612	PRO	CA-C-N	5.69	125.54	119.28
12	M	612	PRO	C-N-CA	5.69	125.54	119.28
35	l	197	ASP	CA-C-N	-5.68	112.74	119.05
35	l	197	ASP	C-N-CA	-5.68	112.74	119.05
40	r	427	LYS	CA-C-N	5.68	125.63	119.78
40	r	427	LYS	C-N-CA	5.68	125.63	119.78
41	s	21	MET	N-CA-C	-5.68	106.20	113.01
33	j	49	VAL	N-CA-C	5.67	114.50	108.95
8	I	17	GLY	N-CA-C	-5.66	107.83	115.36
48	0	129	ALA	CA-C-N	5.65	126.90	119.84
48	0	129	ALA	C-N-CA	5.65	126.90	119.84
24	a	56	VAL	N-CA-C	5.62	117.83	111.88
14	O	236	GLU	CA-C-N	5.61	126.16	120.38
14	O	236	GLU	C-N-CA	5.61	126.16	120.38
25	b	9	LYS	N-CA-C	-5.61	105.07	111.07
35	l	450	LEU	N-CA-C	5.61	122.74	110.80
16	Q	272	THR	N-CA-C	5.60	120.39	113.50
46	y	104	TRP	N-CA-C	5.59	122.72	110.80
50	2	82	CYS	CA-C-N	5.59	125.43	119.28
50	2	82	CYS	C-N-CA	5.59	125.43	119.28
53	5	20	HIS	N-CA-C	5.59	118.14	111.71
35	l	90	ILE	CA-C-N	-5.59	112.85	119.05
35	l	90	ILE	C-N-CA	-5.59	112.85	119.05
30	g	36	LEU	N-CA-C	-5.59	105.29	111.71
35	l	25	ASN	N-CA-C	5.57	118.21	108.75
68	AL	148	GLY	N-CA-C	-5.55	108.56	114.67
12	M	261	ILE	N-CA-C	5.55	116.67	108.45
26	c	120	SER	CA-C-N	5.54	125.49	119.78
26	c	120	SER	C-N-CA	5.54	125.49	119.78
32	i	149	LEU	N-CA-C	5.52	120.02	113.28
24	a	166	GLY	CA-C-N	5.52	125.35	119.28
24	a	166	GLY	C-N-CA	5.52	125.35	119.28
56	8	16	GLU	N-CA-C	5.51	117.37	111.36
36	m	127	TYR	CB-CA-C	-5.51	110.21	116.54
39	p	154	LEU	CA-C-N	5.50	123.62	119.66
39	p	154	LEU	C-N-CA	5.50	123.62	119.66
42	u	171	THR	N-CA-C	-5.50	106.62	113.38
68	AY	355	GLY	N-CA-C	5.49	118.48	110.63
14	O	233	SER	CB-CA-C	-5.49	109.77	117.23
47	z	188	ILE	CB-CA-C	-5.47	104.75	112.14
58	AN	50	VAL	CB-CA-C	-5.45	106.87	114.00
9	J	267	GLY	CA-C-N	5.44	125.26	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	267	GLY	C-N-CA	5.44	125.26	119.28
51	3	72	ASN	CA-C-N	5.43	125.76	119.47
51	3	72	ASN	C-N-CA	5.43	125.76	119.47
26	c	161	TYR	CA-C-N	5.42	125.36	119.78
26	c	161	TYR	C-N-CA	5.42	125.36	119.78
65	AH	246	PRO	CA-C-N	5.42	125.24	119.28
65	AH	246	PRO	C-N-CA	5.42	125.24	119.28
54	6	2	GLU	N-CA-C	5.41	122.33	110.80
66	AJ	153	ILE	CA-C-N	-5.41	112.96	118.85
66	AJ	153	ILE	C-N-CA	-5.41	112.96	118.85
12	M	85	ALA	CA-C-N	5.39	125.21	119.28
12	M	85	ALA	C-N-CA	5.39	125.21	119.28
16	Q	281	GLU	N-CA-C	5.39	117.16	111.28
67	AW	296	GLY	CA-C-N	5.39	125.33	119.78
67	AW	296	GLY	C-N-CA	5.39	125.33	119.78
45	x	159	LEU	N-CA-C	-5.38	105.50	111.36
2	B	78	GLU	CA-C-N	5.37	125.31	119.78
2	B	78	GLU	C-N-CA	5.37	125.31	119.78
34	k	89	TYR	CB-CA-C	-5.36	109.41	115.79
45	x	245	ILE	N-CA-C	-5.36	104.35	111.05
66	AJ	284	VAL	CA-C-N	5.35	125.25	119.85
66	AJ	284	VAL	C-N-CA	5.35	125.25	119.85
26	c	126	TRP	N-CA-C	5.34	116.80	110.97
30	g	22	PRO	O-C-N	5.33	123.65	121.15
35	l	192	HIS	N-CA-C	5.32	117.16	111.36
45	x	305	PHE	N-CA-C	5.31	118.86	112.38
2	B	43	ASP	CA-C-N	5.30	125.24	119.78
2	B	43	ASP	C-N-CA	5.30	125.24	119.78
35	l	270	ASN	CA-C-N	5.29	125.10	119.28
35	l	270	ASN	C-N-CA	5.29	125.10	119.28
45	x	372	TYR	N-CA-C	-5.27	105.43	111.07
58	AA	50	VAL	N-CA-C	5.27	118.67	112.35
47	z	99	TRP	N-CA-C	-5.27	105.44	111.07
45	x	6	TRP	N-CA-C	5.26	119.76	113.23
50	2	38	ALA	N-CA-C	5.25	117.90	110.50
35	l	230	HIS	CA-C-N	-5.24	113.23	119.05
35	l	230	HIS	C-N-CA	-5.24	113.23	119.05
35	l	16	ILE	CB-CA-C	-5.24	108.80	114.35
13	N	83	PRO	CA-C-N	5.23	125.03	119.28
13	N	83	PRO	C-N-CA	5.23	125.03	119.28
32	i	172	GLN	N-CA-C	5.22	117.42	110.53
7	H	12	VAL	N-CA-C	5.22	115.88	110.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	z	107	ALA	CA-C-N	5.20	126.01	119.98
47	z	107	ALA	C-N-CA	5.20	126.01	119.98
12	M	102	ILE	N-CA-C	5.20	114.27	106.42
39	p	145	PRO	CA-C-N	5.20	125.00	119.28
39	p	145	PRO	C-N-CA	5.20	125.00	119.28
64	AG	7	GLY	CA-C-N	5.20	125.00	119.28
64	AG	7	GLY	C-N-CA	5.20	125.00	119.28
35	l	437	PHE	CA-C-N	5.20	125.13	119.78
35	l	437	PHE	C-N-CA	5.20	125.13	119.78
66	AV	318	ARG	CA-C-N	5.20	125.00	119.28
66	AV	318	ARG	C-N-CA	5.20	125.00	119.28
27	d	120	ILE	N-CA-C	5.19	115.91	110.62
63	AF	70	ASN	N-CA-C	5.19	116.93	111.28
45	x	262	SER	N-CA-C	-5.18	106.64	113.17
60	AC	207	LYS	CA-C-N	5.18	124.98	119.28
60	AC	207	LYS	C-N-CA	5.18	124.98	119.28
45	x	353	LEU	N-CA-C	-5.18	105.72	111.36
45	x	401	SER	N-CA-C	5.16	119.71	113.41
45	x	377	PHE	N-CA-C	5.15	119.41	113.18
34	k	1	MET	CA-C-N	-5.15	113.34	119.05
34	k	1	MET	C-N-CA	-5.15	113.34	119.05
4	E	32	VAL	N-CA-C	5.14	115.36	110.42
11	L	126	LEU	N-CA-C	5.14	116.56	107.61
32	i	321	LYS	CA-C-N	5.13	124.92	119.28
32	i	321	LYS	C-N-CA	5.13	124.92	119.28
36	m	114	VAL	CA-C-N	5.12	131.19	121.97
36	m	114	VAL	C-N-CA	5.12	131.19	121.97
68	AY	453	CYS	CA-C-N	5.12	125.03	119.76
68	AY	453	CYS	C-N-CA	5.12	125.03	119.76
19	U	36	SER	CA-C-N	5.12	124.91	119.28
19	U	36	SER	C-N-CA	5.12	124.91	119.28
36	m	137	GLU	N-CA-C	5.11	116.66	111.14
19	U	62	ASN	CB-CA-C	-5.11	109.19	116.34
46	y	165	VAL	CA-C-N	5.11	126.22	119.84
46	y	165	VAL	C-N-CA	5.11	126.22	119.84
53	5	2	THR	N-CA-C	5.11	116.17	108.46
44	w	223	ASP	CA-C-N	5.10	124.89	119.28
44	w	223	ASP	C-N-CA	5.10	124.89	119.28
62	AR	28	ASP	CA-C-N	5.10	124.89	119.28
62	AR	28	ASP	C-N-CA	5.10	124.89	119.28
66	AJ	19	ILE	N-CA-C	5.09	115.81	110.62
20	V	86	ASP	CA-C-N	5.08	124.75	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	V	86	ASP	C-N-CA	5.08	124.75	119.56
32	i	41	ILE	CB-CA-C	-5.08	107.34	114.00
54	6	9	GLN	N-CA-C	-5.08	105.63	111.07
64	AG	45	VAL	CA-C-N	5.08	124.87	119.28
64	AG	45	VAL	C-N-CA	5.08	124.87	119.28
35	l	516	PRO	N-CA-C	5.08	119.06	111.14
45	x	378	HIS	N-CA-C	-5.08	106.25	112.90
15	P	94	ILE	CB-CA-C	-5.08	107.35	114.00
24	a	106	VAL	N-CA-C	5.08	112.58	107.55
52	4	22	ASN	N-CA-C	5.08	117.58	109.81
55	7	35	GLN	N-CA-C	5.07	119.22	113.19
68	AL	421	GLY	N-CA-C	-5.07	103.15	112.62
12	M	681	ALA	N-CA-C	5.06	114.83	108.45
9	J	195	PHE	CA-C-N	5.06	124.85	119.28
9	J	195	PHE	C-N-CA	5.06	124.85	119.28
45	x	2	PHE	N-CA-C	-5.05	105.67	111.07
46	y	12	ALA	N-CA-C	5.04	117.46	109.96
46	y	65	TRP	N-CA-C	5.04	119.14	113.15
45	x	73	ILE	N-CA-C	5.03	115.18	110.30
28	e	58	ASP	CA-C-N	5.03	124.96	119.78
28	e	58	ASP	C-N-CA	5.03	124.96	119.78
21	W	17	GLY	CA-C-N	5.02	124.95	119.78
21	W	17	GLY	C-N-CA	5.02	124.95	119.78
44	w	70	LYS	CB-CA-C	-5.02	109.82	115.79
2	B	67	GLY	N-CA-C	-5.01	106.71	112.73
9	J	242	VAL	N-CA-C	5.01	116.47	111.00
45	x	378	HIS	CB-CG-CD2	-5.01	124.69	131.20
1	A	315	LEU	N-CA-C	-5.01	108.91	114.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	w	338	LYS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3322	0	3289	212	0
2	B	1420	0	1371	121	0
3	C	1249	0	1253	83	0
4	E	968	0	982	66	0
5	F	670	0	679	37	0
6	G	672	0	650	31	0
6	X	686	0	676	33	0
7	H	922	0	950	58	0
8	I	769	0	788	46	0
9	J	2712	0	2757	236	0
10	K	274	0	257	24	0
11	L	964	0	962	63	0
12	M	5274	0	5312	335	0
13	N	1195	0	1155	49	0
14	O	1643	0	1646	114	0
15	P	1730	0	1685	113	0
16	Q	3460	0	3419	310	0
17	S	568	0	567	42	0
18	T	742	0	723	39	0
19	U	647	0	653	16	0
20	V	1038	0	1027	37	0
21	W	1135	0	1129	60	0
22	Y	533	0	475	97	0
23	Z	648	0	627	18	0
24	a	1174	0	1177	106	0
25	b	1059	0	1079	125	0
26	c	1236	0	1092	81	0
27	d	1418	0	1375	121	0
28	e	810	0	772	35	0
29	f	405	0	407	19	0
30	g	1004	0	1008	65	0
31	h	863	0	861	66	0
32	i	2735	0	2893	187	0
33	j	919	0	968	83	0
34	k	740	0	792	90	0
35	l	4717	0	4893	409	0
36	m	1313	0	1330	123	0
37	n	473	0	480	30	0
38	o	1066	0	1086	62	0
39	p	1495	0	1440	101	0
40	r	3629	0	3825	163	0
41	s	2509	0	2617	166	0
42	u	1394	0	1367	60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	v	921	0	892	90	0
44	w	2474	0	2304	115	0
45	x	4025	0	4003	84	0
46	y	1822	0	1834	72	0
47	z	2124	0	2042	52	0
48	0	1195	0	1183	34	0
49	1	878	0	868	18	0
50	2	748	0	728	24	0
51	3	672	0	645	31	0
52	4	628	0	582	22	0
53	5	598	0	612	15	0
54	6	441	0	439	26	0
55	7	384	0	366	13	0
56	8	386	0	388	8	0
57	9	335	0	352	13	0
58	AA	694	0	683	46	0
58	AN	687	0	676	24	0
59	AB	413	0	438	25	0
59	AO	409	0	432	26	0
60	AC	1521	0	1505	54	0
60	AP	1521	0	1505	61	0
61	AD	509	0	511	15	0
61	AQ	509	0	511	24	0
62	AE	580	0	526	52	0
62	AR	580	0	526	34	0
63	AF	921	0	909	73	0
63	AS	921	0	910	30	0
64	AG	425	0	422	14	0
64	AT	425	0	422	30	0
65	AH	1924	0	1874	64	0
65	AU	1924	0	1874	81	0
66	AJ	3009	0	3065	113	0
66	AV	3009	0	3065	176	0
67	AK	3159	0	3130	154	0
67	AW	3162	0	3139	130	0
68	AL	3453	0	3370	154	0
68	AY	3453	0	3368	161	0
69	A	8	0	0	6	0
69	B	16	0	0	3	0
69	C	8	0	0	0	0
69	M	16	0	0	3	0
70	A	31	0	19	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
71	AL	52	0	88	3	0
71	AQ	52	0	88	7	0
71	AT	52	0	88	3	0
71	B	52	0	88	2	0
71	U	52	0	88	3	0
71	V	52	0	88	5	0
71	b	52	0	88	38	0
71	g	156	0	264	13	0
71	r	104	0	176	23	0
72	E	35	0	0	4	0
72	p	35	0	0	12	0
73	J	48	0	26	27	0
74	AC	4	0	0	3	0
74	AP	4	0	0	2	0
74	M	4	0	0	1	0
74	O	4	0	0	2	0
75	AA	64	0	72	1	0
75	AG	64	0	72	29	0
75	AH	64	0	72	6	0
75	AJ	128	0	144	23	0
75	AL	64	0	72	23	0
75	AN	64	0	72	8	0
75	AU	64	0	72	12	0
75	AY	64	0	72	4	0
75	V	63	0	68	8	0
75	i	64	0	72	3	0
75	l	128	0	144	4	0
75	n	64	0	72	10	0
76	AH	49	0	75	31	0
76	AJ	49	0	75	8	0
76	AL	49	0	75	38	0
76	AU	41	0	56	24	0
76	AV	49	0	75	21	0
76	AY	49	0	75	22	0
76	V	51	0	82	21	0
76	W	51	0	82	19	0
76	l	100	0	157	68	0
77	x	1	0	0	0	0
77	y	2	0	0	0	0
78	x	1	0	0	0	0
79	x	120	0	108	5	0
80	2	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	AH	43	0	32	5	0
81	AU	43	0	32	6	0
82	AJ	86	0	60	7	0
82	AV	86	0	60	13	0
All	All	115642	0	115742	5541	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (5541) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:55:PHE:CE2	39:p:118:TYR:CE2	1.82	1.65
68:AY:296:TRP:CD1	68:AY:419:THR:CG2	1.74	1.60
63:AF:29:LYS:CD	63:AF:75:ILE:HD11	1.31	1.58
35:l:533:MET:CE	76:l:702:PEE:H36	1.25	1.58
35:l:37:LYS:HE2	35:l:98:TRP:CD1	1.40	1.56
75:AJ:405:CDL:H112	76:AY:502:PEE:C45	1.18	1.56
24:a:55:PHE:HE2	39:p:118:TYR:CE2	1.17	1.56
63:AF:29:LYS:CG	63:AF:75:ILE:HD11	1.16	1.55
24:a:55:PHE:CE2	39:p:118:TYR:CD2	1.92	1.55
32:i:288:LEU:CD2	76:l:701:PEE:H58	1.37	1.53
24:a:98:LEU:HB3	27:d:57:TYR:CE1	1.45	1.52
68:AY:296:TRP:CD1	68:AY:419:THR:HG23	0.99	1.52
35:l:533:MET:HE1	76:l:702:PEE:C22	1.40	1.51
63:AF:29:LYS:HG2	63:AF:75:ILE:CD1	1.40	1.49
68:AY:296:TRP:NE1	68:AY:419:THR:CG2	1.73	1.49
9:J:130:ILE:HG23	73:J:401:NDP:C8A	1.45	1.46
60:AC:150:ALA:CB	66:AV:168:TYR:HE2	1.29	1.44
35:l:571:ILE:CD1	76:l:701:PEE:O5	1.64	1.43
12:M:134:GLY:HA2	69:M:801:SF4:S3	1.57	1.41
58:AA:78:TYR:CB	62:AE:65:GLU:HG2	1.48	1.41
63:AF:29:LYS:CD	63:AF:75:ILE:CD1	1.97	1.41
35:l:84:TYR:CD1	35:l:88:MET:HE2	1.54	1.40
35:l:84:TYR:CE1	35:l:88:MET:CE	2.05	1.40
63:AF:29:LYS:CG	63:AF:75:ILE:CD1	1.96	1.40
58:AA:78:TYR:HB3	62:AE:65:GLU:CG	1.50	1.39
60:AC:150:ALA:CB	66:AV:168:TYR:CE2	2.05	1.38
38:o:24:ASN:HB3	68:AL:264:THR:CG2	1.54	1.37
24:a:55:PHE:HE2	39:p:118:TYR:CD2	1.32	1.35
66:AV:14:ILE:CD1	76:AY:502:PEE:H41	1.58	1.33

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:262:LEU:HD22	16:Q:268:TRP:CD1	1.64	1.32
67:AK:259:ARG:CG	67:AK:444:LEU:HD13	1.60	1.31
68:AY:296:TRP:HE1	68:AY:419:THR:CB	1.42	1.31
35:l:84:TYR:CE1	35:l:88:MET:HE2	1.64	1.31
60:AC:150:ALA:HB3	66:AV:168:TYR:CE2	1.61	1.31
32:i:288:LEU:HD23	76:l:701:PEE:C36	1.60	1.30
66:AV:10:LEU:HD21	76:AY:502:PEE:C27	1.59	1.30
75:AJ:405:CDL:C11	76:AY:502:PEE:C45	2.08	1.29
75:AL:502:CDL:C57	76:AL:503:PEE:H63	1.61	1.29
38:o:24:ASN:CB	68:AL:264:THR:HG22	1.63	1.28
24:a:98:LEU:CB	27:d:57:TYR:HE1	1.46	1.28
9:J:206:ILE:HA	9:J:240:VAL:O	1.34	1.27
16:Q:82:LEU:O	16:Q:98:VAL:HG13	1.24	1.27
24:a:55:PHE:CD2	39:p:118:TYR:CE2	2.22	1.27
68:AY:296:TRP:NE1	68:AY:419:THR:OG1	1.64	1.27
35:l:188:TRP:CE2	35:l:192:HIS:HD2	1.54	1.26
58:AA:78:TYR:CD1	62:AE:65:GLU:HA	1.69	1.26
9:J:171:ASN:O	9:J:181:LEU:HD21	1.23	1.25
16:Q:271:ARG:NH1	41:s:281:ARG:HB2	1.52	1.24
35:l:447:ASN:OD1	35:l:448:PRO:HD2	1.30	1.24
65:AU:308:ARG:NH1	75:AU:403:CDL:O1	1.70	1.24
9:J:130:ILE:HG23	73:J:401:NDP:N7A	1.52	1.23
76:AU:401:PEE:H17	66:AV:240:MET:CE	1.68	1.22
76:AH:401:PEE:H18	66:AJ:240:MET:CE	1.70	1.21
22:Y:84:PHE:CE2	35:l:483:PRO:HG3	1.74	1.20
35:l:37:LYS:CE	35:l:98:TRP:CD1	2.24	1.20
22:Y:87:PRO:HB3	43:v:103:GLU:OE2	1.38	1.19
22:Y:72:ARG:NH1	35:l:390:TYR:OH	1.76	1.19
24:a:55:PHE:CD2	39:p:118:TYR:CZ	2.30	1.19
63:AF:29:LYS:HD3	63:AF:75:ILE:CD1	1.64	1.19
9:J:206:ILE:O	9:J:211:ASP:OD2	1.61	1.19
9:J:171:ASN:C	9:J:181:LEU:HD21	1.68	1.18
9:J:171:ASN:O	9:J:181:LEU:CD2	1.92	1.18
35:l:226:GLN:HE21	35:l:314:MET:CE	1.56	1.18
25:b:110:ILE:HG23	25:b:111:LEU:HG	1.24	1.17
75:AL:502:CDL:H572	76:AL:503:PEE:C40	1.73	1.17
76:V:202:PEE:C42	76:l:701:PEE:C45	2.23	1.17
24:a:55:PHE:HD2	39:p:118:TYR:CZ	1.61	1.17
76:V:202:PEE:H70	76:l:701:PEE:C45	1.74	1.16
76:W:201:PEE:H75	41:s:77:LEU:CD2	1.75	1.16
68:AY:98:PHE:CE2	68:AY:120:LEU:CD1	2.29	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:188:TRP:CE2	35:l:192:HIS:CD2	2.33	1.15
64:AT:42:LEU:O	64:AT:45:VAL:HG22	1.41	1.15
16:Q:268:TRP:CZ3	16:Q:272:THR:HG21	1.80	1.15
35:l:533:MET:SD	76:l:702:PEE:H36	1.86	1.14
1:A:93:PHE:CE2	1:A:98:LYS:HD3	1.80	1.14
32:i:291:TYR:CE2	76:l:701:PEE:C31	2.29	1.14
68:AY:296:TRP:NE1	68:AY:419:THR:HG21	1.57	1.14
39:p:167:TRP:O	39:p:171:VAL:HG23	1.47	1.14
22:Y:84:PHE:CD1	22:Y:85:PRO:HD3	1.84	1.13
4:E:25:MET:HB3	4:E:29:LYS:CE	1.77	1.13
67:AK:259:ARG:HG3	67:AK:444:LEU:HD13	1.27	1.13
68:AY:296:TRP:NE1	68:AY:419:THR:CB	2.03	1.13
27:d:59:HIS:CE1	28:e:120:ARG:HB3	1.84	1.12
35:l:84:TYR:CE1	35:l:88:MET:HE3	1.74	1.12
66:AV:10:LEU:CD2	76:AY:502:PEE:H46	1.79	1.12
34:k:4:ILE:HD11	36:m:125:MET:SD	1.90	1.11
58:AA:37:ASN:OD1	58:AA:40:ARG:NH2	1.83	1.11
76:W:201:PEE:H75	41:s:77:LEU:HD21	1.19	1.11
64:AT:40:LEU:HD12	64:AT:41:ILE:N	1.63	1.11
75:AG:101:CDL:HA62	75:AG:101:CDL:H332	1.25	1.10
60:AC:150:ALA:HB1	66:AV:168:TYR:CE2	1.80	1.10
75:AL:502:CDL:C57	76:AL:503:PEE:H66	1.80	1.10
75:AL:502:CDL:H571	76:AL:503:PEE:H63	1.12	1.10
76:AL:503:PEE:H19	76:AL:503:PEE:H49	1.11	1.10
68:AY:98:PHE:CE2	68:AY:120:LEU:HD13	1.87	1.10
35:l:54:PHE:CE1	35:l:58:ASP:OD1	2.06	1.08
9:J:130:ILE:HG23	73:J:401:NDP:H8A	1.28	1.08
22:Y:71:TRP:CH2	22:Y:75:HIS:CD2	2.42	1.08
22:Y:84:PHE:CZ	35:l:483:PRO:HG3	1.88	1.08
16:Q:78:LYS:NZ	33:j:48:ARG:HH21	1.49	1.07
35:l:97:THR:HG21	35:l:125:LEU:HD12	1.35	1.07
4:E:25:MET:HB3	4:E:29:LYS:HE3	1.32	1.07
24:a:98:LEU:CB	27:d:57:TYR:CE1	2.25	1.07
26:c:181:VAL:CB	43:v:37:ARG:HH21	1.66	1.07
12:M:134:GLY:CA	69:M:801:SF4:S3	2.42	1.07
24:a:114:LYS:HB2	27:d:57:TYR:CE2	1.88	1.07
35:l:84:TYR:HE1	35:l:88:MET:CE	1.51	1.07
75:AG:101:CDL:H712	75:AG:101:CDL:H531	1.32	1.06
35:l:54:PHE:CZ	35:l:58:ASP:OD1	2.07	1.06
58:AA:78:TYR:HE1	62:AE:64:GLU:O	1.36	1.06
24:a:55:PHE:HD2	39:p:118:TYR:CE1	1.75	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:227:LEU:O	35:l:230:HIS:ND1	1.88	1.05
44:w:332:ARG:O	44:w:338:LYS:HA	1.54	1.05
27:d:81:GLU:OE1	37:n:43:MET:HE3	1.57	1.05
27:d:105:LYS:CE	35:l:197:ASP:OD2	2.04	1.04
58:AA:78:TYR:CE1	62:AE:64:GLU:O	2.09	1.04
34:k:1:MET:N	34:k:1:MET:SD	2.30	1.04
62:AE:34:ARG:HD3	62:AE:78:ARG:NH2	1.71	1.04
63:AF:29:LYS:HG2	63:AF:75:ILE:CG1	1.87	1.04
62:AR:34:ARG:HG3	62:AR:78:ARG:NH1	1.72	1.04
22:Y:71:TRP:CH2	22:Y:75:HIS:HD2	1.76	1.04
34:k:7:ASN:HD21	36:m:9:SER:C	1.65	1.04
9:J:221:HIS:CE1	9:J:222:ARG:HG3	1.91	1.04
6:X:112:SER:CA	72:p:201:8Q1:O2	2.06	1.04
65:AU:288:MET:HB3	76:AU:401:PEE:O4	1.57	1.03
65:AU:296:MET:CE	76:AU:401:PEE:H53	1.86	1.03
16:Q:69:VAL:O	16:Q:72:PRO:HD2	1.58	1.03
32:i:285:ILE:HG12	76:l:701:PEE:H75	1.34	1.03
16:Q:82:LEU:O	16:Q:98:VAL:CG1	2.06	1.03
35:l:84:TYR:CD1	35:l:88:MET:CE	2.30	1.03
67:AK:438:MET:HE2	67:AK:450:VAL:HG13	1.39	1.03
4:E:25:MET:CB	4:E:29:LYS:HE3	1.89	1.03
67:AK:259:ARG:HH21	67:AK:259:ARG:HB2	1.22	1.03
76:AU:401:PEE:H17	66:AV:240:MET:HE1	1.05	1.03
35:l:571:ILE:HD11	76:l:701:PEE:C30	1.89	1.03
66:AV:14:ILE:HD12	76:AY:502:PEE:H41	1.41	1.03
24:a:96:ALA:HB3	27:d:55:TYR:HB2	1.33	1.02
66:AV:10:LEU:CD2	76:AY:502:PEE:C27	2.36	1.02
24:a:96:ALA:CB	27:d:55:TYR:HB2	1.90	1.02
35:l:37:LYS:CE	35:l:98:TRP:HD1	1.64	1.02
35:l:59:GLN:HA	35:l:59:GLN:HE21	1.23	1.02
71:r:502:PLX:H332	71:r:502:PLX:H372	1.37	1.02
75:AG:101:CDL:H712	75:AG:101:CDL:C53	1.90	1.02
9:J:217:PHE:HZ	9:J:322:MET:HE2	1.25	1.02
35:l:25:ASN:ND2	35:l:25:ASN:O	1.91	1.02
27:d:105:LYS:NZ	35:l:197:ASP:OD2	1.91	1.01
35:l:571:ILE:HD11	76:l:701:PEE:O5	0.84	1.01
64:AG:38:TRP:CD1	75:AG:101:CDL:H511	1.94	1.01
9:J:130:ILE:CG2	73:J:401:NDP:N7A	2.24	1.01
16:Q:78:LYS:NZ	33:j:48:ARG:NH2	2.08	1.01
35:l:222:GLY:CA	35:l:229:LEU:HD12	1.91	1.01
35:l:226:GLN:HG3	35:l:280:LEU:CD2	1.91	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:170:ILE:H	39:p:170:ILE:HD12	1.24	1.01
35:l:534:HIS:ND1	76:l:702:PEE:H14	1.74	1.01
62:AR:34:ARG:NH1	62:AR:78:ARG:HH12	1.59	1.00
76:l:701:PEE:H37	40:r:155:VAL:HB	1.42	1.00
39:p:48:PHE:HE1	72:p:201:8Q1:C8	1.73	1.00
32:i:291:TYR:CE2	76:l:701:PEE:H48	1.95	1.00
32:i:291:TYR:CZ	76:l:701:PEE:H49	1.97	1.00
35:l:533:MET:CE	76:l:702:PEE:C22	2.16	1.00
35:l:193:SER:OG	35:l:205:ASN:ND2	1.95	1.00
67:AK:257:GLU:OE2	67:AK:450:VAL:N	1.92	1.00
62:AR:79:ASP:OD2	65:AU:236:TYR:OH	1.79	1.00
65:AH:121:CYS:SG	81:AH:402:HEC:HBB2	2.01	0.99
9:J:130:ILE:CG2	73:J:401:NDP:C8A	2.41	0.99
9:J:141:PHE:CE2	9:J:180:TYR:HA	1.98	0.99
9:J:176:SER:HA	9:J:182:ARG:HH21	1.24	0.99
76:V:202:PEE:C25	76:V:202:PEE:H60	1.92	0.99
35:l:533:MET:HE1	76:l:702:PEE:H35	1.44	0.99
76:AL:503:PEE:H50	76:AL:503:PEE:H16	1.45	0.99
64:AT:39:ARG:HA	64:AT:51:LYS:HE3	1.45	0.99
34:k:7:ASN:HD22	36:m:9:SER:CB	1.75	0.99
16:Q:53:TYR:HE1	76:l:701:PEE:O1P	1.44	0.98
62:AE:30:LEU:HD11	62:AE:34:ARG:HH21	1.26	0.98
1:A:116:ASN:ND2	70:A:502:FMN:C8	2.25	0.98
35:l:51:THR:HG21	35:l:91:PRO:HG2	1.42	0.98
76:AH:401:PEE:H73	76:AH:401:PEE:H64	1.42	0.98
67:AW:351:ILE:HD11	67:AW:448:PRO:HD2	1.44	0.98
35:l:84:TYR:HE1	35:l:88:MET:HE3	1.08	0.98
66:AJ:156:ILE:HG22	66:AJ:160:LEU:HB2	1.42	0.98
25:b:107:GLY:N	25:b:115:GLU:OE1	1.96	0.98
9:J:171:ASN:HB3	9:J:181:LEU:HD11	1.46	0.98
34:k:4:ILE:CD1	36:m:125:MET:SD	2.52	0.98
35:l:231:PRO:O	35:l:234:PRO:HD2	1.64	0.98
25:b:93:LYS:HE3	35:l:65:ASN:O	1.64	0.97
35:l:226:GLN:NE2	35:l:314:MET:CE	2.27	0.97
76:l:701:PEE:C22	40:r:155:VAL:HG11	1.94	0.97
75:AG:101:CDL:HA62	75:AG:101:CDL:C33	1.94	0.97
76:l:701:PEE:H36	40:r:155:VAL:HG11	1.44	0.97
76:AH:401:PEE:C13	66:AJ:240:MET:CE	2.42	0.97
39:p:44:MET:HE1	72:p:201:8Q1:C10	1.94	0.97
67:AK:259:ARG:CG	67:AK:444:LEU:CD1	2.42	0.97
76:l:701:PEE:H37	40:r:155:VAL:CB	1.93	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:AL:502:CDL:C57	76:AL:503:PEE:C38	2.43	0.97
3:C:204:GLU:OE2	3:C:206:ARG:NH1	1.98	0.96
66:AV:14:ILE:HD13	76:AY:502:PEE:H41	1.45	0.96
76:AL:503:PEE:H16	76:AL:503:PEE:C32	1.95	0.96
76:V:202:PEE:H14	32:i:276:LEU:CD1	1.96	0.96
39:p:48:PHE:CE1	72:p:201:8Q1:C8	2.48	0.96
35:l:84:TYR:HD1	35:l:88:MET:HE2	1.20	0.96
16:Q:262:LEU:HD22	16:Q:268:TRP:HD1	1.23	0.95
35:l:74:THR:CG2	35:l:194:ASN:OD1	2.14	0.95
3:C:137:VAL:HG21	16:Q:87:GLN:HE21	1.29	0.95
68:AY:424:ILE:HG23	68:AY:429:TRP:HE1	1.31	0.95
63:AF:67:LEU:HD23	66:AJ:209:LEU:HD12	1.47	0.95
76:AU:401:PEE:C13	66:AV:240:MET:HE1	1.96	0.95
34:k:1:MET:HB3	36:m:125:MET:HB2	1.43	0.95
67:AK:259:ARG:HB2	67:AK:259:ARG:NH2	1.82	0.95
76:V:202:PEE:H14	32:i:276:LEU:HD12	1.47	0.95
24:a:55:PHE:CD2	39:p:118:TYR:CD2	2.49	0.95
24:a:176:LYS:HE2	31:h:42:GLU:HG2	1.49	0.95
9:J:206:ILE:HB	9:J:242:VAL:HG22	1.47	0.95
22:Y:86:TYR:OH	43:v:100:LYS:CE	2.15	0.95
68:AY:98:PHE:CD2	68:AY:120:LEU:HD11	2.01	0.95
76:AL:503:PEE:H49	76:AL:503:PEE:C14	1.95	0.94
1:A:116:ASN:HD22	70:A:502:FMN:C8M	1.78	0.94
16:Q:271:ARG:NH1	41:s:281:ARG:CB	2.30	0.94
76:AL:503:PEE:H19	76:AL:503:PEE:C31	1.96	0.94
26:c:122:THR:OG1	38:o:12:ARG:NH1	1.99	0.94
25:b:88:TYR:CD1	71:b:201:PLX:H1C1	2.02	0.94
71:b:201:PLX:O9	71:r:502:PLX:H1C3	1.67	0.94
60:AC:150:ALA:HB1	66:AV:168:TYR:CD2	2.02	0.94
67:AK:259:ARG:HG3	67:AK:444:LEU:CD1	1.97	0.94
58:AA:78:TYR:CD1	62:AE:65:GLU:CA	2.49	0.94
76:AL:503:PEE:C31	76:AL:503:PEE:H26	1.97	0.94
14:O:177:LEU:N	74:O:301:FES:S1	2.39	0.94
76:AH:401:PEE:H18	66:AJ:240:MET:HE1	1.49	0.94
35:l:226:GLN:CG	35:l:280:LEU:HD21	1.98	0.94
16:Q:85:GLY:HA3	33:j:39:CYS:SG	2.08	0.93
34:k:7:ASN:ND2	36:m:9:SER:CB	2.31	0.93
16:Q:271:ARG:HH11	41:s:281:ARG:HB2	1.18	0.93
66:AV:137:GLN:HE21	66:AV:141:TRP:HE1	1.10	0.93
32:i:291:TYR:CE2	76:l:701:PEE:H49	2.00	0.93
67:AK:257:GLU:CG	67:AK:450:VAL:HG22	1.99	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:118:PRO:O	25:b:120:MET:HG2	1.69	0.93
32:i:167:TRP:CZ3	35:l:573:THR:CB	2.52	0.93
67:AK:259:ARG:HG2	67:AK:444:LEU:HD13	1.49	0.93
16:Q:271:ARG:HH11	41:s:281:ARG:CB	1.82	0.93
22:Y:87:PRO:CB	43:v:103:GLU:OE2	2.17	0.93
60:AC:150:ALA:HB3	66:AV:168:TYR:HE2	0.77	0.93
45:x:365:ILE:HD12	46:y:87:MET:HE1	1.48	0.93
68:AY:98:PHE:CD2	68:AY:120:LEU:CD1	2.52	0.93
76:AH:401:PEE:H66	76:AH:401:PEE:H28	1.50	0.92
27:d:59:HIS:HE1	28:e:120:ARG:HB3	1.24	0.92
1:A:116:ASN:HD22	70:A:502:FMN:C8	1.82	0.92
34:k:3:LEU:CD2	36:m:117:ASN:HD21	1.83	0.92
45:x:449:MET:SD	46:y:5:MET:HE2	2.10	0.92
25:b:110:ILE:HG23	25:b:111:LEU:CG	1.99	0.92
22:Y:83:HIS:O	22:Y:84:PHE:HB2	1.67	0.92
27:d:59:HIS:CE1	28:e:120:ARG:CB	2.53	0.92
62:AE:29:PRO:HD3	65:AH:262:THR:HG21	1.52	0.92
51:3:5:LYS:HZ3	51:3:6:GLY:H	0.93	0.91
16:Q:78:LYS:HZ3	33:j:48:ARG:NH2	1.67	0.91
4:E:25:MET:O	4:E:29:LYS:HG3	1.69	0.91
66:AV:143:ALA:O	66:AV:147:THR:OG1	1.86	0.91
71:b:201:PLX:H1C3	71:b:201:PLX:C3	2.01	0.90
9:J:141:PHE:CZ	9:J:180:TYR:HA	2.07	0.90
22:Y:79:GLU:O	35:l:487:LYS:HE3	1.70	0.90
7:H:45:ARG:NH1	7:H:49:GLU:OE2	2.05	0.90
27:d:60:ARG:HG2	27:d:60:ARG:HH11	1.36	0.90
62:AE:34:ARG:HD3	62:AE:78:ARG:HH22	1.30	0.90
9:J:169:HIS:HD2	73:J:401:NDP:H5N	1.33	0.90
67:AK:257:GLU:OE2	67:AK:450:VAL:HG22	1.70	0.90
65:AU:296:MET:HE1	76:AU:401:PEE:H53	1.51	0.90
32:i:291:TYR:HE2	76:l:701:PEE:H48	1.32	0.89
35:l:226:GLN:CG	35:l:280:LEU:CD2	2.49	0.89
67:AW:450:VAL:HA	67:AW:453:LEU:CD1	2.03	0.89
24:a:114:LYS:HB2	27:d:57:TYR:HE2	1.31	0.89
35:l:51:THR:HG21	35:l:91:PRO:CG	2.02	0.89
35:l:227:LEU:HD12	35:l:230:HIS:ND1	1.85	0.89
66:AV:149:LEU:HD21	66:AV:281:LEU:HD21	1.52	0.89
9:J:360:ARG:HA	36:m:78:TYR:CE1	2.07	0.89
27:d:105:LYS:HE2	35:l:197:ASP:OD2	1.70	0.89
34:k:7:ASN:ND2	36:m:9:SER:HB2	1.86	0.89
66:AV:137:GLN:HE21	66:AV:141:TRP:NE1	1.70	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PHE:HE2	1:A:98:LYS:HD3	1.17	0.89
35:l:78:LEU:HD21	35:l:80:PHE:CE1	2.07	0.89
40:r:78:MET:O	40:r:432:ARG:NH1	2.05	0.89
22:Y:96:GLU:OE2	26:c:185:GLU:O	1.89	0.89
66:AV:14:ILE:CD1	76:AY:502:PEE:C25	2.49	0.89
25:b:110:ILE:C	25:b:111:LEU:HD23	1.98	0.89
9:J:171:ASN:CB	9:J:181:LEU:HD11	2.02	0.89
27:d:110:ARG:HG2	27:d:110:ARG:HH11	1.38	0.89
63:AF:29:LYS:HD2	63:AF:75:ILE:HD11	1.52	0.89
68:AY:99:LYS:O	68:AY:106:GLY:HA3	1.71	0.89
27:d:108:GLN:HG2	35:l:199:GLN:HB3	1.54	0.89
9:J:83:PRO:HB2	9:J:108:TRP:NE1	1.88	0.88
35:l:37:LYS:HE3	35:l:102:GLU:HG3	1.53	0.88
3:C:137:VAL:CG2	16:Q:87:GLN:HE21	1.86	0.88
26:c:169:GLU:OE2	43:v:56:ARG:NH2	2.05	0.88
35:l:193:SER:HB2	35:l:195:SER:OG	1.74	0.88
35:l:226:GLN:HG3	35:l:280:LEU:HD21	1.53	0.88
76:l:701:PEE:H37	40:r:155:VAL:CG1	2.02	0.88
35:l:88:MET:O	35:l:91:PRO:HD2	1.74	0.88
16:Q:400:ILE:HB	16:Q:407:PHE:HB3	1.54	0.88
34:k:23:ARG:H	36:m:22:LYS:HE2	1.39	0.88
43:v:66:LEU:HD11	43:v:84:ARG:HD2	1.55	0.88
76:AH:401:PEE:H18	66:AJ:240:MET:SD	2.12	0.88
9:J:206:ILE:HB	9:J:242:VAL:CG2	2.04	0.88
32:i:288:LEU:CD2	76:l:701:PEE:C36	2.32	0.88
33:j:105:GLU:HG2	36:m:168:ILE:HD11	1.56	0.88
41:s:185:TRP:HE1	41:s:238:THR:HG22	1.39	0.88
65:AU:296:MET:HE2	76:AU:401:PEE:H53	1.53	0.88
24:a:87:THR:HG22	71:b:201:PLX:C13	2.03	0.88
34:k:2:PRO:HG2	36:m:115:VAL:HG21	1.56	0.88
60:AC:150:ALA:CB	66:AV:168:TYR:CD2	2.55	0.88
32:i:167:TRP:HZ3	35:l:570:GLN:HA	1.37	0.88
35:l:78:LEU:HD21	35:l:80:PHE:HE1	1.39	0.88
68:AY:296:TRP:CE2	68:AY:419:THR:HG21	2.08	0.88
22:Y:86:TYR:OH	43:v:100:LYS:CG	2.22	0.87
71:b:201:PLX:H102	71:b:201:PLX:H6	1.56	0.87
58:AA:78:TYR:CE1	62:AE:65:GLU:HA	2.08	0.87
22:Y:84:PHE:CG	22:Y:85:PRO:CD	2.57	0.87
34:k:1:MET:HB2	34:k:4:ILE:CD1	2.04	0.87
26:c:181:VAL:CB	43:v:37:ARG:NH2	2.37	0.87
32:i:224:SER:HB2	32:i:229:LEU:HB3	1.56	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:AG:101:CDL:H712	75:AG:101:CDL:C52	2.03	0.87
35:l:533:MET:SD	76:l:702:PEE:C22	2.62	0.87
35:l:447:ASN:OD1	35:l:448:PRO:CD	2.19	0.87
7:H:36:GLU:HA	7:H:45:ARG:HH21	1.38	0.87
16:Q:194:LEU:HD12	16:Q:268:TRP:CZ2	2.09	0.87
76:V:202:PEE:C43	76:l:701:PEE:C45	2.53	0.87
27:d:59:HIS:CE1	28:e:120:ARG:CG	2.58	0.87
68:AL:70:THR:HG1	68:AL:410:CYS:HG	1.23	0.87
12:M:130:ILE:HD13	18:T:114:TYR:CE1	2.11	0.86
9:J:212:ARG:HG2	9:J:212:ARG:HH11	1.37	0.86
44:w:99:GLY:HA3	44:w:337:ARG:HH12	1.40	0.86
67:AK:183:ARG:NH1	67:AW:451:ASP:OD2	2.08	0.86
67:AK:438:MET:HB3	67:AK:450:VAL:CG1	2.05	0.86
35:l:533:MET:SD	76:l:702:PEE:H37	2.15	0.86
25:b:110:ILE:O	25:b:111:LEU:HD23	1.75	0.86
47:z:112:LEU:HG	47:z:118:PRO:HB3	1.55	0.86
66:AV:137:GLN:NE2	66:AV:141:TRP:HE1	1.73	0.86
22:Y:84:PHE:CD1	22:Y:85:PRO:CD	2.58	0.86
9:J:169:HIS:HD2	73:J:401:NDP:C5N	1.87	0.86
4:E:25:MET:HB3	4:E:29:LYS:HE2	1.55	0.86
76:W:201:PEE:O2P	76:W:201:PEE:N	2.08	0.86
51:3:5:LYS:HZ3	51:3:6:GLY:N	1.73	0.86
34:k:2:PRO:HG2	36:m:115:VAL:CG2	2.04	0.85
67:AK:257:GLU:CD	67:AK:450:VAL:HG22	1.99	0.85
67:AK:438:MET:CB	67:AK:450:VAL:CG1	2.54	0.85
66:AV:10:LEU:HD21	76:AY:502:PEE:H46	0.88	0.85
1:A:126:LYS:HB3	1:A:277:ASN:HD21	1.40	0.85
2:B:81:THR:O	13:N:58:ARG:NH2	2.09	0.85
24:a:96:ALA:HB3	27:d:55:TYR:CB	2.05	0.85
38:o:30:ARG:HE	68:AL:259:GLU:HB3	1.41	0.85
62:AE:21:GLU:O	62:AE:25:GLU:N	2.09	0.85
7:H:102:PRO:HA	15:P:70:PRO:HB2	1.57	0.85
27:d:114:ASN:O	27:d:114:ASN:ND2	2.09	0.85
66:AV:295:LEU:O	66:AV:299:LEU:HD22	1.77	0.85
68:AY:296:TRP:CD1	68:AY:419:THR:HG21	1.91	0.85
62:AE:30:LEU:HD21	65:AH:216:THR:CG2	2.07	0.85
63:AF:71:LEU:HD23	63:AF:71:LEU:H	1.40	0.85
39:p:167:TRP:HE3	39:p:171:VAL:HG21	1.40	0.85
44:w:332:ARG:O	44:w:338:LYS:HG2	1.76	0.85
27:d:111:GLU:OE2	27:d:119:CYS:N	2.10	0.85
1:A:244:ASN:N	70:A:502:FMN:O2P	2.09	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:ARG:HH21	16:Q:208:GLU:HB3	1.39	0.84
16:Q:273:ILE:CD1	16:Q:325:ASP:OD2	2.25	0.84
67:AW:259:ARG:NH1	67:AW:449:PHE:CE1	2.44	0.84
68:AY:412:ASP:O	68:AY:416:SER:HB2	1.76	0.84
46:y:78:LEU:HB2	46:y:79:PRO:HD3	1.58	0.84
16:Q:78:LYS:HZ3	33:j:48:ARG:HH21	1.17	0.84
32:i:54:GLU:OE2	32:i:58:LYS:NZ	2.10	0.84
9:J:176:SER:CA	9:J:182:ARG:HH21	1.89	0.84
24:a:53:ARG:HD2	25:b:28:LEU:HD11	1.57	0.84
16:Q:53:TYR:CE1	76:l:701:PEE:O1P	2.30	0.84
76:V:202:PEE:H74	76:l:701:PEE:C45	2.08	0.84
63:AF:52:PRO:HG2	63:AF:55:LEU:HB2	1.58	0.84
66:AV:344:SER:O	66:AV:348:THR:HG23	1.76	0.84
30:g:1:MET:HE2	30:g:85:ARG:HD3	1.57	0.84
62:AE:30:LEU:HD21	65:AH:216:THR:HG23	1.59	0.84
9:J:85:ARG:HG3	9:J:85:ARG:HH11	1.41	0.84
20:V:84:PRO:O	20:V:89:ASN:ND2	2.10	0.84
35:l:188:TRP:NE1	35:l:192:HIS:CD2	2.45	0.84
32:i:12:THR:HG21	36:m:162:VAL:HG21	1.60	0.83
45:x:187:SER:HB2	45:x:277:MET:HE1	1.60	0.83
63:AF:50:ARG:O	67:AW:148:ARG:NH2	2.11	0.83
4:E:70:ASN:OD1	72:E:201:8Q1:O4	1.95	0.83
24:a:90:ASN:HD22	71:b:201:PLX:H122	1.43	0.83
30:g:62:LEU:HD22	71:g:203:PLX:H91	1.61	0.83
62:AR:34:ARG:NH1	62:AR:78:ARG:NH1	2.25	0.83
26:c:122:THR:HG1	38:o:12:ARG:HH12	1.27	0.83
75:AG:101:CDL:H731	75:AG:101:CDL:H542	1.60	0.83
9:J:206:ILE:CA	9:J:240:VAL:O	2.24	0.83
44:w:160:GLU:HG2	44:w:161:ARG:H	1.43	0.83
59:AB:27:ARG:HE	67:AK:174:ILE:HD12	1.43	0.83
41:s:17:MET:HE1	41:s:232:ILE:HD12	1.61	0.83
75:AG:101:CDL:H332	75:AG:101:CDL:CA6	2.06	0.83
58:AA:25:ARG:HG2	60:AC:91:TYR:O	1.79	0.82
76:AH:401:PEE:H64	76:AH:401:PEE:C43	2.08	0.82
16:Q:145:MET:HE1	16:Q:226:TYR:HB3	1.61	0.82
76:AL:503:PEE:H16	76:AL:503:PEE:C31	2.08	0.82
16:Q:87:GLN:O	16:Q:88:HIS:C	2.22	0.82
24:a:143:GLU:OE1	40:r:175:ASN:ND2	2.11	0.82
27:d:59:HIS:CE1	28:e:120:ARG:HG2	2.14	0.82
12:M:299:ARG:HG2	12:M:300:GLN:H	1.41	0.82
33:j:6:ILE:O	33:j:10:ASN:ND2	2.12	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:AR:86:LEU:O	62:AR:86:LEU:HD23	1.79	0.82
24:a:54:LEU:HD22	25:b:26:GLN:C	2.05	0.82
67:AW:449:PHE:N	67:AW:452:GLU:OE2	2.10	0.82
3:C:156:GLY:HA2	3:C:169:GLY:HA2	1.62	0.82
32:i:235:ASN:ND2	32:i:307:MET:SD	2.53	0.82
62:AR:79:ASP:HB3	65:AU:92:PRO:HG2	1.60	0.82
9:J:169:HIS:CD2	73:J:401:NDP:H5N	2.15	0.82
26:c:93:ASP:OD1	38:o:44:LYS:NZ	2.13	0.82
39:p:124:GLN:O	39:p:128:LEU:HG	1.79	0.82
67:AW:257:GLU:OE2	67:AW:450:VAL:N	2.09	0.82
24:a:87:THR:HG22	71:b:201:PLX:H132	1.61	0.82
71:AL:501:PLX:H71	76:AL:503:PEE:H17	1.60	0.82
65:AH:291:LYS:HD2	76:AH:401:PEE:H8	1.62	0.81
5:F:57:GLU:HB3	12:M:662:ALA:H	1.45	0.81
6:X:112:SER:N	72:p:201:8Q1:O2	2.14	0.81
62:AE:29:PRO:CD	65:AH:262:THR:HG21	2.09	0.81
67:AK:259:ARG:HG2	67:AK:444:LEU:CD1	2.08	0.81
65:AU:307:LYS:NZ	75:AU:403:CDL:OA3	2.12	0.81
22:Y:72:ARG:HH11	35:l:466:PHE:HD1	1.29	0.81
35:l:533:MET:HE1	76:l:702:PEE:H36	0.83	0.81
63:AF:34:ARG:HG2	63:AF:34:ARG:HH11	1.46	0.81
40:r:365:ALA:O	40:r:374:ASN:ND2	2.13	0.81
6:X:99:SER:HG	6:X:102:SER:HG	1.25	0.81
26:c:159:LYS:HA	43:v:98:ARG:HH22	1.46	0.81
30:g:49:ARG:HD3	44:w:339:TYR:HA	1.61	0.81
31:h:88:LYS:HG3	31:h:89:GLU:HG3	1.63	0.81
60:AC:220:LEU:HB2	74:AC:301:FES:S2	2.21	0.81
64:AT:39:ARG:HH21	64:AT:39:ARG:HG2	1.45	0.81
4:E:101:THR:HG22	15:P:218:ARG:HB2	1.60	0.81
32:i:167:TRP:CZ3	35:l:570:GLN:HA	2.14	0.81
62:AE:34:ARG:CD	62:AE:78:ARG:NH2	2.42	0.81
71:AQ:101:PLX:H322	76:AY:502:PEE:H59	1.63	0.81
9:J:226:ILE:HD12	9:J:289:LEU:H	1.45	0.81
43:v:8:ARG:HH11	43:v:106:ARG:HH22	1.29	0.81
35:l:188:TRP:NE1	35:l:192:HIS:HD2	1.78	0.80
66:AV:326:TRP:CZ2	76:AV:403:PEE:H13	2.16	0.80
16:Q:58:THR:HG23	35:l:580:GLN:HE21	1.46	0.80
76:W:201:PEE:C44	41:s:77:LEU:HD21	2.09	0.80
35:l:188:TRP:CZ2	35:l:192:HIS:CD2	2.69	0.80
65:AU:121:CYS:SG	81:AU:402:HEC:HBB2	2.21	0.80
3:C:120:MET:HB3	3:C:147:VAL:HG12	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:74:TRP:HZ3	22:Y:75:HIS:HD1	1.29	0.80
35:l:227:LEU:O	35:l:227:LEU:HD12	1.82	0.80
71:r:502:PLX:H372	71:r:502:PLX:C33	2.09	0.80
62:AE:28:ASP:OD1	62:AE:30:LEU:N	2.15	0.80
65:AU:215:LEU:HD11	81:AU:402:HEC:HMB3	1.63	0.80
34:k:7:ASN:ND2	36:m:9:SER:C	2.38	0.80
35:l:222:GLY:HA2	35:l:229:LEU:HD12	1.63	0.80
76:l:701:PEE:C23	40:r:155:VAL:HG11	2.12	0.80
44:w:332:ARG:O	44:w:338:LYS:CA	2.29	0.80
32:i:91:ASN:OD1	32:i:92:GLN:N	2.13	0.80
34:k:1:MET:HB2	34:k:4:ILE:HD12	1.63	0.80
58:AA:78:TYR:CG	62:AE:65:GLU:HG2	2.15	0.80
66:AV:195:LEU:CD2	66:AV:199:PHE:HE2	1.94	0.80
35:l:226:GLN:NE2	35:l:314:MET:SD	2.53	0.80
66:AJ:262:LEU:HD22	60:AP:216:VAL:HG21	1.64	0.79
22:Y:74:TRP:CE3	22:Y:75:HIS:HA	2.16	0.79
35:l:224:SER:OG	35:l:256:GLY:HA3	1.81	0.79
71:r:502:PLX:H52	71:r:502:PLX:O3	1.82	0.79
68:AY:74:TRP:O	68:AY:418:LEU:HD21	1.82	0.79
9:J:217:PHE:HZ	9:J:322:MET:CE	1.95	0.79
52:4:39:CYS:SG	52:4:53:CYS:CB	2.71	0.79
52:4:75:ARG:HH11	52:4:75:ARG:HG2	1.48	0.79
16:Q:273:ILE:HD13	16:Q:325:ASP:OD2	1.81	0.79
16:Q:294:ARG:O	16:Q:321:GLY:N	2.11	0.79
22:Y:86:TYR:OH	43:v:100:LYS:HE2	1.82	0.79
52:4:39:CYS:SG	52:4:53:CYS:HB3	2.22	0.79
35:l:142:ILE:HG12	40:r:370:PRO:HB2	1.65	0.79
32:i:12:THR:HG22	36:m:158:TRP:HE1	1.47	0.79
39:p:105:ASP:OD1	39:p:122:ARG:NH1	2.16	0.79
16:Q:70:ASP:O	16:Q:74:ASP:OD1	2.00	0.79
25:b:86:MET:O	25:b:90:VAL:HG23	1.83	0.79
25:b:110:ILE:CG2	25:b:111:LEU:HG	2.11	0.79
26:c:166:LEU:HD21	43:v:56:ARG:HG3	1.65	0.79
82:AV:401:HEM:HHD	82:AV:401:HEM:HBC2	1.64	0.79
9:J:177:SER:HB2	9:J:320:GLU:HB3	1.64	0.79
9:J:207:PHE:HA	9:J:211:ASP:OD2	1.82	0.79
9:J:355:ARG:HD2	33:j:31:MET:SD	2.23	0.79
12:M:223:ILE:HD13	12:M:233:SER:HB3	1.64	0.79
27:d:111:GLU:OE1	27:d:115:TYR:HB2	1.82	0.79
35:l:4:HIS:CE1	35:l:87:MET:CE	2.65	0.79
3:C:59:ARG:HH22	3:C:61:GLU:HB3	1.48	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:339:ILE:HG22	32:i:342:PHE:HB3	1.64	0.79
33:j:108:GLN:O	36:m:172:ARG:NH2	2.16	0.79
75:AG:101:CDL:H351	75:AG:101:CDL:H742	1.64	0.78
2:B:133:ARG:HG3	2:B:135:ASP:H	1.47	0.78
32:i:50:PRO:HB3	34:k:84:THR:HG21	1.65	0.78
39:p:143:GLU:OE2	39:p:158:ARG:NH2	2.15	0.78
9:J:206:ILE:HG12	73:J:401:NDP:N7N	1.99	0.78
12:M:647:GLU:HB2	12:M:654:VAL:HG11	1.65	0.78
16:Q:140:ASP:OD2	16:Q:143:SER:OG	2.02	0.78
58:AA:82:LYS:HE2	62:AE:60:ARG:HD3	1.66	0.78
75:AJ:405:CDL:H732	75:AJ:405:CDL:H351	1.65	0.78
64:AT:35:ALA:HB1	76:AY:502:PEE:H75	1.63	0.78
65:AU:315:LYS:HE3	75:AU:403:CDL:H1	1.66	0.78
67:AK:363:GLN:HB2	67:AK:365:ASN:OD1	1.83	0.78
9:J:270:ARG:NH2	9:J:326:ASP:O	2.16	0.78
63:AF:34:ARG:NH1	66:AJ:379:TRP:HE1	1.82	0.78
5:F:63:PRO:HB2	5:F:79:LEU:HB2	1.65	0.78
22:Y:90:SER:HA	43:v:107:ARG:NH1	1.98	0.78
34:k:3:LEU:HD23	36:m:117:ASN:HD21	1.47	0.78
40:r:355:MET:HE1	40:r:437:MET:HE3	1.65	0.78
68:AY:421:GLY:C	68:AY:422:ARG:HG3	2.06	0.78
9:J:86:CYS:O	9:J:87:ASP:HB2	1.83	0.78
32:i:167:TRP:CH2	35:l:570:GLN:HG3	2.19	0.78
39:p:13:GLN:NE2	72:p:201:8Q1:O3	2.15	0.78
51:3:5:LYS:NZ	51:3:6:GLY:H	1.78	0.78
75:AG:101:CDL:H531	75:AG:101:CDL:H731	1.66	0.78
66:AJ:149:LEU:HD21	66:AJ:281:LEU:HD21	1.65	0.78
66:AV:165:TRP:CZ3	66:AV:168:TYR:O	2.37	0.78
9:J:176:SER:HA	9:J:182:ARG:NH2	1.98	0.78
16:Q:83:ASN:HA	16:Q:98:VAL:HG22	1.65	0.78
39:p:167:TRP:O	39:p:171:VAL:CG2	2.28	0.78
67:AK:438:MET:HB3	67:AK:450:VAL:HG11	1.66	0.78
66:AV:148:ASN:O	66:AV:151:SER:HB3	1.84	0.78
34:k:97:GLN:HB2	35:l:579:THR:HG21	1.66	0.78
37:n:55:VAL:HG12	37:n:56:THR:H	1.49	0.78
58:AA:78:TYR:CE1	62:AE:64:GLU:C	2.62	0.78
22:Y:83:HIS:O	22:Y:84:PHE:CB	2.31	0.78
22:Y:84:PHE:CG	22:Y:85:PRO:HD2	2.19	0.77
22:Y:86:TYR:OH	43:v:100:LYS:HG2	1.84	0.77
71:b:201:PLX:H6	71:b:201:PLX:C10	2.13	0.77
26:c:155:PRO:HB3	43:v:5:LEU:HD22	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:111:GLY:HA2	36:m:116:VAL:HA	1.65	0.77
8:I:33:LYS:NZ	8:I:35:THR:O	2.18	0.77
16:Q:194:LEU:CD1	16:Q:268:TRP:CZ2	2.67	0.77
71:b:201:PLX:C6	71:b:201:PLX:H111	2.14	0.77
27:d:63:ARG:NH1	37:n:44:LEU:O	2.18	0.77
34:k:23:ARG:N	36:m:22:LYS:HE2	2.00	0.77
22:Y:81:LEU:HD22	43:v:92:HIS:CD2	2.18	0.77
24:a:54:LEU:CD2	25:b:27:GLU:HA	2.14	0.77
9:J:217:PHE:CB	9:J:280:ILE:HD13	2.15	0.77
15:P:187:ILE:HG22	15:P:188:LEU:HG	1.66	0.77
76:AH:401:PEE:C13	66:AJ:240:MET:HE2	2.14	0.77
9:J:217:PHE:CZ	9:J:322:MET:HE2	2.17	0.77
16:Q:78:LYS:CE	33:j:48:ARG:HH21	1.97	0.77
22:Y:96:GLU:O	22:Y:97:LEU:HD23	1.84	0.77
3:C:59:ARG:NH2	3:C:61:GLU:HB3	1.98	0.77
44:w:64:GLY:O	44:w:161:ARG:NH2	2.17	0.77
76:AL:503:PEE:H26	76:AL:503:PEE:H48	1.66	0.77
62:AR:34:ARG:HH11	62:AR:78:ARG:HH22	1.33	0.77
68:AY:230:VAL:HG21	68:AY:418:LEU:CD1	2.15	0.77
76:AH:401:PEE:H49	76:AH:401:PEE:H14	1.65	0.77
66:AJ:324:LEU:HD11	66:AJ:369:ILE:HD12	1.65	0.77
1:A:64:LYS:NZ	14:O:244:GLY:O	2.18	0.77
32:i:288:LEU:HD23	76:l:701:PEE:H58	0.77	0.77
35:l:74:THR:HG22	35:l:194:ASN:OD1	1.83	0.77
35:l:90:ILE:O	35:l:94:LEU:HD22	1.84	0.77
35:l:226:GLN:HE21	35:l:314:MET:HE1	1.48	0.77
62:AR:78:ARG:O	62:AR:82:VAL:HG23	1.84	0.77
67:AW:375:LYS:NZ	67:AW:416:ILE:O	2.18	0.77
16:Q:268:TRP:CZ3	16:Q:272:THR:CG2	2.66	0.77
63:AF:29:LYS:HD3	63:AF:75:ILE:HD13	1.64	0.77
35:l:226:GLN:NE2	35:l:314:MET:HE3	1.99	0.76
67:AW:277:VAL:HG13	67:AW:278:ALA:HB2	1.66	0.76
44:w:60:ILE:HG13	44:w:203:LEU:HD11	1.68	0.76
63:AF:68:ASP:HA	63:AF:71:LEU:HD21	1.66	0.76
12:M:68:ARG:HD2	12:M:285:TRP:HE1	1.48	0.76
44:w:56:ARG:NH1	44:w:81:LEU:O	2.18	0.76
16:Q:125:GLU:HA	16:Q:419:PRO:HG2	1.67	0.76
3:C:143:GLU:OE1	9:J:89:TYR:OH	2.03	0.76
9:J:130:ILE:CG2	73:J:401:NDP:H8A	2.10	0.76
14:O:182:ASN:ND2	14:O:194:GLU:OE1	2.19	0.76
35:l:190:ILE:H	35:l:190:ILE:HD12	1.49	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:AN:41:ARG:NE	75:AN:101:CDL:OA4	2.19	0.76
46:y:5:MET:HE3	55:7:42:PRO:HA	1.68	0.76
67:AW:450:VAL:HA	67:AW:453:LEU:HD12	1.67	0.76
46:y:59:GLN:H	46:y:62:GLU:HG3	1.51	0.76
4:E:79:VAL:HG22	72:E:201:8Q1:C38	2.16	0.76
15:P:85:GLU:OE2	15:P:142:ARG:NH1	2.19	0.76
67:AW:384:MET:HE2	68:AY:134:LYS:HD3	1.68	0.76
5:F:42:VAL:HG21	12:M:671:LEU:HD12	1.66	0.76
7:H:50:GLN:HE22	8:I:93:LYS:HA	1.50	0.76
39:p:54:GLU:OE2	72:p:201:8Q1:C38	2.34	0.76
1:A:116:ASN:HD22	70:A:502:FMN:HM81	1.51	0.75
4:E:37:ARG:NH2	6:G:123:GLU:OE2	2.19	0.75
12:M:54:GLU:OE2	12:M:62:ARG:NH2	2.19	0.75
36:m:115:VAL:O	36:m:117:ASN:N	2.19	0.75
63:AS:36:ASP:OD2	63:AS:62:ARG:NH1	2.19	0.75
65:AU:125:HIS:NE2	81:AU:402:HEC:NC	2.33	0.75
9:J:221:HIS:ND1	9:J:222:ARG:N	2.34	0.75
12:M:543:LYS:HG3	12:M:565:PHE:HD2	1.50	0.75
24:a:55:PHE:CD2	39:p:118:TYR:CE1	2.64	0.75
62:AE:30:LEU:CD1	62:AE:34:ARG:HH21	2.00	0.75
2:B:68:LEU:HG	41:s:272:TRP:HE1	1.50	0.75
11:L:75:ARG:NH1	11:L:119:ASP:OD2	2.16	0.75
35:l:54:PHE:CD1	35:l:58:ASP:HA	2.21	0.75
35:l:190:ILE:HD11	35:l:196:TRP:NE1	2.02	0.75
68:AL:73:VAL:HG23	68:AL:147:LEU:HD23	1.66	0.75
19:U:82:LYS:NZ	42:u:121:ASP:OD1	2.17	0.75
35:l:228:GLY:C	35:l:229:LEU:HD23	2.11	0.75
59:AB:52:ARG:NH1	68:AL:343:THR:O	2.18	0.75
67:AK:300:LYS:HG2	67:AK:301:ARG:HG2	1.69	0.75
9:J:77:GLY:O	9:J:102:GLN:NE2	2.19	0.75
12:M:128:CYS:HB2	12:M:129:PRO:HD3	1.68	0.75
20:V:40:ARG:HH22	20:V:55:LYS:HD3	1.50	0.75
71:b:201:PLX:O3	71:b:201:PLX:O7	2.05	0.75
1:A:174:ARG:HG3	10:K:91:LEU:HD21	1.69	0.75
2:B:68:LEU:CG	41:s:272:TRP:HE1	1.99	0.75
24:a:189:ASN:ND2	42:u:142:TYR:OH	2.20	0.75
27:d:81:GLU:CD	37:n:43:MET:HE3	2.11	0.75
3:C:105:ARG:HB3	41:s:39:VAL:HG23	1.67	0.75
16:Q:118:ARG:NH2	16:Q:138:ARG:O	2.20	0.75
21:W:31:SER:OG	21:W:35:MET:CE	2.35	0.75
22:Y:84:PHE:CZ	35:l:483:PRO:CG	2.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:AP:234:TYR:HB2	60:AP:243:TYR:HB2	1.69	0.75
22:Y:71:TRP:CZ2	22:Y:75:HIS:CD2	2.74	0.74
22:Y:89:PRO:O	43:v:107:ARG:NH2	2.20	0.74
75:AL:502:CDL:H572	76:AL:503:PEE:H66	0.84	0.74
59:AO:33:THR:HA	59:AO:38:PRO:HG3	1.69	0.74
9:J:54:ILE:HB	9:J:78:SER:HB2	1.68	0.74
35:l:533:MET:SD	76:l:702:PEE:C23	2.75	0.74
44:w:319:ILE:HG23	44:w:323:GLN:HE21	1.53	0.74
59:AB:2:LEU:HD22	67:AK:278:ALA:HB1	1.67	0.74
22:Y:45:ARG:HH21	35:l:439:THR:HG21	1.52	0.74
22:Y:84:PHE:CG	22:Y:85:PRO:HD3	2.22	0.74
71:b:201:PLX:H1C3	71:b:201:PLX:H32	1.68	0.74
75:AG:101:CDL:H521	75:AG:101:CDL:OB8	1.87	0.74
58:AN:67:PHE:HB2	66:AV:346:PRO:HG3	1.69	0.74
66:AV:195:LEU:CD2	66:AV:199:PHE:CE2	2.70	0.74
67:AW:270:ALA:HB2	67:AW:339:TYR:HD1	1.52	0.74
12:M:506:VAL:HG12	12:M:508:GLY:H	1.52	0.74
16:Q:384:LEU:HA	16:Q:388:GLY:HA2	1.68	0.74
24:a:163:ARG:NH2	30:g:99:ASP:OD2	2.20	0.74
46:y:184:LEU:HD11	46:y:211:LEU:HD21	1.69	0.74
67:AK:127:ARG:HB3	68:AL:36:ALA:HB1	1.68	0.74
68:AY:192:PHE:HB3	68:AY:195:THR:HB	1.70	0.74
38:o:24:ASN:HB3	68:AL:264:THR:HG22	0.78	0.74
44:w:98:THR:O	44:w:337:ARG:NH2	2.18	0.74
47:z:187:THR:HG21	51:3:68:THR:HG21	1.68	0.74
63:AF:29:LYS:CG	63:AF:75:ILE:HD13	2.16	0.74
75:AN:101:CDL:OA3	76:AV:403:PEE:H12	1.86	0.74
16:Q:268:TRP:HZ3	16:Q:272:THR:HG21	1.52	0.74
76:V:202:PEE:H60	76:V:202:PEE:H41	1.67	0.74
22:Y:86:TYR:HH	43:v:100:LYS:HE2	1.52	0.74
66:AJ:8:ASN:HD22	66:AJ:11:MET:HG2	1.50	0.74
12:M:50:LEU:HB2	12:M:92:CYS:HA	1.68	0.74
24:a:168:TRP:NE1	30:g:88:GLU:OE1	2.20	0.74
27:d:154:ARG:NH2	30:g:108:TYR:O	2.19	0.74
35:l:78:LEU:HG	35:l:139:GLN:NE2	2.02	0.74
39:p:170:ILE:HD12	39:p:170:ILE:N	2.02	0.74
6:G:79:ILE:HG21	6:G:148:ILE:HG21	1.70	0.74
12:M:406:ASN:HB2	12:M:438:LEU:HD21	1.68	0.74
16:Q:262:LEU:CD2	16:Q:268:TRP:CD1	2.60	0.74
35:l:135:ASN:OD1	35:l:198:PRO:HG3	1.88	0.74
40:r:114:GLU:HG3	42:u:169:PHE:HB3	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AY:171:GLU:OE2	68:AY:175:ASN:ND2	2.21	0.74
4:E:25:MET:C	4:E:29:LYS:HG3	2.13	0.74
26:c:123:PRO:HG3	39:p:75:GLN:HE21	1.52	0.74
33:j:6:ILE:HG13	41:s:6:LEU:HD11	1.68	0.74
66:AV:165:TRP:CE3	66:AV:168:TYR:O	2.41	0.74
9:J:174:ILE:HG13	9:J:182:ARG:HG3	1.70	0.73
41:s:289:LEU:HA	41:s:293:PHE:HB3	1.70	0.73
3:C:88:CYS:SG	16:Q:223:HIS:NE2	2.60	0.73
35:l:4:HIS:NE2	35:l:87:MET:HE1	2.02	0.73
35:l:512:LYS:HG3	54:6:16:ASN:CB	2.17	0.73
39:p:27:LEU:HD11	39:p:44:MET:HG3	1.67	0.73
63:AF:34:ARG:HG2	63:AF:34:ARG:NH1	2.00	0.73
12:M:58:MET:SD	15:P:246:ARG:NH1	2.55	0.73
9:J:201:VAL:HG12	9:J:203:PRO:HD3	1.71	0.73
12:M:128:CYS:HB2	12:M:129:PRO:CD	2.18	0.73
1:A:98:LYS:HD2	1:A:101:PHE:CE2	2.24	0.73
3:C:67:LEU:HD22	3:C:207:LEU:HD21	1.70	0.73
76:V:202:PEE:C44	76:l:701:PEE:C45	2.66	0.73
61:AQ:30:MET:SD	64:AT:34:TRP:HB2	2.29	0.73
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.70	0.73
67:AK:438:MET:CB	67:AK:450:VAL:HG11	2.16	0.73
76:V:202:PEE:H39	76:V:202:PEE:H32	1.70	0.73
67:AW:65:ILE:HG22	67:AW:67:ALA:H	1.53	0.73
9:J:132:ARG:NH2	73:J:401:NDP:C2B	2.52	0.73
16:Q:345:ALA:HB2	21:W:19:ILE:HD11	1.70	0.73
65:AU:290:LEU:HD23	65:AU:290:LEU:C	2.14	0.73
15:P:233:PHE:O	16:Q:418:ARG:NH2	2.22	0.73
18:T:83:ARG:NH1	18:T:102:ASN:OD1	2.22	0.73
63:AF:29:LYS:HG2	63:AF:75:ILE:HG12	1.70	0.73
67:AK:438:MET:CE	67:AK:450:VAL:HG13	2.16	0.73
1:A:158:ILE:HG21	1:A:166:ALA:HB2	1.69	0.73
44:w:209:VAL:HG13	44:w:214:VAL:HG21	1.70	0.73
12:M:121:LEU:HD21	12:M:139:LEU:HD21	1.71	0.72
12:M:198:THR:HG22	14:O:39:PHE:HB3	1.70	0.72
12:M:307:VAL:HG13	12:M:582:VAL:HG22	1.69	0.72
27:d:154:ARG:NH1	30:g:111:ILE:O	2.23	0.72
31:h:70:GLN:HG2	36:m:115:VAL:HG12	1.71	0.72
35:l:571:ILE:CG1	76:l:701:PEE:O5	2.36	0.72
65:AU:296:MET:HE2	76:AU:401:PEE:C33	2.19	0.72
9:J:132:ARG:NH2	73:J:401:NDP:O2B	2.22	0.72
16:Q:232:VAL:HG12	16:Q:234:GLN:H	1.54	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:227:LEU:HD12	35:l:230:HIS:CE1	2.24	0.72
51:3:54:ARG:HD3	51:3:54:ARG:N	2.04	0.72
45:x:176:MET:HE3	45:x:181:THR:HG22	1.72	0.72
48:0:23:PRO:O	49:1:66:ARG:HD3	1.89	0.72
68:AL:280:ASP:HA	68:AL:461:PRO:HB3	1.71	0.72
65:AU:288:MET:CB	76:AU:401:PEE:O4	2.35	0.72
1:A:219:LYS:HA	11:L:174:THR:HG22	1.71	0.72
3:C:129:LYS:NZ	16:Q:113:ILE:O	2.23	0.72
9:J:83:PRO:HB2	9:J:108:TRP:HE1	1.53	0.72
34:k:3:LEU:HD22	36:m:117:ASN:HD21	1.53	0.72
63:AF:29:LYS:HG2	63:AF:75:ILE:HD11	1.02	0.72
67:AK:125:CYS:HB3	67:AK:133:LEU:HD22	1.70	0.72
66:AV:96:LEU:HD23	76:AV:403:PEE:H26	1.69	0.72
14:O:116:ALA:O	14:O:124:ARG:NH1	2.21	0.72
24:a:54:LEU:HD22	25:b:26:GLN:O	1.90	0.72
35:l:384:PRO:O	35:l:389:PHE:HB2	1.89	0.72
35:l:451:LEU:H	35:l:453:PRO:HD2	1.54	0.72
39:p:55:LYS:HE2	39:p:55:LYS:HA	1.70	0.72
63:AF:29:LYS:HZ3	63:AF:29:LYS:HB2	1.54	0.72
76:AU:401:PEE:H61	76:AU:401:PEE:H27	1.70	0.72
1:A:381:GLN:HG2	69:A:501:SF4:S2	2.29	0.72
5:F:17:ARG:HB2	5:F:68:ARG:HE	1.54	0.72
16:Q:333:ARG:NH2	16:Q:453:THR:O	2.22	0.72
33:j:25:PRO:O	33:j:27:LEU:N	2.23	0.72
67:AK:65:ILE:HG22	67:AK:67:ALA:H	1.54	0.72
3:C:143:GLU:OE2	3:C:145:ARG:NH2	2.23	0.72
9:J:212:ARG:NH2	73:J:401:NDP:O2N	2.22	0.72
16:Q:82:LEU:C	16:Q:98:VAL:HG13	2.10	0.72
25:b:109:THR:HB	25:b:113:THR:HA	1.71	0.72
27:d:73:GLU:HG2	30:g:111:ILE:HD11	1.72	0.72
35:l:170:GLN:NE2	76:l:702:PEE:O2P	2.22	0.72
48:0:147:LYS:HE3	48:0:147:LYS:HA	1.72	0.72
75:AJ:405:CDL:H742	75:AJ:405:CDL:C78	2.20	0.72
68:AL:195:THR:HG22	68:AL:197:LEU:H	1.53	0.72
62:AR:34:ARG:HH11	62:AR:78:ARG:NH2	1.87	0.72
16:Q:282:GLU:OE2	16:Q:437:LYS:NZ	2.22	0.72
32:i:167:TRP:CE3	35:l:573:THR:CB	2.72	0.72
35:l:450:LEU:C	35:l:450:LEU:HD22	2.15	0.72
75:AG:101:CDL:H731	75:AG:101:CDL:C54	2.18	0.72
68:AY:296:TRP:HD1	68:AY:419:THR:HG23	0.90	0.72
22:Y:43:ARG:HG3	22:Y:46:GLN:HB2	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:55:PHE:CE2	39:p:118:TYR:HE2	1.96	0.72
35:l:59:GLN:HA	35:l:59:GLN:NE2	2.00	0.72
67:AW:184:ASN:HB3	67:AW:251:ALA:HA	1.72	0.72
12:M:543:LYS:NZ	12:M:563:ASP:OD2	2.23	0.72
16:Q:241:MET:HG3	21:W:11:PRO:HB2	1.72	0.72
1:A:391:TRP:HH2	12:M:153:PHE:HA	1.55	0.71
11:L:137:PHE:O	11:L:141:ASN:ND2	2.15	0.71
15:P:134:SER:HG	15:P:139:SER:HG	1.24	0.71
1:A:124:THR:HG23	1:A:126:LYS:HG2	1.72	0.71
1:A:327:ILE:HG23	1:A:331:VAL:HG13	1.72	0.71
5:F:68:ARG:NH1	12:M:359:ASN:OD1	2.23	0.71
76:V:202:PEE:H60	76:V:202:PEE:H42	1.73	0.71
35:l:78:LEU:CD2	35:l:80:PHE:HE1	2.02	0.71
68:AY:322:VAL:HG12	68:AY:323:HIS:H	1.53	0.71
12:M:374:THR:HB	12:M:377:ALA:HA	1.72	0.71
22:Y:86:TYR:HB3	22:Y:87:PRO:CA	2.19	0.71
16:Q:95:LEU:HD13	16:Q:97:LEU:HD23	1.73	0.71
27:d:136:ARG:NH2	28:e:138:GLU:O	2.23	0.71
75:AG:101:CDL:H712	75:AG:101:CDL:H521	1.72	0.71
61:AQ:22:ALA:HB2	71:AQ:101:PLX:H272	1.72	0.71
1:A:381:GLN:NE2	69:A:501:SF4:S3	2.63	0.71
9:J:221:HIS:CE1	9:J:222:ARG:CG	2.72	0.71
14:O:129:LYS:H	14:O:168:LEU:HA	1.53	0.71
21:W:115:ARG:HH11	31:h:36:PHE:HD1	1.36	0.71
62:AR:34:ARG:HH11	62:AR:78:ARG:NH1	1.88	0.71
12:M:63:PHE:O	12:M:181:ARG:NH2	2.23	0.71
14:O:187:GLN:HE21	14:O:190:ASP:HA	1.56	0.71
15:P:55:HIS:NE2	15:P:78:VAL:O	2.24	0.71
16:Q:80:ILE:O	16:Q:81:THR:HG22	1.90	0.71
71:r:502:PLX:H31	71:r:502:PLX:H72	1.73	0.71
68:AL:470:ARG:NH2	75:AL:502:CDL:OA4	2.22	0.71
12:M:566:ILE:HG13	12:M:580:ALA:HA	1.72	0.71
25:b:106:PRO:HA	25:b:115:GLU:OE2	1.89	0.71
35:l:341:MET:HE2	35:l:457:LEU:HD12	1.72	0.71
35:l:379:ALA:HA	35:l:386:LEU:HD11	1.73	0.71
63:AF:29:LYS:HD3	63:AF:75:ILE:HD12	1.65	0.71
60:AP:155:LYS:HZ3	60:AP:273:VAL:HG21	1.54	0.71
8:I:106:LEU:O	8:I:108:SER:N	2.19	0.71
35:l:567:SER:O	35:l:571:ILE:CD1	2.39	0.71
45:x:11:ASN:HD22	45:x:14:ASP:H	1.38	0.71
1:A:116:ASN:ND2	70:A:502:FMN:C8M	2.52	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:105:ARG:HA	41:s:37:PRO:HA	1.72	0.71
16:Q:432:LEU:HD12	16:Q:461:VAL:HG11	1.73	0.71
21:W:31:SER:OG	21:W:35:MET:HE3	1.91	0.71
67:AW:351:ILE:HD11	67:AW:448:PRO:CD	2.20	0.71
9:J:176:SER:O	9:J:182:ARG:NH2	2.24	0.71
11:L:82:PRO:HG3	11:L:98:LYS:HE3	1.73	0.71
39:p:104:LEU:HD21	39:p:119:PHE:HE1	1.55	0.71
25:b:10:LEU:HD22	39:p:156:PRO:HB2	1.71	0.70
34:k:7:ASN:HD22	36:m:9:SER:HB2	1.47	0.70
35:l:10:LEU:HD22	35:l:46:ILE:HG21	1.72	0.70
35:l:78:LEU:HG	35:l:139:GLN:HE22	1.55	0.70
39:p:170:ILE:H	39:p:170:ILE:CD1	2.02	0.70
63:AF:29:LYS:HB2	63:AF:29:LYS:NZ	2.05	0.70
16:Q:281:GLU:N	16:Q:281:GLU:OE1	2.22	0.70
22:Y:86:TYR:OH	43:v:100:LYS:HE3	1.89	0.70
32:i:298:TYR:O	32:i:303:THR:OG1	2.08	0.70
33:j:67:LEU:HD21	34:k:68:ALA:HB3	1.72	0.70
35:l:71:THR:HG21	40:r:307:TRP:HE1	1.54	0.70
47:z:156:ARG:HG3	47:z:156:ARG:HH11	1.56	0.70
63:AF:29:LYS:CD	63:AF:75:ILE:HD12	2.17	0.70
68:AY:48:THR:HG22	68:AY:62:GLU:HB2	1.73	0.70
1:A:158:ILE:HB	1:A:199:ARG:HG2	1.73	0.70
35:l:135:ASN:HD21	35:l:199:GLN:HE22	1.39	0.70
68:AL:192:PHE:HB3	68:AL:195:THR:HB	1.72	0.70
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.73	0.70
35:l:338:MET:HE3	35:l:372:SER:HB2	1.74	0.70
62:AE:21:GLU:O	62:AE:24:GLU:N	2.24	0.70
62:AR:34:ARG:HH11	62:AR:78:ARG:HH12	1.34	0.70
68:AY:417:LEU:HD23	68:AY:422:ARG:O	1.91	0.70
4:E:70:ASN:O	72:E:201:8Q1:O40	2.10	0.70
5:F:39:LYS:HG3	5:F:40:ARG:H	1.56	0.70
9:J:350:ILE:HD13	9:J:366:ILE:HG12	1.72	0.70
16:Q:48:GLY:HA2	32:i:228:LEU:HD11	1.74	0.70
22:Y:81:LEU:HD23	22:Y:81:LEU:C	2.15	0.70
35:l:190:ILE:HG13	35:l:196:TRP:CD1	2.27	0.70
76:l:701:PEE:H46	40:r:155:VAL:HG12	1.71	0.70
40:r:44:GLN:O	40:r:46:ASN:N	2.24	0.70
46:y:13:THR:HB	46:y:168:LEU:HD23	1.74	0.70
61:AD:48:ASN:HB2	61:AD:51:LYS:HD2	1.74	0.70
66:AV:324:LEU:HD11	66:AV:369:ILE:HD12	1.72	0.70
66:AV:344:SER:OG	66:AV:346:PRO:HD2	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:THR:HG22	12:M:75:CYS:HA	1.72	0.70
2:B:62:THR:HG22	21:W:35:MET:HE1	1.71	0.70
4:E:25:MET:O	4:E:29:LYS:CG	2.38	0.70
12:M:557:ARG:NH1	12:M:579:ILE:O	2.24	0.70
6:X:91:ASP:OD1	23:Z:47:ARG:NH1	2.24	0.70
76:AH:401:PEE:H28	76:AH:401:PEE:C40	2.21	0.70
21:W:108:GLU:OE2	31:h:75:ARG:NH1	2.24	0.70
35:l:78:LEU:CD2	35:l:80:PHE:CE1	2.74	0.70
39:p:55:LYS:HE2	39:p:55:LYS:CA	2.21	0.70
66:AJ:300:ILE:O	66:AJ:303:MET:N	2.25	0.70
1:A:116:ASN:O	1:A:245:VAL:HG23	1.91	0.70
15:P:93:VAL:HB	15:P:154:GLU:HB2	1.72	0.70
27:d:65:VAL:H	27:d:85:GLN:NE2	1.89	0.70
35:l:100:ILE:HD12	35:l:246:LEU:HG	1.72	0.70
35:l:546:GLN:OE1	40:r:278:ARG:NE	2.22	0.70
65:AU:292:MET:HE1	66:AV:241:THR:HG23	1.74	0.70
27:d:59:HIS:HE1	28:e:120:ARG:CB	1.98	0.70
35:l:567:SER:O	35:l:571:ILE:HD12	1.92	0.70
38:o:23:TYR:OH	39:p:68:GLU:OE1	2.09	0.70
2:B:184:ASN:HD21	13:N:127:TYR:H	1.39	0.70
9:J:85:ARG:HD2	9:J:85:ARG:O	1.92	0.70
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.71	0.70
25:b:105:PHE:CE2	43:v:68:LYS:HA	2.27	0.70
67:AW:261:GLN:NE2	67:AW:443:ASN:O	2.25	0.70
68:AY:195:THR:HG22	68:AY:197:LEU:H	1.55	0.70
1:A:214:GLU:OE2	1:A:224:ARG:NH1	2.24	0.69
75:AL:502:CDL:H772	76:AL:503:PEE:H70	1.73	0.69
7:H:12:VAL:HG13	16:Q:280:ALA:H	1.57	0.69
9:J:210:GLU:O	9:J:210:GLU:HG2	1.92	0.69
9:J:233:TRP:HA	9:J:272:LEU:HD21	1.74	0.69
15:P:46:THR:O	16:Q:162:ARG:N	2.16	0.69
21:W:134:LEU:HD11	36:m:2:MET:HB2	1.72	0.69
6:X:84:LEU:HD22	6:X:98:LEU:HD21	1.74	0.69
22:Y:86:TYR:CB	22:Y:87:PRO:HA	2.22	0.69
67:AK:257:GLU:CG	67:AK:450:VAL:CG2	2.70	0.69
67:AW:57:PRO:HG2	68:AY:400:VAL:HG11	1.74	0.69
12:M:299:ARG:HD3	12:M:703:ALA:HB1	1.74	0.69
12:M:472:PRO:O	12:M:510:TRP:NE1	2.25	0.69
30:g:15:ASP:HB2	30:g:18:ARG:HH21	1.57	0.69
41:s:235:ASN:HD22	41:s:267:THR:HG22	1.55	0.69
59:AB:8:SER:OG	59:AB:26:LEU:O	2.09	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:613:PRO:HB2	13:N:134:ILE:HD13	1.73	0.69
16:Q:85:GLY:HA3	33:j:39:CYS:CB	2.22	0.69
34:k:2:PRO:CG	36:m:115:VAL:HG21	2.21	0.69
34:k:66:PHE:HE1	36:m:159:THR:HG21	1.57	0.69
62:AE:34:ARG:CD	62:AE:78:ARG:HH22	2.03	0.69
76:AH:401:PEE:C13	66:AJ:240:MET:HE1	2.12	0.69
16:Q:78:LYS:HZ1	33:j:48:ARG:NH2	1.89	0.69
60:AC:216:VAL:HG21	66:AV:262:LEU:HD22	1.74	0.69
63:AF:14:LEU:O	63:AF:17:ILE:HG13	1.92	0.69
76:AL:503:PEE:H50	76:AL:503:PEE:C12	2.18	0.69
66:AV:80:ARG:NH1	82:AV:401:HEM:O1A	2.25	0.69
12:M:595:THR:HA	12:M:605:GLN:HA	1.74	0.69
25:b:14:GLN:HE22	39:p:157:ALA:HB3	1.56	0.69
25:b:16:ARG:O	25:b:20:ARG:HG2	1.93	0.69
44:w:67:CYS:N	44:w:70:LYS:HD3	2.07	0.69
52:4:39:CYS:HG	52:4:53:CYS:CB	2.05	0.69
65:AU:202:ARG:NH1	65:AU:279:GLU:OE2	2.25	0.69
28:e:129:ARG:NH1	28:e:136:ILE:O	2.24	0.69
64:AG:38:TRP:CD1	75:AG:101:CDL:C51	2.74	0.69
66:AV:332:LEU:CD1	76:AV:403:PEE:H37	2.22	0.69
1:A:60:GLY:HA3	14:O:241:PRO:HB3	1.74	0.69
76:W:201:PEE:H24	76:W:201:PEE:H53	1.73	0.69
24:a:98:LEU:HA	27:d:57:TYR:CD1	2.28	0.69
25:b:54:LYS:HG3	25:b:55:SER:H	1.58	0.69
28:e:76:TYR:O	40:r:82:ARG:NH1	2.21	0.69
35:l:141:PHE:HE2	40:r:375:LEU:HD21	1.58	0.69
35:l:226:GLN:HG3	35:l:280:LEU:HD23	1.74	0.69
75:AG:101:CDL:H542	75:AG:101:CDL:C73	2.22	0.69
66:AJ:156:ILE:CG2	66:AJ:160:LEU:HB2	2.18	0.69
68:AL:171:GLU:OE2	68:AL:175:ASN:ND2	2.26	0.69
66:AV:295:LEU:O	66:AV:299:LEU:CD2	2.40	0.69
9:J:202:LYS:HB2	9:J:264:ALA:HA	1.75	0.69
12:M:124:HIS:HD2	16:Q:375:MET:HE2	1.58	0.69
12:M:144:MET:SD	16:Q:380:HIS:ND1	2.63	0.69
12:M:466:LEU:HD23	12:M:500:ILE:HD11	1.75	0.69
35:l:4:HIS:HE1	35:l:87:MET:HE3	1.57	0.69
44:w:176:GLN:NE2	44:w:236:ASP:OD2	2.24	0.69
63:AF:39:TYR:CD1	63:AF:40:GLU:N	2.61	0.69
75:AG:101:CDL:HA62	75:AG:101:CDL:C34	2.22	0.69
59:AO:35:PRO:HB3	67:AW:320:PRO:HA	1.75	0.69
12:M:225:ILE:HD12	12:M:285:TRP:HH2	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:4:HIS:CE1	35:l:87:MET:HE1	2.28	0.69
35:l:4:HIS:CE1	35:l:87:MET:HE3	2.28	0.69
7:H:12:VAL:HG13	16:Q:280:ALA:N	2.07	0.68
15:P:157:VAL:HG21	15:P:181:HIS:HD2	1.58	0.68
16:Q:190:HIS:HD2	16:Q:452:GLY:HA3	1.58	0.68
25:b:120:MET:SD	43:v:65:ARG:NH2	2.66	0.68
76:l:701:PEE:H37	40:r:155:VAL:HG11	1.70	0.68
76:l:701:PEE:H36	40:r:155:VAL:CG1	2.21	0.68
36:m:121:VAL:O	36:m:123:SER:N	2.26	0.68
65:AH:124:CYS:SG	81:AH:402:HEC:HBC2	2.33	0.68
67:AK:399:GLN:HE22	67:AK:407:MET:HB3	1.56	0.68
67:AK:438:MET:HB2	67:AK:450:VAL:CG1	2.22	0.68
16:Q:450:ILE:O	16:Q:453:THR:OG1	2.07	0.68
25:b:94:PRO:HB3	27:d:5:TRP:HA	1.73	0.68
44:w:63:ASP:OD2	44:w:241:TYR:OH	2.11	0.68
47:z:154:GLY:HA2	50:2:6:VAL:HG22	1.75	0.68
65:AU:288:MET:HE2	66:AV:77:TRP:HH2	1.58	0.68
12:M:289:LYS:NZ	12:M:694:PHE:O	2.25	0.68
33:j:30:TYR:HB2	33:j:33:LYS:HD2	1.75	0.68
63:AS:67:LEU:HD23	66:AV:209:LEU:HD12	1.75	0.68
4:E:25:MET:HB2	4:E:29:LYS:HE3	1.75	0.68
18:T:79:GLU:HG2	18:T:120:ARG:HB3	1.76	0.68
25:b:12:LEU:HB3	25:b:16:ARG:HH12	1.58	0.68
35:l:396:ILE:O	35:l:400:ASN:ND2	2.26	0.68
62:AE:30:LEU:HD12	62:AE:30:LEU:O	1.93	0.68
66:AV:150:LEU:HD23	66:AV:164:ILE:HD13	1.75	0.68
3:C:159:TYR:HE1	16:Q:135:TYR:CZ	2.12	0.68
9:J:171:ASN:O	9:J:181:LEU:CG	2.41	0.68
14:O:137:THR:HG21	14:O:176:CYS:HB2	1.74	0.68
16:Q:271:ARG:NH1	41:s:281:ARG:CA	2.57	0.68
67:AK:100:THR:HG21	68:AL:324:LEU:HB3	1.75	0.68
67:AK:257:GLU:HG3	67:AK:450:VAL:CG2	2.23	0.68
16:Q:262:LEU:HD13	16:Q:268:TRP:NE1	2.08	0.68
20:V:81:ARG:HG2	20:V:83:LYS:HG3	1.75	0.68
24:a:55:PHE:CD2	39:p:118:TYR:CG	2.82	0.68
46:y:186:SER:HB3	46:y:213:LEU:HD22	1.76	0.68
67:AK:183:ARG:HH21	67:AK:183:ARG:HG3	1.57	0.68
38:o:30:ARG:NH2	68:AL:259:GLU:O	2.26	0.68
40:r:144:ASN:O	40:r:147:THR:OG1	2.10	0.68
47:z:12:ASN:HD22	54:6:20:VAL:H	1.39	0.68
1:A:318:ILE:HG22	1:A:326:LEU:HA	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:203:PRO:HA	9:J:265:PHE:HB2	1.75	0.68
9:J:247:LYS:HD2	9:J:340:ILE:HD12	1.74	0.68
76:AH:401:PEE:H15	66:AJ:240:MET:HE1	1.75	0.68
64:AT:24:TRP:CZ3	75:AY:501:CDL:H551	2.28	0.68
70:A:502:FMN:O4'	70:A:502:FMN:H9	1.94	0.68
3:C:128:ASN:ND2	3:C:164:TYR:O	2.24	0.68
6:G:105:MET:HG3	6:G:106:LYS:HG3	1.76	0.68
22:Y:86:TYR:HB3	22:Y:87:PRO:HA	1.75	0.68
71:b:201:PLX:H6	71:b:201:PLX:C11	2.24	0.68
71:b:201:PLX:H6	71:b:201:PLX:H111	1.75	0.68
68:AY:285:ALA:HB3	68:AY:360:CYS:HB2	1.76	0.68
73:J:401:NDP:O2X	73:J:401:NDP:H1B	1.94	0.68
21:W:28:ARG:HG2	21:W:28:ARG:O	1.93	0.68
24:a:98:LEU:HA	27:d:57:TYR:HD1	1.59	0.68
32:i:180:ALA:O	32:i:183:SER:OG	2.08	0.68
35:l:222:GLY:HA3	35:l:229:LEU:HD12	1.74	0.68
35:l:447:ASN:CG	35:l:448:PRO:HD2	2.16	0.68
41:s:85:LEU:HB3	41:s:233:MET:SD	2.34	0.68
45:x:69:MET:HE2	45:x:70:VAL:HG23	1.75	0.68
62:AR:79:ASP:HB3	65:AU:92:PRO:CG	2.23	0.68
1:A:381:GLN:HG3	1:A:382:CYS:H	1.59	0.67
11:L:89:SER:OG	15:P:239:TRP:NE1	2.26	0.67
76:W:201:PEE:H36	33:j:7:LEU:HD22	1.77	0.67
52:4:38:ARG:HG2	52:4:85:ILE:HG23	1.77	0.67
68:AY:165:ARG:NH2	68:AY:211:LEU:O	2.24	0.67
1:A:379:CYS:HA	12:M:200:ARG:HB2	1.74	0.67
12:M:194:ASP:O	12:M:208:THR:OG1	2.10	0.67
26:c:122:THR:O	38:o:12:ARG:NH2	2.27	0.67
39:p:48:PHE:HE1	72:p:201:8Q1:C7	2.06	0.67
42:u:34:ALA:HB2	42:u:120:PRO:HD3	1.75	0.67
66:AJ:66:ILE:HD11	66:AJ:134:PRO:HA	1.77	0.67
60:AP:236:CYS:HB3	60:AP:241:SER:HB2	1.74	0.67
66:AV:111:GLU:HG2	66:AV:199:PHE:CE1	2.28	0.67
9:J:173:ASN:HB2	9:J:327:MET:HE1	1.76	0.67
12:M:476:LEU:HB3	12:M:515:ILE:HG22	1.74	0.67
16:Q:87:GLN:OE1	16:Q:87:GLN:N	2.26	0.67
26:c:62:TYR:OH	26:c:74:ASP:O	2.11	0.67
35:l:188:TRP:CD2	35:l:192:HIS:HD2	2.09	0.67
65:AU:112:ARG:NH1	65:AU:269:ASP:OD2	2.26	0.67
2:B:120:ILE:HD11	16:Q:385:TYR:HB3	1.74	0.67
6:G:145:VAL:HA	6:G:148:ILE:HD12	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:114:TRP:HE1	16:Q:394:GLY:HA2	1.59	0.67
12:M:381:LEU:O	12:M:383:SER:N	2.24	0.67
12:M:500:ILE:O	12:M:503:THR:OG1	2.12	0.67
22:Y:81:LEU:CD2	43:v:92:HIS:CD2	2.77	0.67
25:b:88:TYR:O	25:b:92:GLU:CB	2.42	0.67
34:k:25:HIS:HA	34:k:90:VAL:HG13	1.77	0.67
44:w:132:GLN:HE22	44:w:169:PHE:HD2	1.41	0.67
76:AH:401:PEE:C12	66:AJ:240:MET:HE1	2.24	0.67
1:A:118:ASP:O	1:A:159:ARG:HD2	1.95	0.67
2:B:119:ALA:HA	15:P:233:PHE:HE2	1.60	0.67
24:a:98:LEU:CB	27:d:57:TYR:CD1	2.77	0.67
45:x:151:HIS:O	45:x:155:VAL:HG23	1.94	0.67
47:z:209:ILE:O	47:z:213:THR:HG23	1.95	0.67
63:AF:29:LYS:HD2	63:AF:75:ILE:CD1	2.17	0.67
59:AO:18:THR:OG1	67:AW:110:LEU:O	2.11	0.67
3:C:136:LYS:O	3:C:140:GLN:HG3	1.94	0.67
16:Q:251:PHE:HB2	16:Q:254:ARG:HH21	1.59	0.67
22:Y:84:PHE:CD2	22:Y:85:PRO:HD2	2.30	0.67
33:j:3:PHE:HA	33:j:6:ILE:HD13	1.77	0.67
34:k:83:ASN:ND2	36:m:173:GLY:O	2.27	0.67
35:l:444:ASN:OD1	35:l:445:GLU:N	2.26	0.67
58:AA:12:ARG:HG2	58:AA:13:HIS:ND1	2.10	0.67
1:A:295:PRO:HG2	1:A:298:GLU:HB2	1.77	0.67
10:K:100:SER:HA	14:O:72:GLU:HB3	1.77	0.67
25:b:51:LEU:HD11	25:b:62:HIS:CD2	2.30	0.67
27:d:49:GLN:OE1	27:d:49:GLN:N	2.27	0.67
32:i:170:LEU:HD12	35:l:574:SER:HB3	1.77	0.67
34:k:3:LEU:HD23	36:m:117:ASN:ND2	2.09	0.67
56:8:19:TRP:HZ2	57:9:14:GLU:HG2	1.59	0.67
66:AJ:338:ILE:HD11	66:AJ:350:ILE:HG22	1.76	0.67
76:AJ:403:PEE:H25	76:AJ:403:PEE:H61	1.77	0.67
1:A:43:THR:HG21	14:O:239:LYS:HB2	1.76	0.67
3:C:137:VAL:HG21	16:Q:87:GLN:NE2	2.05	0.67
12:M:173:MET:O	12:M:175:ARG:N	2.24	0.67
14:O:133:GLN:HB2	14:O:174:VAL:HG21	1.75	0.67
16:Q:86:PRO:HG2	33:j:41:PHE:HE2	1.60	0.67
26:c:184:TYR:CB	43:v:37:ARG:HG3	2.25	0.67
41:s:265:LEU:O	41:s:268:SER:OG	2.10	0.67
59:AB:49:PHE:O	68:AL:180:ARG:NH1	2.26	0.67
1:A:89:GLY:HA2	1:A:244:ASN:HD22	1.59	0.67
7:H:32:LEU:HD23	7:H:35:LEU:HD21	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:58:LYS:NZ	11:L:139:GLU:OE1	2.27	0.67
6:X:120:MET:HE1	39:p:24:LEU:HB2	1.77	0.67
33:j:5:LEU:HD13	41:s:3:MET:HE1	1.77	0.67
40:r:15:THR:O	40:r:93:LYS:NZ	2.24	0.67
68:AL:80:ARG:NH1	68:AL:268:CYS:SG	2.67	0.67
10:K:99:PRO:HG2	14:O:71:PRO:HB3	1.76	0.67
14:O:54:ASP:OD1	14:O:60:TYR:OH	2.11	0.67
25:b:93:LYS:CE	35:l:65:ASN:O	2.41	0.67
33:j:36:PRO:HG2	33:j:43:PRO:HG3	1.77	0.67
2:B:111:CYS:O	2:B:139:ARG:NH2	2.28	0.66
16:Q:271:ARG:HD3	41:s:279:ARG:O	1.95	0.66
25:b:38:GLN:OE1	25:b:39:LYS:N	2.28	0.66
25:b:115:GLU:HG2	25:b:116:VAL:N	2.10	0.66
27:d:108:GLN:NE2	35:l:199:GLN:O	2.29	0.66
35:l:190:ILE:HG12	35:l:196:TRP:CE2	2.31	0.66
40:r:369:LEU:O	40:r:372:THR:OG1	2.12	0.66
59:AB:16:SER:OG	59:AB:19:SER:O	2.12	0.66
63:AF:33:MET:HG3	63:AF:62:ARG:NH1	2.09	0.66
75:AG:101:CDL:C53	75:AG:101:CDL:H731	2.24	0.66
67:AK:107:GLY:O	68:AL:397:ASN:ND2	2.28	0.66
68:AL:257:TYR:HD2	68:AL:262:VAL:HG22	1.59	0.66
68:AY:101:THR:HA	68:AY:155:SER:H	1.60	0.66
40:r:150:LEU:O	40:r:153:THR:OG1	2.12	0.66
41:s:169:GLN:HE21	41:s:174:LEU:H	1.42	0.66
68:AY:387:GLU:OE2	68:AY:390:ARG:NH2	2.23	0.66
21:W:86:MET:SD	21:W:128:ARG:NH1	2.66	0.66
27:d:108:GLN:NE2	35:l:203:LEU:HG	2.10	0.66
34:k:51:THR:O	34:k:53:SER:N	2.28	0.66
66:AV:195:LEU:HD21	66:AV:199:PHE:HE2	1.60	0.66
3:C:125:THR:HG21	16:Q:118:ARG:HG2	1.76	0.66
3:C:161:HIS:O	3:C:168:ARG:NH2	2.28	0.66
16:Q:338:ARG:HH22	21:W:23:ARG:HB3	1.58	0.66
35:l:359:MET:O	35:l:436:ARG:NH2	2.29	0.66
9:J:355:ARG:HB3	33:j:31:MET:SD	2.36	0.66
12:M:180:THR:OG1	12:M:184:ARG:NH1	2.29	0.66
35:l:226:GLN:HG2	35:l:280:LEU:CD2	2.25	0.66
35:l:512:LYS:HG3	54:6:16:ASN:HB3	1.78	0.66
41:s:200:LEU:HD12	41:s:285:LEU:HD11	1.78	0.66
1:A:398:ARG:NH1	1:A:408:GLU:OE1	2.25	0.66
22:Y:90:SER:HA	43:v:107:ARG:HH12	1.59	0.66
24:a:58:ARG:HH21	24:a:61:ARG:HD2	1.60	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:332:HIS:HE1	35:l:336:LYS:HZ1	1.44	0.66
40:r:305:THR:O	40:r:308:SER:OG	2.12	0.66
65:AH:277:ALA:O	66:AJ:71:ARG:NH2	2.29	0.66
71:U:101:PLX:HO9	33:j:106:TRP:CD1	2.12	0.66
59:AO:17:ALA:HA	68:AY:319:GLY:H	1.61	0.66
1:A:74:ASP:O	1:A:78:GLY:N	2.27	0.66
1:A:116:ASN:ND2	70:A:502:FMN:C9	2.59	0.66
25:b:105:PHE:CZ	43:v:67:LEU:HB2	2.31	0.66
25:b:114:GLY:O	25:b:115:GLU:HB3	1.95	0.66
62:AE:34:ARG:HH22	65:AH:216:THR:HG22	1.61	0.66
75:AG:101:CDL:H531	75:AG:101:CDL:C71	2.19	0.66
67:AK:176:ASN:ND2	67:AK:260:GLU:OE2	2.29	0.66
64:AT:45:VAL:HG21	64:AT:48:ILE:HB	1.77	0.66
67:AW:60:ARG:HG3	67:AW:124:GLU:HG2	1.78	0.66
4:E:107:PHE:HB3	4:E:109:GLU:HG3	1.78	0.66
9:J:258:ALA:HA	9:J:261:LYS:HD2	1.78	0.66
12:M:254:MET:HB2	12:M:290:THR:HG22	1.78	0.66
34:k:26:LEU:HD11	34:k:78:LEU:HD21	1.78	0.66
67:AK:183:ARG:NH2	67:AK:254:ARG:HB3	2.11	0.66
4:E:23:ARG:N	4:E:27:GLU:OE1	2.24	0.66
11:L:81:VAL:HG11	11:L:150:ARG:HA	1.78	0.66
12:M:300:GLN:HB2	13:N:137:TRP:HA	1.78	0.66
22:Y:85:PRO:HG2	43:v:99:MET:HE2	1.78	0.66
41:s:202:GLU:O	41:s:204:GLU:N	2.29	0.66
75:AG:101:CDL:H521	75:AG:101:CDL:CB7	2.26	0.66
67:AK:407:MET:HE3	67:AK:411:THR:HG22	1.78	0.66
68:AY:121:ASN:ND2	68:AY:132:TYR:OH	2.29	0.66
32:i:12:THR:HG22	36:m:158:TRP:NE1	2.10	0.65
35:l:453:PRO:HA	35:l:456:ARG:NH2	2.11	0.65
43:v:74:PHE:O	43:v:76:ASN:ND2	2.29	0.65
62:AE:27:VAL:O	62:AE:28:ASP:HB3	1.96	0.65
22:Y:81:LEU:HD12	43:v:88:ASP:HB3	1.78	0.65
62:AR:86:LEU:HD23	62:AR:86:LEU:C	2.21	0.65
66:AJ:165:TRP:O	66:AJ:174:THR:OG1	2.14	0.65
41:s:185:TRP:NE1	41:s:238:THR:HG22	2.12	0.65
44:w:58:ARG:NH1	44:w:279:ASP:O	2.29	0.65
67:AK:351:ILE:HD11	67:AK:448:PRO:CG	2.27	0.65
58:AN:12:ARG:HG2	58:AN:13:HIS:ND1	2.12	0.65
67:AW:299:VAL:HG13	68:AY:120:LEU:HD11	1.79	0.65
67:AW:449:PHE:HB2	67:AW:452:GLU:OE1	1.97	0.65
9:J:48:ARG:NH1	9:J:98:GLY:O	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:W:201:PEE:H1	41:s:98:LEU:HD22	1.79	0.65
44:w:188:ASN:HA	44:w:191:LYS:HE2	1.78	0.65
2:B:61:TRP:CH2	41:s:187:ILE:HD11	2.31	0.65
9:J:132:ARG:NH2	73:J:401:NDP:H2B	2.11	0.65
9:J:206:ILE:CB	9:J:242:VAL:HG22	2.25	0.65
12:M:36:VAL:O	12:M:38:GLY:N	2.29	0.65
34:k:11:ALA:HB1	36:m:16:PHE:CD2	2.31	0.65
41:s:20:LEU:HD13	41:s:232:ILE:HD11	1.78	0.65
44:w:249:MET:HB3	44:w:255:VAL:HG11	1.79	0.65
63:AF:36:ASP:OD2	63:AF:62:ARG:NH1	2.28	0.65
67:AK:36:GLN:NE2	67:AK:39:GLU:OE2	2.29	0.65
68:AL:280:ASP:O	68:AL:362:ARG:NH2	2.30	0.65
61:AQ:22:ALA:CB	71:AQ:101:PLX:H272	2.26	0.65
65:AU:308:ARG:HH11	75:AU:403:CDL:H1O1	1.44	0.65
7:H:12:VAL:HG11	16:Q:278:VAL:O	1.96	0.65
15:P:173:MET:HE1	15:P:189:THR:HG23	1.78	0.65
16:Q:80:ILE:O	16:Q:81:THR:CG2	2.45	0.65
34:k:1:MET:HB2	34:k:4:ILE:HD13	1.77	0.65
36:m:147:ASP:OD1	36:m:148:TYR:N	2.30	0.65
45:x:195:LEU:HD23	45:x:245:ILE:HD13	1.79	0.65
46:y:120:SER:OG	46:y:138:VAL:HG21	1.97	0.65
47:z:101:PHE:HZ	47:z:260:GLY:HA3	1.61	0.65
49:1:43:PRO:HB2	49:1:48:ILE:HD11	1.76	0.65
60:AC:162:GLY:O	60:AC:227:ASN:ND2	2.30	0.65
67:AK:230:LEU:HA	67:AK:233:VAL:HG22	1.78	0.65
1:A:424:ILE:HG22	69:A:501:SF4:S4	2.36	0.65
25:b:110:ILE:HG23	25:b:111:LEU:CD2	2.26	0.65
32:i:42:PRO:HG3	36:m:166:ILE:HG23	1.78	0.65
45:x:298:ASP:HB2	45:x:301:THR:HG23	1.77	0.65
56:8:45:LEU:HD21	57:9:40:TYR:HA	1.78	0.65
1:A:244:ASN:OD1	1:A:245:VAL:N	2.29	0.65
7:H:72:LEU:HD22	7:H:77:LEU:HD13	1.78	0.65
8:I:66:PRO:HB3	15:P:79:SER:HB3	1.77	0.65
17:S:53:ARG:NH2	31:h:105:ARG:HD3	2.11	0.65
30:g:27:ASP:OD2	30:g:29:ARG:NH1	2.29	0.65
67:AK:257:GLU:HG3	67:AK:450:VAL:HG22	1.73	0.65
76:AU:401:PEE:C19	76:AU:401:PEE:H64	2.27	0.65
1:A:364:VAL:HG12	1:A:400:VAL:HG12	1.78	0.65
9:J:205:ASP:HB2	9:J:239:PRO:HA	1.79	0.65
12:M:65:TYR:O	12:M:181:ARG:NH2	2.29	0.65
12:M:169:VAL:HG12	12:M:223:ILE:HD11	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:40:THR:OG1	18:T:42:THR:O	2.14	0.65
27:d:110:ARG:HG2	27:d:110:ARG:NH1	2.11	0.65
28:e:76:TYR:H	40:r:432:ARG:HD2	1.61	0.65
67:AK:384:MET:HE2	68:AL:134:LYS:HD3	1.77	0.65
68:AL:48:THR:HG22	68:AL:62:GLU:HB2	1.78	0.65
5:F:56:ARG:NH2	12:M:527:ASP:O	2.29	0.64
16:Q:271:ARG:HH11	41:s:281:ARG:CA	2.09	0.64
21:W:68:ARG:HD3	36:m:134:PHE:CE1	2.32	0.64
22:Y:79:GLU:O	22:Y:80:VAL:HG13	1.96	0.64
34:k:4:ILE:HD13	36:m:125:MET:SD	2.35	0.64
35:l:227:LEU:HD12	35:l:230:HIS:HD1	1.60	0.64
44:w:332:ARG:O	44:w:338:LYS:CG	2.45	0.64
76:AH:401:PEE:H49	76:AH:401:PEE:C11	2.27	0.64
82:AJ:401:HEM:HBC2	82:AJ:401:HEM:HMC1	1.80	0.64
11:L:111:LEU:HG	11:L:112:MET:HG2	1.80	0.64
21:W:68:ARG:HD3	36:m:134:PHE:CZ	2.33	0.64
24:a:94:GLY:O	24:a:96:ALA:N	2.30	0.64
42:u:31:HIS:CE1	42:u:119:ARG:HB3	2.33	0.64
3:C:93:MET:HG2	3:C:110:PHE:HZ	1.62	0.64
16:Q:35:ARG:NH1	28:e:60:GLU:OE2	2.28	0.64
35:l:97:THR:HG21	35:l:125:LEU:CD1	2.20	0.64
76:l:701:PEE:C22	40:r:155:VAL:HG21	2.27	0.64
41:s:228:TYR:HD1	41:s:231:ILE:HD12	1.63	0.64
67:AK:351:ILE:HD11	67:AK:448:PRO:CD	2.27	0.64
62:AR:29:PRO:HD2	65:AU:262:THR:HG21	1.79	0.64
25:b:112:GLU:N	25:b:112:GLU:OE2	2.31	0.64
31:h:91:LYS:HG3	31:h:92:TYR:H	1.62	0.64
35:l:307:SER:HA	35:l:310:LEU:HD12	1.79	0.64
66:AV:129:MET:HE1	66:AV:185:LEU:CD1	2.28	0.64
2:B:51:VAL:HG22	2:B:54:ARG:HH11	1.62	0.64
2:B:151:ILE:HG21	3:C:159:TYR:HD2	1.62	0.64
12:M:618:GLU:OE2	12:M:620:TRP:NE1	2.30	0.64
16:Q:80:ILE:C	16:Q:81:THR:CG2	2.70	0.64
18:T:39:VAL:HG12	18:T:45:VAL:HB	1.79	0.64
21:W:39:GLY:O	21:W:42:THR:OG1	2.15	0.64
32:i:291:TYR:CD2	76:l:701:PEE:H51	2.32	0.64
35:l:226:GLN:OE1	35:l:226:GLN:HA	1.97	0.64
76:l:701:PEE:H36	40:r:155:VAL:HG21	1.79	0.64
67:AK:183:ARG:HH21	67:AK:254:ARG:HB3	1.62	0.64
67:AK:365:ASN:OD1	67:AK:365:ASN:N	2.31	0.64
64:AT:42:LEU:O	64:AT:45:VAL:CG2	2.34	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AV:22:PRO:HB3	66:AV:217:LYS:HB3	1.78	0.64
2:B:52:THR:HG22	21:W:33:TYR:CE1	2.33	0.64
45:x:172:LYS:HB2	45:x:172:LYS:NZ	2.12	0.64
47:z:160:LEU:HD13	47:z:222:GLN:HG2	1.78	0.64
67:AK:422:ALA:O	67:AK:426:ASN:ND2	2.31	0.64
75:AL:502:CDL:C58	76:AL:503:PEE:C38	2.76	0.64
65:AU:202:ARG:NH2	66:AV:256:TYR:OH	2.28	0.64
10:K:81:THR:HB	14:O:88:ARG:HD2	1.79	0.64
12:M:543:LYS:HG3	12:M:565:PHE:CD2	2.33	0.64
25:b:108:ASP:O	25:b:113:THR:HA	1.98	0.64
32:i:197:ASN:HB3	32:i:269:GLU:OE1	1.97	0.64
35:l:67:HIS:CE1	35:l:75:GLN:HG3	2.33	0.64
35:l:405:ASN:OD1	35:l:406:ALA:N	2.31	0.64
75:AJ:405:CDL:C31	75:AJ:405:CDL:HB61	2.27	0.64
64:AT:40:LEU:HD12	64:AT:40:LEU:C	2.21	0.64
1:A:416:SER:HB3	1:A:436:GLN:HE21	1.63	0.64
12:M:591:GLU:OE1	12:M:591:GLU:N	2.30	0.64
26:c:159:LYS:HA	43:v:98:ARG:HH12	1.62	0.64
42:u:140:ASN:ND2	42:u:143:HIS:O	2.31	0.64
45:x:187:SER:CB	45:x:277:MET:HE1	2.28	0.64
63:AF:40:GLU:HG2	63:AF:45:LYS:HG3	1.77	0.64
67:AK:60:ARG:HG3	67:AK:124:GLU:HG2	1.78	0.64
68:AL:75:ILE:HG22	68:AL:77:VAL:H	1.61	0.64
68:AY:75:ILE:HG22	68:AY:77:VAL:H	1.61	0.64
32:i:288:LEU:HD21	76:l:701:PEE:H64	1.80	0.64
35:l:88:MET:O	35:l:92:VAL:HG23	1.98	0.64
45:x:84:PRO:HG3	45:x:92:MET:HE3	1.80	0.64
45:x:273:MET:HG3	45:x:319:LYS:HZ1	1.62	0.64
65:AU:296:MET:HE2	76:AU:401:PEE:H51	1.78	0.64
67:AW:444:LEU:HD23	67:AW:447:THR:HG21	1.79	0.64
5:F:33:VAL:HG22	5:F:87:VAL:HG21	1.78	0.64
20:V:27:SER:O	20:V:30:SER:OG	2.14	0.64
76:W:201:PEE:H75	41:s:77:LEU:HD23	1.75	0.64
24:a:95:GLN:HA	24:a:116:PRO:HD3	1.79	0.64
24:a:96:ALA:CB	27:d:55:TYR:CB	2.70	0.64
31:h:5:ASP:HB3	31:h:8:LYS:HB3	1.80	0.64
58:AA:49:VAL:HG21	76:AJ:403:PEE:O5	1.98	0.64
65:AH:202:ARG:NH2	66:AJ:256:TYR:OH	2.31	0.64
6:G:120:MET:HA	6:G:123:GLU:HG2	1.78	0.63
16:Q:145:MET:H	16:Q:178:THR:HG21	1.63	0.63
24:a:127:ASP:HB3	24:a:131:LYS:HD3	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:190:ILE:HD11	35:l:196:TRP:HE1	1.61	0.63
35:l:501:ALA:O	35:l:505:ASN:ND2	2.29	0.63
35:l:537:ILE:HD11	76:l:702:PEE:H38	1.80	0.63
40:r:112:ALA:O	40:r:113:THR:OG1	2.14	0.63
41:s:280:PHE:HE2	41:s:288:LEU:HD11	1.63	0.63
67:AK:375:LYS:NZ	67:AK:416:ILE:O	2.30	0.63
62:AR:34:ARG:CZ	62:AR:78:ARG:HH12	2.11	0.63
68:AY:424:ILE:CG2	68:AY:429:TRP:HE1	2.09	0.63
68:AY:460:GLY:HA2	68:AY:462:ILE:HD12	1.79	0.63
1:A:414:GLU:OE1	12:M:152:ARG:NH1	2.30	0.63
14:O:245:VAL:O	14:O:247:ALA:N	2.31	0.63
44:w:89:ALA:N	44:w:160:GLU:OE1	2.27	0.63
65:AU:288:MET:SD	76:AU:401:PEE:O4	2.55	0.63
67:AW:313:VAL:HG21	67:AW:323:VAL:HG21	1.80	0.63
1:A:85:LEU:HD21	1:A:247:THR:HG23	1.80	0.63
1:A:98:LYS:HD2	1:A:101:PHE:HE2	1.61	0.63
12:M:266:ARG:HG2	12:M:267:THR:HG23	1.79	0.63
12:M:326:VAL:HG23	12:M:626:LEU:HD13	1.80	0.63
16:Q:171:ARG:HH21	16:Q:231:GLY:HA2	1.61	0.63
24:a:87:THR:HG22	71:b:201:PLX:H131	1.81	0.63
48:O:24:LEU:H	49:1:34:ASN:HD21	1.44	0.63
67:AK:413:LEU:HA	67:AK:416:ILE:HG22	1.79	0.63
8:I:23:LYS:NZ	16:Q:252:SER:OG	2.31	0.63
76:V:202:PEE:H32	76:V:202:PEE:C24	2.25	0.63
27:d:112:GLY:O	27:d:115:TYR:HB3	1.99	0.63
29:f:38:LYS:HB2	29:f:39:PRO:HD3	1.81	0.63
36:m:116:VAL:O	36:m:118:PHE:N	2.31	0.63
42:u:24:VAL:HG22	42:u:86:TRP:NE1	2.12	0.63
65:AH:262:THR:HG22	65:AH:264:SER:H	1.63	0.63
76:AJ:403:PEE:H61	76:AJ:403:PEE:H28	1.81	0.63
16:Q:273:ILE:HD13	16:Q:325:ASP:CG	2.23	0.63
33:j:77:TRP:NE1	41:s:318:THR:O	2.31	0.63
34:k:92:ASN:ND2	35:l:582:GLY:O	2.31	0.63
2:B:57:ARG:O	16:Q:266:ARG:NH2	2.30	0.63
12:M:467:LYS:HG3	12:M:503:THR:HB	1.80	0.63
16:Q:84:PHE:HE2	16:Q:91:ALA:HB2	1.63	0.63
16:Q:136:PHE:HB3	16:Q:147:ASN:HB3	1.79	0.63
22:Y:73:PHE:HA	35:l:385:PHE:CE2	2.33	0.63
22:Y:74:TRP:HE3	22:Y:75:HIS:HA	1.62	0.63
23:Z:32:ILE:HD12	39:p:35:ASP:OD1	1.98	0.63
38:o:56:ARG:HH12	38:o:59:LEU:C	2.06	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:210:TYR:O	40:r:213:HIS:ND1	2.31	0.63
40:r:373:ILE:HG23	40:r:448:SER:HA	1.81	0.63
59:AO:7:ARG:NH1	67:AW:287:SER:OG	2.32	0.63
66:AV:326:TRP:HZ2	76:AV:403:PEE:H13	1.60	0.63
66:AV:333:LEU:HD21	76:AV:403:PEE:C39	2.29	0.63
1:A:207:GLY:O	70:A:502:FMN:C5A	2.47	0.63
12:M:692:LYS:HD2	12:M:715:THR:HG22	1.80	0.63
25:b:105:PHE:CE2	43:v:68:LYS:CA	2.81	0.63
32:i:271:THR:HG22	32:i:276:LEU:HD22	1.81	0.63
62:AR:34:ARG:HG3	62:AR:78:ARG:HH12	1.61	0.63
63:AS:97:GLU:OE1	63:AS:100:ARG:NH2	2.31	0.63
66:AV:200:LEU:HD13	82:AV:402:HEM:HAD2	1.79	0.63
67:AW:450:VAL:O	67:AW:453:LEU:HD13	1.98	0.63
2:B:70:MET:HE2	16:Q:257:GLU:HG2	1.79	0.63
3:C:136:LYS:HD2	33:j:40:GLY:O	1.99	0.63
25:b:88:TYR:CD1	71:b:201:PLX:C1C	2.79	0.63
35:l:534:HIS:ND1	76:l:702:PEE:C11	2.59	0.63
67:AK:185:ALA:HB3	67:AK:251:ALA:HB2	1.81	0.63
1:A:391:TRP:CH2	12:M:153:PHE:HA	2.34	0.63
2:B:99:HIS:NE2	69:B:302:SF4:S1	2.70	0.63
16:Q:72:PRO:HB2	32:i:50:PRO:HG3	1.80	0.63
16:Q:80:ILE:C	16:Q:81:THR:HG23	2.23	0.63
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.81	0.63
26:c:159:LYS:HA	43:v:98:ARG:NH2	2.13	0.63
32:i:72:MET:HE1	34:k:9:MET:HG2	1.81	0.63
36:m:56:PHE:HD2	41:s:107:ALA:HB1	1.64	0.63
41:s:107:ALA:O	41:s:110:SER:OG	2.11	0.63
41:s:169:GLN:NE2	41:s:244:GLY:H	1.96	0.63
43:v:40:VAL:HB	43:v:61:HIS:CE1	2.34	0.63
44:w:117:PHE:HB2	44:w:131:LEU:HD21	1.80	0.63
63:AF:28:ASN:OD1	63:AF:29:LYS:N	2.31	0.63
68:AL:322:VAL:HG12	68:AL:323:HIS:H	1.64	0.63
67:AW:151:VAL:HG12	67:AW:155:GLN:HE21	1.64	0.63
3:C:137:VAL:CG2	16:Q:87:GLN:NE2	2.59	0.62
9:J:141:PHE:CZ	9:J:180:TYR:HD1	2.17	0.62
10:K:82:TYR:HD2	14:O:62:ARG:HH12	1.47	0.62
16:Q:357:LYS:HE3	16:Q:364:SER:HB2	1.81	0.62
71:b:201:PLX:O4	71:b:201:PLX:H11	1.99	0.62
35:l:229:LEU:HD23	35:l:229:LEU:N	2.13	0.62
68:AY:280:ASP:HA	68:AY:461:PRO:HB3	1.79	0.62
1:A:379:CYS:SG	1:A:380:GLY:N	2.68	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:82:SER:HB3	34:k:87:LEU:HD23	1.80	0.62
57:9:13:LYS:HD3	57:9:13:LYS:H	1.65	0.62
58:AA:19:LEU:HD23	68:AL:273:SER:HB3	1.81	0.62
67:AK:70:ARG:NH2	67:AK:332:ASP:OD2	2.31	0.62
12:M:173:MET:C	12:M:175:ARG:H	2.05	0.62
14:O:40:VAL:HG13	14:O:42:ARG:H	1.64	0.62
35:l:124:PHE:HE1	35:l:147:VAL:HG13	1.64	0.62
35:l:450:LEU:O	35:l:450:LEU:HD13	2.00	0.62
45:x:128:VAL:O	45:x:128:VAL:HG22	1.99	0.62
61:AD:53:TRP:NE1	65:AH:139:CYS:O	2.32	0.62
66:AV:138:MET:HB2	66:AV:255:ASN:HD21	1.62	0.62
9:J:83:PRO:HB3	9:J:119:VAL:HG21	1.81	0.62
11:L:75:ARG:HH21	11:L:101:PHE:HB3	1.63	0.62
14:O:158:ILE:HD11	14:O:164:THR:HB	1.81	0.62
25:b:7:ASP:HB2	39:p:156:PRO:HG3	1.79	0.62
32:i:245:PRO:HB3	32:i:297:ILE:HG12	1.80	0.62
48:0:16:TYR:CE1	48:0:25:PRO:HG3	2.34	0.62
75:AG:101:CDL:H551	75:AG:101:CDL:H512	1.81	0.62
66:AV:332:LEU:HD11	76:AV:403:PEE:H37	1.79	0.62
16:Q:150:ALA:HB1	16:Q:400:ILE:HG13	1.80	0.62
22:Y:96:GLU:O	22:Y:97:LEU:HB2	1.98	0.62
43:v:52:ARG:O	43:v:56:ARG:NH1	2.33	0.62
58:AA:78:TYR:HE1	62:AE:64:GLU:C	1.99	0.62
65:AH:202:ARG:HD2	65:AH:279:GLU:HG3	1.81	0.62
67:AW:443:ASN:O	67:AW:444:LEU:HB2	2.00	0.62
1:A:325:PRO:HG3	1:A:433:TRP:HB3	1.81	0.62
6:G:80:GLN:HE22	6:G:100:VAL:HG13	1.63	0.62
42:u:30:HIS:CE1	42:u:119:ARG:HH11	2.17	0.62
65:AH:112:ARG:NH1	65:AH:269:ASP:OD2	2.31	0.62
9:J:48:ARG:HH21	15:P:211:ARG:HD2	1.64	0.62
9:J:241:TYR:CE2	9:J:243:VAL:HB	2.35	0.62
13:N:29:ARG:NH2	13:N:65:THR:O	2.23	0.62
23:Z:24:ILE:HD11	23:Z:47:ARG:HG2	1.80	0.62
38:o:24:ASN:CB	68:AL:264:THR:CG2	2.46	0.62
49:1:82:TYR:HB3	49:1:83:PRO:HD3	1.82	0.62
62:AE:26:LEU:O	62:AE:28:ASP:N	2.27	0.62
68:AL:228:ARG:HH22	68:AL:263:PRO:HG2	1.65	0.62
68:AY:424:ILE:HG23	68:AY:424:ILE:O	2.00	0.62
12:M:627:SER:OG	12:M:632:MET:O	2.17	0.62
15:P:83:GLU:HB3	15:P:142:ARG:HH12	1.65	0.62
36:m:56:PHE:CD2	41:s:107:ALA:HB1	2.35	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:60:ILE:O	44:w:159:LEU:N	2.33	0.62
47:z:154:GLY:HA2	50:2:6:VAL:CG2	2.30	0.62
32:i:37:MET:HE1	32:i:60:PHE:HA	1.82	0.62
35:l:37:LYS:NZ	35:l:98:TRP:NE1	2.47	0.62
35:l:54:PHE:HD2	35:l:55:MET:HE2	1.65	0.62
65:AH:231:LEU:HD21	60:AP:239:HIS:HA	1.81	0.62
67:AK:184:ASN:HB3	67:AK:251:ALA:HA	1.81	0.62
75:AL:502:CDL:C58	76:AL:503:PEE:H63	2.29	0.62
66:AV:119:LEU:HD12	66:AV:192:LEU:HB3	1.81	0.62
10:K:98:GLN:HB3	14:O:71:PRO:HA	1.80	0.62
15:P:154:GLU:HA	15:P:179:ALA:HB2	1.81	0.62
17:S:53:ARG:HB2	31:h:105:ARG:HH12	1.64	0.62
35:l:4:HIS:HE1	35:l:87:MET:CE	2.10	0.62
35:l:216:LEU:HD22	35:l:259:LEU:HD21	1.80	0.62
76:l:701:PEE:H32	40:r:155:VAL:HG21	1.80	0.62
38:o:24:ASN:HB3	68:AL:264:THR:HG23	1.75	0.62
45:x:92:MET:HE2	45:x:167:THR:HG21	1.82	0.62
67:AW:299:VAL:HG21	68:AY:110:GLU:HG3	1.81	0.62
9:J:83:PRO:HB2	9:J:108:TRP:CD1	2.33	0.61
12:M:282:ASN:HA	12:M:413:LEU:HD23	1.81	0.61
14:O:143:ARG:HB3	14:O:184:PRO:HD3	1.82	0.61
16:Q:432:LEU:HG	16:Q:456:ILE:HD13	1.81	0.61
24:a:55:PHE:CD2	39:p:118:TYR:CD1	2.88	0.61
34:k:10:LEU:HD12	36:m:102:LEU:HD12	1.82	0.61
35:l:450:LEU:HD22	35:l:450:LEU:O	2.00	0.61
38:o:26:SER:O	38:o:29:THR:OG1	2.15	0.61
67:AK:295:ALA:HB2	67:AK:325:ALA:HB3	1.82	0.61
62:AR:30:LEU:HD13	62:AR:86:LEU:HD11	1.82	0.61
67:AW:127:ARG:NH1	67:AW:224:GLY:O	2.32	0.61
2:B:36:TYR:HB3	8:I:104:TRP:CE3	2.34	0.61
12:M:387:LEU:HA	12:M:514:ASN:HB2	1.82	0.61
12:M:546:PHE:HB2	12:M:568:TYR:HA	1.81	0.61
16:Q:51:VAL:HG13	32:i:171:ASN:OD1	2.00	0.61
27:d:107:CYS:SG	27:d:119:CYS:HA	2.39	0.61
36:m:118:PHE:CD1	36:m:121:VAL:HB	2.34	0.61
71:r:502:PLX:H31	71:r:502:PLX:C7	2.30	0.61
41:s:186:PHE:O	41:s:189:THR:OG1	2.16	0.61
54:6:3:ASN:C	54:6:3:ASN:HD22	2.08	0.61
1:A:282:VAL:HG21	1:A:304:ALA:HB1	1.83	0.61
35:l:303:ALA:O	35:l:306:THR:OG1	2.17	0.61
50:2:13:ALA:O	50:2:18:ARG:HD2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AK:51:SER:HB2	67:AK:230:LEU:HD12	1.82	0.61
68:AL:96:LEU:HD23	68:AL:164:GLU:HG3	1.80	0.61
61:AQ:34:ARG:HH12	61:AQ:38:GLN:HB3	1.64	0.61
66:AV:141:TRP:HB3	66:AV:268:ILE:HD11	1.82	0.61
67:AW:125:CYS:HB3	67:AW:133:LEU:HD22	1.81	0.61
11:L:109:ASN:ND2	11:L:111:LEU:O	2.33	0.61
16:Q:166:ARG:NH1	16:Q:352:PRO:O	2.30	0.61
27:d:60:ARG:HG2	27:d:60:ARG:NH1	2.12	0.61
38:o:24:ASN:CA	68:AL:264:THR:HG22	2.29	0.61
52:4:57:ARG:HB3	52:4:57:ARG:HH11	1.64	0.61
67:AK:195:TYR:O	67:AK:199:LYS:NZ	2.30	0.61
65:AU:296:MET:CE	76:AU:401:PEE:C33	2.71	0.61
15:P:94:ILE:HG13	15:P:154:GLU:HB3	1.82	0.61
16:Q:428:GLY:HA2	16:Q:431:HIS:HD2	1.66	0.61
22:Y:81:LEU:HD23	22:Y:82:GLY:N	2.14	0.61
35:l:37:LYS:NZ	35:l:98:TRP:CD1	2.69	0.61
40:r:61:LEU:HD22	40:r:241:TYR:HD1	1.64	0.61
40:r:150:LEU:HD21	40:r:154:LEU:HD12	1.79	0.61
45:x:11:ASN:HD21	45:x:13:LYS:HB2	1.65	0.61
63:AF:34:ARG:HH11	63:AF:34:ARG:CG	2.13	0.61
66:AJ:96:LEU:HD23	76:AJ:403:PEE:H26	1.82	0.61
65:AU:133:ARG:O	65:AU:135:LEU:N	2.29	0.61
6:G:76:LEU:HD21	6:G:155:TYR:HA	1.82	0.61
7:H:89:ASN:O	7:H:93:LYS:HG2	2.00	0.61
12:M:177:ILE:HG13	12:M:179:CYS:SG	2.40	0.61
12:M:346:VAL:HB	12:M:548:LEU:HD13	1.82	0.61
16:Q:38:GLN:HE21	32:i:304:LEU:HB2	1.64	0.61
6:X:138:LEU:HD21	6:X:144:ILE:HG12	1.83	0.61
25:b:42:PRO:HA	25:b:45:LYS:HB2	1.81	0.61
35:l:194:ASN:HB2	38:o:125:PHE:O	2.01	0.61
36:m:118:PHE:HE1	36:m:124:TRP:HE1	1.47	0.61
38:o:30:ARG:CZ	68:AL:259:GLU:O	2.48	0.61
44:w:160:GLU:HG2	44:w:161:ARG:N	2.13	0.61
67:AW:116:ARG:NH1	67:AW:188:ASN:O	2.33	0.61
1:A:88:ARG:O	1:A:244:ASN:ND2	2.32	0.61
1:A:161:GLU:O	14:O:192:TYR:OH	2.18	0.61
3:C:184:PRO:HD3	16:Q:223:HIS:HD2	1.65	0.61
9:J:286:ARG:NH2	9:J:356:HIS:O	2.34	0.61
12:M:534:VAL:HG12	12:M:536:ALA:H	1.66	0.61
13:N:130:THR:N	18:T:44:GLN:OE1	2.34	0.61
16:Q:53:TYR:HE1	76:l:701:PEE:P	2.22	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:12:LEU:HB3	25:b:16:ARG:NH1	2.15	0.61
25:b:14:GLN:NE2	39:p:164:PRO:HD3	2.15	0.61
31:h:37:GLU:HB2	31:h:63:PHE:CE1	2.35	0.61
33:j:32:GLU:O	33:j:37:TYR:OH	2.18	0.61
44:w:67:CYS:H	44:w:70:LYS:HD3	1.65	0.61
47:z:6:HIS:HD2	47:z:8:TYR:H	1.49	0.61
64:AT:38:TRP:CE3	64:AT:41:ILE:HD13	2.35	0.61
9:J:226:ILE:HD12	9:J:289:LEU:N	2.16	0.61
12:M:537:ILE:O	12:M:539:LYS:N	2.33	0.61
46:y:59:GLN:HA	46:y:62:GLU:HB2	1.83	0.61
1:A:37:ASP:OD2	14:O:236:GLU:N	2.30	0.61
11:L:75:ARG:HH11	11:L:104:ARG:HE	1.49	0.61
35:l:552:LEU:HD13	38:o:90:GLY:HA2	1.83	0.61
61:AD:48:ASN:HD22	65:AH:104:SER:HB3	1.66	0.61
62:AE:30:LEU:HD21	65:AH:216:THR:HG21	1.83	0.61
63:AF:36:ASP:OD1	63:AF:90:TYR:OH	2.17	0.61
76:AL:503:PEE:H49	76:AL:503:PEE:H26	1.78	0.61
1:A:339:PHE:HB3	1:A:349:LEU:HD13	1.81	0.61
2:B:126:ILE:O	15:P:231:ARG:NH2	2.23	0.61
14:O:137:THR:OG1	14:O:176:CYS:N	2.34	0.61
15:P:212:TYR:HA	15:P:219:VAL:HA	1.83	0.61
75:V:201:CDL:OA7	75:V:201:CDL:O1	2.16	0.61
32:i:58:LYS:HE3	35:l:584:ILE:HG12	1.82	0.61
41:s:280:PHE:CE2	41:s:288:LEU:HD11	2.36	0.61
46:y:122:MET:HB2	46:y:208:PRO:HD2	1.81	0.61
65:AH:315:LYS:NZ	75:AH:403:CDL:OB3	2.21	0.61
75:AL:502:CDL:H572	76:AL:503:PEE:C38	2.24	0.61
62:AR:34:ARG:HH11	62:AR:78:ARG:CZ	2.13	0.61
65:AU:135:LEU:HA	65:AU:138:VAL:HG12	1.82	0.61
65:AU:242:ILE:HG12	65:AU:244:MET:H	1.64	0.61
67:AW:318:GLN:HB3	67:AW:320:PRO:HD2	1.83	0.61
2:B:72:LEU:HB2	41:s:272:TRP:CH2	2.36	0.60
2:B:187:LYS:HB2	13:N:124:TYR:CE1	2.36	0.60
17:S:50:ARG:HA	31:h:105:ARG:CZ	2.30	0.60
22:Y:73:PHE:O	22:Y:73:PHE:HD1	1.84	0.60
30:g:9:PRO:O	30:g:11:ARG:N	2.32	0.60
35:l:427:ILE:HG23	35:l:431:LEU:HD12	1.82	0.60
40:r:447:LEU:HD13	40:r:454:ILE:HD11	1.83	0.60
41:s:28:LEU:O	41:s:32:GLN:HB2	2.01	0.60
75:AJ:404:CDL:HB62	66:AV:13:LEU:HD22	1.83	0.60
67:AK:183:ARG:HH21	67:AK:183:ARG:CG	2.14	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:AL:502:CDL:OA9	76:AL:503:PEE:O5	2.19	0.60
2:B:103:ARG:NH2	18:T:66:ASN:O	2.35	0.60
9:J:319:VAL:O	9:J:323:HIS:ND1	2.28	0.60
11:L:128:PHE:HA	15:P:121:THR:HG22	1.82	0.60
12:M:31:LEU:HD22	12:M:44:GLU:HA	1.83	0.60
12:M:339:ALA:HB3	12:M:544:VAL:HG12	1.82	0.60
21:W:111:PHE:HE2	21:W:117:VAL:HG11	1.66	0.60
27:d:59:HIS:NE2	28:e:121:GLU:HG2	2.16	0.60
33:j:55:PHE:O	33:j:58:VAL:HG12	2.01	0.60
40:r:447:LEU:HD11	71:r:502:PLX:H382	1.82	0.60
60:AC:104:ARG:HH21	68:AL:292:GLU:HG3	1.64	0.60
67:AK:363:GLN:CB	67:AK:365:ASN:OD1	2.49	0.60
68:AL:165:ARG:NH2	68:AL:211:LEU:O	2.32	0.60
8:I:52:ASN:OD1	8:I:57:ARG:NE	2.34	0.60
9:J:272:LEU:HD23	9:J:274:PHE:H	1.65	0.60
12:M:352:VAL:HG21	12:M:646:LEU:HD21	1.82	0.60
25:b:100:LYS:O	25:b:101:LYS:HG2	2.01	0.60
29:f:55:TRP:O	29:f:59:ILE:HG12	2.00	0.60
34:k:3:LEU:CD2	36:m:117:ASN:ND2	2.60	0.60
45:x:92:MET:CE	45:x:167:THR:HG21	2.31	0.60
58:AA:78:TYR:HB3	62:AE:65:GLU:HG2	0.68	0.60
65:AH:124:CYS:CB	81:AH:402:HEC:HBC2	2.31	0.60
66:AV:83:HIS:NE2	82:AV:401:HEM:C4D	2.67	0.60
66:AV:206:ASN:OD1	66:AV:207:ASN:N	2.34	0.60
66:AV:272:TRP:HA	66:AV:275:LEU:HG	1.84	0.60
3:C:205:ARG:HG3	3:C:205:ARG:O	2.02	0.60
12:M:483:ARG:O	12:M:485:ASP:N	2.33	0.60
14:O:87:GLN:O	14:O:91:GLY:N	2.22	0.60
25:b:88:TYR:HD1	25:b:92:GLU:OE2	1.82	0.60
35:l:37:LYS:HE2	35:l:98:TRP:HD1	0.69	0.60
57:9:28:LEU:HB2	57:9:29:PRO:HD3	1.83	0.60
12:M:228:VAL:HG23	12:M:230:ALA:H	1.66	0.60
12:M:345:LEU:HB2	12:M:548:LEU:HD21	1.84	0.60
6:X:72:PRO:HG3	35:l:442:ASN:HD22	1.65	0.60
30:g:32:TYR:OH	32:i:335:LEU:O	2.13	0.60
31:h:49:TYR:HA	31:h:52:ALA:HB3	1.82	0.60
37:n:10:ASP:HB3	40:r:19:LYS:HZ3	1.65	0.60
37:n:50:GLN:HG3	37:n:51:PRO:HD2	1.83	0.60
39:p:55:LYS:HE2	39:p:55:LYS:N	2.17	0.60
43:v:8:ARG:HH11	43:v:106:ARG:NH2	1.98	0.60
46:y:16:ILE:HD12	46:y:17:MET:N	2.15	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:z:192:VAL:O	47:z:196:THR:HB	2.01	0.60
58:AN:73:LYS:O	58:AN:77:ALA:N	2.35	0.60
76:W:201:PEE:C44	41:s:77:LEU:CD2	2.67	0.60
27:d:54:ARG:HD3	27:d:56:TYR:CE1	2.37	0.60
67:AK:101:ARG:NH1	68:AL:325:SER:O	2.33	0.60
68:AY:98:PHE:CZ	68:AY:120:LEU:HD13	2.36	0.60
68:AY:460:GLY:HA2	68:AY:462:ILE:H	1.65	0.60
1:A:164:ASN:ND2	14:O:190:ASP:O	2.34	0.60
1:A:203:ALA:HA	12:M:200:ARG:HH12	1.65	0.60
2:B:74:TYR:HD2	41:s:33:LEU:HG	1.66	0.60
3:C:136:LYS:HD2	33:j:40:GLY:C	2.26	0.60
7:H:77:LEU:O	7:H:80:VAL:HG12	2.01	0.60
9:J:208:GLY:H	9:J:211:ASP:HB2	1.66	0.60
15:P:190:ASP:CG	15:P:191:TYR:H	2.08	0.60
16:Q:179:ARG:CZ	16:Q:303:ARG:HH21	2.13	0.60
16:Q:338:ARG:HH12	21:W:23:ARG:HB3	1.65	0.60
25:b:115:GLU:HG2	25:b:116:VAL:H	1.65	0.60
32:i:291:TYR:CE2	76:l:701:PEE:C32	2.85	0.60
35:l:575:ILE:O	35:l:578:SER:OG	2.16	0.60
64:AT:14:VAL:O	64:AT:18:VAL:HG23	2.02	0.60
66:AV:200:LEU:CD1	82:AV:402:HEM:HAD2	2.32	0.60
4:E:37:ARG:HH21	4:E:41:ARG:NH2	2.00	0.60
9:J:85:ARG:HH11	9:J:85:ARG:CG	2.09	0.60
9:J:188:GLU:HG3	9:J:200:ILE:HG21	1.83	0.60
26:c:84:HIS:CE1	26:c:114:ARG:HA	2.37	0.60
27:d:108:GLN:HG2	35:l:199:GLN:CB	2.31	0.60
40:r:190:TRP:NE1	71:r:501:PLX:H1A2	2.17	0.60
44:w:65:ASN:HD22	44:w:209:VAL:HG21	1.67	0.60
47:z:148:HIS:O	47:z:152:MET:HG3	2.01	0.60
63:AS:71:LEU:O	65:AU:315:LYS:NZ	2.35	0.60
4:E:97:TRP:HH2	15:P:185:ARG:HH11	1.49	0.60
12:M:168:LEU:HD23	12:M:292:PHE:HD2	1.66	0.60
12:M:602:ARG:HE	12:M:659:ILE:HD11	1.67	0.60
13:N:137:TRP:CH2	13:N:140:PRO:HD3	2.36	0.60
71:U:101:PLX:H252	33:j:106:TRP:CD1	2.36	0.60
26:c:105:MET:HE2	38:o:65:LEU:HA	1.83	0.60
35:l:149:ILE:HD12	40:r:369:LEU:HD21	1.83	0.60
58:AA:71:LYS:HE2	65:AH:87:LEU:HD12	1.84	0.60
63:AF:29:LYS:CB	63:AF:75:ILE:HD11	2.22	0.60
66:AJ:282:ARG:HD2	66:AJ:343:VAL:HG22	1.83	0.60
64:AT:39:ARG:HH21	64:AT:39:ARG:CG	2.15	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AY:73:VAL:HG23	68:AY:147:LEU:HD23	1.83	0.60
12:M:387:LEU:HD12	12:M:514:ASN:HB2	1.82	0.60
13:N:129:THR:HA	18:T:44:GLN:HE22	1.67	0.60
75:AL:502:CDL:H761	76:AL:503:PEE:H74	1.82	0.60
9:J:217:PHE:HB2	9:J:280:ILE:HD13	1.83	0.59
12:M:385:TYR:OH	12:M:527:ASP:OD1	2.17	0.59
12:M:460:HIS:CD2	12:M:462:PHE:HB3	2.38	0.59
16:Q:140:ASP:HB3	16:Q:147:ASN:HD21	1.66	0.59
50:2:62:CYS:SG	50:2:84:SER:OG	2.60	0.59
59:AB:33:THR:HA	59:AB:38:PRO:HG3	1.82	0.59
75:AG:101:CDL:H521	75:AG:101:CDL:C71	2.32	0.59
59:AO:34:VAL:HB	59:AO:35:PRO:HD3	1.83	0.59
66:AV:181:PHE:HA	66:AV:184:ILE:HG22	1.83	0.59
68:AY:96:LEU:HA	68:AY:99:LYS:HG2	1.83	0.59
1:A:412:LEU:HA	1:A:415:ILE:HD12	1.84	0.59
12:M:69:LEU:HD21	12:M:184:ARG:HB2	1.83	0.59
13:N:34:LYS:HZ1	13:N:58:ARG:HG2	1.66	0.59
24:a:176:LYS:HB2	31:h:45:HIS:CD2	2.36	0.59
39:p:121:LYS:O	39:p:124:GLN:HG2	2.02	0.59
41:s:172:LEU:HD21	41:s:176:LEU:HB2	1.84	0.59
64:AG:38:TRP:O	64:AG:42:LEU:HD12	2.02	0.59
66:AV:311:LYS:HG3	66:AV:379:TRP:HE1	1.67	0.59
68:AY:89:ALA:O	68:AY:93:LEU:HG	2.02	0.59
1:A:263:ALA:HA	1:A:271:SER:HB3	1.83	0.59
4:E:99:GLN:HE21	33:j:41:PHE:HD1	1.50	0.59
9:J:141:PHE:CZ	9:J:180:TYR:CA	2.84	0.59
26:c:169:GLU:O	26:c:169:GLU:HG2	2.02	0.59
34:k:97:GLN:HG2	35:l:582:GLY:HA2	1.84	0.59
36:m:83:GLY:HA2	36:m:89:LEU:HD21	1.83	0.59
59:AB:7:ARG:NH1	67:AK:287:SER:OG	2.25	0.59
68:AL:79:SER:HB3	68:AL:126:ARG:HA	1.84	0.59
61:AQ:48:ASN:HB2	61:AQ:51:LYS:HD2	1.85	0.59
68:AY:96:LEU:CD2	68:AY:161:ILE:CD1	2.80	0.59
68:AY:326:SER:O	68:AY:330:SER:N	2.30	0.59
1:A:35:LEU:HD22	1:A:290:GLU:HA	1.82	0.59
9:J:207:PHE:HE2	9:J:348:LYS:HB2	1.67	0.59
15:P:204:LEU:HD11	16:Q:123:LEU:HD23	1.83	0.59
21:W:29:GLY:O	21:W:32:GLY:N	2.34	0.59
25:b:79:VAL:HG11	27:d:35:VAL:HG11	1.84	0.59
27:d:54:ARG:HD3	27:d:56:TYR:CZ	2.37	0.59
32:i:8:VAL:HG11	36:m:165:TYR:CE2	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:58:LYS:NZ	34:k:92:ASN:OD1	2.35	0.59
58:AA:40:ARG:HG3	58:AA:41:ARG:N	2.16	0.59
58:AA:78:TYR:CG	62:AE:65:GLU:HA	2.33	0.59
61:AD:34:ARG:NH1	61:AD:38:GLN:OE1	2.35	0.59
60:AP:131:ASN:HD22	76:AU:401:PEE:H7	1.66	0.59
2:B:64:LEU:O	2:B:68:LEU:N	2.30	0.59
2:B:208:LEU:HD22	8:I:39:PRO:HD2	1.85	0.59
12:M:519:ILE:HG12	12:M:521:SER:H	1.68	0.59
16:Q:142:VAL:HG11	16:Q:182:ASN:HA	1.84	0.59
22:Y:45:ARG:HG3	23:Z:52:ARG:HB2	1.84	0.59
32:i:193:VAL:HG21	32:i:266:ILE:HG12	1.82	0.59
35:l:367:PRO:O	35:l:370:SER:OG	2.17	0.59
35:l:512:LYS:HD3	54:6:18:LEU:CD1	2.32	0.59
37:n:31:SER:O	37:n:34:ARG:HG2	2.02	0.59
1:A:123:GLY:HA3	1:A:355:ILE:HD11	1.82	0.59
9:J:172:ALA:O	9:J:185:ALA:HB2	2.03	0.59
12:M:334:GLN:HB2	12:M:361:VAL:HB	1.85	0.59
20:V:40:ARG:HA	75:V:201:CDL:OB3	2.02	0.59
76:V:202:PEE:H71	76:l:701:PEE:C45	2.28	0.59
23:Z:66:VAL:HG22	35:l:363:LEU:HD22	1.85	0.59
32:i:24:SER:O	32:i:86:MET:HG2	2.02	0.59
44:w:304:VAL:HG23	44:w:305:LEU:HG	1.84	0.59
46:y:226:MET:O	46:y:227:LEU:HB2	2.01	0.59
59:AB:37:THR:HA	68:AL:174:GLU:HG2	1.85	0.59
60:AP:79:SER:N	60:AP:82:ASP:OD2	2.35	0.59
62:AR:30:LEU:HD21	65:AU:216:THR:HG23	1.84	0.59
63:AS:43:ASP:OD2	63:AS:102:ARG:NH1	2.35	0.59
4:E:127:ASP:HB3	4:E:128:PRO:HD2	1.84	0.59
7:H:40:LYS:HD3	7:H:45:ARG:NH1	2.18	0.59
21:W:81:ARG:HH22	42:u:64:ASN:ND2	2.01	0.59
25:b:51:LEU:HD21	25:b:62:HIS:HB2	1.83	0.59
25:b:88:TYR:CG	71:b:201:PLX:C1C	2.86	0.59
33:j:54:LYS:HE3	33:j:113:TRP:CD1	2.38	0.59
35:l:227:LEU:HB2	35:l:284:THR:HG22	1.84	0.59
35:l:247:LEU:O	35:l:252:MET:HB3	2.03	0.59
40:r:30:HIS:O	40:r:34:ILE:HD12	2.01	0.59
82:AJ:401:HEM:HBB2	82:AJ:401:HEM:HMB1	1.84	0.59
67:AW:449:PHE:HB2	67:AW:452:GLU:CD	2.27	0.59
68:AY:98:PHE:CD2	68:AY:120:LEU:HD13	2.29	0.59
1:A:220:GLN:NE2	14:O:114:GLU:O	2.35	0.59
25:b:100:LYS:HB2	35:l:60:GLU:HB2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:44:ALA:HA	31:h:47:ILE:HD12	1.85	0.59
31:h:94:PRO:HG2	31:h:95:PRO:HD3	1.85	0.59
35:l:37:LYS:HZ3	35:l:98:TRP:NE1	2.00	0.59
35:l:174:TYR:OH	76:l:702:PEE:H19	2.02	0.59
39:p:112:LYS:HA	39:p:119:PHE:CE2	2.38	0.59
44:w:132:GLN:HG2	44:w:170:LEU:HD12	1.85	0.59
68:AL:387:GLU:OE2	68:AL:390:ARG:NH2	2.27	0.59
1:A:288:VAL:HG11	1:A:303:HIS:CD2	2.38	0.59
2:B:72:LEU:HB2	41:s:272:TRP:HH2	1.68	0.59
31:h:51:ARG:NH1	31:h:55:GLU:OE2	2.36	0.59
35:l:37:LYS:CE	35:l:98:TRP:NE1	2.65	0.59
56:8:46:LYS:O	56:8:47:LYS:HB2	2.03	0.59
62:AE:33:VAL:HG11	62:AE:85:LYS:O	2.03	0.59
60:AP:81:THR:HG21	68:AY:202:GLU:HB2	1.84	0.59
12:M:36:VAL:HG11	12:M:56:VAL:HG11	1.85	0.59
12:M:624:ARG:NE	12:M:636:TYR:O	2.36	0.59
17:S:53:ARG:HB2	31:h:105:ARG:NH1	2.18	0.59
76:V:202:PEE:C11	32:i:276:LEU:HD12	2.28	0.59
26:c:93:ASP:OD2	26:c:101:TRP:N	2.36	0.59
47:z:119:THR:O	51:3:52:HIS:HE1	1.84	0.59
3:C:89:CYS:HB2	3:C:123:ALA:HB1	1.85	0.58
9:J:315:THR:HG23	9:J:318:LYS:H	1.66	0.58
9:J:358:THR:O	9:J:362:LEU:N	2.36	0.58
12:M:126:LEU:HD12	18:T:98:LYS:O	2.03	0.58
76:W:201:PEE:H8	41:s:98:LEU:HD22	1.83	0.58
23:Z:25:GLU:HA	23:Z:30:GLU:HG3	1.84	0.58
25:b:105:PHE:HE2	43:v:68:LYS:N	2.01	0.58
71:b:201:PLX:P1	71:b:201:PLX:H72	2.43	0.58
26:c:94:GLN:O	26:c:98:ARG:N	2.30	0.58
33:j:7:LEU:HA	33:j:10:ASN:HD22	1.67	0.58
35:l:456:ARG:CB	35:l:456:ARG:HH21	2.16	0.58
52:4:57:ARG:HG3	52:4:60:TYR:CE2	2.38	0.58
66:AV:338:ILE:HD11	66:AV:350:ILE:HG22	1.84	0.58
67:AW:357:GLN:O	67:AW:360:THR:OG1	2.17	0.58
4:E:126:HIS:NE2	12:M:612:PRO:O	2.37	0.58
5:F:41:TYR:OH	12:M:380:ASP:OD2	2.20	0.58
9:J:181:LEU:HD23	9:J:181:LEU:O	2.03	0.58
14:O:138:THR:HA	14:O:141:MET:HB3	1.85	0.58
25:b:88:TYR:O	25:b:92:GLU:HB2	2.03	0.58
27:d:134:GLN:NE2	38:o:123:ARG:O	2.35	0.58
33:j:2:ASN:O	33:j:5:LEU:HG	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:170:LEU:HD21	44:w:184:VAL:HG22	1.84	0.58
60:AC:96:VAL:O	68:AL:269:ARG:NH1	2.36	0.58
60:AP:244:ASP:OD1	60:AP:248:ARG:N	2.36	0.58
2:B:186:GLU:OE2	18:T:64:ASN:N	2.36	0.58
9:J:192:ARG:O	9:J:196:PRO:HA	2.02	0.58
9:J:212:ARG:HG2	9:J:212:ARG:NH1	2.15	0.58
14:O:48:ASN:HD22	14:O:94:PRO:HA	1.68	0.58
33:j:32:GLU:HA	33:j:35:THR:HG23	1.84	0.58
42:u:38:LYS:O	42:u:42:GLU:HB2	2.03	0.58
63:AS:7:VAL:HB	63:AS:10:SER:HB2	1.84	0.58
65:AU:288:MET:HE2	66:AV:77:TRP:CH2	2.39	0.58
15:P:147:THR:HG21	15:P:153:ILE:HB	1.84	0.58
16:Q:267:ILE:HG21	41:s:278:PRO:O	2.03	0.58
16:Q:438:MET:HE1	16:Q:454:GLN:NE2	2.18	0.58
21:W:61:GLN:HE22	41:s:317:GLN:HA	1.68	0.58
24:a:67:PHE:HD1	40:r:431:THR:HG23	1.68	0.58
32:i:145:ILE:HD12	32:i:149:LEU:HD11	1.84	0.58
34:k:37:MET:HE1	34:k:63:MET:HB3	1.86	0.58
35:l:227:LEU:CD1	35:l:230:HIS:CE1	2.85	0.58
42:u:96:LEU:HD11	42:u:99:HIS:CD2	2.38	0.58
46:y:145:PRO:CG	46:y:148:MET:HE2	2.33	0.58
46:y:179:LEU:HD21	52:4:65:PRO:HD3	1.84	0.58
46:y:193:TYR:HE1	48:0:126:MET:HE1	1.68	0.58
60:AC:132:ALA:HB2	76:AH:401:PEE:H24	1.84	0.58
76:AU:401:PEE:H17	66:AV:240:MET:HE2	1.76	0.58
2:B:39:VAL:HG22	16:Q:321:GLY:HA2	1.86	0.58
4:E:32:VAL:O	4:E:35:LEU:HB3	2.03	0.58
24:a:53:ARG:HH21	25:b:28:LEU:HD11	1.66	0.58
27:d:153:GLN:O	27:d:157:MET:HG2	2.03	0.58
32:i:249:LEU:HB3	32:i:254:LEU:HD12	1.85	0.58
33:j:72:LEU:HD21	33:j:94:LEU:HD22	1.86	0.58
35:l:88:MET:C	35:l:91:PRO:HD2	2.28	0.58
37:n:10:ASP:HB3	40:r:19:LYS:NZ	2.18	0.58
39:p:98:LYS:HE2	39:p:176:GLU:HA	1.84	0.58
55:7:43:SER:OG	55:7:45:VAL:HG12	2.04	0.58
82:AV:402:HEM:HMB1	82:AV:402:HEM:HBB2	1.85	0.58
1:A:93:PHE:HE2	1:A:98:LYS:CD	2.05	0.58
12:M:330:LEU:HD22	12:M:626:LEU:HD21	1.84	0.58
32:i:277:ILE:O	32:i:280:THR:OG1	2.21	0.58
41:s:294:LEU:O	41:s:297:THR:OG1	2.15	0.58
67:AK:323:VAL:HG13	67:AK:340:THR:HG22	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AV:333:LEU:HD21	76:AV:403:PEE:H62	1.86	0.58
2:B:198:GLU:OE1	13:N:88:ARG:HB2	2.04	0.58
9:J:73:LEU:O	9:J:78:SER:OG	2.21	0.58
12:M:308:ARG:HA	12:M:314:LEU:HA	1.86	0.58
16:Q:251:PHE:HD2	16:Q:341:LEU:HD21	1.69	0.58
6:X:84:LEU:O	6:X:88:LYS:HG2	2.03	0.58
27:d:21:PRO:HG2	27:d:24:ILE:HD12	1.85	0.58
35:l:96:VAL:O	35:l:100:ILE:HG13	2.04	0.58
35:l:512:LYS:O	39:p:40:PHE:CZ	2.56	0.58
44:w:149:HIS:O	44:w:153:THR:OG1	2.16	0.58
49:1:80:GLU:H	49:1:80:GLU:CD	2.10	0.58
66:AJ:283:SER:O	66:AJ:352:GLN:NE2	2.33	0.58
5:F:88:THR:HA	5:F:91:LEU:HD12	1.85	0.58
8:I:23:LYS:HD3	16:Q:250:ASN:HA	1.85	0.58
16:Q:182:ASN:HD21	16:Q:404:LYS:HE3	1.68	0.58
45:x:184:PHE:H	45:x:256:HIS:HE1	1.52	0.58
67:AK:57:PRO:O	67:AK:127:ARG:HG3	2.04	0.58
66:AV:137:GLN:HE21	66:AV:141:TRP:CD1	2.22	0.58
68:AY:98:PHE:CE2	68:AY:120:LEU:HD12	2.36	0.58
1:A:307:VAL:HG11	1:A:314:LEU:HD21	1.86	0.58
8:I:69:ILE:HB	15:P:76:VAL:HB	1.85	0.58
9:J:293:LEU:HD12	9:J:294:PRO:HD2	1.86	0.58
16:Q:251:PHE:HA	16:Q:254:ARG:HE	1.69	0.58
35:l:310:LEU:HA	35:l:313:MET:HE3	1.86	0.58
42:u:124:GLU:OE1	42:u:124:GLU:N	2.37	0.58
58:AA:29:HIS:HD2	58:AA:33:LYS:HB2	1.69	0.58
67:AK:438:MET:HB3	67:AK:450:VAL:HG13	1.86	0.58
10:K:89:LEU:HD11	14:O:61:LYS:HE3	1.86	0.58
12:M:501:ARG:NH1	12:M:666:GLN:HB2	2.18	0.58
17:S:49:GLU:O	31:h:105:ARG:NH2	2.37	0.58
41:s:85:LEU:HD13	41:s:233:MET:HE1	1.85	0.58
66:AJ:100:ARG:NH2	82:AJ:402:HEM:O2A	2.37	0.58
82:AV:402:HEM:HBA1	82:AV:402:HEM:HHA	1.86	0.58
67:AW:70:ARG:NH2	67:AW:332:ASP:OD2	2.21	0.58
1:A:48:ARG:HH12	14:O:231:LEU:HD11	1.69	0.57
1:A:118:ASP:OD1	1:A:120:GLY:N	2.35	0.57
16:Q:412:VAL:HG12	16:Q:420:TYR:HB3	1.86	0.57
24:a:52:LYS:O	24:a:53:ARG:HG2	2.03	0.57
76:l:701:PEE:C23	40:r:155:VAL:CB	2.77	0.57
40:r:126:LEU:O	40:r:129:THR:OG1	2.19	0.57
41:s:169:GLN:NE2	41:s:174:LEU:H	2.02	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:v:113:LYS:HE2	43:v:117:LYS:HE3	1.84	0.57
44:w:332:ARG:O	44:w:338:LYS:CB	2.52	0.57
60:AC:204:ARG:NH1	60:AC:248:ARG:HG3	2.19	0.57
63:AF:41:ASP:N	63:AF:41:ASP:OD1	2.36	0.57
60:AP:183:GLU:HA	60:AP:186:GLN:HG2	1.86	0.57
65:AU:292:MET:HE1	66:AV:241:THR:CG2	2.33	0.57
1:A:159:ARG:NH1	14:O:177:LEU:O	2.33	0.57
1:A:243:ALA:HA	70:A:502:FMN:O2P	2.04	0.57
1:A:438:LEU:HD21	1:A:446:LEU:HD21	1.86	0.57
2:B:36:TYR:HB3	8:I:104:TRP:HE3	1.68	0.57
9:J:212:ARG:HH11	9:J:212:ARG:CG	2.12	0.57
12:M:210:ILE:HG23	12:M:212:LYS:H	1.69	0.57
12:M:222:ILE:O	12:M:225:ILE:HG22	2.04	0.57
12:M:251:ILE:HG22	12:M:260:ASN:HA	1.85	0.57
14:O:160:VAL:HA	14:O:171:LEU:HD23	1.86	0.57
19:U:67:PRO:HB3	19:U:74:GLN:HB2	1.86	0.57
27:d:135:ASP:HB3	27:d:156:ARG:NH2	2.19	0.57
32:i:245:PRO:HA	32:i:248:LEU:HD12	1.85	0.57
66:AJ:163:TRP:CD2	75:AJ:405:CDL:H331	2.39	0.57
67:AK:177:LEU:HD21	67:AK:272:VAL:HG21	1.85	0.57
68:AL:337:LEU:C	68:AL:368:MET:HE2	2.29	0.57
62:AR:37:CYS:SG	62:AR:85:LYS:NZ	2.73	0.57
1:A:201:ALA:HB1	14:O:121:MET:HB2	1.86	0.57
3:C:67:LEU:HD22	3:C:207:LEU:CD2	2.34	0.57
3:C:173:ILE:HG22	3:C:174:VAL:HG13	1.84	0.57
4:E:118:PHE:HA	4:E:121:LYS:HD3	1.86	0.57
9:J:204:SER:O	9:J:240:VAL:HG23	2.04	0.57
12:M:177:ILE:HG13	12:M:177:ILE:O	2.04	0.57
12:M:217:GLU:HB2	12:M:408:ARG:HH21	1.69	0.57
12:M:257:VAL:HG11	12:M:413:LEU:HD22	1.85	0.57
12:M:385:TYR:HB2	12:M:517:HIS:HE2	1.69	0.57
12:M:650:SER:OG	12:M:652:ASN:OD1	2.22	0.57
21:W:47:HIS:CE1	41:s:307:MET:HE1	2.40	0.57
21:W:78:GLU:HB3	31:h:105:ARG:HB3	1.86	0.57
76:W:201:PEE:H1	41:s:98:LEU:CD2	2.34	0.57
22:Y:72:ARG:NH1	35:l:466:PHE:HD1	2.02	0.57
32:i:120:GLN:O	32:i:176:ARG:NH2	2.38	0.57
35:l:286:LEU:HD12	35:l:411:ILE:HG23	1.86	0.57
35:l:453:PRO:HA	35:l:456:ARG:HH22	1.69	0.57
35:l:556:THR:OG1	35:l:557:TRP:N	2.37	0.57
38:o:54:PRO:HA	39:p:129:ARG:HH21	1.67	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:4:75:ARG:HG2	52:4:75:ARG:NH1	2.19	0.57
59:AB:27:ARG:NH1	67:AK:171:THR:HG22	2.19	0.57
68:AL:282:LEU:HB2	68:AL:461:PRO:HD3	1.86	0.57
66:AV:14:ILE:HD13	76:AY:502:PEE:C25	2.22	0.57
1:A:159:ARG:HH22	14:O:177:LEU:HA	1.70	0.57
5:F:63:PRO:HB2	5:F:79:LEU:CB	2.31	0.57
9:J:84:TYR:CB	9:J:91:ILE:HD11	2.34	0.57
12:M:226:CYS:HB2	12:M:231:LEU:HD12	1.85	0.57
12:M:306:MET:HB3	12:M:314:LEU:HD13	1.86	0.57
16:Q:251:PHE:CD2	16:Q:341:LEU:HD21	2.40	0.57
26:c:156:VAL:O	43:v:98:ARG:HG2	2.05	0.57
35:l:27:ASN:HB3	35:l:29:LYS:HG2	1.84	0.57
39:p:176:GLU:HG2	39:p:177:ARG:HG3	1.85	0.57
71:r:502:PLX:H72	71:r:502:PLX:C3	2.31	0.57
66:AV:343:VAL:HG13	66:AV:348:THR:HG22	1.84	0.57
6:G:134:ASP:O	6:G:138:LEU:N	2.38	0.57
9:J:329:LEU:HD13	9:J:332:LEU:HB2	1.84	0.57
20:V:40:ARG:HD3	20:V:59:TYR:HE2	1.68	0.57
22:Y:73:PHE:HA	35:l:385:PHE:HE2	1.70	0.57
25:b:88:TYR:CG	71:b:201:PLX:H1C1	2.38	0.57
30:g:1:MET:SD	32:i:345:MET:HE1	2.44	0.57
32:i:258:THR:HG22	32:i:336:LEU:HB3	1.87	0.57
34:k:2:PRO:HG2	36:m:115:VAL:HG23	1.86	0.57
34:k:8:ILE:HG21	34:k:43:MET:HB2	1.87	0.57
45:x:404:THR:O	45:x:480:ARG:NH1	2.37	0.57
46:y:189:PRO:HD2	53:5:54:TYR:OH	2.05	0.57
46:y:193:TYR:CE1	48:0:126:MET:HE1	2.39	0.57
58:AA:78:TYR:CD1	62:AE:65:GLU:N	2.73	0.57
66:AV:333:LEU:CD2	76:AV:403:PEE:H66	2.35	0.57
68:AY:113:VAL:HG21	68:AY:120:LEU:HD23	1.87	0.57
1:A:209:GLU:HB3	70:A:502:FMN:H3'	1.84	0.57
2:B:66:ARG:NH2	21:W:26:PRO:O	2.38	0.57
8:I:36:GLN:HE22	16:Q:239:GLY:HA2	1.69	0.57
9:J:75:ARG:NH1	15:P:215:GLU:OE2	2.34	0.57
12:M:636:TYR:CE1	12:M:642:VAL:HB	2.39	0.57
25:b:105:PHE:CD2	43:v:68:LYS:HA	2.39	0.57
35:l:272:LEU:O	35:l:275:THR:OG1	2.18	0.57
68:AL:134:LYS:NZ	68:AL:407:THR:OG1	2.38	0.57
71:AL:501:PLX:H71	76:AL:503:PEE:C13	2.33	0.57
60:AP:104:ARG:NH2	68:AY:293:GLY:O	2.37	0.57
68:AY:423:ARG:O	68:AY:424:ILE:HG22	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:GLY:H	2:B:167:GLU:HG3	1.70	0.57
9:J:221:HIS:HE1	9:J:222:ARG:HG3	1.61	0.57
12:M:358:LEU:O	12:M:363:SER:N	2.35	0.57
16:Q:81:THR:HA	16:Q:100:GLU:HA	1.86	0.57
22:Y:39:HIS:ND1	22:Y:40:ILE:HG13	2.20	0.57
22:Y:44:TYR:CD1	35:l:440:LEU:HB2	2.40	0.57
63:AF:97:GLU:OE2	67:AW:147:ARG:NH1	2.38	0.57
65:AU:296:MET:HE2	76:AU:401:PEE:C32	2.34	0.57
67:AW:217:ARG:HE	67:AW:245:GLY:HA3	1.69	0.57
1:A:382:CYS:SG	69:A:501:SF4:S4	3.03	0.57
2:B:74:TYR:OH	16:Q:257:GLU:OE1	2.20	0.57
14:O:148:ILE:HG23	14:O:201:ILE:HD11	1.87	0.57
21:W:111:PHE:HE1	31:h:65:GLU:OE1	1.88	0.57
33:j:57:LEU:O	33:j:61:THR:HG23	2.04	0.57
35:l:35:TYR:CZ	35:l:39:ILE:HD11	2.40	0.57
44:w:124:ASN:HB3	44:w:316:GLU:HG2	1.85	0.57
67:AW:274:GLU:OE2	67:AW:333:SER:OG	2.16	0.57
2:B:87:GLU:HG2	13:N:61:TRP:HB3	1.87	0.57
9:J:220:MET:HB2	9:J:281:PHE:HZ	1.68	0.57
9:J:283:VAL:HG12	9:J:369:VAL:HG21	1.86	0.57
16:Q:306:GLN:O	16:Q:308:TYR:N	2.38	0.57
25:b:88:TYR:CD1	25:b:92:GLU:OE2	2.57	0.57
25:b:111:LEU:O	25:b:112:GLU:HB2	2.05	0.57
45:x:95:PRO:HB2	47:z:11:VAL:HG13	1.87	0.57
66:AJ:206:ASN:OD1	66:AJ:207:ASN:N	2.37	0.57
76:AY:502:PEE:H19	76:AY:502:PEE:O4	2.04	0.57
1:A:126:LYS:HB2	1:A:275:LEU:HD22	1.85	0.57
1:A:235:VAL:HG22	1:A:240:THR:HG21	1.87	0.57
3:C:115:ARG:NH2	33:j:37:TYR:CD2	2.72	0.57
3:C:147:VAL:HG23	3:C:176:VAL:HA	1.86	0.57
8:I:39:PRO:HB2	8:I:41:LEU:HD12	1.87	0.57
8:I:41:LEU:C	21:W:8:GLN:HE22	2.13	0.57
12:M:391:ILE:O	12:M:417:ARG:NH2	2.38	0.57
16:Q:123:LEU:HB3	16:Q:135:TYR:OH	2.05	0.57
6:X:132:ASP:OD2	39:p:18:ARG:HG2	2.05	0.57
24:a:53:ARG:O	24:a:54:LEU:HD23	2.04	0.57
32:i:316:GLN:NE2	44:w:95:ASP:OD1	2.33	0.57
40:r:178:LEU:O	40:r:182:THR:OG1	2.16	0.57
76:AH:401:PEE:H66	76:AH:401:PEE:C18	2.30	0.57
67:AK:378:LEU:HB3	67:AK:416:ILE:HD11	1.87	0.57
63:AS:70:ASN:HD22	66:AV:209:LEU:HG	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AW:449:PHE:HB2	67:AW:452:GLU:OE2	2.04	0.57
12:M:193:ASP:OD2	14:O:111:ARG:NH2	2.38	0.56
12:M:591:GLU:HB3	12:M:612:PRO:HD3	1.87	0.56
16:Q:390:GLN:HE22	16:Q:417:SER:HB3	1.68	0.56
20:V:139:PRO:O	20:V:141:VAL:N	2.38	0.56
71:g:203:PLX:H251	32:i:324:PRO:HB2	1.85	0.56
40:r:210:TYR:HB2	40:r:268:GLY:HA3	1.85	0.56
9:J:64:PHE:HD1	9:J:210:GLU:HB3	1.69	0.56
76:V:202:PEE:H57	76:V:202:PEE:H40	1.87	0.56
24:a:114:LYS:CB	27:d:57:TYR:CE2	2.77	0.56
29:f:72:ARG:HH11	30:g:19:SER:HB3	1.70	0.56
33:j:114:ALA:HB1	41:s:286:MET:HB2	1.87	0.56
35:l:332:HIS:HE1	35:l:336:LYS:NZ	2.02	0.56
49:1:78:HIS:ND1	53:5:12:LEU:HD22	2.21	0.56
65:AH:156:ASP:OD1	65:AH:157:GLY:N	2.37	0.56
68:AY:280:ASP:O	68:AY:362:ARG:NH2	2.37	0.56
6:G:97:LYS:HD3	6:G:108:LEU:HG	1.86	0.56
8:I:46:SER:OG	12:M:150:ARG:NH2	2.38	0.56
9:J:176:SER:C	9:J:182:ARG:HH21	2.13	0.56
9:J:217:PHE:HB3	9:J:280:ILE:HD13	1.87	0.56
12:M:454:ASP:HB3	12:M:460:HIS:HB2	1.85	0.56
16:Q:84:PHE:CE2	16:Q:91:ALA:HB2	2.40	0.56
16:Q:326:CYS:SG	16:Q:453:THR:HG22	2.44	0.56
17:S:59:ARG:O	17:S:61:TYR:N	2.36	0.56
22:Y:86:TYR:OH	43:v:100:LYS:HG3	2.03	0.56
23:Z:51:TRP:O	23:Z:53:TYR:N	2.37	0.56
25:b:110:ILE:HG13	25:b:111:LEU:HD21	1.87	0.56
26:c:153:TYR:HB3	35:l:403:TYR:HD1	1.69	0.56
32:i:237:LEU:HD13	32:i:240:LEU:HD12	1.86	0.56
34:k:7:ASN:ND2	36:m:9:SER:OG	2.31	0.56
35:l:51:THR:HG21	35:l:91:PRO:HG3	1.86	0.56
35:l:452:ASN:HB2	35:l:453:PRO:HD3	1.87	0.56
35:l:564:LYS:O	35:l:567:SER:OG	2.23	0.56
37:n:56:THR:HG1	37:n:57:TRP:CD1	2.23	0.56
44:w:115:GLU:OE2	44:w:225:HIS:ND1	2.39	0.56
47:z:203:PHE:O	47:z:207:HIS:HD2	1.88	0.56
56:8:41:ARG:HG3	57:9:40:TYR:CE2	2.40	0.56
65:AH:242:ILE:HG12	65:AH:244:MET:H	1.70	0.56
66:AJ:24:PRO:HD2	66:AJ:27:ILE:HD11	1.87	0.56
67:AK:259:ARG:CD	67:AK:444:LEU:HD13	2.30	0.56
58:AN:19:LEU:HD23	68:AY:273:SER:HB3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:AP:197:ASP:O	60:AP:257:ASN:ND2	2.37	0.56
60:AP:204:ARG:NH1	60:AP:246:SER:O	2.38	0.56
66:AV:333:LEU:HD22	76:AV:403:PEE:H66	1.87	0.56
68:AY:96:LEU:HD23	68:AY:161:ILE:HD13	1.87	0.56
1:A:86:ARG:HA	1:A:94:PRO:HA	1.88	0.56
1:A:227:PRO:HB3	12:M:95:PRO:HD3	1.87	0.56
5:F:16:LEU:HD11	5:F:19:ILE:HB	1.87	0.56
9:J:84:TYR:O	9:J:107:GLU:HA	2.06	0.56
12:M:225:ILE:HD12	12:M:285:TRP:CH2	2.39	0.56
12:M:492:ALA:O	12:M:495:SER:OG	2.21	0.56
21:W:31:SER:OG	21:W:35:MET:HE2	2.06	0.56
23:Z:22:TRP:CE3	23:Z:51:TRP:HA	2.40	0.56
26:c:127:HIS:O	26:c:131:MET:HG2	2.04	0.56
32:i:230:LEU:HD11	32:i:244:ILE:HG21	1.87	0.56
76:l:702:PEE:O4	76:l:702:PEE:H7	2.05	0.56
41:s:280:PHE:O	41:s:281:ARG:HB3	2.05	0.56
66:AJ:51:LEU:HD13	82:AJ:401:HEM:HBD1	1.88	0.56
58:AN:41:ARG:HE	75:AN:101:CDL:PA1	2.28	0.56
65:AU:133:ARG:NH1	66:AV:72:ASP:OD1	2.32	0.56
2:B:151:ILE:HG21	3:C:159:TYR:CD2	2.41	0.56
9:J:117:ARG:HG2	9:J:155:LEU:HD22	1.86	0.56
9:J:141:PHE:CZ	9:J:180:TYR:CD1	2.93	0.56
15:P:213:ASP:OD1	15:P:214:ASP:N	2.38	0.56
20:V:40:ARG:NH2	20:V:55:LYS:HD3	2.20	0.56
20:V:62:THR:HG22	20:V:104:ARG:HE	1.69	0.56
25:b:88:TYR:O	25:b:92:GLU:HB3	2.05	0.56
35:l:452:ASN:N	35:l:453:PRO:CD	2.68	0.56
36:m:156:THR:O	36:m:159:THR:OG1	2.22	0.56
41:s:156:MET:HE1	41:s:177:PRO:HB2	1.88	0.56
41:s:190:LEU:HD22	41:s:195:ARG:HG2	1.86	0.56
47:z:42:LEU:HD13	54:6:45:TYR:CD2	2.41	0.56
66:AJ:100:ARG:HH22	82:AJ:402:HEM:HBD1	1.71	0.56
67:AK:351:ILE:HD11	67:AK:448:PRO:HD2	1.86	0.56
68:AL:470:ARG:HH22	75:AL:502:CDL:PA1	2.28	0.56
1:A:222:LYS:HE2	1:A:379:CYS:HB2	1.88	0.56
1:A:319:PRO:O	1:A:324:THR:OG1	2.23	0.56
16:Q:390:GLN:OE1	16:Q:417:SER:N	2.39	0.56
6:X:99:SER:OG	6:X:102:SER:OG	2.11	0.56
71:g:203:PLX:H1A2	71:g:203:PLX:H72	1.87	0.56
32:i:250:SER:O	32:i:259:GLY:HA3	2.04	0.56
42:u:35:GLN:O	42:u:37:ASP:N	2.34	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:x:69:MET:HE2	45:x:70:VAL:CG2	2.36	0.56
68:AL:337:LEU:HB3	68:AL:368:MET:HG2	1.87	0.56
58:AN:19:LEU:HD11	60:AP:88:PHE:HB3	1.88	0.56
81:AU:402:HEC:HBB3	81:AU:402:HEC:HHC	1.88	0.56
67:AW:272:VAL:HG11	67:AW:335:LEU:HB3	1.87	0.56
5:F:16:LEU:HB3	5:F:51:LEU:HD13	1.88	0.56
16:Q:94:VAL:HG11	16:Q:458:PHE:HB3	1.87	0.56
22:Y:85:PRO:CG	43:v:99:MET:HE2	2.36	0.56
27:d:59:HIS:ND1	28:e:120:ARG:HG2	2.21	0.56
27:d:60:ARG:HH11	27:d:60:ARG:CG	2.12	0.56
36:m:16:PHE:HA	36:m:19:PHE:CE1	2.40	0.56
39:p:30:TRP:CE2	39:p:76:HIS:HB2	2.40	0.56
46:y:132:GLU:HB3	46:y:137:GLU:HG3	1.87	0.56
63:AF:67:LEU:O	63:AF:71:LEU:HD23	2.05	0.56
67:AW:185:ALA:HB3	67:AW:251:ALA:HB2	1.88	0.56
68:AY:74:TRP:CD2	68:AY:414:GLY:HA3	2.40	0.56
12:M:221:ASN:HB3	12:M:285:TRP:CE3	2.40	0.56
12:M:460:HIS:O	12:M:463:SER:OG	2.13	0.56
24:a:98:LEU:CA	27:d:57:TYR:CE1	2.89	0.56
25:b:105:PHE:HE2	43:v:68:LYS:HA	1.70	0.56
27:d:107:CYS:HG	27:d:119:CYS:HA	1.70	0.56
38:o:8:PRO:HB3	38:o:14:LEU:HG	1.88	0.56
39:p:56:ASP:OD1	39:p:57:MET:N	2.38	0.56
42:u:44:MET:HE3	42:u:48:TRP:CZ3	2.41	0.56
51:3:5:LYS:HD2	51:3:6:GLY:N	2.21	0.56
59:AO:20:ARG:HD2	59:AO:51:SER:HB3	1.88	0.56
66:AV:111:GLU:HG2	66:AV:199:PHE:CD1	2.41	0.56
67:AW:259:ARG:NH2	67:AW:447:THR:OG1	2.38	0.56
9:J:181:LEU:HD13	9:J:324:ILE:HD13	1.88	0.56
11:L:82:PRO:HD3	11:L:98:LYS:HG2	1.87	0.56
25:b:105:PHE:CE2	43:v:68:LYS:N	2.74	0.56
31:h:70:GLN:HG2	36:m:115:VAL:CG1	2.36	0.56
35:l:73:THR:OG1	35:l:74:THR:N	2.39	0.56
35:l:407:TRP:NE1	35:l:411:ILE:HD11	2.21	0.56
36:m:81:ALA:HB3	36:m:84:SER:HB3	1.87	0.56
40:r:346:GLN:HB2	40:r:420:THR:HG23	1.88	0.56
43:v:40:VAL:H	43:v:61:HIS:HE1	1.53	0.56
64:AG:17:TRP:NE1	68:AL:382:SER:OG	2.39	0.56
75:AJ:405:CDL:OB7	75:AJ:405:CDL:HB62	2.05	0.56
64:AT:40:LEU:HD12	64:AT:41:ILE:H	1.64	0.56
66:AV:138:MET:HE1	66:AV:268:ILE:HA	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:17:ARG:HB3	5:F:68:ARG:HH21	1.71	0.56
16:Q:232:VAL:HB	16:Q:356:ILE:HG22	1.88	0.56
52:4:71:THR:O	52:4:75:ARG:HD3	2.05	0.56
60:AP:123:VAL:HG13	61:AQ:29:VAL:HG22	1.88	0.56
66:AV:165:TRP:O	66:AV:174:THR:OG1	2.23	0.56
9:J:132:ARG:HD2	9:J:134:TRP:NE1	2.20	0.55
9:J:168:SER:C	9:J:184:LYS:HE2	2.31	0.55
12:M:476:LEU:HD11	12:M:480:ALA:HB3	1.87	0.55
71:g:201:PLX:H261	32:i:346:ILE:HG23	1.87	0.55
44:w:287:ASP:OD1	44:w:288:ASN:N	2.34	0.55
46:y:111:THR:HG21	52:4:66:ILE:HD11	1.89	0.55
47:z:222:GLN:HA	47:z:222:GLN:HE21	1.71	0.55
67:AK:399:GLN:NE2	67:AK:407:MET:HB3	2.20	0.55
2:B:103:ARG:HH12	18:T:68:ALA:HB2	1.69	0.55
4:E:66:MET:HE3	4:E:106:PHE:HD1	1.71	0.55
12:M:481:LEU:HD11	12:M:515:ILE:HD12	1.88	0.55
12:M:598:ASN:HB3	12:M:602:ARG:HB3	1.89	0.55
13:N:84:PRO:HD3	13:N:113:HIS:CD2	2.41	0.55
16:Q:316:PHE:HB2	16:Q:339:GLN:HE21	1.70	0.55
20:V:47:GLY:O	20:V:48:THR:OG1	2.25	0.55
25:b:75:VAL:O	25:b:79:VAL:HG23	2.06	0.55
25:b:84:TYR:HE1	27:d:43:ARG:HD3	1.71	0.55
30:g:51:PRO:HG2	30:g:55:ALA:HB2	1.87	0.55
31:h:2:PRO:O	31:h:4:LEU:N	2.39	0.55
31:h:74:ARG:HA	36:m:116:VAL:HG21	1.88	0.55
32:i:106:LEU:HD21	32:i:138:PRO:HB2	1.87	0.55
32:i:287:LEU:HD21	40:r:158:LEU:HD11	1.87	0.55
40:r:164:LEU:O	40:r:167:THR:OG1	2.18	0.55
60:AC:83:ILE:HD12	68:AL:189:ALA:HB2	1.87	0.55
66:AJ:181:PHE:HA	66:AJ:184:ILE:HG22	1.88	0.55
67:AK:235:GLU:HA	67:AK:238:LEU:HD13	1.88	0.55
68:AY:424:ILE:HG23	68:AY:429:TRP:NE1	2.12	0.55
1:A:149:MET:HG3	1:A:241:THR:HG21	1.89	0.55
11:L:133:ASP:O	11:L:136:SER:OG	2.20	0.55
14:O:41:HIS:ND1	14:O:41:HIS:O	2.40	0.55
16:Q:66:TRP:NE1	44:w:310:ILE:HD11	2.20	0.55
17:S:50:ARG:HA	31:h:105:ARG:NE	2.21	0.55
20:V:3:PRO:HA	20:V:6:PHE:HB3	1.88	0.55
76:V:202:PEE:H60	76:V:202:PEE:C24	2.36	0.55
21:W:122:GLY:HA3	36:m:124:TRP:CE3	2.41	0.55
30:g:47:ILE:HD12	32:i:327:PRO:HG3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:124:LEU:HD23	32:i:176:ARG:HD3	1.88	0.55
39:p:86:PRO:HA	39:p:91:TYR:CD1	2.41	0.55
40:r:232:ALA:O	40:r:237:LYS:NZ	2.38	0.55
42:u:115:LEU:HB3	42:u:117:TRP:CZ3	2.42	0.55
60:AP:131:ASN:O	60:AP:135:GLN:HG2	2.05	0.55
60:AP:220:LEU:HB2	74:AP:301:FES:S2	2.46	0.55
68:AY:230:VAL:CG2	68:AY:418:LEU:HD11	2.36	0.55
1:A:381:GLN:CG	69:A:501:SF4:S2	2.94	0.55
2:B:145:ILE:HG22	2:B:188:LEU:HD11	1.89	0.55
4:E:75:ASP:HB3	4:E:78:VAL:HG23	1.89	0.55
5:F:80:ASN:OD1	5:F:81:ASN:ND2	2.39	0.55
12:M:128:CYS:N	12:M:129:PRO:HD2	2.21	0.55
12:M:173:MET:C	12:M:175:ARG:N	2.60	0.55
12:M:408:ARG:HB3	12:M:415:ASN:ND2	2.21	0.55
35:l:456:ARG:NH2	35:l:456:ARG:HB2	2.21	0.55
36:m:16:PHE:CD1	36:m:19:PHE:HE1	2.25	0.55
63:AF:29:LYS:HG2	63:AF:75:ILE:HD13	1.67	0.55
66:AJ:316:MET:HA	66:AJ:322:GLN:NE2	2.21	0.55
59:AO:27:ARG:NH1	67:AW:171:THR:HG22	2.21	0.55
68:AY:160:GLN:NE2	68:AY:164:GLU:OE2	2.39	0.55
1:A:342:LEU:HB3	1:A:347:THR:HB	1.87	0.55
4:E:36:TYR:HD1	4:E:67:PHE:CE2	2.25	0.55
11:L:61:ILE:HB	11:L:64:LEU:HB2	1.89	0.55
12:M:50:LEU:N	12:M:91:ALA:O	2.38	0.55
16:Q:273:ILE:HD11	16:Q:325:ASP:OD2	2.04	0.55
19:U:67:PRO:HA	19:U:74:GLN:OE1	2.07	0.55
25:b:83:HIS:CD2	35:l:6:THR:HG21	2.42	0.55
33:j:80:GLN:NE2	41:s:316:PRO:O	2.39	0.55
33:j:92:LEU:O	33:j:96:ILE:HG12	2.06	0.55
39:p:102:TRP:HZ2	40:r:422:HIS:HA	1.70	0.55
62:AE:30:LEU:CD2	65:AH:216:THR:HG23	2.33	0.55
81:AH:402:HEC:HBC3	81:AH:402:HEC:HHD	1.87	0.55
1:A:119:GLU:HB3	1:A:162:PHE:HE2	1.70	0.55
13:N:48:TYR:HB3	13:N:89:TRP:CZ3	2.41	0.55
20:V:40:ARG:HD3	20:V:59:TYR:CE2	2.42	0.55
22:Y:74:TRP:HE3	22:Y:75:HIS:CA	2.19	0.55
22:Y:81:LEU:CD1	43:v:88:ASP:HB3	2.37	0.55
24:a:59:PRO:HD3	39:p:99:VAL:HG21	1.89	0.55
26:c:56:ASN:ND2	38:o:43:LEU:HD11	2.22	0.55
37:n:30:LYS:NZ	75:n:101:CDL:HA31	2.22	0.55
41:s:117:LEU:HD12	41:s:136:VAL:HG21	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:100:CYS:SG	42:u:101:ARG:N	2.78	0.55
65:AH:304:TYR:HE1	75:AH:403:CDL:OA3	1.90	0.55
67:AK:93:GLY:HA3	67:AK:139:ASN:HD21	1.72	0.55
60:AP:204:ARG:NH1	60:AP:248:ARG:HG3	2.21	0.55
68:AY:152:GLN:HE21	68:AY:253:ILE:HG13	1.72	0.55
1:A:418:GLN:O	1:A:422:HIS:ND1	2.39	0.55
9:J:49:SER:HB2	15:P:225:GLU:HB3	1.87	0.55
9:J:141:PHE:CE1	9:J:180:TYR:HD1	2.25	0.55
15:P:51:ASN:HB2	15:P:82:ASN:HD21	1.72	0.55
15:P:235:LEU:HD22	16:Q:387:GLU:HG2	1.87	0.55
27:d:109:GLN:HG2	35:l:62:ILE:HD13	1.88	0.55
34:k:57:ASN:O	34:k:60:PRO:HD2	2.06	0.55
38:o:28:GLU:HA	38:o:31:ARG:HD3	1.88	0.55
40:r:403:THR:HA	40:r:406:TYR:CE2	2.42	0.55
63:AF:49:ARG:HA	63:AF:49:ARG:HE	1.71	0.55
66:AJ:119:LEU:HD11	66:AJ:192:LEU:HB3	1.89	0.55
4:E:25:MET:HE3	4:E:29:LYS:HE2	1.88	0.55
9:J:134:TRP:CZ3	9:J:136:THR:HA	2.42	0.55
9:J:171:ASN:HB2	9:J:181:LEU:HD11	1.84	0.55
12:M:124:HIS:ND1	12:M:125:PRO:HD2	2.22	0.55
25:b:110:ILE:HG13	25:b:111:LEU:CD2	2.37	0.55
46:y:145:PRO:HG3	46:y:148:MET:HE2	1.87	0.55
63:AS:68:ASP:HA	63:AS:71:LEU:HD12	1.89	0.55
5:F:68:ARG:HD2	5:F:72:GLY:HA2	1.87	0.55
9:J:94:LEU:HG	9:J:97:MET:SD	2.46	0.55
12:M:329:MET:HG3	12:M:565:PHE:CE2	2.41	0.55
12:M:620:TRP:HE1	12:M:639:LEU:HD13	1.71	0.55
13:N:57:GLY:H	13:N:59:HIS:CE1	2.24	0.55
16:Q:291:VAL:HA	16:Q:294:ARG:HB2	1.89	0.55
76:W:201:PEE:H4	76:W:201:PEE:P	2.28	0.55
25:b:87:LYS:HE3	27:d:43:ARG:HG2	1.89	0.55
26:c:184:TYR:O	43:v:35:LYS:O	2.25	0.55
27:d:134:GLN:O	27:d:138:GLN:HB2	2.06	0.55
35:l:102:GLU:OE1	35:l:453:PRO:HG3	2.07	0.55
35:l:546:GLN:O	35:l:550:LEU:HB2	2.07	0.55
37:n:7:ILE:O	37:n:11:HIS:N	2.37	0.55
46:y:203:ASN:HD22	46:y:206:PHE:HD2	1.55	0.55
48:0:108:PRO:HG2	48:0:111:PHE:CE2	2.42	0.55
50:2:82:CYS:N	50:2:86:GLY:O	2.40	0.55
59:AB:30:VAL:O	59:AB:33:THR:OG1	2.22	0.55
68:AL:470:ARG:HH12	75:AL:502:CDL:HA31	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:AN:43:ARG:HA	58:AN:46:PHE:HD2	1.72	0.55
61:AQ:48:ASN:HD22	65:AU:104:SER:HB3	1.72	0.55
1:A:278:ILE:HG12	1:A:304:ALA:HB2	1.89	0.55
7:H:16:VAL:HA	7:H:78:GLU:OE2	2.06	0.55
22:Y:74:TRP:CE3	22:Y:74:TRP:C	2.85	0.55
27:d:81:GLU:OE1	37:n:43:MET:CE	2.43	0.55
32:i:288:LEU:HD21	76:l:701:PEE:H58	1.69	0.55
33:j:24:LEU:H	33:j:25:PRO:HD2	1.72	0.55
34:k:1:MET:CB	34:k:4:ILE:HD13	2.36	0.55
36:m:138:ASP:HB2	36:m:139:PRO:HD3	1.89	0.55
40:r:73:LEU:HD12	40:r:103:GLN:HG2	1.89	0.55
66:AV:138:MET:HB2	66:AV:255:ASN:ND2	2.22	0.55
68:AY:161:ILE:O	68:AY:165:ARG:HG3	2.07	0.55
11:L:162:ALA:HA	11:L:168:LYS:NZ	2.23	0.54
25:b:45:LYS:HA	25:b:48:ASN:HB2	1.87	0.54
35:l:3:MET:O	35:l:7:MET:HG2	2.08	0.54
35:l:238:GLU:N	35:l:238:GLU:OE1	2.40	0.54
35:l:452:ASN:N	35:l:452:ASN:OD1	2.36	0.54
40:r:91:ARG:HG2	40:r:136:TRP:HH2	1.72	0.54
45:x:407:ASP:O	45:x:411:LYS:HG3	2.07	0.54
51:3:5:LYS:HD2	51:3:5:LYS:C	2.32	0.54
63:AF:27:PHE:CD1	63:AF:28:ASN:N	2.75	0.54
9:J:141:PHE:HZ	9:J:180:TYR:CD1	2.26	0.54
11:L:61:ILE:HG21	15:P:149:GLU:OE1	2.07	0.54
12:M:241:ARG:HG2	12:M:243:TRP:CZ2	2.42	0.54
12:M:380:ASP:OD1	12:M:381:LEU:N	2.40	0.54
12:M:510:TRP:CD1	12:M:512:VAL:HG22	2.42	0.54
32:i:167:TRP:HH2	35:l:570:GLN:HG3	1.70	0.54
40:r:1:MET:HG3	40:r:2:LEU:H	1.71	0.54
45:x:172:LYS:HB2	45:x:172:LYS:HZ3	1.71	0.54
58:AA:19:LEU:HD11	60:AC:88:PHE:HB3	1.87	0.54
75:AG:101:CDL:H331	66:AV:163:TRP:CD1	2.43	0.54
66:AV:10:LEU:CD2	76:AY:502:PEE:H45	2.34	0.54
68:AY:156:LEU:HB2	68:AY:213:ARG:HE	1.73	0.54
4:E:56:VAL:HG23	9:J:367:GLU:OE2	2.07	0.54
9:J:164:PHE:HE2	9:J:191:VAL:HG13	1.72	0.54
12:M:308:ARG:HD2	12:M:312:GLY:O	2.08	0.54
12:M:341:ILE:HD12	12:M:555:ILE:HG13	1.89	0.54
12:M:697:THR:O	12:M:702:ARG:NH2	2.40	0.54
6:X:84:LEU:HD11	6:X:100:VAL:HG22	1.87	0.54
25:b:105:PHE:HE2	43:v:67:LEU:C	2.15	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:114:ASN:OD1	43:v:50:GLN:HG2	2.07	0.54
30:g:44:ASP:OD2	30:g:63:TYR:OH	2.16	0.54
36:m:48:GLY:HA2	36:m:138:ASP:OD2	2.08	0.54
58:AA:12:ARG:HA	68:AL:279:ASP:HA	1.89	0.54
58:AA:78:TYR:O	58:AA:81:ASP:HB2	2.07	0.54
76:AU:401:PEE:C19	76:AU:401:PEE:C39	2.86	0.54
68:AY:76:ASP:HB3	68:AY:228:ARG:HG3	1.89	0.54
1:A:207:GLY:O	70:A:502:FMN:C9A	2.56	0.54
1:A:328:PRO:HG2	1:A:441:HIS:CD2	2.43	0.54
2:B:71:THR:HG23	41:s:31:MET:CE	2.38	0.54
7:H:12:VAL:HG11	16:Q:296:SER:HB2	1.90	0.54
7:H:31:ILE:HA	7:H:34:VAL:HG12	1.90	0.54
11:L:85:ASN:OD1	11:L:87:MET:N	2.36	0.54
32:i:17:THR:OG1	32:i:36:ASN:ND2	2.39	0.54
35:l:190:ILE:O	35:l:194:ASN:HA	2.08	0.54
40:r:317:ILE:HD12	40:r:454:ILE:HG23	1.88	0.54
40:r:358:TRP:CE3	40:r:441:LEU:HD12	2.42	0.54
60:AC:153:GLU:HB3	60:AC:273:VAL:HB	1.88	0.54
60:AC:173:PRO:HB2	60:AC:215:GLY:HA3	1.90	0.54
68:AL:465:LEU:HD12	68:AL:466:PRO:HD2	1.89	0.54
60:AP:207:LYS:HD3	60:AP:265:PHE:HE2	1.71	0.54
65:AU:98:HIS:NE2	65:AU:208:GLU:OE2	2.38	0.54
66:AV:326:TRP:CH2	76:AV:403:PEE:H51	2.42	0.54
68:AY:79:SER:HB3	68:AY:126:ARG:HA	1.90	0.54
68:AY:96:LEU:C	68:AY:96:LEU:HD12	2.32	0.54
4:E:80:ASP:HA	4:E:83:VAL:HG22	1.90	0.54
9:J:344:PRO:HG2	9:J:347:LEU:HD13	1.89	0.54
15:P:55:HIS:CD2	15:P:78:VAL:HG12	2.42	0.54
15:P:107:GLN:HB3	15:P:109:LYS:HE3	1.89	0.54
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	1.89	0.54
16:Q:198:THR:HA	41:s:32:GLN:OE1	2.07	0.54
22:Y:96:GLU:O	22:Y:97:LEU:CB	2.54	0.54
27:d:115:TYR:CD1	27:d:115:TYR:C	2.85	0.54
30:g:46:LEU:HD11	32:i:239:TRP:HB3	1.88	0.54
35:l:293:LEU:HD23	35:l:422:TYR:HB3	1.90	0.54
36:m:155:VAL:O	36:m:159:THR:HG23	2.08	0.54
40:r:236:LEU:O	40:r:239:GLY:N	2.40	0.54
41:s:145:THR:HG21	41:s:289:LEU:HD22	1.90	0.54
62:AR:80:HIS:C	62:AR:80:HIS:CD2	2.86	0.54
66:AV:140:PHE:CD1	66:AV:140:PHE:C	2.85	0.54
1:A:33:GLY:H	1:A:294:VAL:HG12	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:172:ALA:HA	9:J:181:LEU:CD2	2.38	0.54
9:J:176:SER:C	9:J:182:ARG:NH2	2.65	0.54
9:J:203:PRO:HG2	73:J:401:NDP:C5N	2.37	0.54
12:M:389:THR:OG1	12:M:514:ASN:ND2	2.40	0.54
16:Q:404:LYS:HZ3	16:Q:457:VAL:HB	1.73	0.54
22:Y:96:GLU:O	22:Y:97:LEU:CD2	2.54	0.54
24:a:133:TYR:OH	27:d:81:GLU:HG2	2.08	0.54
35:l:197:ASP:O	35:l:201:MET:HG3	2.08	0.54
48:0:52:SER:OG	48:0:55:GLU:HG3	2.08	0.54
67:AK:364:GLY:HA2	67:AK:425:ILE:HD12	1.89	0.54
68:AL:311:ILE:O	68:AL:326:SER:OG	2.26	0.54
75:AL:502:CDL:H772	76:AL:503:PEE:C42	2.38	0.54
66:AV:150:LEU:CD2	66:AV:164:ILE:HD13	2.37	0.54
1:A:225:LEU:HG	1:A:227:PRO:HD3	1.90	0.54
9:J:168:SER:O	73:J:401:NDP:H6N	2.08	0.54
22:Y:81:LEU:HD22	43:v:92:HIS:HD2	1.70	0.54
35:l:95:PHE:CD1	35:l:95:PHE:C	2.86	0.54
36:m:16:PHE:HD1	36:m:19:PHE:HE1	1.54	0.54
36:m:32:LEU:HD13	36:m:64:MET:HE1	1.88	0.54
44:w:206:TYR:OH	44:w:238:GLU:OE2	2.25	0.54
75:AL:502:CDL:C58	76:AL:503:PEE:H62	2.37	0.54
59:AO:45:LEU:HA	68:AY:284:PHE:HE2	1.71	0.54
67:AW:185:ALA:HB2	67:AW:249:ALA:HB1	1.89	0.54
2:B:61:TRP:HH2	41:s:187:ILE:HD11	1.73	0.54
10:K:92:SER:HB2	14:O:68:LYS:HD2	1.90	0.54
11:L:170:THR:O	11:L:172:VAL:N	2.35	0.54
15:P:160:PHE:C	15:P:162:ALA:H	2.16	0.54
16:Q:149:GLN:CD	16:Q:171:ARG:HB3	2.33	0.54
49:1:41:LEU:HD12	49:1:41:LEU:O	2.08	0.54
59:AB:29:LEU:O	59:AB:31:GLN:N	2.38	0.54
75:AJ:405:CDL:C78	75:AJ:405:CDL:C74	2.86	0.54
3:C:140:GLN:NE2	33:j:40:GLY:HA2	2.23	0.54
8:I:42:PRO:HB3	21:W:10:MET:HE1	1.90	0.54
12:M:47:THR:OG1	12:M:51:GLN:OE1	2.23	0.54
12:M:53:CYS:HB2	12:M:60:ILE:HD11	1.90	0.54
12:M:405:THR:HA	12:M:686:PRO:HG3	1.90	0.54
15:P:85:GLU:HG3	15:P:142:ARG:HB2	1.88	0.54
15:P:235:LEU:HB3	16:Q:387:GLU:HG2	1.90	0.54
16:Q:262:LEU:HD22	16:Q:268:TRP:NE1	2.18	0.54
21:W:81:ARG:HH22	42:u:64:ASN:HD21	1.56	0.54
34:k:87:LEU:HD11	36:m:73:MET:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:61:THR:HG22	44:w:159:LEU:HD23	1.90	0.54
44:w:128:SER:O	44:w:131:LEU:HG	2.08	0.54
63:AF:67:LEU:CD2	66:AJ:209:LEU:HD12	2.28	0.54
68:AL:294:PRO:HG3	68:AL:448:TYR:CZ	2.43	0.54
59:AO:5:ALA:HB1	67:AW:385:SER:HB2	1.90	0.54
1:A:41:ILE:HG23	1:A:253:THR:HG21	1.90	0.54
7:H:111:GLN:NE2	15:P:124:ASN:HB2	2.22	0.54
9:J:167:VAL:HA	9:J:201:VAL:HB	1.88	0.54
12:M:358:LEU:HB3	12:M:363:SER:O	2.07	0.54
12:M:402:LEU:HA	12:M:475:VAL:HB	1.88	0.54
15:P:94:ILE:N	15:P:154:GLU:OE1	2.28	0.54
16:Q:391:VAL:HG12	16:Q:392:PRO:O	2.09	0.54
24:a:54:LEU:HD23	25:b:27:GLU:HA	1.89	0.54
28:e:74:HIS:ND1	28:e:87:MET:HG3	2.23	0.54
35:l:98:TRP:CD1	35:l:98:TRP:C	2.86	0.54
35:l:512:LYS:O	39:p:40:PHE:HZ	1.91	0.54
50:2:51:SER:HB2	50:2:91:LEU:HD11	1.90	0.54
51:3:2:SER:OG	51:3:3:ALA:N	2.41	0.54
60:AC:164:ASN:OD1	60:AC:165:MET:N	2.41	0.54
82:AJ:402:HEM:HMC2	82:AJ:402:HEM:HBC2	1.89	0.54
68:AL:77:VAL:HG21	68:AL:223:HIS:HB3	1.89	0.54
2:B:61:TRP:CD1	16:Q:266:ARG:HH12	2.26	0.53
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.90	0.53
12:M:343:GLY:HA3	12:M:548:LEU:HB2	1.90	0.53
13:N:84:PRO:HA	13:N:87:HIS:HB3	1.90	0.53
17:S:12:MET:HE1	41:s:20:LEU:HD12	1.91	0.53
46:y:165:VAL:HB	46:y:170:LEU:HD12	1.90	0.53
63:AF:29:LYS:CD	63:AF:75:ILE:HD13	2.21	0.53
63:AS:28:ASN:HD22	63:AS:82:THR:HB	1.73	0.53
82:AV:401:HEM:HBB2	82:AV:401:HEM:HMB1	1.91	0.53
8:I:59:GLY:HA2	15:P:47:VAL:HG22	1.90	0.53
9:J:178:SER:OG	9:J:181:LEU:CB	2.57	0.53
9:J:207:PHE:CZ	9:J:345:LEU:HA	2.44	0.53
16:Q:43:TRP:HZ3	32:i:305:LEU:HD21	1.74	0.53
32:i:217:LEU:HB3	32:i:326:LEU:HD12	1.89	0.53
33:j:104:TYR:CG	36:m:165:TYR:HE1	2.26	0.53
41:s:127:TYR:HA	41:s:130:ILE:HD12	1.89	0.53
53:5:63:MET:HB3	53:5:68:ILE:HD11	1.89	0.53
62:AE:21:GLU:O	62:AE:24:GLU:CA	2.57	0.53
67:AK:36:GLN:HG2	67:AK:53:GLU:HB3	1.90	0.53
68:AL:66:GLN:NE2	68:AL:406:THR:OG1	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AY:364:LYS:HB2	68:AY:368:MET:HE3	1.90	0.53
1:A:141:GLY:HA2	1:A:252:PRO:HD3	1.90	0.53
2:B:37:LYS:N	16:Q:318:VAL:O	2.37	0.53
16:Q:85:GLY:HA3	33:j:39:CYS:HG	1.73	0.53
24:a:98:LEU:HB3	27:d:57:TYR:HE1	0.54	0.53
25:b:78:PRO:O	25:b:82:ILE:HD12	2.08	0.53
39:p:102:TRP:NE1	40:r:426:MET:HE1	2.23	0.53
50:2:55:LYS:HA	50:2:74:LEU:O	2.08	0.53
59:AB:31:GLN:NE2	67:AK:297:PRO:HA	2.24	0.53
67:AK:217:ARG:HH21	67:AK:246:LEU:H	1.56	0.53
68:AL:121:ASN:ND2	68:AL:132:TYR:OH	2.36	0.53
63:AS:55:LEU:HD21	63:AS:90:TYR:CD2	2.43	0.53
66:AV:341:GLN:HB3	66:AV:342:PRO:HD2	1.91	0.53
1:A:357:MET:HG2	14:O:142:LEU:HD21	1.91	0.53
1:A:382:CYS:HA	12:M:74:ASN:HA	1.91	0.53
2:B:104:TYR:CE2	2:B:110:ARG:HA	2.43	0.53
4:E:128:PRO:HB3	11:L:104:ARG:HH22	1.73	0.53
9:J:89:TYR:CD1	9:J:89:TYR:C	2.85	0.53
12:M:53:CYS:SG	12:M:102:ILE:HD12	2.48	0.53
12:M:82:ILE:HB	12:M:85:ALA:HB2	1.91	0.53
12:M:124:HIS:CD2	16:Q:375:MET:HE2	2.42	0.53
14:O:204:ILE:O	14:O:208:LEU:HG	2.09	0.53
16:Q:136:PHE:HE2	16:Q:151:TYR:CD1	2.26	0.53
16:Q:265:ASN:OD1	16:Q:266:ARG:N	2.42	0.53
16:Q:449:ALA:O	16:Q:453:THR:HG23	2.08	0.53
76:V:202:PEE:C24	76:V:202:PEE:H57	2.39	0.53
76:W:201:PEE:C3	41:s:98:LEU:HD22	2.38	0.53
23:Z:24:ILE:HG22	23:Z:30:GLU:HB2	1.90	0.53
24:a:98:LEU:CA	27:d:57:TYR:CD1	2.91	0.53
26:c:84:HIS:CD2	26:c:118:ASP:HB3	2.43	0.53
31:h:48:GLY:O	31:h:50:THR:N	2.37	0.53
35:l:525:MET:HE2	39:p:77:PRO:HB3	1.90	0.53
40:r:414:THR:O	40:r:415:GLN:NE2	2.41	0.53
46:y:136:LEU:HB3	46:y:193:TYR:HD2	1.73	0.53
50:2:48:LEU:O	50:2:50:PRO:HD3	2.08	0.53
58:AA:12:ARG:HG2	58:AA:13:HIS:CE1	2.43	0.53
66:AJ:229:ALA:HB1	71:AL:501:PLX:H131	1.89	0.53
67:AW:267:VAL:HG11	67:AW:347:ALA:HB2	1.90	0.53
2:B:68:LEU:O	2:B:71:THR:HG22	2.08	0.53
9:J:64:PHE:CE1	9:J:68:TYR:HE2	2.27	0.53
12:M:215:MET:HE1	12:M:714:VAL:HG23	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:565:PHE:HA	12:M:581:ASP:OD2	2.08	0.53
15:P:88:ILE:HG22	15:P:89:HIS:O	2.09	0.53
17:S:28:ARG:NH1	42:u:91:TYR:OH	2.42	0.53
34:k:66:PHE:CE1	36:m:159:THR:HG21	2.40	0.53
35:l:51:THR:CG2	35:l:91:PRO:HG2	2.30	0.53
41:s:126:ASN:HA	41:s:129:LEU:HD12	1.91	0.53
44:w:138:SER:O	44:w:142:GLN:HG2	2.07	0.53
58:AA:78:TYR:HB3	62:AE:65:GLU:CD	2.30	0.53
61:AD:60:TYR:HD2	65:AH:141:THR:HG21	1.73	0.53
58:AN:12:ARG:HG3	68:AY:279:ASP:HA	1.91	0.53
75:AN:101:CDL:OB9	66:AV:29:ALA:HB3	2.08	0.53
82:AV:402:HEM:HBC2	82:AV:402:HEM:HMC2	1.90	0.53
2:B:61:TRP:O	2:B:63:GLU:N	2.41	0.53
3:C:172:ARG:NH1	15:P:209:GLU:OE2	2.36	0.53
9:J:172:ALA:HA	9:J:181:LEU:HD23	1.91	0.53
9:J:298:TYR:CE2	9:J:319:VAL:HG22	2.44	0.53
12:M:68:ARG:HD2	12:M:285:TRP:NE1	2.21	0.53
14:O:129:LYS:HB3	14:O:168:LEU:HG	1.91	0.53
16:Q:196:ALA:O	16:Q:198:THR:N	2.41	0.53
6:X:93:ILE:HG21	6:X:98:LEU:HD12	1.91	0.53
24:a:112:TYR:HD1	27:d:58:TYR:O	1.92	0.53
41:s:195:ARG:NH1	41:s:270:PHE:HB3	2.24	0.53
42:u:83:THR:O	42:u:86:TRP:HB3	2.08	0.53
44:w:149:HIS:CE1	44:w:155:GLN:HB3	2.43	0.53
45:x:302:ARG:O	45:x:306:THR:HG23	2.09	0.53
63:AF:70:ASN:HB3	66:AJ:26:ASN:HB2	1.91	0.53
67:AK:116:ARG:HH21	67:AK:175:GLU:HG3	1.74	0.53
67:AK:319:GLN:O	67:AK:321:PHE:N	2.41	0.53
1:A:121:GLU:HA	1:A:204:TYR:HE1	1.74	0.53
2:B:65:PHE:O	2:B:69:GLY:N	2.41	0.53
4:E:24:ASP:OD1	4:E:25:MET:N	2.41	0.53
4:E:50:PHE:HB2	4:E:52:LEU:HD12	1.89	0.53
12:M:308:ARG:NH1	12:M:578:PRO:O	2.42	0.53
13:N:94:THR:HG22	13:N:96:ASP:H	1.73	0.53
15:P:172:ASP:OD2	15:P:189:THR:OG1	2.23	0.53
22:Y:84:PHE:CE2	35:l:483:PRO:CG	2.69	0.53
32:i:311:VAL:HG12	32:i:315:TRP:HE1	1.74	0.53
35:l:282:ALA:O	35:l:285:THR:OG1	2.27	0.53
35:l:293:LEU:HD11	35:l:418:LEU:HD22	1.90	0.53
44:w:137:SER:O	44:w:139:ARG:N	2.37	0.53
45:x:268:PHE:CZ	46:y:58:ALA:HA	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:AB:54:SER:HA	68:AL:402:HIS:CE1	2.43	0.53
75:AJ:405:CDL:HB61	75:AJ:405:CDL:H312	1.90	0.53
1:A:117:ALA:HB3	1:A:157:TYR:O	2.08	0.53
1:A:293:SER:HB2	1:A:336:LEU:HD23	1.91	0.53
6:G:75:THR:O	6:G:79:ILE:HG12	2.09	0.53
6:G:105:MET:HE2	6:G:138:LEU:HD23	1.89	0.53
12:M:46:GLY:O	12:M:96:VAL:HG22	2.09	0.53
12:M:168:LEU:HB3	12:M:292:PHE:HE2	1.74	0.53
12:M:394:VAL:HG21	12:M:414:PHE:HE1	1.73	0.53
16:Q:435:LEU:HA	16:Q:438:MET:HE3	1.91	0.53
25:b:95:TYR:HE2	27:d:10:TYR:CD1	2.27	0.53
25:b:110:ILE:N	27:d:17:THR:O	2.41	0.53
32:i:291:TYR:HB2	40:r:151:PHE:CZ	2.44	0.53
41:s:32:GLN:HB3	41:s:34:ARG:HG2	1.91	0.53
63:AF:72:LYS:O	63:AF:73:HIS:HB2	2.09	0.53
67:AK:254:ARG:NH2	67:AW:257:GLU:OE1	2.41	0.53
67:AK:289:LEU:O	67:AK:293:LEU:HD13	2.09	0.53
59:AO:45:LEU:HD13	67:AW:160:ILE:HG23	1.91	0.53
66:AV:149:LEU:HD21	66:AV:281:LEU:CD2	2.31	0.53
1:A:164:ASN:HB3	10:K:77:HIS:HB2	1.91	0.53
1:A:317:VAL:HG13	1:A:356:VAL:HA	1.91	0.53
4:E:81:LEU:HD23	11:L:64:LEU:HD22	1.91	0.53
12:M:351:LEU:HD23	12:M:530:TYR:HE2	1.73	0.53
18:T:52:ARG:HB3	18:T:55:ARG:HH12	1.74	0.53
22:Y:71:TRP:CE3	22:Y:71:TRP:C	2.87	0.53
25:b:105:PHE:HD2	43:v:68:LYS:HG3	1.74	0.53
31:h:99:ILE:HD12	31:h:101:LYS:HD2	1.91	0.53
32:i:229:LEU:HD22	32:i:232:ARG:NH1	2.23	0.53
36:m:19:PHE:CZ	36:m:32:LEU:HD21	2.43	0.53
40:r:272:THR:HA	40:r:275:ILE:HD12	1.90	0.53
47:z:151:LEU:HB2	47:z:159:MET:HG3	1.90	0.53
63:AF:36:ASP:OD1	63:AF:62:ARG:NH1	2.42	0.53
75:AL:502:CDL:C76	76:AL:503:PEE:H74	2.38	0.53
68:AY:473:SER:HB3	76:AY:502:PEE:H10	1.91	0.53
1:A:217:GLU:HB3	11:L:171:ARG:HH22	1.72	0.53
2:B:90:PRO:HD2	3:C:100:ARG:HH11	1.74	0.53
3:C:62:TYR:OH	3:C:66:LYS:NZ	2.29	0.53
3:C:75:ARG:NH2	3:C:144:PRO:HG3	2.24	0.53
7:H:97:TRP:HB3	7:H:100:TRP:CH2	2.43	0.53
9:J:141:PHE:CZ	9:J:180:TYR:CB	2.92	0.53
9:J:141:PHE:HE2	9:J:183:ASN:HB2	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:69:HIS:ND1	19:U:70:PRO:HA	2.24	0.53
31:h:40:TRP:HH2	32:i:83:GLN:HE21	1.57	0.53
40:r:73:LEU:O	40:r:76:THR:OG1	2.18	0.53
40:r:286:ILE:O	40:r:289:SER:OG	2.23	0.53
66:AJ:173:PRO:O	66:AJ:177:ARG:HG2	2.09	0.53
67:AK:57:PRO:HG2	68:AL:400:VAL:HG11	1.91	0.53
1:A:154:ALA:HB3	1:A:195:VAL:HG12	1.91	0.52
11:L:120:PRO:HB2	15:P:203:PRO:HG3	1.91	0.52
15:P:115:THR:HG22	16:Q:423:LYS:HD3	1.92	0.52
25:b:105:PHE:HE2	43:v:68:LYS:CA	2.19	0.52
27:d:57:TYR:HD1	27:d:57:TYR:O	1.91	0.52
32:i:300:THR:OG1	32:i:301:SER:N	2.38	0.52
34:k:11:ALA:HB1	36:m:16:PHE:HD2	1.72	0.52
34:k:62:VAL:HG21	36:m:152:LEU:HD21	1.91	0.52
36:m:23:PRO:O	36:m:24:SER:OG	2.24	0.52
48:0:67:SER:OG	48:0:70:GLU:HG3	2.08	0.52
62:AE:34:ARG:HD3	62:AE:78:ARG:CZ	2.36	0.52
63:AF:36:ASP:CG	63:AF:62:ARG:NH1	2.67	0.52
60:AP:131:ASN:ND2	76:AU:401:PEE:H7	2.24	0.52
1:A:77:LEU:HD21	1:A:100:SER:HA	1.90	0.52
1:A:116:ASN:HD22	70:A:502:FMN:C9	2.22	0.52
3:C:184:PRO:HD3	16:Q:223:HIS:CD2	2.43	0.52
9:J:223:PHE:O	9:J:225:PRO:HD2	2.09	0.52
17:S:54:ILE:HG13	31:h:105:ARG:HH11	1.72	0.52
26:c:101:TRP:NE1	38:o:61:GLU:O	2.43	0.52
27:d:73:GLU:HG3	30:g:106:LYS:O	2.08	0.52
33:j:24:LEU:H	33:j:25:PRO:CD	2.22	0.52
34:k:7:ASN:OD1	36:m:13:VAL:CG2	2.57	0.52
34:k:15:SER:OG	34:k:36:MET:HG2	2.08	0.52
34:k:58:ILE:HG23	36:m:145:LEU:HD12	1.91	0.52
43:v:56:ARG:O	43:v:60:ALA:HB2	2.10	0.52
48:0:40:LEU:HD13	48:0:59:LEU:HD13	1.91	0.52
58:AN:20:SER:HB3	58:AN:23:GLU:HG2	1.91	0.52
64:AT:19:PRO:HA	64:AT:22:TYR:HD2	1.74	0.52
7:H:7:LYS:HG2	7:H:8:THR:HG23	1.92	0.52
12:M:188:GLU:O	12:M:419:ARG:NE	2.40	0.52
12:M:519:ILE:HD13	12:M:522:GLN:HB2	1.90	0.52
12:M:613:PRO:HB3	13:N:134:ILE:HG21	1.91	0.52
35:l:144:TRP:NE1	35:l:179:ASP:OD1	2.42	0.52
35:l:194:ASN:HD22	38:o:127:LEU:HD12	1.74	0.52
35:l:566:ILE:HA	35:l:569:HIS:HD2	1.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:36:GLY:HA3	36:m:60:LEU:HD21	1.90	0.52
71:r:501:PLX:H262	71:r:501:PLX:H6	1.91	0.52
44:w:58:ARG:HB3	44:w:202:HIS:CE1	2.44	0.52
46:y:102:HIS:O	46:y:104:TRP:N	2.42	0.52
60:AC:80:HIS:CE1	68:AL:185:ASN:HD22	2.27	0.52
75:AG:101:CDL:H741	66:AV:156:ILE:HG23	1.91	0.52
67:AK:299:VAL:HG21	68:AL:110:GLU:HG3	1.91	0.52
7:H:32:LEU:O	7:H:36:GLU:HG3	2.10	0.52
9:J:64:PHE:CD1	9:J:210:GLU:HB3	2.44	0.52
11:L:61:ILE:HG22	11:L:64:LEU:HD12	1.91	0.52
15:P:238:PRO:O	15:P:239:TRP:HB2	2.08	0.52
16:Q:159:LEU:HD21	16:Q:391:VAL:HA	1.90	0.52
20:V:124:LEU:HD23	20:V:127:MET:HE3	1.91	0.52
22:Y:61:PHE:CE2	35:l:455:LYS:HG2	2.44	0.52
24:a:90:ASN:ND2	71:b:201:PLX:H122	2.19	0.52
32:i:239:TRP:HA	75:i:401:CDL:HB32	1.91	0.52
34:k:4:ILE:O	34:k:8:ILE:HD13	2.09	0.52
35:l:106:TRP:HB2	35:l:449:THR:OG1	2.09	0.52
35:l:195:SER:O	35:l:196:TRP:HB2	2.08	0.52
36:m:50:TYR:O	36:m:54:MET:HG2	2.10	0.52
36:m:106:VAL:HG11	36:m:117:ASN:HD22	1.75	0.52
40:r:131:ALA:O	40:r:135:ARG:HB3	2.09	0.52
47:z:156:ARG:HG3	47:z:156:ARG:NH1	2.23	0.52
51:3:42:ARG:HH11	51:3:42:ARG:HG3	1.74	0.52
66:AJ:281:LEU:HD11	66:AJ:294:LEU:HD22	1.90	0.52
6:G:123:GLU:HB2	6:G:128:PHE:O	2.09	0.52
12:M:314:LEU:HD11	13:N:140:PRO:HD2	1.92	0.52
15:P:113:ASP:HB3	15:P:115:THR:HG23	1.91	0.52
16:Q:338:ARG:NH2	21:W:23:ARG:HB3	2.24	0.52
17:S:12:MET:CE	41:s:20:LEU:HD12	2.39	0.52
27:d:57:TYR:CD1	27:d:57:TYR:C	2.85	0.52
30:g:27:ASP:OD1	42:u:172:LYS:NZ	2.42	0.52
37:n:40:ASN:ND2	37:n:56:THR:HG23	2.25	0.52
42:u:24:VAL:HG13	42:u:86:TRP:CD1	2.45	0.52
44:w:294:LEU:O	44:w:298:VAL:HG23	2.09	0.52
48:0:23:PRO:HD2	49:1:34:ASN:HD22	1.74	0.52
50:2:8:THR:OG1	50:2:11:GLU:HG2	2.09	0.52
52:4:60:TYR:C	52:4:60:TYR:CD1	2.88	0.52
76:AH:401:PEE:C40	76:AH:401:PEE:C18	2.86	0.52
68:AL:361:ASP:OD1	68:AL:362:ARG:N	2.42	0.52
60:AP:128:ALA:HB1	76:AU:401:PEE:H55	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HD11	1:A:256:ARG:HG2	1.91	0.52
1:A:181:LEU:HA	1:A:187:CYS:HB3	1.91	0.52
1:A:236:PHE:HZ	14:O:77:ALA:HB2	1.73	0.52
6:G:137:LYS:O	6:G:139:MET:N	2.42	0.52
9:J:168:SER:HA	9:J:184:LYS:CE	2.40	0.52
12:M:385:TYR:HB2	12:M:517:HIS:NE2	2.25	0.52
15:P:186:ARG:NH2	15:P:193:PHE:O	2.40	0.52
16:Q:66:TRP:CE2	44:w:310:ILE:HD11	2.45	0.52
21:W:35:MET:HA	21:W:38:ILE:HD12	1.91	0.52
25:b:22:TRP:O	25:b:25:ASP:HB3	2.10	0.52
27:d:110:ARG:NH1	27:d:110:ARG:CG	2.73	0.52
32:i:222:ASN:HD21	32:i:233:THR:HG22	1.75	0.52
32:i:285:ILE:CG1	76:l:701:PEE:H75	2.25	0.52
41:s:139:THR:O	41:s:143:GLU:HG3	2.09	0.52
45:x:225:GLY:HA3	47:z:112:LEU:HD13	1.92	0.52
48:0:40:LEU:HD22	48:0:59:LEU:HD13	1.91	0.52
75:AJ:405:CDL:H111	76:AY:502:PEE:C45	2.30	0.52
68:AL:285:ALA:HB3	68:AL:360:CYS:SG	2.50	0.52
62:AR:37:CYS:SG	62:AR:85:LYS:CE	2.97	0.52
66:AV:333:LEU:HD21	76:AV:403:PEE:C38	2.39	0.52
1:A:281:HIS:NE2	14:O:142:LEU:O	2.38	0.52
5:F:65:LEU:HB2	5:F:79:LEU:HD11	1.92	0.52
12:M:253:VAL:HG23	12:M:345:LEU:HD22	1.91	0.52
16:Q:99:MET:HE2	16:Q:109:CYS:SG	2.49	0.52
20:V:58:GLN:O	20:V:62:THR:HG23	2.10	0.52
21:W:33:TYR:CG	21:W:34:SER:N	2.77	0.52
22:Y:73:PHE:CD1	22:Y:73:PHE:C	2.88	0.52
24:a:153:GLU:OE2	42:u:166:ARG:NH1	2.33	0.52
25:b:105:PHE:CD2	43:v:68:LYS:CB	2.93	0.52
35:l:59:GLN:HE21	35:l:59:GLN:CA	2.09	0.52
36:m:130:GLU:HG2	36:m:131:GLY:O	2.10	0.52
40:r:187:SER:O	40:r:192:ASN:ND2	2.43	0.52
42:u:111:VAL:HG12	42:u:117:TRP:O	2.09	0.52
45:x:398:PRO:O	45:x:498:CYS:HB3	2.09	0.52
46:y:100:MET:CE	46:y:157:GLU:HG3	2.40	0.52
59:AB:26:LEU:HA	59:AB:27:ARG:C	2.35	0.52
75:AJ:405:CDL:H312	75:AJ:405:CDL:OB4	2.10	0.52
60:AP:239:HIS:HB2	74:AP:301:FES:S1	2.50	0.52
12:M:645:ARG:O	12:M:648:GLU:HG2	2.10	0.52
16:Q:55:SER:OG	35:l:580:GLN:NE2	2.42	0.52
17:S:37:ARG:O	21:W:143:TYR:OH	2.27	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:56:PHE:CD1	18:T:61:LYS:HB2	2.45	0.52
26:c:69:GLY:CA	38:o:81:ARG:H	2.23	0.52
27:d:110:ARG:HH11	27:d:110:ARG:CG	2.14	0.52
35:l:190:ILE:CG1	35:l:196:TRP:NE1	2.73	0.52
40:r:20:LYS:HA	40:r:89:LEU:HD13	1.92	0.52
44:w:198:TYR:OH	44:w:304:VAL:HG12	2.10	0.52
46:y:104:TRP:CG	46:y:203:ASN:HB2	2.44	0.52
51:3:8:HIS:O	51:3:10:GLY:N	2.42	0.52
67:AK:116:ARG:NH2	67:AK:175:GLU:HG3	2.24	0.52
68:AY:96:LEU:CD2	68:AY:161:ILE:HD13	2.40	0.52
68:AY:134:LYS:NZ	68:AY:407:THR:OG1	2.42	0.52
1:A:423:THR:OG1	69:A:501:SF4:S4	2.68	0.52
72:E:201:8Q1:C30	72:E:201:8Q1:N36	2.73	0.52
10:K:77:HIS:CD2	14:O:215:LYS:HE2	2.44	0.52
14:O:152:ILE:HG21	14:O:171:LEU:HD13	1.92	0.52
16:Q:39:PRO:HB3	16:Q:43:TRP:CE3	2.45	0.52
17:S:34:LYS:NZ	42:u:90:ASP:HB3	2.25	0.52
24:a:129:PRO:HG2	27:d:60:ARG:HH22	1.75	0.52
25:b:39:LYS:HG3	25:b:41:GLY:H	1.74	0.52
25:b:105:PHE:CD2	43:v:68:LYS:HB2	2.45	0.52
32:i:336:LEU:HD21	32:i:343:MET:SD	2.50	0.52
33:j:18:MET:SD	41:s:72:ILE:HA	2.50	0.52
35:l:190:ILE:CG1	35:l:196:TRP:CD1	2.93	0.52
35:l:512:LYS:HD3	54:6:18:LEU:HD11	1.91	0.52
40:r:5:ILE:O	40:r:8:THR:OG1	2.26	0.52
41:s:13:ILE:HG23	41:s:17:MET:HE3	1.92	0.52
41:s:17:MET:CE	41:s:232:ILE:HD12	2.37	0.52
46:y:68:LEU:HB3	46:y:69:PRO:HD3	1.91	0.52
58:AA:41:ARG:NE	75:AA:101:CDL:OA4	2.35	0.52
66:AJ:191:ALA:O	66:AJ:194:THR:OG1	2.20	0.52
67:AK:146:PHE:HD2	67:AK:206:HIS:CE1	2.28	0.52
67:AK:352:LYS:HE2	67:AK:453:LEU:CB	2.40	0.52
1:A:86:ARG:NE	1:A:92:GLY:O	2.40	0.52
2:B:107:GLY:HA3	18:T:71:LEU:HD23	1.91	0.52
6:G:143:GLU:HA	6:G:146:ASP:HB3	1.92	0.52
7:H:24:LEU:HD21	7:H:81:ILE:HG22	1.92	0.52
12:M:319:TRP:HZ2	12:M:615:LEU:O	1.92	0.52
12:M:634:LEU:HD23	12:M:636:TYR:CZ	2.45	0.52
35:l:244:SER:HA	35:l:248:HIS:HD2	1.73	0.52
35:l:371:THR:O	35:l:374:THR:OG1	2.28	0.52
40:r:130:LEU:HD11	40:r:150:LEU:HD12	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:173:TRP:CZ3	41:s:262:LYS:HE2	2.45	0.52
42:u:31:HIS:CE1	42:u:111:VAL:HG11	2.44	0.52
68:AL:334:ALA:H	68:AL:336:LYS:H	1.58	0.52
68:AL:470:ARG:NH1	75:AL:502:CDL:HA31	2.25	0.52
65:AU:125:HIS:HB3	65:AU:197:LEU:HD13	1.91	0.52
66:AV:173:PRO:HB2	66:AV:177:ARG:HH12	1.74	0.52
68:AY:437:ASP:OD1	68:AY:438:ALA:N	2.43	0.52
68:AY:462:ILE:HG23	68:AY:465:LEU:HB3	1.91	0.52
12:M:61:PRO:HG2	12:M:113:ARG:HE	1.74	0.51
12:M:89:VAL:HB	12:M:94:MET:HG3	1.91	0.51
13:N:34:LYS:NZ	13:N:58:ARG:HG2	2.25	0.51
19:U:84:LEU:O	21:W:59:ARG:NH1	2.41	0.51
24:a:87:THR:CG2	71:b:201:PLX:H131	2.40	0.51
71:b:201:PLX:O3	71:b:201:PLX:H72	2.10	0.51
71:r:502:PLX:C7	71:r:502:PLX:C3	2.88	0.51
46:y:33:LEU:HD23	53:5:28:SER:HB2	1.91	0.51
65:AH:135:LEU:HA	65:AH:138:VAL:HG12	1.91	0.51
1:A:170:GLN:HE21	10:K:91:LEU:HD12	1.74	0.51
3:C:209:ILE:HG21	9:J:86:CYS:O	2.11	0.51
5:F:72:GLY:HA3	12:M:359:ASN:HB3	1.92	0.51
11:L:84:ARG:HG3	11:L:90:GLY:O	2.10	0.51
25:b:105:PHE:HZ	43:v:67:LEU:CB	2.23	0.51
33:j:70:ALA:HB1	36:m:58:ILE:HD11	1.92	0.51
35:l:332:HIS:CE1	35:l:336:LYS:HG3	2.46	0.51
35:l:567:SER:O	35:l:571:ILE:HD13	2.09	0.51
46:y:59:GLN:N	46:y:62:GLU:HG3	2.24	0.51
48:0:128:VAL:O	48:0:134:PHE:HB3	2.09	0.51
60:AC:244:ASP:OD1	60:AC:248:ARG:N	2.44	0.51
61:AD:43:ILE:O	61:AD:47:ILE:HD12	2.10	0.51
75:AJ:405:CDL:H332	75:AJ:405:CDL:OA9	2.10	0.51
60:AP:153:GLU:HB3	60:AP:273:VAL:HB	1.91	0.51
76:AU:401:PEE:H57	66:AV:236:LEU:HD13	1.92	0.51
68:AY:160:GLN:O	68:AY:164:GLU:HG2	2.09	0.51
1:A:342:LEU:O	1:A:347:THR:N	2.42	0.51
8:I:25:GLN:OE1	16:Q:254:ARG:HD3	2.10	0.51
9:J:168:SER:N	9:J:201:VAL:O	2.40	0.51
12:M:50:LEU:HA	12:M:60:ILE:HD13	1.93	0.51
12:M:464:GLN:HE22	12:M:467:LYS:HE2	1.75	0.51
16:Q:304:LYS:HE3	16:Q:316:PHE:CE1	2.46	0.51
21:W:31:SER:C	21:W:32:GLY:O	2.51	0.51
26:c:159:LYS:HA	43:v:98:ARG:NH1	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:137:ALA:HB3	32:i:138:PRO:HD3	1.93	0.51
35:l:135:ASN:OD1	35:l:198:PRO:CG	2.57	0.51
35:l:592:PHE:CE2	35:l:596:ILE:HD11	2.45	0.51
62:AE:30:LEU:HD12	62:AE:30:LEU:C	2.35	0.51
64:AG:9:ARG:HD3	63:AS:109:ALA:O	2.10	0.51
67:AK:438:MET:HB2	67:AK:450:VAL:HG11	1.89	0.51
68:AL:460:GLY:HA2	68:AL:462:ILE:HG13	1.92	0.51
60:AP:194:GLN:O	60:AP:250:ARG:NH1	2.41	0.51
66:AV:97:HIS:CE1	66:AV:100:ARG:HH21	2.27	0.51
67:AW:57:PRO:O	67:AW:127:ARG:HG3	2.11	0.51
67:AW:309:LEU:HD23	67:AW:323:VAL:HG12	1.93	0.51
68:AY:230:VAL:HG21	68:AY:418:LEU:HD11	1.92	0.51
1:A:300:ILE:HA	1:A:304:ALA:HB3	1.93	0.51
2:B:72:LEU:HA	41:s:31:MET:HE1	1.92	0.51
4:E:50:PHE:HB2	4:E:52:LEU:CD1	2.41	0.51
6:G:147:TYR:O	6:G:151:LYS:N	2.43	0.51
11:L:169:ARG:NH1	12:M:426:ASP:HA	2.25	0.51
12:M:278:HIS:CD2	12:M:280:ASP:HB2	2.44	0.51
16:Q:228:ARG:CZ	16:Q:233:HIS:HB2	2.40	0.51
20:V:12:ILE:HG22	20:V:13:PRO:O	2.11	0.51
27:d:135:ASP:C	27:d:156:ARG:HH21	2.18	0.51
34:k:7:ASN:OD1	36:m:13:VAL:HG23	2.10	0.51
35:l:226:GLN:HG2	35:l:280:LEU:HD21	1.84	0.51
35:l:227:LEU:HD12	35:l:227:LEU:C	2.35	0.51
39:p:55:LYS:N	39:p:55:LYS:CE	2.73	0.51
40:r:145:ALA:HA	40:r:148:TYR:HB3	1.91	0.51
44:w:98:THR:HG23	44:w:337:ARG:NH2	2.25	0.51
46:y:186:SER:CB	46:y:213:LEU:HD22	2.41	0.51
49:1:63:SER:O	49:1:67:ILE:HG13	2.10	0.51
63:AF:109:ALA:O	64:AT:9:ARG:HD3	2.11	0.51
75:AG:101:CDL:C54	75:AG:101:CDL:C73	2.85	0.51
75:AL:502:CDL:H772	76:AL:503:PEE:C43	2.41	0.51
61:AQ:51:LYS:O	65:AU:107:HIS:ND1	2.32	0.51
67:AW:101:ARG:NH1	68:AY:325:SER:O	2.44	0.51
1:A:62:TRP:CE2	1:A:181:LEU:HD13	2.45	0.51
12:M:430:ALA:HA	12:M:442:TYR:HB2	1.93	0.51
14:O:135:CYS:O	14:O:145:SER:OG	2.25	0.51
27:d:76:ILE:O	27:d:80:TYR:N	2.41	0.51
32:i:37:MET:HE3	32:i:41:ILE:HD11	1.93	0.51
35:l:419:THR:HA	35:l:422:TYR:CE2	2.45	0.51
36:m:27:TYR:HB3	36:m:82:TRP:CZ2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:114:VAL:O	36:m:115:VAL:HG13	2.11	0.51
42:u:142:TYR:O	42:u:144:SER:N	2.44	0.51
44:w:115:GLU:HA	44:w:118:TYR:HD2	1.76	0.51
47:z:119:THR:O	51:3:52:HIS:CE1	2.64	0.51
60:AC:183:GLU:HA	60:AC:186:GLN:HG2	1.93	0.51
76:AH:401:PEE:H17	66:AJ:240:MET:HE2	1.93	0.51
67:AK:159:LYS:HG3	67:AK:197:ILE:HG21	1.92	0.51
2:B:79:PRO:HD2	17:S:1:MET:SD	2.50	0.51
2:B:127:THR:HB	2:B:144:ASP:OD1	2.10	0.51
3:C:162:TYR:O	16:Q:123:LEU:HD21	2.10	0.51
16:Q:203:LEU:HD11	16:Q:258:LEU:HD11	1.93	0.51
6:X:77:GLU:HB2	23:Z:13:LYS:HE2	1.93	0.51
25:b:108:ASP:O	25:b:109:THR:HB	2.10	0.51
28:e:56:GLN:HG2	44:w:320:GLY:HA3	1.93	0.51
28:e:87:MET:HE1	40:r:431:THR:HG21	1.92	0.51
35:l:119:LYS:O	35:l:123:ILE:HG12	2.11	0.51
35:l:485:TYR:O	35:l:489:THR:HG23	2.10	0.51
35:l:563:PRO:HG3	40:r:148:TYR:OH	2.10	0.51
40:r:281:ASP:HB2	40:r:284:SER:OG	2.10	0.51
44:w:54:THR:C	44:w:56:ARG:H	2.19	0.51
62:AE:21:GLU:O	62:AE:24:GLU:CB	2.59	0.51
66:AV:263:ASN:OD1	66:AV:264:THR:N	2.44	0.51
68:AY:304:LEU:HD13	68:AY:354:LEU:HD11	1.93	0.51
1:A:113:LEU:HD23	1:A:113:LEU:C	2.35	0.51
1:A:126:LYS:HZ3	1:A:246:GLU:HG3	1.75	0.51
2:B:138:ARG:NH1	12:M:238:PHE:HA	2.26	0.51
3:C:112:ALA:O	3:C:113:SER:OG	2.29	0.51
4:E:19:PRO:HA	4:E:77:ARG:HD3	1.93	0.51
11:L:107:TRP:HZ3	11:L:118:ALA:HB2	1.76	0.51
24:a:160:MET:HE2	24:a:168:TRP:HB2	1.92	0.51
34:k:8:ILE:CD1	34:k:8:ILE:N	2.73	0.51
35:l:87:MET:O	35:l:91:PRO:HD3	2.11	0.51
38:o:17:THR:O	38:o:23:TYR:OH	2.21	0.51
40:r:104:ILE:O	40:r:108:MET:HG2	2.10	0.51
44:w:128:SER:OG	44:w:173:MET:SD	2.69	0.51
63:AF:43:ASP:OD2	63:AF:102:ARG:NH1	2.44	0.51
66:AJ:103:TYR:O	66:AJ:315:MET:HB2	2.10	0.51
67:AK:65:ILE:HG13	67:AK:218:MET:HG2	1.92	0.51
67:AW:107:GLY:O	68:AY:397:ASN:ND2	2.41	0.51
67:AW:214:THR:HG22	67:AW:216:ALA:H	1.75	0.51
68:AY:230:VAL:HG21	68:AY:418:LEU:HD13	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:76:ARG:HE	12:M:79:LEU:HD21	1.74	0.51
12:M:573:GLY:HA3	13:N:137:TRP:NE1	2.25	0.51
13:N:18:GLY:O	13:N:20:LEU:N	2.44	0.51
13:N:30:THR:HG21	13:N:63:VAL:HG22	1.91	0.51
15:P:168:ARG:NH1	15:P:185:ARG:HG3	2.26	0.51
16:Q:381:HIS:O	16:Q:385:TYR:HD2	1.93	0.51
18:T:83:ARG:NH1	18:T:103:LEU:H	2.08	0.51
27:d:111:GLU:HB3	27:d:115:TYR:CB	2.41	0.51
32:i:128:LEU:HD11	32:i:213:THR:HG22	1.93	0.51
35:l:593:PHE:HB2	35:l:594:PRO:HD3	1.93	0.51
41:s:154:LEU:HD13	41:s:160:PHE:CD1	2.46	0.51
45:x:184:PHE:H	45:x:256:HIS:CE1	2.29	0.51
45:x:377:PHE:HA	45:x:380:VAL:HG22	1.93	0.51
62:AE:75:LEU:HD23	62:AE:78:ARG:HD3	1.92	0.51
63:AF:63:ILE:HD13	66:AJ:211:ILE:HG21	1.93	0.51
66:AV:47:THR:HG23	66:AV:79:ILE:HG23	1.93	0.51
66:AV:141:TRP:HZ2	66:AV:260:ASN:O	1.93	0.51
66:AV:326:TRP:CH2	76:AV:403:PEE:H13	2.46	0.51
67:AW:95:SER:O	67:AW:99:ILE:HD12	2.11	0.51
67:AW:180:ALA:HA	67:AW:254:ARG:NH1	2.26	0.51
2:B:109:GLU:OE2	2:B:139:ARG:HD2	2.10	0.51
9:J:84:TYR:HB2	9:J:91:ILE:HD11	1.92	0.51
12:M:372:PHE:CD1	12:M:481:LEU:HD13	2.46	0.51
6:X:155:TYR:CD1	25:b:23:LEU:HB3	2.46	0.51
25:b:86:MET:HA	25:b:89:HIS:HB3	1.92	0.51
71:g:202:PLX:H1C2	71:g:202:PLX:H31	1.93	0.51
33:j:65:PHE:HA	33:j:68:GLU:HB2	1.93	0.51
35:l:343:SER:O	35:l:347:ILE:HD12	2.11	0.51
40:r:271:MET:O	40:r:275:ILE:HG13	2.11	0.51
41:s:223:PHE:O	41:s:227:GLU:HG3	2.11	0.51
60:AC:219:HIS:ND1	74:AC:301:FES:S1	2.74	0.51
64:AG:16:ASN:ND2	68:AL:442:ARG:HH12	2.09	0.51
67:AK:92:LYS:HD2	67:AK:143:ALA:HB1	1.93	0.51
66:AV:96:LEU:CD2	76:AV:403:PEE:H26	2.40	0.51
66:AV:151:SER:HB2	66:AV:161:VAL:HG21	1.92	0.51
68:AY:182:VAL:HG12	68:AY:186:TYR:CE2	2.46	0.51
2:B:99:HIS:HE1	2:B:150:CYS:SG	2.34	0.51
2:B:201:ALA:HB1	13:N:88:ARG:NH1	2.26	0.51
3:C:137:VAL:HA	3:C:140:GLN:CD	2.36	0.51
7:H:107:PRO:HB2	7:H:111:GLN:HB2	1.93	0.51
8:I:9:GLN:O	8:I:13:ASN:ND2	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:61:ILE:HG12	11:L:140:LYS:O	2.10	0.51
12:M:81:GLU:CD	12:M:108:LYS:HB3	2.36	0.51
12:M:532:PRO:HB2	12:M:534:VAL:HG23	1.93	0.51
13:N:40:GLY:HA3	13:N:48:TYR:HB2	1.92	0.51
17:S:24:ALA:HA	41:s:93:ASN:HD22	1.76	0.51
18:T:80:VAL:HG12	18:T:82:THR:H	1.76	0.51
19:U:58:ARG:NH2	42:u:49:GLU:OE1	2.43	0.51
71:V:203:PLX:H151	38:o:91:ALA:HB2	1.93	0.51
6:X:85:TYR:HE2	22:Y:45:ARG:NH1	2.09	0.51
25:b:19:ARG:NH2	39:p:173:ARG:HB2	2.26	0.51
25:b:92:GLU:HG2	25:b:93:LYS:HG3	1.94	0.51
25:b:113:THR:OG1	25:b:114:GLY:N	2.44	0.51
29:f:55:TRP:CE2	30:g:65:THR:HG22	2.46	0.51
31:h:99:ILE:HD12	31:h:101:LYS:HB2	1.93	0.51
32:i:234:TRP:O	32:i:238:THR:HG22	2.11	0.51
32:i:243:LEU:HD21	75:i:401:CDL:H752	1.92	0.51
32:i:268:GLU:OE2	42:u:168:TYR:OH	2.24	0.51
35:l:42:SER:O	35:l:46:ILE:HG12	2.11	0.51
46:y:1:MET:SD	46:y:133:LEU:CD1	2.99	0.51
46:y:139:ASP:OD1	46:y:140:ASN:N	2.44	0.51
64:AG:39:ARG:HB2	75:AG:101:CDL:HB31	1.93	0.51
68:AL:364:LYS:HB2	68:AL:368:MET:HE3	1.93	0.51
67:AW:288:VAL:O	67:AW:292:VAL:HG23	2.11	0.51
2:B:37:LYS:O	16:Q:320:VAL:N	2.38	0.50
2:B:113:ALA:HB1	2:B:130:ALA:HB2	1.94	0.50
7:H:111:GLN:NE2	15:P:122:ARG:HB3	2.26	0.50
9:J:142:GLU:OE2	9:J:146:VAL:HG21	2.11	0.50
9:J:178:SER:OG	9:J:181:LEU:HB3	2.11	0.50
12:M:302:LEU:HB3	12:M:585:PRO:HB3	1.93	0.50
12:M:308:ARG:HD3	12:M:314:LEU:HB3	1.92	0.50
12:M:506:VAL:HG12	12:M:508:GLY:N	2.24	0.50
22:Y:86:TYR:HB3	22:Y:87:PRO:HB3	1.93	0.50
32:i:139:ILE:HD11	32:i:187:MET:HE1	1.92	0.50
34:k:81:ILE:HG22	34:k:87:LEU:HA	1.92	0.50
39:p:104:LEU:HD21	39:p:119:PHE:CE1	2.41	0.50
40:r:144:ASN:OD1	40:r:145:ALA:N	2.45	0.50
44:w:121:PRO:HG2	44:w:178:PHE:HB3	1.93	0.50
45:x:250:GLY:O	45:x:254:ILE:HG12	2.11	0.50
45:x:347:LEU:HG	45:x:383:MET:HE3	1.93	0.50
81:AH:402:HEC:HHC	81:AH:402:HEC:HBB3	1.92	0.50
58:AN:29:HIS:ND1	58:AN:33:LYS:HB2	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:AP:242:HIS:HB2	60:AP:251:LEU:HB2	1.92	0.50
66:AV:282:ARG:NH1	66:AV:343:VAL:HG22	2.27	0.50
68:AY:412:ASP:O	68:AY:416:SER:CB	2.56	0.50
7:H:83:GLN:HG2	15:P:107:GLN:NE2	2.26	0.50
13:N:137:TRP:HH2	13:N:140:PRO:HD3	1.75	0.50
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.76	0.50
15:P:74:GLN:HB2	15:P:87:CYS:HB2	1.93	0.50
23:Z:29:LEU:HD23	39:p:35:ASP:OD1	2.12	0.50
24:a:184:LYS:O	24:a:186:THR:N	2.45	0.50
71:b:201:PLX:H21	27:d:43:ARG:HH22	1.77	0.50
30:g:29:ARG:HH21	42:u:172:LYS:HB3	1.76	0.50
31:h:80:ARG:NH1	36:m:121:VAL:HG22	2.26	0.50
35:l:15:LEU:O	35:l:18:PRO:HD2	2.11	0.50
36:m:67:PHE:O	36:m:71:THR:HG23	2.11	0.50
40:r:120:ILE:O	40:r:124:THR:HG23	2.11	0.50
40:r:134:THR:O	40:r:142:ARG:NE	2.33	0.50
40:r:423:ILE:HD12	40:r:425:ASN:H	1.75	0.50
45:x:75:ILE:O	45:x:79:GLY:HA3	2.11	0.50
45:x:232:GLN:HB2	45:x:292:MET:HE3	1.93	0.50
45:x:240:HIS:HB3	45:x:241:PRO:HD3	1.92	0.50
60:AC:197:ASP:O	60:AC:257:ASN:ND2	2.45	0.50
67:AK:183:ARG:NH2	67:AK:183:ARG:CG	2.73	0.50
68:AL:285:ALA:HB2	68:AL:461:PRO:O	2.11	0.50
58:AN:42:ILE:HG22	58:AN:46:PHE:CE2	2.47	0.50
66:AV:173:PRO:HB2	66:AV:177:ARG:NH1	2.27	0.50
1:A:63:TYR:CE2	1:A:64:LYS:HG3	2.47	0.50
1:A:87:GLY:N	1:A:93:PHE:O	2.44	0.50
5:F:30:SER:OG	5:F:63:PRO:HG3	2.11	0.50
5:F:36:PHE:HB2	5:F:84:ALA:HB1	1.92	0.50
9:J:54:ILE:HA	9:J:124:ASN:HD21	1.76	0.50
9:J:62:THR:HB	73:J:401:NDP:HO3A	1.76	0.50
12:M:151:SER:OG	16:Q:374:SER:HB2	2.11	0.50
12:M:381:LEU:C	12:M:383:SER:H	2.16	0.50
13:N:119:GLY:O	13:N:120:THR:OG1	2.27	0.50
31:h:6:ILE:HB	32:i:22:LEU:HD22	1.93	0.50
35:l:428:LEU:HD23	35:l:432:THR:HG21	1.93	0.50
45:x:40:GLU:HG2	45:x:54:TYR:CD1	2.47	0.50
60:AC:132:ALA:CB	76:AH:401:PEE:H24	2.41	0.50
63:AF:39:TYR:HD1	63:AF:40:GLU:H	1.59	0.50
67:AK:309:LEU:HD23	67:AK:323:VAL:HG12	1.92	0.50
63:AS:71:LEU:HD21	66:AV:25:SER:HB2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:AT:40:LEU:CD1	64:AT:41:ILE:N	2.56	0.50
65:AU:193:LEU:HD12	65:AU:194:PRO:HD2	1.93	0.50
66:AV:87:ALA:HB2	82:AV:401:HEM:HHB	1.92	0.50
2:B:37:LYS:HE2	8:I:110:GLN:O	2.11	0.50
2:B:108:GLU:OE1	18:T:68:ALA:HB1	2.12	0.50
12:M:213:MET:HG3	12:M:215:MET:HG3	1.93	0.50
14:O:63:ILE:HA	14:O:66:ILE:HD12	1.92	0.50
16:Q:82:LEU:N	16:Q:99:MET:O	2.41	0.50
16:Q:85:GLY:H	16:Q:88:HIS:HE2	1.58	0.50
71:V:203:PLX:H201	38:o:95:PHE:CZ	2.47	0.50
22:Y:51:THR:HG21	35:l:446:ASN:HD21	1.76	0.50
27:d:156:ARG:NH1	28:e:139:SER:O	2.37	0.50
29:f:47:THR:HG22	71:g:203:PLX:H1A1	1.94	0.50
32:i:150:ASN:HD21	35:l:602:ILE:HD13	1.76	0.50
32:i:315:TRP:HZ3	44:w:327:VAL:HG12	1.76	0.50
35:l:68:TRP:HB2	35:l:76:LEU:CD1	2.41	0.50
35:l:594:PRO:O	35:l:598:THR:HG23	2.12	0.50
38:o:6:TYR:OH	38:o:12:ARG:HG2	2.11	0.50
71:r:502:PLX:C33	71:r:502:PLX:C37	2.85	0.50
43:v:5:LEU:O	43:v:8:ARG:HG2	2.11	0.50
44:w:218:ILE:HD11	44:w:226:GLU:HB3	1.93	0.50
46:y:136:LEU:HB3	46:y:193:TYR:CD2	2.46	0.50
51:3:5:LYS:NZ	51:3:5:LYS:HB3	2.27	0.50
51:3:44:ARG:HD2	51:3:74:ARG:O	2.11	0.50
58:AA:74:ASN:N	58:AA:75:PRO:HD2	2.27	0.50
66:AJ:326:TRP:CH2	76:AJ:403:PEE:H50	2.46	0.50
68:AL:161:ILE:O	68:AL:165:ARG:HG3	2.12	0.50
65:AU:104:SER:OG	65:AU:283:ASP:OD1	2.27	0.50
68:AY:168:ILE:O	68:AY:172:MET:HG2	2.11	0.50
7:H:90:LEU:HD11	15:P:99:PHE:HD1	1.76	0.50
9:J:141:PHE:CZ	9:J:180:TYR:HB2	2.47	0.50
9:J:159:ALA:HB3	9:J:161:VAL:HG23	1.93	0.50
9:J:161:VAL:HG12	9:J:163:LYS:H	1.76	0.50
12:M:77:MET:HA	12:M:116:VAL:HG21	1.92	0.50
12:M:92:CYS:SG	74:M:803:FES:S2	3.10	0.50
12:M:307:VAL:HB	12:M:317:THR:HG21	1.93	0.50
15:P:202:PHE:HB2	15:P:203:PRO:HD2	1.92	0.50
16:Q:69:VAL:HG12	16:Q:72:PRO:CD	2.41	0.50
6:X:88:LYS:HZ1	6:X:98:LEU:HD22	1.76	0.50
22:Y:86:TYR:HB3	22:Y:87:PRO:CB	2.40	0.50
24:a:54:LEU:CD2	25:b:27:GLU:CA	2.89	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:60:ARG:NH1	27:d:60:ARG:CG	2.73	0.50
29:f:30:TYR:HD2	44:w:98:THR:HA	1.77	0.50
31:h:101:LYS:C	31:h:104:PRO:HD2	2.37	0.50
32:i:244:ILE:HB	32:i:245:PRO:HD3	1.93	0.50
32:i:309:ASN:OD1	44:w:319:ILE:HD11	2.11	0.50
35:l:44:PHE:O	35:l:47:SER:OG	2.24	0.50
35:l:136:ASN:OD1	35:l:137:LEU:N	2.44	0.50
35:l:306:THR:HA	35:l:336:LYS:NZ	2.27	0.50
37:n:50:GLN:OE1	37:n:51:PRO:HD2	2.11	0.50
39:p:170:ILE:O	39:p:173:ARG:HG3	2.11	0.50
41:s:230:ASN:O	41:s:234:MET:HG2	2.11	0.50
41:s:303:TRP:NE1	41:s:307:MET:SD	2.85	0.50
44:w:139:ARG:HD2	44:w:166:ASP:OD2	2.12	0.50
44:w:248:GLU:OE1	44:w:252:LYS:NZ	2.45	0.50
60:AC:123:VAL:HG13	61:AD:29:VAL:HG22	1.94	0.50
82:AJ:402:HEM:HBB2	82:AJ:402:HEM:HMB1	1.92	0.50
4:E:25:MET:CB	4:E:29:LYS:CE	2.59	0.50
12:M:569:GLN:NE2	12:M:622:ILE:HD12	2.26	0.50
16:Q:143:SER:HB2	16:Q:178:THR:HB	1.93	0.50
16:Q:145:MET:HB3	16:Q:227:ILE:HD12	1.92	0.50
16:Q:394:GLY:O	16:Q:413:SER:OG	2.24	0.50
28:e:112:TYR:O	40:r:45:ILE:HG23	2.11	0.50
32:i:98:ILE:O	32:i:102:MET:HG2	2.12	0.50
39:p:55:LYS:CA	39:p:55:LYS:CE	2.89	0.50
44:w:331:PHE:CZ	44:w:337:ARG:HB3	2.46	0.50
45:x:11:ASN:ND2	45:x:14:ASP:H	2.07	0.50
63:AF:71:LEU:HD23	63:AF:71:LEU:N	2.20	0.50
75:AL:502:CDL:H572	76:AL:503:PEE:C39	2.38	0.50
60:AP:160:PRO:HD2	60:AP:163:LYS:HD3	1.94	0.50
66:AV:254:ASP:O	66:AV:257:THR:OG1	2.28	0.50
1:A:118:ASP:O	1:A:159:ARG:CD	2.60	0.50
15:P:74:GLN:HB2	15:P:87:CYS:SG	2.52	0.50
35:l:49:PHE:O	35:l:52:THR:OG1	2.22	0.50
75:n:101:CDL:HB62	42:u:172:LYS:HB2	1.93	0.50
40:r:355:MET:HA	40:r:358:TRP:HD1	1.77	0.50
41:s:180:PRO:O	41:s:184:MET:HG2	2.11	0.50
48:0:64:PHE:CE1	49:1:66:ARG:HD2	2.46	0.50
62:AE:29:PRO:HD2	65:AH:262:THR:HG21	1.91	0.50
59:AO:28:PRO:HG3	67:AW:324:SER:OG	2.10	0.50
67:AW:254:ARG:HG2	67:AW:256:GLY:H	1.77	0.50
1:A:112:TYR:CD1	1:A:155:TYR:HE2	2.29	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ARG:HB3	1:A:444:PRO:HD3	1.94	0.50
2:B:36:TYR:HD2	8:I:104:TRP:HB2	1.76	0.50
2:B:74:TYR:CD2	41:s:33:LEU:HG	2.45	0.50
2:B:175:THR:HA	13:N:118:THR:HG21	1.94	0.50
4:E:50:PHE:HE1	4:E:96:VAL:HG13	1.76	0.50
9:J:268:PRO:HG3	9:J:344:PRO:HA	1.94	0.50
12:M:88:VAL:HG13	12:M:108:LYS:HE2	1.94	0.50
12:M:381:LEU:HB2	12:M:384:ASN:OD1	2.12	0.50
12:M:464:GLN:NE2	12:M:467:LYS:HE2	2.27	0.50
16:Q:65:PRO:HG2	16:Q:69:VAL:HG22	1.94	0.50
16:Q:133:LEU:HD12	16:Q:229:PRO:HD3	1.93	0.50
6:X:103:HIS:HB2	6:X:106:LYS:HB3	1.94	0.50
35:l:190:ILE:CD1	35:l:196:TRP:NE1	2.73	0.50
35:l:512:LYS:HB2	54:6:16:ASN:HB2	1.94	0.50
41:s:203:GLY:O	41:s:205:SER:N	2.43	0.50
45:x:145:LEU:HD21	47:z:32:THR:HG21	1.93	0.50
50:2:37:LYS:N	50:2:37:LYS:HD3	2.27	0.50
58:AA:28:PRO:HB2	58:AA:29:HIS:CE1	2.47	0.50
65:AH:125:HIS:HB3	65:AH:197:LEU:HD13	1.94	0.50
65:AH:323:PRO:HB2	65:AH:325:LYS:HG2	1.93	0.50
67:AK:185:ALA:HB2	67:AK:249:ALA:HB1	1.92	0.50
67:AK:299:VAL:HG13	68:AL:120:LEU:HD11	1.94	0.50
68:AL:308:ASN:HD21	68:AL:345:SER:HB3	1.77	0.50
64:AT:38:TRP:CD2	64:AT:41:ILE:HD13	2.47	0.50
1:A:152:ARG:HH12	10:K:99:PRO:HB3	1.76	0.50
6:G:112:SER:O	6:G:115:GLN:HB3	2.11	0.50
7:H:114:TRP:NE1	16:Q:394:GLY:HA2	2.25	0.50
7:H:115:PRO:O	15:P:247:GLN:NE2	2.45	0.50
9:J:206:ILE:HB	9:J:242:VAL:HG23	1.90	0.50
16:Q:87:GLN:O	16:Q:88:HIS:O	2.30	0.50
16:Q:291:VAL:N	16:Q:294:ARG:HH21	2.09	0.50
25:b:89:HIS:C	25:b:89:HIS:CD2	2.90	0.50
35:l:70:THR:HG23	35:l:75:GLN:HB3	1.94	0.50
40:r:220:HIS:HE1	40:r:232:ALA:HB2	1.77	0.50
41:s:9:LEU:HD13	41:s:95:LEU:HD12	1.94	0.50
41:s:167:THR:C	41:s:169:GLN:H	2.18	0.50
44:w:57:SER:OG	44:w:154:GLY:O	2.28	0.50
47:z:42:LEU:HD13	54:6:45:TYR:HD2	1.77	0.50
58:AA:20:SER:HB3	58:AA:23:GLU:HG2	1.94	0.50
1:A:63:TYR:HD2	1:A:256:ARG:HD2	1.76	0.49
11:L:92:ASN:HB2	15:P:239:TRP:H	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:168:LEU:HD23	12:M:292:PHE:CD2	2.46	0.49
16:Q:85:GLY:CA	33:j:39:CYS:CB	2.90	0.49
16:Q:428:GLY:HA2	16:Q:431:HIS:CD2	2.44	0.49
18:T:89:GLY:HA2	18:T:115:CYS:SG	2.52	0.49
24:a:99:ALA:O	27:d:58:TYR:HD1	1.95	0.49
25:b:33:PRO:HD2	39:p:114:MET:O	2.12	0.49
25:b:61:VAL:HA	25:b:64:VAL:HG12	1.93	0.49
26:c:55:TYR:OH	26:c:74:ASP:OD2	2.24	0.49
26:c:69:GLY:HA3	38:o:81:ARG:O	2.12	0.49
30:g:38:TYR:CE2	30:g:42:LEU:HD11	2.47	0.49
33:j:109:LYS:HA	33:j:112:ASP:HB2	1.94	0.49
35:l:74:THR:HG23	35:l:194:ASN:OD1	2.08	0.49
35:l:332:HIS:HA	35:l:335:PHE:CE2	2.46	0.49
35:l:566:ILE:HA	35:l:569:HIS:CD2	2.47	0.49
36:m:33:ILE:HA	36:m:60:LEU:HD22	1.94	0.49
43:v:39:MET:SD	43:v:58:TYR:HD1	2.34	0.49
68:AL:257:TYR:CD2	68:AL:262:VAL:HG22	2.45	0.49
60:AP:126:ALA:HA	76:AY:502:PEE:H61	1.95	0.49
61:AQ:34:ARG:NH1	61:AQ:38:GLN:HB3	2.26	0.49
65:AU:155:GLN:HA	65:AU:166:MET:HA	1.94	0.49
68:AY:164:GLU:O	68:AY:168:ILE:HG12	2.12	0.49
2:B:68:LEU:CD1	41:s:272:TRP:HE1	2.24	0.49
5:F:21:ILE:HG12	5:F:55:ILE:HG12	1.93	0.49
6:G:99:SER:OG	6:G:102:SER:OG	2.29	0.49
7:H:107:PRO:HD3	15:P:74:GLN:HE22	1.76	0.49
10:K:104:GLU:OE1	10:K:104:GLU:N	2.46	0.49
13:N:87:HIS:O	13:N:91:HIS:HD2	1.96	0.49
26:c:111:MET:HG3	40:r:278:ARG:HH12	1.77	0.49
35:l:188:TRP:CD2	35:l:212:PRO:HG3	2.48	0.49
41:s:195:ARG:HG3	41:s:197:PRO:HD2	1.93	0.49
44:w:149:HIS:HE1	44:w:155:GLN:HB3	1.76	0.49
44:w:335:PRO:HA	44:w:338:LYS:HG3	1.94	0.49
45:x:508:PRO:HG3	47:z:6:HIS:HB3	1.94	0.49
47:z:18:LEU:HD22	47:z:22:LEU:HD22	1.92	0.49
51:3:42:ARG:HD2	51:3:42:ARG:O	2.13	0.49
67:AK:299:VAL:HG22	68:AL:120:LEU:HG	1.94	0.49
62:AR:66:ASP:OD1	62:AR:67:CYS:N	2.44	0.49
63:AS:54:ASN:OD1	63:AS:55:LEU:N	2.45	0.49
64:AT:39:ARG:HG2	64:AT:39:ARG:NH2	2.19	0.49
66:AV:186:PRO:HA	66:AV:189:ILE:HD12	1.94	0.49
68:AY:119:HIS:HB2	68:AY:134:LYS:HB3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:115:PRO:HG3	16:Q:393:PRO:HB2	1.94	0.49
9:J:85:ARG:CG	9:J:85:ARG:NH1	2.72	0.49
12:M:209:TYR:O	12:M:210:ILE:HG22	2.12	0.49
12:M:385:TYR:O	12:M:517:HIS:NE2	2.43	0.49
15:P:113:ASP:OD1	16:Q:425:LYS:HD2	2.13	0.49
76:V:202:PEE:H40	76:V:202:PEE:C35	2.42	0.49
25:b:77:VAL:HB	25:b:78:PRO:HD3	1.94	0.49
30:g:4:ARG:NH1	30:g:6:ASN:HB3	2.28	0.49
32:i:9:ILE:O	32:i:12:THR:OG1	2.30	0.49
32:i:234:TRP:C	32:i:238:THR:HG22	2.37	0.49
35:l:37:LYS:HZ3	35:l:98:TRP:CD1	2.30	0.49
35:l:450:LEU:C	35:l:450:LEU:CD2	2.85	0.49
38:o:8:PRO:HD3	38:o:14:LEU:HD21	1.95	0.49
41:s:228:TYR:CD1	41:s:231:ILE:HD12	2.43	0.49
44:w:305:LEU:O	44:w:308:THR:HG22	2.12	0.49
46:y:13:THR:O	46:y:13:THR:HG22	2.12	0.49
65:AH:289:GLY:HA2	65:AH:292:MET:HG2	1.93	0.49
67:AK:239:ASN:OD1	67:AK:240:MET:N	2.45	0.49
68:AL:168:ILE:O	68:AL:172:MET:HG2	2.13	0.49
67:AW:105:ALA:HA	68:AY:390:ARG:HG3	1.94	0.49
3:C:73:TRP:HD1	3:C:76:ARG:NH2	2.10	0.49
3:C:79:LEU:HB2	3:C:108:VAL:HG12	1.95	0.49
7:H:111:GLN:HE22	15:P:122:ARG:HB3	1.77	0.49
9:J:201:VAL:HG13	9:J:265:PHE:CE2	2.47	0.49
12:M:61:PRO:HG2	12:M:113:ARG:NE	2.26	0.49
16:Q:334:VAL:O	16:Q:338:ARG:HG2	2.12	0.49
6:X:90:TYR:HD2	6:X:93:ILE:HD12	1.77	0.49
24:a:115:HIS:HE1	24:a:117:ILE:HD12	1.77	0.49
32:i:329:LEU:O	32:i:333:THR:HG23	2.11	0.49
39:p:167:TRP:CE3	39:p:171:VAL:HG21	2.32	0.49
61:AD:16:ARG:NH1	68:AL:446:SER:OG	2.42	0.49
67:AK:49:ILE:HG12	67:AK:50:ALA:N	2.26	0.49
64:AT:40:LEU:C	64:AT:40:LEU:CD1	2.85	0.49
67:AW:230:LEU:HA	67:AW:233:VAL:HG22	1.94	0.49
68:AY:296:TRP:CD1	68:AY:419:THR:CB	2.67	0.49
2:B:36:TYR:CD2	8:I:104:TRP:HB2	2.48	0.49
9:J:179:ARG:HB3	9:J:179:ARG:NH1	2.27	0.49
12:M:32:ILE:HG23	12:M:98:LYS:HB2	1.93	0.49
12:M:126:LEU:HD23	16:Q:375:MET:SD	2.52	0.49
12:M:300:GLN:HA	13:N:135:GLN:O	2.12	0.49
12:M:348:ALA:O	12:M:352:VAL:HG23	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:194:LEU:HD12	16:Q:268:TRP:CE2	2.45	0.49
16:Q:424:ILE:O	16:Q:463:ARG:NE	2.45	0.49
20:V:62:THR:HG22	20:V:104:ARG:NE	2.27	0.49
22:Y:78:GLU:HG2	35:l:385:PHE:HE1	1.78	0.49
25:b:13:GLN:O	25:b:17:GLU:HG2	2.12	0.49
30:g:27:ASP:OD1	30:g:28:PRO:HD2	2.13	0.49
32:i:232:ARG:NH2	44:w:306:ASN:OD1	2.29	0.49
33:j:28:ASN:HB2	33:j:30:TYR:CZ	2.47	0.49
35:l:189:PHE:CD1	35:l:201:MET:HE3	2.48	0.49
42:u:131:VAL:HG12	42:u:133:THR:HG23	1.95	0.49
65:AH:93:SER:HB2	65:AH:99:ARG:HH12	1.77	0.49
68:AL:75:ILE:HG21	68:AL:224:TYR:CD1	2.48	0.49
66:AV:150:LEU:HD23	66:AV:164:ILE:CD1	2.43	0.49
68:AY:75:ILE:HG12	68:AY:229:MET:SD	2.52	0.49
1:A:71:LYS:HA	1:A:147:ARG:HH21	1.77	0.49
1:A:102:MET:SD	1:A:149:MET:HB3	2.52	0.49
1:A:202:GLY:O	12:M:200:ARG:NH2	2.42	0.49
9:J:217:PHE:CZ	9:J:322:MET:CE	2.86	0.49
9:J:221:HIS:HE1	9:J:222:ARG:CG	2.20	0.49
9:J:350:ILE:HG21	9:J:366:ILE:HG12	1.95	0.49
12:M:123:ASN:HA	12:M:157:LYS:HG2	1.94	0.49
14:O:193:TYR:HB3	14:O:196:LEU:HD11	1.94	0.49
15:P:190:ASP:OD1	15:P:191:TYR:N	2.45	0.49
16:Q:323:ARG:N	16:Q:328:ASP:OD2	2.46	0.49
26:c:108:HIS:HE1	35:l:546:GLN:HG2	1.77	0.49
76:l:701:PEE:C23	40:r:155:VAL:HB	2.29	0.49
36:m:130:GLU:OE1	36:m:130:GLU:N	2.39	0.49
51:3:42:ARG:NH1	51:3:74:ARG:HH21	2.10	0.49
75:AG:101:CDL:H741	66:AV:156:ILE:CG2	2.43	0.49
65:AH:291:LYS:HD2	76:AH:401:PEE:C3	2.37	0.49
66:AJ:131:TYR:O	66:AJ:134:PRO:HD2	2.11	0.49
66:AJ:186:PRO:HA	66:AJ:189:ILE:HD12	1.94	0.49
67:AK:173:VAL:HG11	67:AK:339:TYR:HE1	1.77	0.49
61:AQ:53:TRP:NE1	65:AU:139:CYS:O	2.45	0.49
65:AU:288:MET:CG	76:AU:401:PEE:O4	2.61	0.49
66:AV:281:LEU:HD11	66:AV:294:LEU:HD22	1.94	0.49
4:E:49:GLN:HE21	4:E:96:VAL:HG21	1.78	0.49
9:J:62:THR:HB	73:J:401:NDP:O2X	2.12	0.49
9:J:209:ARG:HD2	15:P:217:LYS:HE2	1.93	0.49
12:M:64:CYS:O	12:M:184:ARG:NH2	2.46	0.49
12:M:66:HIS:HE1	12:M:68:ARG:HG2	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:711:VAL:HA	12:M:714:VAL:HG12	1.94	0.49
16:Q:360:ASP:O	16:Q:364:SER:OG	2.29	0.49
20:V:39:TYR:HD2	75:V:201:CDL:H721	1.76	0.49
21:W:101:VAL:HG21	31:h:82:GLN:NE2	2.28	0.49
22:Y:86:TYR:HH	43:v:100:LYS:HG2	1.78	0.49
30:g:29:ARG:NH2	42:u:172:LYS:HD2	2.28	0.49
34:k:60:PRO:O	34:k:63:MET:HB2	2.12	0.49
35:l:75:GLN:HG2	35:l:75:GLN:O	2.13	0.49
35:l:286:LEU:HB2	35:l:411:ILE:HG23	1.95	0.49
39:p:136:GLU:HG2	39:p:165:PRO:HA	1.94	0.49
40:r:113:THR:O	40:r:176:ILE:HG13	2.12	0.49
41:s:79:LEU:HD11	41:s:222:LEU:HD22	1.94	0.49
41:s:141:SER:HB2	41:s:290:TRP:HE1	1.77	0.49
46:y:59:GLN:O	46:y:62:GLU:HB2	2.13	0.49
66:AJ:126:THR:O	66:AJ:182:HIS:ND1	2.46	0.49
67:AK:64:PHE:CE2	67:AK:397:GLY:HA3	2.48	0.49
67:AK:305:THR:HA	67:AK:311:GLN:HE21	1.78	0.49
67:AK:378:LEU:HD13	67:AK:416:ILE:HD11	1.94	0.49
68:AL:75:ILE:HG21	68:AL:224:TYR:HD1	1.77	0.49
61:AQ:43:ILE:O	61:AQ:47:ILE:HD12	2.13	0.49
1:A:160:GLY:HA2	1:A:199:ARG:NH1	2.27	0.49
9:J:64:PHE:HE2	9:J:242:VAL:HG21	1.77	0.49
11:L:75:ARG:HH11	11:L:104:ARG:NE	2.09	0.49
16:Q:175:GLY:O	16:Q:178:THR:OG1	2.29	0.49
16:Q:358:VAL:HG12	16:Q:360:ASP:H	1.78	0.49
24:a:101:ILE:HG13	27:d:58:TYR:HB3	1.94	0.49
26:c:52:ALA:CB	26:c:59:VAL:HA	2.42	0.49
32:i:41:ILE:HD11	32:i:60:PHE:HD1	1.78	0.49
36:m:22:LYS:N	36:m:23:PRO:HD3	2.28	0.49
43:v:113:LYS:HA	43:v:116:GLU:OE1	2.13	0.49
44:w:217:ARG:HA	44:w:220:LYS:HD2	1.94	0.49
68:AL:426:LEU:HA	68:AL:429:TRP:HD1	1.78	0.49
66:AV:10:LEU:CD2	76:AY:502:PEE:C26	2.91	0.49
66:AV:286:ASN:OD1	66:AV:287:LYS:N	2.46	0.49
68:AY:294:PRO:HG3	68:AY:448:TYR:CE1	2.48	0.49
1:A:274:LYS:HB2	1:A:292:MET:SD	2.53	0.49
2:B:51:VAL:HG22	2:B:54:ARG:NH1	2.26	0.49
6:G:123:GLU:OE1	6:G:130:ILE:N	2.39	0.49
9:J:212:ARG:NH1	9:J:212:ARG:CG	2.73	0.49
12:M:610:VAL:O	12:M:611:THR:OG1	2.25	0.49
16:Q:179:ARG:HG2	16:Q:183:HIS:CD2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:V:202:PEE:H41	76:V:202:PEE:C37	2.40	0.49
6:X:76:LEU:HD12	6:X:156:GLU:HB2	1.94	0.49
35:l:51:THR:CG2	35:l:91:PRO:CG	2.84	0.49
35:l:100:ILE:HD12	35:l:246:LEU:CG	2.39	0.49
35:l:386:LEU:HD12	35:l:387:THR:N	2.28	0.49
36:m:118:PHE:HZ	36:m:124:TRP:HZ2	1.61	0.49
40:r:220:HIS:CE1	40:r:232:ALA:HB2	2.47	0.49
46:y:16:ILE:HD12	46:y:17:MET:H	1.77	0.49
58:AA:11:MET:HE2	68:AL:278:ARG:HH11	1.78	0.49
75:AJ:405:CDL:H762	75:AJ:405:CDL:H132	1.95	0.49
67:AK:116:ARG:NH1	67:AK:188:ASN:O	2.46	0.49
66:AV:254:ASP:OD2	66:AV:267:HIS:NE2	2.46	0.49
68:AY:101:THR:OG1	68:AY:149:ASP:OD1	2.31	0.49
1:A:378:SER:O	1:A:380:GLY:N	2.45	0.49
9:J:238:GLN:NE2	9:J:267:GLY:O	2.43	0.49
11:L:95:LYS:NZ	15:P:240:GLU:OE2	2.45	0.49
14:O:197:THR:H	14:O:200:ASP:HB3	1.77	0.49
26:c:111:MET:HG3	40:r:278:ARG:NH1	2.27	0.49
32:i:334:THR:OG1	32:i:335:LEU:N	2.45	0.49
34:k:81:ILE:CG2	34:k:87:LEU:HA	2.43	0.49
35:l:47:SER:O	35:l:50:PRO:HD2	2.13	0.49
50:2:49:VAL:HG21	50:2:74:LEU:HD12	1.95	0.49
66:AJ:97:HIS:HE1	66:AJ:100:ARG:HH21	1.58	0.49
68:AL:192:PHE:HB2	68:AL:198:ALA:HB2	1.95	0.49
63:AS:34:ARG:NH2	63:AS:92:GLU:OE2	2.45	0.49
66:AV:366:MET:HB3	66:AV:367:PRO:HD3	1.95	0.49
7:H:46:LYS:HE3	8:I:90:THR:OG1	2.13	0.48
12:M:136:GLU:OE1	12:M:136:GLU:N	2.46	0.48
12:M:372:PHE:CE1	12:M:481:LEU:HD13	2.48	0.48
13:N:11:LEU:HA	13:N:14:ILE:HD12	1.94	0.48
16:Q:438:MET:HE1	16:Q:454:GLN:HE22	1.78	0.48
20:V:62:THR:HG22	20:V:104:ARG:HD3	1.95	0.48
22:Y:44:TYR:HD1	35:l:440:LEU:HB2	1.78	0.48
23:Z:28:PRO:O	23:Z:31:THR:OG1	2.22	0.48
31:h:32:ARG:NH2	34:k:50:ASN:O	2.42	0.48
32:i:337:LEU:O	32:i:339:ILE:N	2.46	0.48
35:l:119:LYS:HD2	75:l:703:CDL:HB32	1.95	0.48
40:r:18:SER:OG	40:r:23:ILE:HG12	2.13	0.48
71:r:502:PLX:H52	71:r:502:PLX:P1	2.53	0.48
41:s:106:LEU:HD21	41:s:150:LEU:HD12	1.94	0.48
44:w:242:LYS:HA	44:w:246:LEU:HG	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:323:GLN:O	44:w:326:ARG:HB3	2.13	0.48
48:0:68:PHE:HA	48:0:71:MET:HG2	1.95	0.48
67:AK:259:ARG:HH12	67:AK:438:MET:CE	2.26	0.48
67:AK:438:MET:HB2	67:AK:450:VAL:HG12	1.94	0.48
68:AL:304:LEU:HD13	68:AL:354:LEU:HD11	1.95	0.48
75:AN:101:CDL:C58	76:AV:403:PEE:H52	2.42	0.48
64:AT:39:ARG:CG	64:AT:39:ARG:NH2	2.73	0.48
66:AV:195:LEU:HD22	66:AV:199:PHE:CE2	2.48	0.48
1:A:256:ARG:O	14:O:246:GLN:HB3	2.13	0.48
3:C:140:GLN:HE22	33:j:40:GLY:HA2	1.78	0.48
4:E:47:VAL:HG11	4:E:56:VAL:HG22	1.95	0.48
12:M:36:VAL:HG23	12:M:41:VAL:HG21	1.96	0.48
12:M:171:THR:HB	12:M:173:MET:HE3	1.94	0.48
17:S:50:ARG:CZ	17:S:54:ILE:HD11	2.43	0.48
19:U:58:ARG:HH12	42:u:137:LEU:N	2.10	0.48
25:b:39:LYS:O	25:b:42:PRO:HD2	2.13	0.48
30:g:38:TYR:O	30:g:42:LEU:HG	2.13	0.48
35:l:383:MET:SD	35:l:384:PRO:HD2	2.52	0.48
37:n:55:VAL:HG12	37:n:56:THR:N	2.24	0.48
43:v:41:ALA:O	43:v:42:THR:OG1	2.31	0.48
63:AF:29:LYS:NZ	63:AF:29:LYS:CB	2.73	0.48
61:AQ:27:VAL:O	61:AQ:30:MET:HB2	2.13	0.48
68:AY:187:LEU:HD11	68:AY:290:ALA:HB3	1.94	0.48
68:AY:424:ILE:HG13	68:AY:429:TRP:NE1	2.27	0.48
1:A:130:ILE:HD11	1:A:275:LEU:HD21	1.94	0.48
1:A:274:LYS:HZ2	1:A:352:ALA:HB3	1.78	0.48
9:J:93:HIS:O	9:J:96:PRO:HD2	2.14	0.48
12:M:37:ASP:OD1	12:M:38:GLY:N	2.41	0.48
12:M:200:ARG:HH21	14:O:120:THR:HG23	1.78	0.48
12:M:392:ALA:HA	12:M:417:ARG:HH22	1.78	0.48
14:O:115:VAL:O	14:O:119:TYR:HD2	1.96	0.48
21:W:141:MET:SD	36:m:47:GLY:HA2	2.53	0.48
28:e:107:ALA:O	71:r:502:PLX:H1B3	2.13	0.48
30:g:119:ARG:HD3	38:o:116:ILE:HD13	1.96	0.48
32:i:18:LEU:O	32:i:22:LEU:HG	2.14	0.48
32:i:59:TYR:CZ	32:i:63:GLN:OE1	2.67	0.48
32:i:115:VAL:HG12	32:i:180:ALA:HB1	1.95	0.48
34:k:51:THR:O	34:k:51:THR:OG1	2.28	0.48
35:l:347:ILE:HG12	35:l:354:GLN:HG2	1.96	0.48
40:r:188:ASN:CG	40:r:189:SER:H	2.21	0.48
41:s:73:THR:O	41:s:76:THR:OG1	2.19	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:109:ASN:HD21	44:w:111:ASN:HD22	1.61	0.48
44:w:335:PRO:HA	44:w:338:LYS:NZ	2.29	0.48
60:AC:136:PHE:CE2	76:AH:401:PEE:H34	2.48	0.48
65:AU:307:LYS:HE2	75:AU:403:CDL:CA3	2.43	0.48
66:AV:131:TYR:O	66:AV:134:PRO:HD2	2.13	0.48
68:AY:96:LEU:C	68:AY:96:LEU:CD1	2.86	0.48
68:AY:98:PHE:N	68:AY:98:PHE:CD1	2.79	0.48
1:A:36:LYS:HB2	1:A:39:ASP:CG	2.38	0.48
1:A:111:LYS:O	1:A:152:ARG:N	2.34	0.48
1:A:118:ASP:O	1:A:119:GLU:C	2.55	0.48
1:A:318:ILE:HD11	1:A:355:ILE:HD13	1.94	0.48
9:J:64:PHE:CE2	9:J:242:VAL:HG21	2.48	0.48
9:J:197:GLU:OE1	9:J:197:GLU:N	2.45	0.48
12:M:365:THR:HG22	12:M:537:ILE:HD11	1.95	0.48
16:Q:140:ASP:HB3	16:Q:147:ASN:ND2	2.28	0.48
17:S:53:ARG:HH21	31:h:105:ARG:HD3	1.77	0.48
20:V:29:ALA:O	20:V:63:ALA:HB1	2.14	0.48
21:W:47:HIS:O	21:W:51:MET:HG3	2.13	0.48
24:a:54:LEU:HD21	25:b:27:GLU:HA	1.91	0.48
35:l:173:LEU:HD21	40:r:405:LEU:HD21	1.96	0.48
45:x:87:ILE:O	45:x:173:PRO:HD3	2.13	0.48
45:x:168:ILE:HG21	45:x:189:MET:HG3	1.94	0.48
47:z:65:SER:HB3	47:z:71:HIS:CE1	2.49	0.48
63:AF:83:LYS:HB2	63:AF:86:GLU:HB2	1.95	0.48
66:AJ:22:PRO:HB3	66:AJ:217:LYS:HB3	1.94	0.48
67:AK:82:LEU:HD21	67:AK:151:VAL:HG13	1.94	0.48
67:AK:207:TYR:HA	67:AK:210:GLN:NE2	2.28	0.48
62:AR:34:ARG:CG	62:AR:78:ARG:NH1	2.61	0.48
66:AV:246:SER:HB3	66:AV:249:LEU:HD23	1.95	0.48
68:AY:119:HIS:HB2	68:AY:134:LYS:HD2	1.93	0.48
1:A:158:ILE:N	1:A:198:VAL:O	2.47	0.48
2:B:94:ARG:CZ	16:Q:237:PRO:HG3	2.44	0.48
9:J:152:ILE:HG22	9:J:164:PHE:HE1	1.77	0.48
9:J:360:ARG:HA	36:m:78:TYR:CZ	2.47	0.48
12:M:266:ARG:NE	12:M:271:MET:HE3	2.29	0.48
12:M:636:TYR:HB2	12:M:641:GLN:HB3	1.95	0.48
13:N:129:THR:HA	18:T:44:GLN:NE2	2.28	0.48
17:S:28:ARG:O	17:S:33:GLY:N	2.47	0.48
24:a:114:LYS:CA	27:d:57:TYR:CD2	2.97	0.48
24:a:160:MET:HE3	24:a:166:GLY:HA3	1.96	0.48
32:i:117:GLU:OE1	32:i:117:GLU:N	2.41	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:282:MET:O	32:i:286:THR:HG23	2.14	0.48
32:i:326:LEU:HB3	32:i:327:PRO:HD3	1.95	0.48
35:l:224:SER:OG	35:l:256:GLY:CA	2.59	0.48
41:s:226:ALA:O	41:s:230:ASN:ND2	2.40	0.48
44:w:139:ARG:HH12	44:w:160:GLU:CD	2.21	0.48
45:x:476:PHE:CD1	56:8:15:VAL:HG21	2.48	0.48
46:y:186:SER:HB3	46:y:213:LEU:CD2	2.42	0.48
66:AJ:223:TYR:OH	68:AL:469:ASN:ND2	2.44	0.48
64:AT:17:TRP:NE1	68:AY:382:SER:OG	2.41	0.48
65:AU:284:HIS:O	65:AU:288:MET:HG3	2.13	0.48
67:AW:384:MET:SD	68:AY:68:THR:HG21	2.54	0.48
67:AW:413:LEU:HA	67:AW:416:ILE:HG22	1.94	0.48
1:A:132:ARG:HG2	1:A:165:GLU:OE1	2.13	0.48
2:B:142:ARG:NH2	11:L:112:MET:O	2.47	0.48
4:E:128:PRO:HG3	11:L:74:THR:OG1	2.14	0.48
9:J:141:PHE:HE2	9:J:183:ASN:HD22	1.62	0.48
11:L:75:ARG:NH2	11:L:101:PHE:HB3	2.29	0.48
11:L:98:LYS:HA	11:L:126:LEU:O	2.13	0.48
12:M:124:HIS:CG	12:M:125:PRO:HD2	2.48	0.48
12:M:302:LEU:N	12:M:571:HIS:O	2.33	0.48
12:M:564:CYS:O	12:M:566:ILE:HG12	2.14	0.48
14:O:233:SER:OG	14:O:234:LEU:N	2.47	0.48
16:Q:149:GLN:HG3	16:Q:171:ARG:HD3	1.94	0.48
27:d:34:ILE:HG13	27:d:35:VAL:HG13	1.95	0.48
32:i:128:LEU:HD13	32:i:216:PHE:HD2	1.78	0.48
35:l:302:VAL:O	35:l:305:SER:OG	2.24	0.48
40:r:61:LEU:HD22	40:r:241:TYR:CD1	2.45	0.48
45:x:397:PHE:HB3	45:x:398:PRO:HD3	1.95	0.48
52:4:24:ASN:ND2	52:4:26:THR:H	2.11	0.48
63:AF:51:LEU:HD22	63:AF:55:LEU:HB3	1.96	0.48
68:AL:179:MET:O	68:AL:181:ASP:N	2.45	0.48
65:AU:315:LYS:HZ2	75:AU:403:CDL:HB22	1.77	0.48
66:AV:96:LEU:HD23	76:AV:403:PEE:C17	2.39	0.48
4:E:20:ILE:H	4:E:77:ARG:HG2	1.78	0.48
8:I:11:LEU:O	8:I:14:TRP:HB3	2.13	0.48
40:r:127:ILE:HB	40:r:128:PRO:HD3	1.94	0.48
42:u:24:VAL:HG22	42:u:86:TRP:HE1	1.76	0.48
53:5:39:VAL:O	53:5:42:LYS:HE2	2.14	0.48
66:AJ:177:ARG:NH2	60:AP:140:MET:O	2.47	0.48
65:AU:115:GLN:HA	65:AU:118:LYS:HE2	1.96	0.48
66:AV:45:ILE:HA	82:AV:401:HEM:CMC	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AY:377:MET:HE2	68:AY:477:TRP:H	1.78	0.48
3:C:106:PHE:CD1	41:s:39:VAL:HG21	2.49	0.48
4:E:52:LEU:HB3	4:E:54:ILE:HG13	1.96	0.48
7:H:35:LEU:O	7:H:45:ARG:NE	2.43	0.48
9:J:250:VAL:O	9:J:254:LYS:HG2	2.13	0.48
16:Q:124:ILE:HG22	16:Q:419:PRO:HG3	1.96	0.48
16:Q:301:ASP:OD1	16:Q:302:LEU:N	2.47	0.48
32:i:106:LEU:HB3	32:i:187:MET:HE2	1.95	0.48
33:j:54:LYS:HB3	33:j:113:TRP:NE1	2.29	0.48
35:l:213:LEU:HB3	35:l:273:ILE:HD13	1.96	0.48
40:r:1:MET:HG3	40:r:2:LEU:N	2.29	0.48
44:w:258:TYR:CE1	44:w:267:LYS:HA	2.49	0.48
46:y:4:PRO:HB2	55:7:43:SER:HA	1.96	0.48
46:y:22:HIS:CE1	53:5:44:LYS:HD3	2.49	0.48
68:AL:183:VAL:HG21	68:AL:286:HIS:HD2	1.79	0.48
68:AL:186:TYR:CD1	68:AL:275:ILE:HG21	2.48	0.48
61:AQ:56:ILE:O	61:AQ:59:LYS:HG2	2.14	0.48
1:A:370:LEU:O	1:A:373:PHE:HB3	2.14	0.48
7:H:40:LYS:HA	7:H:45:ARG:HD3	1.94	0.48
9:J:357:ARG:HG3	9:J:362:LEU:HA	1.94	0.48
12:M:262:VAL:HG23	12:M:276:ARG:HB2	1.95	0.48
14:O:207:GLU:HA	14:O:210:ALA:HB3	1.96	0.48
16:Q:201:PHE:CB	41:s:32:GLN:HG3	2.43	0.48
6:X:102:SER:O	6:X:140:CYS:HA	2.14	0.48
24:a:55:PHE:CE2	39:p:118:TYR:CG	2.82	0.48
25:b:108:ASP:CG	25:b:109:THR:H	2.20	0.48
32:i:37:MET:CE	32:i:60:PHE:HA	2.44	0.48
35:l:591:PHE:O	35:l:594:PRO:HD2	2.13	0.48
38:o:30:ARG:NE	68:AL:259:GLU:HB3	2.20	0.48
38:o:73:THR:OG1	38:o:74:ILE:N	2.47	0.48
41:s:42:PRO:HD2	41:s:45:LEU:HD12	1.95	0.48
45:x:197:LEU:O	47:z:92:LEU:HD22	2.13	0.48
46:y:90:ILE:H	46:y:90:ILE:HD12	1.77	0.48
54:6:8:LYS:HB3	54:6:8:LYS:NZ	2.28	0.48
58:AA:66:GLU:HG2	66:AJ:346:PRO:HB3	1.96	0.48
66:AJ:13:LEU:HD11	66:AV:198:LEU:HD11	1.95	0.48
66:AJ:140:PHE:O	66:AJ:144:THR:OG1	2.26	0.48
68:AL:101:THR:HA	68:AL:154:CYS:HA	1.95	0.48
68:AL:326:SER:O	68:AL:330:SER:N	2.43	0.48
60:AP:88:PHE:O	60:AP:92:ARG:HG3	2.14	0.48
62:AR:86:LEU:C	62:AR:86:LEU:CD2	2.86	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:AT:40:LEU:HD12	64:AT:41:ILE:CA	2.36	0.48
68:AY:286:HIS:ND1	68:AY:359:VAL:HG22	2.29	0.48
1:A:208:GLU:OE1	1:A:211:ALA:N	2.38	0.48
4:E:36:TYR:HD1	4:E:67:PHE:HE2	1.62	0.48
8:I:44:GLY:HA2	16:Q:355:GLU:HG3	1.95	0.48
8:I:96:THR:OG1	8:I:98:ALA:O	2.19	0.48
9:J:203:PRO:O	73:J:401:NDP:H5N	2.14	0.48
10:K:96:MET:HE3	10:K:97:PRO:HD2	1.96	0.48
19:U:52:ASN:HD21	31:h:27:TYR:C	2.20	0.48
20:V:37:ALA:HB1	20:V:56:VAL:HG22	1.95	0.48
22:Y:41:GLU:HG2	35:l:442:ASN:HB2	1.96	0.48
24:a:95:GLN:OE1	24:a:114:LYS:NZ	2.46	0.48
71:b:201:PLX:O7	71:b:201:PLX:H31	2.13	0.48
71:b:201:PLX:H171	71:b:201:PLX:H141	1.69	0.48
31:h:91:LYS:HG3	31:h:92:TYR:N	2.28	0.48
32:i:237:LEU:HD22	32:i:240:LEU:HD12	1.96	0.48
32:i:288:LEU:HD22	76:l:701:PEE:H58	1.69	0.48
35:l:500:THR:HG22	54:6:33:ARG:HD2	1.95	0.48
40:r:94:LEU:O	40:r:97:SER:OG	2.21	0.48
41:s:205:SER:OG	41:s:279:ARG:NH1	2.47	0.48
45:x:507:GLU:O	45:x:508:PRO:O	2.32	0.48
54:6:16:ASN:ND2	54:6:16:ASN:H	2.12	0.48
65:AH:96:TRP:CZ3	65:AH:208:GLU:HG3	2.49	0.48
67:AK:38:LEU:HB3	67:AK:52:LEU:HB2	1.94	0.48
67:AK:267:VAL:HG21	67:AK:447:THR:HG21	1.95	0.48
76:AL:503:PEE:H26	76:AL:503:PEE:C33	2.44	0.48
59:AO:26:LEU:HA	59:AO:27:ARG:O	2.14	0.48
62:AR:34:ARG:NH1	62:AR:78:ARG:CZ	2.76	0.48
66:AV:278:TYR:CE2	66:AV:282:ARG:HD2	2.48	0.48
2:B:52:THR:CG2	21:W:33:TYR:CE1	2.98	0.47
2:B:198:GLU:OE2	2:B:202:ASN:ND2	2.46	0.47
5:F:68:ARG:HA	5:F:74:GLU:HG2	1.95	0.47
12:M:383:SER:HA	12:M:386:LEU:HD12	1.96	0.47
16:Q:103:GLY:HA3	33:j:52:SER:HB3	1.95	0.47
20:V:40:ARG:HG3	75:V:201:CDL:HB22	1.96	0.47
75:V:201:CDL:H552	75:V:201:CDL:H522	1.70	0.47
25:b:109:THR:HG22	25:b:111:LEU:H	1.79	0.47
71:b:201:PLX:H111	71:b:201:PLX:C7	2.43	0.47
34:k:97:GLN:HG2	35:l:587:TYR:OH	2.14	0.47
35:l:19:ILE:HD11	35:l:126:ILE:HD11	1.96	0.47
47:z:173:PHE:CD1	47:z:173:PHE:C	2.92	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:3:5:LYS:HZ3	51:3:5:LYS:HB3	1.79	0.47
65:AH:249:TYR:O	65:AH:252:VAL:HG23	2.14	0.47
67:AK:425:ILE:HG22	67:AK:429:LYS:HE2	1.95	0.47
58:AN:28:PRO:HB2	58:AN:29:HIS:CD2	2.50	0.47
60:AP:138:SER:O	66:AV:74:ASN:ND2	2.44	0.47
66:AV:65:SER:O	66:AV:68:HIS:HB3	2.14	0.47
67:AW:443:ASN:OD1	67:AW:445:GLY:N	2.43	0.47
1:A:119:GLU:OE1	1:A:127:ASP:HB2	2.14	0.47
2:B:40:ASN:O	2:B:42:GLN:N	2.43	0.47
5:F:35:ASP:O	5:F:39:LYS:HG2	2.14	0.47
9:J:91:ILE:HA	9:J:93:HIS:CE1	2.49	0.47
9:J:176:SER:CA	9:J:182:ARG:NH2	2.67	0.47
12:M:704:SER:OG	12:M:706:THR:HG22	2.14	0.47
6:X:80:GLN:HG3	6:X:145:VAL:HG11	1.95	0.47
27:d:18:PRO:HG2	43:v:71:ARG:NH1	2.29	0.47
27:d:20:GLN:OE1	43:v:71:ARG:NH1	2.48	0.47
28:e:89:LEU:HD13	40:r:29:THR:HG21	1.95	0.47
33:j:67:LEU:HD23	34:k:65:VAL:HG13	1.95	0.47
40:r:44:GLN:O	40:r:46:ASN:ND2	2.47	0.47
42:u:85:TYR:OH	42:u:104:GLN:NE2	2.45	0.47
46:y:83:ILE:O	46:y:87:MET:HG3	2.14	0.47
47:z:80:ARG:O	47:z:84:ILE:HG12	2.14	0.47
58:AA:78:TYR:CD1	62:AE:64:GLU:C	2.91	0.47
66:AJ:62:ALA:O	66:AJ:65:SER:OG	2.22	0.47
75:AJ:405:CDL:OB9	75:AJ:405:CDL:HA4	2.13	0.47
68:AL:113:VAL:HG11	68:AL:120:LEU:HD23	1.95	0.47
68:AL:133:ILE:HG22	68:AL:134:LYS:H	1.79	0.47
68:AL:437:ASP:OD1	68:AL:438:ALA:N	2.44	0.47
60:AP:124:GLY:HA3	65:AU:299:LEU:HD21	1.94	0.47
67:AW:136:PHE:O	67:AW:140:VAL:HG23	2.13	0.47
1:A:99:TRP:HH2	1:A:248:VAL:HA	1.78	0.47
1:A:114:VAL:O	1:A:242:VAL:HA	2.13	0.47
3:C:95:HIS:HE1	16:Q:211:PHE:CE2	2.32	0.47
4:E:98:LYS:HG2	15:P:191:TYR:HB3	1.96	0.47
9:J:218:ALA:HB2	9:J:353:LEU:HD22	1.96	0.47
12:M:287:SER:HB3	12:M:290:THR:HG23	1.96	0.47
13:N:38:LEU:HD22	13:N:50:GLU:HB2	1.96	0.47
13:N:85:GLU:HG2	13:N:86:TRP:N	2.29	0.47
16:Q:136:PHE:CE2	16:Q:151:TYR:HB2	2.49	0.47
17:S:21:LEU:HD21	41:s:253:GLU:HA	1.96	0.47
25:b:42:PRO:HA	25:b:45:LYS:HD2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:105:PHE:CZ	43:v:67:LEU:CB	2.96	0.47
26:c:38:PRO:HG2	38:o:71:ALA:HB2	1.95	0.47
29:f:31:VAL:O	29:f:34:PRO:HD2	2.15	0.47
30:g:20:LEU:HD21	42:u:158:LEU:HB3	1.96	0.47
32:i:17:THR:HG23	32:i:137:ALA:HB2	1.96	0.47
32:i:135:LYS:O	32:i:139:ILE:HG12	2.14	0.47
32:i:149:LEU:HD23	32:i:154:LEU:HD13	1.96	0.47
32:i:198:PRO:O	32:i:201:THR:OG1	2.23	0.47
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.96	0.47
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.96	0.47
39:p:54:GLU:OE2	72:p:201:8Q1:C37	2.61	0.47
41:s:253:GLU:O	41:s:257:THR:HG23	2.13	0.47
66:AJ:47:THR:HG23	66:AJ:79:ILE:HG23	1.96	0.47
66:AJ:82:LEU:HD23	66:AJ:243:THR:HG21	1.96	0.47
67:AK:115:THR:HG23	67:AK:118:ASN:H	1.80	0.47
60:AP:236:CYS:HA	60:AP:237:PRO:HD2	1.75	0.47
61:AQ:56:ILE:HG23	61:AQ:59:LYS:HE3	1.96	0.47
63:AS:14:LEU:HA	63:AS:17:ILE:HG12	1.96	0.47
65:AU:128:ASP:OD1	65:AU:177:LYS:NZ	2.47	0.47
68:AY:294:PRO:HG3	68:AY:448:TYR:CZ	2.50	0.47
2:B:133:ARG:NH1	2:B:139:ARG:HG3	2.29	0.47
7:H:34:VAL:HG23	7:H:95:ARG:CZ	2.44	0.47
7:H:108:PRO:HG2	7:H:111:GLN:HG2	1.97	0.47
8:I:97:PRO:HG3	15:P:61:PHE:CG	2.49	0.47
9:J:41:MET:HE3	9:J:42:PRO:HD2	1.96	0.47
9:J:221:HIS:ND1	9:J:221:HIS:C	2.73	0.47
10:K:91:LEU:HA	10:K:94:PHE:HD2	1.79	0.47
12:M:360:ARG:NH1	12:M:635:PRO:HD3	2.29	0.47
16:Q:390:GLN:NE2	16:Q:417:SER:HB3	2.29	0.47
17:S:53:ARG:HB2	31:h:105:ARG:NH2	2.30	0.47
20:V:96:ALA:HA	20:V:99:LEU:HD12	1.95	0.47
24:a:114:LYS:N	27:d:57:TYR:HD2	2.12	0.47
24:a:126:TYR:OH	28:e:109:LEU:HD22	2.14	0.47
30:g:67:PHE:CE1	71:g:203:PLX:H172	2.49	0.47
31:h:18:LEU:HD21	34:k:59:MET:HE3	1.96	0.47
31:h:22:SER:HB3	31:h:37:GLU:OE1	2.13	0.47
35:l:95:PHE:C	35:l:95:PHE:HD1	2.23	0.47
39:p:157:ALA:HB2	39:p:164:PRO:N	2.30	0.47
40:r:132:ILE:O	40:r:136:TRP:HB2	2.14	0.47
45:x:266:GLU:HB2	45:x:267:PRO:HD2	1.94	0.47
64:AG:14:VAL:O	64:AG:18:VAL:HG23	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:AL:503:PEE:H16	76:AL:503:PEE:C30	2.44	0.47
60:AP:136:PHE:HB3	66:AV:50:PHE:CE2	2.49	0.47
62:AR:71:LEU:HD22	65:AU:222:PRO:HG3	1.97	0.47
65:AU:214:LEU:O	65:AU:234:ASN:ND2	2.44	0.47
67:AW:138:LEU:O	67:AW:142:THR:OG1	2.25	0.47
67:AW:157:GLN:NE2	68:AY:317:THR:O	2.45	0.47
2:B:151:ILE:HD13	3:C:159:TYR:CD2	2.50	0.47
11:L:92:ASN:O	11:L:95:LYS:HG2	2.15	0.47
11:L:115:ALA:O	15:P:228:GLN:N	2.44	0.47
11:L:121:LEU:HA	15:P:203:PRO:HB3	1.97	0.47
11:L:162:ALA:HA	11:L:168:LYS:HZ2	1.79	0.47
16:Q:194:LEU:CD1	16:Q:268:TRP:CE2	2.97	0.47
18:T:109:THR:HB	18:T:118:GLN:HB3	1.95	0.47
22:Y:50:LEU:O	22:Y:51:THR:OG1	2.27	0.47
24:a:113:TYR:C	27:d:57:TYR:HD2	2.23	0.47
26:c:156:VAL:HG12	43:v:98:ARG:CD	2.44	0.47
34:k:83:ASN:HD21	36:m:174:ASN:HA	1.78	0.47
35:l:159:TYR:HB2	40:r:416:TRP:CG	2.49	0.47
35:l:549:PRO:HG3	40:r:271:MET:HE3	1.96	0.47
41:s:65:THR:O	41:s:124:ASN:ND2	2.46	0.47
41:s:126:ASN:O	41:s:130:ILE:HG13	2.14	0.47
44:w:332:ARG:HA	44:w:332:ARG:HD3	1.61	0.47
45:x:115:SER:O	45:x:121:GLY:HA2	2.14	0.47
45:x:172:LYS:HB3	45:x:176:MET:HE2	1.96	0.47
46:y:148:MET:HE3	46:y:148:MET:HB3	1.77	0.47
47:z:164:PHE:O	47:z:168:THR:HG23	2.14	0.47
67:AK:84:ARG:HH11	67:AK:114:ALA:HB3	1.79	0.47
68:AL:376:TRP:HB3	68:AL:449:ILE:HG21	1.95	0.47
65:AU:242:ILE:HD13	65:AU:244:MET:HE2	1.95	0.47
67:AW:301:ARG:HD2	68:AY:95:HIS:CD2	2.49	0.47
68:AY:296:TRP:HB3	68:AY:349:ALA:HA	1.96	0.47
2:B:84:TYR:CE2	2:B:85:PRO:HB3	2.49	0.47
3:C:100:ARG:NH2	16:Q:208:GLU:HB3	2.18	0.47
7:H:32:LEU:HG	7:H:52:THR:HG21	1.97	0.47
10:K:89:LEU:HD13	14:O:65:ALA:HB2	1.95	0.47
12:M:236:TYR:CZ	12:M:272:ARG:HD3	2.50	0.47
16:Q:99:MET:HE1	16:Q:447:VAL:HG21	1.97	0.47
17:S:50:ARG:HD3	31:h:105:ARG:HG2	1.97	0.47
20:V:14:ASP:O	20:V:21:LYS:NZ	2.45	0.47
24:a:168:TRP:HZ2	30:g:85:ARG:HG3	1.80	0.47
26:c:184:TYR:HA	43:v:36:GLU:C	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:71:PRO:O	28:e:72:ASP:HB2	2.15	0.47
32:i:256:PRO:HG2	32:i:257:LEU:HG	1.97	0.47
32:i:319:HIS:CE1	44:w:302:PHE:CD2	3.02	0.47
32:i:319:HIS:CE1	44:w:302:PHE:HD2	2.32	0.47
35:l:95:PHE:CZ	35:l:456:ARG:HG2	2.50	0.47
35:l:194:ASN:ND2	38:o:127:LEU:HB2	2.29	0.47
46:y:78:LEU:HB2	46:y:79:PRO:CD	2.38	0.47
51:3:67:HIS:CD2	51:3:78:LEU:HD11	2.50	0.47
59:AB:34:VAL:HB	59:AB:35:PRO:HD3	1.95	0.47
61:AD:38:GLN:NE2	64:AG:47:TYR:OH	2.48	0.47
63:AF:28:ASN:O	63:AF:31:GLY:N	2.42	0.47
76:AH:401:PEE:C11	76:AH:401:PEE:C30	2.92	0.47
75:AJ:405:CDL:H341	75:AJ:405:CDL:H371	1.67	0.47
67:AK:183:ARG:NH2	67:AK:254:ARG:CB	2.78	0.47
66:AV:141:TRP:CZ2	66:AV:260:ASN:O	2.67	0.47
68:AY:322:VAL:HG12	68:AY:323:HIS:N	2.27	0.47
1:A:276:PHE:CE2	1:A:290:GLU:HB3	2.50	0.47
2:B:78:GLU:HA	17:S:1:MET:SD	2.53	0.47
2:B:138:ARG:HG2	12:M:238:PHE:CG	2.48	0.47
71:B:303:PLX:H272	41:s:280:PHE:HZ	1.79	0.47
3:C:96:MET:HG2	3:C:103:MET:HB3	1.96	0.47
8:I:69:ILE:O	8:I:71:SER:N	2.48	0.47
9:J:41:MET:HB3	9:J:42:PRO:HD2	1.97	0.47
9:J:99:ASP:O	9:J:102:GLN:HG2	2.14	0.47
9:J:220:MET:SD	9:J:223:PHE:CD2	3.08	0.47
12:M:198:THR:HG23	14:O:117:THR:HG21	1.97	0.47
12:M:303:THR:O	12:M:615:LEU:HB2	2.15	0.47
12:M:546:PHE:CE2	12:M:566:ILE:HD12	2.50	0.47
16:Q:57:GLU:HB2	35:l:580:GLN:CD	2.40	0.47
16:Q:97:LEU:HA	16:Q:110:ASP:O	2.14	0.47
16:Q:205:GLU:HG3	16:Q:209:LYS:NZ	2.29	0.47
17:S:34:LYS:HZ1	42:u:90:ASP:HB3	1.80	0.47
21:W:101:VAL:HG13	21:W:102:PRO:HD2	1.96	0.47
24:a:114:LYS:HA	27:d:57:TYR:CD2	2.50	0.47
24:a:182:SER:O	24:a:184:LYS:HG3	2.15	0.47
71:b:201:PLX:H72	71:b:201:PLX:O2	2.14	0.47
29:f:60:LYS:O	29:f:64:GLU:HG3	2.14	0.47
71:g:203:PLX:H72	71:g:203:PLX:H11	1.96	0.47
32:i:241:THR:OG1	32:i:242:PRO:HD3	2.15	0.47
75:n:101:CDL:H312	75:n:101:CDL:H341	1.56	0.47
40:r:61:LEU:O	40:r:64:PRO:HD2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:66:LEU:HA	40:r:66:LEU:HD23	1.76	0.47
41:s:231:ILE:HG23	41:s:270:PHE:HD2	1.79	0.47
45:x:195:LEU:CD2	45:x:245:ILE:HD13	2.45	0.47
48:0:33:LEU:HD22	48:0:37:GLN:HB3	1.97	0.47
50:2:31:TYR:HE1	50:2:98:HIS:HE1	1.62	0.47
59:AB:35:PRO:HB3	67:AK:320:PRO:HA	1.96	0.47
63:AF:70:ASN:HD22	66:AJ:209:LEU:HG	1.80	0.47
67:AK:64:PHE:CE1	67:AK:120:ALA:HB1	2.49	0.47
67:AK:277:VAL:HG22	67:AK:278:ALA:HA	1.96	0.47
68:AL:96:LEU:HA	68:AL:99:LYS:HG2	1.96	0.47
68:AL:373:GLN:HE22	68:AL:471:ILE:HG23	1.80	0.47
62:AR:30:LEU:HD13	62:AR:86:LEU:CD1	2.44	0.47
66:AV:14:ILE:HD11	76:AY:502:PEE:H41	1.80	0.47
67:AW:444:LEU:HD23	67:AW:447:THR:CG2	2.42	0.47
5:F:48:ASN:HD21	5:F:53:ILE:HD11	1.77	0.47
12:M:535:GLU:O	12:M:538:ARG:HG2	2.15	0.47
16:Q:281:GLU:N	16:Q:281:GLU:CD	2.73	0.47
17:S:35:GLU:HG2	17:S:35:GLU:O	2.14	0.47
21:W:48:TRP:O	21:W:51:MET:HB2	2.15	0.47
76:W:201:PEE:H28	76:W:201:PEE:H22	1.50	0.47
24:a:82:VAL:HG11	28:e:104:THR:HG21	1.96	0.47
25:b:108:ASP:CG	25:b:109:THR:N	2.73	0.47
35:l:190:ILE:CG1	35:l:196:TRP:CE2	2.96	0.47
35:l:315:VAL:O	35:l:318:GLY:N	2.48	0.47
41:s:142:TYR:CE1	41:s:289:LEU:HD21	2.49	0.47
44:w:46:GLY:HA2	44:w:51:LYS:HE3	1.97	0.47
45:x:11:ASN:ND2	45:x:13:LYS:HB2	2.28	0.47
45:x:306:THR:HB	45:x:359:ALA:O	2.15	0.47
48:0:23:PRO:HB3	49:1:70:VAL:CG2	2.45	0.47
58:AA:27:TYR:HE2	65:AH:305:THR:HG22	1.80	0.47
60:AC:207:LYS:HD3	60:AC:265:PHE:CE2	2.50	0.47
66:AV:111:GLU:O	66:AV:115:ILE:HG12	2.15	0.47
1:A:69:LEU:HD11	1:A:143:LEU:HD21	1.96	0.47
1:A:123:GLY:N	14:O:180:CYS:SG	2.72	0.47
6:G:104:PHE:CD1	6:G:108:LEU:HD22	2.49	0.47
7:H:28:TYR:HD1	7:H:52:THR:HG23	1.80	0.47
9:J:229:GLY:HA2	9:J:293:LEU:O	2.15	0.47
12:M:69:LEU:HD22	12:M:181:ARG:HG3	1.95	0.47
15:P:186:ARG:NH2	15:P:193:PHE:HB3	2.30	0.47
16:Q:46:GLN:NE2	76:l:701:PEE:H11	2.29	0.47
16:Q:57:GLU:HB2	35:l:580:GLN:NE2	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:338:ARG:NH1	21:W:23:ARG:HB3	2.29	0.47
22:Y:88:ASP:N	22:Y:89:PRO:CD	2.78	0.47
26:c:159:LYS:CA	43:v:98:ARG:HH12	2.27	0.47
27:d:141:GLY:HA3	30:g:118:ILE:HD12	1.97	0.47
32:i:274:ASN:O	32:i:275:SER:OG	2.30	0.47
40:r:130:LEU:O	40:r:134:THR:OG1	2.25	0.47
58:AA:78:TYR:CE1	62:AE:65:GLU:CA	2.87	0.47
63:AF:45:LYS:HZ2	63:AF:45:LYS:HB3	1.80	0.47
66:AJ:138:MET:HE1	66:AJ:268:ILE:HA	1.97	0.47
59:AO:11:PHE:H	59:AO:27:ARG:CZ	2.27	0.47
75:AU:403:CDL:HB62	75:AU:403:CDL:H732	1.96	0.47
2:B:91:LEU:HG	16:Q:215:GLU:OE2	2.15	0.47
2:B:160:CYS:O	16:Q:368:ARG:NH1	2.41	0.47
9:J:238:GLN:HG3	9:J:269:SER:O	2.15	0.47
9:J:281:PHE:HA	9:J:284:ALA:HB3	1.97	0.47
9:J:365:GLU:N	9:J:365:GLU:OE1	2.45	0.47
11:L:77:VAL:HG22	11:L:78:ARG:H	1.80	0.47
14:O:54:ASP:OD1	14:O:55:PHE:N	2.47	0.47
15:P:201:ASP:OD1	15:P:202:PHE:N	2.48	0.47
17:S:4:GLU:O	17:S:7:PRO:HD2	2.15	0.47
6:X:82:ARG:O	6:X:86:VAL:HG23	2.15	0.47
33:j:3:PHE:O	33:j:6:ILE:HB	2.14	0.47
35:l:140:LEU:O	35:l:144:TRP:HB2	2.15	0.47
35:l:189:PHE:CG	35:l:201:MET:HE3	2.50	0.47
35:l:527:GLY:C	35:l:529:TYR:H	2.22	0.47
35:l:548:LEU:HB2	35:l:549:PRO:HD3	1.95	0.47
40:r:58:SER:HB2	40:r:63:THR:HG22	1.97	0.47
40:r:80:SER:HB3	40:r:226:ALA:HB2	1.97	0.47
76:AH:401:PEE:C11	76:AH:401:PEE:C31	2.93	0.47
66:AJ:221:HIS:HB3	66:AJ:222:PRO:HD3	1.97	0.47
68:AL:164:GLU:O	68:AL:168:ILE:HG12	2.14	0.47
60:AP:177:ARG:HB3	60:AP:211:VAL:HG13	1.97	0.47
63:AS:44:VAL:O	63:AS:48:ILE:HG12	2.14	0.47
64:AT:24:TRP:CH2	75:AY:501:CDL:H551	2.50	0.47
65:AU:262:THR:HG22	65:AU:264:SER:H	1.78	0.47
66:AV:129:MET:HE1	66:AV:185:LEU:HD12	1.97	0.47
67:AW:450:VAL:HA	67:AW:453:LEU:HD13	1.94	0.47
16:Q:71:PRO:N	16:Q:72:PRO:CD	2.78	0.46
16:Q:113:ILE:HG12	16:Q:114:GLY:H	1.80	0.46
16:Q:408:GLY:HA3	16:Q:425:LYS:HB3	1.97	0.46
22:Y:74:TRP:CE3	22:Y:75:HIS:CA	2.91	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:b:201:PLX:C3	71:b:201:PLX:C1C	2.86	0.46
26:c:163:TYR:OH	43:v:42:THR:O	2.11	0.46
29:f:28:LYS:HE2	44:w:100:ASP:HA	1.97	0.46
46:y:63:THR:O	46:y:66:THR:HG22	2.15	0.46
46:y:108:TYR:N	46:y:108:TYR:CD1	2.83	0.46
48:0:79:LYS:HZ3	55:7:15:ASN:HD21	1.63	0.46
60:AC:164:ASN:HD21	60:AC:175:PHE:HB3	1.80	0.46
66:AJ:97:HIS:CE1	66:AJ:100:ARG:HH21	2.32	0.46
59:AO:43:LEU:HD11	68:AY:179:MET:HG3	1.97	0.46
60:AP:199:GLN:NE2	60:AP:204:ARG:HG2	2.29	0.46
64:AT:9:ARG:HH22	71:AT:101:PLX:H1A1	1.79	0.46
65:AU:131:ALA:HA	65:AU:174:TYR:HA	1.97	0.46
2:B:40:ASN:C	2:B:42:GLN:H	2.21	0.46
3:C:147:VAL:CG2	3:C:176:VAL:HA	2.46	0.46
9:J:141:PHE:CE2	9:J:183:ASN:ND2	2.83	0.46
12:M:616:ALA:O	12:M:617:ARG:NH1	2.44	0.46
14:O:138:THR:OG1	14:O:139:PRO:HD3	2.15	0.46
14:O:182:ASN:HD21	14:O:218:PRO:HB3	1.79	0.46
16:Q:156:GLU:OE2	16:Q:163:PRO:HG3	2.15	0.46
17:S:53:ARG:HB2	31:h:105:ARG:HH22	1.80	0.46
21:W:77:ALA:O	21:W:80:ASP:HB3	2.16	0.46
24:a:168:TRP:CZ2	30:g:85:ARG:HG3	2.50	0.46
29:f:28:LYS:HB3	29:f:31:VAL:HB	1.96	0.46
34:k:12:PHE:O	34:k:15:SER:OG	2.25	0.46
37:n:34:ARG:CZ	75:n:101:CDL:HB22	2.45	0.46
40:r:63:THR:OG1	40:r:64:PRO:HD3	2.15	0.46
41:s:236:THR:HG22	41:s:263:THR:HG21	1.96	0.46
43:v:104:ARG:O	43:v:108:LEU:HG	2.15	0.46
45:x:435:GLY:O	45:x:437:PRO:HD3	2.16	0.46
64:AG:16:ASN:CG	68:AL:442:ARG:HH12	2.23	0.46
65:AH:133:ARG:O	65:AH:135:LEU:N	2.37	0.46
66:AJ:171:ASP:CG	66:AJ:172:SER:H	2.23	0.46
62:AR:62:HIS:ND1	62:AR:62:HIS:O	2.48	0.46
66:AV:343:VAL:CG1	66:AV:348:THR:HG22	2.46	0.46
68:AY:377:MET:HE1	68:AY:450:TYR:CE1	2.51	0.46
1:A:119:GLU:O	1:A:159:ARG:NH1	2.45	0.46
1:A:275:LEU:HA	1:A:289:GLU:HA	1.97	0.46
1:A:311:TRP:CD1	1:A:314:LEU:HD12	2.50	0.46
2:B:94:ARG:NH2	16:Q:237:PRO:HG3	2.30	0.46
3:C:106:PHE:CE2	3:C:191:LEU:HD11	2.51	0.46
6:G:84:LEU:HD23	6:G:87:LEU:HD12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:620:TRP:NE1	12:M:639:LEU:HD13	2.30	0.46
12:M:645:ARG:HG3	12:M:648:GLU:OE2	2.16	0.46
14:O:200:ASP:O	14:O:204:ILE:HG12	2.16	0.46
16:Q:159:LEU:O	16:Q:161:ILE:HG13	2.16	0.46
16:Q:241:MET:HE3	21:W:16:TYR:OH	2.15	0.46
17:S:47:LEU:HA	17:S:50:ARG:HB3	1.98	0.46
25:b:106:PRO:HG2	25:b:118:PRO:HD3	1.96	0.46
25:b:111:LEU:HB2	25:b:112:GLU:OE1	2.14	0.46
27:d:120:ILE:O	27:d:123:VAL:N	2.48	0.46
27:d:133:TYR:O	27:d:136:ARG:N	2.48	0.46
30:g:33:ILE:HG22	30:g:67:PHE:HB3	1.97	0.46
32:i:332:LEU:HD22	32:i:336:LEU:HD12	1.97	0.46
40:r:35:SER:O	40:r:38:PRO:HD2	2.15	0.46
40:r:73:LEU:HB3	40:r:74:PRO:HD3	1.97	0.46
58:AA:16:SER:HA	65:AH:319:LEU:HA	1.98	0.46
65:AH:321:TYR:CD2	65:AH:323:PRO:HD3	2.51	0.46
67:AK:214:THR:HG22	67:AK:216:ALA:H	1.80	0.46
67:AK:305:THR:HA	67:AK:311:GLN:NE2	2.30	0.46
76:AL:503:PEE:H49	76:AL:503:PEE:C17	2.44	0.46
63:AS:55:LEU:HD11	63:AS:90:TYR:HB2	1.97	0.46
1:A:177:TYR:CE2	10:K:91:LEU:HD13	2.50	0.46
1:A:203:ALA:HB2	14:O:119:TYR:CE1	2.49	0.46
3:C:59:ARG:HH22	3:C:61:GLU:CB	2.25	0.46
9:J:168:SER:HA	9:J:184:LYS:HE3	1.97	0.46
11:L:109:ASN:OD1	11:L:110:PRO:HD2	2.16	0.46
12:M:292:PHE:HB3	12:M:706:THR:HG21	1.96	0.46
15:P:124:ASN:HB3	15:P:146:TYR:HB2	1.98	0.46
16:Q:97:LEU:HD12	16:Q:97:LEU:O	2.15	0.46
16:Q:131:GLN:O	16:Q:134:PRO:HD2	2.16	0.46
20:V:121:ALA:O	20:V:125:VAL:HG23	2.16	0.46
24:a:170:TYR:HE2	24:a:172:GLU:HG2	1.80	0.46
27:d:120:ILE:O	27:d:121:LYS:C	2.57	0.46
29:f:55:TRP:CZ2	30:g:65:THR:HG22	2.51	0.46
34:k:2:PRO:CG	36:m:115:VAL:CG2	2.84	0.46
35:l:100:ILE:CD1	35:l:246:LEU:HG	2.40	0.46
35:l:512:LYS:HD3	54:6:18:LEU:HD12	1.97	0.46
35:l:559:GLU:O	35:l:564:LYS:HG2	2.15	0.46
36:m:10:VAL:O	36:m:14:MET:HG2	2.16	0.46
37:n:42:SER:O	37:n:46:LYS:HB2	2.16	0.46
75:n:101:CDL:H342	75:n:101:CDL:HA62	1.97	0.46
40:r:367:LEU:HD13	40:r:404:ALA:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:294:LEU:HB3	41:s:295:PRO:HD3	1.97	0.46
45:x:273:MET:HG3	45:x:319:LYS:NZ	2.31	0.46
48:0:102:TYR:CD2	57:9:35:TYR:HE1	2.33	0.46
54:6:11:LEU:HD23	54:6:11:LEU:O	2.15	0.46
65:AH:296:MET:HE3	66:AJ:237:LEU:HA	1.96	0.46
1:A:89:GLY:HA2	1:A:244:ASN:ND2	2.28	0.46
6:G:77:GLU:OE1	6:G:77:GLU:N	2.38	0.46
9:J:299:ARG:HE	9:J:316:ARG:HH11	1.62	0.46
11:L:69:GLU:HB2	11:L:73:LYS:NZ	2.30	0.46
12:M:68:ARG:NH2	12:M:284:GLU:OE1	2.33	0.46
12:M:299:ARG:O	12:M:301:ARG:HG2	2.15	0.46
16:Q:412:VAL:O	16:Q:420:TYR:N	2.43	0.46
24:a:66:ARG:NH1	28:e:74:HIS:NE2	2.63	0.46
25:b:105:PHE:CD2	43:v:68:LYS:CA	2.98	0.46
27:d:65:VAL:HG11	27:d:81:GLU:HB3	1.96	0.46
27:d:121:LYS:O	27:d:125:GLN:HG3	2.15	0.46
71:g:202:PLX:H101	71:g:202:PLX:H132	1.45	0.46
33:j:56:PHE:CE1	36:m:70:THR:HG21	2.51	0.46
33:j:62:PHE:CG	41:s:140:ILE:HG23	2.50	0.46
35:l:32:TYR:HB3	35:l:33:PRO:HD3	1.96	0.46
35:l:512:LYS:HG3	54:6:16:ASN:HB2	1.95	0.46
44:w:270:VAL:O	44:w:275:TYR:N	2.47	0.46
48:0:33:LEU:HD13	48:0:41:LYS:HG3	1.97	0.46
76:AJ:403:PEE:H61	76:AJ:403:PEE:C17	2.42	0.46
68:AL:101:THR:HA	68:AL:155:SER:H	1.81	0.46
68:AL:166:ASP:OD1	68:AL:167:VAL:N	2.49	0.46
63:AS:35:ASP:O	63:AS:38:ILE:HG22	2.15	0.46
1:A:86:ARG:HB3	1:A:92:GLY:O	2.16	0.46
2:B:151:ILE:HD13	3:C:159:TYR:CE2	2.51	0.46
2:B:192:GLY:O	2:B:196:GLU:HB2	2.15	0.46
5:F:14:LEU:N	5:F:17:ARG:HH22	2.13	0.46
7:H:36:GLU:HA	7:H:45:ARG:NH2	2.19	0.46
14:O:78:ALA:O	14:O:82:VAL:HG23	2.15	0.46
15:P:64:TYR:CE2	15:P:68:ILE:HD11	2.50	0.46
16:Q:216:ARG:HE	16:Q:240:LEU:HD23	1.80	0.46
23:Z:49:GLU:OE2	39:p:38:ARG:NH2	2.33	0.46
24:a:187:PRO:HB3	42:u:47:ARG:HG3	1.96	0.46
25:b:38:GLN:OE1	25:b:38:GLN:HA	2.14	0.46
25:b:111:LEU:HB2	25:b:112:GLU:CD	2.41	0.46
26:c:44:THR:HB	26:c:47:GLU:HG2	1.97	0.46
26:c:168:LEU:HD12	26:c:169:GLU:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:32:TYR:HB2	75:n:101:CDL:H732	1.97	0.46
32:i:39:ALA:O	32:i:42:PRO:HD2	2.16	0.46
35:l:211:THR:HG21	75:l:704:CDL:HA4	1.96	0.46
36:m:19:PHE:HB3	36:m:31:VAL:HB	1.98	0.46
37:n:34:ARG:HH22	75:n:101:CDL:PA1	2.38	0.46
38:o:52:ASN:HD22	39:p:166:LEU:HG	1.81	0.46
38:o:52:ASN:O	39:p:129:ARG:NH2	2.49	0.46
45:x:484:THR:HB	57:9:2:THR:OG1	2.15	0.46
48:0:41:LYS:HD3	48:0:62:LEU:HD23	1.97	0.46
59:AB:11:PHE:CD1	59:AB:24:GLY:HA3	2.50	0.46
67:AK:370:ASP:OD1	67:AK:371:VAL:N	2.49	0.46
68:AL:332:ALA:O	68:AL:337:LEU:N	2.43	0.46
59:AO:11:PHE:CD1	59:AO:27:ARG:HD2	2.51	0.46
60:AP:136:PHE:HD1	66:AV:50:PHE:HD2	1.62	0.46
62:AR:75:LEU:HD23	62:AR:75:LEU:HA	1.80	0.46
67:AW:152:ALA:HA	67:AW:155:GLN:HG2	1.98	0.46
67:AW:298:HIS:HE1	67:AW:377:LYS:HG2	1.81	0.46
67:AW:306:THR:OG1	68:AY:111:LYS:NZ	2.45	0.46
4:E:62:LYS:HE3	4:E:66:MET:HE2	1.98	0.46
8:I:33:LYS:NZ	8:I:36:GLN:HA	2.30	0.46
9:J:207:PHE:CE2	9:J:348:LYS:HB2	2.49	0.46
11:L:107:TRP:O	11:L:116:SER:HB2	2.16	0.46
13:N:49:TYR:HD2	13:N:61:TRP:CZ3	2.33	0.46
13:N:83:PRO:HG2	13:N:86:TRP:HB2	1.98	0.46
14:O:84:ASP:O	14:O:88:ARG:N	2.47	0.46
15:P:83:GLU:HB3	15:P:142:ARG:NH1	2.29	0.46
16:Q:205:GLU:O	16:Q:209:LYS:HG3	2.16	0.46
16:Q:255:LEU:HD11	16:Q:337:MET:HG2	1.98	0.46
16:Q:315:GLU:HB2	16:Q:346:GLN:HE22	1.80	0.46
17:S:38:VAL:HG21	42:u:94:GLN:HG2	1.97	0.46
17:S:43:TYR:CZ	21:W:68:ARG:HD2	2.51	0.46
26:c:123:PRO:HG3	39:p:75:GLN:NE2	2.25	0.46
34:k:37:MET:HE1	34:k:63:MET:HE3	1.97	0.46
35:l:79:SER:OG	35:l:135:ASN:HB3	2.16	0.46
35:l:370:SER:O	35:l:374:THR:HG23	2.16	0.46
40:r:267:TRP:O	40:r:271:MET:HG2	2.15	0.46
41:s:7:LEU:HD23	41:s:7:LEU:HA	1.78	0.46
41:s:248:ASP:OD1	41:s:249:ALA:N	2.49	0.46
44:w:86:PHE:CE2	44:w:157:VAL:HG11	2.50	0.46
44:w:91:ILE:HG23	44:w:134:TRP:CD1	2.51	0.46
44:w:137:SER:C	44:w:139:ARG:H	2.18	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:2:40:SER:OG	50:2:45:ASP:HB3	2.16	0.46
58:AA:74:ASN:OD1	58:AA:78:TYR:HE2	1.99	0.46
76:AL:503:PEE:H49	76:AL:503:PEE:H16	1.95	0.46
60:AP:181:GLN:HA	60:AP:184:ILE:HD12	1.98	0.46
61:AQ:14:LEU:O	61:AQ:20:THR:OG1	2.33	0.46
3:C:81:PRO:HA	3:C:119:VAL:O	2.15	0.46
5:F:36:PHE:CE1	5:F:40:ARG:HB2	2.51	0.46
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.51	0.46
12:M:457:SER:O	12:M:499:LYS:NZ	2.49	0.46
21:W:115:ARG:NH1	31:h:36:PHE:HD1	2.08	0.46
22:Y:89:PRO:O	43:v:107:ARG:NH1	2.49	0.46
23:Z:31:THR:O	23:Z:34:LYS:HB3	2.16	0.46
25:b:89:HIS:CE1	25:b:97:ILE:HG13	2.51	0.46
25:b:104:ILE:HB	43:v:48:ASP:HB3	1.98	0.46
25:b:106:PRO:HA	25:b:115:GLU:CD	2.41	0.46
25:b:112:GLU:N	25:b:112:GLU:CD	2.74	0.46
28:e:113:ARG:HH21	40:r:459:SER:HB2	1.80	0.46
32:i:92:GLN:O	32:i:95:SER:OG	2.21	0.46
32:i:146:SER:O	32:i:149:LEU:HD13	2.16	0.46
32:i:335:LEU:O	32:i:338:PRO:HD2	2.16	0.46
32:i:339:ILE:HG22	32:i:342:PHE:CB	2.42	0.46
35:l:306:THR:HA	35:l:336:LYS:HZ3	1.79	0.46
35:l:367:PRO:O	35:l:371:THR:HG23	2.16	0.46
44:w:212:PRO:O	44:w:215:GLN:HB2	2.14	0.46
45:x:147:ILE:HD11	45:x:209:LEU:HD23	1.98	0.46
48:0:108:PRO:HG2	48:0:111:PHE:CD2	2.50	0.46
62:AE:74:PHE:CZ	62:AE:78:ARG:HD2	2.51	0.46
66:AJ:246:SER:HB3	66:AJ:249:LEU:HD23	1.98	0.46
68:AL:125:THR:HG22	68:AL:126:ARG:H	1.81	0.46
58:AN:67:PHE:CB	66:AV:346:PRO:HG3	2.42	0.46
63:AS:93:PRO:O	63:AS:97:GLU:HG2	2.15	0.46
66:AV:171:ASP:CG	66:AV:172:SER:H	2.23	0.46
1:A:174:ARG:HB2	10:K:91:LEU:HD11	1.96	0.46
1:A:369:ARG:NH2	14:O:175:GLU:OE2	2.33	0.46
4:E:40:TYR:CE1	4:E:60:ARG:HD3	2.51	0.46
9:J:220:MET:O	9:J:223:PHE:HB2	2.16	0.46
9:J:311:GLU:HA	9:J:312:PRO:HD3	1.79	0.46
11:L:78:ARG:HA	11:L:146:ASP:OD1	2.16	0.46
12:M:589:TYR:CE2	12:M:590:THR:HG23	2.50	0.46
14:O:236:GLU:C	14:O:238:PRO:HD2	2.41	0.46
16:Q:446:ASP:O	16:Q:450:ILE:HG13	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:V:203:PLX:H221	38:o:95:PHE:CE1	2.51	0.46
32:i:291:TYR:CZ	76:l:701:PEE:C31	2.71	0.46
33:j:86:LEU:HD21	36:m:150:ARG:HD3	1.96	0.46
35:l:369:THR:O	35:l:372:SER:OG	2.27	0.46
39:p:51:HIS:O	72:p:201:8Q1:C38	2.64	0.46
40:r:1:MET:HE1	40:r:53:SER:HB3	1.98	0.46
40:r:405:LEU:HA	40:r:405:LEU:HD23	1.73	0.46
45:x:449:MET:HE3	55:7:40:TRP:HB3	1.98	0.46
46:y:1:MET:SD	46:y:133:LEU:HD11	2.56	0.46
46:y:76:ILE:O	46:y:79:PRO:HD2	2.16	0.46
58:AA:12:ARG:NH1	68:AL:279:ASP:OD1	2.49	0.46
76:AH:401:PEE:C30	76:AH:401:PEE:C10	2.93	0.46
67:AK:178:HIS:HE1	67:AK:330:TYR:CE2	2.34	0.46
67:AK:277:VAL:HG11	67:AK:329:SER:HA	1.97	0.46
60:AP:136:PHE:HB3	66:AV:50:PHE:HE2	1.81	0.46
60:AP:167:PHE:HB2	60:AP:174:LEU:HB3	1.97	0.46
67:AW:259:ARG:NH1	67:AW:449:PHE:CZ	2.83	0.46
68:AY:148:GLY:O	68:AY:152:GLN:N	2.43	0.46
1:A:392:MET:O	1:A:396:MET:HG2	2.16	0.46
7:H:35:LEU:HA	7:H:38:ILE:HD12	1.96	0.46
12:M:164:ASN:OD1	12:M:165:ILE:N	2.49	0.46
12:M:692:LYS:HG3	12:M:714:VAL:HG13	1.98	0.46
14:O:58:GLU:O	14:O:62:ARG:HG3	2.15	0.46
25:b:109:THR:HA	27:d:18:PRO:HA	1.97	0.46
26:c:101:TRP:CD1	38:o:62:ASN:ND2	2.84	0.46
26:c:153:TYR:HB3	35:l:403:TYR:CD1	2.48	0.46
29:f:47:THR:OG1	29:f:48:LEU:N	2.48	0.46
29:f:47:THR:O	29:f:51:THR:HG23	2.16	0.46
35:l:302:VAL:O	35:l:306:THR:HG23	2.16	0.46
35:l:587:TYR:O	35:l:590:SER:OG	2.27	0.46
36:m:118:PHE:HD1	36:m:121:VAL:HB	1.79	0.46
40:r:339:SER:O	40:r:340:ARG:HB2	2.16	0.46
42:u:25:LEU:O	42:u:29:ALA:HB2	2.15	0.46
44:w:124:ASN:O	44:w:126:GLY:N	2.41	0.46
46:y:185:MET:SD	46:y:185:MET:C	2.98	0.46
48:0:66:GLU:O	49:1:66:ARG:NH2	2.49	0.46
57:9:1:ILE:HG23	57:9:1:ILE:O	2.15	0.46
66:AJ:300:ILE:H	66:AJ:300:ILE:HG13	1.57	0.46
66:AV:24:PRO:HD2	66:AV:27:ILE:HD11	1.97	0.46
67:AW:63:LEU:HD21	67:AW:218:MET:HE3	1.96	0.46
1:A:128:ARG:O	1:A:132:ARG:HG3	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:ARG:HD3	12:M:130:ILE:HG22	1.98	0.45
6:G:133:ILE:O	6:G:136:GLU:HB2	2.15	0.45
9:J:220:MET:SD	9:J:223:PHE:HD2	2.39	0.45
14:O:218:PRO:HG2	14:O:222:ARG:O	2.16	0.45
18:T:68:ALA:O	18:T:72:ILE:HG13	2.16	0.45
6:X:132:ASP:HA	6:X:135:ALA:HB3	1.97	0.45
6:X:140:CYS:HB2	6:X:143:GLU:CD	2.41	0.45
22:Y:42:PRO:HD2	23:Z:14:MET:HG3	1.98	0.45
26:c:41:TYR:CE1	26:c:67:ASP:HB3	2.51	0.45
26:c:174:PRO:O	26:c:175:SER:OG	2.26	0.45
27:d:43:ARG:O	27:d:47:GLU:HG2	2.15	0.45
30:g:48:ARG:O	30:g:50:ARG:HG3	2.16	0.45
71:g:202:PLX:H1B3	71:g:202:PLX:H22	1.58	0.45
35:l:319:ILE:HG22	35:l:319:ILE:O	2.17	0.45
35:l:512:LYS:CB	54:6:16:ASN:HB2	2.46	0.45
76:l:701:PEE:H33	76:l:701:PEE:H27	1.62	0.45
36:m:109:TYR:O	36:m:112:VAL:HG23	2.16	0.45
37:n:50:GLN:CG	37:n:51:PRO:HD2	2.46	0.45
43:v:60:ALA:O	43:v:61:HIS:C	2.59	0.45
43:v:62:HIS:CD2	43:v:90:CYS:HG	2.33	0.45
60:AC:164:ASN:HB3	60:AC:226:ALA:HB1	1.98	0.45
65:AH:291:LYS:CD	76:AH:401:PEE:H8	2.42	0.45
67:AK:57:PRO:HG2	68:AL:400:VAL:CG1	2.47	0.45
68:AL:70:THR:OG1	68:AL:410:CYS:SG	2.50	0.45
58:AN:41:ARG:HH21	75:AN:101:CDL:H1	1.81	0.45
67:AW:38:LEU:HD21	67:AW:406:TYR:CD1	2.51	0.45
1:A:116:ASN:HD21	70:A:502:FMN:C8	2.22	0.45
1:A:321:GLY:HA2	1:A:353:ALA:HB3	1.97	0.45
12:M:64:CYS:SG	12:M:75:CYS:HB3	2.55	0.45
12:M:323:LEU:HG	12:M:629:ILE:HD12	1.98	0.45
16:Q:94:VAL:HG21	16:Q:458:PHE:HB2	1.99	0.45
17:S:16:LEU:O	17:S:19:PRO:HD2	2.16	0.45
25:b:88:TYR:CG	71:b:201:PLX:H1C2	2.51	0.45
27:d:20:GLN:NE2	35:l:57:LEU:HD21	2.30	0.45
29:f:32:ARG:O	29:f:35:PRO:HD2	2.16	0.45
30:g:32:TYR:CD2	32:i:339:ILE:HD11	2.51	0.45
32:i:46:LYS:O	32:i:47:LYS:HB2	2.16	0.45
32:i:102:MET:HE3	32:i:138:PRO:HB3	1.98	0.45
35:l:508:THR:O	39:p:36:LYS:NZ	2.30	0.45
38:o:17:THR:HG21	39:p:22:ARG:HH12	1.82	0.45
60:AC:135:GLN:HG3	66:AJ:75:TYR:CD2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AF:34:ARG:HH11	66:AJ:379:TRP:HE1	1.60	0.45
66:AJ:362:ILE:HG13	66:AJ:363:LEU:HD12	1.98	0.45
58:AN:67:PHE:HD1	66:AV:344:SER:HG	1.61	0.45
60:AP:150:ALA:C	60:AP:152:ILE:H	2.24	0.45
60:AP:159:ILE:HA	60:AP:160:PRO:HD3	1.76	0.45
65:AU:204:ARG:HE	81:AU:402:HEC:CGA	2.29	0.45
68:AY:192:PHE:HB2	68:AY:198:ALA:HB2	1.98	0.45
68:AY:424:ILE:HD12	68:AY:424:ILE:HA	1.85	0.45
3:C:163:SER:H	3:C:168:ARG:HH22	1.64	0.45
4:E:59:GLY:O	4:E:63:VAL:HG23	2.16	0.45
7:H:31:ILE:HG12	7:H:88:LEU:HA	1.99	0.45
12:M:221:ASN:OD1	12:M:291:ARG:NH2	2.35	0.45
17:S:53:ARG:HB3	31:h:102:GLY:HA2	1.99	0.45
17:S:54:ILE:HG13	31:h:105:ARG:NH1	2.32	0.45
20:V:17:ASP:OD1	58:AA:69:ARG:NH2	2.48	0.45
21:W:57:ARG:CZ	41:s:168:THR:HG22	2.47	0.45
26:c:69:GLY:HA2	38:o:81:ARG:H	1.80	0.45
32:i:25:HIS:CE1	32:i:84:TRP:CE3	3.04	0.45
35:l:286:LEU:O	35:l:290:VAL:HG23	2.17	0.45
42:u:23:ALA:HB1	42:u:90:ASP:OD1	2.16	0.45
44:w:79:GLU:OE1	44:w:79:GLU:N	2.43	0.45
44:w:139:ARG:O	44:w:142:GLN:HB2	2.15	0.45
45:x:240:HIS:NE2	45:x:244:TYR:CE2	2.81	0.45
45:x:299:VAL:HA	45:x:302:ARG:NH1	2.31	0.45
46:y:58:ALA:O	46:y:60:GLU:HG3	2.16	0.45
49:1:70:VAL:HG12	49:1:71:VAL:N	2.31	0.45
60:AC:178:HIS:HD2	60:AC:209:GLU:O	1.99	0.45
64:AG:39:ARG:HE	64:AG:51:LYS:HD2	1.80	0.45
66:AJ:366:MET:HB3	66:AJ:367:PRO:HD3	1.98	0.45
68:AL:286:HIS:ND1	68:AL:359:VAL:HG22	2.31	0.45
68:AL:294:PRO:HB2	68:AL:301:ASN:HD21	1.82	0.45
65:AU:313:VAL:HG13	65:AU:314:LEU:HD12	1.97	0.45
67:AW:49:ILE:HD11	67:AW:230:LEU:HB3	1.98	0.45
67:AW:449:PHE:N	67:AW:452:GLU:CD	2.73	0.45
68:AY:66:GLN:OE1	68:AY:67:PRO:HD2	2.16	0.45
1:A:371:ILE:HD11	1:A:435:VAL:HB	1.97	0.45
11:L:69:GLU:HB2	11:L:73:LYS:HZ2	1.80	0.45
14:O:196:LEU:HD21	14:O:204:ILE:HG13	1.98	0.45
15:P:170:ILE:HG23	15:P:174:PHE:CD2	2.52	0.45
16:Q:136:PHE:CD2	16:Q:151:TYR:HB2	2.52	0.45
18:T:52:ARG:HB3	18:T:55:ARG:NH1	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:111:PHE:CD2	21:W:117:VAL:HG21	2.51	0.45
24:a:175:ASP:OD1	24:a:176:LYS:N	2.49	0.45
27:d:59:HIS:HD2	28:e:121:GLU:OE2	1.99	0.45
29:f:34:PRO:O	29:f:38:LYS:HG3	2.16	0.45
30:g:39:CYS:O	30:g:43:ILE:HG13	2.17	0.45
31:h:36:PHE:HD2	31:h:66:CYS:HB2	1.82	0.45
32:i:2:ASN:HD21	32:i:4:LEU:HB2	1.81	0.45
36:m:32:LEU:HB3	36:m:64:MET:HE3	1.99	0.45
41:s:89:LEU:HA	41:s:90:PRO:HD3	1.65	0.45
44:w:108:TYR:HD1	44:w:327:VAL:HG13	1.82	0.45
44:w:168:VAL:HG11	44:w:241:TYR:HA	1.97	0.45
45:x:365:ILE:HD12	46:y:87:MET:CE	2.34	0.45
47:z:223:LEU:HD23	47:z:223:LEU:HA	1.79	0.45
52:4:57:ARG:HB3	52:4:57:ARG:NH1	2.31	0.45
53:5:21:ILE:HD12	53:5:21:ILE:HA	1.81	0.45
65:AH:242:ILE:HD13	65:AH:244:MET:HE2	1.97	0.45
68:AL:140:LEU:HD21	68:AL:237:VAL:HG13	1.99	0.45
63:AS:83:LYS:HB2	63:AS:86:GLU:HB2	1.98	0.45
1:A:201:ALA:O	14:O:119:TYR:HB3	2.17	0.45
3:C:161:HIS:CE1	3:C:168:ARG:HD2	2.51	0.45
4:E:43:VAL:HB	4:E:44:PRO:HD3	1.98	0.45
4:E:120:SER:O	4:E:124:VAL:HG23	2.17	0.45
8:I:30:GLU:HG2	8:I:31:ILE:N	2.32	0.45
12:M:197:THR:O	14:O:114:GLU:HG2	2.17	0.45
12:M:688:GLN:O	12:M:690:THR:N	2.50	0.45
14:O:80:LEU:HB2	14:O:81:PRO:HD3	1.99	0.45
14:O:153:GLN:HG3	14:O:158:ILE:O	2.15	0.45
16:Q:70:ASP:N	16:Q:71:PRO:CD	2.80	0.45
16:Q:145:MET:HG3	16:Q:174:PHE:HB3	1.99	0.45
16:Q:399:ALA:HB1	16:Q:406:GLU:HG3	1.98	0.45
26:c:56:ASN:HD21	38:o:43:LEU:HD11	1.81	0.45
71:g:203:PLX:H101	71:g:203:PLX:H291	1.98	0.45
32:i:324:PRO:C	32:i:326:LEU:H	2.24	0.45
32:i:337:LEU:C	32:i:339:ILE:H	2.23	0.45
34:k:22:TYR:CG	34:k:22:TYR:O	2.69	0.45
35:l:166:THR:CG2	76:l:702:PEE:H2	2.46	0.45
35:l:173:LEU:HA	35:l:173:LEU:HD23	1.73	0.45
35:l:222:GLY:N	35:l:229:LEU:HD12	2.31	0.45
35:l:533:MET:HE3	76:l:702:PEE:H32	1.97	0.45
35:l:558:LEU:HD23	35:l:558:LEU:HA	1.71	0.45
36:m:13:VAL:HG11	36:m:99:GLU:HG2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:118:PHE:HZ	36:m:124:TRP:CZ2	2.34	0.45
37:n:7:ILE:HG23	37:n:11:HIS:HB2	1.98	0.45
40:r:13:PRO:HA	40:r:16:TRP:HB2	1.98	0.45
44:w:211:VAL:HG13	44:w:212:PRO:HD3	1.98	0.45
62:AE:53:CYS:O	62:AE:57:VAL:HG23	2.17	0.45
67:AK:259:ARG:HH21	67:AK:259:ARG:CB	2.10	0.45
59:AO:36:ALA:HB3	67:AW:320:PRO:HB3	1.97	0.45
66:AV:25:SER:HB3	66:AV:218:ILE:HD12	1.98	0.45
67:AW:312:ALA:HA	67:AW:315:LYS:HE3	1.98	0.45
68:AY:465:LEU:HD12	68:AY:466:PRO:HD2	1.97	0.45
1:A:44:ASN:HD22	1:A:59:ARG:NH2	2.14	0.45
3:C:168:ARG:HG3	3:C:172:ARG:NH1	2.31	0.45
8:I:55:CYS:HB3	12:M:110:LYS:HE3	1.98	0.45
9:J:99:ASP:H	9:J:102:GLN:HB2	1.82	0.45
12:M:158:ARG:HH21	12:M:178:GLN:HE22	1.64	0.45
12:M:446:GLY:N	12:M:451:ILE:HD11	2.32	0.45
13:N:48:TYR:HB3	13:N:89:TRP:HZ3	1.81	0.45
15:P:164:ASN:HA	15:P:181:HIS:HE2	1.82	0.45
16:Q:304:LYS:HE3	16:Q:316:PHE:CZ	2.52	0.45
16:Q:316:PHE:HD1	16:Q:339:GLN:NE2	2.14	0.45
19:U:18:VAL:HG11	41:s:292:ASN:O	2.17	0.45
75:V:201:CDL:H541	75:V:201:CDL:H572	1.46	0.45
24:a:55:PHE:HE2	39:p:118:TYR:HE2	1.26	0.45
35:l:30:ASN:O	35:l:33:PRO:HD2	2.17	0.45
35:l:595:LEU:O	35:l:598:THR:OG1	2.31	0.45
45:x:431:LEU:HD21	45:x:450:TRP:HB2	1.98	0.45
63:AF:38:ILE:HG12	63:AF:39:TYR:N	2.30	0.45
75:AG:101:CDL:H371	75:AG:101:CDL:H341	1.78	0.45
65:AH:158:PRO:HG3	65:AU:181:ASN:HD22	1.82	0.45
68:AL:126:ARG:NH1	68:AL:199:GLN:O	2.50	0.45
65:AU:88:GLU:HB3	65:AU:238:PRO:HA	1.97	0.45
66:AV:18:PHE:O	66:AV:220:PHE:HB3	2.17	0.45
66:AV:333:LEU:CD2	76:AV:403:PEE:C40	2.94	0.45
3:C:140:GLN:HG2	33:j:37:TYR:CG	2.51	0.45
4:E:53:ASP:OD2	9:J:351:GLU:HB3	2.17	0.45
6:G:123:GLU:O	6:G:127:GLY:N	2.50	0.45
9:J:319:VAL:C	9:J:323:HIS:HD1	2.22	0.45
11:L:102:ASP:OD1	11:L:102:ASP:N	2.50	0.45
12:M:421:SER:O	12:M:425:ASN:N	2.49	0.45
12:M:471:LYS:HB3	12:M:510:TRP:CH2	2.52	0.45
12:M:546:PHE:CZ	12:M:566:ILE:HD12	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:602:ARG:NE	12:M:659:ILE:HD11	2.30	0.45
15:P:97:LEU:HD23	15:P:100:LEU:HD12	1.97	0.45
25:b:116:VAL:HG12	25:b:117:ILE:N	2.32	0.45
71:b:201:PLX:H1C3	71:b:201:PLX:H31	1.94	0.45
32:i:146:SER:OG	32:i:147:PRO:HD3	2.17	0.45
33:j:75:LEU:N	33:j:76:PRO:HD2	2.32	0.45
35:l:18:PRO:HG3	35:l:39:ILE:HD12	1.99	0.45
35:l:194:ASN:ND2	38:o:127:LEU:HD12	2.32	0.45
40:r:56:PHE:HZ	40:r:108:MET:HE1	1.82	0.45
40:r:145:ALA:HB3	40:r:222:GLU:OE2	2.17	0.45
41:s:288:LEU:O	41:s:293:PHE:N	2.50	0.45
45:x:240:HIS:O	45:x:243:VAL:HG22	2.16	0.45
50:2:31:TYR:HE1	50:2:98:HIS:CE1	2.34	0.45
51:3:3:ALA:O	51:3:4:ALA:HB2	2.17	0.45
51:3:42:ARG:HG3	51:3:42:ARG:NH1	2.32	0.45
56:8:35:ALA:HB3	56:8:36:PRO:HD3	1.99	0.45
59:AB:46:LYS:HD2	59:AB:49:PHE:CZ	2.52	0.45
65:AH:218:TYR:OH	65:AH:244:MET:HE3	2.17	0.45
65:AH:288:MET:SD	76:AH:401:PEE:O4	2.75	0.45
66:AJ:372:ILE:O	66:AJ:376:MET:HG2	2.17	0.45
68:AL:332:ALA:HA	68:AL:337:LEU:HB2	1.98	0.45
65:AU:201:VAL:O	65:AU:207:GLY:HA2	2.17	0.45
66:AV:10:LEU:HD21	76:AY:502:PEE:H45	1.77	0.45
68:AY:166:ASP:OD1	68:AY:167:VAL:N	2.49	0.45
68:AY:296:TRP:HB2	68:AY:348:TYR:C	2.42	0.45
1:A:440:ARG:HE	1:A:441:HIS:CE1	2.35	0.45
2:B:94:ARG:HE	16:Q:234:GLN:NE2	2.15	0.45
9:J:108:TRP:HZ3	9:J:110:ALA:HA	1.82	0.45
9:J:178:SER:OG	9:J:181:LEU:HB2	2.17	0.45
9:J:273:LEU:O	9:J:276:LEU:HB3	2.17	0.45
13:N:29:ARG:HH22	13:N:65:THR:C	2.17	0.45
15:P:167:GLU:HG2	15:P:181:HIS:CD2	2.52	0.45
15:P:214:ASP:O	15:P:217:LYS:HD2	2.16	0.45
16:Q:235:ASP:OD1	16:Q:356:ILE:HD12	2.17	0.45
16:Q:369:ALA:HA	18:T:93:ALA:HB2	1.99	0.45
22:Y:74:TRP:HE3	22:Y:75:HIS:N	2.15	0.45
22:Y:78:GLU:CG	35:l:385:PHE:HE1	2.30	0.45
25:b:90:VAL:HG22	25:b:97:ILE:HD12	1.98	0.45
35:l:304:PHE:HZ	35:l:526:LEU:HD22	1.82	0.45
35:l:434:GLN:HB3	35:l:435:PRO:HD2	1.99	0.45
41:s:234:MET:O	41:s:238:THR:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:y:41:ILE:O	46:y:45:MET:HG2	2.16	0.45
47:z:183:GLU:O	51:3:42:ARG:NH2	2.50	0.45
50:2:33:ILE:HG22	50:2:34:LEU:HD12	1.98	0.45
50:2:98:HIS:ND1	50:2:98:HIS:N	2.64	0.45
75:AJ:404:CDL:OB9	75:AJ:404:CDL:O1	2.33	0.45
68:AL:42:LEU:HD11	68:AL:430:GLU:OE1	2.17	0.45
61:AQ:53:TRP:HA	61:AQ:56:ILE:HB	1.99	0.45
68:AY:337:LEU:C	68:AY:368:MET:HE2	2.41	0.45
1:A:319:PRO:HB2	1:A:347:THR:HG21	1.98	0.45
2:B:90:PRO:HG2	13:N:56:PHE:CE2	2.52	0.45
5:F:22:HIS:HB2	5:F:64:LYS:HB3	1.97	0.45
7:H:28:TYR:CD2	7:H:56:LEU:HD13	2.52	0.45
9:J:163:LYS:HE2	9:J:253:VAL:HA	1.98	0.45
14:O:207:GLU:HG2	14:O:213:ILE:HG13	1.99	0.45
15:P:97:LEU:HA	15:P:100:LEU:HD12	1.97	0.45
16:Q:201:PHE:HB2	41:s:32:GLN:HG3	1.99	0.45
16:Q:259:GLU:O	16:Q:263:THR:OG1	2.34	0.45
20:V:2:ALA:O	20:V:6:PHE:N	2.45	0.45
22:Y:73:PHE:HD1	22:Y:73:PHE:C	2.24	0.45
26:c:177:GLU:O	26:c:178:PRO:C	2.59	0.45
32:i:20:THR:O	32:i:23:SER:OG	2.34	0.45
35:l:33:PRO:HA	35:l:118:PHE:HD2	1.82	0.45
35:l:481:THR:HG22	43:v:92:HIS:CD2	2.52	0.45
38:o:6:TYR:HE1	38:o:12:ARG:NH2	2.15	0.45
44:w:58:ARG:HB3	44:w:202:HIS:HE1	1.82	0.45
44:w:92:HIS:HB3	44:w:103:PRO:HB3	1.99	0.45
66:AJ:278:TYR:O	66:AJ:281:LEU:HB2	2.17	0.45
67:AK:148:ARG:NH1	63:AS:50:ARG:O	2.50	0.45
68:AL:75:ILE:HD13	68:AL:224:TYR:CD1	2.51	0.45
68:AL:113:VAL:HG21	68:AL:120:LEU:HD23	1.99	0.45
61:AQ:26:ILE:HD12	64:AT:27:VAL:HG13	1.98	0.45
66:AV:191:ALA:O	66:AV:194:THR:OG1	2.24	0.45
67:AW:444:LEU:HA	67:AW:447:THR:HG23	1.99	0.45
68:AY:101:THR:HA	68:AY:155:SER:N	2.30	0.45
68:AY:479:ARG:HH11	75:AY:501:CDL:HB62	1.82	0.45
1:A:63:TYR:HE2	1:A:64:LYS:NZ	2.15	0.45
3:C:88:CYS:SG	16:Q:223:HIS:CE1	3.10	0.45
12:M:382:ARG:O	12:M:386:LEU:HG	2.16	0.45
12:M:498:GLN:HE22	12:M:501:ARG:HD2	1.82	0.45
14:O:198:ALA:HA	14:O:201:ILE:HD12	1.99	0.45
34:k:31:LEU:HD23	34:k:31:LEU:HA	1.75	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:42:ILE:O	34:k:46:LEU:HG	2.17	0.45
35:l:399:ALA:O	35:l:402:SER:OG	2.33	0.45
38:o:24:ASN:HA	68:AL:262:VAL:O	2.16	0.45
42:u:82:PHE:CE2	42:u:86:TRP:HD1	2.35	0.45
45:x:32:ALA:HB3	56:8:36:PRO:HG2	1.98	0.45
48:0:79:LYS:NZ	55:7:15:ASN:HD21	2.15	0.45
59:AB:26:LEU:HG	59:AB:28:PRO:HA	1.99	0.45
65:AH:304:TYR:CE1	75:AH:403:CDL:OA3	2.70	0.45
66:AJ:16:HIS:O	66:AJ:21:LEU:HB3	2.16	0.45
68:AL:63:GLN:HE22	68:AL:238:GLU:HA	1.81	0.45
67:AW:328:ALA:HB3	67:AW:335:LEU:HB2	1.99	0.45
68:AY:96:LEU:HD23	68:AY:161:ILE:CD1	2.47	0.45
7:H:50:GLN:NE2	8:I:93:LYS:HD2	2.32	0.44
12:M:307:VAL:HG22	12:M:582:VAL:HG13	1.99	0.44
12:M:546:PHE:HD2	12:M:568:TYR:HD1	1.63	0.44
14:O:145:SER:O	14:O:148:ILE:HB	2.18	0.44
18:T:96:HIS:NE2	18:T:115:CYS:SG	2.90	0.44
76:V:202:PEE:H60	76:V:202:PEE:H40	1.99	0.44
6:X:138:LEU:CD2	6:X:144:ILE:HG12	2.47	0.44
22:Y:81:LEU:HD12	43:v:88:ASP:CB	2.45	0.44
22:Y:81:LEU:HD11	43:v:89:TYR:HA	1.98	0.44
32:i:4:LEU:HG	44:w:43:PHE:HE2	1.82	0.44
41:s:40:VAL:CG1	41:s:46:LEU:HB2	2.47	0.44
44:w:351:TRP:HA	44:w:353:TRP:CZ3	2.52	0.44
45:x:70:VAL:HG11	45:x:246:LEU:HD22	1.99	0.44
45:x:158:ILE:O	45:x:162:ILE:HG13	2.17	0.44
48:0:40:LEU:HD22	48:0:59:LEU:CD1	2.47	0.44
60:AC:80:HIS:CE1	68:AL:182:VAL:HG22	2.52	0.44
60:AC:81:THR:O	60:AC:83:ILE:N	2.48	0.44
60:AC:140:MET:HA	66:AV:177:ARG:HH21	1.81	0.44
60:AC:195:LEU:HD13	60:AC:248:ARG:HD2	1.99	0.44
61:AD:34:ARG:NH1	61:AD:38:GLN:HB3	2.32	0.44
63:AF:34:ARG:NH1	66:AJ:379:TRP:NE1	2.60	0.44
65:AH:221:PRO:HA	65:AH:222:PRO:HD3	1.77	0.44
66:AJ:265:PRO:HA	66:AJ:266:PRO:HD3	1.82	0.44
66:AV:7:THR:O	66:AV:12:LYS:HE3	2.17	0.44
66:AV:155:TYR:CD1	66:AV:155:TYR:C	2.94	0.44
68:AY:421:GLY:O	68:AY:422:ARG:HG3	2.16	0.44
1:A:157:TYR:HB2	1:A:212:LEU:HD21	1.99	0.44
7:H:23:ARG:HH22	7:H:27:LEU:HD21	1.83	0.44
7:H:32:LEU:HA	7:H:35:LEU:HG	1.97	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:38:PRO:HA	8:I:39:PRO:HD3	1.58	0.44
73:J:401:NDP:O2X	73:J:401:NDP:O3B	2.33	0.44
11:L:136:SER:O	11:L:140:LYS:HG3	2.16	0.44
12:M:157:LYS:HB2	18:T:100:TYR:CD2	2.52	0.44
12:M:255:ASP:HB3	12:M:257:VAL:HG23	1.98	0.44
14:O:205:ILE:HA	14:O:208:LEU:HD12	1.98	0.44
20:V:69:VAL:HG21	20:V:100:THR:HG21	1.98	0.44
21:W:111:PHE:CE2	21:W:117:VAL:HG11	2.49	0.44
30:g:78:GLU:OE1	32:i:342:PHE:HD1	2.01	0.44
32:i:291:TYR:CE2	76:l:701:PEE:H51	2.52	0.44
34:k:59:MET:HB2	34:k:60:PRO:HD3	1.99	0.44
71:r:501:PLX:H101	71:r:501:PLX:H132	1.59	0.44
41:s:257:THR:O	41:s:261:THR:HG23	2.17	0.44
42:u:100:CYS:O	42:u:102:LYS:N	2.49	0.44
45:x:51:ASP:O	45:x:55:ASN:HB2	2.18	0.44
59:AB:41:PRO:HB2	67:AK:167:GLN:NE2	2.31	0.44
61:AD:27:VAL:O	61:AD:30:MET:HB2	2.17	0.44
68:AL:373:GLN:NE2	68:AL:471:ILE:HG23	2.31	0.44
63:AS:51:LEU:HD22	63:AS:55:LEU:HD22	1.99	0.44
63:AS:71:LEU:HD21	66:AV:25:SER:CB	2.48	0.44
66:AV:160:LEU:O	66:AV:164:ILE:HD12	2.17	0.44
67:AW:277:VAL:HA	67:AW:278:ALA:HA	1.73	0.44
1:A:317:VAL:HG22	1:A:356:VAL:HA	1.99	0.44
2:B:127:THR:HA	15:P:231:ARG:HH12	1.81	0.44
3:C:160:TYR:HE1	16:Q:120:THR:HG22	1.81	0.44
9:J:329:LEU:HD12	9:J:329:LEU:O	2.17	0.44
11:L:62:THR:HG23	11:L:72:ILE:HD13	1.99	0.44
15:P:63:GLU:O	15:P:67:GLU:HG3	2.17	0.44
17:S:31:ASN:HD21	17:S:36:LYS:HD3	1.83	0.44
20:V:40:ARG:HE	75:V:201:CDL:CA2	2.30	0.44
22:Y:55:VAL:O	22:Y:58:SER:OG	2.33	0.44
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.58	0.44
22:Y:72:ARG:NH1	35:l:390:TYR:CZ	2.79	0.44
25:b:105:PHE:HZ	43:v:67:LEU:HB2	1.75	0.44
26:c:52:ALA:HB2	26:c:62:TYR:HB2	1.99	0.44
30:g:45:ASN:HD21	30:g:60:GLN:HE21	1.65	0.44
31:h:80:ARG:NH1	36:m:1:MET:SD	2.89	0.44
40:r:246:LEU:HD23	40:r:246:LEU:HA	1.81	0.44
41:s:142:TYR:CD2	41:s:289:LEU:HD11	2.52	0.44
46:y:60:GLU:CD	46:y:61:VAL:H	2.24	0.44
59:AB:50:LEU:O	59:AB:51:SER:OG	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:AH:301:PRO:O	65:AH:305:THR:HG23	2.17	0.44
66:AJ:8:ASN:HB3	66:AJ:11:MET:HB2	2.00	0.44
67:AK:155:GLN:NE2	67:AK:200:VAL:O	2.50	0.44
65:AU:249:TYR:O	65:AU:252:VAL:HG23	2.17	0.44
65:AU:253:LEU:HD23	65:AU:254:GLU:N	2.32	0.44
66:AV:155:TYR:CD1	66:AV:155:TYR:O	2.70	0.44
67:AW:108:GLY:HA2	68:AY:397:ASN:ND2	2.33	0.44
68:AY:333:VAL:HG13	68:AY:336:LYS:HD2	1.99	0.44
2:B:69:GLY:O	2:B:72:LEU:HB3	2.17	0.44
2:B:91:LEU:HD23	2:B:95:PHE:CD2	2.52	0.44
8:I:97:PRO:HG3	15:P:61:PHE:CD1	2.52	0.44
9:J:169:HIS:CD2	73:J:401:NDP:C5N	2.79	0.44
12:M:221:ASN:HB3	12:M:285:TRP:HE3	1.82	0.44
12:M:275:PRO:HB3	12:M:286:ILE:HB	1.99	0.44
12:M:306:MET:HA	12:M:315:THR:O	2.18	0.44
12:M:371:VAL:HG12	12:M:533:GLY:O	2.17	0.44
12:M:501:ARG:HH12	12:M:666:GLN:HB2	1.82	0.44
12:M:541:PRO:HA	12:M:542:PRO:HD2	1.77	0.44
12:M:612:PRO:HB3	12:M:616:ALA:HB3	1.99	0.44
14:O:76:ALA:HA	14:O:79:VAL:HG23	1.98	0.44
14:O:195:ASP:HB2	14:O:219:ARG:H	1.83	0.44
18:T:67:PHE:O	18:T:71:LEU:HD13	2.17	0.44
18:T:81:GLU:HA	18:T:122:HIS:O	2.17	0.44
22:Y:85:PRO:O	22:Y:86:TYR:CD1	2.71	0.44
26:c:101:TRP:CD1	38:o:47:TYR:CD1	3.06	0.44
27:d:107:CYS:HG	27:d:119:CYS:CA	2.31	0.44
32:i:2:ASN:HA	32:i:3:PRO:HD2	1.87	0.44
35:l:567:SER:C	35:l:571:ILE:HD13	2.42	0.44
38:o:6:TYR:CD2	38:o:14:LEU:HD23	2.53	0.44
40:r:325:LEU:HD12	40:r:440:HIS:HB3	1.98	0.44
40:r:339:SER:HB2	40:r:344:LEU:HD12	2.00	0.44
71:r:502:PLX:H192	71:r:502:PLX:H162	1.44	0.44
41:s:89:LEU:HD12	41:s:91:MET:HE2	1.98	0.44
43:v:49:ALA:O	43:v:51:LEU:N	2.46	0.44
44:w:238:GLU:O	44:w:242:LYS:HG3	2.17	0.44
46:y:59:GLN:CA	46:y:62:GLU:HB2	2.46	0.44
46:y:162:SER:HB2	46:y:198:GLU:HB2	1.99	0.44
61:AD:25:ILE:O	61:AD:29:VAL:HG23	2.18	0.44
63:AF:44:VAL:O	63:AF:48:ILE:HG12	2.17	0.44
66:AJ:198:LEU:CD1	75:AJ:404:CDL:H332	2.48	0.44
68:AL:225:LYS:HD2	68:AL:257:TYR:CE1	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:AN:17:TYR:HD1	68:AY:275:ILE:HG12	1.83	0.44
66:AV:315:MET:SD	66:AV:318:ARG:NH2	2.90	0.44
67:AW:104:GLU:OE1	68:AY:325:SER:HA	2.17	0.44
68:AY:64:SER:HB3	68:AY:235:GLY:HA2	1.99	0.44
68:AY:92:PHE:O	68:AY:92:PHE:HD1	2.00	0.44
68:AY:112:GLU:HG3	68:AY:116:MET:HE2	2.00	0.44
1:A:99:TRP:HA	1:A:149:MET:HE1	2.00	0.44
1:A:194:ASP:OD2	10:K:96:MET:N	2.41	0.44
2:B:61:TRP:HB2	2:B:65:PHE:HE2	1.82	0.44
7:H:13:GLY:HA2	16:Q:279:THR:HG22	2.00	0.44
7:H:23:ARG:O	7:H:26:ILE:HB	2.18	0.44
9:J:72:HIS:O	9:J:75:ARG:HG2	2.18	0.44
9:J:141:PHE:CD2	9:J:183:ASN:ND2	2.86	0.44
11:L:72:ILE:HA	11:L:143:TRP:NE1	2.33	0.44
12:M:219:SER:O	12:M:222:ILE:HG12	2.16	0.44
12:M:229:GLY:O	12:M:232:THR:HG23	2.18	0.44
16:Q:174:PHE:HD1	16:Q:214:TYR:HE1	1.65	0.44
26:c:166:LEU:HB2	26:c:170:ARG:NH2	2.33	0.44
31:h:3:PHE:HB2	32:i:144:GLN:HE21	1.83	0.44
33:j:48:ARG:HD2	33:j:49:VAL:H	1.83	0.44
35:l:37:LYS:HE3	35:l:102:GLU:CG	2.37	0.44
76:l:701:PEE:H51	76:l:701:PEE:H56	1.55	0.44
40:r:109:THR:HG22	40:r:121:PHE:HB2	2.00	0.44
44:w:246:LEU:HB2	44:w:247:PRO:HD3	1.99	0.44
66:AJ:156:ILE:HG21	66:AJ:160:LEU:HD13	2.00	0.44
67:AK:126:LEU:HB3	68:AL:38:PHE:CZ	2.52	0.44
68:AL:125:THR:HG22	68:AL:126:ARG:N	2.31	0.44
68:AL:286:HIS:CE1	68:AL:359:VAL:HG22	2.52	0.44
63:AS:99:ILE:O	63:AS:103:LYS:HG2	2.17	0.44
65:AU:114:PHE:CE2	65:AU:148:LEU:HD21	2.52	0.44
65:AU:197:LEU:HD23	65:AU:274:LEU:HD21	1.99	0.44
67:AW:323:VAL:HG13	67:AW:340:THR:HG22	1.99	0.44
67:AW:452:GLU:HG2	67:AW:453:LEU:N	2.31	0.44
1:A:173:ILE:HG22	1:A:177:TYR:CE2	2.52	0.44
1:A:225:LEU:HB2	1:A:424:ILE:HD11	1.99	0.44
7:H:12:VAL:HG13	7:H:13:GLY:N	2.33	0.44
9:J:71:ASN:ND2	15:P:214:ASP:HB3	2.33	0.44
9:J:168:SER:CA	9:J:184:LYS:HE3	2.47	0.44
12:M:385:TYR:HB2	12:M:517:HIS:CE1	2.53	0.44
15:P:188:LEU:HD22	16:Q:117:HIS:HB2	2.00	0.44
16:Q:190:HIS:HD2	16:Q:452:GLY:CA	2.26	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:W:201:PEE:N	76:W:201:PEE:P	2.87	0.44
26:c:63:GLU:O	26:c:77:LYS:N	2.43	0.44
28:e:54:PRO:O	28:e:56:GLN:HG3	2.18	0.44
29:f:32:ARG:C	29:f:35:PRO:HD2	2.42	0.44
32:i:8:VAL:O	32:i:12:THR:HG23	2.18	0.44
33:j:34:SER:HB2	41:s:63:PRO:HA	2.00	0.44
35:l:98:TRP:CD1	35:l:98:TRP:O	2.71	0.44
40:r:36:ILE:O	40:r:39:LEU:HB3	2.18	0.44
41:s:92:PRO:HB3	41:s:255:TYR:CD2	2.53	0.44
41:s:215:TYR:HD1	41:s:219:PRO:HB2	1.83	0.44
41:s:266:LEU:HA	41:s:266:LEU:HD23	1.73	0.44
49:1:78:HIS:CE1	53:5:12:LEU:HD22	2.52	0.44
75:AL:502:CDL:H511	76:AL:503:PEE:H67	1.98	0.44
75:AN:101:CDL:C58	76:AV:403:PEE:C33	2.96	0.44
68:AY:225:LYS:NZ	68:AY:258:ALA:H	2.15	0.44
1:A:167:SER:O	1:A:171:VAL:HG23	2.18	0.44
2:B:128:ILE:HG12	2:B:143:TYR:HD1	1.83	0.44
4:E:35:LEU:HD11	4:E:39:TRP:HE1	1.81	0.44
9:J:130:ILE:HG21	73:J:401:NDP:N7A	2.23	0.44
9:J:220:MET:HA	9:J:223:PHE:CD2	2.53	0.44
12:M:510:TRP:HD1	12:M:512:VAL:HG22	1.82	0.44
16:Q:106:VAL:HG11	16:Q:109:CYS:HB2	2.00	0.44
21:W:120:LEU:HG	31:h:69:ARG:NH1	2.32	0.44
76:W:201:PEE:C2	41:s:98:LEU:HD22	2.47	0.44
33:j:30:TYR:HB2	33:j:33:LYS:CD	2.47	0.44
34:k:46:LEU:HD22	36:m:46:PHE:CD2	2.53	0.44
45:x:379:TYR:CE2	45:x:383:MET:HE2	2.52	0.44
53:5:61:GLU:OE1	53:5:64:ARG:NH1	2.51	0.44
53:5:68:ILE:HG13	53:5:69:PHE:N	2.33	0.44
54:6:3:ASN:ND2	54:6:5:VAL:HG13	2.33	0.44
62:AE:26:LEU:C	62:AE:28:ASP:H	2.22	0.44
63:AF:34:ARG:HD2	66:AJ:377:LEU:HB3	2.00	0.44
66:AJ:105:GLY:HA2	66:AJ:107:PHE:CE2	2.53	0.44
68:AL:279:ASP:OD2	68:AL:282:LEU:HG	2.17	0.44
75:AU:403:CDL:H112	66:AV:234:LEU:HD12	2.00	0.44
2:B:131:GLU:OE1	2:B:141:THR:HG21	2.18	0.44
2:B:169:PRO:HG3	2:B:198:GLU:HG2	2.00	0.44
8:I:37:PRO:HA	8:I:38:PRO:HD3	1.81	0.44
12:M:37:ASP:HA	12:M:103:LEU:HD23	1.98	0.44
14:O:132:ILE:O	14:O:172:ILE:HG22	2.18	0.44
16:Q:55:SER:N	16:Q:58:THR:OG1	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:W:201:PEE:H51	76:W:201:PEE:H56	1.33	0.44
26:c:108:HIS:CE1	35:l:546:GLN:HG2	2.53	0.44
71:g:201:PLX:H1B1	31:h:2:PRO:HG2	1.99	0.44
36:m:2:MET:N	36:m:123:SER:OG	2.50	0.44
37:n:27:LEU:HD12	40:r:2:LEU:HD21	1.99	0.44
39:p:25:ARG:HA	39:p:25:ARG:HD3	1.80	0.44
39:p:173:ARG:HA	39:p:174:PRO:HD3	1.83	0.44
40:r:72:LEU:O	40:r:76:THR:HG23	2.18	0.44
71:r:502:PLX:H151	71:r:502:PLX:H122	1.83	0.44
43:v:63:LEU:O	43:v:67:LEU:HG	2.18	0.44
44:w:86:PHE:HD2	44:w:159:LEU:HD13	1.83	0.44
79:x:604:HEA:O11	79:x:604:HEA:HHC	2.17	0.44
47:z:41:THR:O	47:z:45:ILE:HG13	2.18	0.44
55:7:9:PHE:HD1	55:7:10:HIS:HD2	1.64	0.44
58:AA:27:TYR:CE2	65:AH:305:THR:HG22	2.53	0.44
76:AJ:403:PEE:H61	76:AJ:403:PEE:C18	2.45	0.44
68:AL:231:LEU:HD22	68:AL:250:LEU:HD12	2.00	0.44
62:AR:43:CYS:SG	62:AR:78:ARG:HA	2.57	0.44
67:AW:81:HIS:CD2	67:AW:158:LEU:HD22	2.53	0.44
2:B:81:THR:HG23	41:s:35:LYS:H	1.83	0.44
4:E:39:TRP:O	4:E:43:VAL:HG23	2.18	0.44
4:E:50:PHE:CD2	4:E:103:VAL:HG21	2.52	0.44
8:I:60:ARG:HD3	16:Q:159:LEU:HD22	1.99	0.44
12:M:278:HIS:NE2	12:M:280:ASP:HB2	2.33	0.44
12:M:358:LEU:HD22	12:M:363:SER:HB2	1.99	0.44
12:M:639:LEU:O	12:M:642:VAL:HG12	2.18	0.44
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.49	0.44
16:Q:265:ASN:OD1	16:Q:267:ILE:HD12	2.17	0.44
16:Q:271:ARG:NH1	41:s:281:ARG:HA	2.31	0.44
32:i:79:MET:SD	34:k:43:MET:HE1	2.58	0.44
32:i:197:ASN:HA	32:i:198:PRO:HD3	1.79	0.44
35:l:122:LEU:HD23	35:l:122:LEU:HA	1.85	0.44
38:o:100:PHE:CZ	38:o:104:ILE:HD11	2.53	0.44
41:s:224:PHE:CZ	41:s:228:TYR:HE2	2.36	0.44
42:u:104:GLN:O	42:u:108:ASP:N	2.41	0.44
51:3:78:LEU:HA	51:3:78:LEU:HD12	1.75	0.44
60:AC:145:ASP:OD1	60:AC:146:VAL:N	2.51	0.44
60:AC:179:ARG:NE	60:AC:208:PRO:O	2.43	0.44
9:J:81:ILE:HG22	9:J:83:PRO:HD3	2.00	0.43
12:M:299:ARG:HG2	12:M:300:GLN:N	2.19	0.43
12:M:385:TYR:HE1	12:M:523:VAL:HG23	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:147:SER:HA	14:O:150:GLU:OE1	2.18	0.43
14:O:236:GLU:HB3	14:O:238:PRO:HD2	2.00	0.43
16:Q:307:PRO:HB2	16:Q:312:ASP:HB3	2.00	0.43
17:S:12:MET:HE1	41:s:19:PHE:C	2.43	0.43
24:a:150:ARG:NH1	40:r:168:HIS:CE1	2.86	0.43
26:c:139:PHE:O	26:c:143:MET:HG2	2.18	0.43
27:d:111:GLU:OE1	27:d:119:CYS:HB2	2.18	0.43
30:g:87:ARG:HD2	42:u:156:GLY:C	2.42	0.43
32:i:309:ASN:HD21	44:w:130:ARG:HD3	1.82	0.43
33:j:34:SER:HB2	41:s:64:ALA:H	1.82	0.43
33:j:49:VAL:HG12	36:m:75:ILE:H	1.82	0.43
34:k:8:ILE:N	34:k:8:ILE:HD12	2.33	0.43
40:r:237:LYS:HD2	40:r:237:LYS:N	2.33	0.43
71:r:501:PLX:H211	71:r:501:PLX:H182	1.66	0.43
43:v:93:ARG:O	43:v:97:MET:HG2	2.18	0.43
46:y:1:MET:SD	46:y:133:LEU:HD13	2.58	0.43
46:y:121:TYR:C	46:y:138:VAL:HG23	2.42	0.43
47:z:137:LEU:HA	47:z:137:LEU:HD12	1.70	0.43
53:5:26:MET:N	53:5:26:MET:SD	2.91	0.43
54:6:2:GLU:CG	54:6:3:ASN:H	2.30	0.43
62:AE:34:ARG:HE	62:AE:34:ARG:HB2	1.62	0.43
67:AK:158:LEU:HB2	67:AK:197:ILE:HG23	1.99	0.43
68:AL:152:GLN:NE2	68:AL:249:HIS:O	2.51	0.43
68:AL:414:GLY:O	68:AL:418:LEU:HD13	2.18	0.43
67:AW:228:PRO:O	67:AW:231:LYS:HB2	2.18	0.43
2:B:178:HIS:HB2	3:C:179:TYR:CZ	2.53	0.43
3:C:88:CYS:HB3	16:Q:141:TYR:CG	2.54	0.43
3:C:211:TYR:CD1	3:C:211:TYR:C	2.96	0.43
4:E:53:ASP:HA	9:J:366:ILE:HD11	2.00	0.43
9:J:83:PRO:HA	9:J:106:LEU:O	2.18	0.43
9:J:168:SER:O	9:J:203:PRO:HD2	2.18	0.43
12:M:646:LEU:HD13	12:M:653:LEU:HB3	2.00	0.43
14:O:143:ARG:CB	14:O:184:PRO:HD3	2.47	0.43
15:P:55:HIS:NE2	15:P:78:VAL:HG12	2.33	0.43
16:Q:391:VAL:O	16:Q:415:GLY:HA2	2.18	0.43
20:V:51:GLU:HB3	20:V:55:LYS:NZ	2.34	0.43
25:b:79:VAL:HG22	35:l:10:LEU:CD1	2.48	0.43
25:b:111:LEU:C	25:b:112:GLU:CD	2.85	0.43
31:h:56:CYS:HA	42:u:145:ARG:NH1	2.33	0.43
35:l:208:PRO:HG2	35:l:266:LEU:HB3	1.99	0.43
35:l:356:ILE:CG2	35:l:429:LEU:HB3	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:o:9:SER:OG	38:o:12:ARG:HB3	2.18	0.43
39:p:30:TRP:O	39:p:32:VAL:HG23	2.18	0.43
40:r:345:SER:O	40:r:348:LEU:HG	2.18	0.43
42:u:18:VAL:HG12	42:u:20:ILE:H	1.83	0.43
42:u:121:ASP:HB3	42:u:124:GLU:OE2	2.18	0.43
47:z:19:THR:CG2	47:z:53:THR:OG1	2.66	0.43
47:z:19:THR:HG22	47:z:53:THR:OG1	2.18	0.43
52:4:84:LYS:HA	52:4:84:LYS:HD2	1.83	0.43
59:AB:1:MET:SD	67:AK:412:VAL:HG13	2.58	0.43
63:AF:39:TYR:CD1	63:AF:39:TYR:C	2.95	0.43
65:AH:288:MET:HE1	66:AJ:78:ILE:HD11	2.00	0.43
75:AJ:404:CDL:H121	75:AJ:404:CDL:H152	1.70	0.43
67:AK:155:GLN:N	67:AK:156:PRO:HD2	2.33	0.43
67:AK:257:GLU:HG3	67:AK:450:VAL:HG21	1.98	0.43
68:AL:360:CYS:HB3	68:AL:368:MET:SD	2.59	0.43
65:AU:202:ARG:NH2	66:AV:248:ASP:OD1	2.51	0.43
2:B:35:THR:N	8:I:105:GLU:O	2.51	0.43
12:M:455:ILE:HG12	12:M:463:SER:HB3	1.99	0.43
12:M:566:ILE:HD11	12:M:579:ILE:HG22	1.99	0.43
17:S:43:TYR:CE2	21:W:68:ARG:HD2	2.53	0.43
24:a:150:ARG:NH1	40:r:168:HIS:HE1	2.16	0.43
26:c:41:TYR:CZ	26:c:67:ASP:HB3	2.54	0.43
27:d:57:TYR:CD1	27:d:57:TYR:O	2.70	0.43
28:e:115:LYS:O	28:e:118:SER:OG	2.30	0.43
31:h:82:GLN:HA	31:h:85:LYS:HE3	1.99	0.43
32:i:232:ARG:NH1	44:w:306:ASN:O	2.50	0.43
32:i:237:LEU:HB3	32:i:240:LEU:HB2	2.00	0.43
35:l:81:LYS:HD3	35:l:83:ASP:OD2	2.18	0.43
35:l:533:MET:CE	76:l:702:PEE:H32	2.48	0.43
40:r:115:LEU:O	40:r:118:PHE:HB3	2.19	0.43
41:s:59:GLU:OE1	41:s:59:GLU:N	2.52	0.43
41:s:289:LEU:HA	41:s:289:LEU:HD23	1.82	0.43
44:w:217:ARG:O	44:w:221:LYS:HG2	2.18	0.43
47:z:148:HIS:CE1	47:z:152:MET:HE3	2.53	0.43
53:5:19:PHE:CD1	53:5:19:PHE:C	2.94	0.43
66:AJ:155:TYR:HE2	64:AT:38:TRP:CZ2	2.35	0.43
67:AK:60:ARG:HB3	67:AK:223:LEU:HD12	2.00	0.43
67:AW:379:LYS:HG2	67:AW:413:LEU:HG	2.00	0.43
67:AW:444:LEU:HD23	67:AW:444:LEU:HA	1.78	0.43
1:A:73:PRO:HB2	1:A:74:ASP:H	1.58	0.43
1:A:88:ARG:C	1:A:244:ASN:HD22	2.26	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ARG:NH1	10:K:99:PRO:HB3	2.33	0.43
3:C:163:SER:HB3	16:Q:123:LEU:HD11	2.00	0.43
5:F:39:LYS:HG3	5:F:40:ARG:N	2.29	0.43
5:F:65:LEU:O	5:F:76:ASN:HA	2.18	0.43
6:G:115:GLN:NE2	6:G:135:ALA:HB1	2.34	0.43
11:L:72:ILE:HA	11:L:143:TRP:CD1	2.53	0.43
12:M:136:GLU:HB3	12:M:242:PRO:HG2	2.00	0.43
12:M:323:LEU:HA	12:M:326:VAL:HG22	1.99	0.43
13:N:5:GLN:O	13:N:9:ARG:HG2	2.17	0.43
16:Q:147:ASN:O	16:Q:150:ALA:HB3	2.17	0.43
17:S:53:ARG:HH21	31:h:105:ARG:HA	1.82	0.43
19:U:52:ASN:ND2	31:h:27:TYR:O	2.42	0.43
21:W:110:VAL:HG11	31:h:71:LYS:HB2	2.01	0.43
30:g:15:ASP:OD1	30:g:16:GLU:N	2.52	0.43
34:k:87:LEU:HD13	36:m:74:ALA:HB2	2.00	0.43
35:l:151:SER:HA	35:l:247:LEU:HD13	2.01	0.43
35:l:227:LEU:HA	35:l:230:HIS:HB3	2.00	0.43
40:r:408:LEU:HD23	40:r:408:LEU:HA	1.70	0.43
46:y:162:SER:HB3	46:y:197:SER:C	2.44	0.43
48:0:37:GLN:O	48:0:41:LYS:HG2	2.18	0.43
49:1:27:TRP:CH2	50:2:86:GLY:HA2	2.54	0.43
51:3:5:LYS:CD	51:3:6:GLY:N	2.82	0.43
65:AH:131:ALA:HB3	65:AH:133:ARG:HG2	2.00	0.43
65:AH:131:ALA:HA	65:AH:174:TYR:HA	2.00	0.43
59:AO:37:THR:N	68:AY:174:GLU:OE2	2.41	0.43
60:AP:127:TYR:HE1	61:AQ:33:GLU:HG2	1.83	0.43
60:AP:214:ILE:HG22	60:AP:216:VAL:H	1.83	0.43
63:AS:36:ASP:OD1	63:AS:90:TYR:OH	2.37	0.43
65:AU:291:LYS:HE3	76:AU:401:PEE:O1P	2.18	0.43
66:AV:129:MET:CE	66:AV:185:LEU:CD1	2.95	0.43
68:AY:57:LEU:HD13	68:AY:250:LEU:HB3	1.99	0.43
2:B:166:VAL:HG11	2:B:199:ILE:HG23	2.00	0.43
6:G:138:LEU:O	6:G:143:GLU:HB2	2.18	0.43
10:K:78:ASP:HA	14:O:215:LYS:HD3	2.00	0.43
10:K:86:ASP:O	10:K:90:GLU:HG3	2.18	0.43
12:M:221:ASN:HB3	12:M:285:TRP:CZ3	2.53	0.43
12:M:341:ILE:HD13	12:M:367:CYS:SG	2.59	0.43
15:P:55:HIS:HD2	15:P:79:SER:O	2.01	0.43
15:P:188:LEU:HA	16:Q:114:GLY:HA3	2.00	0.43
6:X:123:GLU:HB2	6:X:128:PHE:O	2.18	0.43
23:Z:65:ASP:O	23:Z:69:LYS:HB2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:57:GLU:HB2	44:w:323:GLN:HB3	2.00	0.43
32:i:218:LEU:HD23	32:i:218:LEU:HA	1.81	0.43
33:j:53:MET:HG3	34:k:79:VAL:HG13	1.99	0.43
33:j:64:LEU:O	33:j:68:GLU:HG2	2.18	0.43
34:k:32:CYS:O	34:k:36:MET:HG3	2.18	0.43
35:l:210:LEU:HD21	35:l:214:LEU:HD13	2.01	0.43
39:p:54:GLU:OE1	39:p:54:GLU:N	2.51	0.43
40:r:105:SER:O	40:r:109:THR:HG23	2.18	0.43
41:s:142:TYR:CE2	41:s:289:LEU:HD11	2.54	0.43
42:u:149:ASP:HA	42:u:150:PRO:HD3	1.88	0.43
43:v:50:GLN:O	43:v:56:ARG:NH1	2.41	0.43
62:AE:40:LEU:O	62:AE:44:VAL:HG23	2.19	0.43
67:AK:227:HIS:N	67:AK:228:PRO:HD2	2.33	0.43
60:AP:125:VAL:CG2	71:AQ:101:PLX:H141	2.49	0.43
65:AU:91:PRO:HA	65:AU:92:PRO:HD3	1.84	0.43
67:AW:79:THR:HG23	67:AW:205:LEU:HD23	2.00	0.43
67:AW:346:ALA:O	67:AW:350:VAL:HG23	2.19	0.43
3:C:150:MET:HE3	3:C:185:PRO:HG2	1.99	0.43
12:M:66:HIS:CE1	12:M:68:ARG:HG2	2.53	0.43
12:M:200:ARG:HB3	14:O:118:PHE:CD1	2.54	0.43
14:O:104:VAL:HG12	14:O:105:LEU:HD12	2.00	0.43
22:Y:58:SER:HB2	35:l:371:THR:HG21	2.01	0.43
24:a:185:ALA:O	42:u:48:TRP:HZ2	2.01	0.43
25:b:115:GLU:CG	25:b:116:VAL:N	2.82	0.43
30:g:82:TYR:OH	32:i:341:PRO:O	2.35	0.43
33:j:106:TRP:HZ3	41:s:291:LYS:HA	1.84	0.43
37:n:39:ARG:HB2	37:n:57:TRP:CZ2	2.53	0.43
40:r:87:GLU:O	40:r:92:LYS:HE3	2.18	0.43
42:u:80:GLU:N	42:u:81:PRO:HD2	2.33	0.43
45:x:106:PRO:HB2	45:x:107:PRO:HD3	2.01	0.43
45:x:377:PHE:CD2	79:x:604:HEA:HAD1	2.54	0.43
48:0:126:MET:HG3	48:0:128:VAL:HG23	2.00	0.43
54:6:11:LEU:HD23	54:6:11:LEU:C	2.44	0.43
54:6:36:MET:O	54:6:40:LEU:HG	2.18	0.43
63:AF:99:ILE:O	63:AF:103:LYS:HG2	2.19	0.43
66:AJ:8:ASN:OD1	66:AJ:9:PRO:HD2	2.19	0.43
66:AJ:331:ASP:HA	66:AJ:334:ILE:HD12	2.01	0.43
67:AK:127:ARG:NH1	67:AK:224:GLY:O	2.49	0.43
68:AL:58:ARG:HB2	68:AL:230:VAL:HG22	2.01	0.43
68:AL:133:ILE:HG22	68:AL:134:LYS:N	2.33	0.43
65:AU:156:ASP:OD1	65:AU:157:GLY:N	2.43	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AY:287:VAL:HG12	68:AY:458:GLY:HA2	2.01	0.43
4:E:126:HIS:HD2	12:M:612:PRO:HD2	1.84	0.43
5:F:67:ALA:HB3	5:F:75:THR:OG1	2.18	0.43
9:J:56:ALA:HA	9:J:125:VAL:HG23	2.01	0.43
9:J:167:VAL:HG22	9:J:201:VAL:HB	2.00	0.43
11:L:77:VAL:HG22	11:L:78:ARG:N	2.33	0.43
12:M:381:LEU:C	12:M:383:SER:N	2.77	0.43
16:Q:164:PRO:HA	16:Q:165:PRO:HD3	1.83	0.43
71:V:203:PLX:H332	71:V:203:PLX:H141	2.01	0.43
25:b:71:VAL:O	25:b:75:VAL:HB	2.18	0.43
26:c:154:GLN:C	26:c:156:VAL:HG23	2.44	0.43
32:i:71:LEU:HA	32:i:71:LEU:HD23	1.73	0.43
35:l:280:LEU:O	35:l:284:THR:HG23	2.19	0.43
75:n:101:CDL:H741	75:n:101:CDL:H711	1.60	0.43
46:y:52:HIS:CD2	49:l:40:ASP:HB2	2.54	0.43
46:y:122:MET:HB2	46:y:208:PRO:CD	2.47	0.43
57:9:37:LEU:HD23	57:9:37:LEU:HA	1.84	0.43
63:AF:70:ASN:ND2	66:AJ:209:LEU:HG	2.33	0.43
64:AG:45:VAL:HA	64:AG:46:PRO:HD3	1.80	0.43
75:AH:403:CDL:OB8	75:AH:403:CDL:O1	2.35	0.43
67:AK:293:LEU:HD21	67:AK:358:VAL:HG22	2.00	0.43
67:AK:326:PHE:HB3	67:AK:337:GLY:O	2.19	0.43
68:AL:322:VAL:HG12	68:AL:323:HIS:N	2.31	0.43
60:AP:80:HIS:CD2	60:AP:81:THR:HG23	2.54	0.43
60:AP:82:ASP:OD1	60:AP:83:ILE:N	2.51	0.43
66:AV:171:ASP:OD1	66:AV:172:SER:N	2.50	0.43
66:AV:206:ASN:H	82:AV:402:HEM:CGD	2.31	0.43
67:AW:262:ASN:O	67:AW:443:ASN:HA	2.18	0.43
67:AW:323:VAL:HG22	67:AW:340:THR:HG22	1.99	0.43
68:AY:295:GLY:HA2	68:AY:351:THR:O	2.19	0.43
1:A:40:ARG:NH1	1:A:289:GLU:O	2.40	0.43
2:B:99:HIS:ND1	2:B:147:MET:HE1	2.34	0.43
3:C:156:GLY:O	3:C:161:HIS:ND1	2.52	0.43
4:E:43:VAL:O	4:E:47:VAL:HG23	2.19	0.43
4:E:80:ASP:OD1	4:E:81:LEU:N	2.52	0.43
9:J:125:VAL:HG12	9:J:163:LYS:HB2	2.00	0.43
12:M:243:TRP:CD1	12:M:244:GLU:HG3	2.54	0.43
15:P:163:ALA:O	15:P:167:GLU:HB2	2.17	0.43
16:Q:82:LEU:HD23	16:Q:82:LEU:HA	1.78	0.43
16:Q:144:MET:HA	16:Q:147:ASN:HD22	1.84	0.43
20:V:19:HIS:CD2	20:V:20:ARG:HG3	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:66:ARG:O	24:a:70:LEU:HG	2.19	0.43
29:f:28:LYS:HE3	44:w:101:GLY:H	1.83	0.43
32:i:76:PHE:CZ	32:i:80:LEU:HD11	2.54	0.43
34:k:97:GLN:CD	35:l:587:TYR:HE1	2.27	0.43
35:l:209:SER:O	35:l:212:PRO:HD2	2.19	0.43
35:l:217:LEU:O	35:l:217:LEU:HD23	2.19	0.43
35:l:222:GLY:HA2	35:l:229:LEU:CD1	2.43	0.43
39:p:49:GLU:O	39:p:52:LYS:HG2	2.19	0.43
44:w:163:ILE:HD12	44:w:166:ASP:OD2	2.19	0.43
50:2:53:THR:HG22	50:2:54:ASN:OD1	2.19	0.43
55:7:44:PRO:HA	55:7:47:ARG:NH1	2.34	0.43
58:AA:74:ASN:OD1	58:AA:78:TYR:CE2	2.72	0.43
60:AC:200:HIS:O	60:AC:204:ARG:HG3	2.18	0.43
68:AL:121:ASN:HB3	68:AL:132:TYR:CZ	2.54	0.43
68:AL:350:GLU:HG2	68:AL:351:THR:HG23	2.00	0.43
61:AQ:44:TYR:HB2	65:AU:290:LEU:HD13	2.01	0.43
75:AU:403:CDL:H742	75:AU:403:CDL:H711	1.77	0.43
66:AV:333:LEU:HD21	76:AV:403:PEE:C40	2.48	0.43
2:B:175:THR:HB	2:B:180:GLU:OE1	2.19	0.43
8:I:5:THR:HB	8:I:8:ILE:HD12	2.00	0.43
9:J:61:ALA:HA	9:J:66:GLY:HA3	2.00	0.43
9:J:204:SER:OG	9:J:240:VAL:HG23	2.18	0.43
9:J:283:VAL:O	9:J:357:ARG:NH2	2.51	0.43
12:M:153:PHE:C	12:M:154:LEU:HD12	2.44	0.43
13:N:106:ARG:O	13:N:109:ILE:HG12	2.18	0.43
15:P:129:VAL:HG22	15:P:144:LYS:HB3	2.01	0.43
15:P:171:TRP:CZ3	15:P:177:PHE:HA	2.54	0.43
16:Q:119:GLY:H	16:Q:463:ARG:C	2.27	0.43
16:Q:410:TYR:O	16:Q:422:CYS:HA	2.19	0.43
24:a:170:TYR:CD1	30:g:5:ARG:HD3	2.54	0.43
31:h:73:MET:HG2	36:m:124:TRP:CH2	2.54	0.43
33:j:68:GLU:HG3	33:j:98:LEU:HD21	2.01	0.43
35:l:67:HIS:ND1	35:l:75:GLN:HG3	2.33	0.43
35:l:68:TRP:HB2	35:l:76:LEU:HD12	2.01	0.43
35:l:95:PHE:HZ	35:l:456:ARG:HG2	1.82	0.43
36:m:26:ILE:HD13	41:s:121:TRP:CE2	2.54	0.43
36:m:56:PHE:CZ	41:s:111:LEU:HD11	2.54	0.43
39:p:104:LEU:HD22	39:p:122:ARG:NH2	2.33	0.43
40:r:45:ILE:O	40:r:45:ILE:HG22	2.19	0.43
40:r:122:PHE:CE1	40:r:238:LEU:HD21	2.54	0.43
41:s:251:SER:HA	41:s:252:PRO:HD2	1.85	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AF:27:PHE:HD1	63:AF:28:ASN:N	2.17	0.43
67:AK:105:ALA:HA	68:AL:390:ARG:HG3	2.00	0.43
75:AU:403:CDL:OA6	66:AV:230:LEU:HD23	2.19	0.43
67:AW:61:ILE:HG22	67:AW:222:GLY:HA2	1.99	0.43
1:A:134:ASP:N	1:A:135:PRO:HD3	2.34	0.43
1:A:418:GLN:CD	12:M:115:GLY:HA2	2.44	0.43
4:E:48:HIS:HE1	9:J:363:SER:O	2.02	0.43
4:E:118:PHE:HZ	12:M:621:LYS:HG3	1.83	0.43
5:F:87:VAL:O	5:F:91:LEU:HG	2.18	0.43
9:J:131:GLY:HA3	73:J:401:NDP:O3D	2.19	0.43
9:J:293:LEU:HD23	9:J:298:TYR:HD1	1.84	0.43
12:M:342:ALA:O	12:M:369:GLU:HG2	2.19	0.43
13:N:73:THR:HG22	13:N:74:PHE:N	2.34	0.43
14:O:108:PRO:HA	14:O:109:PRO:HD3	1.78	0.43
16:Q:295:GLY:HA2	16:Q:321:GLY:HA3	2.01	0.43
21:W:33:TYR:O	21:W:34:SER:OG	2.27	0.43
21:W:72:LEU:HD23	21:W:72:LEU:HA	1.84	0.43
22:Y:74:TRP:C	22:Y:74:TRP:CD2	2.97	0.43
26:c:44:THR:HB	26:c:47:GLU:CG	2.49	0.43
26:c:102:GLY:HA3	38:o:43:LEU:HD13	2.00	0.43
30:g:51:PRO:HG2	30:g:55:ALA:CA	2.49	0.43
32:i:214:THR:HG22	32:i:329:LEU:HB3	2.01	0.43
32:i:258:THR:CG2	32:i:336:LEU:HB3	2.48	0.43
34:k:39:SER:HB3	36:m:16:PHE:HE2	1.84	0.43
35:l:227:LEU:HD22	35:l:283:ILE:HG22	2.00	0.43
35:l:548:LEU:O	35:l:552:LEU:HB2	2.18	0.43
35:l:550:LEU:HA	35:l:554:ASP:HB3	2.01	0.43
76:l:701:PEE:H36	40:r:155:VAL:CG2	2.46	0.43
41:s:55:LEU:HD13	41:s:221:ALA:HB2	2.01	0.43
41:s:150:LEU:O	41:s:154:LEU:HG	2.19	0.43
45:x:131:PRO:HB2	46:y:159:VAL:HA	2.00	0.43
45:x:247:ILE:HB	79:x:604:HEA:HBC1	2.01	0.43
53:5:21:ILE:O	53:5:25:PHE:HD2	2.02	0.43
62:AE:21:GLU:HA	62:AE:24:GLU:CB	2.49	0.43
63:AF:51:LEU:CD2	63:AF:55:LEU:HD13	2.49	0.43
59:AO:28:PRO:O	67:AW:170:GLN:NE2	2.52	0.43
65:AU:114:PHE:HE2	65:AU:148:LEU:HD21	1.83	0.43
68:AY:74:TRP:CG	68:AY:414:GLY:HA3	2.54	0.43
1:A:403:ASP:HA	1:A:453:PHE:CE2	2.54	0.42
2:B:78:GLU:HG3	17:S:1:MET:SD	2.59	0.42
2:B:84:TYR:OH	3:C:192:TYR:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:28:ALA:HA	4:E:31:ARG:HG3	1.99	0.42
9:J:124:ASN:OD1	9:J:125:VAL:N	2.51	0.42
9:J:180:TYR:O	9:J:184:LYS:HG3	2.19	0.42
9:J:221:HIS:ND1	9:J:222:ARG:HG3	2.31	0.42
14:O:163:THR:HG22	14:O:170:THR:HG22	2.01	0.42
16:Q:372:LYS:HD2	18:T:93:ALA:HA	2.00	0.42
20:V:62:THR:HG22	20:V:104:ARG:CD	2.49	0.42
20:V:95:CYS:O	20:V:99:LEU:HG	2.19	0.42
71:b:201:PLX:C2	27:d:43:ARG:HH22	2.31	0.42
26:c:61:ASP:O	26:c:63:GLU:HG3	2.19	0.42
30:g:15:ASP:HB2	30:g:18:ARG:NH2	2.29	0.42
30:g:32:TYR:CE2	32:i:339:ILE:HD11	2.54	0.42
30:g:51:PRO:HB2	30:g:54:THR:OG1	2.19	0.42
32:i:234:TRP:HH2	32:i:305:LEU:HB2	1.83	0.42
32:i:298:TYR:HE2	40:r:147:THR:HG23	1.83	0.42
33:j:64:LEU:HD23	33:j:64:LEU:HA	1.81	0.42
34:k:7:ASN:ND2	36:m:9:SER:CA	2.83	0.42
36:m:27:TYR:HA	36:m:30:LEU:HD12	2.01	0.42
36:m:43:ILE:HG22	36:m:48:GLY:HA3	2.00	0.42
39:p:48:PHE:CZ	72:p:201:8Q1:C8	2.99	0.42
40:r:308:SER:HB3	40:r:384:THR:HG21	2.01	0.42
46:y:63:THR:HA	46:y:66:THR:HG22	2.00	0.42
47:z:60:ASP:O	47:z:64:GLU:HG3	2.18	0.42
47:z:63:ARG:HA	47:z:67:PHE:CD2	2.53	0.42
63:AF:110:LYS:HG3	63:AF:111:LYS:HG3	2.02	0.42
75:AH:403:CDL:H122	66:AJ:234:LEU:HD12	2.01	0.42
66:AJ:197:LEU:HD22	75:AJ:404:CDL:H162	2.01	0.42
67:AK:82:LEU:O	67:AK:86:THR:HG23	2.20	0.42
67:AK:178:HIS:HE1	67:AK:330:TYR:HE2	1.66	0.42
67:AK:355:TYR:CE2	67:AK:359:LYS:HD2	2.54	0.42
76:AL:503:PEE:H1	76:AL:503:PEE:H13	1.74	0.42
59:AO:46:LYS:HG2	59:AO:47:ARG:O	2.18	0.42
65:AU:292:MET:CE	66:AV:241:THR:CG2	2.96	0.42
1:A:274:LYS:NZ	1:A:351:THR:O	2.51	0.42
2:B:117:CYS:HB2	69:B:301:SF4:S1	2.59	0.42
2:B:158:GLU:O	16:Q:368:ARG:NH2	2.52	0.42
3:C:175:PRO:HB3	9:J:96:PRO:HD3	2.01	0.42
8:I:42:PRO:HG3	16:Q:354:GLY:O	2.19	0.42
10:K:82:TYR:HB3	14:O:62:ARG:HH22	1.84	0.42
12:M:133:GLN:HA	12:M:136:GLU:OE2	2.17	0.42
12:M:153:PHE:O	12:M:154:LEU:HD12	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:573:GLY:HA3	13:N:137:TRP:CD1	2.54	0.42
12:M:651:PRO:O	12:M:654:VAL:HG22	2.19	0.42
16:Q:86:PRO:CG	33:j:41:PHE:HE2	2.29	0.42
16:Q:267:ILE:HB	41:s:278:PRO:HG2	2.02	0.42
18:T:102:ASN:HD21	18:T:104:ASP:HB2	1.84	0.42
20:V:133:TRP:CG	76:V:202:PEE:H7	2.54	0.42
24:a:78:THR:OG1	28:e:96:SER:O	2.24	0.42
24:a:87:THR:CG2	71:b:201:PLX:C13	2.87	0.42
30:g:61:LEU:O	30:g:65:THR:HG23	2.19	0.42
31:h:58:ILE:HD12	42:u:145:ARG:NH2	2.34	0.42
33:j:49:VAL:CG1	36:m:75:ILE:H	2.32	0.42
40:r:179:LEU:O	40:r:248:LEU:HD13	2.19	0.42
41:s:195:ARG:O	41:s:198:PHE:N	2.52	0.42
46:y:5:MET:CE	55:7:42:PRO:HA	2.45	0.42
76:AH:401:PEE:H61	66:AJ:236:LEU:HD13	2.01	0.42
66:AJ:312:GLN:HG3	66:AJ:379:TRP:HH2	1.84	0.42
67:AK:138:LEU:O	67:AK:142:THR:N	2.52	0.42
67:AK:195:TYR:CE2	67:AK:196:ARG:HG2	2.54	0.42
68:AL:156:LEU:HB3	68:AL:161:ILE:HD11	2.01	0.42
68:AL:267:PRO:HA	68:AL:350:GLU:OE1	2.18	0.42
63:AS:8:SER:OG	63:AS:9:ALA:N	2.51	0.42
66:AV:326:TRP:CZ2	76:AV:403:PEE:O5	2.72	0.42
67:AW:82:LEU:O	67:AW:86:THR:HG23	2.19	0.42
68:AY:64:SER:N	68:AY:235:GLY:O	2.49	0.42
1:A:37:ASP:OD2	14:O:235:THR:N	2.49	0.42
1:A:257:ARG:HH12	14:O:239:LYS:NZ	2.17	0.42
70:A:502:FMN:H4'	70:A:502:FMN:H1'2	1.63	0.42
15:P:90:PRO:O	15:P:93:VAL:HG23	2.18	0.42
15:P:97:LEU:HD11	15:P:130:TYR:CE2	2.54	0.42
15:P:109:LYS:O	15:P:110:SER:OG	2.31	0.42
16:Q:116:LEU:O	16:Q:118:ARG:HG3	2.19	0.42
16:Q:167:ALA:O	16:Q:171:ARG:HG3	2.18	0.42
16:Q:338:ARG:O	16:Q:341:LEU:HB2	2.19	0.42
17:S:53:ARG:HB2	31:h:105:ARG:CZ	2.49	0.42
18:T:79:GLU:OE1	18:T:122:HIS:HB3	2.19	0.42
22:Y:40:ILE:HD11	35:l:446:ASN:ND2	2.34	0.42
23:Z:18:ASP:OD1	23:Z:19:TYR:N	2.52	0.42
28:e:87:MET:HE3	28:e:87:MET:HB3	1.77	0.42
35:l:149:ILE:HD12	40:r:369:LEU:HD11	2.01	0.42
35:l:548:LEU:HD22	38:o:93:CYS:HB3	2.01	0.42
36:m:86:VAL:O	36:m:90:VAL:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:67:ALA:O	42:u:70:PHE:HB3	2.19	0.42
43:v:5:LEU:HG	43:v:6:VAL:N	2.34	0.42
46:y:100:MET:HE3	46:y:157:GLU:HG3	2.02	0.42
58:AA:3:ARG:HH12	66:AJ:217:LYS:CE	2.32	0.42
59:AB:50:LEU:HD23	59:AB:51:SER:O	2.20	0.42
62:AE:78:ARG:O	62:AE:82:VAL:HG23	2.19	0.42
67:AK:407:MET:HE2	67:AK:412:VAL:HA	2.01	0.42
67:AK:449:PHE:CE2	67:AW:183:ARG:HB3	2.54	0.42
60:AP:244:ASP:OD2	60:AP:248:ARG:HB2	2.18	0.42
65:AU:292:MET:CE	66:AV:241:THR:HG22	2.49	0.42
66:AV:123:THR:HG22	66:AV:189:ILE:HD13	2.00	0.42
67:AW:90:THR:HG22	67:AW:150:GLU:OE1	2.19	0.42
1:A:129:GLU:OE1	1:A:132:ARG:NH1	2.49	0.42
1:A:220:GLN:NE2	14:O:114:GLU:HB3	2.34	0.42
1:A:227:PRO:HB2	1:A:228:PRO:HD3	2.00	0.42
1:A:282:VAL:HA	1:A:307:VAL:HA	2.00	0.42
1:A:314:LEU:O	1:A:315:LEU:HD12	2.19	0.42
4:E:99:GLN:NE2	33:j:41:PHE:CD1	2.82	0.42
6:G:93:ILE:HG12	6:G:94:ASP:O	2.19	0.42
7:H:21:HIS:NE2	7:H:63:PRO:O	2.52	0.42
7:H:47:TYR:OH	8:I:92:LYS:HG3	2.20	0.42
8:I:40:LYS:HG2	21:W:8:GLN:HA	2.00	0.42
11:L:79:ILE:HD12	11:L:145:TYR:CD2	2.54	0.42
12:M:307:VAL:HA	12:M:582:VAL:HA	2.01	0.42
12:M:559:ASP:OD1	12:M:560:LEU:N	2.51	0.42
13:N:66:THR:HG23	13:N:74:PHE:H	1.85	0.42
14:O:164:THR:HG23	14:O:167:LYS:N	2.34	0.42
15:P:200:LYS:HE2	16:Q:420:TYR:CE1	2.55	0.42
16:Q:116:LEU:HD11	16:Q:141:TYR:OH	2.20	0.42
18:T:52:ARG:O	18:T:55:ARG:HG2	2.20	0.42
19:U:40:LYS:O	19:U:44:MET:HG2	2.18	0.42
30:g:37:GLY:O	30:g:40:SER:OG	2.28	0.42
31:h:17:TRP:CZ3	31:h:18:LEU:HB2	2.55	0.42
32:i:109:ALA:CB	32:i:112:HIS:HD2	2.33	0.42
37:n:51:PRO:O	37:n:53:GLU:HG3	2.20	0.42
39:p:90:SER:HB2	39:p:93:ARG:HE	1.84	0.42
41:s:169:GLN:NE2	41:s:241:ILE:O	2.42	0.42
41:s:231:ILE:HG23	41:s:270:PHE:CD2	2.53	0.42
53:5:35:TYR:O	53:5:39:VAL:HB	2.19	0.42
54:6:31:LEU:HA	54:6:31:LEU:HD23	1.83	0.42
60:AC:132:ALA:HB1	76:AH:401:PEE:H27	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:AC:239:HIS:HB2	74:AC:301:FES:S1	2.59	0.42
68:AL:51:SER:HB2	68:AL:59:VAL:HB	2.01	0.42
68:AL:87:ASN:HD21	68:AL:199:GLN:HB2	1.85	0.42
68:AL:294:PRO:HB2	68:AL:301:ASN:ND2	2.34	0.42
76:AL:503:PEE:C33	76:AL:503:PEE:C17	2.97	0.42
60:AP:207:LYS:HA	60:AP:208:PRO:HD3	1.84	0.42
65:AU:290:LEU:HD23	65:AU:290:LEU:O	2.19	0.42
67:AW:373:ALA:O	67:AW:377:LYS:HG3	2.19	0.42
68:AY:88:GLY:O	68:AY:92:PHE:HB2	2.19	0.42
1:A:52:ARG:O	1:A:55:GLY:N	2.51	0.42
1:A:270:ASN:CG	1:A:338:ASP:HB2	2.44	0.42
2:B:176:GLU:OE1	3:C:200:LYS:HD2	2.20	0.42
7:H:83:GLN:HG2	15:P:107:GLN:HE21	1.84	0.42
9:J:128:ASN:O	9:J:129:LEU:HD12	2.19	0.42
11:L:170:THR:HG22	12:M:423:LEU:O	2.18	0.42
12:M:542:PRO:HB2	12:M:543:LYS:HD3	2.01	0.42
14:O:46:GLU:C	14:O:49:PRO:HD3	2.44	0.42
16:Q:39:PRO:HD2	32:i:304:LEU:O	2.19	0.42
6:X:105:MET:HE2	6:X:139:MET:HE3	2.00	0.42
25:b:51:LEU:HD22	25:b:59:LYS:HA	2.01	0.42
26:c:119:THR:HB	38:o:13:THR:HG23	2.02	0.42
30:g:87:ARG:HD2	42:u:156:GLY:O	2.19	0.42
32:i:26:TRP:HD1	32:i:84:TRP:O	2.02	0.42
37:n:40:ASN:HD22	37:n:56:THR:HG23	1.82	0.42
75:n:101:CDL:H712	75:n:101:CDL:H512	2.01	0.42
40:r:10:MET:O	40:r:13:PRO:HD2	2.20	0.42
40:r:398:LEU:HA	40:r:398:LEU:HD23	1.81	0.42
71:r:502:PLX:H311	71:r:502:PLX:H282	1.75	0.42
41:s:18:ALA:O	41:s:21:MET:HG2	2.19	0.42
41:s:90:PRO:HB2	41:s:92:PRO:O	2.18	0.42
50:2:86:GLY:O	50:2:87:THR:O	2.37	0.42
51:3:54:ARG:N	51:3:54:ARG:CD	2.80	0.42
56:8:41:ARG:HD2	57:9:40:TYR:CZ	2.54	0.42
65:AH:214:LEU:O	65:AH:234:ASN:ND2	2.41	0.42
66:AJ:214:HIS:ND1	66:AJ:217:LYS:NZ	2.68	0.42
67:AK:330:TYR:HB2	67:AK:333:SER:O	2.20	0.42
58:AN:82:LYS:HE2	62:AR:65:GLU:HB2	2.02	0.42
59:AO:14:VAL:HA	67:AW:113:THR:HA	2.01	0.42
60:AP:217:CYS:SG	60:AP:243:TYR:OH	2.59	0.42
66:AV:346:PRO:O	66:AV:349:ILE:HG22	2.19	0.42
1:A:32:PHE:HB3	1:A:294:VAL:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:ARG:NH2	33:j:37:TYR:HD2	2.17	0.42
6:G:116:VAL:HA	6:G:119:ILE:HG22	2.01	0.42
9:J:336:GLU:C	9:J:339:GLY:H	2.28	0.42
11:L:154:LYS:HG2	12:M:279:GLU:HG3	2.02	0.42
12:M:319:TRP:HH2	12:M:617:ARG:NE	2.18	0.42
17:S:55:SER:C	17:S:64:LYS:HZ1	2.28	0.42
24:a:54:LEU:CD2	25:b:26:GLN:C	2.87	0.42
24:a:101:ILE:HG13	27:d:58:TYR:CB	2.49	0.42
25:b:117:ILE:CG2	25:b:118:PRO:HD2	2.50	0.42
71:b:201:PLX:C6	71:b:201:PLX:C11	2.85	0.42
26:c:101:TRP:CD1	38:o:62:ASN:HD22	2.38	0.42
31:h:74:ARG:HG2	36:m:116:VAL:HG13	2.02	0.42
35:l:14:SER:O	35:l:17:PRO:HD2	2.20	0.42
35:l:93:ALA:O	35:l:97:THR:OG1	2.38	0.42
37:n:50:GLN:HG3	37:n:51:PRO:CD	2.50	0.42
43:v:79:ALA:C	43:v:81:LYS:H	2.26	0.42
44:w:143:TYR:OH	44:w:162:SER:HB2	2.20	0.42
45:x:495:LEU:HA	45:x:495:LEU:HD23	1.68	0.42
68:AL:233:ALA:HB3	68:AL:242:LEU:HD22	2.01	0.42
68:AL:324:LEU:O	68:AL:325:SER:OG	2.32	0.42
58:AN:49:VAL:HG21	76:AV:403:PEE:H7	2.02	0.42
65:AU:221:PRO:HA	65:AU:222:PRO:HD3	1.85	0.42
75:AU:403:CDL:O1	75:AU:403:CDL:HB61	2.20	0.42
68:AY:284:PHE:C	68:AY:461:PRO:HD2	2.45	0.42
3:C:150:MET:SD	3:C:190:LEU:HD13	2.60	0.42
4:E:102:HIS:HA	4:E:105:ARG:HG3	2.02	0.42
12:M:254:MET:CB	12:M:290:THR:HG22	2.46	0.42
12:M:492:ALA:O	12:M:496:ILE:HG13	2.19	0.42
16:Q:70:ASP:HB2	16:Q:71:PRO:HD3	2.02	0.42
16:Q:275:ILE:HD13	16:Q:446:ASP:OD1	2.20	0.42
16:Q:358:VAL:O	16:Q:364:SER:OG	2.24	0.42
19:U:69:HIS:CE1	19:U:70:PRO:HA	2.54	0.42
6:X:155:TYR:CD2	6:X:155:TYR:O	2.73	0.42
26:c:94:GLN:OE1	26:c:99:LEU:HB2	2.20	0.42
26:c:125:SER:O	26:c:129:MET:HG3	2.20	0.42
26:c:183:HIS:CB	43:v:37:ARG:HA	2.50	0.42
27:d:134:GLN:OE1	38:o:124:THR:HA	2.20	0.42
31:h:94:PRO:O	31:h:97:HIS:N	2.52	0.42
35:l:158:TRP:CH2	35:l:240:PRO:HB3	2.55	0.42
35:l:404:THR:HB	35:l:405:ASN:H	1.66	0.42
39:p:31:CYS:HB3	39:p:36:LYS:HD2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:48:PHE:HE1	72:p:201:8Q1:C6	2.33	0.42
40:r:374:ASN:OD1	40:r:374:ASN:N	2.52	0.42
45:x:462:LEU:O	45:x:466:MET:HG3	2.20	0.42
47:z:40:MET:O	47:z:41:THR:C	2.62	0.42
55:7:9:PHE:CD1	55:7:9:PHE:C	2.97	0.42
61:AD:39:GLY:O	61:AD:43:ILE:HG12	2.19	0.42
76:AH:401:PEE:C12	66:AJ:240:MET:CE	2.91	0.42
58:AN:48:ARG:HE	66:AV:319:PRO:HB3	1.84	0.42
1:A:159:ARG:HD3	1:A:162:PHE:CE2	2.55	0.42
2:B:133:ARG:NH2	18:T:69:ILE:HG13	2.34	0.42
4:E:25:MET:O	4:E:29:LYS:N	2.44	0.42
4:E:78:VAL:O	4:E:82:LEU:HD13	2.20	0.42
5:F:62:GLN:HE21	5:F:64:LYS:NZ	2.17	0.42
6:G:87:LEU:HA	6:G:90:TYR:HB3	2.00	0.42
7:H:7:LYS:O	7:H:8:THR:OG1	2.29	0.42
8:I:60:ARG:HD2	16:Q:390:GLN:O	2.19	0.42
9:J:98:GLY:HA3	9:J:103:LEU:HG	2.01	0.42
9:J:171:ASN:O	9:J:181:LEU:HG	2.18	0.42
9:J:240:VAL:HG22	9:J:266:VAL:C	2.45	0.42
9:J:283:VAL:HG13	9:J:369:VAL:HG11	2.02	0.42
12:M:33:GLU:O	12:M:98:LYS:HA	2.20	0.42
12:M:49:VAL:HG23	12:M:94:MET:O	2.20	0.42
13:N:10:GLY:O	13:N:14:ILE:HG13	2.20	0.42
14:O:100:LYS:O	14:O:104:VAL:HG23	2.20	0.42
16:Q:371:MET:HA	16:Q:377:SER:OG	2.20	0.42
18:T:83:ARG:HH12	18:T:103:LEU:H	1.68	0.42
21:W:57:ARG:NH2	41:s:316:PRO:HG3	2.35	0.42
76:W:201:PEE:H36	33:j:7:LEU:CD2	2.47	0.42
76:W:201:PEE:H60	36:m:56:PHE:HZ	1.84	0.42
24:a:57:ILE:HA	39:p:104:LEU:HD12	2.01	0.42
25:b:117:ILE:HG23	25:b:118:PRO:HD2	2.01	0.42
26:c:81:ARG:HD3	26:c:85:GLU:OE1	2.20	0.42
26:c:100:ASN:HB2	26:c:103:GLU:HG3	2.02	0.42
27:d:24:ILE:HD11	35:l:56:CYS:HB3	2.02	0.42
27:d:162:LYS:O	27:d:165:LYS:HB3	2.20	0.42
32:i:79:MET:HE3	34:k:5:TYR:CD2	2.55	0.42
32:i:120:GLN:HA	32:i:176:ARG:HE	1.85	0.42
32:i:217:LEU:HD23	32:i:217:LEU:HA	1.86	0.42
36:m:33:ILE:HD11	41:s:114:TYR:CE1	2.55	0.42
36:m:40:CYS:O	36:m:44:LEU:HG	2.19	0.42
41:s:11:VAL:N	41:s:12:PRO:HD2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:6:30:ILE:HG13	54:6:31:LEU:N	2.33	0.42
66:AJ:163:TRP:CG	75:AJ:405:CDL:H331	2.55	0.42
67:AK:347:ALA:O	67:AK:351:ILE:HG12	2.20	0.42
58:AN:11:MET:SD	63:AS:64:LYS:HD2	2.60	0.42
58:AN:19:LEU:HD11	60:AP:88:PHE:CB	2.50	0.42
61:AQ:18:THR:HG22	68:AY:480:PHE:OXT	2.19	0.42
71:AT:101:PLX:H1A2	71:AT:101:PLX:H21	1.78	0.42
67:AW:271:PHE:CZ	67:AW:338:ILE:HB	2.55	0.42
68:AY:58:ARG:HH11	68:AY:230:VAL:HG22	1.85	0.42
1:A:453:PHE:O	1:A:456:GLN:HG2	2.20	0.42
2:B:166:VAL:HG11	2:B:199:ILE:CG2	2.49	0.42
7:H:81:ILE:HG13	7:H:82:LEU:N	2.34	0.42
9:J:209:ARG:HD2	15:P:217:LYS:CE	2.50	0.42
9:J:263:PHE:CE1	9:J:333:PRO:HG2	2.55	0.42
11:L:130:THR:O	11:L:133:ASP:HB3	2.19	0.42
12:M:198:THR:CG2	14:O:39:PHE:HB3	2.47	0.42
12:M:314:LEU:HD22	12:M:583:ILE:HD12	2.02	0.42
12:M:342:ALA:HA	12:M:547:LEU:HB2	2.00	0.42
12:M:560:LEU:HD12	12:M:561:PRO:HD2	2.02	0.42
12:M:589:TYR:O	12:M:606:THR:HG21	2.19	0.42
12:M:598:ASN:N	12:M:602:ARG:O	2.48	0.42
14:O:176:CYS:HA	74:O:301:FES:S1	2.60	0.42
15:P:210:LEU:HA	15:P:221:ALA:HA	2.01	0.42
16:Q:190:HIS:CE1	16:Q:268:TRP:CH2	3.08	0.42
16:Q:233:HIS:CD2	16:Q:234:GLN:HB2	2.55	0.42
16:Q:235:ASP:HA	16:Q:356:ILE:HD12	2.01	0.42
22:Y:95:GLU:CD	22:Y:95:GLU:N	2.77	0.42
71:b:201:PLX:C10	71:b:201:PLX:C6	2.85	0.42
26:c:133:LEU:HD13	35:l:532:ILE:HD12	2.00	0.42
33:j:71:LEU:O	33:j:74:PRO:HD2	2.20	0.42
35:l:310:LEU:HD23	35:l:313:MET:HE3	2.01	0.42
37:n:16:LEU:HD21	40:r:10:MET:HE3	2.02	0.42
39:p:174:PRO:O	39:p:175:ARG:HB3	2.19	0.42
40:r:344:LEU:O	40:r:420:THR:HG21	2.20	0.42
43:v:59:CYS:O	43:v:87:TRP:HZ3	2.03	0.42
46:y:146:MET:SD	46:y:189:PRO:HB3	2.60	0.42
47:z:80:ARG:HG2	47:z:233:PHE:CE1	2.54	0.42
48:0:102:TYR:HD2	57:9:35:TYR:HE1	1.68	0.42
51:3:42:ARG:NH1	51:3:74:ARG:NH2	2.68	0.42
52:4:24:ASN:HD22	52:4:25:GLN:N	2.18	0.42
66:AJ:316:MET:HB3	76:AJ:403:PEE:O2P	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:AJ:405:CDL:H741	75:AJ:405:CDL:H711	1.59	0.42
67:AK:65:ILE:HG21	67:AK:213:PHE:HD1	1.83	0.42
76:AL:503:PEE:H19	76:AL:503:PEE:C30	2.47	0.42
59:AO:50:LEU:O	59:AO:51:SER:OG	2.33	0.42
60:AP:145:ASP:OD1	60:AP:146:VAL:N	2.53	0.42
81:AU:402:HEC:HBC3	81:AU:402:HEC:HHD	2.01	0.42
1:A:47:GLY:HA2	1:A:133:HIS:HB3	2.00	0.42
1:A:122:PRO:HB2	1:A:322:SER:HB2	2.01	0.42
11:L:131:LYS:HD2	11:L:147:ILE:CG2	2.49	0.42
12:M:357:LEU:O	12:M:361:VAL:HG22	2.20	0.42
12:M:543:LYS:N	12:M:543:LYS:HD2	2.35	0.42
12:M:711:VAL:O	12:M:715:THR:HG23	2.19	0.42
14:O:93:LEU:HA	14:O:94:PRO:HD2	1.86	0.42
14:O:144:ASN:O	14:O:147:SER:OG	2.35	0.42
15:P:202:PHE:HB2	15:P:207:TYR:CE2	2.55	0.42
15:P:240:GLU:OE1	15:P:246:ARG:NE	2.51	0.42
17:S:53:ARG:CZ	31:h:105:ARG:NH2	2.83	0.42
18:T:40:THR:OG1	18:T:44:GLN:HG2	2.20	0.42
20:V:23:TYR:O	20:V:24:SER:HB2	2.20	0.42
24:a:149:LEU:HD23	24:a:149:LEU:HA	1.79	0.42
24:a:180:ASP:HB3	31:h:24:GLU:HG3	2.02	0.42
30:g:44:ASP:OD1	32:i:327:PRO:HG2	2.20	0.42
32:i:2:ASN:ND2	32:i:4:LEU:HB2	2.35	0.42
32:i:294:LEU:HD23	32:i:294:LEU:HA	1.74	0.42
33:j:12:LEU:O	33:j:16:LEU:HB2	2.20	0.42
35:l:7:MET:O	35:l:11:THR:HG23	2.20	0.42
35:l:305:SER:O	35:l:309:GLN:HG2	2.20	0.42
35:l:414:ILE:O	35:l:417:SER:OG	2.29	0.42
35:l:536:THR:O	35:l:539:TYR:HB3	2.20	0.42
35:l:558:LEU:HB3	40:r:214:LEU:HD11	2.02	0.42
44:w:223:ASP:HA	44:w:224:PRO:HD3	1.85	0.42
44:w:240:ALA:O	44:w:244:THR:OG1	2.14	0.42
60:AC:200:HIS:CE1	60:AC:202:LEU:HB3	2.55	0.42
63:AF:39:TYR:CE2	66:AJ:108:LEU:HD13	2.55	0.42
66:AJ:320:LEU:HB2	66:AJ:373:GLU:OE2	2.20	0.42
67:AK:79:THR:HG23	67:AK:205:LEU:HD23	2.02	0.42
68:AL:233:ALA:HB1	68:AL:237:VAL:HG21	2.01	0.42
68:AL:424:ILE:HA	68:AL:425:PRO:HD2	1.91	0.42
66:AV:271:GLU:HG3	66:AV:273:TYR:CZ	2.55	0.42
2:B:96:ARG:HB3	2:B:167:GLU:HG2	2.01	0.41
6:G:103:HIS:N	6:G:107:ASP:HB2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:179:ARG:HB3	9:J:179:ARG:HH11	1.84	0.41
11:L:86:ASN:ND2	12:M:224:ASP:OD2	2.53	0.41
12:M:83:GLU:HB2	12:M:101:ASN:HB3	2.02	0.41
12:M:433:GLY:HA3	12:M:684:LEU:HD23	2.01	0.41
14:O:53:PHE:HE2	14:O:55:PHE:CE1	2.38	0.41
14:O:213:ILE:HG22	14:O:214:PRO:O	2.20	0.41
16:Q:83:ASN:CA	16:Q:98:VAL:HG22	2.44	0.41
16:Q:199:PRO:HB3	16:Q:258:LEU:HD21	2.01	0.41
16:Q:368:ARG:HA	16:Q:371:MET:HG2	2.01	0.41
18:T:80:VAL:O	18:T:121:GLN:HA	2.20	0.41
24:a:129:PRO:CG	27:d:60:ARG:HH22	2.33	0.41
26:c:49:ALA:O	26:c:53:LYS:HG2	2.21	0.41
27:d:74:GLU:HB2	30:g:105:LYS:HD2	2.01	0.41
28:e:62:GLU:OE2	38:o:57:ARG:NH2	2.53	0.41
71:g:203:PLX:H22	71:g:203:PLX:H1B3	1.74	0.41
35:l:154:LEU:HD23	35:l:154:LEU:HA	1.85	0.41
40:r:245:ARG:HA	40:r:245:ARG:HD3	1.86	0.41
47:z:110:PRO:HB3	52:4:30:TRP:CD2	2.54	0.41
57:9:19:LEU:HD23	57:9:19:LEU:C	2.45	0.41
60:AC:200:HIS:HE1	60:AC:202:LEU:HB3	1.84	0.41
60:AC:246:SER:OG	60:AC:248:ARG:NE	2.47	0.41
61:AD:30:MET:SD	64:AG:34:TRP:HB2	2.60	0.41
63:AF:63:ILE:HD13	66:AJ:211:ILE:CG2	2.50	0.41
68:AL:240:GLN:HE22	68:AL:243:LEU:HD23	1.84	0.41
68:AL:407:THR:HB	68:AL:408:PRO:HD3	2.02	0.41
64:AT:24:TRP:HZ3	75:AY:501:CDL:H551	1.79	0.41
66:AV:149:LEU:O	66:AV:152:ALA:HB3	2.19	0.41
67:AW:43:LEU:HD13	67:AW:238:LEU:HD11	2.01	0.41
67:AW:257:GLU:HG2	67:AW:450:VAL:HB	2.02	0.41
68:AY:40:GLN:HB3	68:AY:44:PHE:HE2	1.84	0.41
68:AY:407:THR:HB	68:AY:408:PRO:HD3	2.01	0.41
1:A:27:PRO:HB2	1:A:28:LYS:H	1.65	0.41
2:B:128:ILE:HG12	2:B:143:TYR:CD1	2.55	0.41
7:H:44:TYR:CD2	7:H:94:MET:HE2	2.54	0.41
9:J:157:LYS:HA	9:J:195:PHE:HE1	1.85	0.41
15:P:96:VAL:O	15:P:100:LEU:HG	2.20	0.41
16:Q:290:GLY:C	16:Q:294:ARG:HE	2.28	0.41
16:Q:341:LEU:HA	16:Q:341:LEU:HD23	1.88	0.41
19:U:19:LEU:O	19:U:22:SER:OG	2.29	0.41
20:V:126:LYS:HE3	20:V:130:LEU:HD11	2.02	0.41
24:a:98:LEU:HB2	27:d:57:TYR:CE1	2.40	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:119:PRO:HB2	43:v:40:VAL:HG13	2.01	0.41
71:b:201:PLX:P1	71:b:201:PLX:O6	2.79	0.41
31:h:56:CYS:HA	42:u:145:ARG:HH12	1.84	0.41
35:l:106:TRP:CZ2	35:l:348:HIS:HD2	2.38	0.41
37:n:28:ASP:OD1	40:r:2:LEU:HB3	2.19	0.41
37:n:43:MET:HE3	37:n:43:MET:HB2	1.87	0.41
40:r:188:ASN:O	40:r:189:SER:OG	2.21	0.41
41:s:275:THR:OG1	41:s:276:ALA:N	2.53	0.41
44:w:93:TYR:CZ	44:w:142:GLN:OE1	2.73	0.41
45:x:264:LYS:NZ	46:y:56:MET:HE2	2.35	0.41
45:x:501:PRO:O	45:x:502:TYR:C	2.63	0.41
79:x:603:HEA:HHC	79:x:603:HEA:H122	2.02	0.41
51:3:77:PRO:HA	51:3:82:TYR:HA	2.01	0.41
60:AC:181:GLN:HA	60:AC:184:ILE:HD12	2.01	0.41
62:AE:29:PRO:HD3	65:AH:262:THR:CG2	2.37	0.41
63:AF:76:LEU:HD12	63:AF:77:PRO:HD2	2.02	0.41
66:AJ:9:PRO:HB3	66:AV:202:GLU:OE1	2.20	0.41
66:AJ:160:LEU:O	66:AJ:164:ILE:HD12	2.20	0.41
67:AK:80:THR:HA	67:AK:83:LEU:HB3	2.03	0.41
68:AL:35:THR:OG1	68:AL:36:ALA:N	2.52	0.41
58:AN:13:HIS:H	68:AY:279:ASP:H	1.67	0.41
66:AV:10:LEU:HD22	76:AY:502:PEE:C27	2.41	0.41
66:AV:320:LEU:O	66:AV:323:SER:OG	2.30	0.41
68:AY:373:GLN:NE2	68:AY:471:ILE:HG23	2.35	0.41
68:AY:392:LYS:O	68:AY:396:ARG:HG3	2.20	0.41
1:A:413:TRP:HZ3	1:A:436:GLN:HB3	1.84	0.41
2:B:140:THR:HG1	2:B:185:LYS:HZ2	1.60	0.41
3:C:118:ASP:CG	3:C:119:VAL:H	2.28	0.41
7:H:50:GLN:HE22	8:I:93:LYS:HD2	1.85	0.41
8:I:23:LYS:NZ	16:Q:252:SER:HG	2.18	0.41
8:I:94:ALA:HB1	15:P:105:ASN:HD21	1.84	0.41
9:J:152:ILE:HG22	9:J:164:PHE:CE1	2.55	0.41
13:N:117:VAL:HG11	13:N:122:GLU:HB2	2.02	0.41
16:Q:149:GLN:OE1	16:Q:171:ARG:HB3	2.20	0.41
16:Q:271:ARG:HH11	41:s:281:ARG:N	2.18	0.41
18:T:32:VAL:HG22	18:T:38:LYS:HE3	2.02	0.41
25:b:118:PRO:HA	25:b:119:PRO:HD3	1.94	0.41
30:g:51:PRO:HG2	30:g:55:ALA:CB	2.50	0.41
32:i:108:MET:SD	32:i:191:MET:HG3	2.60	0.41
32:i:307:MET:O	44:w:319:ILE:HD12	2.20	0.41
35:l:188:TRP:O	35:l:192:HIS:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:248:LEU:HD12	40:r:249:ILE:N	2.35	0.41
71:r:501:PLX:H282	71:r:501:PLX:H251	1.77	0.41
41:s:173:TRP:HZ3	41:s:262:LYS:HE2	1.86	0.41
42:u:104:GLN:HB3	42:u:108:ASP:OD2	2.20	0.41
44:w:62:VAL:HG21	44:w:74:ALA:HB2	2.02	0.41
44:w:77:ILE:HG23	44:w:81:LEU:HD13	2.03	0.41
44:w:86:PHE:HE2	44:w:146:ALA:HB2	1.86	0.41
45:x:314:ILE:HB	45:x:315:PRO:CD	2.50	0.41
46:y:98:LYS:HE3	46:y:98:LYS:HB2	1.80	0.41
47:z:42:LEU:HA	47:z:42:LEU:HD12	1.66	0.41
47:z:146:TRP:NE1	51:3:17:ARG:HB2	2.35	0.41
59:AB:53:GLU:O	68:AL:402:HIS:ND1	2.47	0.41
75:AG:101:CDL:C52	75:AG:101:CDL:C71	2.86	0.41
65:AH:266:ILE:O	65:AH:270:VAL:HG23	2.20	0.41
66:AJ:9:PRO:HG2	66:AV:199:PHE:CE1	2.55	0.41
66:AJ:147:THR:HG22	66:AJ:161:VAL:HG13	2.02	0.41
68:AL:360:CYS:SG	68:AL:365:ILE:HG12	2.60	0.41
60:AP:207:LYS:HE3	60:AP:209:GLU:OE2	2.20	0.41
62:AR:34:ARG:NH1	62:AR:78:ARG:NH2	2.63	0.41
66:AV:33:PHE:HA	66:AV:36:LEU:HD12	2.01	0.41
67:AW:125:CYS:SG	67:AW:130:VAL:HG22	2.60	0.41
67:AW:195:TYR:CE2	67:AW:196:ARG:HG2	2.55	0.41
1:A:223:PRO:HB2	1:A:425:CYS:SG	2.60	0.41
2:B:62:THR:OG1	2:B:63:GLU:N	2.53	0.41
2:B:133:ARG:C	2:B:136:GLY:H	2.29	0.41
10:K:101:SER:OG	10:K:102:GLY:N	2.53	0.41
11:L:131:LYS:HD2	11:L:147:ILE:HG23	2.03	0.41
12:M:234:LYS:N	12:M:235:PRO:HD2	2.36	0.41
12:M:598:ASN:HD22	12:M:602:ARG:NH1	2.19	0.41
13:N:34:LYS:NZ	13:N:54:GLN:HG2	2.36	0.41
15:P:157:VAL:HG21	15:P:181:HIS:CD2	2.46	0.41
16:Q:371:MET:HE1	16:Q:381:HIS:CE1	2.55	0.41
6:X:105:MET:CE	6:X:139:MET:HG3	2.50	0.41
6:X:115:GLN:HE21	6:X:119:ILE:HD11	1.84	0.41
22:Y:81:LEU:HB3	35:l:480:THR:OG1	2.20	0.41
25:b:111:LEU:C	25:b:113:THR:N	2.78	0.41
30:g:46:LEU:CD1	32:i:239:TRP:HB3	2.49	0.41
32:i:69:ILE:HD12	32:i:104:MET:HE1	2.01	0.41
33:j:70:ALA:HA	33:j:73:LEU:HD13	2.01	0.41
33:j:94:LEU:HD12	36:m:153:VAL:HG13	2.02	0.41
34:k:10:LEU:O	34:k:14:ILE:HG13	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:37:LYS:NZ	35:l:98:TRP:HE1	2.18	0.41
35:l:174:TYR:OH	35:l:534:HIS:HE1	2.03	0.41
35:l:197:ASP:O	35:l:201:MET:CG	2.68	0.41
35:l:562:LEU:O	35:l:566:ILE:HD12	2.21	0.41
75:l:703:CDL:HA61	75:l:703:CDL:H1	2.02	0.41
36:m:5:LEU:HD23	36:m:8:LEU:HD12	2.02	0.41
39:p:76:HIS:HA	39:p:77:PRO:HD3	1.86	0.41
40:r:121:PHE:O	40:r:125:THR:HG23	2.20	0.41
79:x:603:HEA:H272	79:x:603:HEA:H172	1.90	0.41
48:0:130:PRO:O	48:0:136:ALA:HB2	2.21	0.41
52:4:57:ARG:HA	52:4:60:TYR:CD2	2.55	0.41
64:AG:45:VAL:HG21	64:AG:48:ILE:HB	2.02	0.41
67:AK:261:GLN:H	67:AK:444:LEU:HD12	1.86	0.41
75:AN:101:CDL:OB4	63:AS:73:HIS:CE1	2.73	0.41
63:AS:42:GLU:HA	63:AS:45:LYS:HD3	2.03	0.41
68:AY:314:TYR:HB3	68:AY:341:PHE:CE1	2.56	0.41
1:A:184:LYS:C	1:A:186:ALA:H	2.27	0.41
1:A:222:LYS:NZ	12:M:197:THR:HG21	2.35	0.41
1:A:262:PHE:CZ	1:A:272:GLY:HA3	2.54	0.41
1:A:329:LYS:HA	1:A:332:CYS:HB3	2.02	0.41
1:A:382:CYS:HA	12:M:75:CYS:H	1.86	0.41
2:B:184:ASN:ND2	13:N:126:PRO:HA	2.35	0.41
7:H:19:THR:N	7:H:20:PRO:HD3	2.35	0.41
12:M:557:ARG:HE	12:M:579:ILE:HG23	1.86	0.41
23:Z:53:TYR:HA	35:l:435:PRO:HG2	2.02	0.41
26:c:151:PRO:O	26:c:153:TYR:HD1	2.03	0.41
26:c:163:TYR:HB3	26:c:168:LEU:HD21	2.02	0.41
30:g:27:ASP:O	30:g:31:LEU:HG	2.19	0.41
39:p:135:ARG:HD3	39:p:162:ASP:OD1	2.21	0.41
42:u:83:THR:O	42:u:87:THR:HG23	2.20	0.41
45:x:354:THR:HG21	45:x:376:HIS:HA	2.03	0.41
46:y:3:TYR:CD1	46:y:3:TYR:N	2.87	0.41
46:y:86:MET:HE3	46:y:86:MET:HB2	1.80	0.41
50:2:49:VAL:O	50:2:91:LEU:HD12	2.21	0.41
63:AF:76:LEU:O	63:AF:81:TRP:NE1	2.37	0.41
66:AJ:146:ILE:HA	66:AJ:149:LEU:HD13	2.02	0.41
67:AK:81:HIS:CD2	67:AK:158:LEU:HD22	2.55	0.41
61:AQ:4:ALA:HB3	61:AQ:9:LYS:HE3	2.02	0.41
65:AU:177:LYS:HA	65:AU:178:PRO:HD3	1.87	0.41
66:AV:105:GLY:HA2	66:AV:107:PHE:CE2	2.56	0.41
67:AW:64:PHE:HZ	67:AW:393:LEU:HD23	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HD22	1:A:332:CYS:SG	2.61	0.41
3:C:187:ALA:O	3:C:190:LEU:HB3	2.20	0.41
4:E:84:ILE:HD13	15:P:177:PHE:CE1	2.56	0.41
9:J:50:SER:O	9:J:77:GLY:HA3	2.20	0.41
9:J:201:VAL:HG13	9:J:265:PHE:CD2	2.55	0.41
14:O:156:LEU:HD13	14:O:158:ILE:HD12	2.03	0.41
6:X:131:PRO:HG3	26:c:89:TRP:CE3	2.55	0.41
26:c:65:TYR:CE2	26:c:77:LYS:HG3	2.55	0.41
27:d:76:ILE:HG22	27:d:77:MET:HE2	2.02	0.41
30:g:73:TYR:O	30:g:76:LYS:HB3	2.21	0.41
32:i:210:ILE:O	32:i:214:THR:HG23	2.20	0.41
32:i:256:PRO:HB3	40:r:124:THR:HG22	2.01	0.41
35:l:452:ASN:CB	35:l:453:PRO:HD3	2.51	0.41
40:r:355:MET:HA	40:r:358:TRP:CD1	2.54	0.41
54:6:5:VAL:O	54:6:9:GLN:HG3	2.21	0.41
60:AC:88:PHE:O	60:AC:92:ARG:HG3	2.20	0.41
60:AC:248:ARG:HG2	60:AC:257:ASN:ND2	2.36	0.41
65:AH:197:LEU:HA	65:AH:200:ILE:HB	2.03	0.41
68:AL:156:LEU:HB2	68:AL:213:ARG:HE	1.85	0.41
76:AL:503:PEE:H25	76:AL:503:PEE:H53	2.01	0.41
58:AN:17:TYR:CD1	68:AY:275:ILE:HG12	2.55	0.41
67:AW:290:GLN:HB3	67:AW:336:PHE:HE1	1.86	0.41
67:AW:450:VAL:CA	67:AW:453:LEU:CD1	2.89	0.41
68:AY:225:LYS:O	68:AY:228:ARG:HB3	2.20	0.41
68:AY:274:GLU:OE2	68:AY:468:TYR:HB2	2.20	0.41
1:A:63:TYR:CD2	1:A:64:LYS:HG3	2.55	0.41
3:C:109:VAL:HG21	41:s:25:ARG:HH12	1.85	0.41
24:a:62:PHE:HB2	39:p:111:GLU:OE2	2.19	0.41
25:b:111:LEU:C	25:b:113:THR:H	2.27	0.41
71:b:201:PLX:C6	71:b:201:PLX:P1	3.08	0.41
26:c:73:GLY:C	26:c:75:TYR:H	2.28	0.41
26:c:159:LYS:HA	43:v:98:ARG:CZ	2.50	0.41
26:c:162:PRO:O	26:c:166:LEU:HD12	2.21	0.41
27:d:35:VAL:C	27:d:38:PRO:HD2	2.46	0.41
33:j:36:PRO:HA	41:s:214:GLU:OE2	2.21	0.41
36:m:33:ILE:O	36:m:37:VAL:HG23	2.19	0.41
39:p:124:GLN:HA	39:p:127:LYS:NZ	2.36	0.41
42:u:24:VAL:CG2	42:u:86:TRP:HE1	2.34	0.41
45:x:240:HIS:O	45:x:241:PRO:C	2.64	0.41
45:x:276:ALA:O	45:x:280:ILE:HG13	2.21	0.41
48:0:11:TYR:CD1	48:0:11:TYR:C	2.99	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:O:86:MET:O	55:7:25:CYS:HB2	2.20	0.41
63:AF:51:LEU:C	67:AW:148:ARG:HH22	2.29	0.41
66:AJ:132:VAL:HG22	66:AJ:143:ALA:HB2	2.03	0.41
59:AO:13:PRO:HB2	67:AW:84:ARG:HH12	1.86	0.41
59:AO:20:ARG:NH2	59:AO:48:PRO:HG2	2.36	0.41
60:AP:218:THR:HG21	60:AP:256:LEU:HD12	2.02	0.41
65:AU:201:VAL:HG13	65:AU:208:GLU:N	2.36	0.41
76:AU:401:PEE:H55	76:AU:401:PEE:H49	1.81	0.41
66:AV:87:ALA:HB2	82:AV:401:HEM:CHB	2.50	0.41
66:AV:249:LEU:CD1	66:AV:250:LEU:HD12	2.50	0.41
67:AW:88:SER:O	67:AW:96:SER:OG	2.33	0.41
67:AW:214:THR:HG21	67:AW:244:LEU:N	2.34	0.41
1:A:98:LYS:HD2	1:A:98:LYS:HA	1.92	0.41
1:A:244:ASN:ND2	70:A:502:FMN:HM82	2.36	0.41
1:A:387:GLU:HG2	12:M:119:PHE:O	2.20	0.41
3:C:98:ALA:HB1	3:C:99:PRO:HD2	2.03	0.41
5:F:23:LEU:HD21	5:F:34:ARG:HG2	2.03	0.41
9:J:62:THR:HG21	73:J:401:NDP:O1X	2.21	0.41
11:L:117:THR:OG1	15:P:229:GLU:OE1	2.39	0.41
12:M:646:LEU:O	12:M:651:PRO:HA	2.20	0.41
14:O:87:GLN:OE1	14:O:122:TYR:HA	2.21	0.41
15:P:77:GLN:HB2	15:P:85:GLU:HB2	2.03	0.41
19:U:56:PRO:HB3	42:u:129:THR:OG1	2.20	0.41
24:a:106:VAL:HA	24:a:107:PRO:HD2	1.82	0.41
27:d:123:VAL:O	27:d:127:THR:HG23	2.21	0.41
31:h:6:ILE:HD12	32:i:22:LEU:HD21	2.02	0.41
32:i:19:ILE:HD12	32:i:35:MET:HE1	2.02	0.41
33:j:54:LYS:HB3	33:j:113:TRP:HE1	1.85	0.41
35:l:396:ILE:HG22	35:l:400:ASN:HD21	1.85	0.41
35:l:536:THR:OG1	35:l:537:ILE:N	2.53	0.41
38:o:112:LYS:NZ	40:r:389:SER:HA	2.36	0.41
39:p:134:GLU:O	39:p:138:LYS:HG3	2.21	0.41
39:p:145:PRO:HA	39:p:146:PRO:HD3	1.84	0.41
40:r:153:THR:O	40:r:157:SER:N	2.54	0.41
71:r:502:PLX:H392	71:r:502:PLX:H361	1.64	0.41
41:s:86:TRP:HH2	41:s:232:ILE:HG22	1.85	0.41
41:s:150:LEU:HD23	41:s:150:LEU:HA	1.88	0.41
41:s:154:LEU:HA	41:s:154:LEU:HD23	1.73	0.41
41:s:164:THR:O	41:s:167:THR:OG1	2.38	0.41
47:z:146:TRP:CE2	51:3:17:ARG:HB2	2.56	0.41
47:z:233:PHE:HA	47:z:236:GLU:HG3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:3:44:ARG:HA	51:3:45:PRO:HD2	1.76	0.41
52:4:65:PRO:HG2	52:4:68:TRP:CG	2.56	0.41
58:AA:64:THR:HG23	66:AJ:337:TRP:HZ2	1.86	0.41
60:AC:127:TYR:HE1	61:AD:33:GLU:HG2	1.85	0.41
65:AH:112:ARG:O	65:AH:116:VAL:HG23	2.21	0.41
66:AJ:2:THR:HG21	68:AL:335:ASN:HD22	1.86	0.41
66:AJ:111:GLU:O	66:AJ:115:ILE:HG12	2.20	0.41
66:AJ:138:MET:HE1	66:AJ:269:LYS:H	1.86	0.41
67:AK:67:ALA:HB2	67:AK:212:HIS:HB3	2.03	0.41
64:AT:9:ARG:HH22	71:AT:101:PLX:C1A	2.33	0.41
65:AU:266:ILE:O	65:AU:270:VAL:HG23	2.20	0.41
66:AV:156:ILE:HG22	66:AV:160:LEU:HB2	2.01	0.41
67:AW:51:SER:HB2	67:AW:230:LEU:HD12	2.02	0.41
67:AW:299:VAL:HG22	68:AY:120:LEU:HG	2.03	0.41
68:AY:282:LEU:HB2	68:AY:461:PRO:HD3	2.03	0.41
1:A:113:LEU:HD23	1:A:114:VAL:N	2.35	0.41
1:A:123:GLY:CA	1:A:355:ILE:HD11	2.48	0.41
1:A:249:ALA:O	1:A:252:PRO:HD2	2.21	0.41
1:A:284:HIS:CE1	14:O:229:GLY:HA3	2.56	0.41
1:A:339:PHE:HA	1:A:342:LEU:HD12	2.03	0.41
2:B:57:ARG:HG2	2:B:62:THR:OG1	2.21	0.41
2:B:143:TYR:HB3	2:B:185:LYS:HB2	2.03	0.41
2:B:146:ASP:OD2	2:B:149:LYS:HE2	2.21	0.41
2:B:160:CYS:HA	2:B:161:PRO:HD2	1.83	0.41
71:B:303:PLX:H332	71:B:303:PLX:H301	1.80	0.41
3:C:137:VAL:HA	3:C:140:GLN:OE1	2.20	0.41
3:C:213:ARG:O	3:C:213:ARG:HG2	2.19	0.41
7:H:45:ARG:O	7:H:49:GLU:HG3	2.21	0.41
9:J:130:ILE:HA	73:J:401:NDP:H8A	2.03	0.41
9:J:271:TYR:HE1	9:J:374:THR:HB	1.85	0.41
9:J:329:LEU:HD22	9:J:332:LEU:HD12	2.01	0.41
12:M:236:TYR:CE1	12:M:272:ARG:HB3	2.55	0.41
12:M:246:ARG:NH2	15:P:229:GLU:OE2	2.54	0.41
12:M:522:GLN:HE21	12:M:526:LEU:HG	1.85	0.41
12:M:568:TYR:HB2	12:M:580:ALA:CB	2.51	0.41
15:P:227:ALA:O	15:P:229:GLU:N	2.47	0.41
16:Q:35:ARG:HH21	44:w:322:HIS:HB3	1.86	0.41
16:Q:80:ILE:HG22	16:Q:81:THR:N	2.35	0.41
16:Q:204:PHE:CE1	16:Q:207:ARG:HD3	2.56	0.41
16:Q:316:PHE:HD1	16:Q:339:GLN:HE21	1.67	0.41
17:S:47:LEU:O	17:S:50:ARG:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:110:GLY:N	18:T:119:PHE:O	2.28	0.41
20:V:114:ALA:HB1	20:V:118:PHE:CE2	2.56	0.41
21:W:86:MET:HG2	21:W:128:ARG:HH22	1.86	0.41
22:Y:62:SER:O	22:Y:65:MET:HB3	2.21	0.41
24:a:112:TYR:CD1	27:d:58:TYR:O	2.72	0.41
24:a:115:HIS:CG	24:a:116:PRO:HD2	2.56	0.41
24:a:130:GLU:HA	37:n:45:PHE:CD2	2.56	0.41
28:e:150:PRO:HD3	30:g:112:PHE:CD1	2.56	0.41
29:f:34:PRO:HG3	44:w:342:GLY:HA2	2.03	0.41
30:g:37:GLY:HA2	30:g:67:PHE:CE2	2.56	0.41
30:g:45:ASN:HD21	30:g:60:GLN:NE2	2.19	0.41
32:i:112:HIS:HB2	32:i:184:ILE:HD13	2.03	0.41
32:i:167:TRP:HZ3	35:l:570:GLN:CA	2.20	0.41
34:k:3:LEU:O	34:k:3:LEU:HD13	2.20	0.41
34:k:10:LEU:CD1	36:m:102:LEU:HD12	2.49	0.41
34:k:14:ILE:HD13	36:m:17:VAL:HG22	2.02	0.41
35:l:452:ASN:N	35:l:453:PRO:HD2	2.36	0.41
36:m:106:VAL:HG11	36:m:117:ASN:ND2	2.34	0.41
36:m:114:VAL:O	36:m:115:VAL:HG22	2.20	0.41
38:o:124:THR:C	38:o:126:HIS:H	2.29	0.41
39:p:31:CYS:O	39:p:33:GLN:N	2.54	0.41
39:p:158:ARG:O	39:p:162:ASP:HB2	2.21	0.41
40:r:130:LEU:HD21	40:r:149:PHE:HD2	1.86	0.41
40:r:229:MET:HE2	40:r:229:MET:HB3	1.90	0.41
41:s:311:ILE:O	41:s:312:SER:OG	2.28	0.41
44:w:42:HIS:O	44:w:46:GLY:N	2.54	0.41
45:x:168:ILE:CG2	45:x:189:MET:HG3	2.51	0.41
45:x:474:GLU:HG3	45:x:475:ALA:N	2.35	0.41
47:z:6:HIS:CD2	47:z:8:TYR:HB2	2.56	0.41
47:z:122:HIS:HA	47:z:123:PRO:HD2	1.91	0.41
47:z:228:THR:O	47:z:232:HIS:HD2	2.04	0.41
48:0:24:LEU:HB3	49:1:30:ARG:HG2	2.03	0.41
48:0:137:LYS:O	48:0:145:TRP:HE3	2.03	0.41
49:1:21:LYS:O	49:1:57:ARG:NH1	2.53	0.41
50:2:10:GLU:HG2	50:2:25:ARG:HH22	1.86	0.41
51:3:25:LEU:HD23	51:3:25:LEU:HA	1.91	0.41
53:5:42:LYS:HE2	53:5:42:LYS:HB3	1.83	0.41
58:AA:78:TYR:CD1	62:AE:65:GLU:CG	3.04	0.41
60:AC:196:ARG:HB3	60:AC:249:ILE:HG23	2.01	0.41
60:AC:209:GLU:HG2	60:AC:210:TRP:CD1	2.56	0.41
65:AH:85:SER:OG	65:AH:86:ASP:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:AH:128:ASP:OD1	65:AH:177:LYS:HE2	2.20	0.41
65:AH:284:HIS:CG	65:AH:288:MET:HE2	2.56	0.41
66:AJ:221:HIS:HA	66:AJ:225:THR:HG23	2.02	0.41
67:AK:239:ASN:OD1	67:AK:240:MET:HG2	2.21	0.41
67:AK:449:PHE:HE2	67:AW:183:ARG:HB3	1.86	0.41
68:AL:91:TYR:O	68:AL:94:GLU:HB3	2.21	0.41
68:AL:141:PRO:HA	68:AL:245:LEU:HD13	2.03	0.41
68:AL:170:ARG:O	68:AL:174:GLU:HG3	2.20	0.41
68:AL:462:ILE:HG23	68:AL:465:LEU:HB3	2.03	0.41
60:AP:111:LYS:NZ	68:AY:451:ASP:O	2.32	0.41
60:AP:186:GLN:O	60:AP:190:VAL:HG23	2.20	0.41
61:AQ:21:PHE:CE2	61:AQ:25:ILE:HD11	2.56	0.41
62:AR:34:ARG:NH1	62:AR:78:ARG:HH22	2.10	0.41
65:AU:156:ASP:HB2	65:AU:167:ARG:HB2	2.03	0.41
65:AU:199:TYR:OH	66:AV:71:ARG:NH1	2.53	0.41
66:AV:146:ILE:O	66:AV:149:LEU:HB2	2.21	0.41
67:AW:155:GLN:N	67:AW:156:PRO:HD2	2.35	0.41
67:AW:205:LEU:O	67:AW:209:VAL:HG23	2.21	0.41
67:AW:209:VAL:HG13	67:AW:213:PHE:CD2	2.55	0.41
67:AW:305:THR:HA	67:AW:311:GLN:NE2	2.36	0.41
67:AW:352:LYS:O	67:AW:356:ASN:ND2	2.54	0.41
2:B:101:LEU:O	2:B:192:GLY:HA3	2.21	0.41
9:J:168:SER:CA	9:J:184:LYS:CE	2.99	0.41
9:J:202:LYS:N	9:J:263:PHE:O	2.54	0.41
11:L:123:ASN:HB3	15:P:232:LYS:HD2	2.02	0.41
12:M:128:CYS:CB	12:M:129:PRO:CD	2.86	0.41
14:O:148:ILE:O	14:O:152:ILE:HG13	2.21	0.41
14:O:198:ALA:O	14:O:202:GLU:HG2	2.21	0.41
15:P:148:ASP:HB2	15:P:151:THR:HG23	2.02	0.41
16:Q:153:LEU:O	16:Q:157:LYS:HG3	2.21	0.41
16:Q:169:TRP:C	16:Q:351:MET:HE2	2.46	0.41
18:T:33:SER:HB3	18:T:45:VAL:HG21	2.03	0.41
6:X:113:LEU:HD12	6:X:114:ASP:N	2.36	0.41
24:a:96:ALA:CB	27:d:55:TYR:H	2.34	0.41
26:c:154:GLN:HE22	43:v:3:ALA:HB2	1.86	0.41
35:l:100:ILE:HD12	35:l:246:LEU:CD2	2.51	0.41
35:l:218:LEU:C	35:l:218:LEU:CD2	2.94	0.41
35:l:244:SER:HA	35:l:248:HIS:CD2	2.56	0.41
35:l:272:LEU:HD11	75:l:704:CDL:HB61	2.02	0.41
35:l:311:GLY:O	35:l:315:VAL:HG23	2.21	0.41
35:l:362:LEU:HA	35:l:365:THR:OG1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:493:VAL:O	35:l:496:LEU:HB3	2.21	0.41
40:r:170:THR:OG1	40:r:171:LEU:N	2.53	0.41
41:s:195:ARG:HG3	41:s:196:ALA:N	2.36	0.41
45:x:23:GLY:HA3	45:x:73:ILE:HG13	2.03	0.41
50:2:30:PRO:HG2	50:2:31:TYR:CD1	2.56	0.41
52:4:20:PHE:N	52:4:21:PRO:HD3	2.35	0.41
55:7:24:PHE:CE1	55:7:28:VAL:HG21	2.56	0.41
60:AC:176:VAL:HG22	60:AC:212:ILE:HG12	2.02	0.41
65:AH:91:PRO:HA	65:AH:92:PRO:HD3	1.91	0.41
76:AH:401:PEE:C30	76:AH:401:PEE:H13	2.50	0.41
66:AJ:3:PRO:HB2	66:AJ:5:ARG:HG2	2.03	0.41
66:AJ:103:TYR:OH	66:AJ:322:GLN:NE2	2.54	0.41
66:AJ:198:LEU:HD12	75:AJ:404:CDL:H311	2.02	0.41
67:AK:58:VAL:HG23	68:AL:400:VAL:HG11	2.03	0.41
68:AL:234:ALA:HB2	68:AL:413:ILE:HD12	2.03	0.41
71:AQ:101:PLX:H1C3	71:AQ:101:PLX:H21	1.84	0.41
67:AW:67:ALA:HA	67:AW:71:TYR:CD2	2.56	0.41
68:AY:98:PHE:HE2	68:AY:120:LEU:CD1	2.19	0.41
68:AY:113:VAL:HG13	68:AY:118:ALA:HB3	2.03	0.41
2:B:90:PRO:O	2:B:91:LEU:HD12	2.21	0.40
2:B:120:ILE:O	2:B:121:CYS:C	2.64	0.40
2:B:155:PHE:HB2	69:B:302:SF4:S2	2.61	0.40
2:B:169:PRO:HG3	2:B:198:GLU:CG	2.51	0.40
3:C:81:PRO:HA	3:C:119:VAL:HG13	2.03	0.40
3:C:140:GLN:HG2	33:j:37:TYR:CD1	2.56	0.40
4:E:42:GLU:OE2	4:E:46:THR:OG1	2.40	0.40
5:F:89:ARG:HD2	5:F:92:GLU:OE2	2.21	0.40
73:J:401:NDP:O3B	73:J:401:NDP:P2B	2.79	0.40
12:M:209:TYR:H	14:O:110:MET:HE1	1.86	0.40
12:M:382:ARG:NE	12:M:527:ASP:OD1	2.54	0.40
12:M:401:LEU:HD13	12:M:462:PHE:CE2	2.56	0.40
12:M:483:ARG:O	12:M:483:ARG:HG3	2.21	0.40
16:Q:65:PRO:CG	16:Q:69:VAL:HG22	2.51	0.40
16:Q:71:PRO:HB2	16:Q:72:PRO:HD3	2.03	0.40
75:V:201:CDL:H722	75:V:201:CDL:H752	1.75	0.40
22:Y:43:ARG:HH11	22:Y:49:GLN:HG2	1.86	0.40
26:c:88:PRO:HB2	39:p:86:PRO:HG2	2.03	0.40
27:d:72:LYS:HE3	30:g:105:LYS:O	2.20	0.40
32:i:58:LYS:HZ1	34:k:92:ASN:CG	2.28	0.40
32:i:189:TRP:HE1	32:i:286:THR:HG21	1.85	0.40
34:k:3:LEU:C	34:k:3:LEU:CD1	2.94	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:31:LEU:HD21	36:m:67:PHE:CE2	2.56	0.40
34:k:97:GLN:N	35:l:579:THR:OG1	2.41	0.40
35:l:39:ILE:O	35:l:43:THR:HG23	2.21	0.40
35:l:522:PHE:HA	35:l:528:PHE:CE2	2.56	0.40
37:n:30:LYS:HZ2	75:n:101:CDL:HA31	1.86	0.40
38:o:6:TYR:HE2	38:o:14:LEU:HA	1.85	0.40
40:r:196:TRP:NE1	40:r:250:LEU:HD13	2.36	0.40
40:r:375:LEU:HD12	40:r:375:LEU:HA	1.85	0.40
43:v:75:PRO:O	43:v:77:PHE:N	2.43	0.40
45:x:442:ASP:OD2	46:y:134:ARG:NH2	2.54	0.40
50:2:74:LEU:HD23	50:2:74:LEU:HA	1.86	0.40
65:AH:89:LEU:HD23	65:AH:236:TYR:CZ	2.56	0.40
75:AL:502:CDL:H712	75:AL:502:CDL:HB62	1.75	0.40
60:AP:173:PRO:HD2	60:AP:216:VAL:HG23	2.03	0.40
60:AP:248:ARG:HG2	60:AP:257:ASN:ND2	2.36	0.40
61:AQ:15:PHE:O	71:AQ:101:PLX:H1A1	2.21	0.40
61:AQ:25:ILE:O	61:AQ:29:VAL:HG23	2.21	0.40
67:AW:177:LEU:HD21	67:AW:272:VAL:HG21	2.02	0.40
67:AW:261:GLN:H	67:AW:444:LEU:HD12	1.85	0.40
68:AY:334:ALA:H	68:AY:336:LYS:H	1.68	0.40
1:A:314:LEU:O	1:A:329:LYS:HD2	2.21	0.40
6:G:154:VAL:O	6:G:156:GLU:HG3	2.22	0.40
7:H:75:GLY:CA	8:I:103:ARG:HH11	2.34	0.40
12:M:128:CYS:HA	69:M:801:SF4:S4	2.61	0.40
12:M:436:VAL:HG21	12:M:686:PRO:HG2	2.02	0.40
12:M:460:HIS:HA	12:M:461:PRO:HD3	1.96	0.40
14:O:99:ASN:O	14:O:103:GLU:HG3	2.21	0.40
15:P:61:PHE:O	15:P:64:TYR:HB3	2.20	0.40
15:P:81:PHE:HE1	16:Q:157:LYS:O	2.03	0.40
15:P:100:LEU:O	15:P:108:PHE:HD2	2.05	0.40
16:Q:52:MET:HE2	32:i:295:ARG:HH21	1.86	0.40
71:U:101:PLX:H22	71:U:101:PLX:H1B3	1.86	0.40
20:V:124:LEU:HA	20:V:127:MET:HE3	2.03	0.40
71:V:203:PLX:H371	71:V:203:PLX:H342	1.76	0.40
22:Y:74:TRP:CZ3	22:Y:75:HIS:HA	2.53	0.40
24:a:54:LEU:HD23	24:a:54:LEU:HA	1.81	0.40
24:a:109:HIS:O	24:a:112:TYR:HD2	2.03	0.40
25:b:105:PHE:HD2	43:v:68:LYS:CB	2.34	0.40
27:d:56:TYR:HD1	27:d:56:TYR:HA	1.78	0.40
28:e:67:TYR:CE2	40:r:428:PRO:HG2	2.56	0.40
32:i:61:LEU:O	32:i:65:THR:HG23	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:70:THR:HA	35:l:75:GLN:HB2	2.04	0.40
35:l:550:LEU:HD23	35:l:554:ASP:OD2	2.22	0.40
39:p:30:TRP:NE1	39:p:76:HIS:HB2	2.36	0.40
41:s:2:PRO:O	41:s:5:ASN:HB2	2.20	0.40
41:s:116:ILE:O	41:s:119:SER:OG	2.34	0.40
41:s:193:THR:O	41:s:194:ASN:HB2	2.20	0.40
41:s:273:ILE:HG23	41:s:277:TYR:HD2	1.86	0.40
44:w:72:LYS:HD2	44:w:75:LYS:HD2	2.03	0.40
47:z:182:TYR:O	51:3:72:ASN:HB2	2.21	0.40
54:6:12:PHE:O	54:6:23:LYS:HE2	2.21	0.40
54:6:21:HIS:CD2	54:6:22:LEU:HG	2.57	0.40
58:AA:17:TYR:CD1	68:AL:275:ILE:HG12	2.56	0.40
60:AC:246:SER:HG	60:AC:248:ARG:HE	1.66	0.40
75:AG:101:CDL:H512	75:AG:101:CDL:C55	2.43	0.40
75:AH:403:CDL:H311	75:AH:403:CDL:H341	1.79	0.40
67:AK:288:VAL:O	67:AK:292:VAL:HG23	2.21	0.40
68:AL:314:TYR:HB3	68:AL:341:PHE:CZ	2.55	0.40
60:AP:155:LYS:HB2	60:AP:271:VAL:HG13	2.04	0.40
63:AS:76:LEU:O	63:AS:81:TRP:NE1	2.37	0.40
66:AV:3:PRO:HG2	66:AV:6:LYS:HG2	2.03	0.40
66:AV:128:PHE:O	66:AV:132:VAL:HG23	2.22	0.40
67:AW:317:THR:HB	67:AW:318:GLN:H	1.69	0.40
1:A:55:GLY:O	1:A:58:SER:OG	2.32	0.40
2:B:84:TYR:CD1	2:B:85:PRO:HA	2.56	0.40
2:B:96:ARG:HD2	2:B:154:GLY:HA3	2.03	0.40
5:F:57:GLU:HB3	12:M:662:ALA:N	2.24	0.40
9:J:329:LEU:HD13	9:J:332:LEU:HD12	2.03	0.40
11:L:78:ARG:HD2	12:M:607:LYS:HE2	2.02	0.40
11:L:163:ASN:O	11:L:171:ARG:N	2.55	0.40
14:O:110:MET:HA	14:O:113:TYR:CD2	2.57	0.40
14:O:197:THR:N	14:O:200:ASP:HB3	2.36	0.40
16:Q:120:THR:O	16:Q:124:ILE:HG13	2.22	0.40
16:Q:310:VAL:O	16:Q:314:VAL:HG23	2.21	0.40
21:W:93:GLU:OE1	31:h:93:THR:HG21	2.21	0.40
21:W:111:PHE:CE2	21:W:117:VAL:HG21	2.56	0.40
22:Y:45:ARG:O	22:Y:45:ARG:HG2	2.22	0.40
22:Y:68:TRP:CZ3	35:l:386:LEU:HA	2.56	0.40
32:i:70:LEU:HD23	32:i:70:LEU:HA	1.76	0.40
32:i:342:PHE:CD2	32:i:343:MET:HE2	2.57	0.40
34:k:46:LEU:HD22	36:m:46:PHE:CE2	2.56	0.40
39:p:158:ARG:O	39:p:159:LYS:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:89:LEU:O	40:r:93:LYS:HG3	2.20	0.40
44:w:68:THR:OG1	44:w:69:GLY:N	2.54	0.40
44:w:86:PHE:HA	44:w:87:PRO:HD2	1.85	0.40
45:x:398:PRO:HB3	45:x:482:VAL:HG21	2.03	0.40
47:z:224:LYS:NZ	47:z:226:HIS:HE2	2.18	0.40
50:2:16:LEU:O	50:2:20:VAL:HG13	2.21	0.40
55:7:13:TYR:O	55:7:14:GLY:C	2.63	0.40
57:9:35:TYR:HD2	57:9:36:HIS:CE1	2.39	0.40
65:AH:175:PHE:HA	65:AH:176:PRO:HD3	1.84	0.40
66:AJ:150:LEU:HA	66:AJ:150:LEU:HD12	1.87	0.40
66:AJ:345:TYR:N	66:AJ:346:PRO:HD2	2.36	0.40
68:AL:294:PRO:HG3	68:AL:448:TYR:CE1	2.56	0.40
68:AL:301:ASN:O	68:AL:305:GLN:HG2	2.21	0.40
59:AO:35:PRO:CB	67:AW:320:PRO:HA	2.48	0.40
60:AP:125:VAL:HG21	71:AQ:101:PLX:H141	2.03	0.40
66:AV:21:LEU:O	66:AV:21:LEU:HD12	2.22	0.40
67:AW:126:LEU:HB3	68:AY:38:PHE:HZ	1.85	0.40
68:AY:61:SER:HA	68:AY:233:ALA:O	2.21	0.40
68:AY:61:SER:HB2	68:AY:242:LEU:HD23	2.03	0.40
68:AY:331:GLY:O	68:AY:337:LEU:HD12	2.21	0.40
2:B:104:TYR:N	2:B:108:GLU:O	2.33	0.40
5:F:14:LEU:N	5:F:17:ARG:HH12	2.20	0.40
5:F:66:TRP:CZ2	12:M:648:GLU:HB2	2.57	0.40
12:M:645:ARG:O	12:M:649:VAL:HG12	2.21	0.40
13:N:39:VAL:HG12	13:N:40:GLY:O	2.21	0.40
16:Q:267:ILE:HG23	41:s:280:PHE:HD1	1.87	0.40
16:Q:316:PHE:HB2	16:Q:339:GLN:CG	2.51	0.40
16:Q:331:LEU:O	16:Q:335:GLU:HG3	2.20	0.40
19:U:50:PRO:HB2	21:W:69:ILE:HD11	2.03	0.40
25:b:31:ARG:HH12	39:p:116:PRO:HG2	1.85	0.40
71:b:201:PLX:C11	71:b:201:PLX:C7	3.00	0.40
27:d:138:GLN:HG2	27:d:139:ASP:OD1	2.22	0.40
75:i:401:CDL:H311	75:i:401:CDL:H341	1.83	0.40
35:l:84:TYR:HD1	35:l:88:MET:CE	2.01	0.40
35:l:417:SER:HB3	35:l:493:VAL:CG1	2.51	0.40
35:l:512:LYS:CG	54:6:16:ASN:HB2	2.51	0.40
40:r:80:SER:O	40:r:81:GLN:C	2.64	0.40
40:r:235:LEU:O	40:r:238:LEU:HB3	2.22	0.40
45:x:198:SER:HB2	45:x:238:PHE:HA	2.03	0.40
45:x:461:SER:O	45:x:465:VAL:HG13	2.21	0.40
46:y:193:TYR:CD1	46:y:193:TYR:N	2.88	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:z:22:LEU:HD12	47:z:22:LEU:HA	1.87	0.40
60:AC:207:LYS:HA	60:AC:208:PRO:HD3	1.86	0.40
65:AH:228:ARG:NH1	65:AH:229:GLU:HB3	2.36	0.40
67:AK:452:GLU:O	67:AK:452:GLU:HG3	2.20	0.40
59:AO:37:THR:O	67:AW:266:LEU:HD21	2.22	0.40
60:AP:184:ILE:HD13	60:AP:208:PRO:HB2	2.04	0.40
65:AU:304:TYR:OH	75:AU:403:CDL:H732	2.22	0.40
68:AY:53:LEU:HD12	68:AY:57:LEU:HB3	2.04	0.40
68:AY:71:VAL:HG22	68:AY:233:ALA:HB2	2.02	0.40
1:A:53:LEU:O	1:A:56:SER:OG	2.24	0.40
1:A:86:ARG:C	1:A:95:THR:HG23	2.46	0.40
1:A:122:PRO:HA	14:O:176:CYS:SG	2.61	0.40
2:B:102:ARG:HB2	2:B:196:GLU:OE2	2.21	0.40
3:C:104:ASP:OD2	41:s:37:PRO:HD3	2.20	0.40
4:E:37:ARG:HH21	4:E:41:ARG:HH22	1.68	0.40
6:G:123:GLU:HB3	6:G:130:ILE:HG12	2.04	0.40
14:O:186:VAL:HG12	14:O:188:ILE:HG13	2.03	0.40
16:Q:50:ALA:HB2	16:Q:63:PRO:HB3	2.03	0.40
16:Q:198:THR:HG22	41:s:32:GLN:HE22	1.87	0.40
16:Q:314:VAL:HG12	16:Q:316:PHE:HD2	1.87	0.40
17:S:37:ARG:NH1	17:S:51:ASP:OD2	2.51	0.40
18:T:105:LYS:HB3	18:T:107:THR:HG22	2.04	0.40
19:U:8:PHE:O	19:U:11:ASN:HB3	2.21	0.40
24:a:170:TYR:CD2	30:g:5:ARG:HB3	2.56	0.40
25:b:33:PRO:HG2	39:p:116:PRO:HD3	2.03	0.40
25:b:88:TYR:HB2	71:b:201:PLX:C1B	2.51	0.40
26:c:168:LEU:HD12	26:c:169:GLU:N	2.36	0.40
27:d:107:CYS:HB2	27:d:122:GLU:OE1	2.22	0.40
28:e:74:HIS:HB3	28:e:87:MET:SD	2.62	0.40
29:f:63:ASN:O	29:f:67:LEU:HG	2.22	0.40
30:g:11:ARG:O	30:g:13:LEU:N	2.54	0.40
30:g:86:ASP:CG	42:u:166:ARG:HH22	2.27	0.40
32:i:73:ALA:HA	32:i:97:MET:HE3	2.03	0.40
32:i:86:MET:HE2	32:i:144:GLN:OE1	2.21	0.40
32:i:124:LEU:HD13	32:i:219:LEU:HG	2.03	0.40
32:i:146:SER:HA	32:i:149:LEU:HD13	2.04	0.40
32:i:193:VAL:HB	32:i:201:THR:HG22	2.02	0.40
35:l:121:LEU:HD23	35:l:121:LEU:HA	1.92	0.40
35:l:564:LYS:HG3	38:o:77:TYR:OH	2.21	0.40
76:l:701:PEE:H65	76:l:701:PEE:H71	1.79	0.40
40:r:346:GLN:HA	40:r:413:THR:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:r:501:PLX:H301	71:r:501:PLX:H271	1.66	0.40
71:r:502:PLX:H1B2	71:r:502:PLX:H22	1.53	0.40
44:w:246:LEU:O	44:w:249:MET:HB2	2.22	0.40
48:0:127:LYS:O	48:0:130:PRO:HD3	2.20	0.40
52:4:33:TYR:O	52:4:37:HIS:HD2	2.05	0.40
52:4:54:GLU:CD	52:4:57:ARG:HH12	2.30	0.40
65:AH:162:GLY:C	65:AH:164:MET:H	2.26	0.40
66:AJ:171:ASP:OD1	66:AJ:172:SER:N	2.51	0.40
67:AK:104:GLU:OE1	68:AL:325:SER:HA	2.21	0.40
67:AK:159:LYS:HG2	67:AK:197:ILE:HD13	2.03	0.40
60:AP:151:LYS:O	60:AP:153:GLU:N	2.51	0.40
64:AT:38:TRP:CD1	64:AT:40:LEU:HG	2.56	0.40
65:AU:281:GLU:HG3	66:AV:77:TRP:CD2	2.56	0.40
66:AV:132:VAL:HG11	66:AV:178:PHE:HD2	1.87	0.40
66:AV:186:PRO:O	66:AV:189:ILE:HB	2.21	0.40
66:AV:222:PRO:HG3	68:AY:470:ARG:HD3	2.04	0.40
67:AW:438:MET:HB2	67:AW:450:VAL:HG23	2.03	0.40
68:AY:163:LYS:O	68:AY:167:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	5	31
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	21	55
3	C	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	3	25
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	6	34
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	4	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	X	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	18
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	2	19
8	I	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	14
9	J	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	5	31
10	K	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	0	8
11	L	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	3	24
12	M	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	3	24
13	N	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	1	18
14	O	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	3	24
15	P	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	1	17
16	Q	428/430 (100%)	398 (93%)	23 (5%)	7 (2%)	7	36
17	S	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	3	26
18	T	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	2	20
19	U	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	10	41
20	V	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	5	31
21	W	136/138 (99%)	127 (93%)	4 (3%)	5 (4%)	2	22
22	Y	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	6
23	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
24	a	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	5	31
25	b	122/124 (98%)	107 (88%)	10 (8%)	5 (4%)	2	20
26	c	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	2	19
27	d	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	21	55
28	e	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	3	25
29	f	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	5	31
30	g	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	1	17
31	h	102/104 (98%)	86 (84%)	10 (10%)	6 (6%)	1	15
32	i	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	7	35
33	j	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	4	28
34	k	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	3	25
35	l	601/603 (100%)	553 (92%)	38 (6%)	10 (2%)	7	35
36	m	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	1	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	n	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	2	22
38	o	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	3	25
39	p	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	6	34
40	r	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	6	32
41	s	316/318 (99%)	285 (90%)	22 (7%)	9 (3%)	4	27
42	u	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	3	26
43	v	107/122 (88%)	90 (84%)	14 (13%)	3 (3%)	4	27
44	w	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	4	27
45	x	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	50
46	y	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	40
47	z	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
48	0	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
49	1	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
50	2	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	2	20
51	3	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	15
52	4	73/75 (97%)	64 (88%)	8 (11%)	1 (1%)	9	38
53	5	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
54	6	54/56 (96%)	47 (87%)	5 (9%)	2 (4%)	2	22
55	7	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
56	8	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
57	9	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
58	AA	79/81 (98%)	71 (90%)	6 (8%)	2 (2%)	4	29
58	AN	79/81 (98%)	74 (94%)	4 (5%)	1 (1%)	9	40
59	AB	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	1	17
59	AO	55/57 (96%)	43 (78%)	6 (11%)	6 (11%)	0	6
60	AC	194/196 (99%)	179 (92%)	10 (5%)	5 (3%)	4	28
60	AP	194/196 (99%)	178 (92%)	13 (7%)	3 (2%)	8	37
61	AD	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
61	AQ	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
62	AE	72/74 (97%)	65 (90%)	5 (7%)	2 (3%)	4	27
62	AR	72/74 (97%)	69 (96%)	2 (3%)	1 (1%)	9	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	AF	104/106 (98%)	100 (96%)	3 (3%)	1 (1%)	12	45
63	AS	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
64	AG	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
64	AT	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
65	AH	239/241 (99%)	225 (94%)	12 (5%)	2 (1%)	16	50
65	AU	239/241 (99%)	230 (96%)	7 (3%)	2 (1%)	16	50
66	AJ	376/378 (100%)	363 (96%)	10 (3%)	3 (1%)	16	50
66	AV	376/378 (100%)	359 (96%)	14 (4%)	3 (1%)	16	50
67	AK	417/419 (100%)	390 (94%)	22 (5%)	5 (1%)	10	41
67	AW	417/419 (100%)	397 (95%)	15 (4%)	5 (1%)	10	41
68	AL	444/446 (100%)	405 (91%)	33 (7%)	6 (1%)	9	38
68	AY	444/446 (100%)	413 (93%)	24 (5%)	7 (2%)	7	36
All	All	14029/14219 (99%)	12872 (92%)	849 (6%)	308 (2%)	7	31

All (308) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	73	PRO
1	A	379	CYS
2	B	62	THR
12	M	37	ASP
12	M	47	THR
12	M	178	GLN
12	M	210	ILE
12	M	369	GLU
13	N	115	PHE
14	O	232	THR
14	O	246	GLN
15	P	167	GLU
17	S	60	TYR
18	T	82	THR
19	U	71	GLN
21	W	34	SER
6	X	155	TYR
22	Y	84	PHE
24	a	58	ARG
26	c	115	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	c	178	PRO
27	d	2	PRO
31	h	20	ILE
32	i	91	ASN
32	i	323	THR
33	j	24	LEU
33	j	26	GLN
34	k	52	HIS
35	l	450	LEU
36	m	115	VAL
36	m	116	VAL
36	m	118	PHE
37	n	55	VAL
40	r	52	CYS
40	r	346	GLN
44	w	57	SER
44	w	282	PRO
44	w	347	VAL
45	x	328	HIS
45	x	508	PRO
50	2	2	SER
50	2	87	THR
50	2	95	GLN
51	3	4	ALA
51	3	9	GLY
52	4	46	LYS
54	6	2	GLU
66	AJ	268	ILE
67	AK	241	ARG
59	AO	23	ALA
60	AP	141	SER
68	AY	424	ILE
3	C	84	PHE
3	C	165	SER
4	E	20	ILE
4	E	127	ASP
6	G	138	LEU
7	H	105	GLU
8	I	31	ILE
8	I	93	LYS
8	I	107	SER
9	J	87	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	L	173	SER
12	M	250	SER
12	M	482	GLN
12	M	484	ASN
12	M	562	LYS
12	M	663	ASN
12	M	676	ASN
13	N	19	GLY
13	N	76	ASP
14	O	49	PRO
14	O	160	VAL
16	Q	104	GLU
16	Q	117	HIS
18	T	44	GLN
20	V	135	VAL
20	V	140	LYS
21	W	11	PRO
22	Y	44	TYR
22	Y	51	THR
24	a	57	ILE
24	a	185	ALA
25	b	101	LYS
26	c	170	ARG
30	g	9	PRO
31	h	3	PHE
31	h	24	GLU
31	h	43	CYS
33	j	2	ASN
35	l	73	THR
36	m	122	GLY
37	n	52	SER
40	r	45	ILE
40	r	188	ASN
40	r	250	LEU
40	r	421	HIS
41	s	203	GLY
41	s	213	ILE
41	s	217	ALA
41	s	316	PRO
43	v	56	ARG
44	w	264	GLN
44	w	285	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	5	LYS
60	AC	153	GLU
60	AC	255	PRO
66	AJ	157	GLY
67	AK	176	ASN
59	AO	38	PRO
60	AP	255	PRO
66	AV	157	GLY
66	AV	254	ASP
66	AV	266	PRO
67	AW	244	LEU
68	AY	312	GLY
68	AY	322	VAL
1	A	74	ASP
7	H	8	THR
7	H	63	PRO
8	I	52	ASN
9	J	135	GLU
9	J	178	SER
10	K	101	SER
11	L	165	SER
12	M	538	ARG
12	M	677	GLN
12	M	689	LEU
12	M	715	THR
13	N	113	HIS
14	O	238	PRO
15	P	44	ARG
15	P	179	ALA
15	P	214	ASP
15	P	229	GLU
16	Q	36	GLN
16	Q	197	MET
18	T	83	ARG
6	X	140	CYS
22	Y	85	PRO
25	b	37	PRO
25	b	109	THR
26	c	164	ASN
28	e	61	PRO
28	e	111	ASP
30	g	10	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	g	12	PHE
30	g	50	ARG
32	i	87	THR
34	k	83	ASN
34	k	96	LEU
35	l	65	ASN
35	l	451	LEU
35	l	549	PRO
35	l	554	ASP
35	l	563	PRO
36	m	4	ALA
36	m	76	GLU
36	m	110	ASP
38	o	5	LYS
38	o	12	ARG
40	r	139	GLN
41	s	38	ASN
42	u	36	CYS
42	u	101	ARG
42	u	143	HIS
43	v	73	SER
44	w	351	TRP
46	y	104	TRP
51	3	61	SER
58	AA	13	HIS
58	AA	29	HIS
59	AB	38	PRO
63	AF	8	SER
65	AH	133	ARG
67	AK	244	LEU
68	AL	180	ARG
68	AL	312	GLY
68	AL	322	VAL
58	AN	46	PHE
59	AO	51	SER
67	AW	241	ARG
67	AW	261	GLN
68	AY	382	SER
1	A	50	ASP
1	A	186	ALA
3	C	156	GLY
7	H	76	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	I	108	SER
9	J	100	LEU
9	J	330	PRO
9	J	370	LYS
10	K	78	ASP
11	L	172	VAL
12	M	377	ALA
12	M	426	ASP
13	N	42	ASP
13	N	130	THR
14	O	216	PRO
14	O	230	GLY
15	P	175	GLY
15	P	246	ARG
17	S	36	LYS
21	W	16	TYR
6	X	74	LEU
22	Y	42	PRO
22	Y	87	PRO
25	b	115	GLU
26	c	40	PRO
26	c	41	TYR
30	g	49	ARG
30	g	56	GLY
31	h	32	ARG
31	h	45	HIS
32	i	150	ASN
35	l	249	SER
35	l	387	THR
35	l	562	LEU
38	o	59	LEU
38	o	120	LYS
39	p	76	HIS
40	r	251	ASN
41	s	208	VAL
41	s	288	LEU
41	s	289	LEU
42	u	167	PHE
43	v	36	GLU
45	x	51	ASP
59	AB	51	SER
60	AC	142	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
60	AC	204	ARG
60	AC	219	HIS
62	AE	86	LEU
67	AK	261	GLN
68	AL	193	GLN
62	AR	28	ASP
65	AU	133	ARG
67	AW	144	PRO
67	AW	403	ALA
68	AY	193	GLN
68	AY	461	PRO
1	A	228	PRO
1	A	420	GLU
7	H	103	LEU
9	J	259	ASN
12	M	281	ILE
12	M	548	LEU
12	M	667	GLN
15	P	110	SER
15	P	202	PHE
15	P	239	TRP
15	P	245	TYR
16	Q	102	SER
20	V	48	THR
6	X	153	ASP
26	c	171	GLY
32	i	92	GLN
36	m	113	VAL
39	p	175	ARG
42	u	144	SER
44	w	58	ARG
44	w	121	PRO
44	w	160	GLU
46	y	103	GLN
54	6	3	ASN
59	AB	40	GLN
62	AE	28	ASP
68	AL	463	GLU
59	AO	27	ARG
59	AO	40	GLN
60	AP	204	ARG
65	AU	246	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
68	AY	463	GLU
3	C	102	ASP
6	G	137	LYS
8	I	70	MET
11	L	96	LYS
12	M	446	GLY
13	N	135	GLN
18	T	90	GLY
25	b	41	GLY
29	f	39	PRO
36	m	24	SER
39	p	32	VAL
40	r	205	VAL
45	x	91	ASP
46	y	158	ASP
51	3	49	PRO
65	AH	246	PRO
66	AJ	286	ASN
68	AL	279	ASP
12	M	435	PRO
21	W	10	MET
41	s	241	ILE
1	A	94	PRO
12	M	575	VAL
36	m	23	PRO
50	2	15	GLY
59	AO	30	VAL
3	C	144	PRO
16	Q	307	PRO
21	W	32	GLY
16	Q	69	VAL
67	AK	320	PRO
10	K	102	GLY
32	i	338	PRO
28	e	135	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	106/106 (100%)	106 (100%)	0	100	100
5	F	74/74 (100%)	74 (100%)	0	100	100
6	G	74/79 (94%)	74 (100%)	0	100	100
6	X	78/79 (99%)	78 (100%)	0	100	100
7	H	100/100 (100%)	99 (99%)	1 (1%)	68	75
8	I	87/96 (91%)	87 (100%)	0	100	100
9	J	292/292 (100%)	288 (99%)	4 (1%)	59	71
10	K	32/32 (100%)	32 (100%)	0	100	100
11	L	107/107 (100%)	107 (100%)	0	100	100
12	M	576/577 (100%)	574 (100%)	2 (0%)	86	85
13	N	129/129 (100%)	129 (100%)	0	100	100
14	O	181/181 (100%)	181 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	371/371 (100%)	368 (99%)	3 (1%)	73	77
17	S	59/59 (100%)	59 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	72/72 (100%)	72 (100%)	0	100	100
20	V	102/102 (100%)	102 (100%)	0	100	100
21	W	119/119 (100%)	119 (100%)	0	100	100
22	Y	57/57 (100%)	50 (88%)	7 (12%)	4	20
23	Z	62/63 (98%)	62 (100%)	0	100	100
24	a	124/124 (100%)	123 (99%)	1 (1%)	73	77
25	b	118/118 (100%)	113 (96%)	5 (4%)	26	50
26	c	124/137 (90%)	124 (100%)	0	100	100
27	d	145/154 (94%)	137 (94%)	8 (6%)	19	45
28	e	90/90 (100%)	90 (100%)	0	100	100
29	f	43/43 (100%)	43 (100%)	0	100	100
30	g	105/105 (100%)	105 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	h	90/90 (100%)	90 (100%)	0	100	100
32	i	314/314 (100%)	313 (100%)	1 (0%)	86	85
33	j	102/103 (99%)	101 (99%)	1 (1%)	68	75
34	k	85/85 (100%)	81 (95%)	4 (5%)	23	48
35	l	531/532 (100%)	511 (96%)	20 (4%)	29	52
36	m	137/137 (100%)	137 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	114/114 (100%)	114 (100%)	0	100	100
39	p	157/157 (100%)	155 (99%)	2 (1%)	61	71
40	r	416/416 (100%)	416 (100%)	0	100	100
41	s	278/278 (100%)	278 (100%)	0	100	100
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	89/111 (80%)	89 (100%)	0	100	100
44	w	249/288 (86%)	249 (100%)	0	100	100
45	x	427/427 (100%)	387 (91%)	40 (9%)	8	29
46	y	211/211 (100%)	191 (90%)	20 (10%)	8	29
47	z	226/226 (100%)	199 (88%)	27 (12%)	5	21
48	0	128/128 (100%)	118 (92%)	10 (8%)	11	36
49	1	95/95 (100%)	89 (94%)	6 (6%)	16	42
50	2	81/81 (100%)	73 (90%)	8 (10%)	7	28
51	3	68/68 (100%)	52 (76%)	16 (24%)	1	5
52	4	67/67 (100%)	58 (87%)	9 (13%)	4	19
53	5	58/58 (100%)	51 (88%)	7 (12%)	5	21
54	6	47/47 (100%)	41 (87%)	6 (13%)	4	20
55	7	39/39 (100%)	36 (92%)	3 (8%)	12	37
56	8	40/40 (100%)	37 (92%)	3 (8%)	12	38
57	9	37/37 (100%)	34 (92%)	3 (8%)	11	35
58	AA	74/74 (100%)	68 (92%)	6 (8%)	11	35
58	AN	73/74 (99%)	73 (100%)	0	100	100
59	AB	46/46 (100%)	46 (100%)	0	100	100
59	AO	45/46 (98%)	45 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	AC	166/166 (100%)	166 (100%)	0	100	100
60	AP	166/166 (100%)	166 (100%)	0	100	100
61	AD	52/52 (100%)	52 (100%)	0	100	100
61	AQ	52/52 (100%)	51 (98%)	1 (2%)	50	66
62	AE	61/71 (86%)	59 (97%)	2 (3%)	33	56
62	AR	61/71 (86%)	58 (95%)	3 (5%)	22	47
63	AF	95/95 (100%)	83 (87%)	12 (13%)	4	20
63	AS	95/95 (100%)	95 (100%)	0	100	100
64	AG	42/42 (100%)	42 (100%)	0	100	100
64	AT	42/42 (100%)	40 (95%)	2 (5%)	23	48
65	AH	207/207 (100%)	207 (100%)	0	100	100
65	AU	207/207 (100%)	206 (100%)	1 (0%)	81	82
66	AJ	330/330 (100%)	326 (99%)	4 (1%)	63	72
66	AV	330/330 (100%)	321 (97%)	9 (3%)	39	60
67	AK	334/335 (100%)	330 (99%)	4 (1%)	63	72
67	AW	335/335 (100%)	331 (99%)	4 (1%)	63	72
68	AL	367/367 (100%)	367 (100%)	0	100	100
68	AY	367/367 (100%)	362 (99%)	5 (1%)	59	71
All	All	12164/12289 (99%)	11894 (98%)	270 (2%)	45	64

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	H	81	ILE
9	J	85	ARG
9	J	91	ILE
9	J	206	ILE
9	J	212	ARG
12	M	130	ILE
12	M	174	THR
16	Q	268	TRP
16	Q	273	ILE
16	Q	275	ILE
22	Y	75	HIS
22	Y	78	GLU
22	Y	80	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	Y	81	LEU
22	Y	87	PRO
22	Y	95	GLU
22	Y	97	LEU
24	a	53	ARG
25	b	21	ARG
25	b	38	GLN
25	b	82	ILE
25	b	111	LEU
25	b	112	GLU
27	d	54	ARG
27	d	55	TYR
27	d	57	TYR
27	d	60	ARG
27	d	61	GLN
27	d	113	GLN
27	d	116	GLN
27	d	117	GLN
32	i	149	LEU
33	j	86	LEU
34	k	1	MET
34	k	3	LEU
34	k	6	MET
34	k	8	ILE
35	l	25	ASN
35	l	59	GLN
35	l	87	MET
35	l	94	LEU
35	l	97	THR
35	l	99	SER
35	l	191	LEU
35	l	193	SER
35	l	195	SER
35	l	196	TRP
35	l	197	ASP
35	l	217	LEU
35	l	218	LEU
35	l	223	LYS
35	l	226	GLN
35	l	229	LEU
35	l	447	ASN
35	l	450	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	l	452	ASN
35	l	513	MET
39	p	124	GLN
39	p	170	ILE
45	x	18	LEU
45	x	35	LEU
45	x	92	MET
45	x	96	ARG
45	x	105	LEU
45	x	115	SER
45	x	136	LEU
45	x	138	HIS
45	x	150	LEU
45	x	158	ILE
45	x	159	LEU
45	x	187	SER
45	x	188	VAL
45	x	189	MET
45	x	194	LEU
45	x	199	LEU
45	x	213	ARG
45	x	241	PRO
45	x	273	MET
45	x	295	VAL
45	x	301	THR
45	x	306	THR
45	x	318	VAL
45	x	324	LEU
45	x	347	LEU
45	x	353	LEU
45	x	354	THR
45	x	365	ILE
45	x	369	ASP
45	x	373	VAL
45	x	383	MET
45	x	417	MET
45	x	444	PRO
45	x	465	VAL
45	x	467	LEU
45	x	474	GLU
45	x	492	LEU
45	x	508	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	x	509	THR
45	x	512	ASN
46	y	7	LEU
46	y	16	ILE
46	y	31	VAL
46	y	33	LEU
46	y	52	HIS
46	y	60	GLU
46	y	63	THR
46	y	67	ILE
46	y	88	ASP
46	y	92	ASN
46	y	125	THR
46	y	130	PRO
46	y	134	ARG
46	y	142	VAL
46	y	147	GLU
46	y	170	LEU
46	y	171	LYS
46	y	185	MET
46	y	205	SER
46	y	216	LEU
47	z	1	MET
47	z	11	VAL
47	z	13	PRO
47	z	14	SER
47	z	18	LEU
47	z	19	THR
47	z	22	LEU
47	z	26	LEU
47	z	38	ASN
47	z	39	SER
47	z	85	LEU
47	z	92	LEU
47	z	112	LEU
47	z	127	LEU
47	z	128	GLU
47	z	131	LEU
47	z	132	LEU
47	z	137	LEU
47	z	142	VAL
47	z	160	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	z	163	LEU
47	z	188	ILE
47	z	196	THR
47	z	199	VAL
47	z	213	THR
47	z	222	GLN
47	z	230	ASN
48	0	9	GLU
48	0	27	VAL
48	0	31	LYS
48	0	36	SER
48	0	40	LEU
48	0	59	LEU
48	0	62	LEU
48	0	107	ILE
48	0	143	ASN
48	0	147	LYS
49	1	7	THR
49	1	29	LEU
49	1	70	VAL
49	1	79	LYS
49	1	80	GLU
49	1	90	ARG
50	2	6	VAL
50	2	20	VAL
50	2	37	LYS
50	2	52	ILE
50	2	53	THR
50	2	74	LEU
50	2	95	GLN
50	2	98	HIS
51	3	5	LYS
51	3	7	ASP
51	3	8	HIS
51	3	14	ARG
51	3	17	ARG
51	3	33	LEU
51	3	34	ASN
51	3	37	LEU
51	3	41	HIS
51	3	42	ARG
51	3	43	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	48	ILE
51	3	54	ARG
51	3	56	ARG
51	3	68	THR
51	3	78	LEU
52	4	19	ARG
52	4	29	CYS
52	4	41	LYS
52	4	51	SER
52	4	53	CYS
52	4	57	ARG
52	4	60	TYR
52	4	67	SER
52	4	75	ARG
53	5	2	THR
53	5	4	LEU
53	5	8	GLN
53	5	22	VAL
53	5	26	MET
53	5	44	LYS
53	5	64	ARG
54	6	2	GLU
54	6	5	VAL
54	6	8	LYS
54	6	16	ASN
54	6	23	LYS
54	6	27	THR
55	7	45	VAL
55	7	48	VAL
55	7	49	THR
56	8	15	VAL
56	8	22	LEU
56	8	26	THR
57	9	13	LYS
57	9	24	LEU
57	9	42	LYS
58	AA	25	ARG
58	AA	40	ARG
58	AA	48	ARG
58	AA	61	THR
58	AA	64	THR
58	AA	66	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
62	AE	28	ASP
62	AE	30	LEU
63	AF	14	LEU
63	AF	17	ILE
63	AF	29	LYS
63	AF	33	MET
63	AF	34	ARG
63	AF	38	ILE
63	AF	40	GLU
63	AF	41	ASP
63	AF	49	ARG
63	AF	60	MET
63	AF	71	LEU
63	AF	74	GLN
66	AJ	124	MET
66	AJ	150	LEU
66	AJ	164	ILE
66	AJ	300	ILE
67	AK	49	ILE
67	AK	259	ARG
67	AK	365	ASN
67	AK	451	ASP
61	AQ	47	ILE
62	AR	30	LEU
62	AR	78	ARG
62	AR	81	CYS
64	AT	39	ARG
64	AT	40	LEU
65	AU	292	MET
66	AV	42	ILE
66	AV	147	THR
66	AV	149	LEU
66	AV	150	LEU
66	AV	164	ILE
66	AV	185	LEU
66	AV	192	LEU
66	AV	195	LEU
66	AV	299	LEU
67	AW	138	LEU
67	AW	254	ARG
67	AW	451	ASP
67	AW	453	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
68	AY	96	LEU
68	AY	418	LEU
68	AY	422	ARG
68	AY	423	ARG
68	AY	462	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (274) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	49	HIS
1	A	116	ASN
1	A	164	ASN
1	A	170	GLN
1	A	220	GLN
1	A	270	ASN
1	A	284	HIS
1	A	313	ASN
1	A	441	HIS
2	B	184	ASN
3	C	72	ASN
3	C	95	HIS
4	E	48	HIS
4	E	49	GLN
4	E	51	GLN
4	E	70	ASN
4	E	108	HIS
5	F	62	GLN
5	F	81	ASN
6	G	80	GLN
6	G	142	GLN
7	H	50	GLN
7	H	76	GLN
7	H	83	GLN
7	H	111	GLN
9	J	71	ASN
9	J	93	HIS
9	J	102	GLN
9	J	183	ASN
10	K	77	HIS
11	L	86	ASN
12	M	142	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	M	425	ASN
12	M	460	HIS
12	M	464	GLN
12	M	498	GLN
12	M	514	ASN
12	M	663	ASN
12	M	666	GLN
12	M	669	ASN
13	N	72	ASN
13	N	91	HIS
13	N	113	HIS
13	N	123	GLN
13	N	135	GLN
14	O	69	ASN
14	O	187	GLN
14	O	189	ASN
14	O	191	ASN
15	P	74	GLN
15	P	82	ASN
15	P	105	ASN
16	Q	38	GLN
16	Q	147	ASN
16	Q	182	ASN
16	Q	183	HIS
16	Q	190	HIS
16	Q	233	HIS
16	Q	234	GLN
16	Q	339	GLN
16	Q	431	HIS
16	Q	442	HIS
16	Q	454	GLN
17	S	44	HIS
18	T	64	ASN
20	V	44	ASN
21	W	8	GLN
21	W	61	GLN
21	W	112	HIS
21	W	135	HIS
6	X	142	GLN
22	Y	75	HIS
23	Z	33	GLN
24	a	90	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	a	109	HIS
24	a	115	HIS
24	a	189	ASN
25	b	14	GLN
25	b	83	HIS
25	b	89	HIS
26	c	56	ASN
26	c	84	HIS
26	c	127	HIS
26	c	154	GLN
26	c	165	ASN
27	d	59	HIS
27	d	61	GLN
27	d	85	GLN
27	d	108	GLN
27	d	113	GLN
27	d	116	GLN
27	d	117	GLN
28	e	140	ASN
30	g	45	ASN
30	g	58	HIS
30	g	96	HIS
32	i	83	GLN
32	i	112	HIS
32	i	150	ASN
32	i	186	HIS
32	i	222	ASN
33	j	10	ASN
34	k	7	ASN
34	k	94	ASN
35	l	4	HIS
35	l	59	GLN
35	l	113	ASN
35	l	139	GLN
35	l	192	HIS
35	l	199	GLN
35	l	205	ASN
35	l	226	GLN
35	l	248	HIS
35	l	274	GLN
35	l	296	ASN
35	l	323	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	l	332	HIS
35	l	348	HIS
35	l	394	HIS
35	l	400	ASN
35	l	442	ASN
35	l	446	ASN
35	l	534	HIS
35	l	569	HIS
35	l	580	GLN
36	m	117	ASN
37	n	40	ASN
38	o	52	ASN
38	o	62	ASN
38	o	126	HIS
39	p	26	HIS
39	p	75	GLN
40	r	21	HIS
40	r	46	ASN
40	r	168	HIS
40	r	390	ASN
40	r	415	GLN
40	r	425	ASN
41	s	93	ASN
41	s	97	ASN
41	s	169	GLN
41	s	235	ASN
42	u	30	HIS
42	u	31	HIS
42	u	64	ASN
42	u	77	HIS
42	u	99	HIS
42	u	104	GLN
42	u	140	ASN
42	u	143	HIS
43	v	43	GLN
43	v	61	HIS
43	v	85	HIS
43	v	92	HIS
44	w	92	HIS
44	w	111	ASN
44	w	132	GLN
44	w	149	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	w	257	GLN
44	w	323	GLN
45	x	4	ASN
45	x	11	ASN
45	x	12	HIS
45	x	55	ASN
45	x	99	ASN
45	x	170	ASN
45	x	256	HIS
45	x	360	ASN
45	x	368	HIS
45	x	413	HIS
45	x	503	HIS
45	x	512	ASN
46	y	52	HIS
46	y	91	ASN
46	y	102	HIS
46	y	195	GLN
46	y	203	ASN
47	z	3	HIS
47	z	6	HIS
47	z	12	ASN
47	z	133	ASN
47	z	148	HIS
47	z	158	HIS
47	z	204	HIS
47	z	207	HIS
47	z	222	GLN
47	z	232	HIS
48	0	32	ASN
48	0	109	HIS
49	1	34	ASN
50	2	66	ASN
51	3	51	HIS
51	3	52	HIS
52	4	23	GLN
52	4	24	ASN
52	4	25	GLN
52	4	28	ASN
52	4	32	ASN
52	4	37	HIS
54	6	3	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	6	16	ASN
55	7	10	HIS
55	7	15	ASN
55	7	35	GLN
55	7	41	ASN
57	9	39	ASN
58	AA	29	HIS
60	AC	80	HIS
63	AF	23	ASN
63	AF	70	ASN
63	AF	73	HIS
64	AG	16	ASN
65	AH	107	HIS
65	AH	205	HIS
65	AH	265	GLN
65	AH	282	HIS
66	AJ	8	ASN
66	AJ	16	HIS
66	AJ	54	HIS
66	AJ	97	HIS
66	AJ	313	GLN
66	AJ	322	GLN
67	AK	139	ASN
67	AK	155	GLN
67	AK	178	HIS
67	AK	206	HIS
67	AK	310	HIS
67	AK	311	GLN
67	AK	399	GLN
68	AL	63	GLN
68	AL	66	GLN
68	AL	87	ASN
68	AL	207	ASN
68	AL	239	HIS
68	AL	240	GLN
68	AL	301	ASN
68	AL	308	ASN
68	AL	335	ASN
68	AL	452	GLN
60	AP	178	HIS
60	AP	199	GLN
61	AQ	38	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
62	AR	80	HIS
63	AS	23	ASN
63	AS	28	ASN
63	AS	70	ASN
63	AS	73	HIS
64	AT	16	ASN
65	AU	282	HIS
66	AV	97	HIS
66	AV	137	GLN
66	AV	255	ASN
66	AV	341	GLN
67	AW	81	HIS
67	AW	155	GLN
67	AW	176	ASN
67	AW	206	HIS
67	AW	227	HIS
67	AW	284	ASN
67	AW	298	HIS
67	AW	310	HIS
67	AW	311	GLN
67	AW	421	ASN
67	AW	426	ASN
67	AW	446	HIS
68	AY	87	ASN
68	AY	121	ASN
68	AY	152	GLN
68	AY	223	HIS
68	AY	301	ASN
68	AY	342	GLN
68	AY	375	GLN
68	AY	469	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 63 ligands modelled in this entry, 5 are monoatomic - leaving 58 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	SF4	B	301	2	0,12,12	-	-	-		
70	FMN	A	502	-	33,33,33	1.39	6 (18%)	48,50,50	1.34	8 (16%)
71	PLX	AL	501	-	51,51,51	0.77	1 (1%)	55,59,59	0.63	1 (1%)
71	PLX	V	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.60	1 (1%)
75	CDL	V	201	-	61,61,99	1.21	5 (8%)	64,71,111	0.94	3 (4%)
75	CDL	AJ	405	-	63,63,99	1.13	4 (6%)	69,75,111	1.22	5 (7%)
76	PEE	W	201	-	50,50,50	1.14	6 (12%)	53,55,55	0.97	2 (3%)
71	PLX	b	201	-	51,51,51	0.57	0	55,59,59	0.64	0
76	PEE	AU	401	-	40,40,50	1.46	4 (10%)	43,45,55	0.95	3 (6%)
79	HEA	x	604	45	66,67,67	1.22	7 (10%)	78,103,103	1.36	11 (14%)
69	SF4	M	801	12	0,12,12	-	-	-		
71	PLX	g	202	-	51,51,51	0.74	1 (1%)	55,59,59	0.61	1 (1%)
81	HEC	AU	402	65	50,50,50	1.73	6 (12%)	68,82,82	1.49	11 (16%)
74	FES	O	301	14	0,4,4	-	-	-		
69	SF4	M	802	12	0,12,12	-	-	-		
75	CDL	AG	101	-	63,63,99	1.15	4 (6%)	69,75,111	1.16	6 (8%)
73	NDP	J	401	-	49,52,52	1.20	5 (10%)	66,80,80	1.75	11 (16%)
82	HEM	AV	401	66	50,50,50	1.81	8 (16%)	66,82,82	1.34	5 (7%)
75	CDL	AJ	404	-	63,63,99	1.24	5 (7%)	69,75,111	1.03	4 (5%)
82	HEM	AV	402	66	50,50,50	1.78	7 (14%)	66,82,82	1.39	8 (12%)
75	CDL	AU	403	-	63,63,99	1.24	6 (9%)	69,75,111	1.04	4 (5%)
76	PEE	AV	403	-	48,48,50	1.34	4 (8%)	51,53,55	1.04	2 (3%)
74	FES	AC	301	60	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	CDL	l	703	-	63,63,99	1.21	5 (7%)	69,75,111	1.07	4 (5%)
76	PEE	AH	401	-	48,48,50	1.35	4 (8%)	51,53,55	0.95	2 (3%)
76	PEE	V	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.91	2 (3%)
71	PLX	B	303	-	51,51,51	0.77	1 (1%)	55,59,59	0.68	1 (1%)
69	SF4	B	302	2	0,12,12	-	-	-		
75	CDL	n	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.07	4 (5%)
72	8Q1	p	201	-	31,34,34	1.67	5 (16%)	40,43,43	1.57	5 (12%)
75	CDL	AN	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.02	4 (5%)
71	PLX	r	502	-	51,51,51	0.64	0	55,59,59	0.67	1 (1%)
75	CDL	i	401	-	63,63,99	1.21	5 (7%)	69,75,111	1.04	5 (7%)
71	PLX	U	101	-	51,51,51	0.74	1 (1%)	55,59,59	0.72	2 (3%)
79	HEA	x	603	45	66,67,67	1.09	3 (4%)	78,103,103	1.37	12 (15%)
69	SF4	C	301	3	0,12,12	-	-	-		
75	CDL	AA	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.07	4 (5%)
81	HEC	AH	402	65	50,50,50	1.68	5 (10%)	68,82,82	1.55	10 (14%)
71	PLX	AQ	101	-	51,51,51	0.77	1 (1%)	55,59,59	0.61	2 (3%)
75	CDL	l	704	-	63,63,99	1.26	5 (7%)	69,75,111	1.01	4 (5%)
76	PEE	AL	503	-	48,48,50	1.38	4 (8%)	51,53,55	0.92	2 (3%)
82	HEM	AJ	402	66	50,50,50	1.82	7 (14%)	66,82,82	1.35	7 (10%)
76	PEE	AY	502	-	48,48,50	1.39	4 (8%)	51,53,55	0.96	2 (3%)
82	HEM	AJ	401	66	50,50,50	1.80	8 (16%)	66,82,82	1.32	5 (7%)
74	FES	AP	301	60	0,4,4	-	-	-		
69	SF4	A	501	1	0,12,12	-	-	-		
71	PLX	AT	101	-	51,51,51	0.75	1 (1%)	55,59,59	0.60	1 (1%)
76	PEE	l	701	-	48,48,50	1.34	4 (8%)	51,53,55	0.96	2 (3%)
75	CDL	AL	502	-	63,63,99	1.24	5 (7%)	69,75,111	1.05	4 (5%)
75	CDL	AH	403	-	63,63,99	1.25	5 (7%)	69,75,111	1.03	4 (5%)
71	PLX	g	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.58	1 (1%)
74	FES	M	803	-	0,4,4	-	-	-		
76	PEE	AJ	403	-	48,48,50	1.33	4 (8%)	51,53,55	0.99	2 (3%)
71	PLX	g	201	-	51,51,51	0.82	1 (1%)	55,59,59	0.69	1 (1%)
71	PLX	r	501	-	51,51,51	0.74	1 (1%)	55,59,59	0.65	1 (1%)
75	CDL	AY	501	-	63,63,99	1.24	5 (7%)	69,75,111	1.01	4 (5%)
72	8Q1	E	201	-	31,34,34	1.64	6 (19%)	40,43,43	1.39	7 (17%)
76	PEE	l	702	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	SF4	B	301	2	-	-	0/6/5/5
70	FMN	A	502	-	-	7/18/18/18	0/3/3/3
71	PLX	AL	501	-	-	23/55/55/55	-
71	PLX	V	203	-	-	26/55/55/55	-
75	CDL	V	201	-	-	41/69/69/110	-
75	CDL	AJ	405	-	-	28/74/74/110	-
76	PEE	W	201	-	-	32/54/54/54	-
71	PLX	b	201	-	-	27/55/55/55	-
76	PEE	AU	401	-	-	17/44/44/54	-
79	HEA	x	604	45	-	7/36/76/76	-
81	HEC	AU	402	65	-	2/14/54/54	-
71	PLX	g	202	-	-	25/55/55/55	-
69	SF4	M	801	12	-	-	0/6/5/5
74	FES	O	301	14	-	-	0/1/1/1
69	SF4	M	802	12	-	-	0/6/5/5
75	CDL	AG	101	-	-	38/74/74/110	-
73	NDP	J	401	-	-	15/34/77/77	0/5/5/5
82	HEM	AV	401	66	-	5/14/54/54	-
75	CDL	AJ	404	-	-	33/74/74/110	-
82	HEM	AV	402	66	-	4/14/54/54	-
75	CDL	AU	403	-	-	48/74/74/110	-
76	PEE	AV	403	-	-	30/52/52/54	-
75	CDL	l	703	-	-	38/74/74/110	-
76	PEE	AH	401	-	-	27/52/52/54	-
74	FES	AC	301	60	-	-	0/1/1/1
76	PEE	V	202	-	-	27/54/54/54	-
71	PLX	B	303	-	-	21/55/55/55	-
75	CDL	n	101	-	-	33/74/74/110	-
75	CDL	AN	101	-	-	40/74/74/110	-
72	8Q1	p	201	-	-	19/41/41/41	-
69	SF4	B	302	2	-	-	0/6/5/5
71	PLX	r	502	-	-	36/55/55/55	-
75	CDL	i	401	-	-	39/74/74/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	PLX	U	101	-	-	22/55/55/55	-
79	HEA	x	603	45	-	9/36/76/76	-
69	SF4	C	301	3	-	-	0/6/5/5
75	CDL	AA	101	-	-	35/74/74/110	-
81	HEC	AH	402	65	-	6/14/54/54	-
71	PLX	AQ	101	-	-	25/55/55/55	-
75	CDL	l	704	-	-	44/74/74/110	-
76	PEE	AL	503	-	-	22/52/52/54	-
82	HEM	AJ	402	66	-	2/14/54/54	-
76	PEE	AY	502	-	-	20/52/52/54	-
82	HEM	AJ	401	66	-	1/14/54/54	-
76	PEE	l	701	-	-	32/52/52/54	-
69	SF4	A	501	1	-	-	0/6/5/5
71	PLX	AT	101	-	-	23/55/55/55	-
74	FES	AP	301	60	-	-	0/1/1/1
75	CDL	AL	502	-	-	43/74/74/110	-
75	CDL	AH	403	-	-	42/74/74/110	-
71	PLX	g	203	-	-	24/55/55/55	-
74	FES	M	803	-	-	-	0/1/1/1
76	PEE	AJ	403	-	-	20/52/52/54	-
71	PLX	g	201	-	-	25/55/55/55	-
71	PLX	r	501	-	-	28/55/55/55	-
75	CDL	AY	501	-	-	36/74/74/110	-
72	8Q1	E	201	-	-	18/41/41/41	-
76	PEE	l	702	-	-	27/54/54/54	-

All (198) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	AU	402	HEC	C3D-C2D	8.00	1.53	1.36
81	AH	402	HEC	C3D-C2D	7.93	1.53	1.36
82	AJ	401	HEM	C3D-C2D	7.85	1.53	1.36
82	AV	402	HEM	C3D-C2D	7.85	1.53	1.36
82	AJ	402	HEM	C3D-C2D	7.80	1.53	1.36
82	AV	401	HEM	C3D-C2D	7.75	1.53	1.36
72	p	201	8Q1	C34-N36	5.33	1.45	1.33
72	E	201	8Q1	C34-N36	5.26	1.45	1.33
72	p	201	8Q1	C39-N41	5.24	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	E	201	8Q1	C39-N41	4.91	1.44	1.33
82	AV	401	HEM	FE-ND	4.80	2.09	1.94
70	A	502	FMN	C9A-C5A	4.40	1.48	1.41
75	l	704	CDL	OB8-CB7	4.35	1.46	1.33
75	AH	403	CDL	OA6-CA5	4.34	1.46	1.34
75	AL	502	CDL	OA6-CA5	4.32	1.46	1.34
75	AH	403	CDL	OB8-CB7	4.31	1.45	1.33
75	n	101	CDL	OA6-CA5	4.30	1.46	1.34
76	AY	502	PEE	C39-C38	4.30	1.56	1.31
75	AY	501	CDL	OA6-CA5	4.30	1.46	1.34
75	AG	101	CDL	OB8-CB7	4.30	1.45	1.33
75	AU	403	CDL	OA6-CA5	4.28	1.46	1.34
75	AJ	405	CDL	OA8-CA7	4.28	1.45	1.33
76	AU	401	PEE	C39-C38	4.27	1.56	1.31
75	V	201	CDL	OA6-CA5	4.27	1.46	1.34
75	AJ	404	CDL	OA6-CA5	4.27	1.46	1.34
75	l	703	CDL	OA6-CA5	4.26	1.46	1.34
76	AL	503	PEE	C39-C38	4.26	1.56	1.31
76	AV	403	PEE	C39-C38	4.25	1.56	1.31
76	AL	503	PEE	O3-C30	4.25	1.45	1.33
75	AU	403	CDL	OB8-CB7	4.24	1.45	1.33
76	AJ	403	PEE	C39-C38	4.24	1.56	1.31
75	AG	101	CDL	OA6-CA5	4.23	1.46	1.34
75	l	703	CDL	OB8-CB7	4.23	1.45	1.33
75	AL	502	CDL	OB8-CB7	4.23	1.45	1.33
76	AH	401	PEE	C39-C38	4.23	1.56	1.31
75	AG	101	CDL	OA8-CA7	4.22	1.45	1.33
75	AY	501	CDL	OB8-CB7	4.22	1.45	1.33
76	AY	502	PEE	O3-C30	4.22	1.45	1.33
76	AY	502	PEE	C18-C19	4.21	1.56	1.31
76	AH	401	PEE	C18-C19	4.20	1.56	1.31
75	V	201	CDL	OB8-CB7	4.20	1.45	1.33
76	AL	503	PEE	C18-C19	4.20	1.56	1.31
76	AH	401	PEE	O3-C30	4.20	1.45	1.33
75	AA	101	CDL	OB8-CB7	4.19	1.45	1.33
75	AJ	404	CDL	OB8-CB7	4.19	1.45	1.33
76	l	701	PEE	C39-C38	4.17	1.56	1.31
75	AA	101	CDL	OA6-CA5	4.17	1.46	1.34
75	AJ	405	CDL	OB8-CB7	4.16	1.45	1.33
75	AN	101	CDL	OA6-CA5	4.16	1.46	1.34
75	l	704	CDL	OA8-CA7	4.15	1.45	1.33
76	AJ	403	PEE	C18-C19	4.15	1.55	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	l	704	CDL	OA6-CA5	4.15	1.46	1.34
76	l	701	PEE	O3-C30	4.13	1.45	1.33
76	AV	403	PEE	C18-C19	4.13	1.55	1.31
75	AN	101	CDL	OB8-CB7	4.13	1.45	1.33
76	l	701	PEE	C18-C19	4.13	1.55	1.31
76	AV	403	PEE	O3-C30	4.12	1.45	1.33
76	AU	401	PEE	O3-C30	4.12	1.45	1.33
75	n	101	CDL	OB8-CB7	4.11	1.45	1.33
82	AJ	401	HEM	FE-NB	4.11	2.07	1.94
82	AJ	402	HEM	FE-ND	4.09	2.07	1.94
75	AJ	405	CDL	OB6-CB5	4.09	1.45	1.34
76	AU	401	PEE	C19-C18	4.07	1.56	1.28
75	i	401	CDL	OB8-CB7	4.06	1.45	1.33
75	AG	101	CDL	OB6-CB5	4.03	1.45	1.34
75	i	401	CDL	OA6-CA5	3.99	1.45	1.34
76	AJ	403	PEE	O3-C30	3.98	1.45	1.33
75	AJ	405	CDL	OA6-CA5	3.98	1.45	1.34
75	AJ	404	CDL	OA8-CA7	3.97	1.44	1.33
75	AY	501	CDL	OA8-CA7	3.96	1.44	1.33
75	AH	403	CDL	OA8-CA7	3.94	1.44	1.33
75	AU	403	CDL	OA8-CA7	3.94	1.44	1.33
73	J	401	NDP	C5A-C4A	3.92	1.46	1.39
75	n	101	CDL	OA8-CA7	3.91	1.44	1.33
75	AL	502	CDL	OA8-CA7	3.91	1.44	1.33
75	AN	101	CDL	OA8-CA7	3.91	1.44	1.33
82	AJ	401	HEM	FE-ND	3.91	2.07	1.94
75	AA	101	CDL	OA8-CA7	3.90	1.44	1.33
82	AV	402	HEM	FE-ND	3.87	2.06	1.94
81	AU	402	HEC	FE-NB	3.86	2.06	1.94
75	l	703	CDL	OA8-CA7	3.82	1.44	1.33
76	l	702	PEE	C18-C19	3.77	1.53	1.31
76	V	202	PEE	C18-C19	3.77	1.53	1.31
79	x	604	HEA	CMA-C3A	-3.75	1.37	1.45
76	W	201	PEE	C18-C19	3.74	1.53	1.31
75	i	401	CDL	OA8-CA7	3.71	1.44	1.33
76	V	202	PEE	C39-C38	3.71	1.53	1.31
76	l	702	PEE	C39-C38	3.69	1.53	1.31
76	W	201	PEE	C39-C38	3.68	1.53	1.31
81	AU	402	HEC	FE-ND	3.59	2.06	1.94
81	AH	402	HEC	FE-NB	3.59	2.06	1.94
76	AY	502	PEE	O2-C10	3.46	1.44	1.34
82	AJ	402	HEM	FE-NC	3.46	2.06	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	AL	503	PEE	O2-C10	3.45	1.44	1.34
75	l	704	CDL	OB6-CB5	3.35	1.43	1.34
76	l	701	PEE	O2-C10	3.33	1.43	1.34
75	AY	501	CDL	OB6-CB5	3.29	1.43	1.34
75	n	101	CDL	OB6-CB5	3.27	1.43	1.34
75	AJ	404	CDL	OB6-CB5	3.24	1.43	1.34
76	AJ	403	PEE	O2-C10	3.23	1.43	1.34
75	AN	101	CDL	OB6-CB5	3.22	1.43	1.34
75	l	703	CDL	OB6-CB5	3.22	1.43	1.34
75	AH	403	CDL	OB6-CB5	3.20	1.43	1.34
76	AU	401	PEE	O2-C10	3.18	1.43	1.34
75	AA	101	CDL	OB6-CB5	3.15	1.43	1.34
76	AV	403	PEE	O2-C10	3.15	1.43	1.34
75	AU	403	CDL	OB6-CB5	3.14	1.43	1.34
82	AJ	402	HEM	FE-NA	3.14	2.05	1.95
73	J	401	NDP	C6N-C5N	3.13	1.38	1.33
76	AH	401	PEE	O2-C10	3.11	1.43	1.34
75	V	201	CDL	OB6-CB5	3.11	1.43	1.34
81	AH	402	HEC	FE-ND	3.10	2.04	1.94
75	AL	502	CDL	OB6-CB5	3.10	1.43	1.34
70	A	502	FMN	C8-C7	3.07	1.48	1.40
75	i	401	CDL	OB6-CB5	3.07	1.43	1.34
70	A	502	FMN	C4-N3	-3.03	1.33	1.38
75	V	201	CDL	OA8-CA7	3.01	1.45	1.33
82	AV	402	HEM	FE-NC	2.98	2.05	1.95
82	AV	402	HEM	CAC-C3C	2.98	1.55	1.47
82	AJ	402	HEM	CAB-C3B	2.97	1.55	1.47
71	B	303	PLX	O6-C4	-2.97	1.40	1.44
82	AV	401	HEM	CAB-C3B	2.97	1.55	1.47
82	AJ	402	HEM	FE-NB	2.95	2.04	1.94
81	AU	402	HEC	FE-NC	2.94	2.05	1.95
79	x	604	HEA	FE-NA	2.93	2.05	1.95
82	AJ	401	HEM	CAC-C3C	2.93	1.55	1.47
82	AJ	401	HEM	CAB-C3B	2.93	1.55	1.47
82	AV	402	HEM	CAB-C3B	2.91	1.55	1.47
71	g	203	PLX	O6-C4	-2.90	1.40	1.44
73	J	401	NDP	C5A-N7A	-2.86	1.33	1.39
82	AV	401	HEM	FE-NC	2.86	2.04	1.95
82	AV	402	HEM	FE-NB	2.85	2.03	1.94
82	AJ	402	HEM	CAC-C3C	2.84	1.55	1.47
82	AV	402	HEM	FE-NA	2.82	2.04	1.95
82	AV	401	HEM	FE-NA	2.79	2.04	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	g	201	PLX	O6-C4	-2.76	1.40	1.44
75	n	101	CDL	OB6-CB4	-2.76	1.39	1.46
81	AH	402	HEC	FE-NC	2.75	2.04	1.95
71	V	203	PLX	O6-C4	-2.75	1.40	1.44
82	AV	401	HEM	CAC-C3C	2.70	1.54	1.47
71	AL	501	PLX	O6-C4	-2.68	1.41	1.44
79	x	603	HEA	C1A-C2A	-2.68	1.40	1.45
75	AL	502	CDL	OB6-CB4	-2.63	1.40	1.46
79	x	604	HEA	C3A-C2A	-2.62	1.31	1.36
79	x	604	HEA	C1D-C2D	2.62	1.49	1.44
75	V	201	CDL	OB6-CB4	-2.62	1.40	1.46
75	AH	403	CDL	OB6-CB4	-2.60	1.40	1.46
82	AV	401	HEM	FE-NB	2.60	2.02	1.94
79	x	603	HEA	CMA-C3A	-2.60	1.39	1.45
82	AJ	401	HEM	FE-NA	2.59	2.03	1.95
75	AA	101	CDL	OB6-CB4	-2.58	1.40	1.46
71	AQ	101	PLX	O6-C4	-2.58	1.41	1.44
79	x	604	HEA	C1D-ND	-2.57	1.35	1.40
71	U	101	PLX	O6-C4	-2.57	1.41	1.44
75	AJ	404	CDL	OB6-CB4	-2.55	1.40	1.46
75	AN	101	CDL	OB6-CB4	-2.54	1.40	1.46
81	AH	402	HEC	FE-NA	2.53	2.03	1.95
75	AU	403	CDL	OB6-CB4	-2.52	1.40	1.46
75	i	401	CDL	OB6-CB4	-2.50	1.40	1.46
72	E	201	8Q1	O35-C34	-2.49	1.18	1.23
72	p	201	8Q1	O35-C34	-2.49	1.18	1.23
71	AT	101	PLX	O6-C4	-2.47	1.41	1.44
75	AY	501	CDL	OB6-CB4	-2.46	1.40	1.46
71	g	202	PLX	O6-C4	-2.43	1.41	1.44
76	V	202	PEE	O2-C10	2.39	1.41	1.34
71	r	501	PLX	O6-C4	-2.38	1.41	1.44
76	l	702	PEE	O2-C10	2.38	1.41	1.34
72	E	201	8Q1	C1-S44	2.36	1.81	1.76
75	l	704	CDL	OB6-CB4	-2.36	1.40	1.46
75	l	703	CDL	OB6-CB4	-2.34	1.40	1.46
72	E	201	8Q1	O40-C39	-2.34	1.18	1.23
72	p	201	8Q1	O40-C39	-2.33	1.18	1.23
76	l	702	PEE	O3-C30	2.33	1.40	1.33
79	x	603	HEA	C3A-C4A	-2.31	1.42	1.46
70	A	502	FMN	C5A-N5	-2.30	1.35	1.39
81	AU	402	HEC	FE-NA	2.30	2.02	1.95
76	V	202	PEE	O3-C30	2.25	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	l	702	PEE	O2-C2	-2.25	1.41	1.46
76	V	202	PEE	O2-C2	-2.24	1.41	1.46
76	W	201	PEE	O3-C30	2.24	1.39	1.33
79	x	604	HEA	CMD-C2D	2.24	1.55	1.50
72	p	201	8Q1	C1-S44	2.22	1.81	1.76
76	V	202	PEE	O3-C3	-2.22	1.40	1.45
82	AV	401	HEM	C3C-C2C	-2.22	1.32	1.37
76	W	201	PEE	O2-C10	2.22	1.40	1.34
76	l	702	PEE	O3-C3	-2.20	1.40	1.45
72	E	201	8Q1	C6-C1	2.20	1.53	1.50
76	W	201	PEE	O2-C2	-2.18	1.41	1.46
73	J	401	NDP	C5A-C6A	2.17	1.47	1.41
70	A	502	FMN	C4A-N5	2.16	1.34	1.30
76	W	201	PEE	O3-C3	-2.14	1.40	1.45
82	AJ	401	HEM	C2A-C3A	-2.07	1.33	1.38
82	AJ	401	HEM	FE-NC	2.07	2.02	1.95
73	J	401	NDP	C8A-N7A	2.06	1.35	1.31
70	A	502	FMN	C2-N3	-2.04	1.34	1.39
75	AU	403	CDL	C11-CA5	2.04	1.56	1.50
79	x	604	HEA	FE-NC	2.04	2.02	1.95
81	AU	402	HEC	C3C-C2C	-2.01	1.33	1.38

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	AH	402	HEC	C1D-ND-C4D	6.46	111.74	105.07
81	AU	402	HEC	C1D-ND-C4D	6.29	111.56	105.07
82	AV	402	HEM	C4D-ND-C1D	6.20	111.47	105.07
73	J	401	NDP	C5A-C4A-N3A	-6.18	118.69	126.75
82	AJ	401	HEM	C4D-ND-C1D	6.12	111.39	105.07
82	AJ	402	HEM	C4D-ND-C1D	6.02	111.30	105.07
72	p	201	8Q1	C6-C1-S44	6.02	120.47	113.46
82	AV	401	HEM	C4D-ND-C1D	5.32	110.57	105.07
73	J	401	NDP	PN-O3-PA	-5.21	114.95	132.83
73	J	401	NDP	N3A-C4A-N9A	4.97	135.28	127.08
72	E	201	8Q1	C6-C1-S44	4.57	118.77	113.46
76	l	702	PEE	O2-C10-C11	4.38	120.95	111.50
76	AY	502	PEE	O2-C10-C11	4.31	120.78	111.50
75	AJ	405	CDL	OB6-CB5-C51	4.29	120.74	111.50
75	AL	502	CDL	OA6-CA5-C11	4.26	120.69	111.50
75	AY	501	CDL	OA6-CA5-C11	4.20	120.55	111.50
75	l	703	CDL	OA6-CA5-C11	4.19	120.54	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	AG	101	CDL	OB6-CB5-C51	4.19	120.53	111.50
75	AH	403	CDL	OA6-CA5-C11	4.16	120.47	111.50
75	AU	403	CDL	OA6-CA5-C11	4.15	120.45	111.50
75	i	401	CDL	OA6-CA5-C11	4.13	120.41	111.50
75	AJ	404	CDL	OA6-CA5-C11	4.12	120.39	111.50
75	V	201	CDL	OB6-CB5-C51	4.09	120.31	111.50
75	l	704	CDL	OA6-CA5-C11	4.09	120.31	111.50
75	AA	101	CDL	OA6-CA5-C11	4.08	120.30	111.50
75	n	101	CDL	OB6-CB5-C51	4.08	120.30	111.50
75	AU	403	CDL	OB6-CB5-C51	4.04	120.20	111.50
75	AJ	404	CDL	OB6-CB5-C51	4.03	120.19	111.50
76	AJ	403	PEE	O2-C10-C11	4.03	120.19	111.50
73	J	401	NDP	C2A-N3A-C4A	4.03	121.27	111.75
76	l	701	PEE	O2-C10-C11	4.00	120.13	111.50
75	AA	101	CDL	OB6-CB5-C51	3.99	120.10	111.50
79	x	603	HEA	C17-C18-C19	-3.98	118.09	127.66
75	l	703	CDL	OB6-CB5-C51	3.95	120.02	111.50
75	AN	101	CDL	OA6-CA5-C11	3.95	120.01	111.50
75	n	101	CDL	OA6-CA5-C11	3.93	119.97	111.50
75	AH	403	CDL	OB6-CB5-C51	3.92	119.95	111.50
75	l	704	CDL	OB6-CB5-C51	3.92	119.95	111.50
76	AV	403	PEE	O2-C10-C11	3.91	119.93	111.50
75	AY	501	CDL	OB6-CB5-C51	3.88	119.87	111.50
75	AN	101	CDL	OB6-CB5-C51	3.87	119.83	111.50
75	AL	502	CDL	OB6-CB5-C51	3.85	119.79	111.50
73	J	401	NDP	N3A-C2A-N1A	-3.70	122.81	128.60
76	W	201	PEE	O2-C10-C11	3.69	119.45	111.50
72	p	201	8Q1	O4-C1-C6	-3.65	119.68	123.99
76	V	202	PEE	O2-C10-C11	3.61	119.28	111.50
75	AG	101	CDL	OA6-CA5-C11	3.58	119.21	111.50
76	AH	401	PEE	O2-C10-C11	3.55	119.16	111.50
75	AJ	405	CDL	OA6-CA5-C11	3.55	119.15	111.50
76	AL	503	PEE	O2-C10-C11	3.51	119.06	111.50
75	i	401	CDL	OB6-CB5-C51	3.49	119.03	111.50
75	V	201	CDL	OA6-CA5-C11	3.45	118.93	111.50
75	AJ	405	CDL	OB8-CB7-C71	3.25	122.11	111.91
79	x	604	HEA	CHA-C1A-NA	-3.23	120.94	124.44
76	AU	401	PEE	O2-C10-C11	3.23	118.46	111.50
81	AH	402	HEC	C4A-CHB-C1B	-3.13	119.30	126.06
79	x	603	HEA	C13-C14-C15	-3.13	120.13	127.66
73	J	401	NDP	C4A-C5A-N7A	-3.09	106.86	110.62
76	AV	403	PEE	O3-C30-C31	3.06	121.52	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	l	703	CDL	OA8-CA7-C31	2.99	121.29	111.91
82	AV	401	HEM	CAD-CBD-CGD	-2.98	107.20	113.60
75	AA	101	CDL	OA8-CA7-C31	2.97	121.22	111.91
79	x	603	HEA	C1B-C2B-C3B	2.93	110.30	106.80
75	AG	101	CDL	CB4-OB6-CB5	-2.90	110.64	117.79
73	J	401	NDP	C5A-N7A-C8A	2.86	107.57	103.51
76	V	202	PEE	O3-C30-C31	2.85	120.85	111.91
81	AH	402	HEC	C4A-NA-C1A	2.84	108.13	105.35
76	l	702	PEE	O3-C30-C31	2.84	120.82	111.91
70	A	502	FMN	C4-C4A-N5	2.80	122.22	118.23
72	E	201	8Q1	C43-S44-C1	2.79	110.57	101.87
75	i	401	CDL	OB8-CB7-C71	2.76	120.57	111.91
70	A	502	FMN	C4A-C10-N1	-2.75	118.34	124.73
75	n	101	CDL	OA8-CA7-C31	2.75	120.54	111.91
75	AG	101	CDL	OB8-CB7-C71	2.74	120.51	111.91
72	E	201	8Q1	C32-C34-N36	2.74	122.03	116.58
75	AL	502	CDL	OA8-CA7-C31	2.72	120.46	111.91
75	l	704	CDL	OA8-CA7-C31	2.72	120.45	111.91
72	p	201	8Q1	C43-S44-C1	2.72	110.34	101.87
82	AJ	402	HEM	C4A-NA-C1A	2.72	108.01	105.35
82	AV	402	HEM	C4A-NA-C1A	2.72	108.01	105.35
75	AJ	405	CDL	OA8-CA7-C31	2.70	120.40	111.91
73	J	401	NDP	C4A-N9A-C8A	2.70	108.65	105.73
75	l	703	CDL	OB8-CB7-C71	2.69	120.36	111.91
75	AL	502	CDL	OB8-CB7-C71	2.69	120.36	111.91
75	n	101	CDL	OB8-CB7-C71	2.69	120.34	111.91
75	AN	101	CDL	OA8-CA7-C31	2.68	120.33	111.91
76	W	201	PEE	O3-C30-C31	2.68	120.33	111.91
75	AH	403	CDL	OB8-CB7-C71	2.67	120.30	111.91
75	l	704	CDL	OB8-CB7-C71	2.67	120.28	111.91
75	AU	403	CDL	OA8-CA7-C31	2.66	120.25	111.91
75	AJ	404	CDL	OA8-CA7-C31	2.66	120.25	111.91
81	AU	402	HEC	CAB-C3B-C4B	2.66	128.26	124.81
76	AH	401	PEE	O3-C30-C31	2.65	120.23	111.91
81	AU	402	HEC	C4B-NB-C1B	2.63	107.79	105.07
79	x	604	HEA	C4A-C3A-C2A	2.63	108.91	106.75
81	AU	402	HEC	C4C-NC-C1C	2.63	107.92	105.35
82	AJ	402	HEM	C1B-NB-C4B	2.63	107.79	105.07
81	AH	402	HEC	C4B-NB-C1B	2.62	107.78	105.07
79	x	604	HEA	CMD-C2D-C1D	2.62	129.03	125.04
75	AA	101	CDL	OB8-CB7-C71	2.61	120.11	111.91
75	AU	403	CDL	OB8-CB7-C71	2.59	120.05	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	AU	402	HEC	C4A-NA-C1A	2.59	107.88	105.35
81	AH	402	HEC	C4C-NC-C1C	2.58	107.87	105.35
75	AG	101	CDL	OA8-CA7-C31	2.57	119.96	111.91
72	p	201	8Q1	C38-C39-N41	2.55	120.71	116.42
75	AJ	404	CDL	OB8-CB7-C71	2.54	119.87	111.91
75	V	201	CDL	OB8-CB7-C71	2.54	119.86	111.91
75	AY	501	CDL	OA8-CA7-C31	2.52	119.82	111.91
72	E	201	8Q1	O4-C1-C6	-2.52	121.01	123.99
75	AY	501	CDL	OB8-CB7-C71	2.52	119.81	111.91
75	AN	101	CDL	OB8-CB7-C71	2.52	119.81	111.91
75	AH	403	CDL	OA8-CA7-C31	2.50	119.76	111.91
81	AH	402	HEC	CAB-C3B-C4B	2.47	128.02	124.81
76	AL	503	PEE	O3-C30-C31	2.47	119.66	111.91
82	AV	401	HEM	C1B-NB-C4B	2.46	107.62	105.07
82	AV	402	HEM	C1B-NB-C4B	2.46	107.61	105.07
82	AV	401	HEM	C4C-NC-C1C	2.45	107.75	105.35
71	AT	101	PLX	C1C-N1-C1	2.43	119.87	109.92
75	i	401	CDL	OA8-CA7-C31	2.42	119.49	111.91
79	x	603	HEA	C17-C16-C15	-2.41	105.04	112.98
70	A	502	FMN	C4A-C10-N10	2.41	120.01	116.48
81	AU	402	HEC	C2A-C1A-NA	-2.41	107.98	110.32
72	E	201	8Q1	C42-N41-C39	-2.41	118.36	122.84
81	AU	402	HEC	C4A-CHB-C1B	-2.40	120.88	126.06
76	AJ	403	PEE	O3-C30-C31	2.38	119.39	111.91
81	AH	402	HEC	C2A-C1A-NA	-2.38	108.01	110.32
79	x	604	HEA	C1D-C2D-C3D	-2.37	104.46	106.96
79	x	603	HEA	C3C-C4C-NC	2.37	111.71	110.25
72	E	201	8Q1	C37-N36-C34	-2.37	118.36	122.59
79	x	603	HEA	C16-C17-C18	-2.37	104.10	111.88
79	x	604	HEA	C25-C23-C24	2.36	119.82	114.60
79	x	604	HEA	CMB-C2B-C3B	-2.36	125.84	130.34
71	B	303	PLX	C1C-N1-C1	2.36	119.58	109.92
82	AV	402	HEM	CAD-C3D-C4D	2.35	128.77	124.66
71	AL	501	PLX	C1C-N1-C1	2.35	119.53	109.92
79	x	604	HEA	CAA-C2A-C1A	2.35	129.32	124.89
79	x	603	HEA	C20-C19-C18	2.35	125.87	121.12
81	AU	402	HEC	CAA-CBA-CGA	-2.33	108.59	113.60
79	x	603	HEA	CAD-C3D-C4D	2.33	128.72	124.66
71	V	203	PLX	C1C-N1-C1	2.32	119.40	109.92
70	A	502	FMN	O2-C2-N1	-2.31	118.00	121.83
76	AU	401	PEE	O3-C30-C31	2.31	119.16	111.91
76	AY	502	PEE	O3-C30-C31	2.30	119.11	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
71	U	101	PLX	C1C-N1-C1	2.29	119.30	109.92
76	l	701	PEE	O3-C30-C31	2.29	119.09	111.91
82	AJ	402	HEM	CAD-C3D-C4D	2.27	128.63	124.66
71	g	203	PLX	C1C-N1-C1	2.27	119.20	109.92
82	AV	402	HEM	C4C-NC-C1C	2.26	107.56	105.35
79	x	604	HEA	C13-C14-C15	-2.25	122.25	127.66
70	A	502	FMN	C4-N3-C2	-2.24	121.51	125.64
73	J	401	NDP	N9A-C8A-N7A	-2.22	110.88	113.91
79	x	604	HEA	C26-C15-C16	2.22	119.00	115.27
81	AH	402	HEC	CAA-CBA-CGA	-2.21	108.84	113.60
75	AJ	405	CDL	OB8-CB7-OB9	-2.21	118.02	123.59
82	AJ	401	HEM	CAD-CBD-CGD	-2.20	108.86	113.60
71	g	201	PLX	C1C-N1-C1	2.20	118.91	109.92
79	x	603	HEA	C4B-C3B-C2B	-2.20	103.66	107.41
73	J	401	NDP	C3D-C2D-C1D	2.19	105.59	101.43
71	g	202	PLX	C1C-N1-C1	2.19	118.89	109.92
79	x	603	HEA	C12-C13-C14	-2.18	106.47	112.23
82	AV	402	HEM	CAD-CBD-CGD	-2.18	108.92	113.60
82	AJ	401	HEM	C4C-NC-C1C	2.17	107.47	105.35
82	AJ	401	HEM	C4A-NA-C1A	2.17	107.47	105.35
73	J	401	NDP	C6A-C5A-N7A	2.16	136.04	132.02
76	AU	401	PEE	C17-C18-C19	-2.15	112.22	126.84
70	A	502	FMN	C4A-C4-N3	2.15	118.65	113.19
72	E	201	8Q1	O35-C34-N36	-2.14	118.40	122.99
70	A	502	FMN	C10-N1-C2	2.13	121.16	116.90
70	A	502	FMN	N3-C2-N1	2.13	123.56	119.38
72	p	201	8Q1	O4-C1-S44	-2.13	119.85	122.61
81	AH	402	HEC	C3C-C4C-NC	-2.11	107.78	110.15
82	AV	401	HEM	C4A-NA-C1A	2.11	107.42	105.35
71	r	502	PLX	C2-C1-N1	-2.09	108.79	115.78
82	AJ	401	HEM	CHC-C1C-NC	2.08	126.69	124.44
81	AH	402	HEC	C3B-C4B-NB	-2.08	107.85	110.17
71	U	101	PLX	C5-C4-C3	-2.07	106.88	111.79
81	AU	402	HEC	C3B-C4B-NB	-2.07	107.86	110.17
82	AJ	402	HEM	C2A-C1A-NA	-2.07	107.83	110.15
82	AV	402	HEM	CAA-C2A-C1A	2.07	128.96	124.89
71	r	501	PLX	C1C-N1-C1	2.06	118.36	109.92
79	x	603	HEA	C27-C19-C18	-2.06	118.41	123.68
82	AJ	402	HEM	C3B-C2B-C1B	2.05	108.01	106.49
82	AV	402	HEM	C2A-C1A-NA	-2.05	107.86	110.15
75	AG	101	CDL	OB6-CB5-OB7	-2.05	118.76	123.70
71	AQ	101	PLX	C2-C1-N1	-2.04	108.95	115.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	AU	402	HEC	CAB-C3B-C2B	-2.04	124.04	127.53
79	x	604	HEA	CBD-CAD-C3D	2.03	118.28	112.63
81	AU	402	HEC	C3C-C4C-NC	-2.03	107.88	110.15
71	AQ	101	PLX	C1C-N1-C1	2.03	118.22	109.92
82	AJ	402	HEM	CHD-C1D-ND	2.02	126.61	124.42
75	i	401	CDL	OA6-CA5-OA7	-2.01	118.83	123.70
79	x	603	HEA	OMA-CMA-C3A	-2.01	121.14	125.69
79	x	604	HEA	C3A-C2A-C1A	-2.01	105.16	107.08

There are no chirality outliers.

All (1192) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	A	502	FMN	C1'-C2'-C3'-O3'
70	A	502	FMN	C1'-C2'-C3'-C4'
70	A	502	FMN	C3'-C4'-C5'-O5'
70	A	502	FMN	O4'-C4'-C5'-O5'
71	B	303	PLX	C2-O1-P1-O2
71	B	303	PLX	N1-C1-C2-O1
71	U	101	PLX	O7-C6-C7-C8
71	U	101	PLX	O7-C6-O6-C4
71	U	101	PLX	C3-O4-P1-O2
71	U	101	PLX	N1-C1-C2-O1
71	U	101	PLX	O9-C24-C25-C26
71	V	203	PLX	O7-C6-C7-C8
71	V	203	PLX	N1-C1-C2-O1
71	V	203	PLX	O9-C24-C25-C26
71	b	201	PLX	O7-C6-O6-C4
71	b	201	PLX	N1-C1-C2-O1
71	b	201	PLX	O9-C24-O8-C5
71	g	201	PLX	O7-C6-C7-C8
71	g	201	PLX	O7-C6-O6-C4
71	g	201	PLX	C3-C4-O6-C6
71	g	202	PLX	C2-O1-P1-O4
71	g	202	PLX	C2-O1-P1-O2
71	g	202	PLX	C2-O1-P1-O3
71	g	202	PLX	O9-C24-O8-C5
71	g	203	PLX	O7-C6-O6-C4
71	g	203	PLX	C2-O1-P1-O2
71	g	203	PLX	C25-C24-O8-C5
71	r	501	PLX	C3-O4-P1-O1
71	r	501	PLX	C3-O4-P1-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	r	501	PLX	C3-O4-P1-O3
71	r	501	PLX	O8-C24-C25-C26
71	r	502	PLX	C7-C6-O6-C4
71	r	502	PLX	C3-O4-P1-O1
71	r	502	PLX	C3-O4-P1-O2
71	r	502	PLX	C3-O4-P1-O3
71	r	502	PLX	C2-O1-P1-O2
71	r	502	PLX	N1-C1-C2-O1
71	r	502	PLX	O9-C24-C25-C26
71	AL	501	PLX	O7-C6-C7-C8
71	AQ	101	PLX	O7-C6-O6-C4
71	AQ	101	PLX	O6-C4-C5-O8
71	AQ	101	PLX	N1-C1-C2-O1
71	AQ	101	PLX	C25-C24-O8-C5
71	AQ	101	PLX	O9-C24-C25-C26
71	AT	101	PLX	C2-O1-P1-O4
71	AT	101	PLX	O9-C24-O8-C5
72	E	201	8Q1	C1-C6-C7-C8
72	E	201	8Q1	O4-C1-S44-C43
72	E	201	8Q1	C6-C1-S44-C43
72	E	201	8Q1	C29-C32-C34-N36
72	E	201	8Q1	C29-C32-C34-O35
72	E	201	8Q1	C42-C43-S44-C1
72	E	201	8Q1	C28-O27-P24-O3
72	E	201	8Q1	C28-O27-P24-O2
72	E	201	8Q1	C28-O27-P24-O1
72	p	201	8Q1	C1-C6-C7-C8
72	p	201	8Q1	O4-C1-S44-C43
72	p	201	8Q1	C6-C1-S44-C43
72	p	201	8Q1	C28-C29-C32-C34
72	p	201	8Q1	C28-C29-C32-O33
72	p	201	8Q1	C30-C29-C32-C34
72	p	201	8Q1	C31-C29-C32-C34
72	p	201	8Q1	C31-C29-C32-O33
72	p	201	8Q1	C28-O27-P24-O2
72	p	201	8Q1	C28-O27-P24-O1
73	J	401	NDP	C5B-O5B-PA-O1A
73	J	401	NDP	C5D-O5D-PN-O1N
75	V	201	CDL	CB2-C1-CA2-OA2
75	V	201	CDL	CA2-OA2-PA1-OA3
75	V	201	CDL	CA2-OA2-PA1-OA4
75	V	201	CDL	CA2-OA2-PA1-OA5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	V	201	CDL	CA3-OA5-PA1-OA3
75	V	201	CDL	CA3-OA5-PA1-OA4
75	V	201	CDL	OA9-CA7-OA8-CA6
75	V	201	CDL	C51-CB5-OB6-CB4
75	i	401	CDL	O1-C1-CA2-OA2
75	i	401	CDL	CB2-C1-CA2-OA2
75	i	401	CDL	CA2-OA2-PA1-OA3
75	i	401	CDL	CA2-OA2-PA1-OA4
75	i	401	CDL	CA2-OA2-PA1-OA5
75	i	401	CDL	CA3-OA5-PA1-OA3
75	i	401	CDL	CA3-OA5-PA1-OA4
75	i	401	CDL	OA6-CA4-CA6-OA8
75	i	401	CDL	CB2-OB2-PB2-OB4
75	i	401	CDL	CB3-OB5-PB2-OB3
75	i	401	CDL	CB3-OB5-PB2-OB4
75	l	703	CDL	CA2-OA2-PA1-OA3
75	l	703	CDL	OB7-CB5-OB6-CB4
75	l	704	CDL	CA2-OA2-PA1-OA3
75	l	704	CDL	CA2-OA2-PA1-OA4
75	l	704	CDL	CA3-OA5-PA1-OA2
75	l	704	CDL	CA3-OA5-PA1-OA4
75	l	704	CDL	C11-CA5-OA6-CA4
75	l	704	CDL	CB2-OB2-PB2-OB3
75	n	101	CDL	CA2-OA2-PA1-OA3
75	n	101	CDL	CA2-OA2-PA1-OA4
75	n	101	CDL	CA2-OA2-PA1-OA5
75	n	101	CDL	OA7-CA5-OA6-CA4
75	n	101	CDL	C11-CA5-OA6-CA4
75	n	101	CDL	CB2-OB2-PB2-OB3
75	n	101	CDL	CB2-OB2-PB2-OB4
75	n	101	CDL	C51-CB5-OB6-CB4
75	AA	101	CDL	O1-C1-CB2-OB2
75	AA	101	CDL	CB2-OB2-PB2-OB4
75	AA	101	CDL	CB2-OB2-PB2-OB5
75	AG	101	CDL	OA9-CA7-OA8-CA6
75	AG	101	CDL	CB2-OB2-PB2-OB4
75	AH	403	CDL	CA2-OA2-PA1-OA3
75	AH	403	CDL	CA2-OA2-PA1-OA4
75	AH	403	CDL	CA3-OA5-PA1-OA2
75	AH	403	CDL	C11-CA5-OA6-CA4
75	AH	403	CDL	CB3-OB5-PB2-OB3
75	AH	403	CDL	OB7-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	AJ	404	CDL	CA3-OA5-PA1-OA2
75	AJ	404	CDL	CA3-OA5-PA1-OA3
75	AJ	404	CDL	CA3-OA5-PA1-OA4
75	AJ	404	CDL	C11-CA5-OA6-CA4
75	AJ	404	CDL	CB3-OB5-PB2-OB2
75	AJ	404	CDL	CB3-OB5-PB2-OB3
75	AJ	404	CDL	CB3-OB5-PB2-OB4
75	AJ	405	CDL	CA3-OA5-PA1-OA4
75	AJ	405	CDL	C51-CB5-OB6-CB4
75	AL	502	CDL	O1-C1-CA2-OA2
75	AL	502	CDL	CA3-OA5-PA1-OA2
75	AL	502	CDL	C11-CA5-OA6-CA4
75	AL	502	CDL	CB2-OB2-PB2-OB3
75	AL	502	CDL	CB2-OB2-PB2-OB4
75	AL	502	CDL	C71-CB7-OB8-CB6
75	AN	101	CDL	CA3-OA5-PA1-OA3
75	AN	101	CDL	OA7-CA5-OA6-CA4
75	AN	101	CDL	C11-CA5-OA6-CA4
75	AN	101	CDL	CB2-OB2-PB2-OB4
75	AN	101	CDL	CB2-OB2-PB2-OB5
75	AU	403	CDL	CA3-OA5-PA1-OA2
75	AU	403	CDL	CA3-OA5-PA1-OA3
75	AU	403	CDL	C11-CA5-OA6-CA4
75	AU	403	CDL	CB3-OB5-PB2-OB2
75	AU	403	CDL	CB3-OB5-PB2-OB3
75	AU	403	CDL	OB7-CB5-OB6-CB4
75	AY	501	CDL	CB2-C1-CA2-OA2
75	AY	501	CDL	C11-CA5-OA6-CA4
76	V	202	PEE	C2-C1-O3P-P
76	V	202	PEE	O4P-C4-C5-N
76	W	201	PEE	C4-O4P-P-O3P
76	W	201	PEE	C4-O4P-P-O1P
76	l	701	PEE	C11-C10-O2-C2
76	l	701	PEE	C4-O4P-P-O2P
76	l	701	PEE	C4-O4P-P-O1P
76	AH	401	PEE	C4-O4P-P-O2P
76	AJ	403	PEE	C37-C38-C39-C40
76	AL	503	PEE	C11-C10-O2-C2
76	AL	503	PEE	O4-C10-O2-C2
76	AU	401	PEE	C11-C10-O2-C2
76	AU	401	PEE	C1-O3P-P-O2P
76	AU	401	PEE	C1-O3P-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
76	AU	401	PEE	C4-O4P-P-O2P
76	AV	403	PEE	O4P-C4-C5-N
76	AV	403	PEE	C39-C40-C41-C42
76	AY	502	PEE	C1-O3P-P-O2P
76	AY	502	PEE	C4-O4P-P-O3P
76	AY	502	PEE	C4-O4P-P-O2P
76	AY	502	PEE	C4-O4P-P-O1P
79	x	603	HEA	C2A-C3A-CMA-OMA
79	x	603	HEA	C4A-C3A-CMA-OMA
79	x	603	HEA	C12-C11-C3B-C2B
79	x	604	HEA	C2A-C3A-CMA-OMA
79	x	604	HEA	C4A-C3A-CMA-OMA
82	AV	402	HEM	C1A-C2A-CAA-CBA
75	AL	502	CDL	OB9-CB7-OB8-CB6
75	l	704	CDL	OA9-CA7-OA8-CA6
75	l	704	CDL	OB9-CB7-OB8-CB6
75	n	101	CDL	OA9-CA7-OA8-CA6
75	AA	101	CDL	OB9-CB7-OB8-CB6
75	AN	101	CDL	OB9-CB7-OB8-CB6
75	AU	403	CDL	OB9-CB7-OB8-CB6
75	V	201	CDL	OB7-CB5-OB6-CB4
75	l	704	CDL	OA7-CA5-OA6-CA4
75	n	101	CDL	OB7-CB5-OB6-CB4
75	AJ	404	CDL	OA7-CA5-OA6-CA4
75	AJ	405	CDL	OB7-CB5-OB6-CB4
75	AL	502	CDL	OA7-CA5-OA6-CA4
75	AU	403	CDL	OA7-CA5-OA6-CA4
75	AY	501	CDL	OA7-CA5-OA6-CA4
75	AY	501	CDL	OB7-CB5-OB6-CB4
76	l	701	PEE	O4-C10-O2-C2
76	AU	401	PEE	O4-C10-O2-C2
75	l	704	CDL	C31-CA7-OA8-CA6
75	l	704	CDL	C71-CB7-OB8-CB6
75	n	101	CDL	C31-CA7-OA8-CA6
75	n	101	CDL	C71-CB7-OB8-CB6
75	AG	101	CDL	C31-CA7-OA8-CA6
75	AN	101	CDL	C71-CB7-OB8-CB6
75	AU	403	CDL	C71-CB7-OB8-CB6
75	l	703	CDL	C51-CB5-OB6-CB4
75	AH	403	CDL	C51-CB5-OB6-CB4
75	AU	403	CDL	C51-CB5-OB6-CB4
75	AY	501	CDL	C51-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
72	E	201	8Q1	C38-C39-N41-C42
75	AA	101	CDL	C71-CB7-OB8-CB6
75	AH	403	CDL	C71-CB7-OB8-CB6
75	AL	502	CDL	C31-CA7-OA8-CA6
76	W	201	PEE	C17-C18-C19-C20
76	l	701	PEE	C37-C38-C39-C40
76	l	702	PEE	C37-C38-C39-C40
75	AH	403	CDL	OA7-CA5-OA6-CA4
75	n	101	CDL	OB9-CB7-OB8-CB6
76	l	702	PEE	O5-C30-O3-C3
71	AL	501	PLX	C2-C1-N1-C1C
81	AU	402	HEC	C2B-C3B-CAB-CBB
75	l	703	CDL	O1-C1-CA2-OA2
75	l	704	CDL	O1-C1-CA2-OA2
75	AG	101	CDL	O1-C1-CB2-OB2
75	AY	501	CDL	O1-C1-CA2-OA2
75	AY	501	CDL	O1-C1-CB2-OB2
75	AJ	405	CDL	C31-CA7-OA8-CA6
75	AU	403	CDL	C31-CA7-OA8-CA6
75	AH	403	CDL	OB9-CB7-OB8-CB6
75	i	401	CDL	C11-CA5-OA6-CA4
75	AA	101	CDL	C51-CB5-OB6-CB4
76	W	201	PEE	C21-C22-C23-C24
75	AU	403	CDL	OA9-CA7-OA8-CA6
76	V	202	PEE	C20-C21-C22-C23
76	AU	401	PEE	C31-C32-C33-C34
71	r	502	PLX	C16-C17-C18-C19
75	AH	403	CDL	C31-C32-C33-C34
76	l	701	PEE	C32-C33-C34-C35
73	J	401	NDP	O4B-C4B-C5B-O5B
73	J	401	NDP	C3B-C4B-C5B-O5B
76	l	702	PEE	C31-C30-O3-C3
71	r	501	PLX	C10-C11-C12-C13
71	b	201	PLX	C4-C3-O4-P1
75	AJ	405	CDL	OA9-CA7-OA8-CA6
75	AL	502	CDL	OA9-CA7-OA8-CA6
71	g	203	PLX	C26-C27-C28-C29
79	x	603	HEA	C15-C16-C17-C18
71	b	201	PLX	C14-C15-C16-C17
71	g	203	PLX	C30-C31-C32-C33
71	r	502	PLX	C30-C31-C32-C33
75	AJ	405	CDL	C71-C72-C73-C74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	AY	501	CDL	C12-C13-C14-C15
76	W	201	PEE	C32-C33-C34-C35
73	J	401	NDP	C1B-C2B-O2B-P2B
75	AY	501	CDL	C31-CA7-OA8-CA6
71	g	202	PLX	C10-C11-C12-C13
72	E	201	8Q1	O40-C39-N41-C42
75	l	703	CDL	CB2-C1-CA2-OA2
75	AA	101	CDL	CA2-C1-CB2-OB2
75	AJ	404	CDL	CB2-C1-CA2-OA2
75	AL	502	CDL	CB2-C1-CA2-OA2
75	AL	502	CDL	CA2-C1-CB2-OB2
71	r	502	PLX	C12-C13-C14-C15
75	i	401	CDL	C31-C32-C33-C34
75	AH	403	CDL	C31-CA7-OA8-CA6
76	W	201	PEE	C31-C30-O3-C3
75	l	703	CDL	C73-C74-C75-C76
75	l	703	CDL	OB5-CB3-CB4-OB6
76	W	201	PEE	C12-C13-C14-C15
76	l	701	PEE	C34-C35-C36-C37
75	V	201	CDL	O1-C1-CA2-OA2
75	l	703	CDL	O1-C1-CB2-OB2
75	AA	101	CDL	O1-C1-CA2-OA2
75	AJ	404	CDL	O1-C1-CA2-OA2
75	AY	501	CDL	CB5-C51-C52-C53
71	AT	101	PLX	O6-C4-C5-O8
71	r	501	PLX	C12-C13-C14-C15
75	AH	403	CDL	OA9-CA7-OA8-CA6
76	W	201	PEE	O5-C30-O3-C3
82	AV	402	HEM	C3A-C2A-CAA-CBA
75	V	201	CDL	C54-C55-C56-C57
75	i	401	CDL	OA7-CA5-OA6-CA4
71	V	203	PLX	C13-C14-C15-C16
75	l	704	CDL	CB5-C51-C52-C53
75	n	101	CDL	CA7-C31-C32-C33
75	AH	403	CDL	CB5-C51-C52-C53
75	AN	101	CDL	CA5-C11-C12-C13
75	AY	501	CDL	CA7-C31-C32-C33
76	l	702	PEE	C10-C11-C12-C13
76	l	702	PEE	C17-C18-C19-C20
76	AH	401	PEE	C37-C38-C39-C40
75	AN	101	CDL	C71-C72-C73-C74
81	AH	402	HEC	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
76	W	201	PEE	C15-C16-C17-C18
75	i	401	CDL	CA5-C11-C12-C13
75	AJ	404	CDL	CA7-C31-C32-C33
75	AL	502	CDL	CA5-C11-C12-C13
75	AU	403	CDL	CA5-C11-C12-C13
76	V	202	PEE	C10-C11-C12-C13
76	l	701	PEE	C30-C31-C32-C33
76	AV	403	PEE	C10-C11-C12-C13
81	AU	402	HEC	C4B-C3B-CAB-CBB
71	r	501	PLX	C27-C28-C29-C30
75	AL	502	CDL	C52-C53-C54-C55
82	AJ	402	HEM	C1A-C2A-CAA-CBA
75	AA	101	CDL	OB7-CB5-OB6-CB4
75	AA	101	CDL	CB7-C71-C72-C73
75	AG	101	CDL	CB7-C71-C72-C73
75	AJ	405	CDL	CB7-C71-C72-C73
82	AJ	401	HEM	C3D-CAD-CBD-CGD
82	AV	401	HEM	C3D-CAD-CBD-CGD
75	n	101	CDL	C31-C32-C33-C34
76	AL	503	PEE	C30-C31-C32-C33
75	AL	502	CDL	O1-C1-CB2-OB2
75	i	401	CDL	C31-CA7-OA8-CA6
73	J	401	NDP	C3B-C2B-O2B-P2B
75	AN	101	CDL	C14-C15-C16-C17
75	AY	501	CDL	OA9-CA7-OA8-CA6
76	l	701	PEE	C39-C40-C41-C42
76	V	202	PEE	C17-C18-C19-C20
76	l	701	PEE	C17-C18-C19-C20
75	AH	403	CDL	C33-C34-C35-C36
71	B	303	PLX	C2-O1-P1-O4
71	U	101	PLX	C3-O4-P1-O1
71	b	201	PLX	C3-O4-P1-O1
71	g	201	PLX	C3-O4-P1-O1
71	g	202	PLX	C3-O4-P1-O1
71	g	203	PLX	C2-O1-P1-O4
71	r	502	PLX	C2-O1-P1-O4
75	V	201	CDL	CA3-OA5-PA1-OA2
75	V	201	CDL	CB3-OB5-PB2-OB2
75	i	401	CDL	CA3-OA5-PA1-OA2
75	i	401	CDL	CB2-OB2-PB2-OB5
75	i	401	CDL	CB3-OB5-PB2-OB2
75	l	703	CDL	CB3-OB5-PB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	l	704	CDL	CA2-OA2-PA1-OA5
75	n	101	CDL	CB2-OB2-PB2-OB5
75	AG	101	CDL	CA2-OA2-PA1-OA5
75	AG	101	CDL	CB2-OB2-PB2-OB5
75	AH	403	CDL	CA2-OA2-PA1-OA5
75	AH	403	CDL	CB3-OB5-PB2-OB2
75	AJ	405	CDL	CA3-OA5-PA1-OA2
75	AL	502	CDL	CB2-OB2-PB2-OB5
75	AL	502	CDL	CB3-OB5-PB2-OB2
75	AN	101	CDL	CA3-OA5-PA1-OA2
75	AY	501	CDL	CA3-OA5-PA1-OA2
76	V	202	PEE	C1-O3P-P-O4P
76	W	201	PEE	C1-O3P-P-O4P
76	l	701	PEE	C4-O4P-P-O3P
76	AH	401	PEE	C4-O4P-P-O3P
76	AU	401	PEE	C1-O3P-P-O4P
76	AU	401	PEE	C4-O4P-P-O3P
76	AY	502	PEE	C1-O3P-P-O4P
75	AY	501	CDL	C71-CB7-OB8-CB6
76	V	202	PEE	C31-C30-O3-C3
71	AL	501	PLX	C12-C13-C14-C15
75	l	703	CDL	CA2-C1-CB2-OB2
75	AG	101	CDL	CA2-C1-CB2-OB2
75	AY	501	CDL	CA2-C1-CB2-OB2
71	AL	501	PLX	C2-C1-N1-C1A
75	l	703	CDL	C71-CB7-OB8-CB6
71	B	303	PLX	O6-C6-C7-C8
71	U	101	PLX	O6-C6-C7-C8
71	g	203	PLX	O8-C24-C25-C26
71	AQ	101	PLX	O8-C24-C25-C26
75	n	101	CDL	C13-C14-C15-C16
75	l	704	CDL	C51-CB5-OB6-CB4
75	AG	101	CDL	C51-CB5-OB6-CB4
71	B	303	PLX	C27-C28-C29-C30
71	g	201	PLX	C13-C14-C15-C16
71	g	201	PLX	C7-C8-C9-C10
71	g	202	PLX	C7-C8-C9-C10
71	g	203	PLX	C29-C30-C31-C32
71	AQ	101	PLX	C19-C20-C21-C22
71	AT	101	PLX	C7-C8-C9-C10
75	l	704	CDL	C31-C32-C33-C34
75	n	101	CDL	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	AG	101	CDL	C33-C34-C35-C36
75	AJ	405	CDL	C12-C13-C14-C15
75	AY	501	CDL	C32-C33-C34-C35
76	W	201	PEE	C14-C15-C16-C17
76	l	701	PEE	C22-C23-C24-C25
71	g	203	PLX	C34-C35-C36-C37
71	AT	101	PLX	C9-C10-C11-C12
75	AU	403	CDL	C13-C14-C15-C16
76	l	702	PEE	C20-C21-C22-C23
76	AJ	403	PEE	C20-C21-C22-C23
76	AY	502	PEE	C11-C12-C13-C14
75	AL	502	CDL	CA6-CA4-OA6-CA5
75	l	704	CDL	OB7-CB5-OB6-CB4
75	AG	101	CDL	OB7-CB5-OB6-CB4
75	n	101	CDL	CB5-C51-C52-C53
71	AQ	101	PLX	C10-C11-C12-C13
72	p	201	8Q1	C11-C12-C13-C14
76	l	701	PEE	C21-C22-C23-C24
75	AJ	404	CDL	C1-CB2-OB2-PB2
75	AY	501	CDL	OA5-CA3-CA4-OA6
71	AQ	101	PLX	C12-C13-C14-C15
75	V	201	CDL	C71-C72-C73-C74
75	AA	101	CDL	C51-C52-C53-C54
75	AG	101	CDL	C14-C15-C16-C17
75	AL	502	CDL	C51-C52-C53-C54
75	AU	403	CDL	C54-C55-C56-C57
71	r	501	PLX	C13-C14-C15-C16
71	r	502	PLX	C14-C15-C16-C17
75	l	704	CDL	C51-C52-C53-C54
76	V	202	PEE	C12-C13-C14-C15
75	l	703	CDL	CB7-C71-C72-C73
75	l	704	CDL	CB7-C71-C72-C73
75	AA	101	CDL	CA5-C11-C12-C13
71	U	101	PLX	C33-C34-C35-C36
71	b	201	PLX	C16-C17-C18-C19
71	AL	501	PLX	C15-C16-C17-C18
71	AL	501	PLX	C13-C14-C15-C16
75	AA	101	CDL	C31-C32-C33-C34
76	V	202	PEE	C40-C41-C42-C43
76	l	702	PEE	C33-C34-C35-C36
76	AJ	403	PEE	C13-C14-C15-C16
76	AJ	403	PEE	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	U	101	PLX	C19-C20-C21-C22
71	U	101	PLX	C10-C11-C12-C13
71	U	101	PLX	C35-C36-C37-C38
71	g	203	PLX	C15-C16-C17-C18
71	r	502	PLX	C11-C12-C13-C14
71	r	502	PLX	C10-C11-C12-C13
72	p	201	8Q1	C6-C7-C8-C9
76	AH	401	PEE	C21-C22-C23-C24
75	AN	101	CDL	CB4-CB6-OB8-CB7
71	U	101	PLX	C12-C13-C14-C15
71	U	101	PLX	C9-C10-C11-C12
71	V	203	PLX	C10-C11-C12-C13
71	b	201	PLX	C27-C28-C29-C30
71	b	201	PLX	C29-C30-C31-C32
71	g	202	PLX	C14-C15-C16-C17
71	AQ	101	PLX	C34-C35-C36-C37
72	E	201	8Q1	C12-C13-C14-C15
75	i	401	CDL	C13-C14-C15-C16
75	AL	502	CDL	C32-C33-C34-C35
76	l	702	PEE	C40-C41-C42-C43
76	AL	503	PEE	C32-C33-C34-C35
71	B	303	PLX	C9-C10-C11-C12
71	B	303	PLX	C28-C29-C30-C31
71	r	502	PLX	C9-C10-C11-C12
75	l	704	CDL	C32-C33-C34-C35
75	AJ	405	CDL	C33-C34-C35-C36
75	AU	403	CDL	C31-C32-C33-C34
76	V	202	PEE	C14-C15-C16-C17
76	AH	401	PEE	C11-C12-C13-C14
71	V	203	PLX	C25-C26-C27-C28
71	g	201	PLX	C16-C17-C18-C19
71	AL	501	PLX	C10-C11-C12-C13
75	AY	501	CDL	C14-C15-C16-C17
76	l	702	PEE	C34-C35-C36-C37
76	AH	401	PEE	C22-C23-C24-C25
76	AJ	403	PEE	C22-C23-C24-C25
76	AL	503	PEE	C11-C12-C13-C14
76	AU	401	PEE	C11-C12-C13-C14
76	AV	403	PEE	C35-C36-C37-C38
76	AY	502	PEE	C19-C20-C21-C22
75	l	704	CDL	CA7-C31-C32-C33
75	AG	101	CDL	CA5-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	AL	502	CDL	CA7-C31-C32-C33
75	AU	403	CDL	CB7-C71-C72-C73
71	U	101	PLX	C7-C8-C9-C10
71	b	201	PLX	C18-C19-C20-C21
71	g	201	PLX	C10-C11-C12-C13
75	l	703	CDL	C51-C52-C53-C54
76	l	702	PEE	C21-C22-C23-C24
71	AL	501	PLX	C2-C1-N1-C1B
71	b	201	PLX	C25-C26-C27-C28
75	l	703	CDL	C11-C12-C13-C14
76	AY	502	PEE	C22-C23-C24-C25
71	V	203	PLX	C32-C33-C34-C35
71	g	202	PLX	C9-C10-C11-C12
75	n	101	CDL	C51-C52-C53-C54
75	AG	101	CDL	C73-C74-C75-C76
75	n	101	CDL	CB7-C71-C72-C73
71	AQ	101	PLX	C15-C16-C17-C18
76	l	701	PEE	C20-C21-C22-C23
71	r	502	PLX	C32-C33-C34-C35
76	AJ	403	PEE	C32-C33-C34-C35
76	AL	503	PEE	C34-C35-C36-C37
72	E	201	8Q1	N41-C42-C43-S44
71	g	203	PLX	C10-C11-C12-C13
71	r	502	PLX	C26-C27-C28-C29
75	AU	403	CDL	C14-C15-C16-C17
76	V	202	PEE	C34-C35-C36-C37
76	AV	403	PEE	C32-C33-C34-C35
76	V	202	PEE	O5-C30-O3-C3
71	B	303	PLX	C12-C13-C14-C15
71	g	203	PLX	C17-C18-C19-C20
75	AG	101	CDL	C72-C73-C74-C75
75	AY	501	CDL	C33-C34-C35-C36
76	W	201	PEE	C37-C38-C39-C40
71	g	203	PLX	C7-C8-C9-C10
71	r	502	PLX	C25-C26-C27-C28
76	AH	401	PEE	C32-C33-C34-C35
71	g	202	PLX	C11-C12-C13-C14
75	i	401	CDL	C34-C35-C36-C37
75	i	401	CDL	OA9-CA7-OA8-CA6
75	AY	501	CDL	OB9-CB7-OB8-CB6
75	AL	502	CDL	C51-CB5-OB6-CB4
72	p	201	8Q1	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	AH	403	CDL	C32-C33-C34-C35
71	B	303	PLX	O7-C6-C7-C8
71	g	203	PLX	O9-C24-C25-C26
71	r	501	PLX	O9-C24-C25-C26
71	r	502	PLX	O7-C6-C7-C8
71	AT	101	PLX	O9-C24-C25-C26
71	g	203	PLX	C14-C15-C16-C17
71	r	501	PLX	C7-C8-C9-C10
75	i	401	CDL	C11-C12-C13-C14
75	l	703	CDL	C33-C34-C35-C36
75	AU	403	CDL	C53-C54-C55-C56
70	A	502	FMN	O2'-C2'-C3'-O3'
71	AT	101	PLX	C11-C12-C13-C14
75	i	401	CDL	C32-C33-C34-C35
71	r	501	PLX	C35-C36-C37-C38
75	AJ	405	CDL	C52-C53-C54-C55
75	l	703	CDL	OB9-CB7-OB8-CB6
75	AJ	404	CDL	C11-C12-C13-C14
75	AJ	404	CDL	C14-C15-C16-C17
75	AY	501	CDL	C13-C14-C15-C16
76	V	202	PEE	C43-C44-C45-C46
76	l	701	PEE	C13-C14-C15-C16
76	l	701	PEE	C41-C42-C43-C44
75	V	201	CDL	OA7-CA5-OA6-CA4
70	A	502	FMN	O2'-C2'-C3'-C4'
71	V	203	PLX	C11-C12-C13-C14
75	AG	101	CDL	C31-C32-C33-C34
72	p	201	8Q1	C12-C13-C14-C15
76	AV	403	PEE	C41-C42-C43-C44
75	i	401	CDL	CB5-C51-C52-C53
76	AV	403	PEE	C30-C31-C32-C33
76	W	201	PEE	C23-C24-C25-C26
75	l	703	CDL	C31-CA7-OA8-CA6
75	V	201	CDL	C11-CA5-OA6-CA4
76	AH	401	PEE	C11-C10-O2-C2
71	g	201	PLX	C32-C33-C34-C35
71	r	501	PLX	C26-C27-C28-C29
75	AA	101	CDL	C33-C34-C35-C36
75	AG	101	CDL	C52-C53-C54-C55
75	V	201	CDL	CB5-C51-C52-C53
76	AL	503	PEE	C10-C11-C12-C13
75	n	101	CDL	C55-C56-C57-C58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	AN	101	CDL	C31-C32-C33-C34
76	AV	403	PEE	C12-C13-C14-C15
76	AU	401	PEE	C33-C34-C35-C36
76	AL	503	PEE	C37-C38-C39-C40
71	r	502	PLX	C36-C37-C38-C39
75	i	401	CDL	C73-C74-C75-C76
76	W	201	PEE	C41-C42-C43-C44
76	l	701	PEE	C15-C16-C17-C18
76	l	702	PEE	C19-C20-C21-C22
75	AL	502	CDL	OB7-CB5-OB6-CB4
76	AV	403	PEE	O4-C10-O2-C2
75	AJ	405	CDL	CB5-C51-C52-C53
75	i	401	CDL	C71-CB7-OB8-CB6
71	r	502	PLX	C20-C21-C22-C23
71	r	502	PLX	C7-C8-C9-C10
76	V	202	PEE	C31-C32-C33-C34
71	AT	101	PLX	C33-C34-C35-C36
75	n	101	CDL	C71-C72-C73-C74
76	l	702	PEE	C31-C32-C33-C34
76	AY	502	PEE	C20-C21-C22-C23
71	b	201	PLX	C30-C31-C32-C33
71	g	202	PLX	C26-C27-C28-C29
76	W	201	PEE	C43-C44-C45-C46
75	i	401	CDL	C51-CB5-OB6-CB4
76	AV	403	PEE	C11-C10-O2-C2
75	AL	502	CDL	OA5-CA3-CA4-OA6
75	AL	502	CDL	OB5-CB3-CB4-OB6
71	AQ	101	PLX	C13-C14-C15-C16
75	AA	101	CDL	C12-C13-C14-C15
71	r	502	PLX	C35-C36-C37-C38
76	AV	403	PEE	C40-C41-C42-C43
76	AH	401	PEE	O4-C10-O2-C2
71	AQ	101	PLX	C18-C19-C20-C21
75	V	201	CDL	C14-C15-C16-C17
71	AL	501	PLX	O6-C4-C5-O8
71	b	201	PLX	C32-C33-C34-C35
75	AH	403	CDL	C53-C54-C55-C56
76	AL	503	PEE	C12-C13-C14-C15
76	AU	401	PEE	C34-C35-C36-C37
71	B	303	PLX	C29-C30-C31-C32
71	g	203	PLX	C35-C36-C37-C38
76	V	202	PEE	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
76	W	201	PEE	C19-C20-C21-C22
76	AV	403	PEE	C19-C20-C21-C22
71	r	501	PLX	C9-C10-C11-C12
71	b	201	PLX	C11-C12-C13-C14
75	l	703	CDL	OA9-CA7-OA8-CA6
71	g	202	PLX	C11-C10-C9-C8
71	r	502	PLX	C17-C18-C19-C20
71	AQ	101	PLX	C7-C8-C9-C10
75	l	704	CDL	C13-C14-C15-C16
75	AU	403	CDL	C73-C74-C75-C76
76	l	701	PEE	C23-C24-C25-C26
76	l	701	PEE	C40-C41-C42-C43
76	l	701	PEE	C16-C17-C18-C19
71	g	201	PLX	C2-O1-P1-O4
75	l	703	CDL	CA2-OA2-PA1-OA5
75	AL	502	CDL	CA2-OA2-PA1-OA5
76	AV	403	PEE	C1-O3P-P-O4P
71	B	303	PLX	C15-C16-C17-C18
75	n	101	CDL	C34-C35-C36-C37
76	AV	403	PEE	C33-C34-C35-C36
76	AH	401	PEE	C2-C1-O3P-P
71	AL	501	PLX	C7-C8-C9-C10
75	AG	101	CDL	C34-C35-C36-C37
71	AL	501	PLX	O4-C3-C4-C5
75	l	704	CDL	OB5-CB3-CB4-CB6
76	l	701	PEE	O3P-C1-C2-C3
76	AJ	403	PEE	O3P-C1-C2-C3
71	r	502	PLX	C15-C16-C17-C18
71	AT	101	PLX	C32-C33-C34-C35
75	AG	101	CDL	CA7-C31-C32-C33
75	AY	501	CDL	CB7-C71-C72-C73
71	AQ	101	PLX	C26-C27-C28-C29
71	AT	101	PLX	C18-C19-C20-C21
76	l	702	PEE	C42-C43-C44-C45
71	B	303	PLX	C11-C10-C9-C8
71	AT	101	PLX	C13-C14-C15-C16
71	AT	101	PLX	C34-C35-C36-C37
76	AL	503	PEE	C21-C22-C23-C24
81	AH	402	HEC	C4B-C3B-CAB-CBB
75	l	704	CDL	CB2-C1-CA2-OA2
75	i	401	CDL	OB7-CB5-OB6-CB4
75	V	201	CDL	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	AL	502	CDL	C14-C15-C16-C17
75	n	101	CDL	C33-C34-C35-C36
76	W	201	PEE	C33-C34-C35-C36
71	r	501	PLX	C3-C4-C5-O8
75	l	703	CDL	CA3-CA4-CA6-OA8
75	AH	403	CDL	CA3-CA4-CA6-OA8
75	AJ	405	CDL	CB3-CB4-CB6-OB8
75	AL	502	CDL	CA3-CA4-CA6-OA8
75	AL	502	CDL	CB3-CB4-CB6-OB8
75	AN	101	CDL	CB3-CB4-CB6-OB8
75	AU	403	CDL	CA3-CA4-CA6-OA8
76	AV	403	PEE	C1-C2-C3-O3
75	AL	502	CDL	C13-C14-C15-C16
76	AY	502	PEE	C33-C34-C35-C36
71	r	501	PLX	C18-C19-C20-C21
75	AG	101	CDL	C75-C76-C77-C78
76	V	202	PEE	C41-C42-C43-C44
71	g	201	PLX	C26-C27-C28-C29
75	AJ	404	CDL	C15-C16-C17-C18
76	W	201	PEE	C44-C45-C46-C47
76	AJ	403	PEE	C41-C42-C43-C44
75	AJ	404	CDL	CA5-C11-C12-C13
71	U	101	PLX	O8-C24-C25-C26
75	AY	501	CDL	C15-C16-C17-C18
75	AH	403	CDL	C55-C56-C57-C58
75	AL	502	CDL	C31-C32-C33-C34
75	AU	403	CDL	C15-C16-C17-C18
76	l	702	PEE	C12-C13-C14-C15
76	AJ	403	PEE	C35-C36-C37-C38
76	AJ	403	PEE	C39-C40-C41-C42
76	AU	401	PEE	C15-C16-C17-C18
76	AV	403	PEE	C15-C16-C17-C18
75	i	401	CDL	OB9-CB7-OB8-CB6
72	p	201	8Q1	C13-C14-C15-C16
71	AQ	101	PLX	C36-C37-C38-C39
75	AJ	404	CDL	C74-C75-C76-C77
71	b	201	PLX	C20-C21-C22-C23
76	AY	502	PEE	C42-C43-C44-C45
75	AU	403	CDL	CB5-C51-C52-C53
75	AJ	405	CDL	C55-C56-C57-C58
71	V	203	PLX	C7-C8-C9-C10
75	AN	101	CDL	C55-C56-C57-C58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
76	l	701	PEE	C42-C43-C44-C45
75	AJ	404	CDL	CA3-CA4-OA6-CA5
75	AJ	405	CDL	CB6-CB4-OB6-CB5
71	AQ	101	PLX	C31-C32-C33-C34
76	l	702	PEE	C44-C45-C46-C47
76	l	701	PEE	C2-C1-O3P-P
71	AQ	101	PLX	C9-C10-C11-C12
75	V	201	CDL	OA5-CA3-CA4-OA6
71	U	101	PLX	C26-C27-C28-C29
75	AN	101	CDL	C15-C16-C17-C18
75	AJ	405	CDL	CA7-C31-C32-C33
76	AH	401	PEE	C30-C31-C32-C33
71	AL	501	PLX	C34-C35-C36-C37
75	AH	403	CDL	C32-C31-CA7-OA8
76	W	201	PEE	O2-C2-C3-O3
75	l	703	CDL	C75-C76-C77-C78
76	AH	401	PEE	C34-C35-C36-C37
72	p	201	8Q1	C30-C29-C32-O33
75	i	401	CDL	C52-C51-CB5-OB6
71	V	203	PLX	C16-C17-C18-C19
75	AA	101	CDL	C71-C72-C73-C74
76	AV	403	PEE	C13-C14-C15-C16
75	AG	101	CDL	C71-CB7-OB8-CB6
76	AH	401	PEE	C24-C25-C26-C27
75	i	401	CDL	C35-C36-C37-C38
71	U	101	PLX	C11-C10-C9-C8
75	V	201	CDL	C72-C73-C74-C75
75	AH	403	CDL	C15-C16-C17-C18
76	W	201	PEE	C34-C35-C36-C37
75	AJ	405	CDL	C32-C33-C34-C35
71	V	203	PLX	C12-C13-C14-C15
71	g	201	PLX	C17-C18-C19-C20
71	g	201	PLX	C27-C28-C29-C30
75	AJ	404	CDL	C73-C74-C75-C76
75	l	703	CDL	OB5-CB3-CB4-CB6
75	AL	502	CDL	OA5-CA3-CA4-CA6
75	AU	403	CDL	OA5-CA3-CA4-CA6
75	AY	501	CDL	OA5-CA3-CA4-CA6
75	AY	501	CDL	OB5-CB3-CB4-CB6
76	W	201	PEE	O3P-C1-C2-C3
76	AH	401	PEE	C20-C21-C22-C23
71	V	203	PLX	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	AJ	404	CDL	C12-C13-C14-C15
71	B	303	PLX	C30-C31-C32-C33
71	r	501	PLX	C25-C26-C27-C28
75	V	201	CDL	C52-C53-C54-C55
71	U	101	PLX	C28-C29-C30-C31
71	b	201	PLX	C13-C14-C15-C16
71	b	201	PLX	C11-C10-C9-C8
71	b	201	PLX	C36-C37-C38-C39
76	AJ	403	PEE	C40-C41-C42-C43
81	AH	402	HEC	C4C-C3C-CAC-CBC
75	AA	101	CDL	C75-C76-C77-C78
71	U	101	PLX	C27-C28-C29-C30
71	g	201	PLX	C3-C4-C5-O8
71	AL	501	PLX	C3-C4-C5-O8
71	AQ	101	PLX	C3-C4-C5-O8
71	AT	101	PLX	C3-C4-C5-O8
75	V	201	CDL	CB3-CB4-CB6-OB8
75	i	401	CDL	CA3-CA4-CA6-OA8
75	AA	101	CDL	CB3-CB4-CB6-OB8
76	W	201	PEE	C1-C2-C3-O3
71	r	502	PLX	C27-C28-C29-C30
72	p	201	8Q1	C10-C11-C12-C13
72	E	201	8Q1	C7-C8-C9-C10
76	AV	403	PEE	C22-C23-C24-C25
71	r	501	PLX	C28-C29-C30-C31
76	W	201	PEE	C13-C14-C15-C16
76	l	702	PEE	C11-C10-O2-C2
71	AQ	101	PLX	C14-C15-C16-C17
75	V	201	CDL	C53-C54-C55-C56
71	b	201	PLX	C5-C4-O6-C6
71	g	202	PLX	C5-C4-O6-C6
71	AT	101	PLX	C3-O4-P1-O1
76	AV	403	PEE	C4-O4P-P-O3P
75	AJ	404	CDL	C71-C72-C73-C74
71	r	501	PLX	O7-C6-C7-C8
71	b	201	PLX	C35-C36-C37-C38
75	AH	403	CDL	C52-C53-C54-C55
75	l	704	CDL	OA5-CA3-CA4-OA6
75	AN	101	CDL	OA5-CA3-CA4-OA6
76	AJ	403	PEE	O3P-C1-C2-O2
71	AL	501	PLX	C32-C33-C34-C35
71	V	203	PLX	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	AG	101	CDL	OB9-CB7-OB8-CB6
75	l	703	CDL	OA6-CA4-CA6-OA8
75	AG	101	CDL	OB6-CB4-CB6-OB8
75	AH	403	CDL	OB6-CB4-CB6-OB8
75	AL	502	CDL	OA6-CA4-CA6-OA8
75	AL	502	CDL	OB6-CB4-CB6-OB8
75	AU	403	CDL	OA6-CA4-CA6-OA8
75	V	201	CDL	C12-C11-CA5-OA6
75	AJ	404	CDL	C31-C32-C33-C34
76	AL	503	PEE	C14-C15-C16-C17
71	g	201	PLX	C20-C21-C22-C23
81	AH	402	HEC	C1A-C2A-CAA-CBA
75	AG	101	CDL	C74-C75-C76-C77
75	AN	101	CDL	C52-C53-C54-C55
71	g	203	PLX	C4-C3-O4-P1
71	r	501	PLX	C4-C3-O4-P1
75	AA	101	CDL	C1-CA2-OA2-PA1
75	AA	101	CDL	C1-CB2-OB2-PB2
75	AA	101	CDL	CB4-CB3-OB5-PB2
75	AH	403	CDL	C1-CA2-OA2-PA1
75	AN	101	CDL	CB4-CB3-OB5-PB2
75	l	704	CDL	C73-C74-C75-C76
76	AV	403	PEE	C34-C35-C36-C37
71	r	501	PLX	C19-C20-C21-C22
75	AU	403	CDL	C74-C75-C76-C77
75	l	703	CDL	C15-C16-C17-C18
75	n	101	CDL	CA5-C11-C12-C13
76	W	201	PEE	O4-C10-O2-C2
76	W	201	PEE	C11-C10-O2-C2
75	AL	502	CDL	C53-C54-C55-C56
71	B	303	PLX	C11-C12-C13-C14
76	AV	403	PEE	C20-C21-C22-C23
75	V	201	CDL	OB5-CB3-CB4-CB6
75	AA	101	CDL	OA5-CA3-CA4-CA6
75	AJ	404	CDL	OB5-CB3-CB4-CB6
75	AN	101	CDL	OA5-CA3-CA4-CA6
75	AU	403	CDL	OB5-CB3-CB4-CB6
76	AY	502	PEE	C14-C15-C16-C17
76	AV	403	PEE	C16-C17-C18-C19
76	AH	401	PEE	C39-C40-C41-C42
76	l	702	PEE	O4-C10-O2-C2
75	AU	403	CDL	C55-C56-C57-C58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
76	AV	403	PEE	C11-C12-C13-C14
75	AA	101	CDL	C35-C36-C37-C38
71	B	303	PLX	C32-C33-C34-C35
76	l	701	PEE	C31-C32-C33-C34
71	r	501	PLX	C30-C31-C32-C33
75	V	201	CDL	C75-C76-C77-C78
75	AU	403	CDL	C71-C72-C73-C74
71	AT	101	PLX	C26-C27-C28-C29
75	AJ	405	CDL	CA6-CA4-OA6-CA5
75	AU	403	CDL	CA6-CA4-OA6-CA5
75	AY	501	CDL	CA6-CA4-OA6-CA5
75	AY	501	CDL	CB3-CB4-OB6-CB5
71	g	202	PLX	C30-C31-C32-C33
75	AG	101	CDL	C11-C12-C13-C14
76	AL	503	PEE	C31-C32-C33-C34
75	AA	101	CDL	CA3-CA4-CA6-OA8
75	AH	403	CDL	C1-CB2-OB2-PB2
75	AN	101	CDL	CA3-CA4-CA6-OA8
75	AU	403	CDL	C1-CB2-OB2-PB2
75	AY	501	CDL	CA3-CA4-CA6-OA8
71	g	202	PLX	O4-C3-C4-O6
71	AL	501	PLX	O4-C3-C4-O6
71	AQ	101	PLX	O4-C3-C4-O6
75	V	201	CDL	OB5-CB3-CB4-OB6
75	l	703	CDL	OA5-CA3-CA4-OA6
75	AJ	404	CDL	OB5-CB3-CB4-OB6
75	AU	403	CDL	OA5-CA3-CA4-OA6
82	AV	401	HEM	C4C-C3C-CAC-CBC
76	V	202	PEE	C33-C34-C35-C36
71	AL	501	PLX	C6-C7-C8-C9
81	AH	402	HEC	C2C-C3C-CAC-CBC
76	V	202	PEE	C32-C33-C34-C35
71	b	201	PLX	O6-C4-C5-O8
71	r	501	PLX	O6-C4-C5-O8
75	V	201	CDL	OA6-CA4-CA6-OA8
75	V	201	CDL	OB6-CB4-CB6-OB8
75	AA	101	CDL	OA6-CA4-CA6-OA8
75	AG	101	CDL	OA6-CA4-CA6-OA8
75	AJ	405	CDL	OA6-CA4-CA6-OA8
75	AJ	405	CDL	OB6-CB4-CB6-OB8
75	AN	101	CDL	OA6-CA4-CA6-OA8
75	AA	101	CDL	C32-C31-CA7-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
72	E	201	8Q1	C6-C7-C8-C9
75	AH	403	CDL	C12-C13-C14-C15
73	J	401	NDP	C5B-O5B-PA-O3
73	J	401	NDP	C5D-O5D-PN-O3
76	AH	401	PEE	C15-C16-C17-C18
75	l	704	CDL	C12-C13-C14-C15
76	AJ	403	PEE	O4-C10-O2-C2
71	r	502	PLX	C24-C25-C26-C27
75	AJ	404	CDL	C33-C34-C35-C36
71	r	502	PLX	C34-C35-C36-C37
71	g	201	PLX	C35-C36-C37-C38
76	l	701	PEE	C24-C25-C26-C27
76	l	702	PEE	C11-C12-C13-C14
75	AL	502	CDL	C11-C12-C13-C14
75	n	101	CDL	C35-C36-C37-C38
75	n	101	CDL	C11-C12-C13-C14
75	l	704	CDL	CB2-OB2-PB2-OB5
75	AJ	405	CDL	CB2-OB2-PB2-OB5
71	r	501	PLX	C31-C32-C33-C34
76	W	201	PEE	C31-C32-C33-C34
71	r	502	PLX	C4-C3-O4-P1
75	l	704	CDL	CA4-CA3-OA5-PA1
75	AH	403	CDL	CA4-CA3-OA5-PA1
75	AN	101	CDL	C1-CA2-OA2-PA1
75	AN	101	CDL	C1-CB2-OB2-PB2
71	b	201	PLX	C3-O4-P1-O2
71	g	201	PLX	C3-O4-P1-O3
71	g	202	PLX	C3-O4-P1-O2
71	g	202	PLX	C3-O4-P1-O3
71	r	502	PLX	C2-O1-P1-O3
71	AQ	101	PLX	C3-O4-P1-O3
71	AT	101	PLX	C2-O1-P1-O3
73	J	401	NDP	C5B-O5B-PA-O2A
73	J	401	NDP	C5D-O5D-PN-O2N
75	V	201	CDL	CB3-OB5-PB2-OB4
75	i	401	CDL	CB2-OB2-PB2-OB3
75	l	703	CDL	CA2-OA2-PA1-OA4
75	l	703	CDL	CB3-OB5-PB2-OB4
75	l	704	CDL	CA3-OA5-PA1-OA3
75	n	101	CDL	CA3-OA5-PA1-OA3
75	AA	101	CDL	CB2-OB2-PB2-OB3
75	AG	101	CDL	CA2-OA2-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	AG	101	CDL	CB2-OB2-PB2-OB3
75	AL	502	CDL	CA2-OA2-PA1-OA4
75	AL	502	CDL	CB3-OB5-PB2-OB3
75	AL	502	CDL	CB3-OB5-PB2-OB4
75	AN	101	CDL	CA2-OA2-PA1-OA3
75	AN	101	CDL	CB2-OB2-PB2-OB3
75	AY	501	CDL	CA3-OA5-PA1-OA4
76	V	202	PEE	C1-O3P-P-O1P
76	AH	401	PEE	C4-O4P-P-O1P
76	AU	401	PEE	C4-O4P-P-O1P
76	AV	403	PEE	C1-O3P-P-O2P
76	AV	403	PEE	C1-O3P-P-O1P
76	AY	502	PEE	C1-O3P-P-O1P
71	g	202	PLX	O4-C3-C4-C5
71	AQ	101	PLX	O4-C3-C4-C5
75	V	201	CDL	OA5-CA3-CA4-CA6
75	l	703	CDL	OA5-CA3-CA4-CA6
75	l	704	CDL	OA5-CA3-CA4-CA6
75	AL	502	CDL	OB5-CB3-CB4-CB6
71	r	501	PLX	C15-C16-C17-C18
75	AL	502	CDL	C33-C34-C35-C36
76	AH	401	PEE	C17-C18-C19-C20
76	AV	403	PEE	C17-C18-C19-C20
71	V	203	PLX	C19-C20-C21-C22
71	U	101	PLX	C25-C24-O8-C5
71	b	201	PLX	C1-C2-O1-P1
71	g	203	PLX	C1-C2-O1-P1
71	r	501	PLX	C25-C24-O8-C5
71	AT	101	PLX	C1-C2-O1-P1
71	AT	101	PLX	C25-C24-O8-C5
76	AH	401	PEE	C5-C4-O4P-P
76	W	201	PEE	C10-C11-C12-C13
71	g	203	PLX	C19-C20-C21-C22
75	V	201	CDL	C74-C75-C76-C77
75	AN	101	CDL	CA2-C1-CB2-OB2
75	AU	403	CDL	CA2-C1-CB2-OB2
75	l	704	CDL	OB5-CB3-CB4-OB6
75	AU	403	CDL	OB5-CB3-CB4-OB6
75	AY	501	CDL	OB5-CB3-CB4-OB6
76	l	701	PEE	O3P-C1-C2-O2
71	AL	501	PLX	C19-C20-C21-C22
76	AJ	403	PEE	C11-C10-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	V	203	PLX	C14-C15-C16-C17
76	AH	401	PEE	C14-C15-C16-C17
71	g	203	PLX	C3-C4-C5-O8
71	r	502	PLX	C3-C4-C5-O8
71	AL	501	PLX	N1-C1-C2-O1
75	AG	101	CDL	CA3-CA4-CA6-OA8
71	g	203	PLX	O6-C4-C5-O8
71	r	502	PLX	O6-C4-C5-O8
75	l	704	CDL	OA6-CA4-CA6-OA8
75	AH	403	CDL	OA6-CA4-CA6-OA8
75	AY	501	CDL	OA6-CA4-CA6-OA8
76	AV	403	PEE	O2-C2-C3-O3
75	AJ	404	CDL	C55-C56-C57-C58
75	AJ	404	CDL	CA4-CA3-OA5-PA1
71	g	201	PLX	C24-C25-C26-C27
75	AJ	404	CDL	C13-C14-C15-C16
71	r	502	PLX	O8-C24-C25-C26
72	E	201	8Q1	O33-C32-C34-O35
71	g	202	PLX	O7-C6-C7-C8
71	B	303	PLX	C20-C21-C22-C23
71	U	101	PLX	C36-C37-C38-C39
75	l	704	CDL	C15-C16-C17-C18
73	J	401	NDP	O4D-C1D-N1N-C6N
76	AL	503	PEE	C33-C34-C35-C36
71	r	502	PLX	C11-C10-C9-C8
75	AH	403	CDL	O1-C1-CB2-OB2
75	AH	403	CDL	C13-C14-C15-C16
75	n	101	CDL	C73-C74-C75-C76
71	g	201	PLX	C14-C15-C16-C17
75	AH	403	CDL	C54-C55-C56-C57
75	V	201	CDL	CA3-CA4-OA6-CA5
75	l	703	CDL	CB6-CB4-OB6-CB5
75	l	704	CDL	CA6-CA4-OA6-CA5
75	AH	403	CDL	CA3-CA4-OA6-CA5
76	l	701	PEE	C3-C2-O2-C10
76	l	702	PEE	C3-C2-O2-C10
82	AV	401	HEM	C1A-C2A-CAA-CBA
75	AA	101	CDL	CB2-C1-CA2-OA2
75	V	201	CDL	CB7-C71-C72-C73
75	i	401	CDL	C32-C31-CA7-OA8
75	AJ	404	CDL	CB4-CB3-OB5-PB2
75	V	201	CDL	C55-C56-C57-C58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	n	101	CDL	C53-C54-C55-C56
75	AA	101	CDL	OA5-CA3-CA4-OA6
75	l	703	CDL	CA7-C31-C32-C33
76	V	202	PEE	C11-C10-O2-C2
75	n	101	CDL	C15-C16-C17-C18
76	AH	401	PEE	C31-C32-C33-C34
76	AY	502	PEE	C38-C39-C40-C41
75	AN	101	CDL	OB6-CB4-CB6-OB8
71	U	101	PLX	C2-O1-P1-O4
71	V	203	PLX	C3-O4-P1-O1
71	g	203	PLX	C3-O4-P1-O1
75	V	201	CDL	CB2-OB2-PB2-OB5
75	l	703	CDL	CB2-OB2-PB2-OB5
75	AG	101	CDL	CB3-OB5-PB2-OB2
75	AJ	405	CDL	CA2-OA2-PA1-OA5
75	AJ	405	CDL	CB3-OB5-PB2-OB2
75	AU	403	CDL	CA2-OA2-PA1-OA5
76	V	202	PEE	C4-O4P-P-O3P
76	l	701	PEE	C1-O3P-P-O4P
76	l	702	PEE	C4-O4P-P-O3P
76	AH	401	PEE	C1-O3P-P-O4P
76	AL	503	PEE	C4-O4P-P-O3P
71	V	203	PLX	C3-C4-C5-O8
75	AG	101	CDL	CB3-CB4-CB6-OB8
71	V	203	PLX	C29-C30-C31-C32
71	b	201	PLX	C28-C29-C30-C31
81	AH	402	HEC	C3A-C2A-CAA-CBA
71	r	501	PLX	C11-C10-C9-C8
82	AJ	402	HEM	C3A-C2A-CAA-CBA
82	AV	402	HEM	C4D-C3D-CAD-CBD
76	AV	403	PEE	C31-C32-C33-C34
76	AY	502	PEE	C40-C41-C42-C43
76	V	202	PEE	C23-C24-C25-C26
75	AN	101	CDL	CB5-C51-C52-C53
75	l	703	CDL	C34-C35-C36-C37
75	l	704	CDL	C1-CB2-OB2-PB2
75	AG	101	CDL	C1-CA2-OA2-PA1
75	AU	403	CDL	CB4-CB3-OB5-PB2
75	AJ	405	CDL	C34-C35-C36-C37
75	AJ	405	CDL	C14-C15-C16-C17
76	V	202	PEE	O4-C10-O2-C2
76	V	202	PEE	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
73	J	401	NDP	C2D-C1D-N1N-C6N
75	AG	101	CDL	C51-C52-C53-C54
76	l	702	PEE	C23-C24-C25-C26
76	l	701	PEE	O4P-C4-C5-N
76	AY	502	PEE	O4P-C4-C5-N
71	g	202	PLX	C15-C16-C17-C18
75	AL	502	CDL	C54-C55-C56-C57
75	AY	501	CDL	C52-C53-C54-C55
71	g	201	PLX	C19-C20-C21-C22
75	AJ	405	CDL	C15-C16-C17-C18
71	V	203	PLX	O6-C6-C7-C8
71	g	201	PLX	O6-C6-C7-C8
75	i	401	CDL	C1-CB2-OB2-PB2
75	i	401	CDL	CB4-CB3-OB5-PB2
75	l	703	CDL	CA4-CA3-OA5-PA1
75	AN	101	CDL	C32-C33-C34-C35
71	g	201	PLX	C25-C26-C27-C28
76	W	201	PEE	C11-C12-C13-C14
71	B	303	PLX	C6-C7-C8-C9
71	V	203	PLX	C6-C7-C8-C9
75	l	703	CDL	CB5-C51-C52-C53
75	AG	101	CDL	C71-C72-C73-C74
79	x	603	HEA	CAD-CBD-CGD-O1D
72	E	201	8Q1	O27-C28-C29-C30
72	p	201	8Q1	O27-C28-C29-C31
76	AJ	403	PEE	C15-C16-C17-C18
75	AU	403	CDL	CB3-CB4-OB6-CB5
71	g	203	PLX	C3-C4-O6-C6
71	r	501	PLX	C5-C4-O6-C6
71	AQ	101	PLX	C5-C4-O6-C6
75	AN	101	CDL	CA2-OA2-PA1-OA5
75	V	201	CDL	C11-C12-C13-C14
75	i	401	CDL	C72-C71-CB7-OB8
82	AV	402	HEM	C2D-C3D-CAD-CBD
75	AN	101	CDL	C31-CA7-OA8-CA6
76	V	202	PEE	C21-C22-C23-C24
76	AL	503	PEE	C19-C20-C21-C22
75	AH	403	CDL	C51-C52-C53-C54
79	x	604	HEA	CAD-CBD-CGD-O1D
82	AV	401	HEM	C2A-CAA-CBA-CGA
76	AU	401	PEE	C30-C31-C32-C33
71	V	203	PLX	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
72	p	201	8Q1	C42-C43-S44-C1
71	g	201	PLX	O6-C4-C5-O8
75	AA	101	CDL	OB6-CB4-CB6-OB8
76	AL	503	PEE	C16-C17-C18-C19
79	x	604	HEA	CAD-CBD-CGD-O2D
75	AH	403	CDL	C14-C15-C16-C17
76	AV	403	PEE	C14-C15-C16-C17
76	AL	503	PEE	C40-C41-C42-C43
79	x	603	HEA	CAA-CBA-CGA-O1A
75	AH	403	CDL	C32-C31-CA7-OA9
75	AN	101	CDL	OA9-CA7-OA8-CA6
79	x	603	HEA	CAD-CBD-CGD-O2D
75	AU	403	CDL	O1-C1-CA2-OA2
71	B	303	PLX	C7-C8-C9-C10
75	i	401	CDL	C52-C51-CB5-OB7
75	V	201	CDL	C73-C74-C75-C76
75	l	704	CDL	CA3-CA4-CA6-OA8
75	AN	101	CDL	C53-C54-C55-C56
75	AN	101	CDL	C35-C36-C37-C38
71	g	202	PLX	C16-C17-C18-C19
71	r	502	PLX	C28-C29-C30-C31
76	AJ	403	PEE	C36-C37-C38-C39
71	g	201	PLX	O4-C3-C4-O6
75	AH	403	CDL	CB7-C71-C72-C73
71	V	203	PLX	C24-C25-C26-C27
75	AY	501	CDL	C72-C71-CB7-OB8
71	AL	501	PLX	O6-C6-C7-C8
75	AU	403	CDL	C34-C35-C36-C37
76	AL	503	PEE	C23-C24-C25-C26
76	AU	401	PEE	C14-C15-C16-C17
76	AU	401	PEE	C38-C39-C40-C41
76	AY	502	PEE	C36-C37-C38-C39
71	AT	101	PLX	C30-C31-C32-C33
72	E	201	8Q1	O33-C32-C34-N36
76	AU	401	PEE	C42-C43-C44-C45
75	AH	403	CDL	C73-C74-C75-C76
76	W	201	PEE	C35-C36-C37-C38
76	AJ	403	PEE	C19-C20-C21-C22
75	l	703	CDL	C32-C31-CA7-OA8
75	l	704	CDL	C32-C31-CA7-OA8
76	W	201	PEE	C1-C2-O2-C10
76	V	202	PEE	C30-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	g	202	PLX	C27-C28-C29-C30
75	AA	101	CDL	C15-C16-C17-C18
71	B	303	PLX	C14-C15-C16-C17
71	V	203	PLX	C35-C36-C37-C38
75	AG	101	CDL	C32-C31-CA7-OA8
75	AJ	404	CDL	C52-C51-CB5-OB6
76	AH	401	PEE	C40-C41-C42-C43
76	AV	403	PEE	C36-C37-C38-C39
71	b	201	PLX	C3-C4-C5-O8
75	V	201	CDL	CA3-CA4-CA6-OA8
75	AH	403	CDL	CB3-CB4-CB6-OB8
75	AJ	405	CDL	CA3-CA4-CA6-OA8
76	AH	401	PEE	O3P-C1-C2-O2
75	AN	101	CDL	C12-C11-CA5-OA6
71	AT	101	PLX	C10-C11-C12-C13
73	J	401	NDP	O4D-C4D-C5D-O5D
79	x	604	HEA	CAA-CBA-CGA-O2A
71	r	502	PLX	C33-C34-C35-C36
73	J	401	NDP	O4D-C1D-N1N-C2N
75	l	704	CDL	C35-C36-C37-C38
76	AH	401	PEE	C36-C37-C38-C39
79	x	604	HEA	CAA-CBA-CGA-O1A
71	B	303	PLX	O9-C24-C25-C26
71	AL	501	PLX	C11-C12-C13-C14
76	l	701	PEE	C38-C39-C40-C41
75	AU	403	CDL	O1-C1-CB2-OB2
71	AL	501	PLX	C29-C30-C31-C32
75	l	703	CDL	C32-C31-CA7-OA9
75	AA	101	CDL	C32-C33-C34-C35
76	AL	503	PEE	O2-C10-C11-C12
76	l	702	PEE	C18-C19-C20-C21
75	l	703	CDL	C32-C33-C34-C35
75	AG	101	CDL	C32-C31-CA7-OA9
75	AN	101	CDL	C12-C11-CA5-OA7
75	AU	403	CDL	CB3-CB4-CB6-OB8
76	l	702	PEE	C1-C2-C3-O3
71	b	201	PLX	C24-C25-C26-C27
75	AU	403	CDL	C72-C71-CB7-OB8
76	AL	503	PEE	C41-C42-C43-C44
71	AL	501	PLX	C33-C34-C35-C36
75	AG	101	CDL	C15-C16-C17-C18
76	l	702	PEE	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	AN	101	CDL	C72-C71-CB7-OB8
71	B	303	PLX	C4-C3-O4-P1
75	AU	403	CDL	C1-CA2-OA2-PA1
75	AJ	404	CDL	C52-C51-CB5-OB7
71	V	203	PLX	C17-C18-C19-C20
79	x	603	HEA	CAA-CBA-CGA-O2A
71	V	203	PLX	C3-O4-P1-O2
71	g	201	PLX	C3-O4-P1-O2
71	AT	101	PLX	C3-O4-P1-O3
75	l	703	CDL	CA3-OA5-PA1-OA3
75	l	704	CDL	CB3-OB5-PB2-OB3
75	n	101	CDL	CB3-OB5-PB2-OB3
75	AJ	405	CDL	CA2-OA2-PA1-OA3
75	AL	502	CDL	CA2-OA2-PA1-OA3
75	AU	403	CDL	CA2-OA2-PA1-OA3
75	AU	403	CDL	CB2-OB2-PB2-OB3
75	AY	501	CDL	CA2-OA2-PA1-OA3
76	l	702	PEE	C4-O4P-P-O1P
76	AH	401	PEE	C1-O3P-P-O1P
76	AJ	403	PEE	C4-O4P-P-O2P
75	AU	403	CDL	OB6-CB4-CB6-OB8
76	l	701	PEE	C33-C34-C35-C36
75	V	201	CDL	C12-C11-CA5-OA7
75	l	704	CDL	C32-C31-CA7-OA9
75	AU	403	CDL	C75-C76-C77-C78
76	AY	502	PEE	C21-C22-C23-C24
82	AV	401	HEM	CAA-CBA-CGA-O2A
76	AJ	403	PEE	O4P-C4-C5-N
71	AT	101	PLX	C25-C26-C27-C28
75	AA	101	CDL	C12-C11-CA5-OA6
71	r	501	PLX	C14-C15-C16-C17
71	b	201	PLX	C25-C24-O8-C5
71	g	202	PLX	C25-C24-O8-C5
71	AL	501	PLX	C1-C2-O1-P1
76	W	201	PEE	C5-C4-O4P-P
76	AJ	403	PEE	C10-C11-C12-C13
75	AY	501	CDL	C51-C52-C53-C54
73	J	401	NDP	C2D-C1D-N1N-C2N
76	l	702	PEE	C41-C42-C43-C44
76	V	202	PEE	C39-C40-C41-C42
75	l	704	CDL	C74-C75-C76-C77
76	l	702	PEE	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	l	704	CDL	C52-C51-CB5-OB6
75	AG	101	CDL	C52-C51-CB5-OB6
75	AJ	404	CDL	C12-C11-CA5-OA6
76	AH	401	PEE	O2-C10-C11-C12
76	AL	503	PEE	O3-C30-C31-C32
76	AY	502	PEE	O3-C30-C31-C32
76	AL	503	PEE	O4-C10-C11-C12
71	g	202	PLX	C6-C7-C8-C9
71	g	202	PLX	C24-C25-C26-C27
71	AQ	101	PLX	C6-C7-C8-C9
79	x	604	HEA	C26-C15-C16-C17
70	A	502	FMN	N10-C1'-C2'-O2'
79	x	603	HEA	O11-C11-C3B-C2B
75	AU	403	CDL	C72-C71-CB7-OB9
76	l	701	PEE	C11-C12-C13-C14
75	AH	403	CDL	C12-C11-CA5-OA6
71	V	203	PLX	C15-C16-C17-C18
75	AH	403	CDL	C12-C11-CA5-OA7
76	AY	502	PEE	O5-C30-C31-C32
75	AA	101	CDL	C12-C11-CA5-OA7
71	g	203	PLX	C36-C37-C38-C39
75	AN	101	CDL	O1-C1-CB2-OB2
75	l	704	CDL	C52-C51-CB5-OB7
75	AJ	404	CDL	C12-C11-CA5-OA7
75	AN	101	CDL	C72-C71-CB7-OB9
71	AT	101	PLX	C17-C18-C19-C20
76	W	201	PEE	C42-C43-C44-C45
75	AY	501	CDL	CA5-C11-C12-C13
75	AA	101	CDL	C52-C51-CB5-OB6

There are no ring outliers.

56 monomers are involved in 561 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	B	301	SF4	1	0
70	A	502	FMN	16	0
71	AL	501	PLX	3	0
71	V	203	PLX	5	0
75	V	201	CDL	8	0
75	AJ	405	CDL	17	0
76	W	201	PEE	19	0
71	b	201	PLX	38	0

Continued on next page...

Continued from previous page...

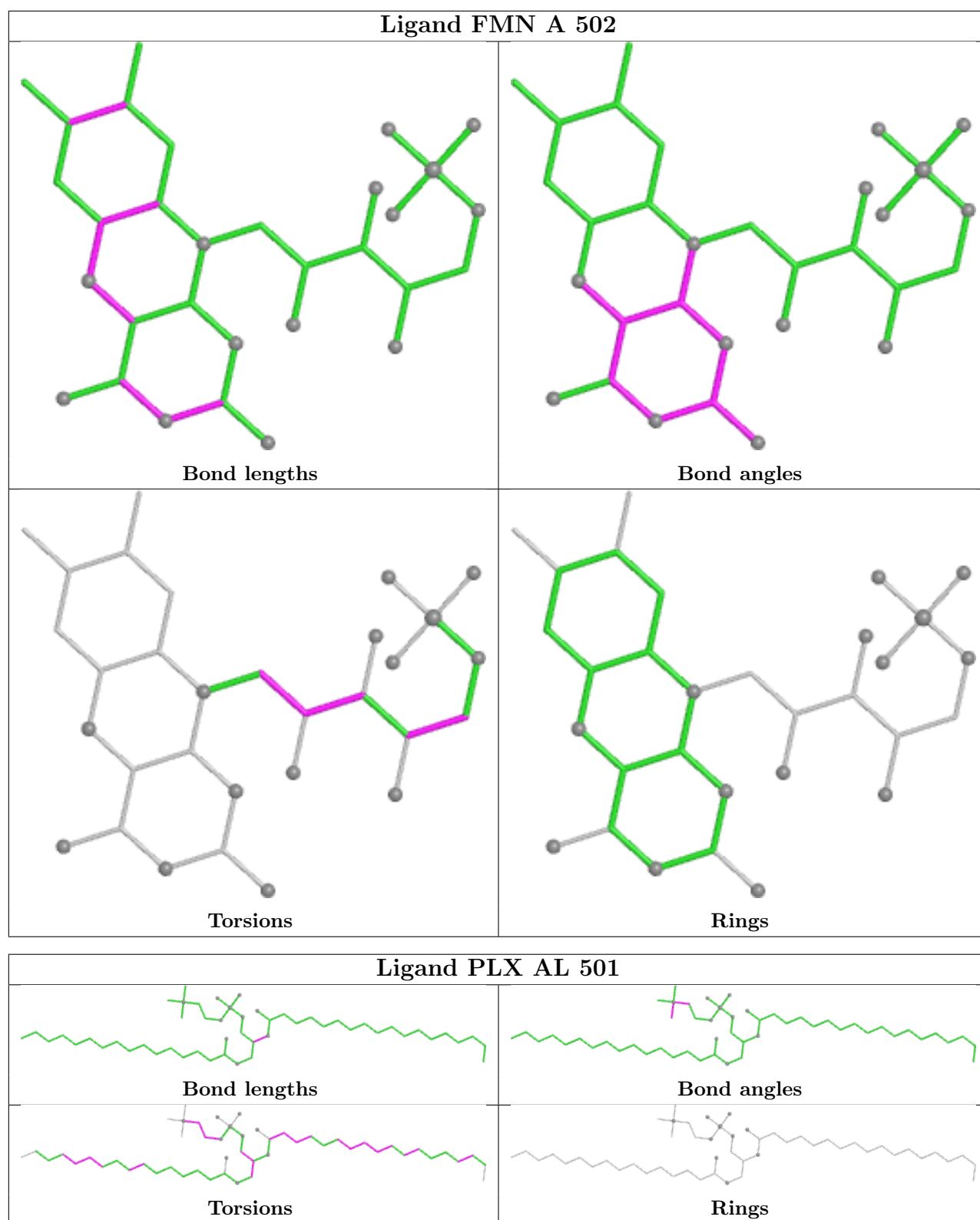
Mol	Chain	Res	Type	Clashes	Symm-Clashes
76	AU	401	PEE	24	0
79	x	604	HEA	3	0
69	M	801	SF4	3	0
71	g	202	PLX	3	0
81	AU	402	HEC	6	0
74	O	301	FES	2	0
75	AG	101	CDL	29	0
73	J	401	NDP	27	0
82	AV	401	HEM	7	0
75	AJ	404	CDL	6	0
82	AV	402	HEM	6	0
75	AU	403	CDL	12	0
76	AV	403	PEE	21	0
74	AC	301	FES	3	0
75	l	703	CDL	2	0
76	AH	401	PEE	31	0
76	V	202	PEE	21	0
71	B	303	PLX	2	0
69	B	302	SF4	2	0
75	n	101	CDL	10	0
72	p	201	8Q1	12	0
75	AN	101	CDL	8	0
71	r	502	PLX	17	0
75	i	401	CDL	3	0
71	U	101	PLX	3	0
79	x	603	HEA	2	0
75	AA	101	CDL	1	0
81	AH	402	HEC	5	0
71	AQ	101	PLX	7	0
75	l	704	CDL	2	0
76	AL	503	PEE	38	0
82	AJ	402	HEM	4	0
76	AY	502	PEE	22	0
82	AJ	401	HEM	3	0
74	AP	301	FES	2	0
69	A	501	SF4	6	0
71	AT	101	PLX	3	0
76	l	701	PEE	50	0
75	AL	502	CDL	23	0
75	AH	403	CDL	6	0
71	g	203	PLX	8	0
74	M	803	FES	1	0

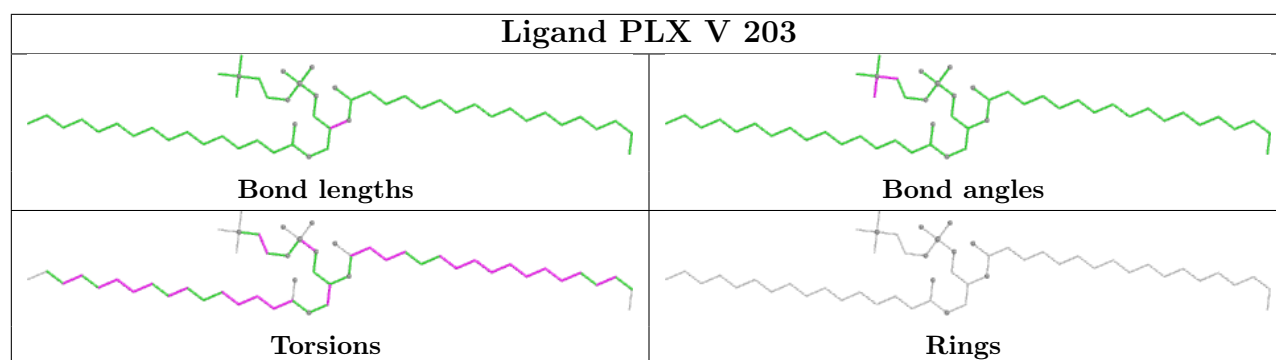
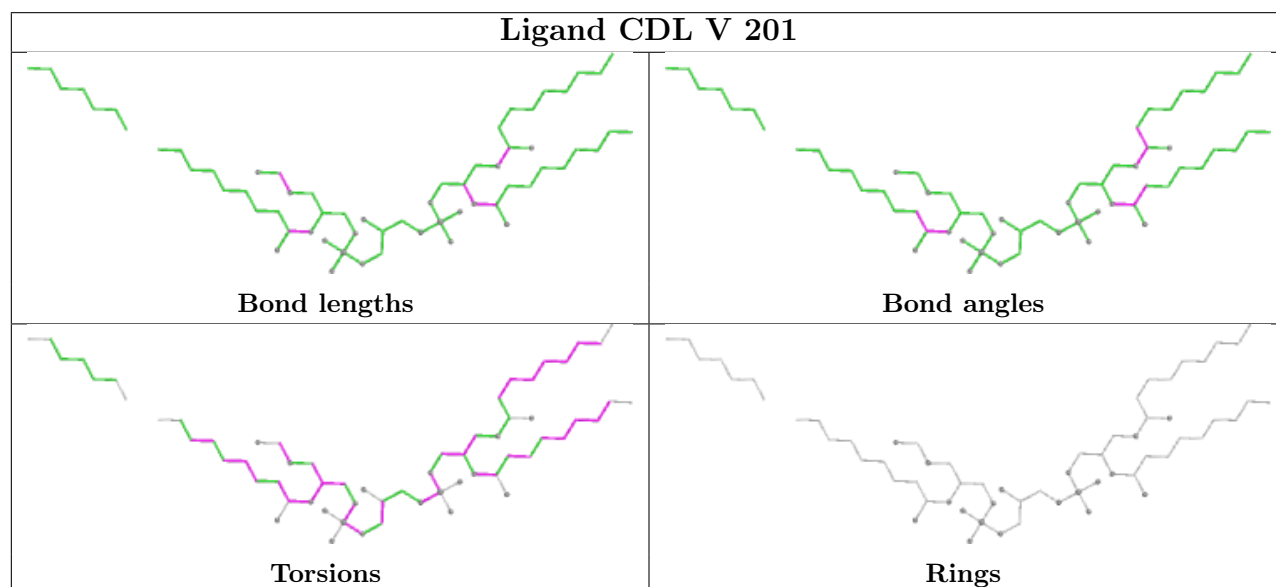
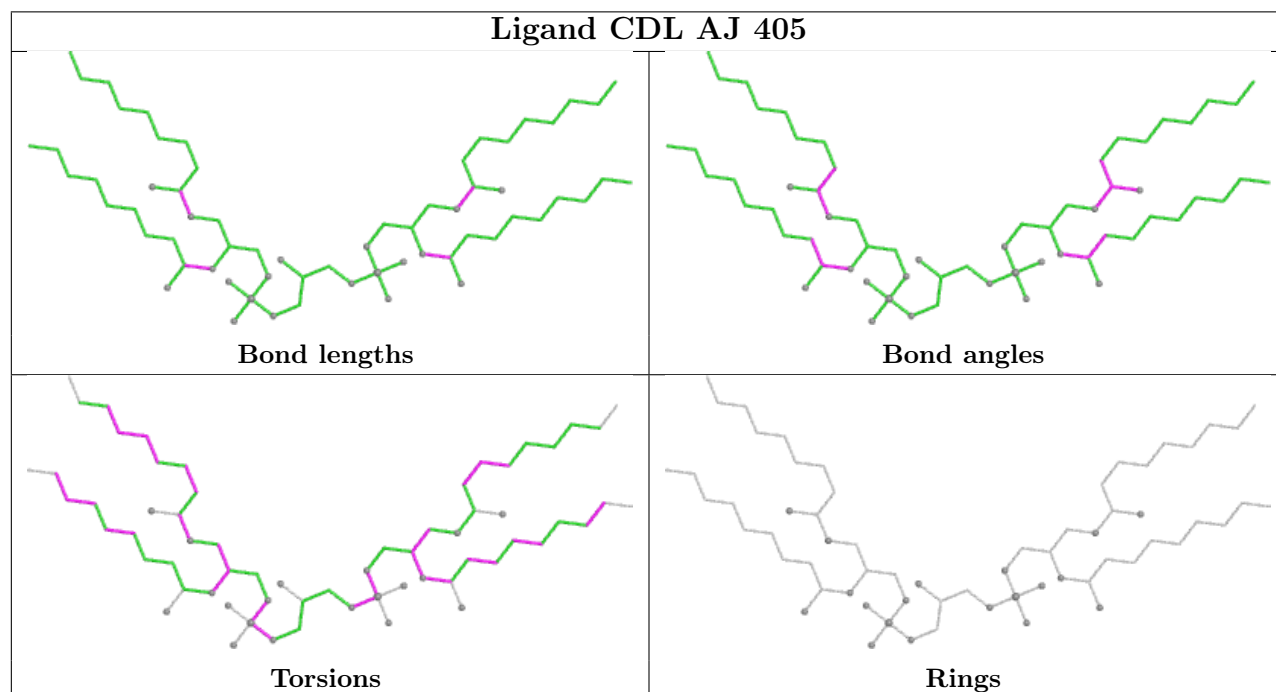
Continued on next page...

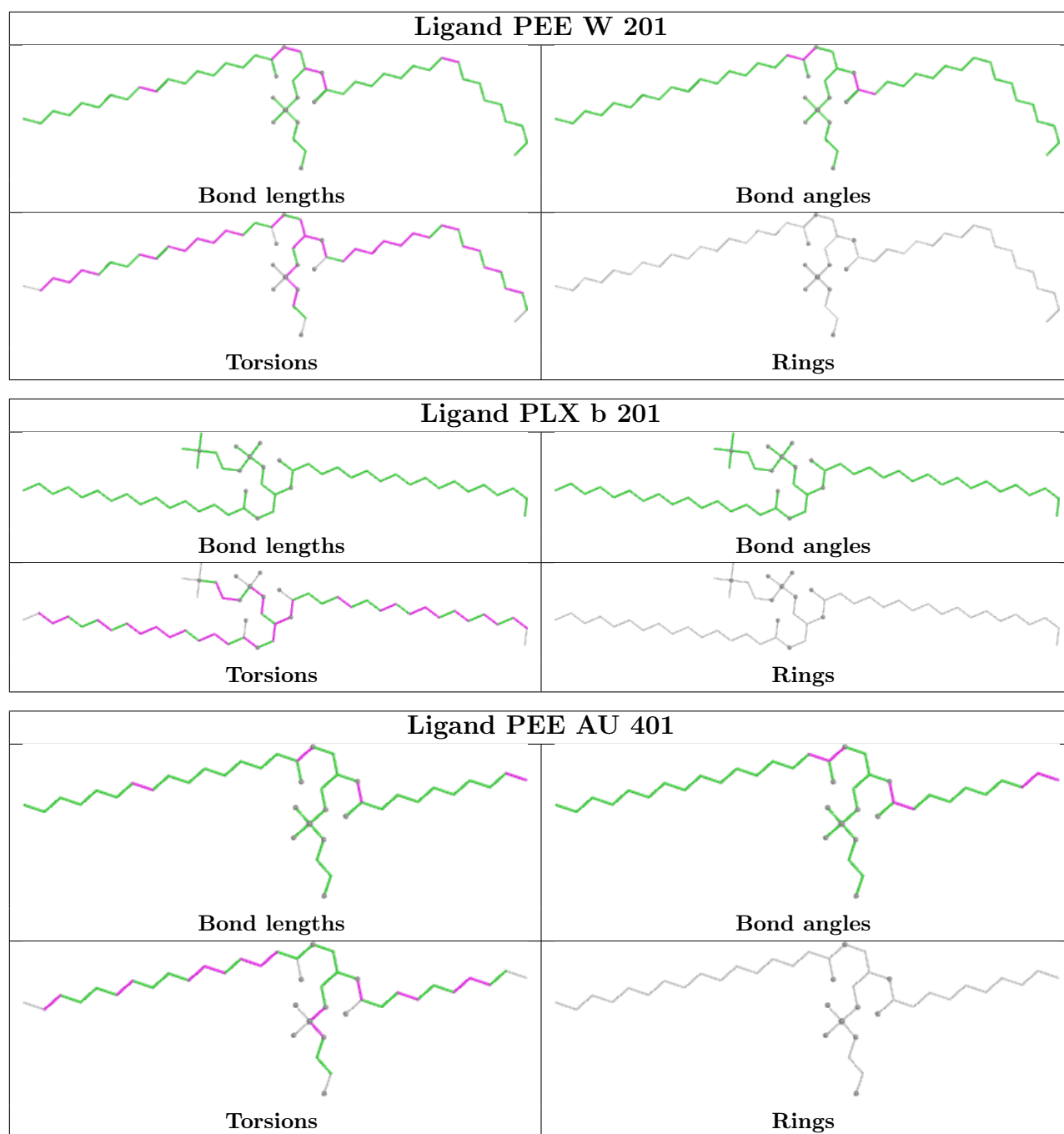
Continued from previous page...

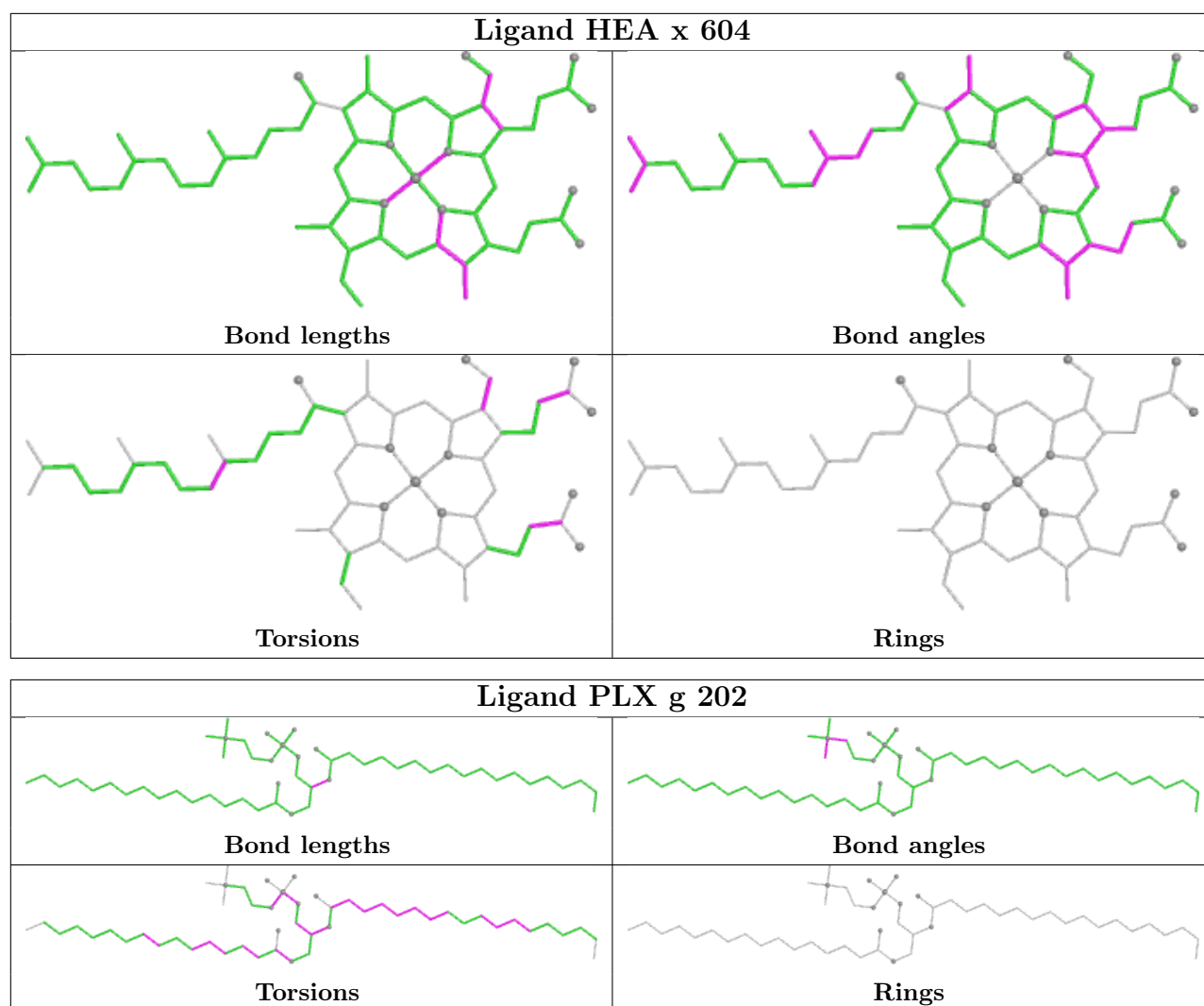
Mol	Chain	Res	Type	Clashes	Symm-Clashes
76	AJ	403	PEE	8	0
71	g	201	PLX	2	0
71	r	501	PLX	6	0
75	AY	501	CDL	4	0
72	E	201	8Q1	4	0
76	l	702	PEE	18	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

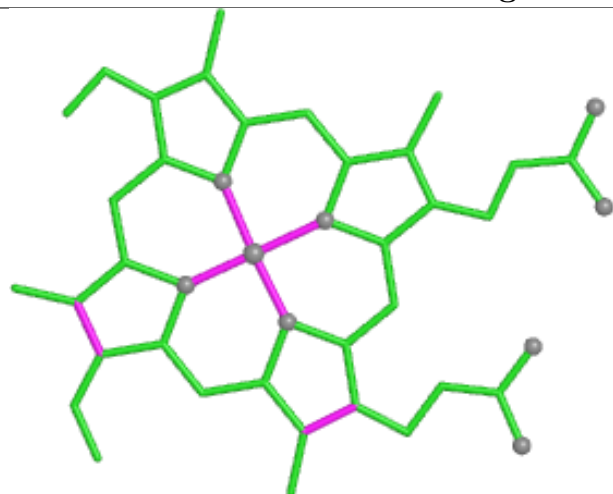




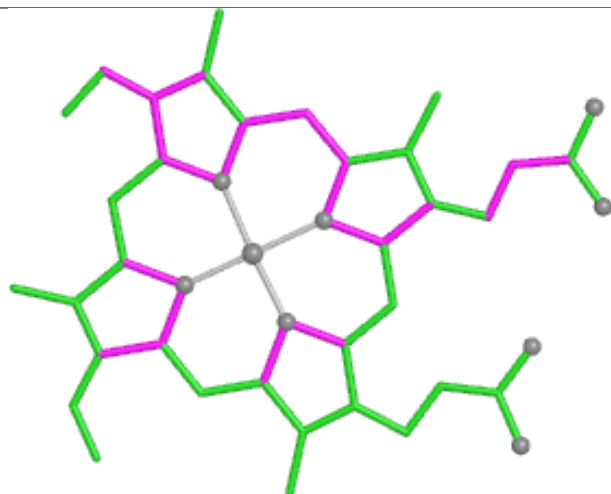




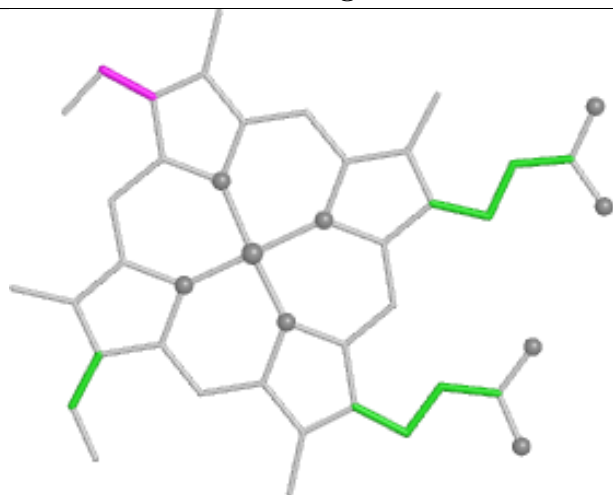
Ligand HEC AU 402



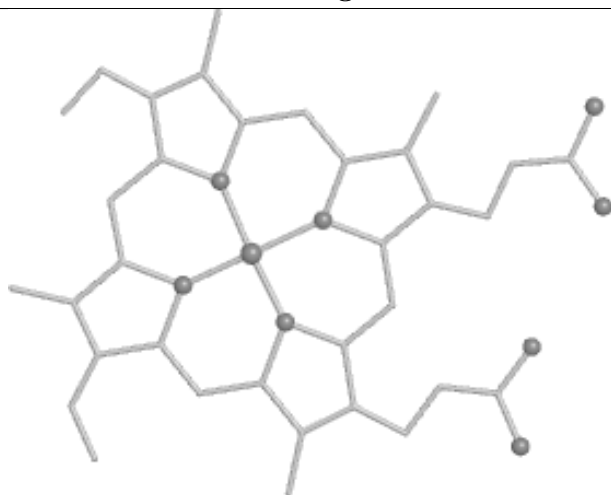
Bond lengths



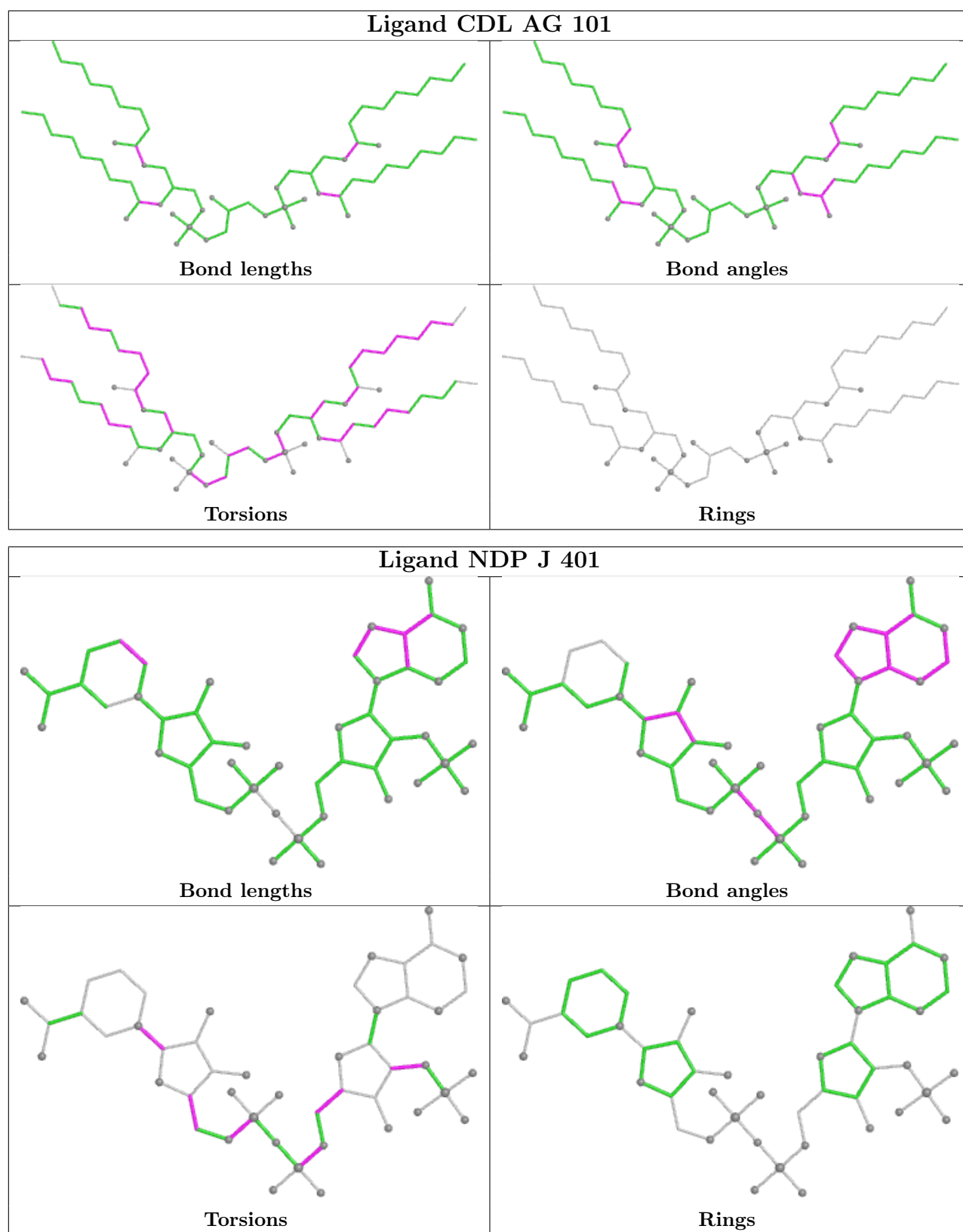
Bond angles



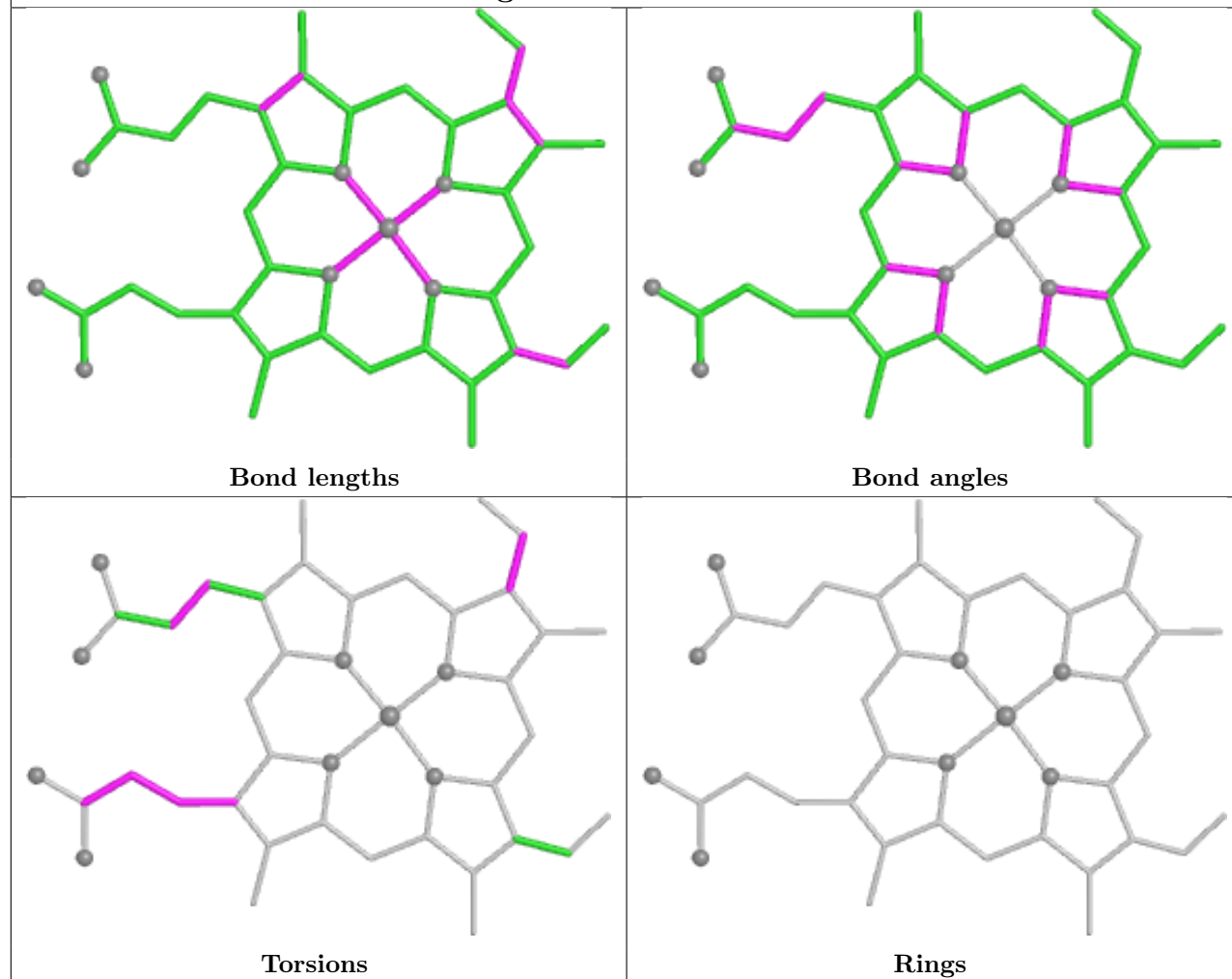
Torsions



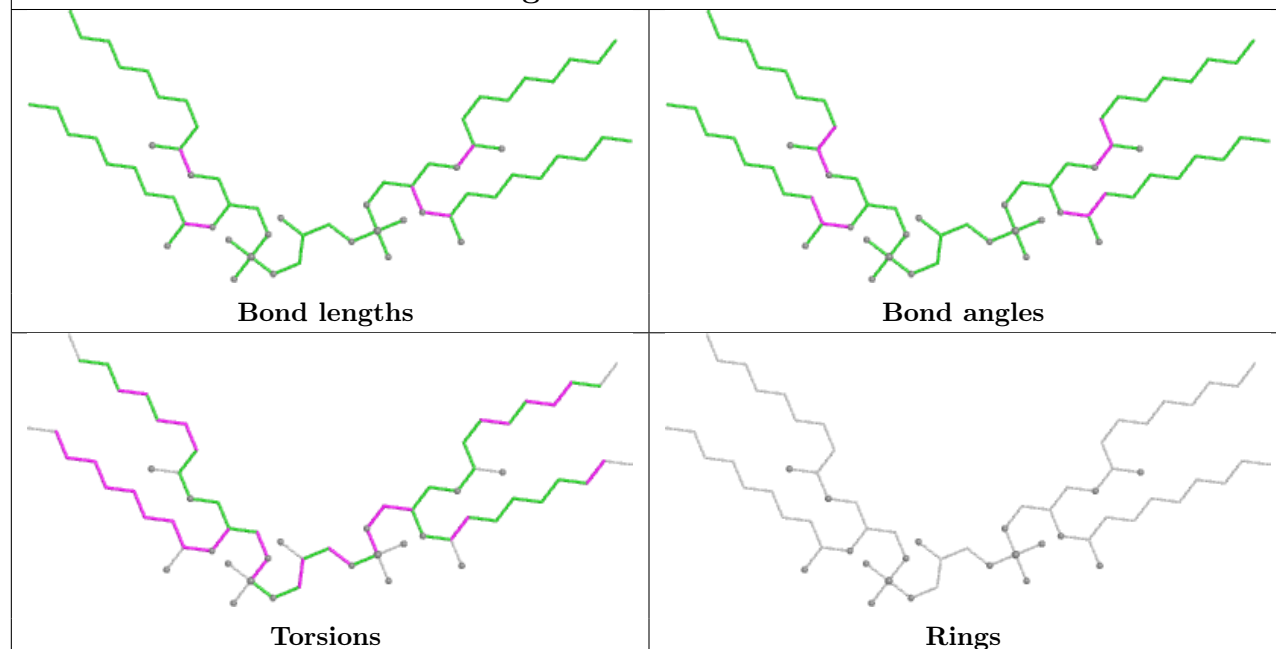
Rings



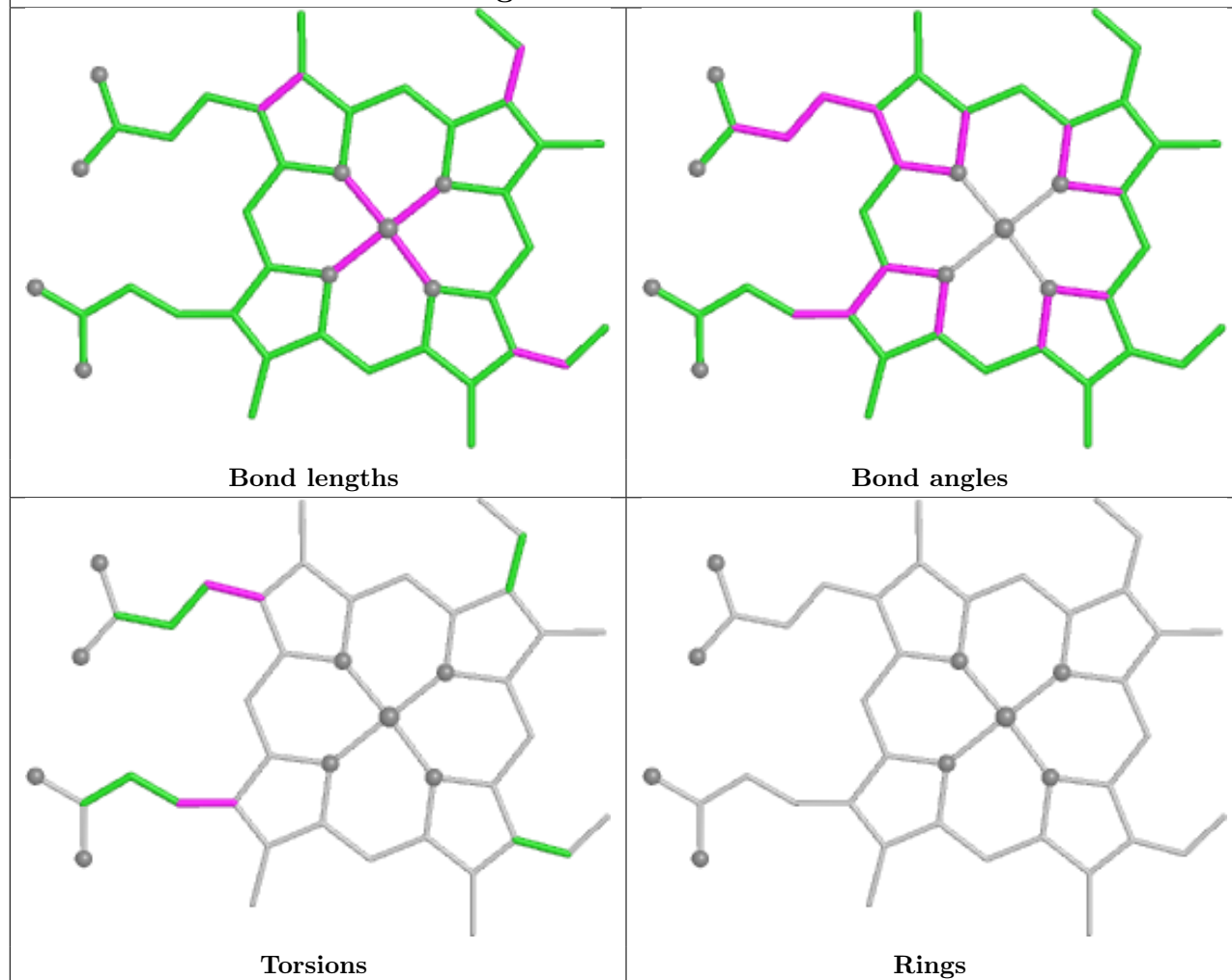
Ligand HEM AV 401



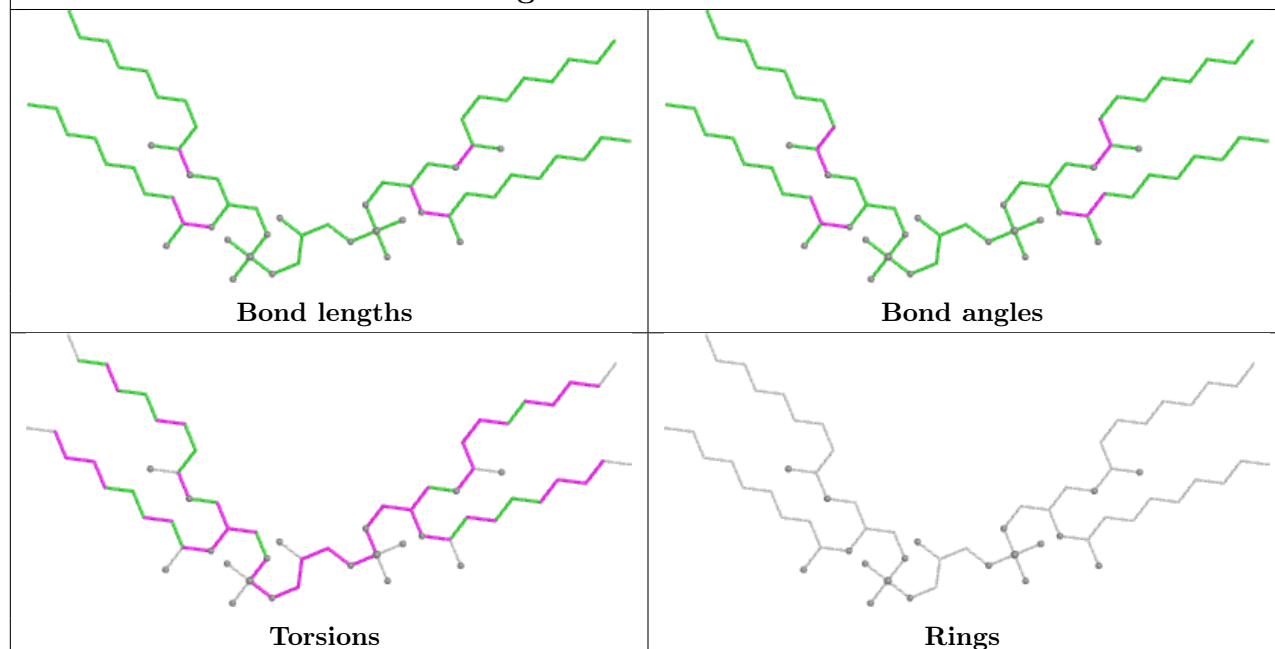
Ligand CDL AJ 404

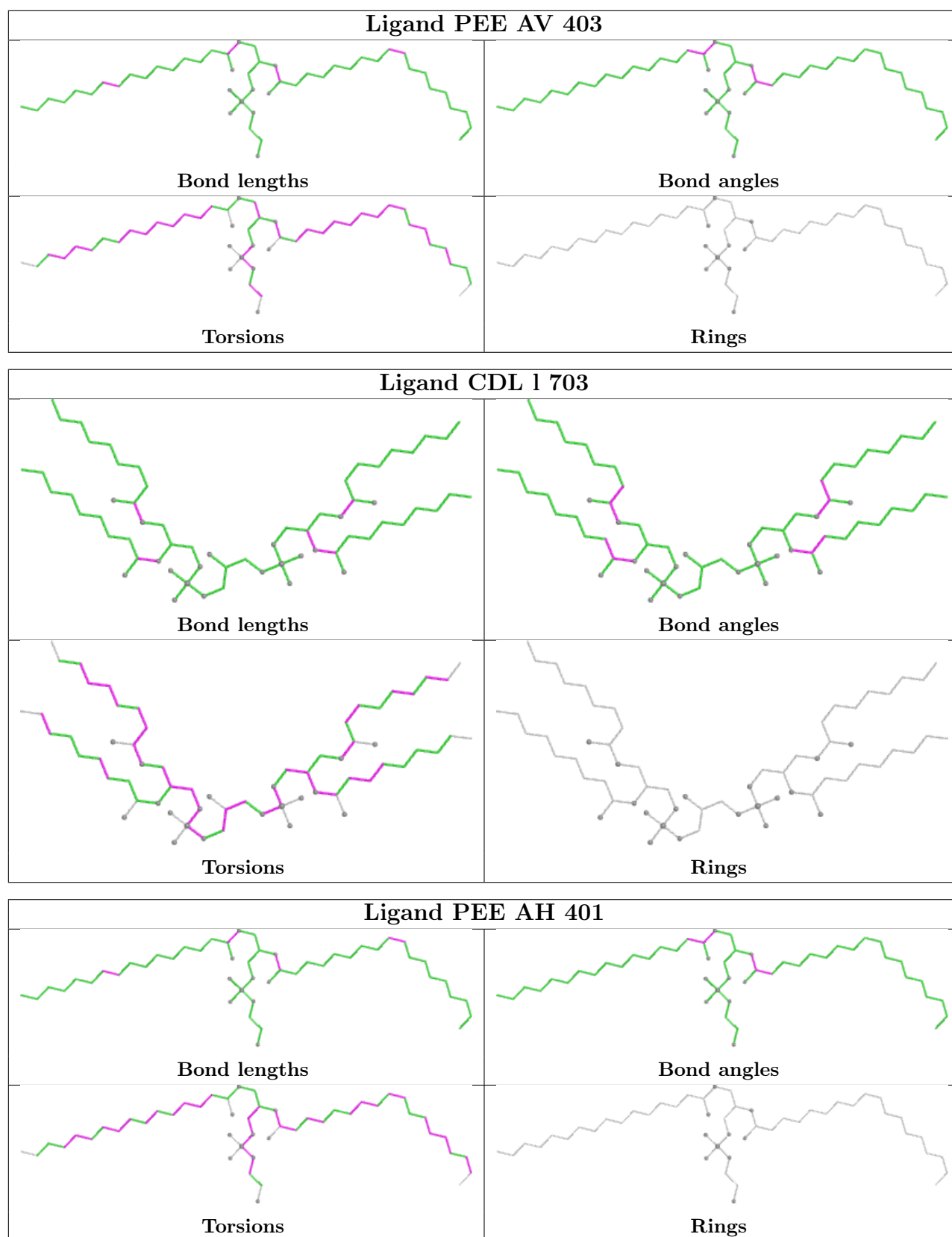


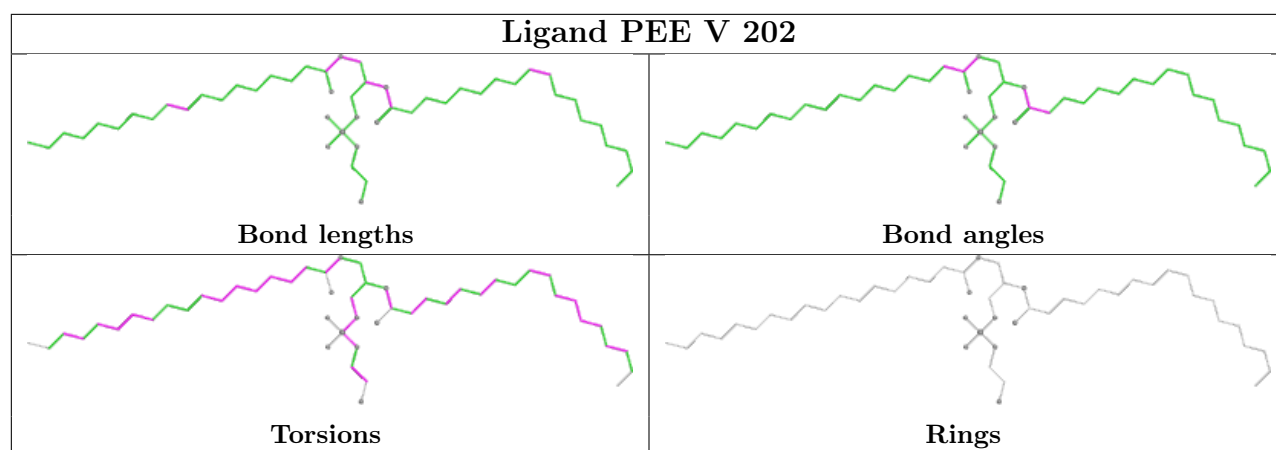
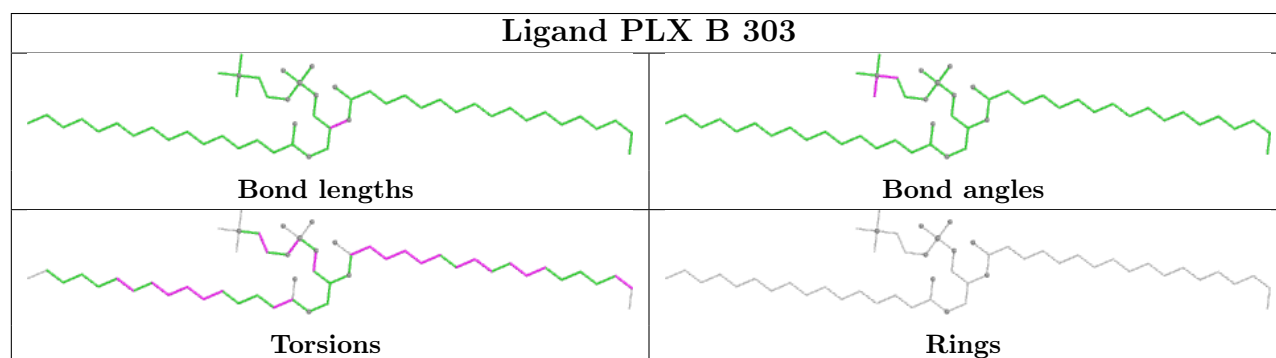
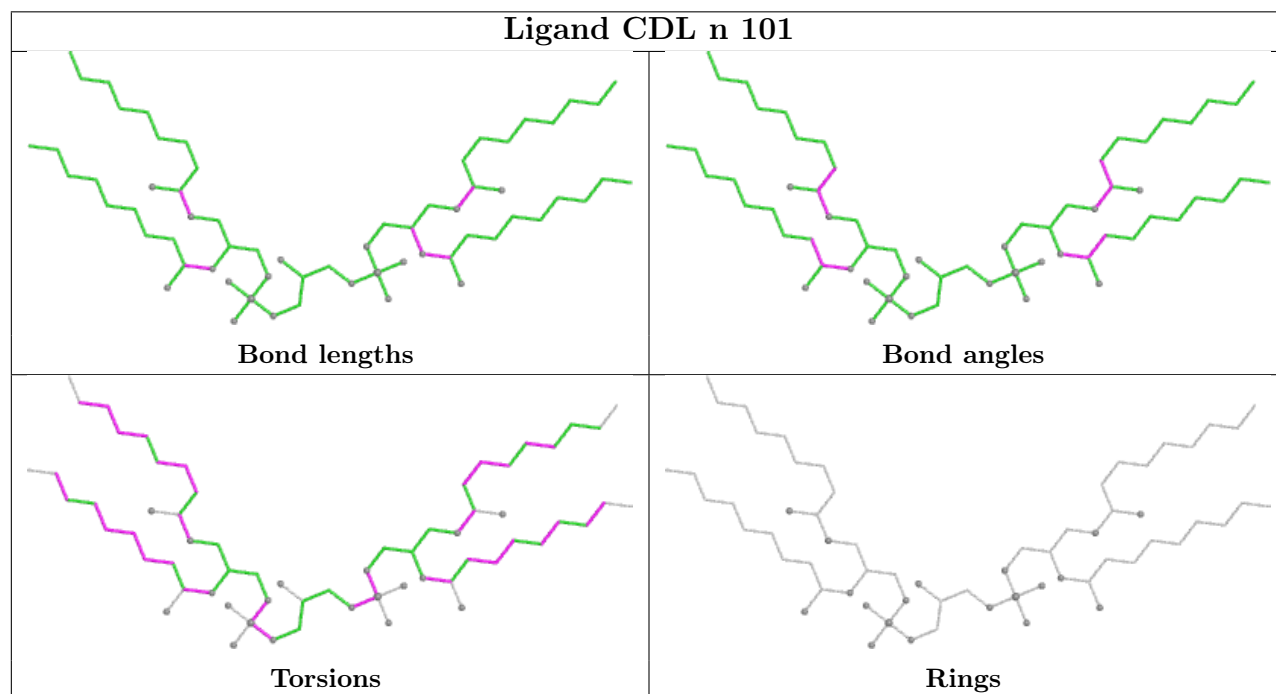
Ligand HEM AV 402

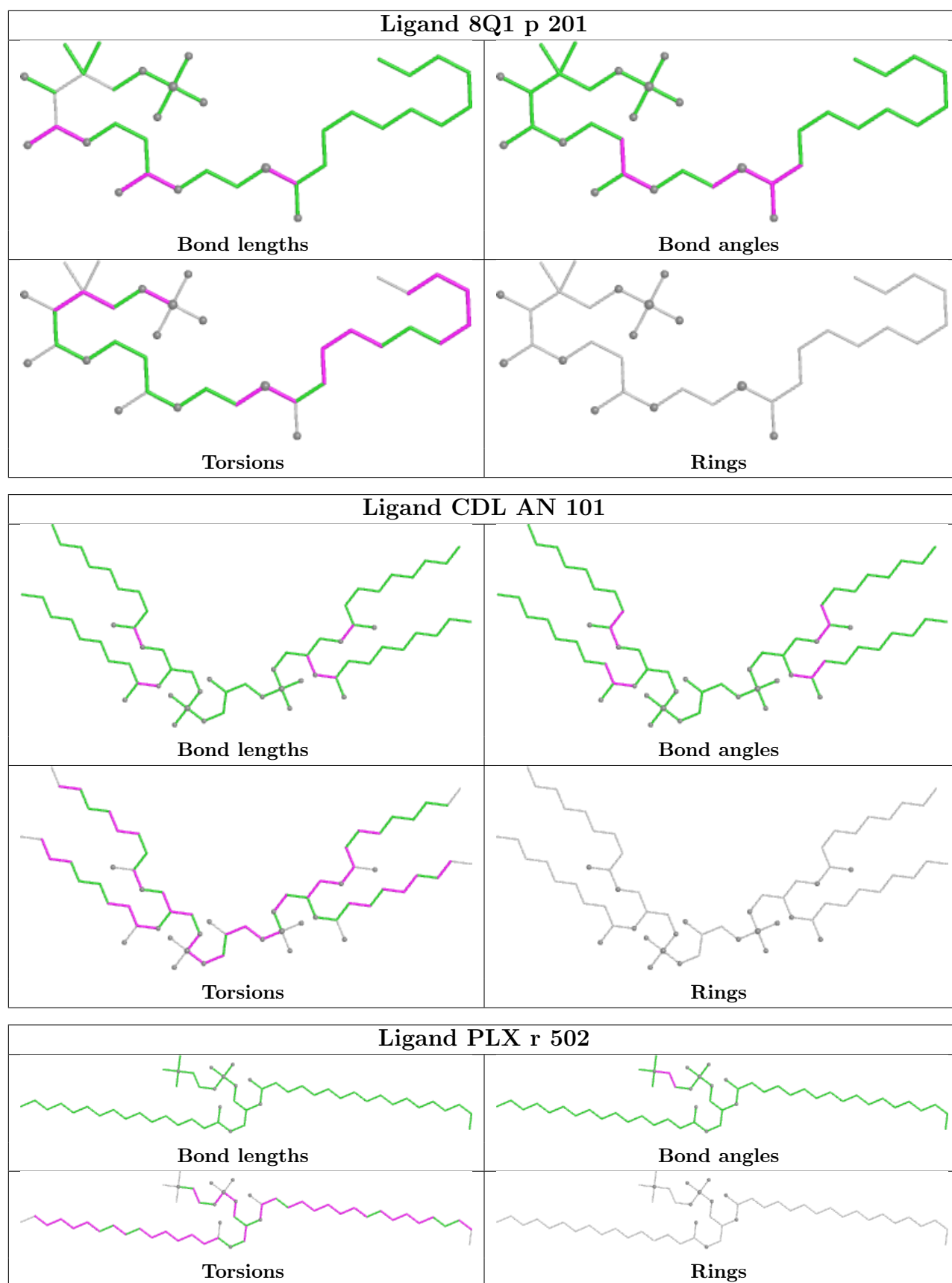


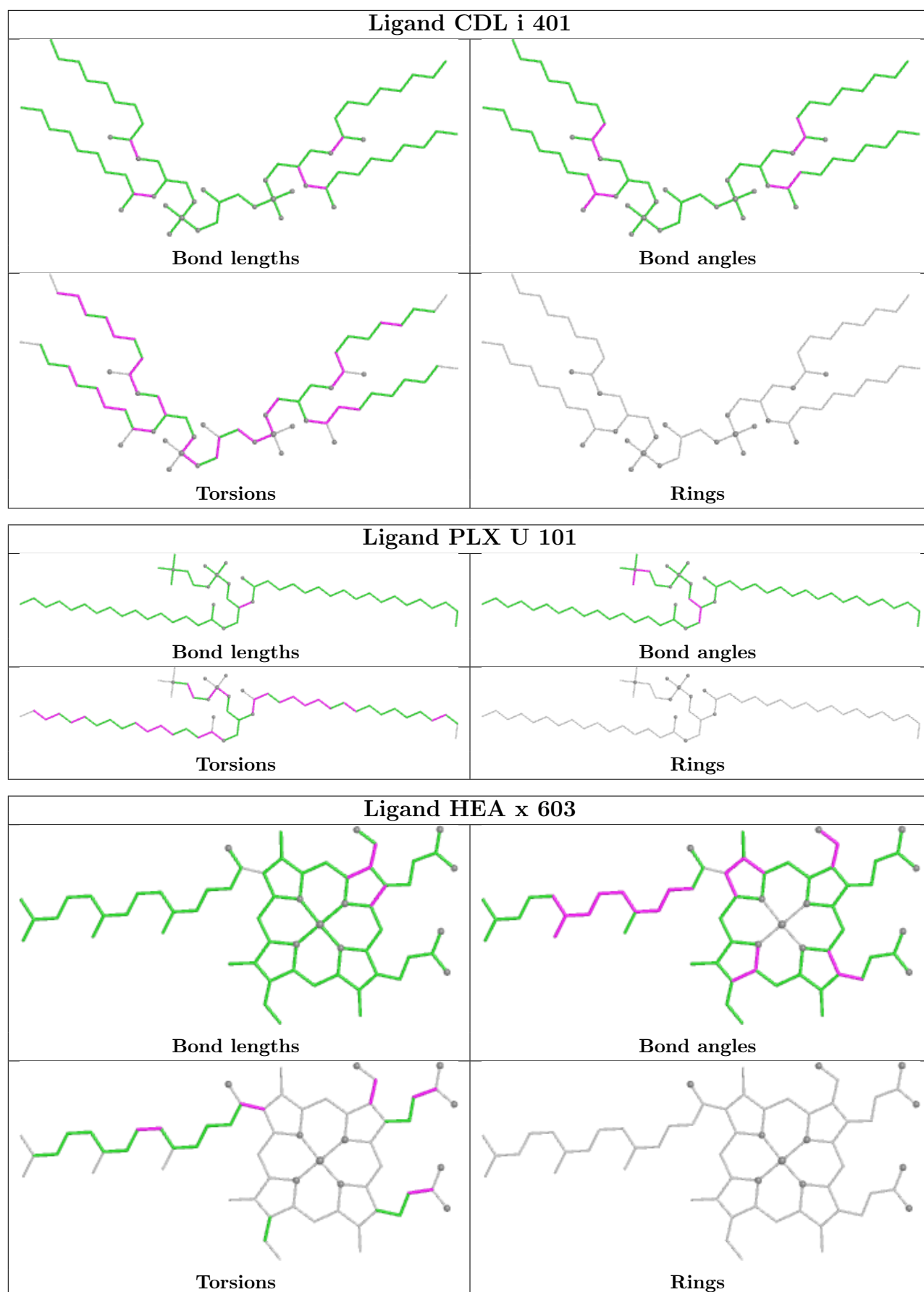
Ligand CDL AU 403

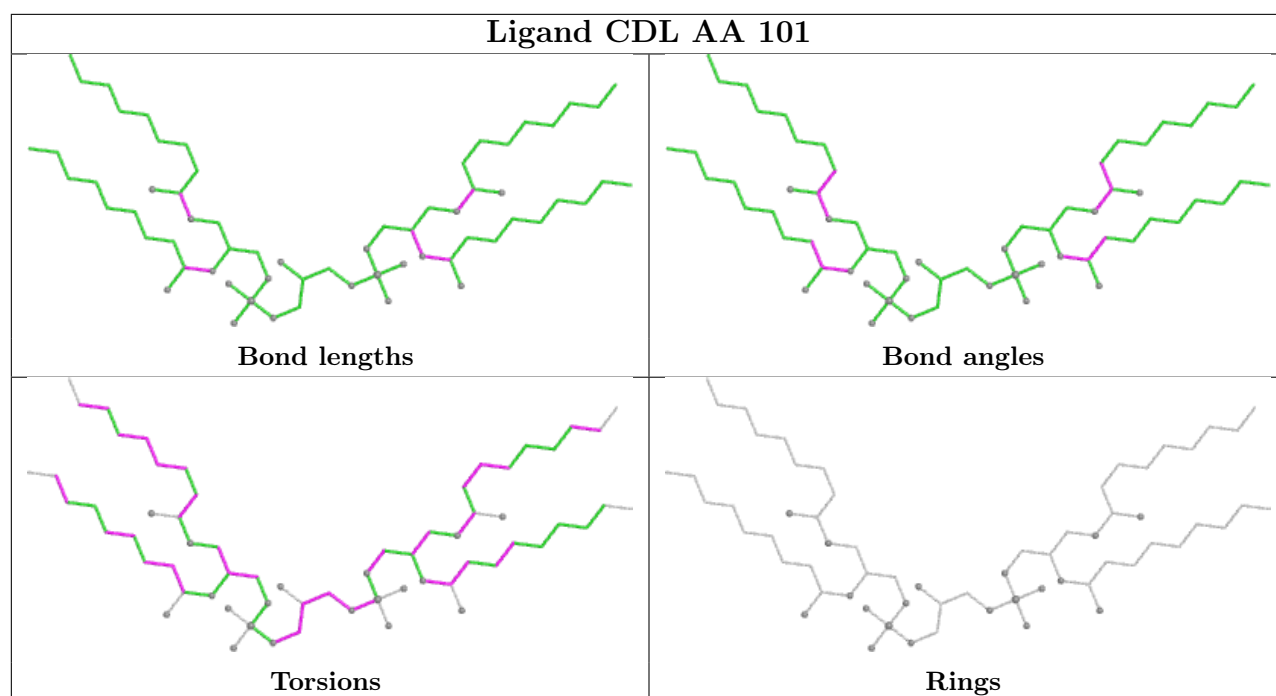




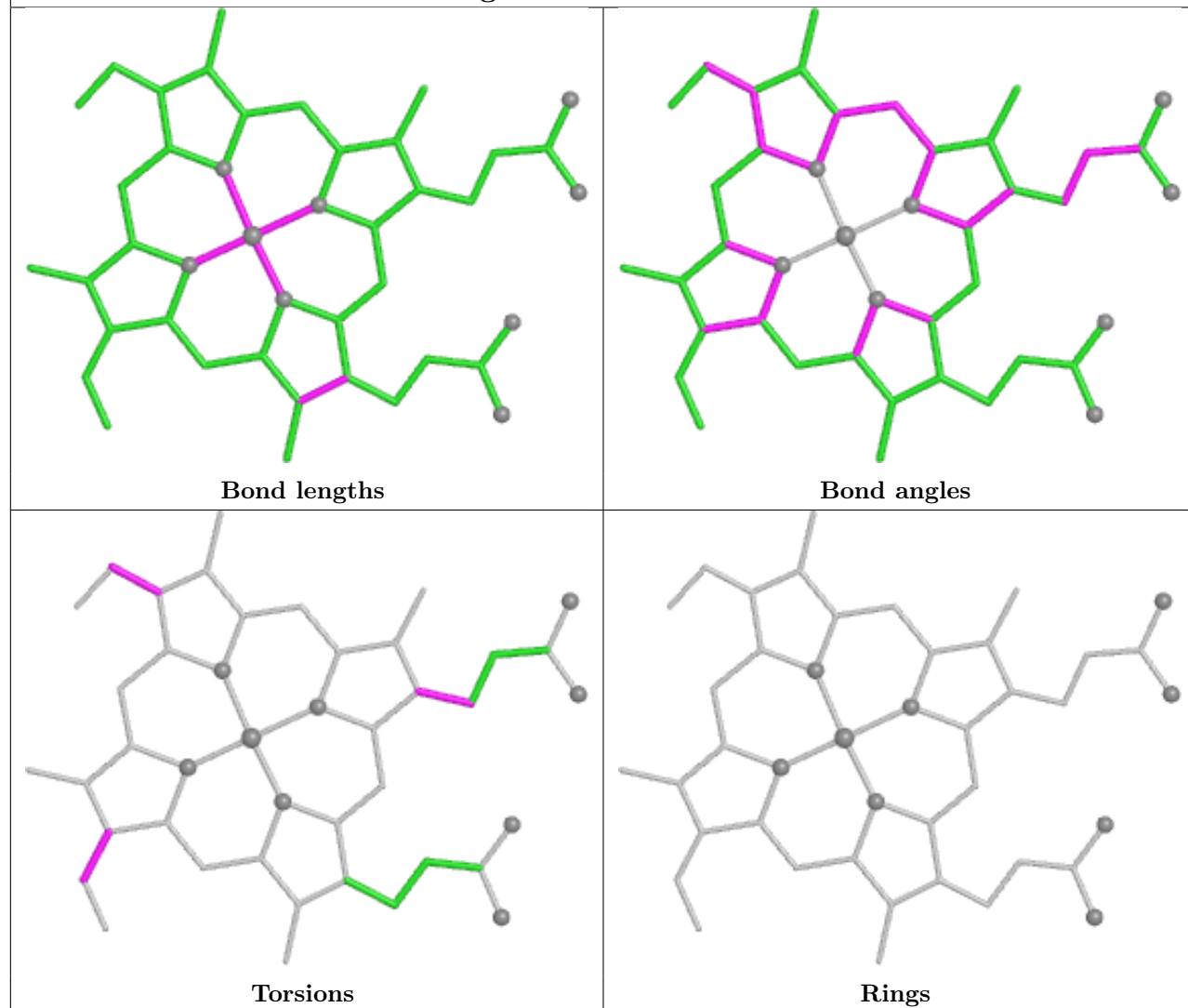




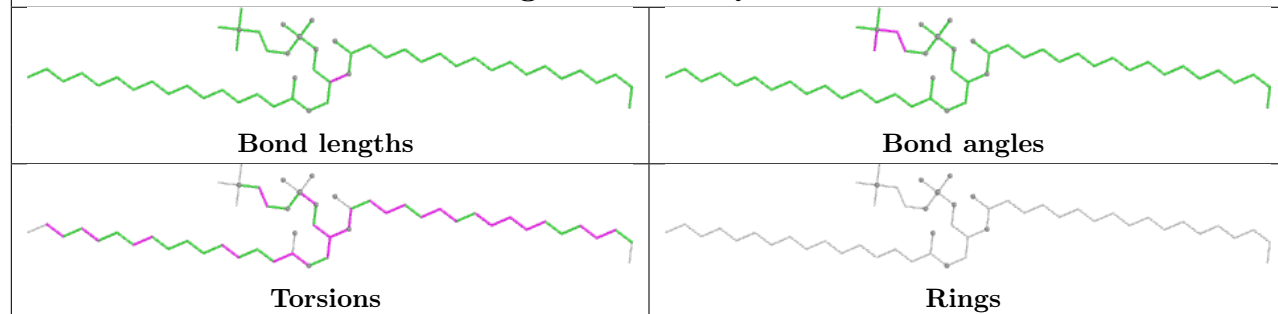


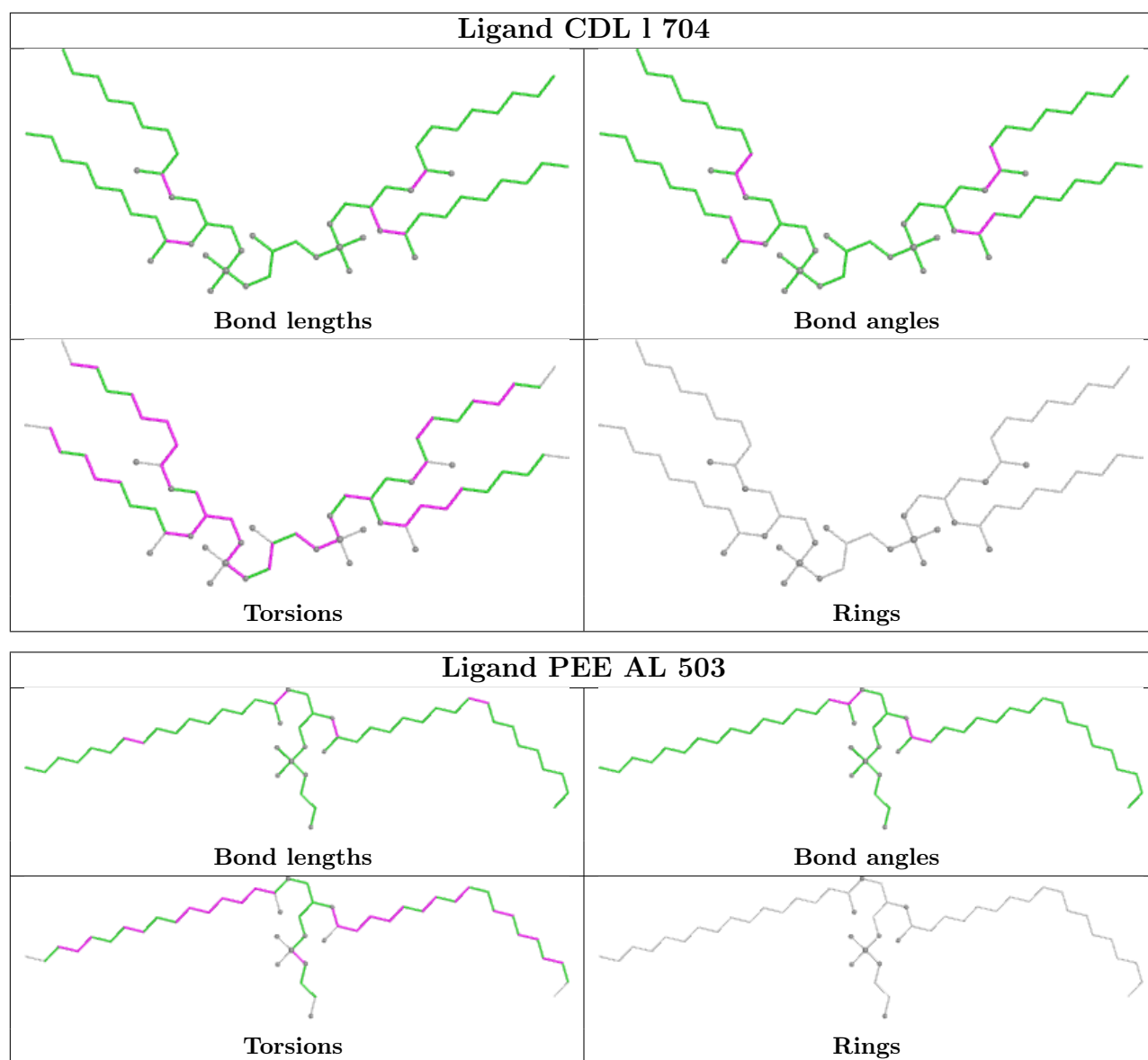


Ligand HEC AH 402

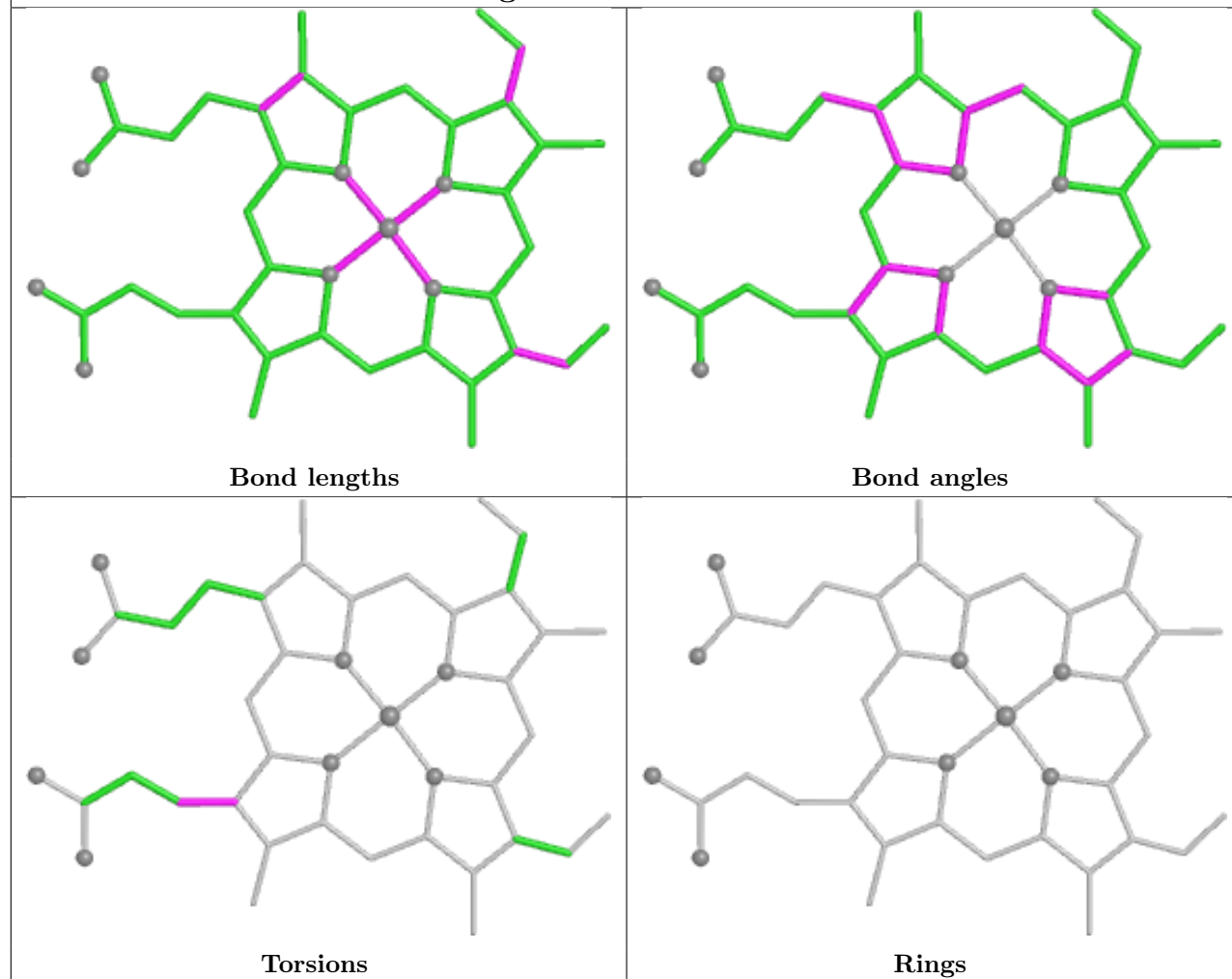


Ligand PLX AQ 101

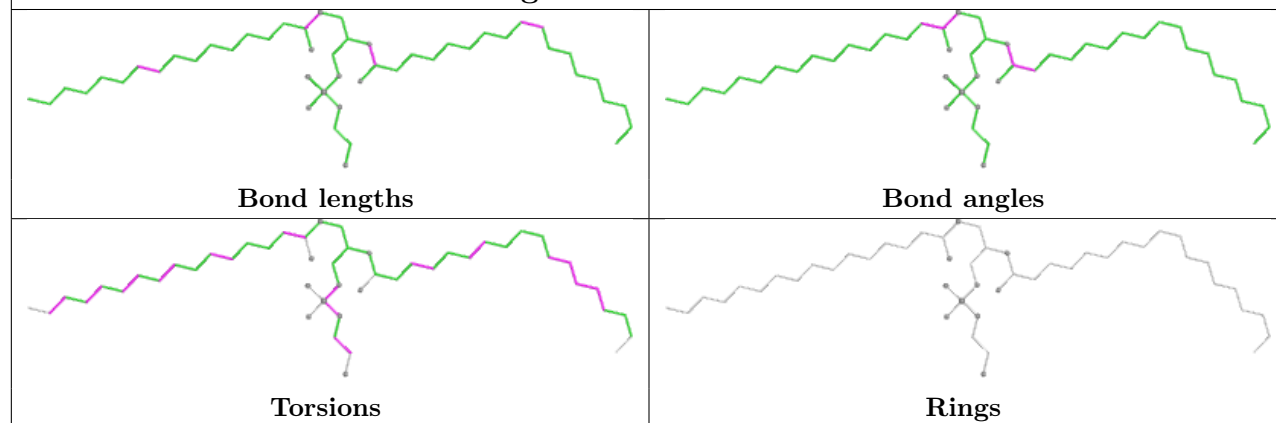




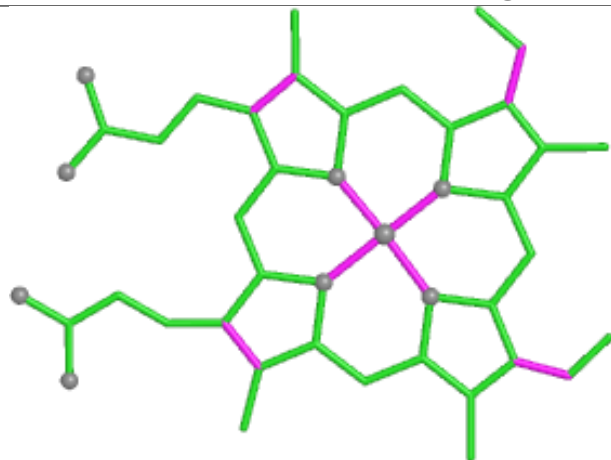
Ligand HEM AJ 402



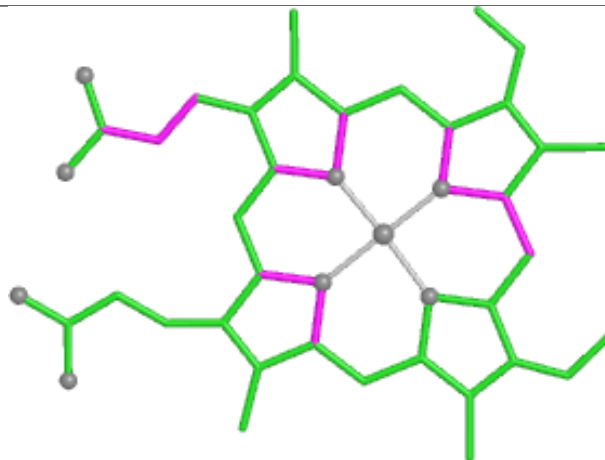
Ligand PEE AY 502



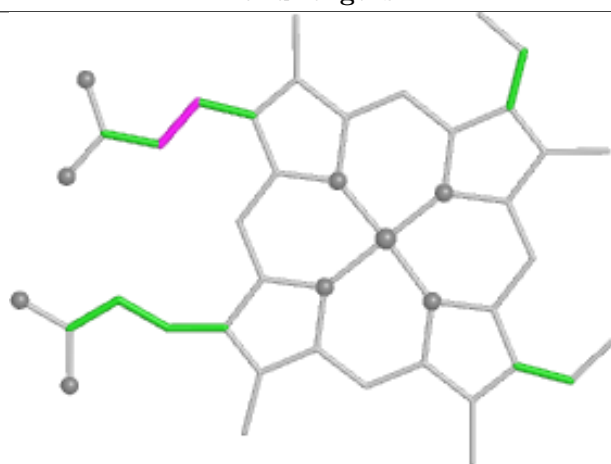
Ligand HEM AJ 401



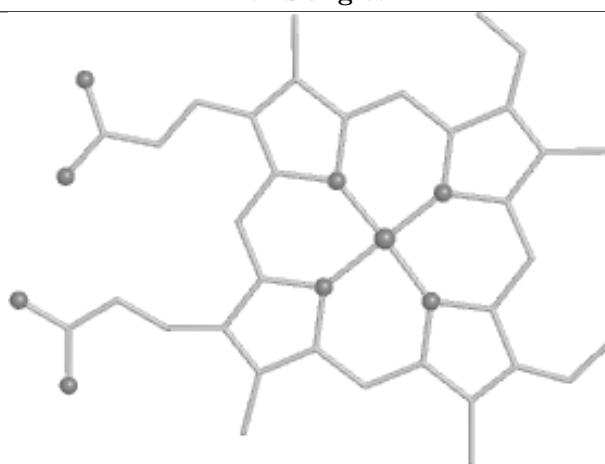
Bond lengths



Bond angles

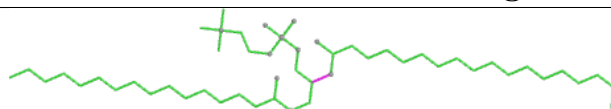


Torsions

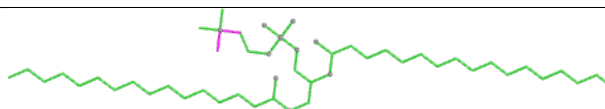


Rings

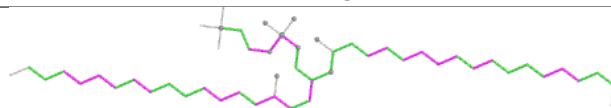
Ligand PLX AT 101



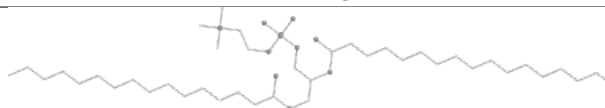
Bond lengths



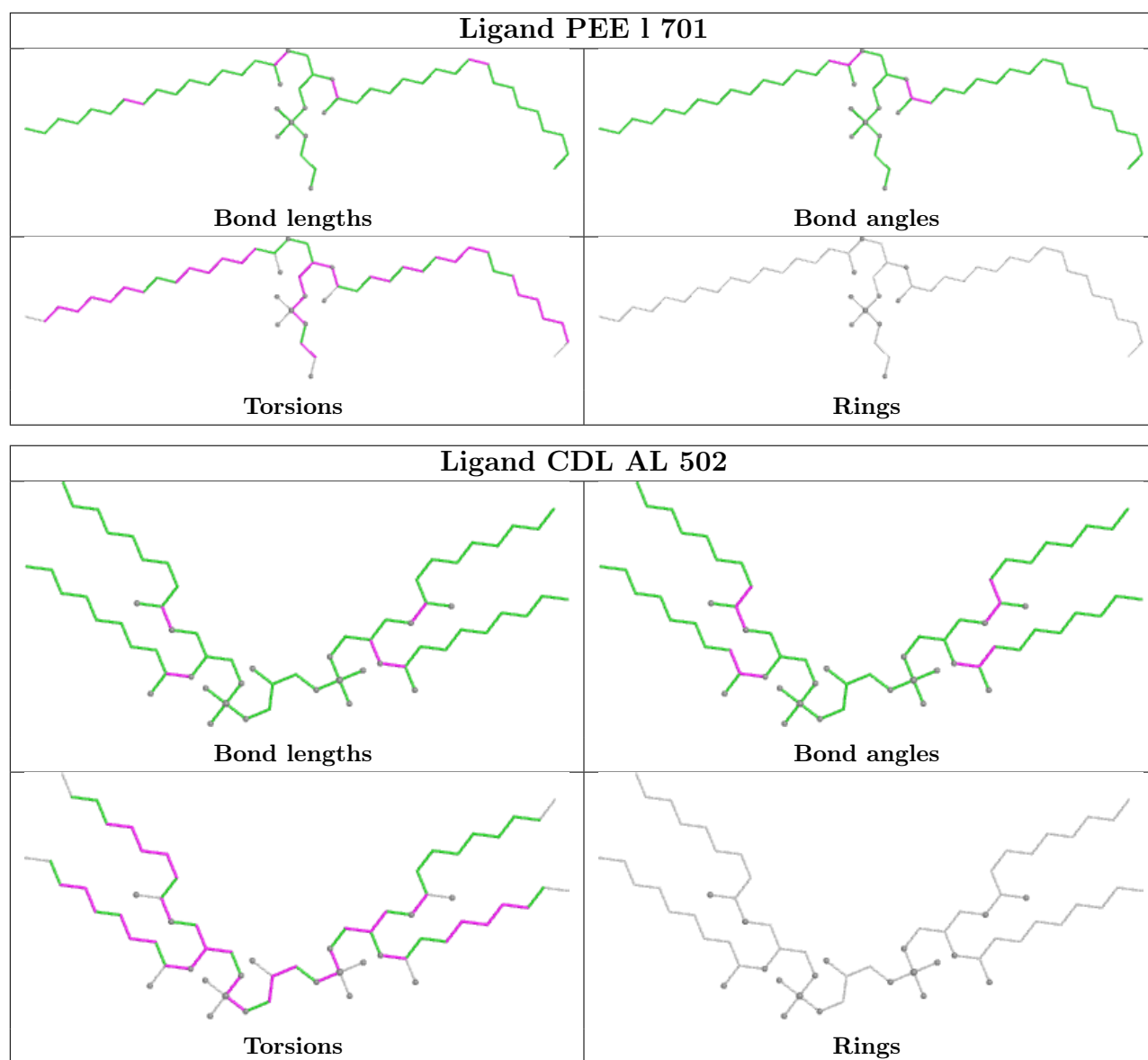
Bond angles

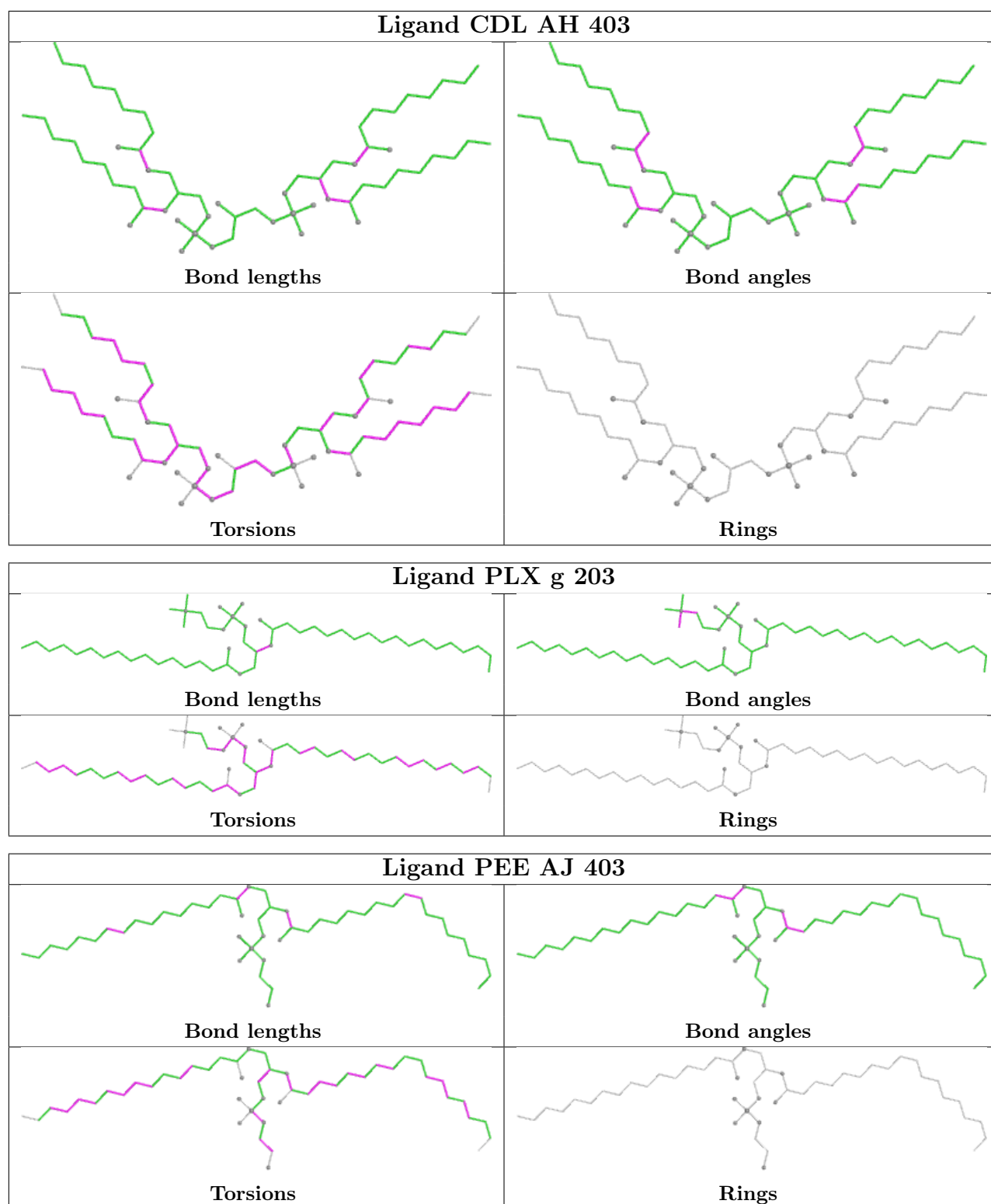


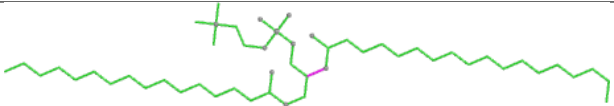
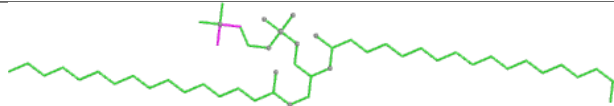
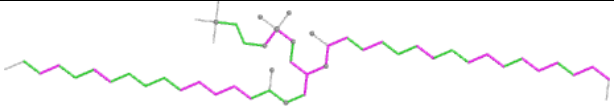
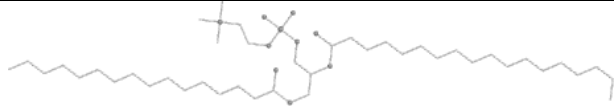
Torsions

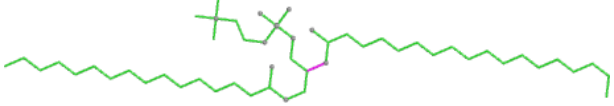
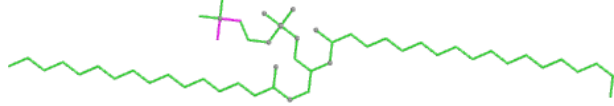
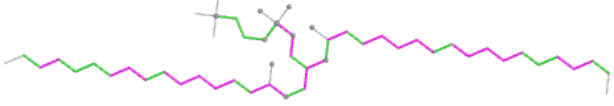
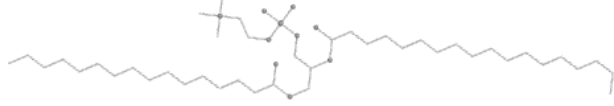


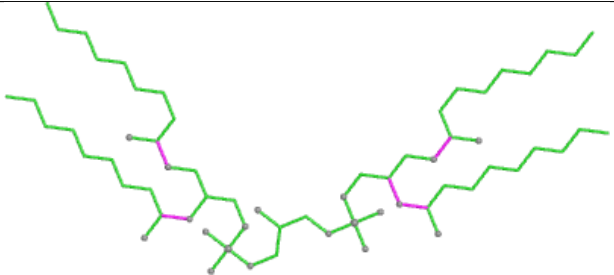
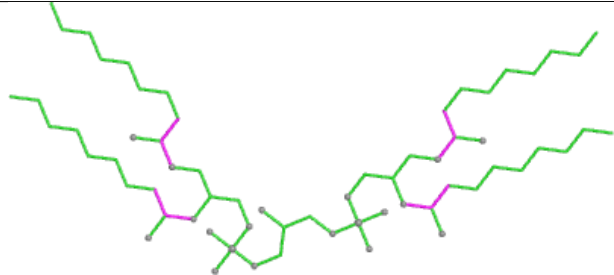
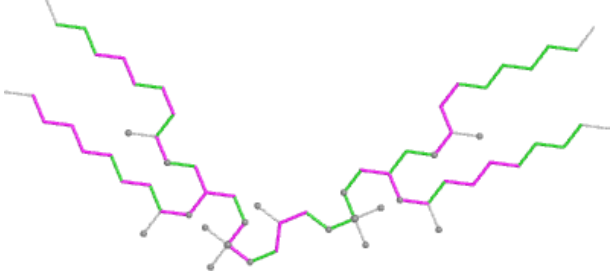
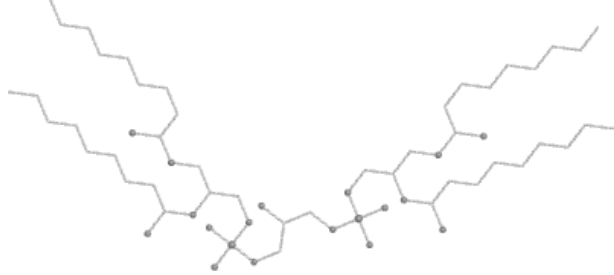
Rings

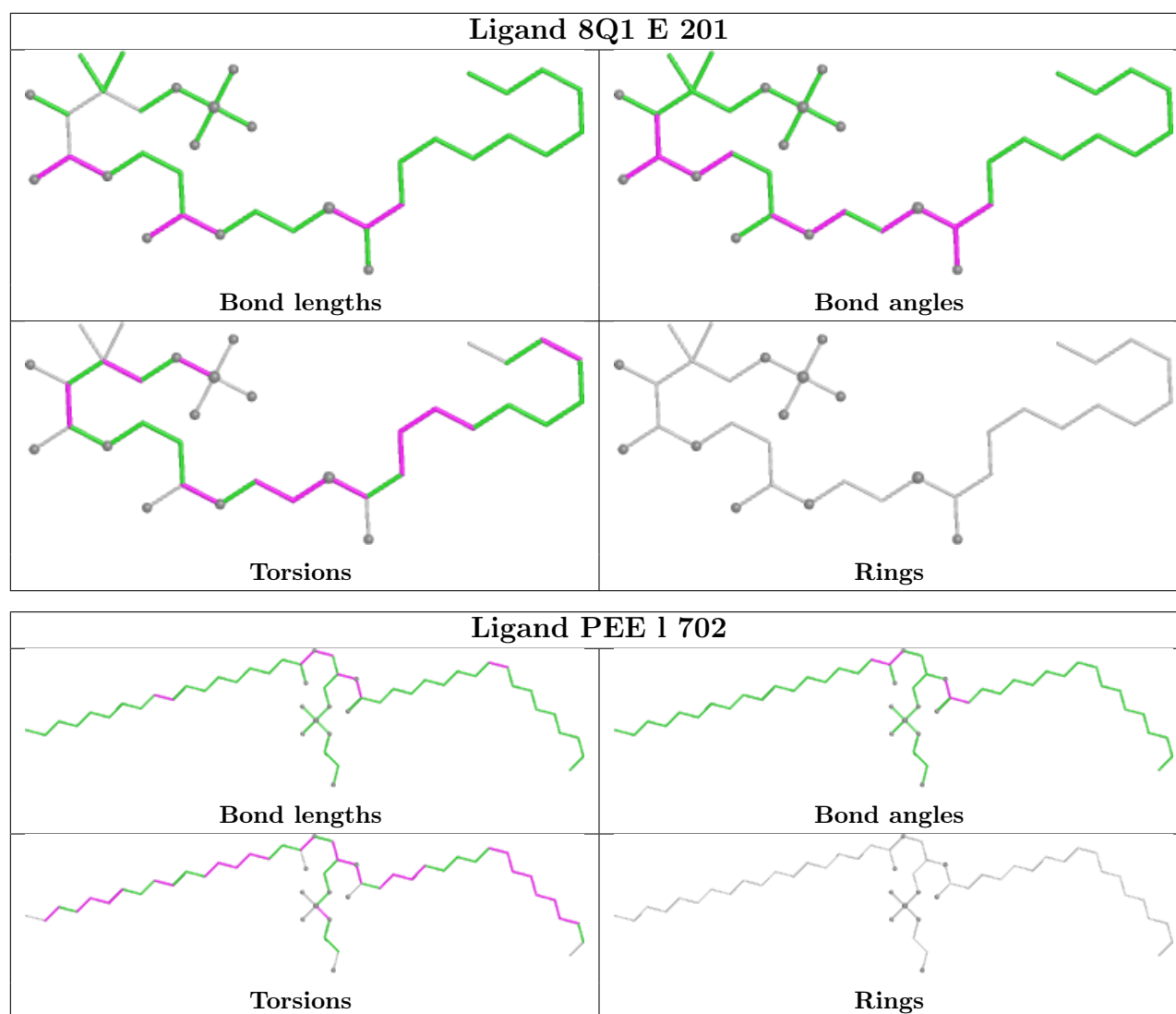




Ligand PLX g 201	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

Ligand PLX r 501	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

Ligand CDL AY 501	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

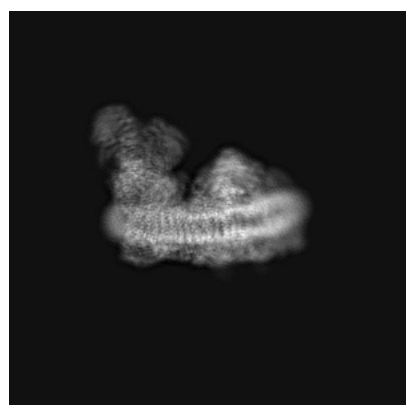
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6775. These allow visual inspection of the internal detail of the map and identification of artifacts.

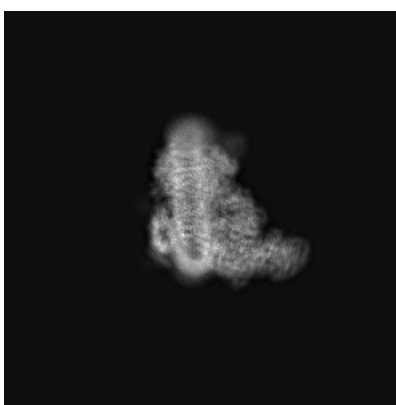
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

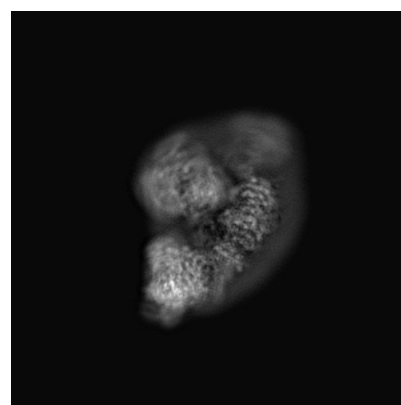
6.1.1 Primary map



X



Y

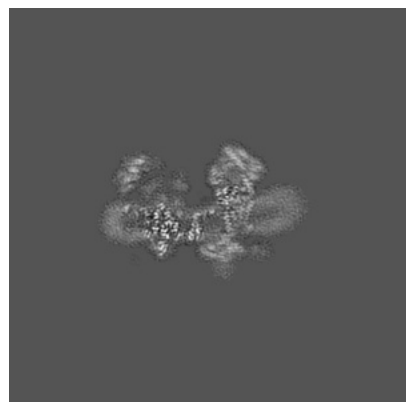


Z

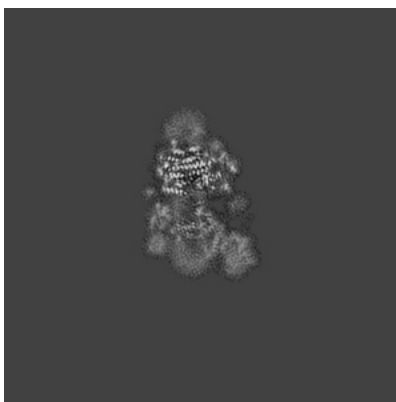
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

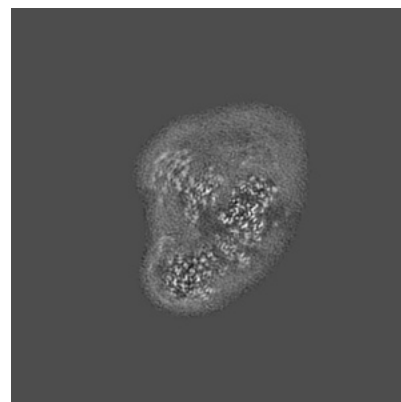
6.2.1 Primary map



X Index: 240



Y Index: 240



Z Index: 240

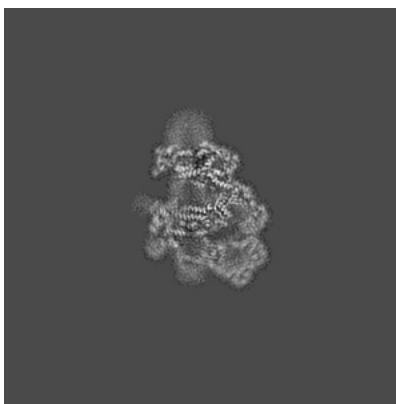
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

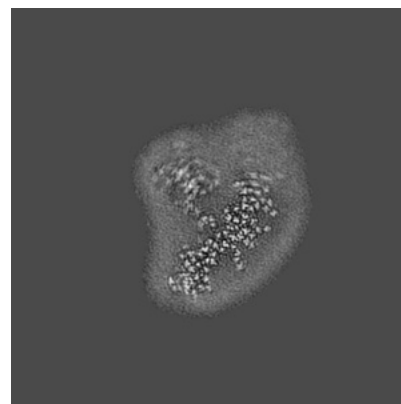
6.3.1 Primary map



X Index: 194



Y Index: 261

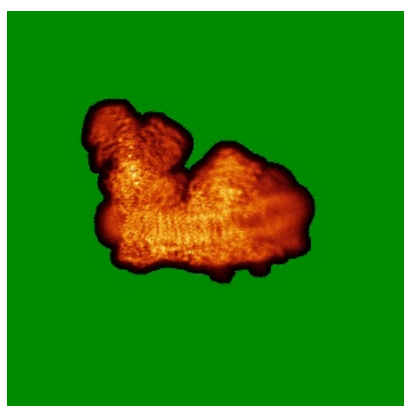


Z Index: 214

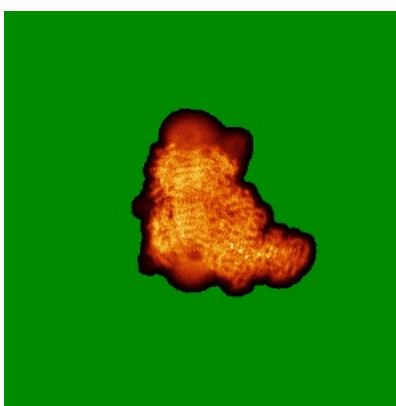
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

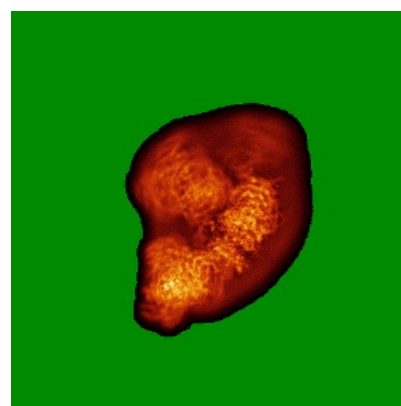
6.4.1 Primary map



X



Y

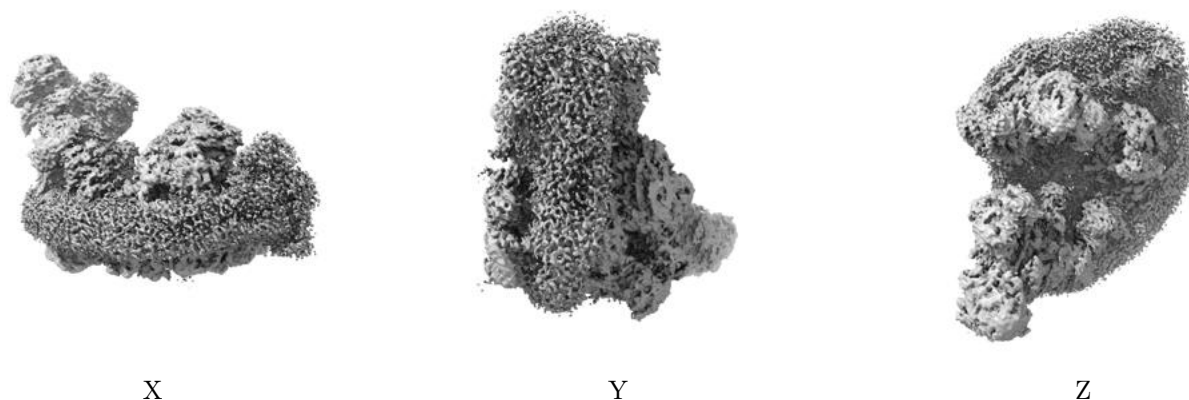


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0354. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

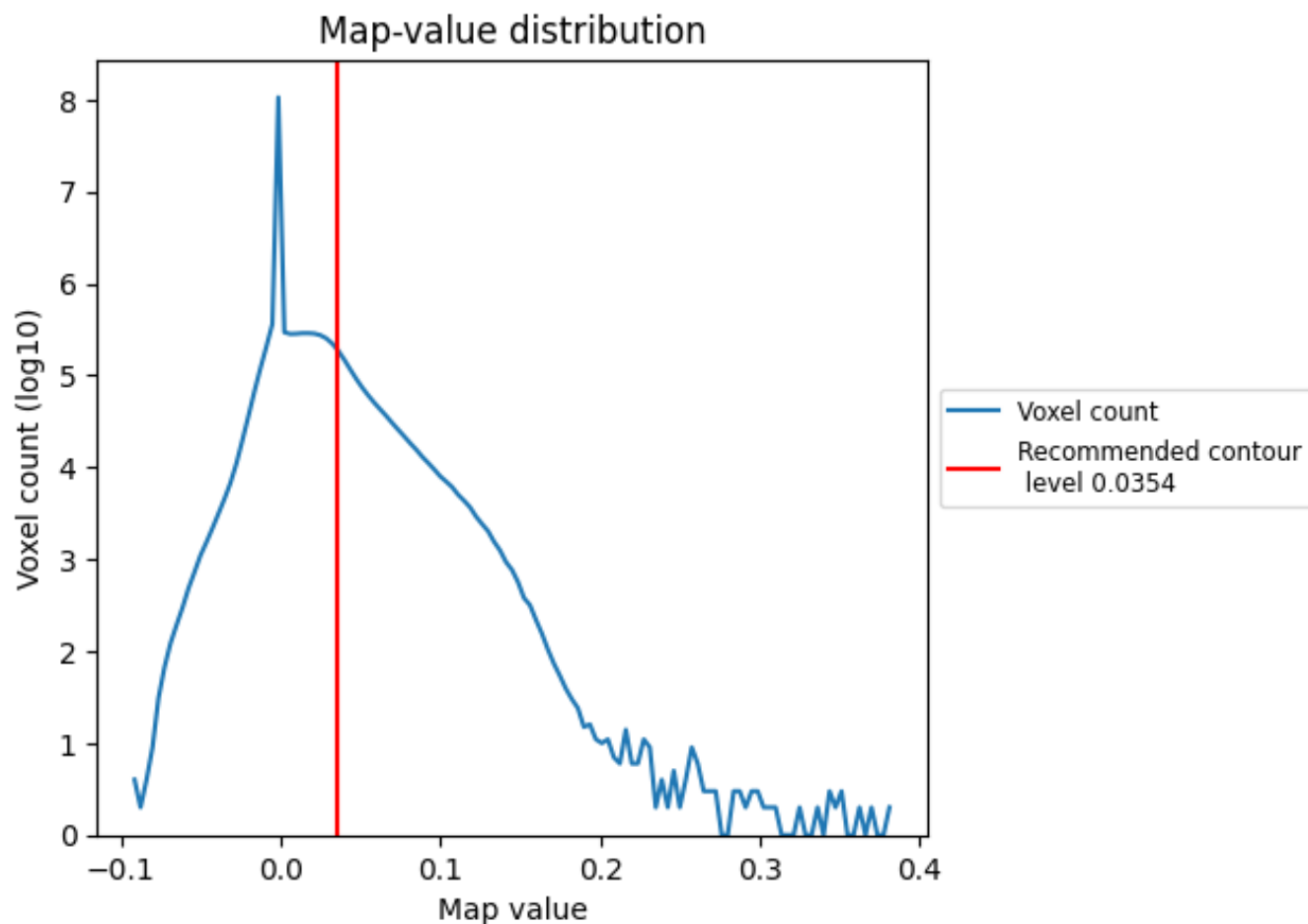
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

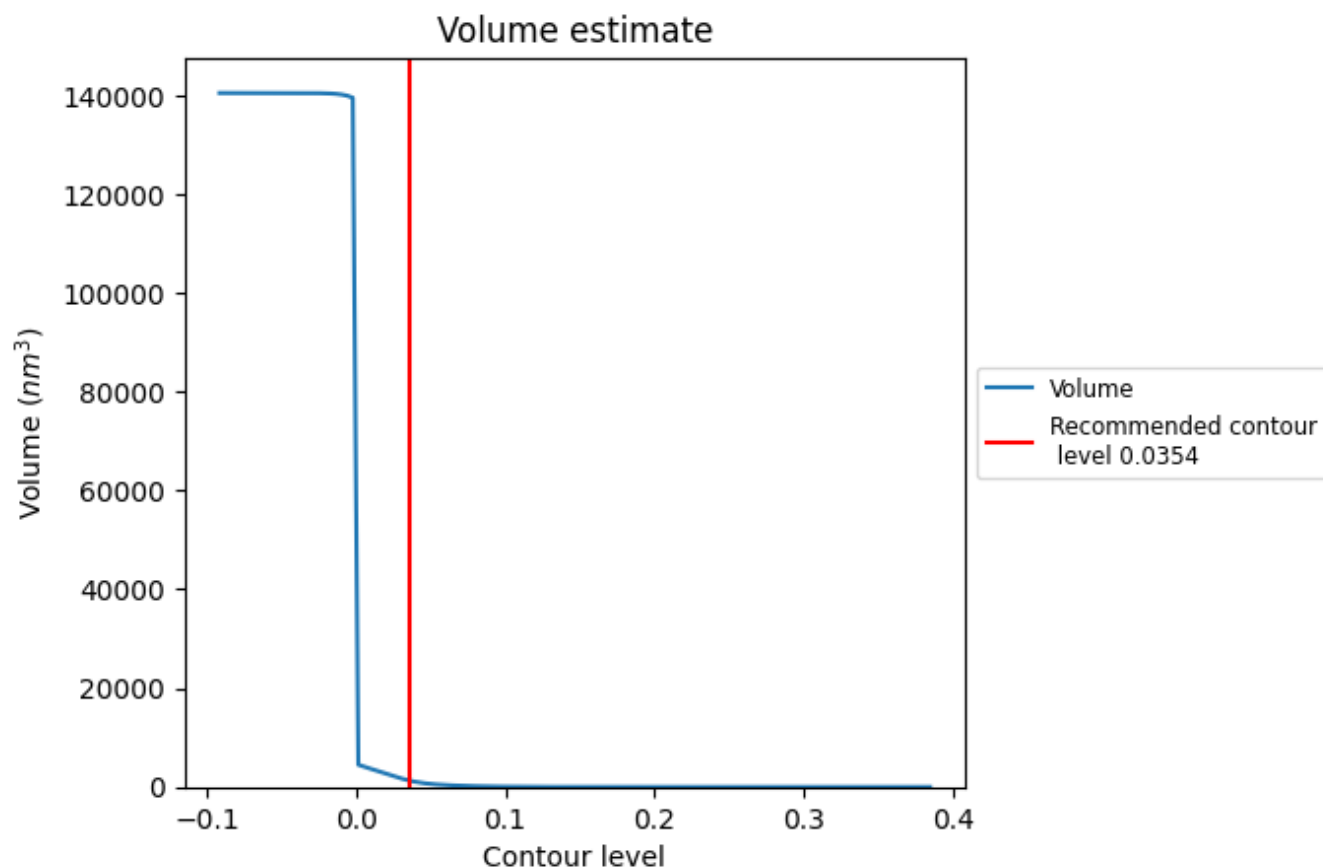
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

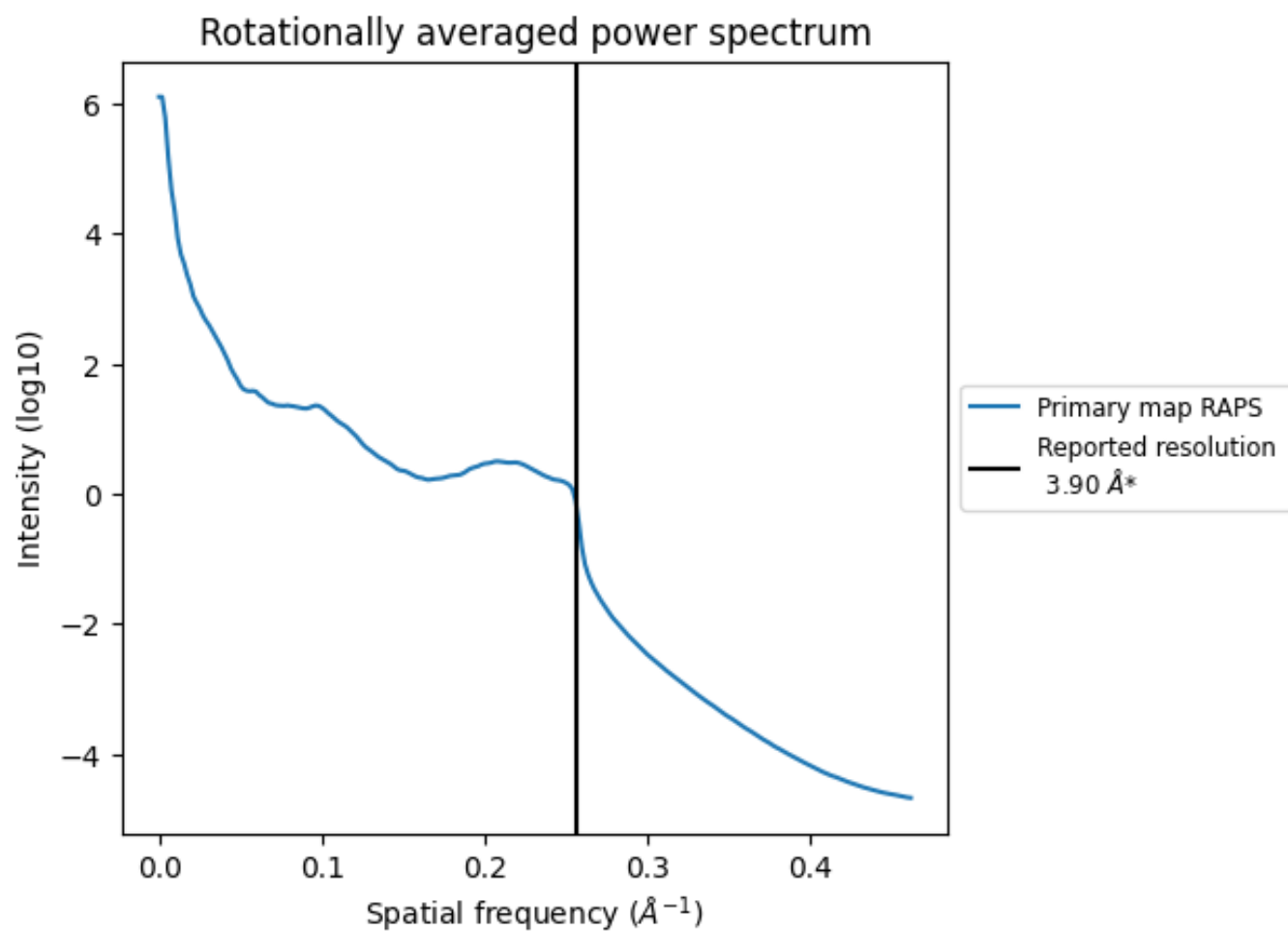
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1319 nm^3 ; this corresponds to an approximate mass of 1191 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

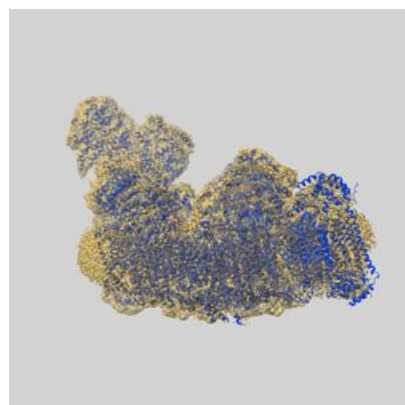
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

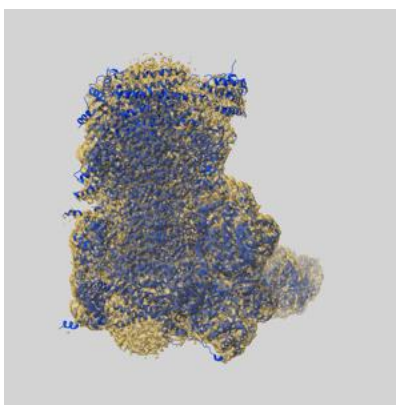
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6775 and PDB model 5XTH. Per-residue inclusion information can be found in section [3](#) on page [27](#).

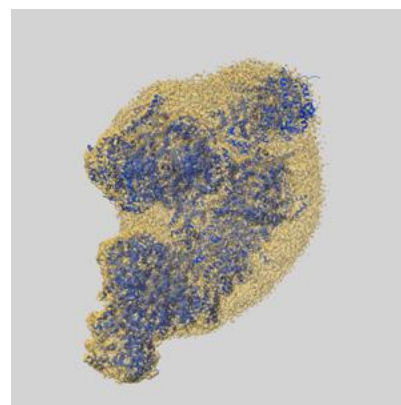
9.1 Map-model overlay [i](#)



X



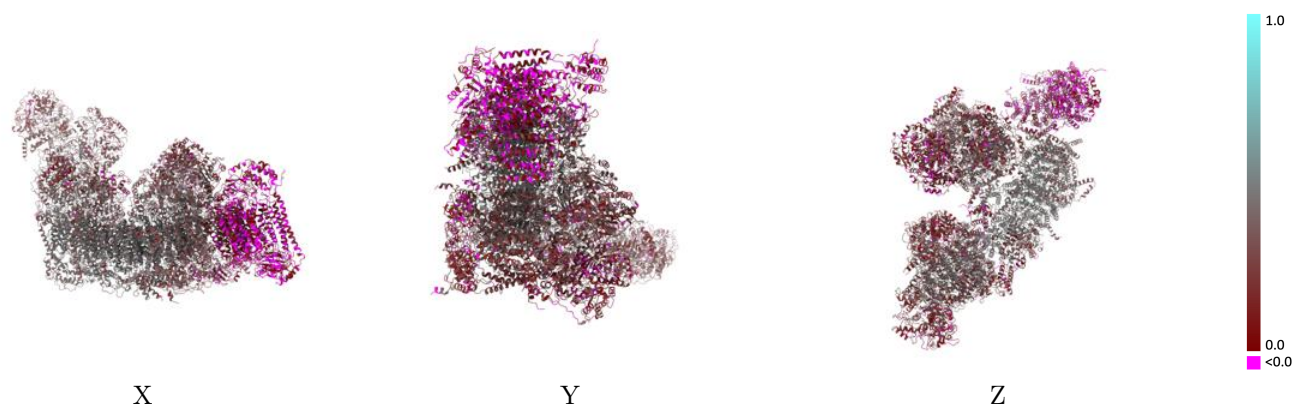
Y



Z

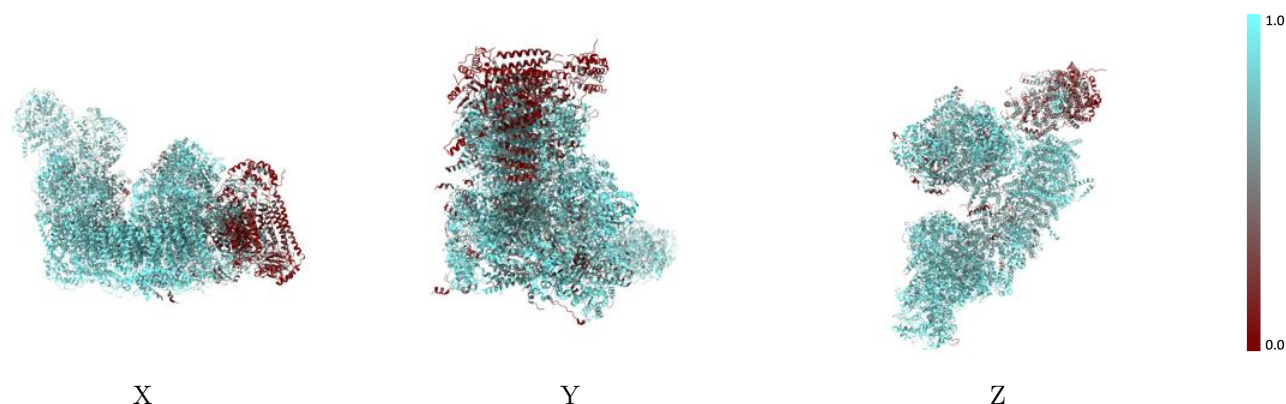
The images above show the 3D surface view of the map at the recommended contour level 0.0354 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



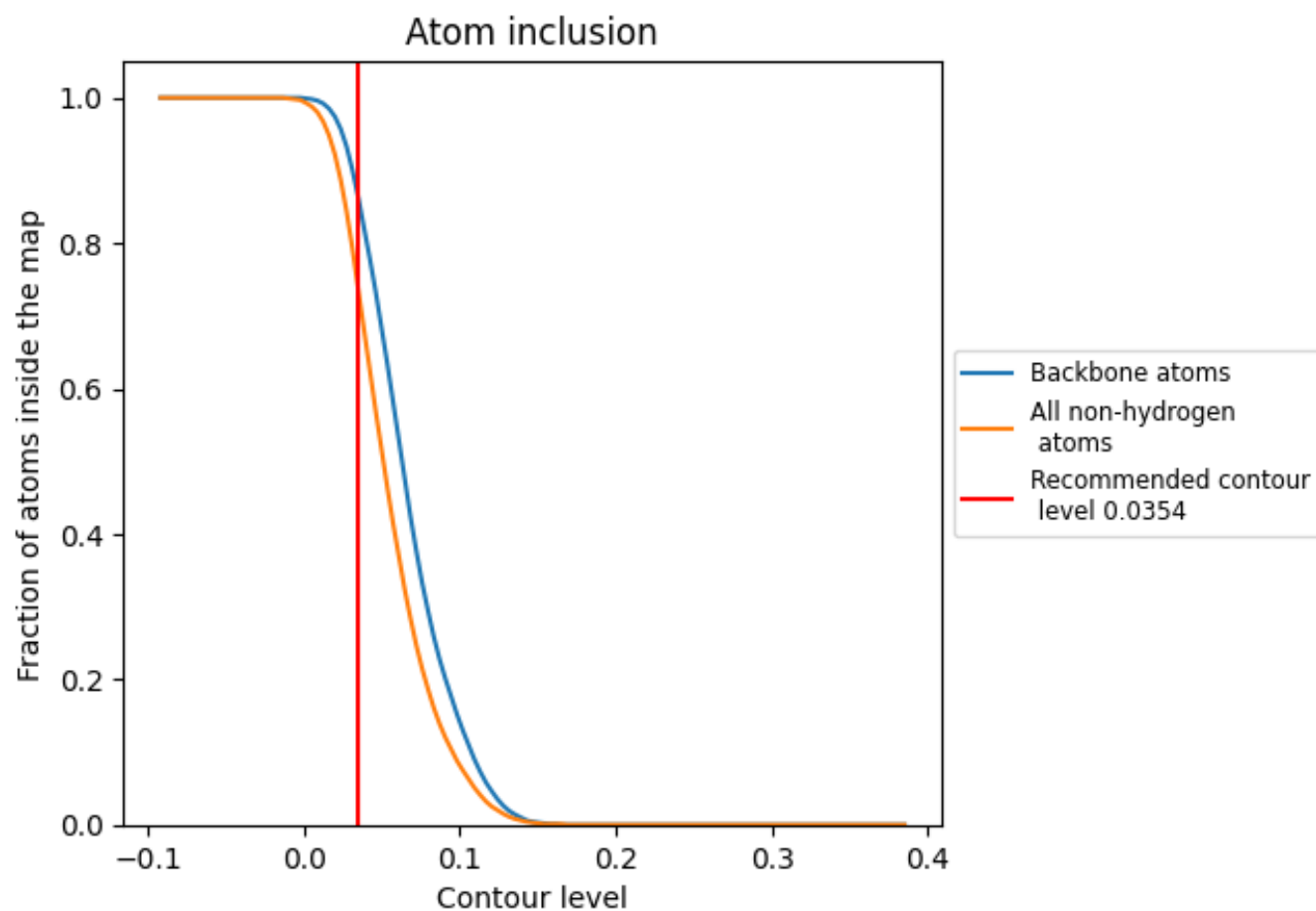
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0354).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0354) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7320	 0.2930
0	 0.1290	 0.0250
1	 0.1760	 0.0530
2	 0.4300	 0.0700
3	 0.2680	 0.0410
4	 0.3500	 0.0370
5	 0.0950	 0.0310
6	 0.3420	 0.0880
7	 0.1040	 0.0240
8	 0.2820	 0.0120
9	 0.1360	 0.0240
A	 0.7830	 0.2470
AA	 0.7190	 0.3250
AB	 0.2280	 0.0740
AC	 0.6510	 0.2070
AD	 0.6410	 0.2820
AE	 0.7310	 0.2250
AF	 0.7020	 0.2830
AG	 0.6360	 0.2600
AH	 0.7730	 0.2990
AJ	 0.7420	 0.3490
AK	 0.8260	 0.2600
AL	 0.7960	 0.3320
AN	 0.6850	 0.1970
AO	 0.1150	 -0.0360
AP	 0.6980	 0.1840
AQ	 0.6500	 0.1980
AR	 0.7170	 0.1870
AS	 0.7790	 0.2640
AT	 0.6440	 0.1700
AU	 0.7820	 0.2360
AV	 0.7580	 0.3070
AW	 0.6950	 0.1790
AY	 0.7270	 0.1890
B	 0.8840	 0.4270



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
C	 0.9010	 0.4360
E	 0.6870	 0.2550
F	 0.7820	 0.1840
G	 0.4550	 0.1620
H	 0.7200	 0.2130
I	 0.7930	 0.3150
J	 0.8070	 0.2950
K	 0.7540	 0.2440
L	 0.7280	 0.3180
M	 0.7950	 0.2910
N	 0.8210	 0.3440
O	 0.8010	 0.2630
P	 0.7980	 0.3200
Q	 0.8200	 0.3830
S	 0.9090	 0.4250
T	 0.7840	 0.3430
U	 0.8790	 0.4120
V	 0.7820	 0.4030
W	 0.8900	 0.4140
X	 0.8660	 0.3870
Y	 0.8900	 0.3530
Z	 0.8520	 0.3550
a	 0.9170	 0.4530
b	 0.8370	 0.3440
c	 0.8960	 0.4430
d	 0.8900	 0.4060
e	 0.8320	 0.4170
f	 0.7970	 0.3270
g	 0.8480	 0.4350
h	 0.8830	 0.4310
i	 0.8500	 0.4610
j	 0.7550	 0.3810
k	 0.7920	 0.4260
l	 0.8170	 0.4190
m	 0.7980	 0.4080
n	 0.8530	 0.3850
o	 0.8560	 0.4240
p	 0.8950	 0.4010
r	 0.8720	 0.4660
s	 0.8480	 0.4340
u	 0.9120	 0.4080
v	 0.8310	 0.3020

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
w	 0.8350	 0.3410
x	 0.3690	 0.0410
y	 0.2580	 0.0090
z	 0.4570	 0.0910