



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 02:23 AM JST

PDB ID : 5GUP / pdb_00005gup
EMDB ID : EMD-9539
Title : Cryo-EM structure of mammalian respiratory supercomplex I1III2IV1
Authors : Gu, J.; Wu, M.; Guo, R.; Yang, M.
Deposited on : 2016-08-30
Resolution : 4.00 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:

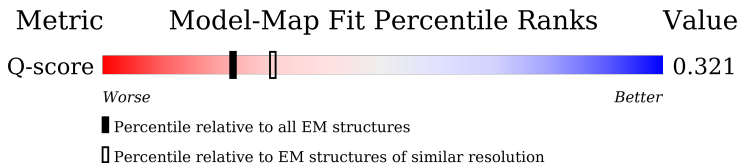
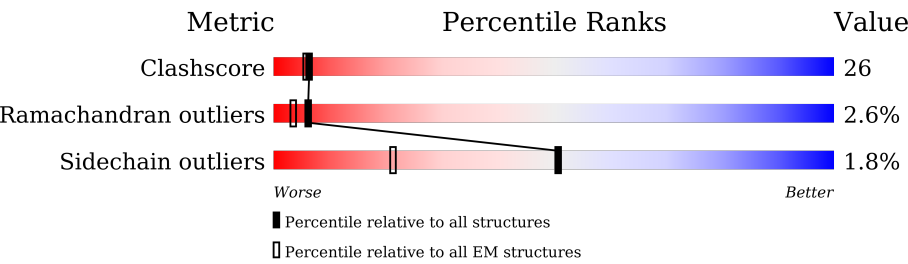
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 4.00 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.



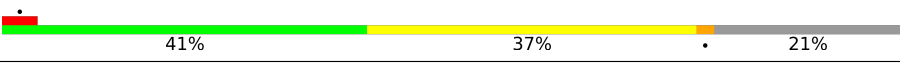
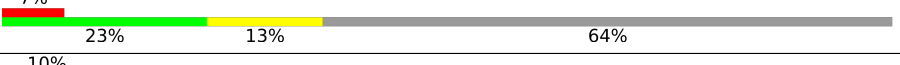
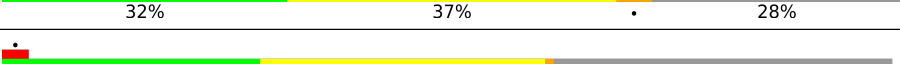
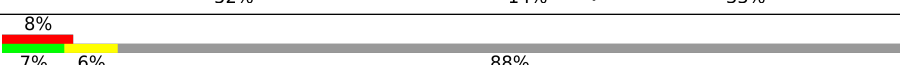
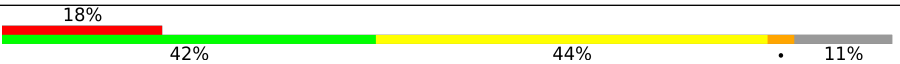
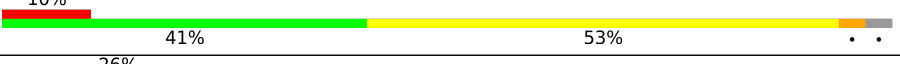
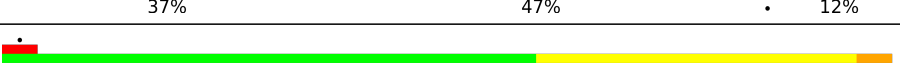
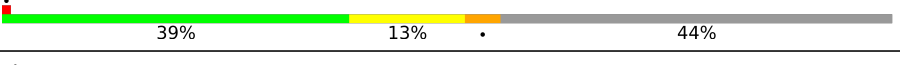
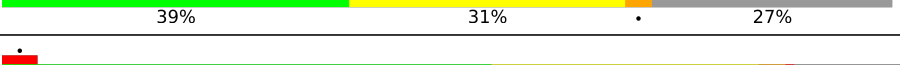
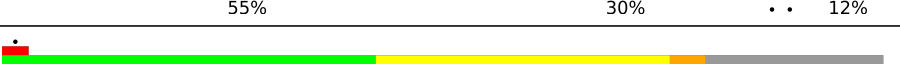
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	73	100% 71%23%5%
2	B	464	9% 42%43%12%
3	C	463	45%46%7%
4	D	264	33%41%5%21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	249	
6	F	123	
7	G	727	
8	H	212	
9	I	216	
10	J	175	
11	K	145	
11	R	145	
12	L	377	
13	M	113	
14	N	116	
15	O	156	
15	X	156	
16	P	99	
17	Q	128	
18	S	70	
19	T	84	
20	U	357	
21	V	141	
22	W	144	
23	Y	105	
24	Z	98	
25	a	189	
26	b	128	
27	c	186	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	d	176	
29	e	154	
30	f	76	
31	g	122	
32	h	106	
33	i	347	
34	j	115	
35	k	98	
36	l	606	
37	m	175	
38	n	58	
39	o	129	
40	p	179	
41	q	459	
42	r	318	
43	s	172	
44	t	137	
45	5	480	
45	u	480	
46	6	453	
46	v	453	
47	7	379	
47	w	379	
48	8	326	
48	x	326	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
49	9	111	
49	y	111	
50	Aa	82	
50	z	82	
51	0	91	
51	Ab	91	
52	1	64	
52	Ac	64	
53	2	274	
53	4	274	
54	3	56	
54	Ad	56	
55	Ae	78	
55	Af	78	
56	Ag	46	
57	Ah	59	
58	Ai	56	
59	Aj	47	
60	Ak	514	
61	Al	227	
62	Am	261	
63	An	147	
64	Ao	109	
65	Ap	98	
66	Aq	84	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
67	Ar	85	84% 54% 29% 5% 12%

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
68	SF4	B	501	-	-	X	-
68	SF4	G	801	-	-	X	-
68	SF4	H	301	-	-	X	-
68	SF4	H	302	-	-	X	-
69	FMN	B	502	-	-	X	-
70	FES	2	303	-	-	X	-
71	PLX	2	301	-	-	X	-
73	ZMP	Q	201	-	-	X	-
75	PEE	2	302	-	-	X	-
75	PEE	7	402	-	-	X	-
75	PEE	u	502	-	-	X	-
75	PEE	w	403	-	-	X	-
77	HEC	8	402	X	-	-	-
77	HEC	x	401	X	-	-	-

2 Entry composition

There are 81 unique types of molecules in this entry. The entry contains 109982 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 Cytochrome c oxidase subunit 6C.

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

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	410	Total	C	N	O	S	0	0
			3128	1975	558	575	20		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	430	Total	C	N	O	S	0	0
			3391	2167	583	617	24		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1679	1088	290	299	2		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	197	Total	C	N	O	S	0	0
			1463	935	246	273	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	44	Total	C	N	O	S	0	0
			242	145	49	47	1		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	673	Total	C	N	O	S	0	0
			5005	3133	875	959	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	176	Total	C	N	O	S	0	0
			1408	884	242	269	13		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	156	Total	C	N	O	S	0	0
			1241	792	227	208	14		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	109	Total	C	N	O	S	0	0
			877	557	154	163	3		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	97	Total	C	N	O		0	0
			520	314	104	102			
11	R	18	Total	C	N	O		0	0
			90	54	18	18			

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	337	Total	C	N	O	S	0	0
			2665	1726	462	468	9		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	94	Total	C	N	O	S	0	0
			685	433	129	121	2		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	112	Total	C	N	O	S	0	0
			895	577	152	163	3		

- Molecule 15 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	85	Total	C	N	O	S	0	0
			647	417	97	128	5		
15	X	85	Total	C	N	O	S	0	0
			663	428	98	132	5		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	83	Total	C	N	O	S	0	0
			673	423	125	123	2		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	112	Total	C	N	O	S	0	0
			942	600	174	163	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	70	Total	C	N	O	S	0	0
			567	364	104	94	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	82	Total	C	N	O	S	0	0
			622	404	104	113	1		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	281	Total	C	N	O	S	0	0
			1941	1228	342	366	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	140	Total	C	N	O	S	0	0
			1009	644	172	187	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	138	Total	C	N	O	S	0	0
			1122	724	193	197	8		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	59	Total	C	N	O	S	0	0
			400	262	70	67	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Z	78	Total	C	N	O	0	0
			550	363	92	95		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	138	Total	C	N	O	S	0	0
			1124	736	190	195	3		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	b	113	Total	C	N	O	0	0
			741	478	137	126		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	148	Total	C	N	O	S	0	0
			1073	696	185	185	7		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	169	Total	C	N	O	S	0	0
			1233	763	233	229	8		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	97	Total	C	N	O	S	0	0
			757	490	127	136	4		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	f	36	Total	C	N	O	0	0
			300	201	51	48		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	121	Total	C	N	O	S	0	0
			996	648	173	169	6		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	104	Total	C	N	O	S	0	0
			798	501	150	141	6		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	347	Total	C	N	O	S	0	0
			2706	1779	419	462	46		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	114	Total	C	N	O	S	0	0
			893	601	130	155	7		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	k	97	Total	C	N	O	S	0	0
			718	473	109	123	13		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	l	606	Total	C	N	O	S	0	0
			4790	3177	742	821	50		

- Molecule 37 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	m	174	Total	C	N	O	S	0	0
			1280	855	187	226	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	n	47	Total	C	N	O	S	0	0
			359	233	66	59	1		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	o	128	Total	C	N	O	S	0	0
			1021	666	179	176			

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	p	171	Total	C	N	O	S	0	0
			1415	904	263	240	8		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	q	459	Total	C	N	O	S	0	0
			3627	2408	572	609	38		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	169	Total	C	N	O	S	0	0
			1350	858	247	235	10		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	115	Total	C	N	O	S	0	0
			749	463	151	130	5		

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	u	446	Total	C	N	O	S	0	0
			3452	2157	603	673	19		
45	5	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	v	418	Total	C	N	O	S	0	0
			3127	1956	556	606	9		
46	6	418	Total	C	N	O	S	0	0
			3127	1956	556	606	9		

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	w	378	Total	C	N	O	S	0	0
			3017	2026	470	501	20		
47	7	378	Total	C	N	O	S	0	0
			3017	2026	470	501	20		

- Molecule 48 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	x	241	Total	C	N	O	S	0	0
			1918	1223	330	350	15		
48	8	241	Total	C	N	O	S	0	0
			1918	1223	330	350	15		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	y	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
49	9	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	z	79	Total	C	N	O	S	0	0
			666	434	122	108	2		
50	Aa	80	Total	C	N	O	S	0	0
			679	442	124	111	2		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	0	64	Total	C	N	O	S	0	0
			528	320	97	106	5		
51	Ab	64	Total	C	N	O	S	0	0
			528	320	97	106	5		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	62	Total	C	N	O	S	0	0
			507	331	90	86			
52	Ac	62	Total	C	N	O	S	0	0
			507	331	90	86			

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	196	Total	C	N	O	S	0	0
			1517	954	265	291	7		
53	4	196	Total	C	N	O	S	0	0
			1517	954	265	291	7		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	51	Total	C	N	O	S	0	0
			414	277	74	63			
54	Ad	49	Total	C	N	O	S	0	0
			395	262	71	61	1		

- Molecule 55 is a protein called Cytochrome b-c1 complex subunit Rieske transit peptide, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Ae	57	Total	C	N	O	S	0	0
			394	243	74	75	2		
55	Af	57	Total	C	N	O	S	0	0
			389	240	71	76	2		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

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

- Molecule 57 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Ah	56	Total	C	N	O	S	0	0
			431	277	73	78	3		

- Molecule 58 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

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

- Molecule 59 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

- Molecule 60 is a protein called Cytochrome c oxidase subunit 1.

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

- Molecule 61 is a protein called Cytochrome c oxidase subunit 2.

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

- Molecule 62 is a protein called Cytochrome c oxidase subunit 3.

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

- Molecule 63 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

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

- Molecule 64 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

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

- Molecule 65 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

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

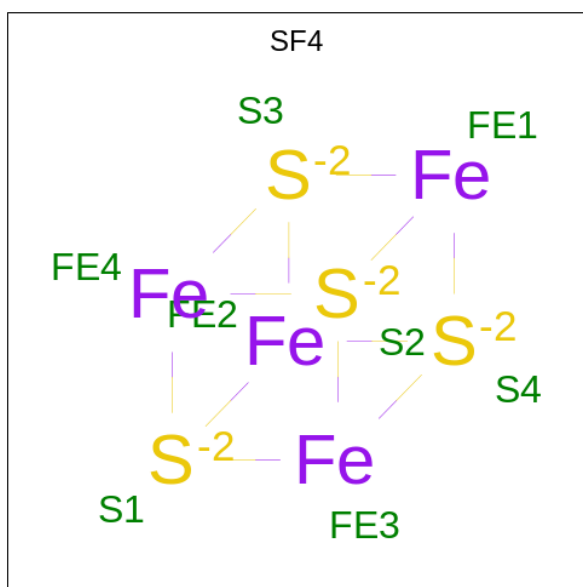
- Molecule 66 is a protein called Cytochrome c oxidase subunit 6A, mitochondrial.

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

- Molecule 67 is a protein called Cytochrome c oxidase subunit 6B1.

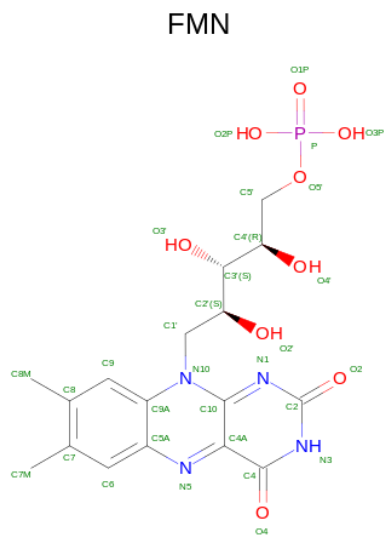
Mol	Chain	Residues	Atoms					AltConf	Trace
67	Ar	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 68 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



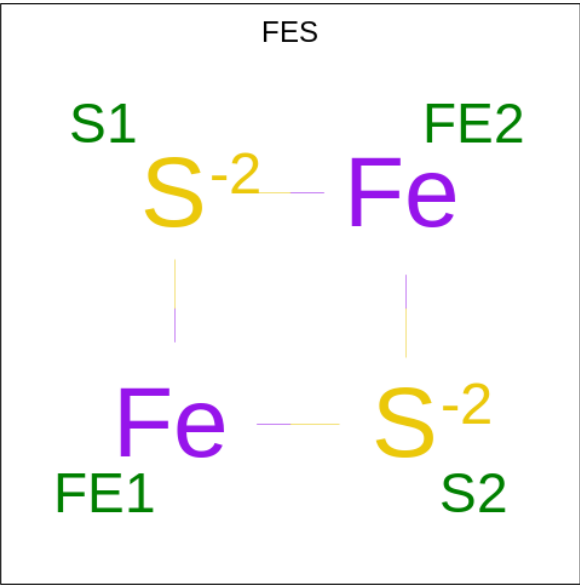
Mol	Chain	Residues	Atoms			AltConf
68	B	1	Total	Fe	S	0
			8	4	4	
68	G	1	Total	Fe	S	
			8	4	4	
68	G	1	Total	Fe	S	
			8	4	4	
68	H	1	Total	Fe	S	0
			8	4	4	
68	H	1	Total	Fe	S	0
			8	4	4	
68	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 69 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 70 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



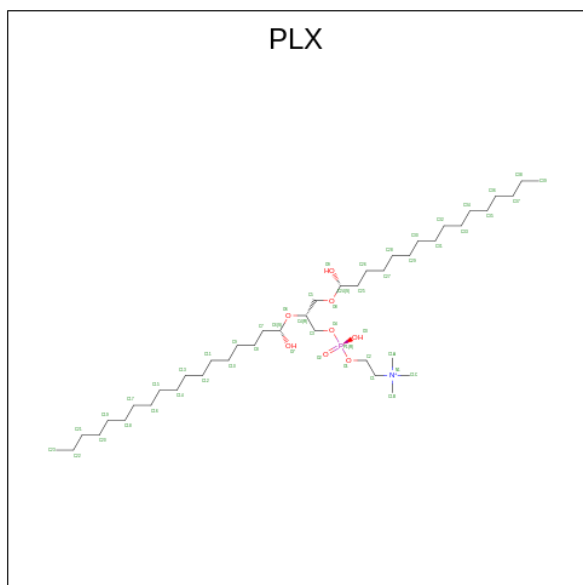
Mol	Chain	Residues	Atoms			AltConf
70	E	1	Total 4	Fe 2	S 2	0
70	G	1	Total 4	Fe 2	S 2	0
70	2	1	Total 4	Fe 2	S 2	0

Continued on next page...

Continued from previous page...

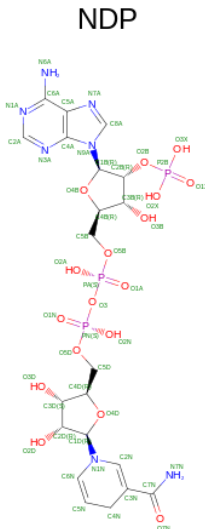
Mol	Chain	Residues	Atoms			AltConf
70	4	1	Total	Fe	S	0
			4	2	2	

- 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).



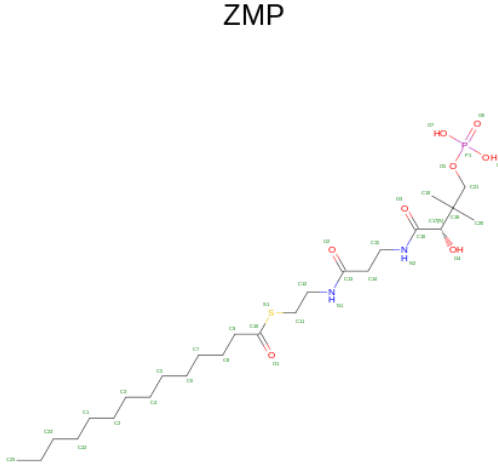
Mol	Chain	Residues	Atoms					AltConf
71	H	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	V	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	i	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	2	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	4	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 72 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



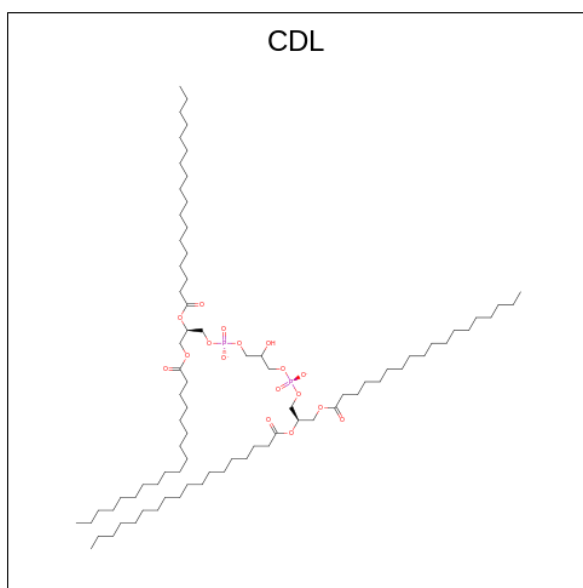
Mol	Chain	Residues	Atoms					AltConf
72	L	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 73 is S-[2-($\{N-[(2S)-2\text{-hydroxy-}3,3\text{-dimethyl-}4\text{-(phosphonooxy)butanoyl]-}\beta\text{-alaninyl}\}$ amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



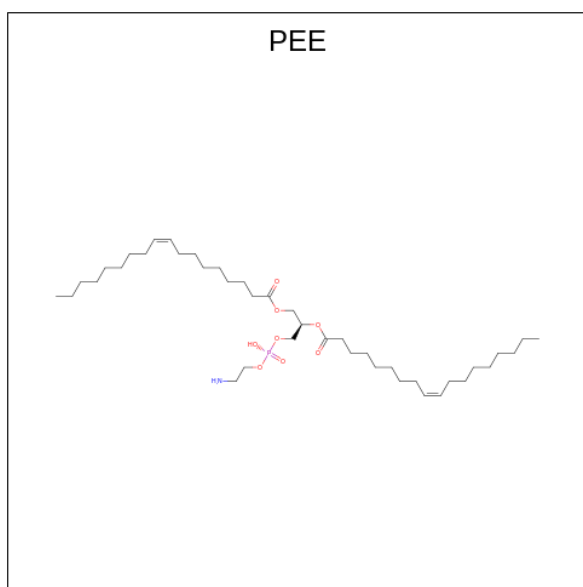
Mol	Chain	Residues	Atoms						AltConf
73	Q	1	Total 34	C 23	N 2	O 7	P 1	S 1	0
73	X	1	Total 34	C 23	N 2	O 7	P 1	S 1	0

- Molecule 74 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



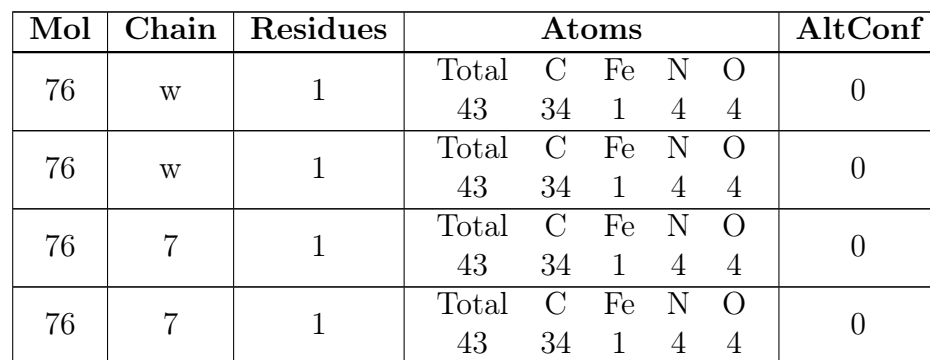
Mol	Chain	Residues	Atoms				AltConf
74	V	1	Total	C	O	P	0
			63	44	17	2	
74	i	1	Total	C	O	P	0
			64	45	17	2	
74	l	1	Total	C	O	P	0
			64	45	17	2	
74	s	1	Total	C	O	P	0
			64	45	17	2	
74	u	1	Total	C	O	P	0
			64	45	17	2	
74	x	1	Total	C	O	P	0
			64	45	17	2	
74	z	1	Total	C	O	P	0
			64	45	17	2	
74	5	1	Total	C	O	P	0
			64	45	17	2	
74	8	1	Total	C	O	P	0
			64	45	17	2	
74	Aa	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 75 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
75	W	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	i	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	l	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	q	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	u	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	w	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	2	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	5	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	7	1	Total	C	N	O	P	0
			41	31	1	8	1	
75	7	1	Total	C	N	O	P	0
			49	39	1	8	1	

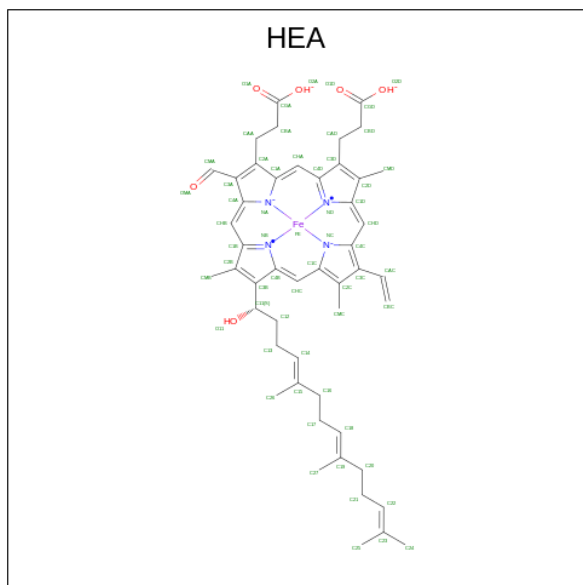
- Molecule 76 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



- # HEC
-
- The chemical structure of HEC (Hexaethylchlorin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with various side chains: CMC, CAC, CBC, CBB, CMB, CHB, CMA, CAA, CBA, CAD, CBD, CGD, CGA, and CBA. Two carboxylic acid groups are attached to the ring, labeled HO-C(=O)-O1D and HO-C(=O)-O1A. The structure is labeled HEC at the top.

Mol	Chain	Residues	Atoms					AltConf
77	x	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
77	8	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 78 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

- Molecule 79 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
79	Ak	1	Total	Cu	0
			1	1	
79	Al	2	Total	Cu	0
			2	2	

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	Ak	1	Total	Mg	0
			1	1	

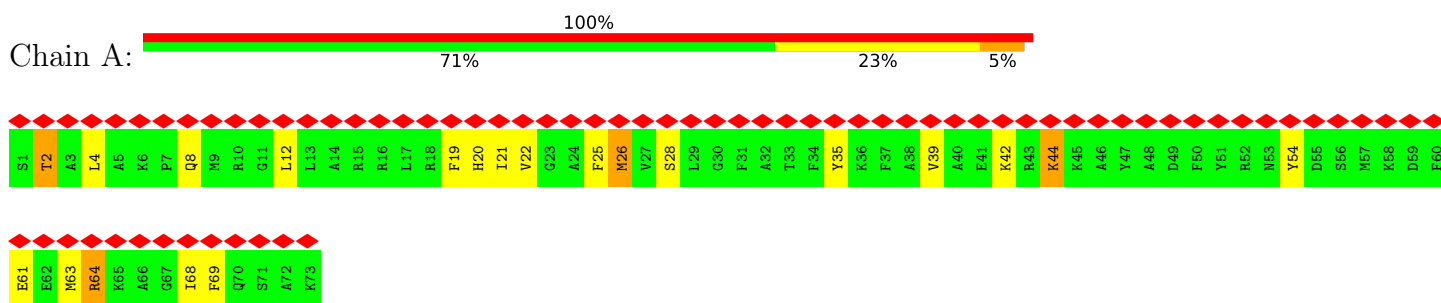
- Molecule 81 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
81	Ap	1	Total	Zn	0
			1	1	

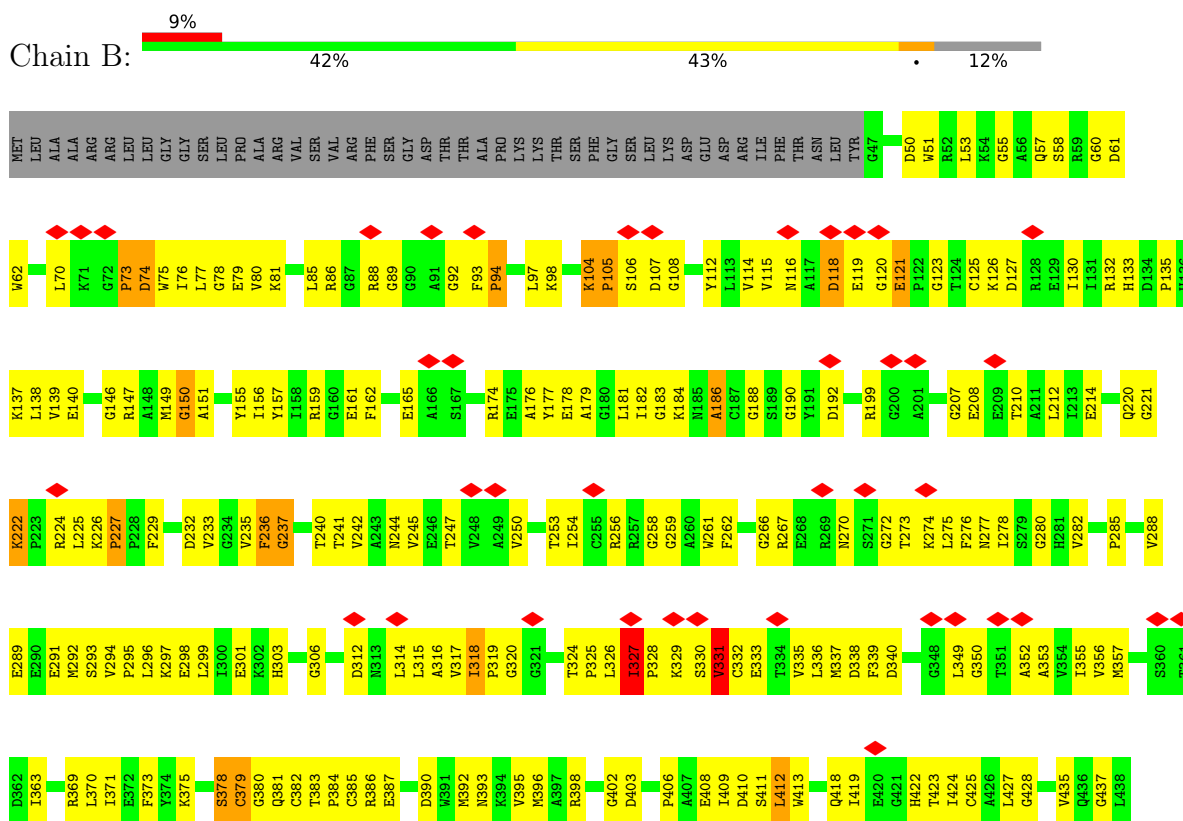
3 Residue-property plots

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: Cytochrome c oxidase subunit 6C

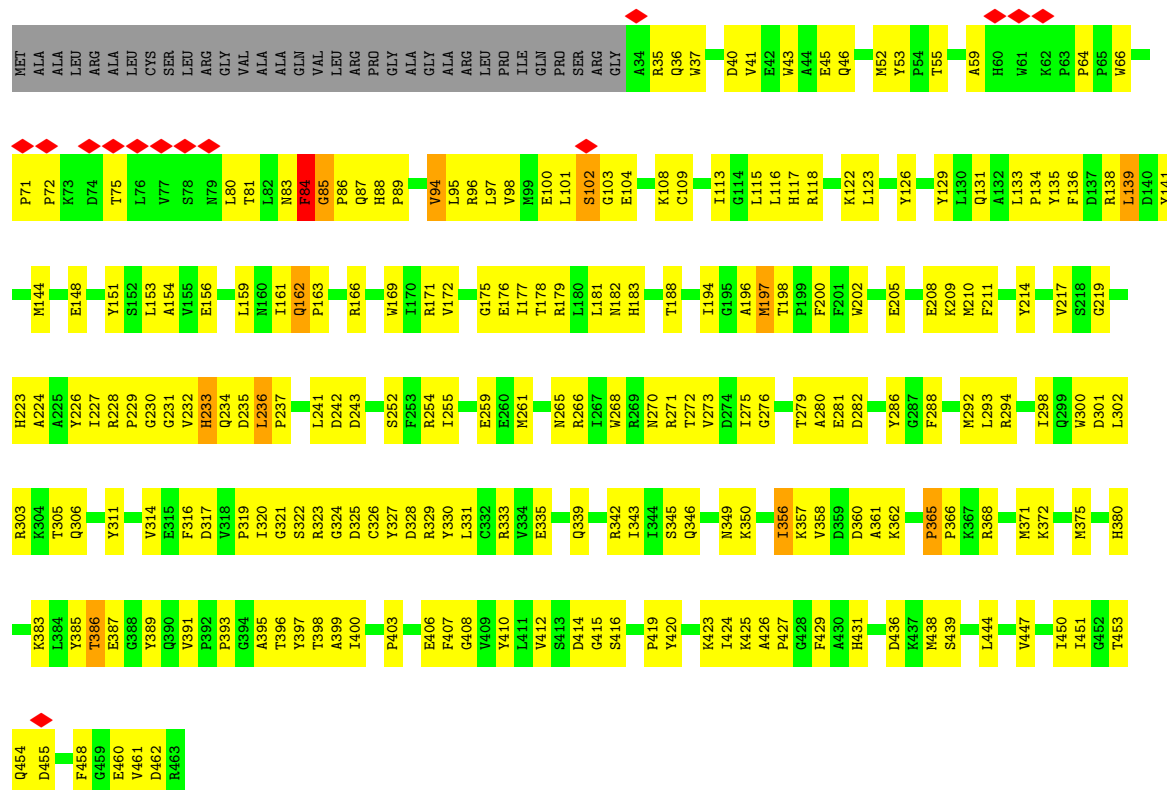


- Molecule 2: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

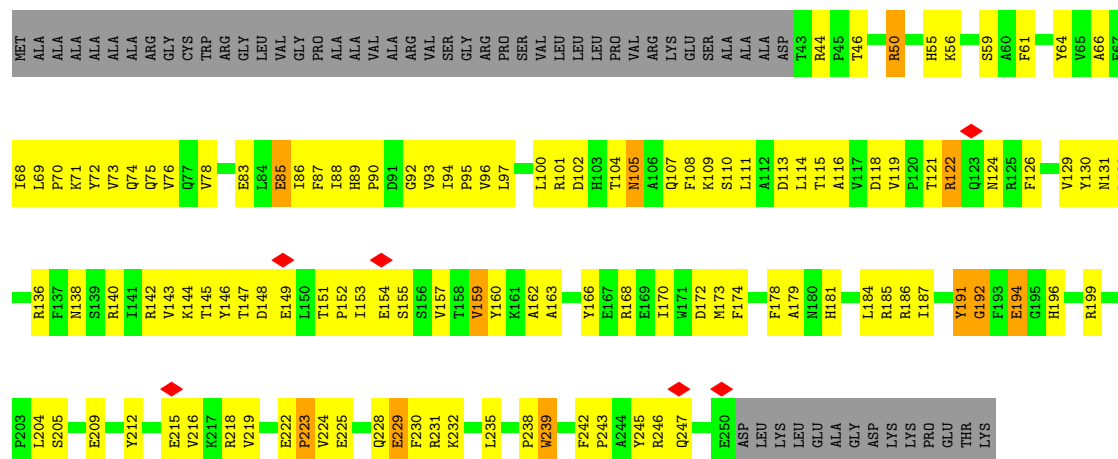




- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

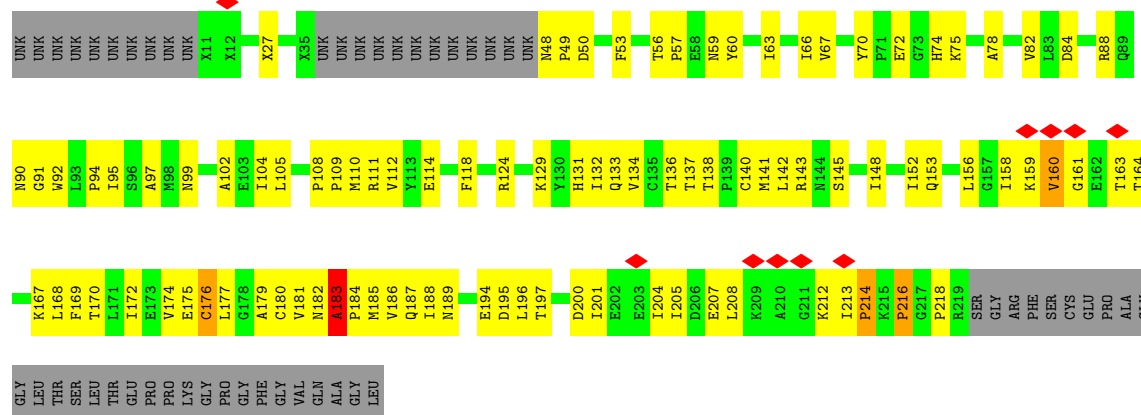


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



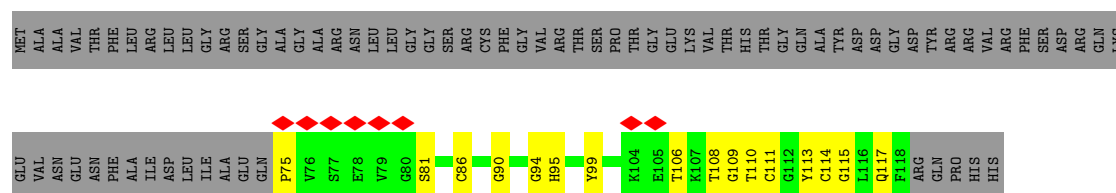
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E: 



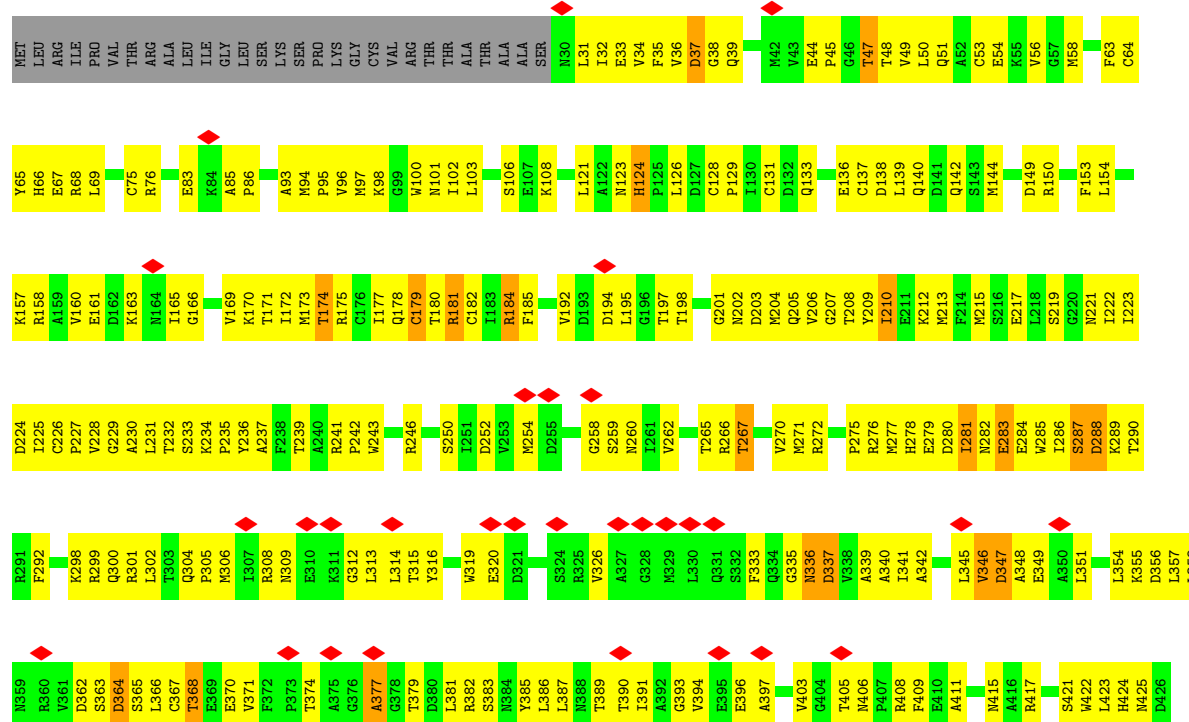
- Molecule 6: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

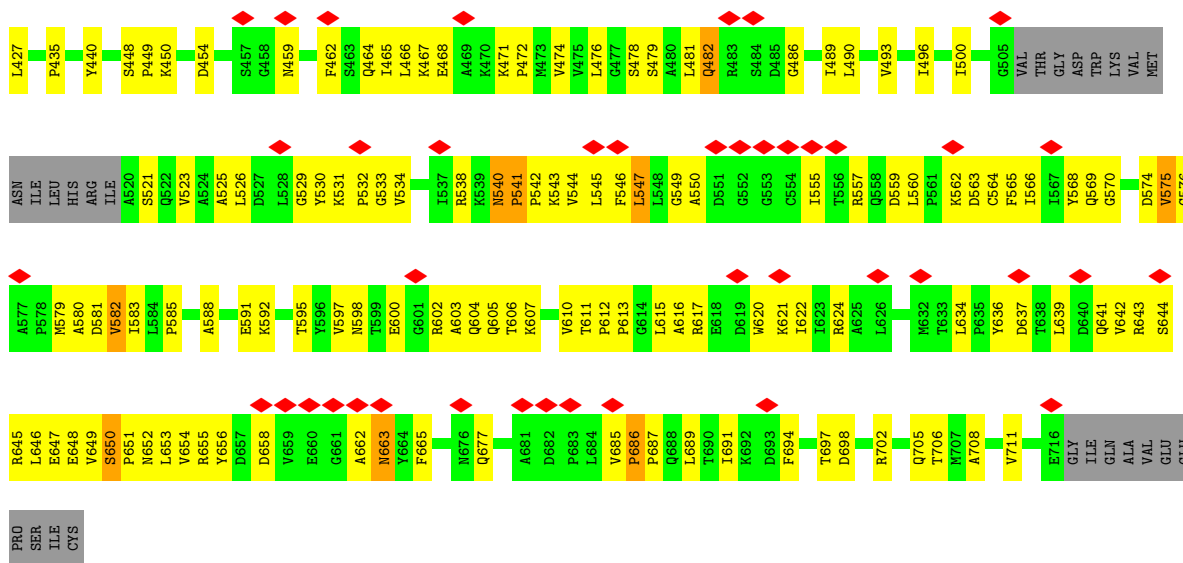
Chain F: 



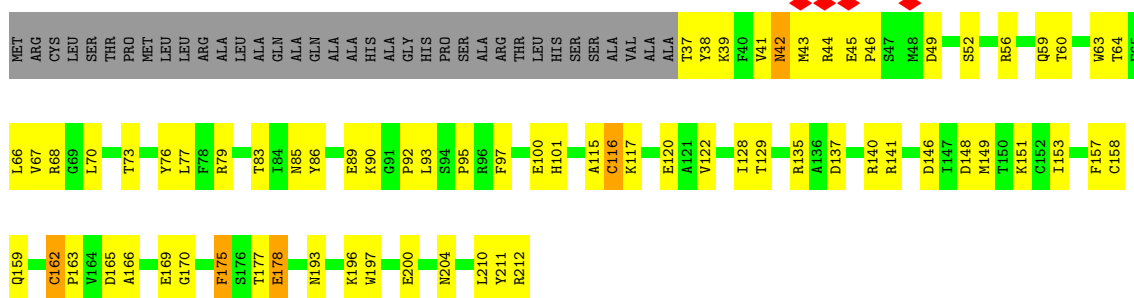
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G: 

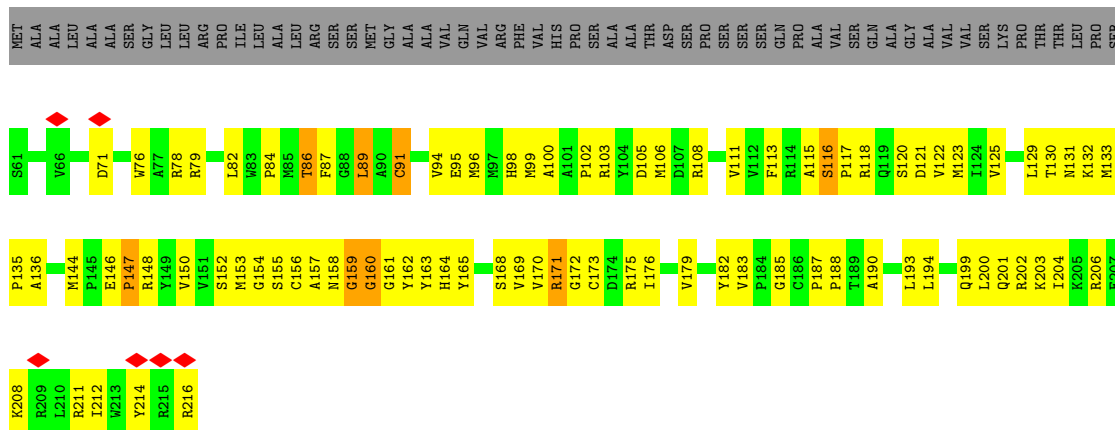
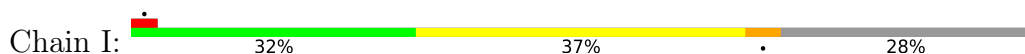




- Molecule 8: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

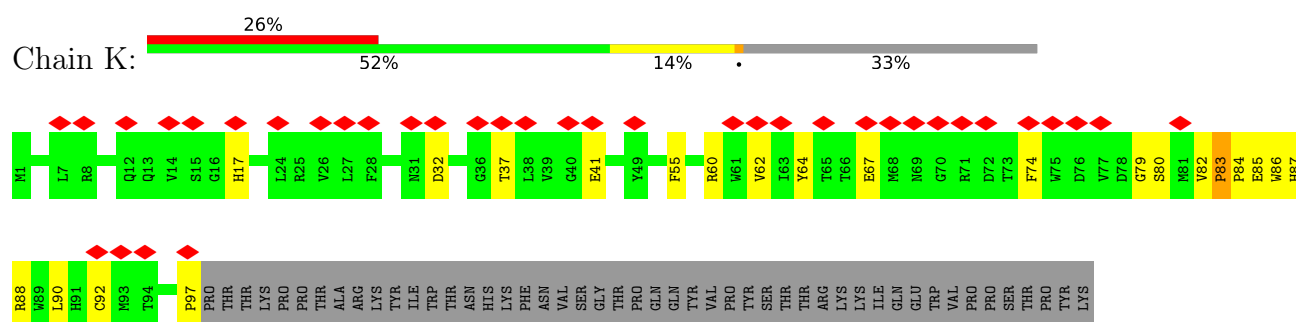


- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

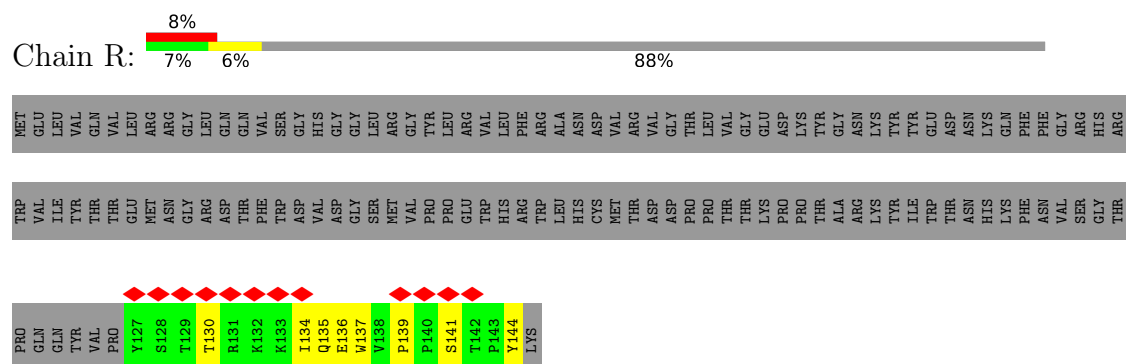


- Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

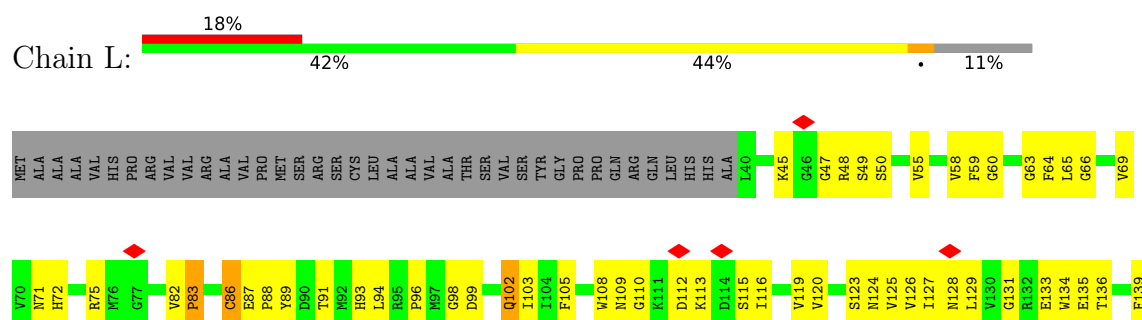
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

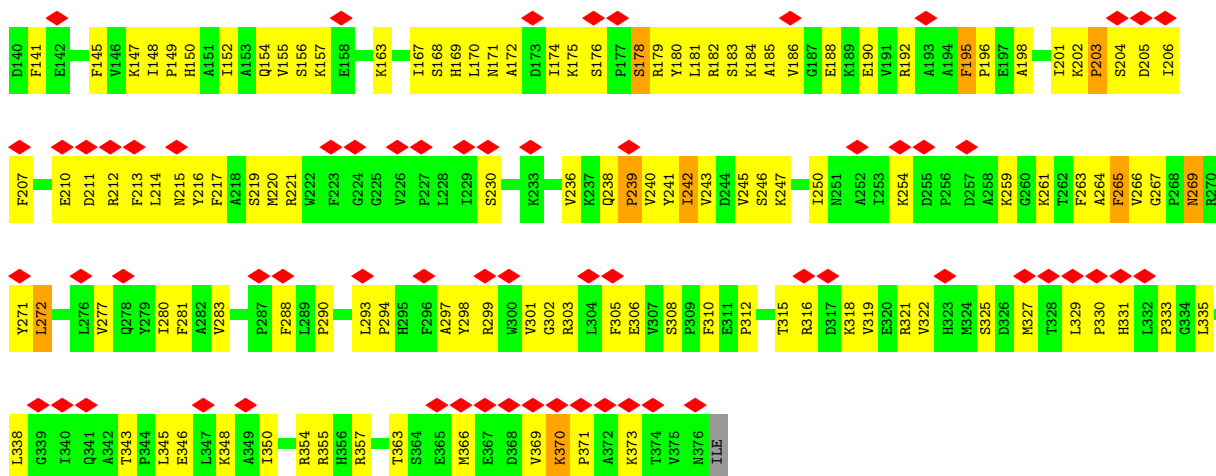


- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

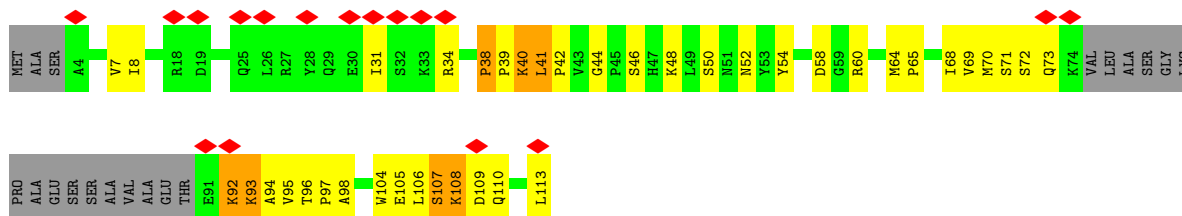


- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

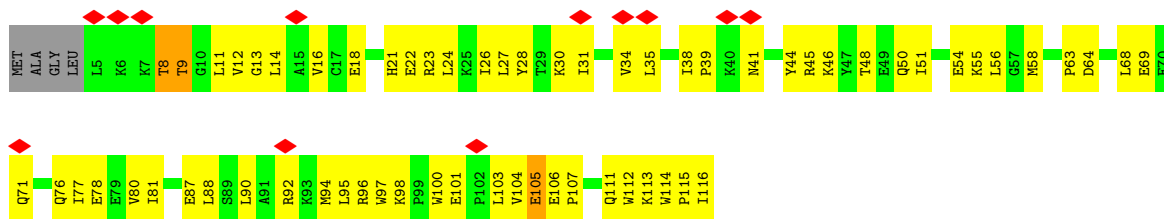




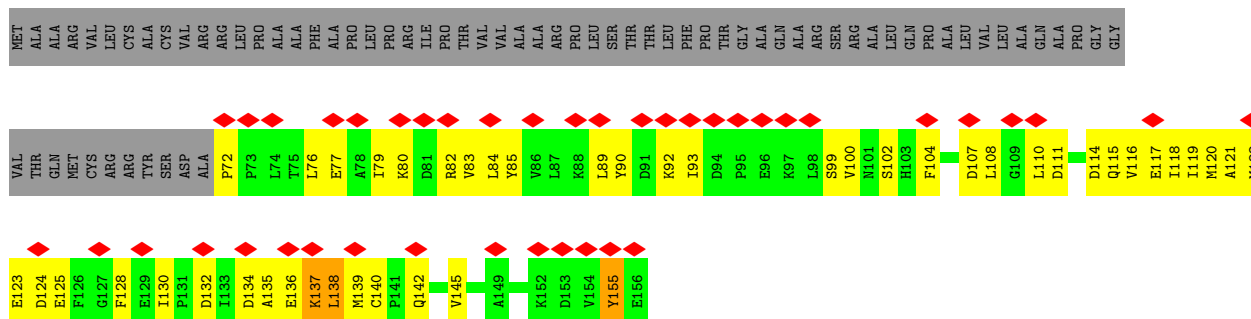
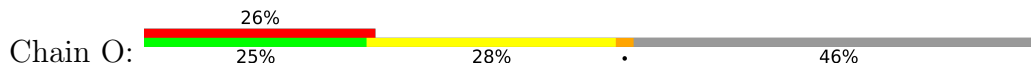
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



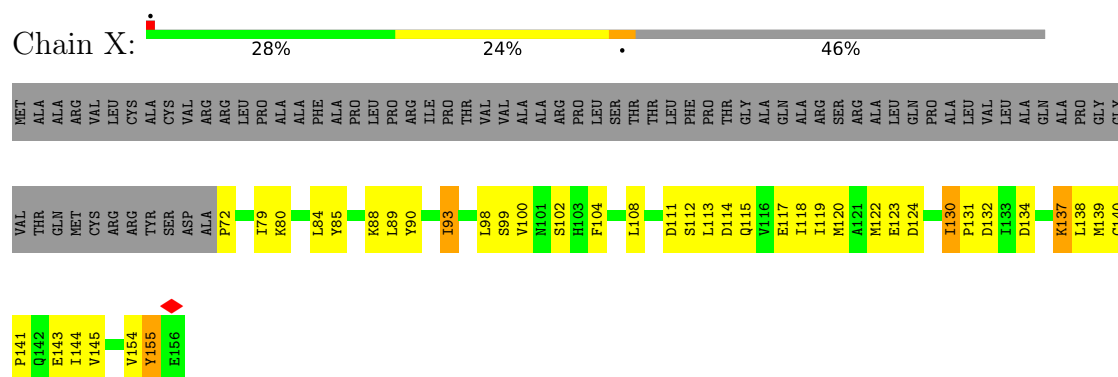
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



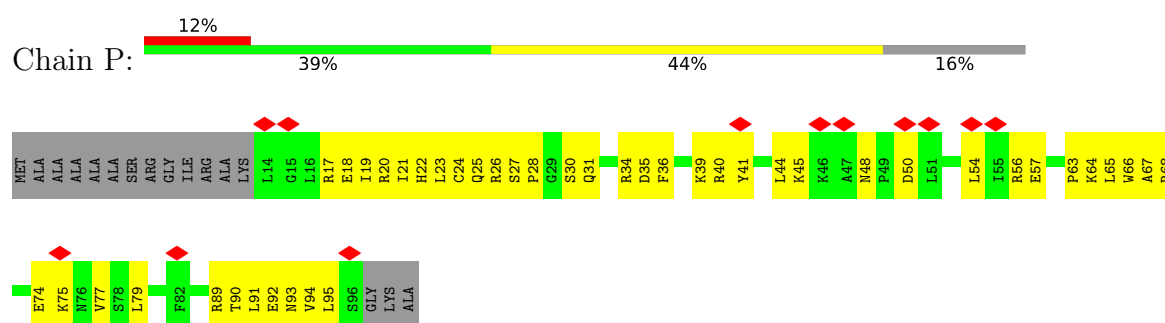
- Molecule 15: Acyl carrier protein, mitochondrial



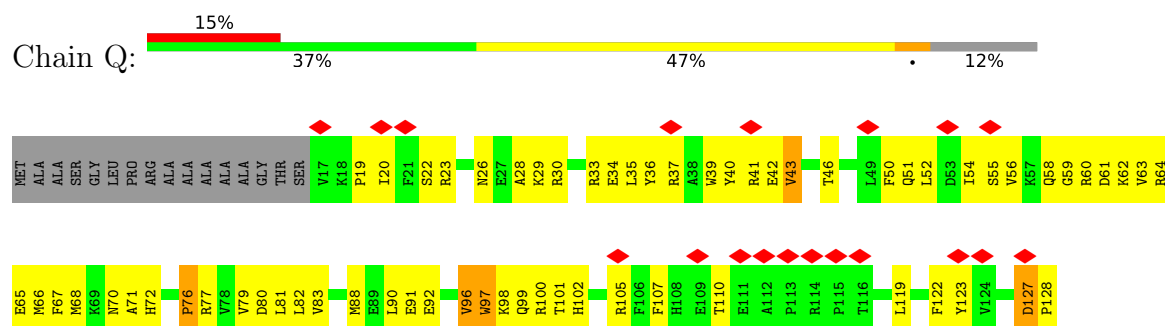
- Molecule 15: Acyl carrier protein, mitochondrial



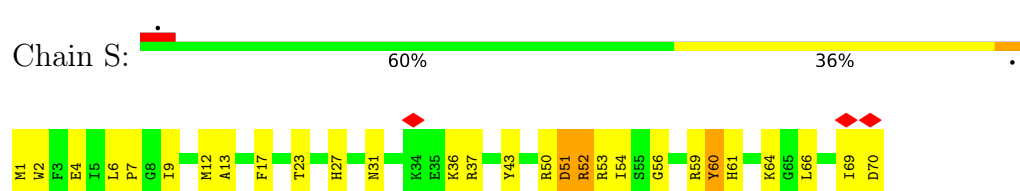
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



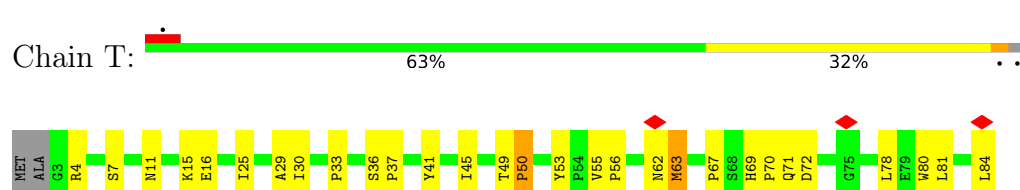
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

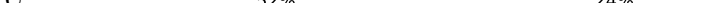


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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

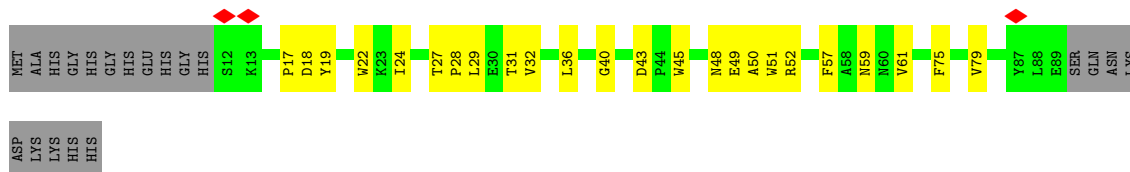


- Chain U:  52% 24% 21%

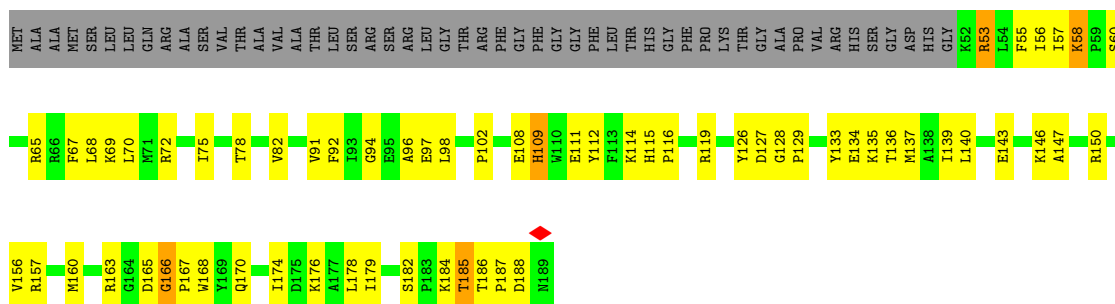




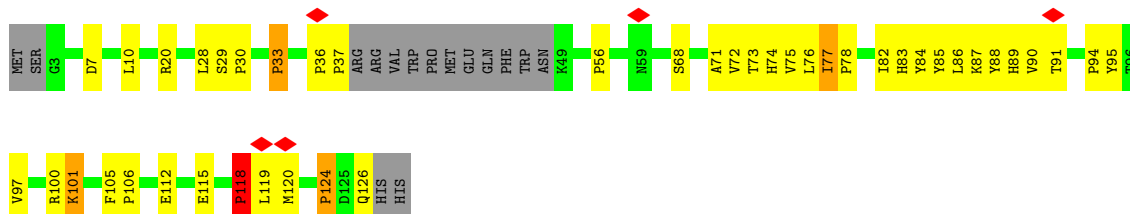
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



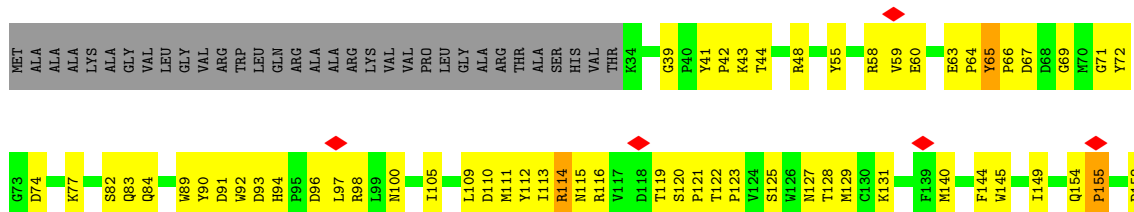
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



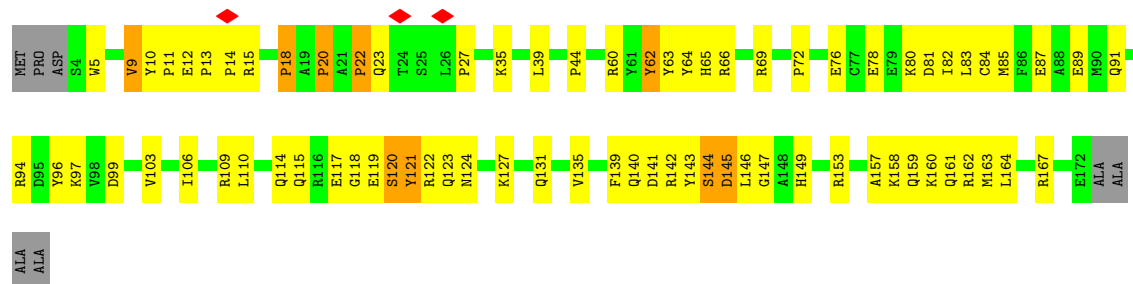
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial





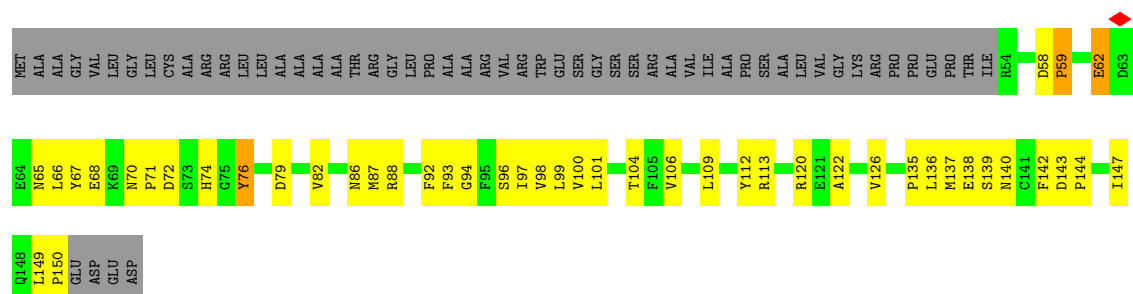
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d: 53% 38% 5%



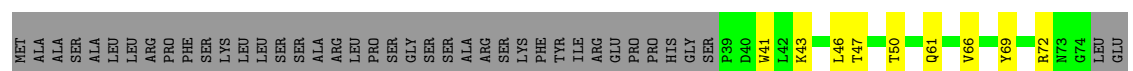
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e: 33% 28% 37%



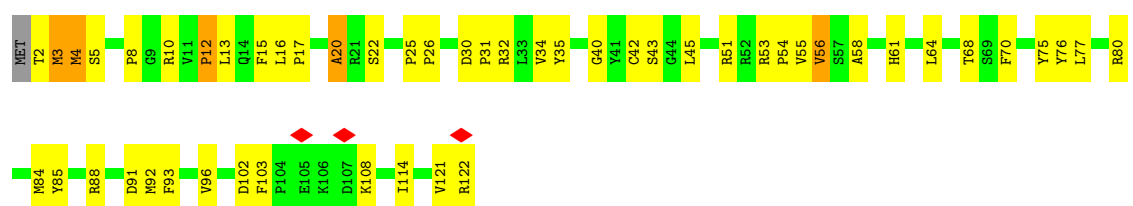
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f: 36% 12% 53%

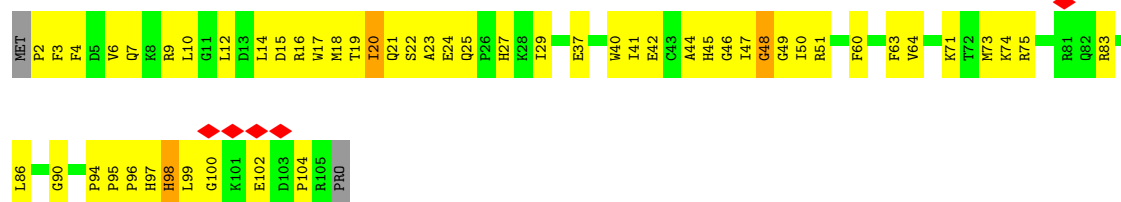


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 subunit C2

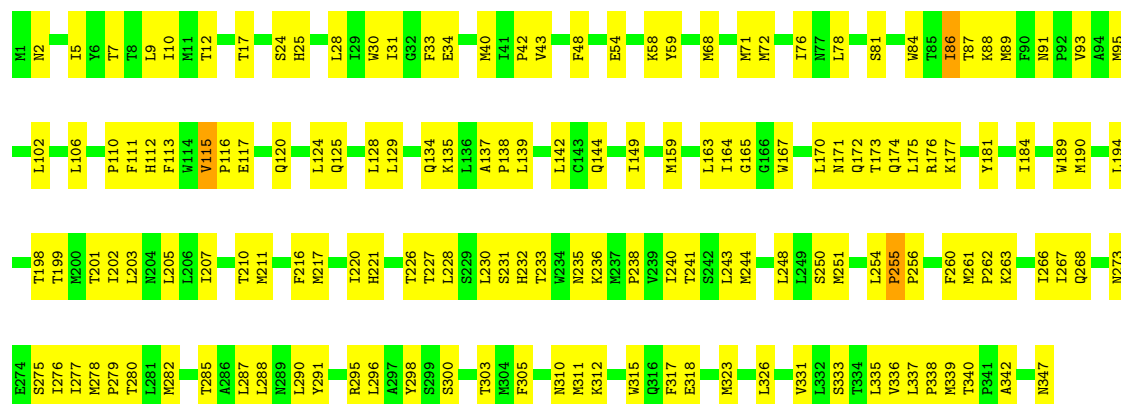
Chain g: 57% 38% 5%



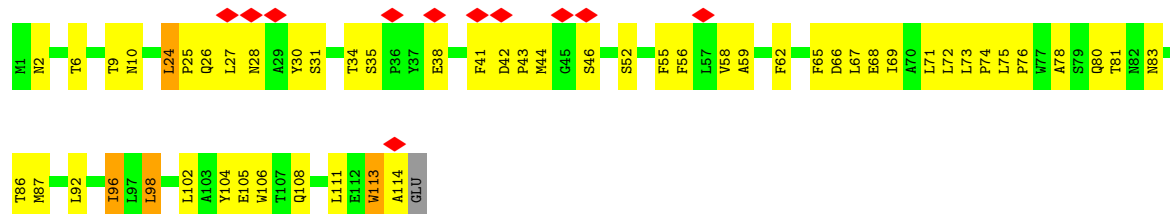
- Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



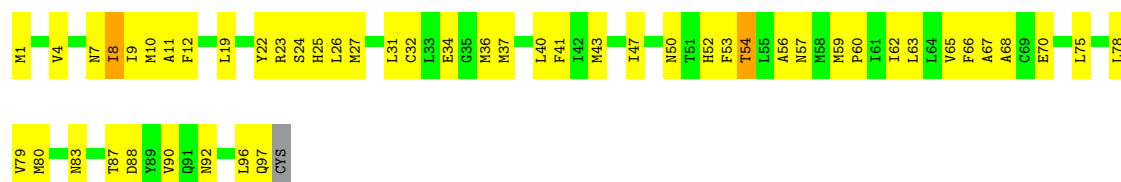
- Molecule 33: NADH-ubiquinone oxidoreductase chain 2



- Molecule 34: NADH-ubiquinone oxidoreductase chain 3

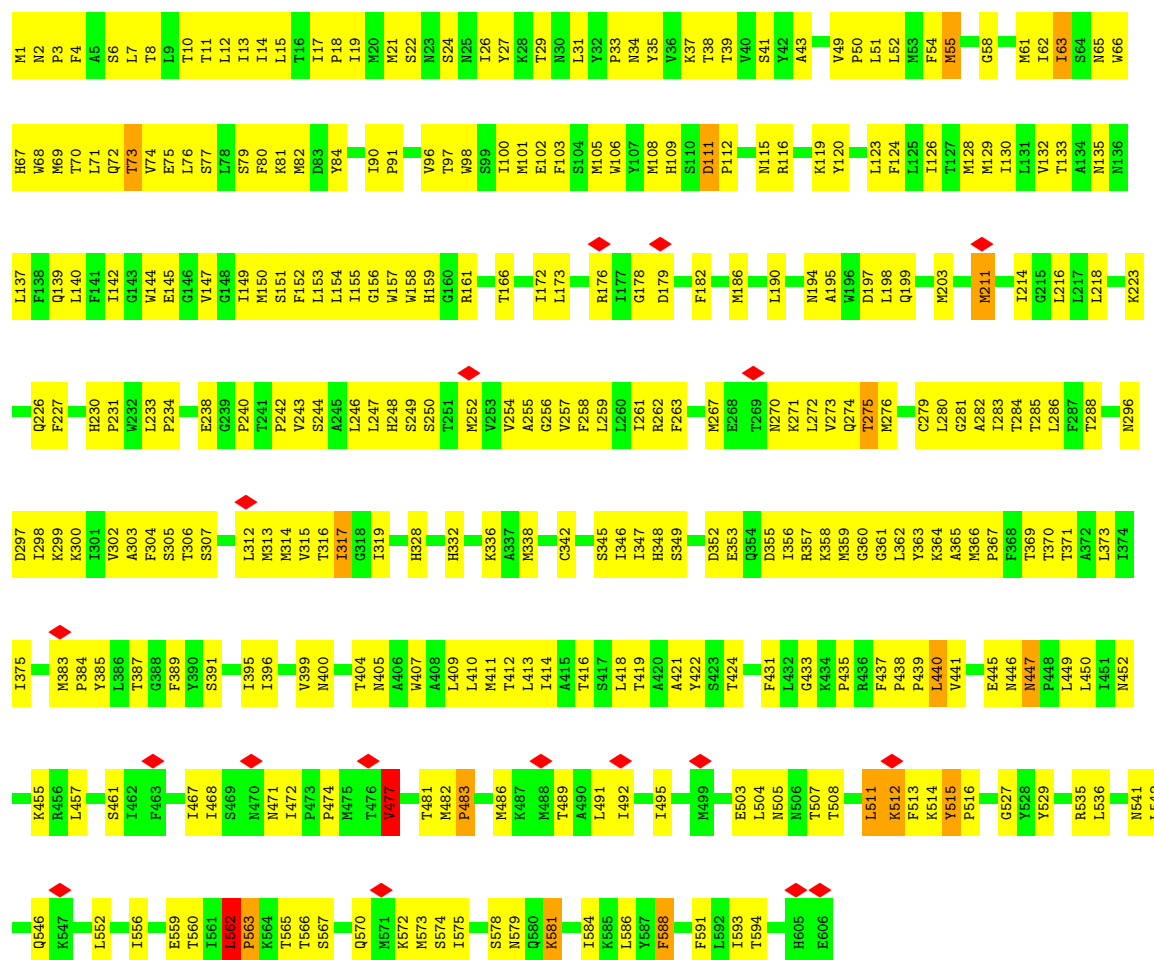


- Molecule 35: NADH-ubiquinone oxidoreductase chain 4L



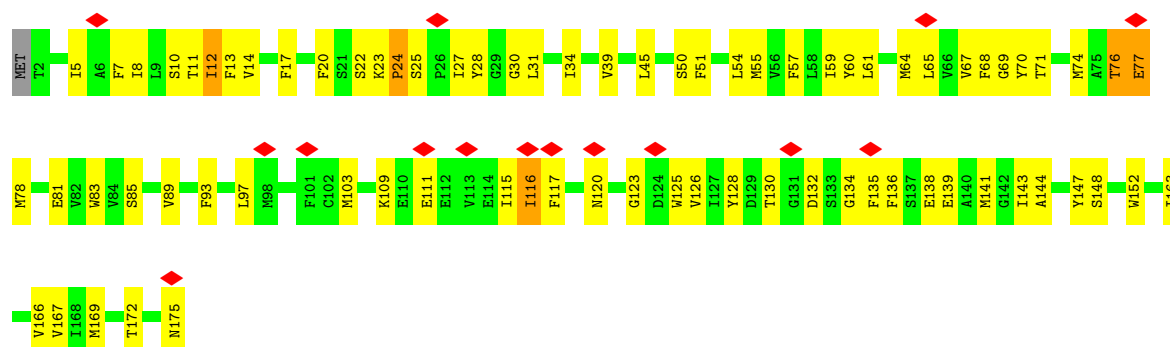
- Molecule 36: NADH-ubiquinone oxidoreductase chain 5

Chain l: 



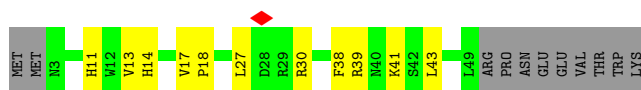
• Molecule 37: NADH-ubiquinone oxidoreductase chain 6

Chain m: 

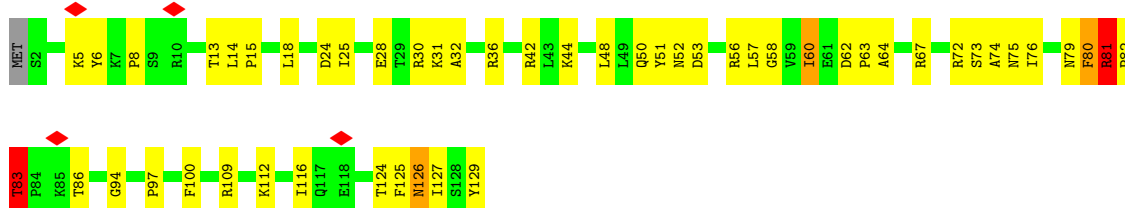


• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n: 



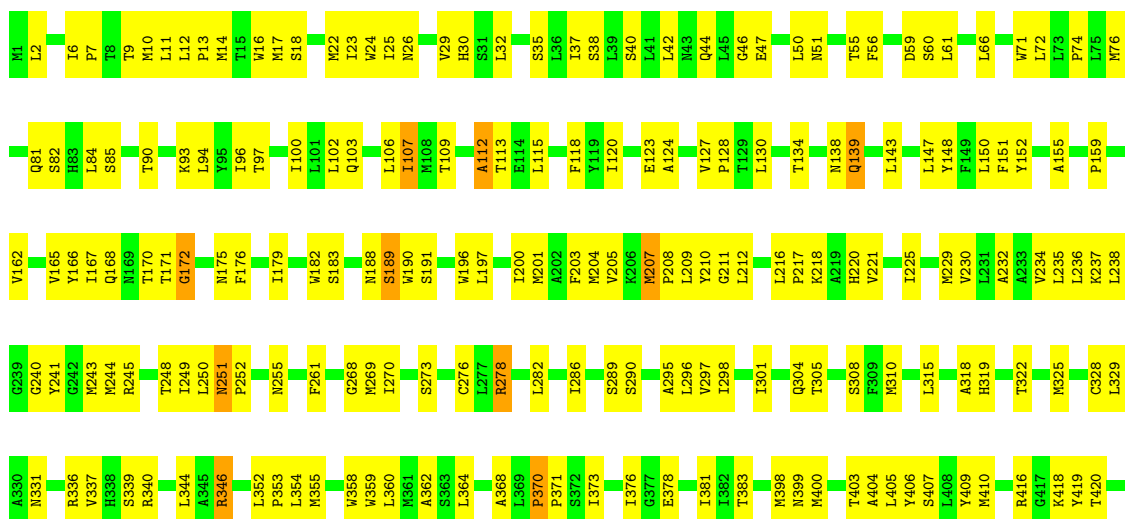
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

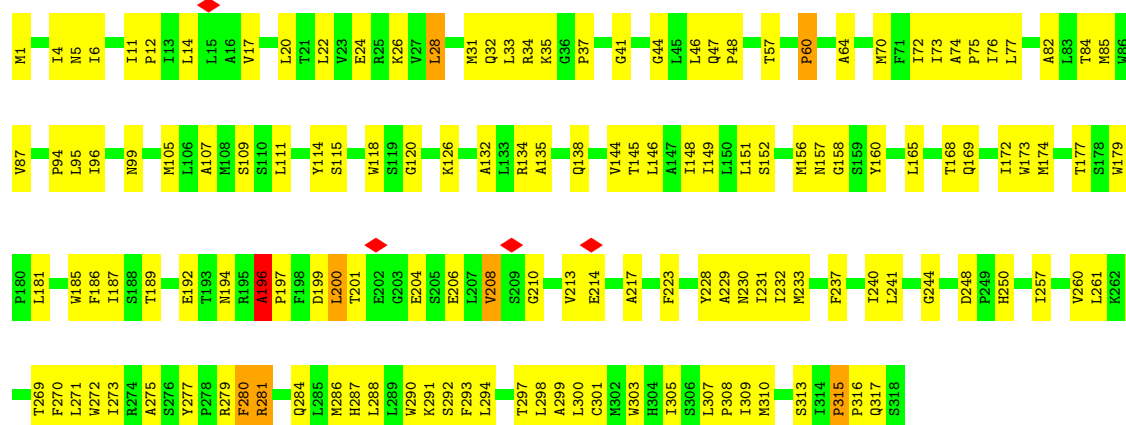


- Molecule 41: NADH-ubiquinone oxidoreductase chain 4

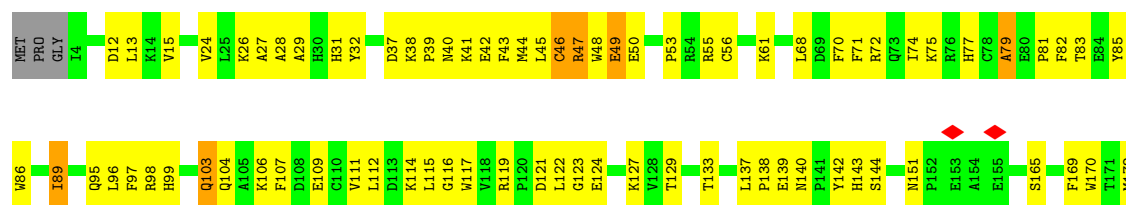




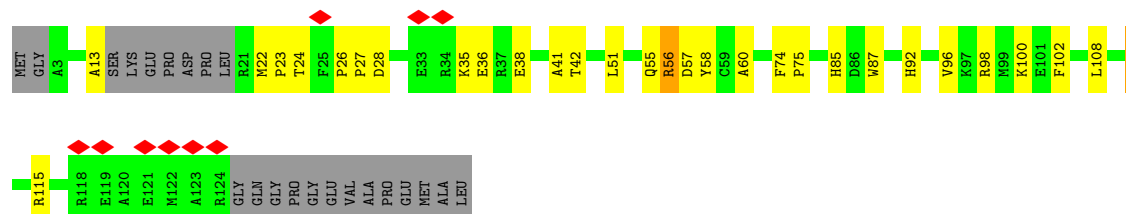
• Molecule 42: NADH-ubiquinone oxidoreductase chain 1



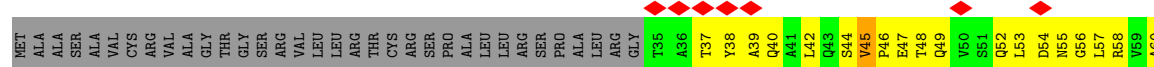
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

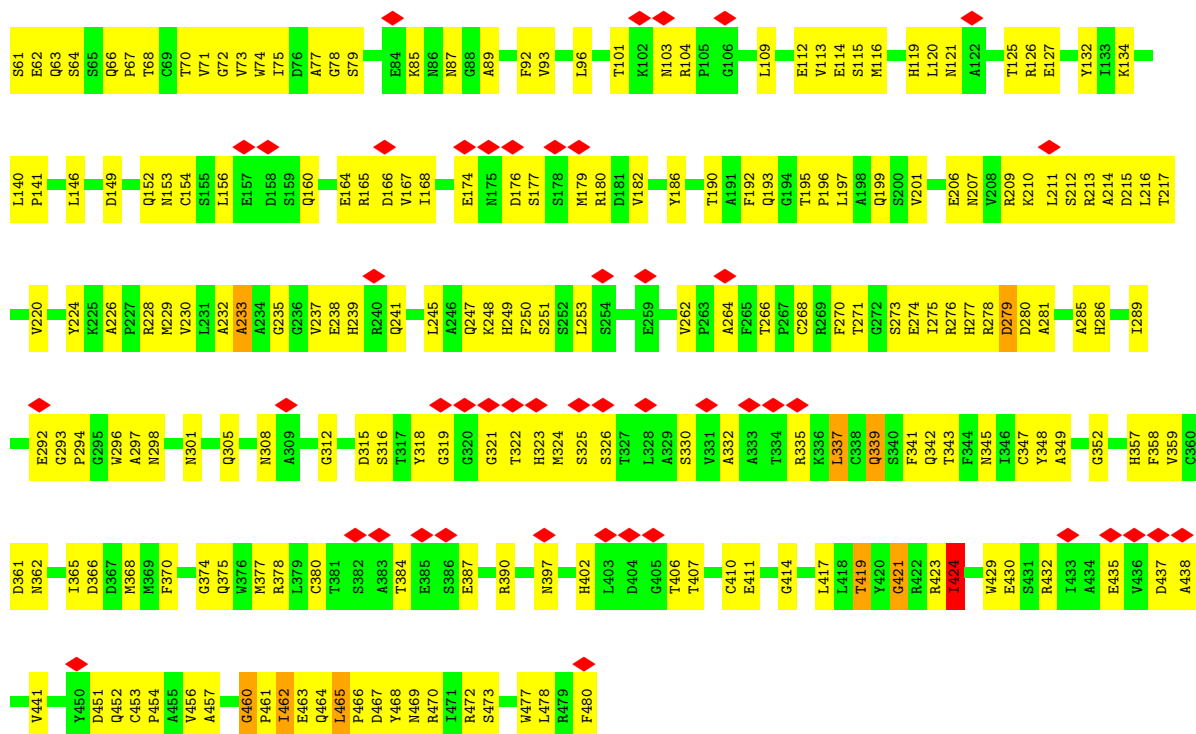


• Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

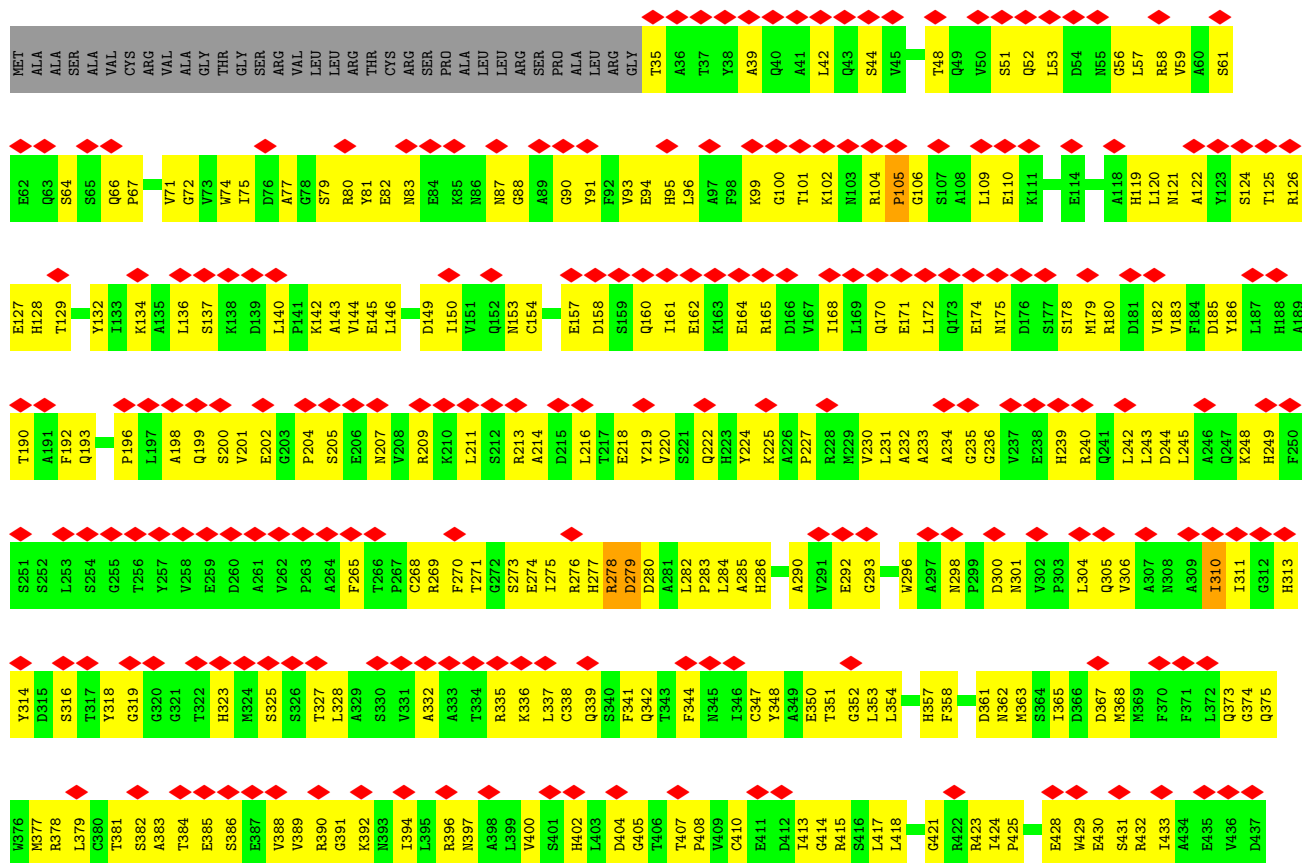
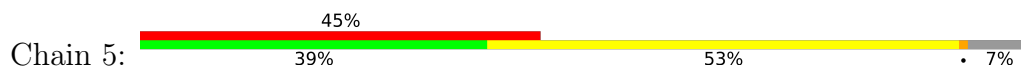


• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial



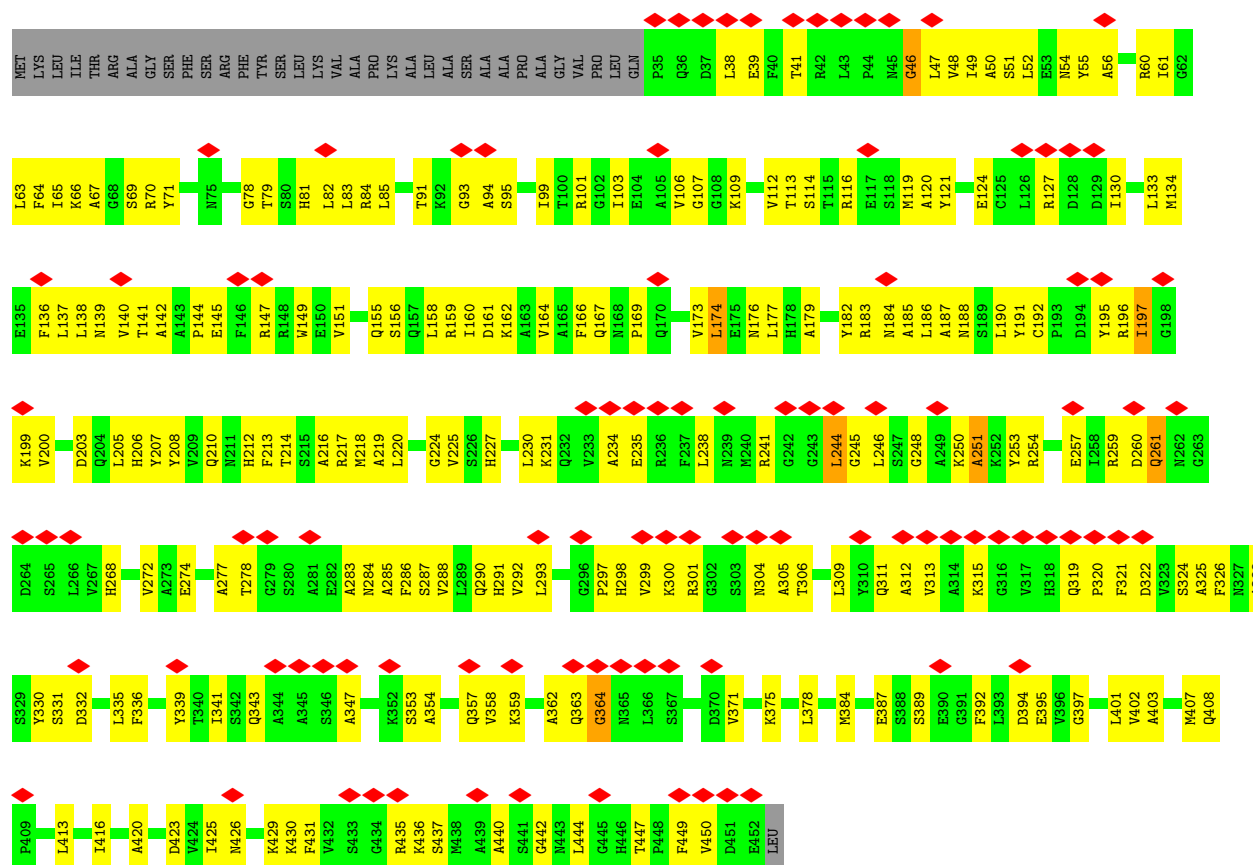
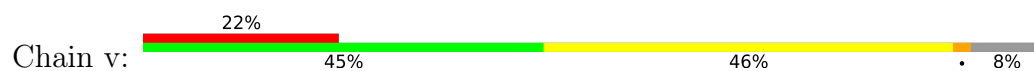


• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

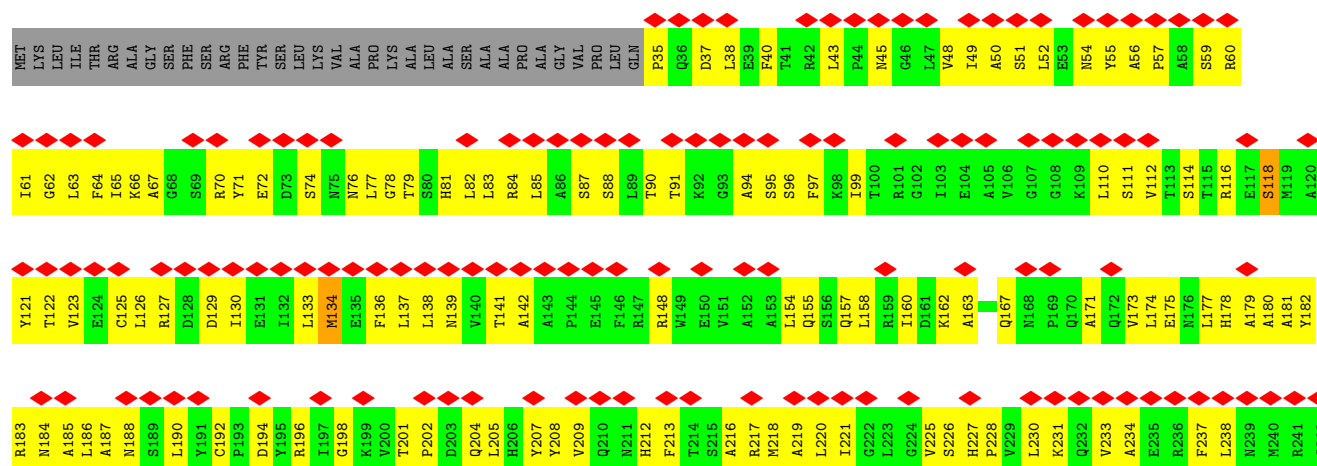


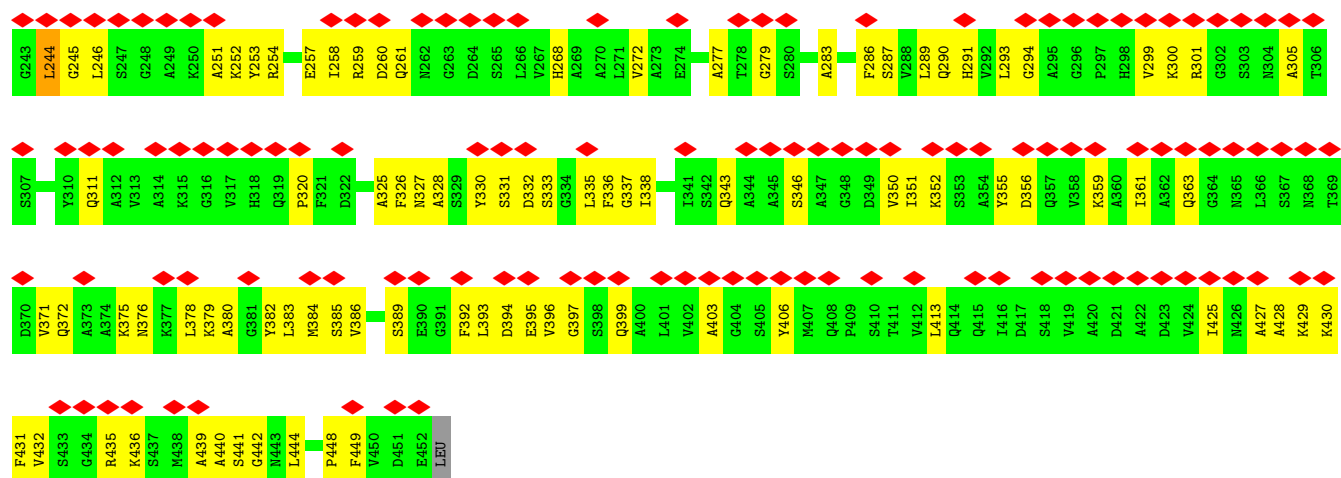


• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

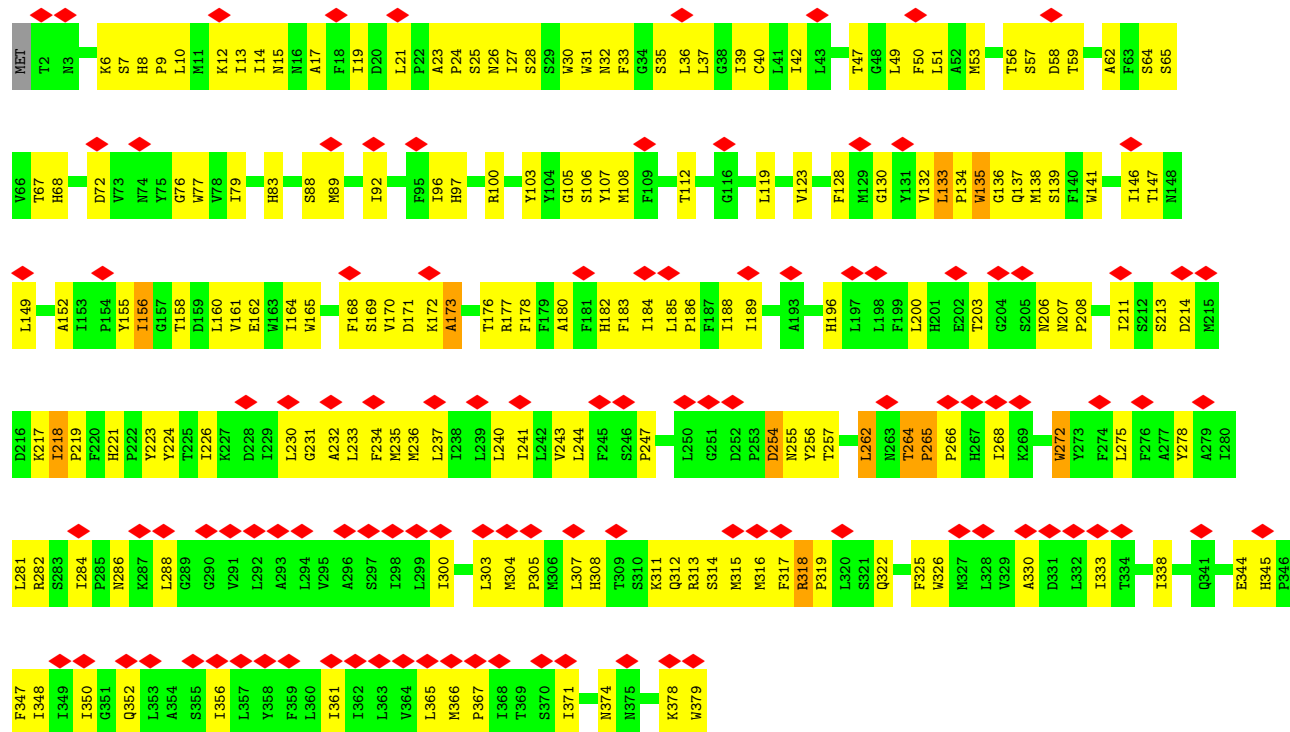


• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

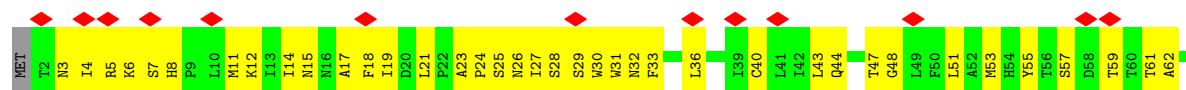
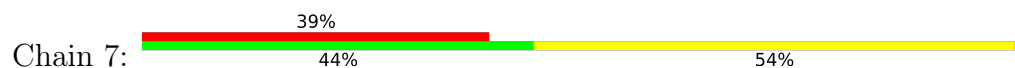


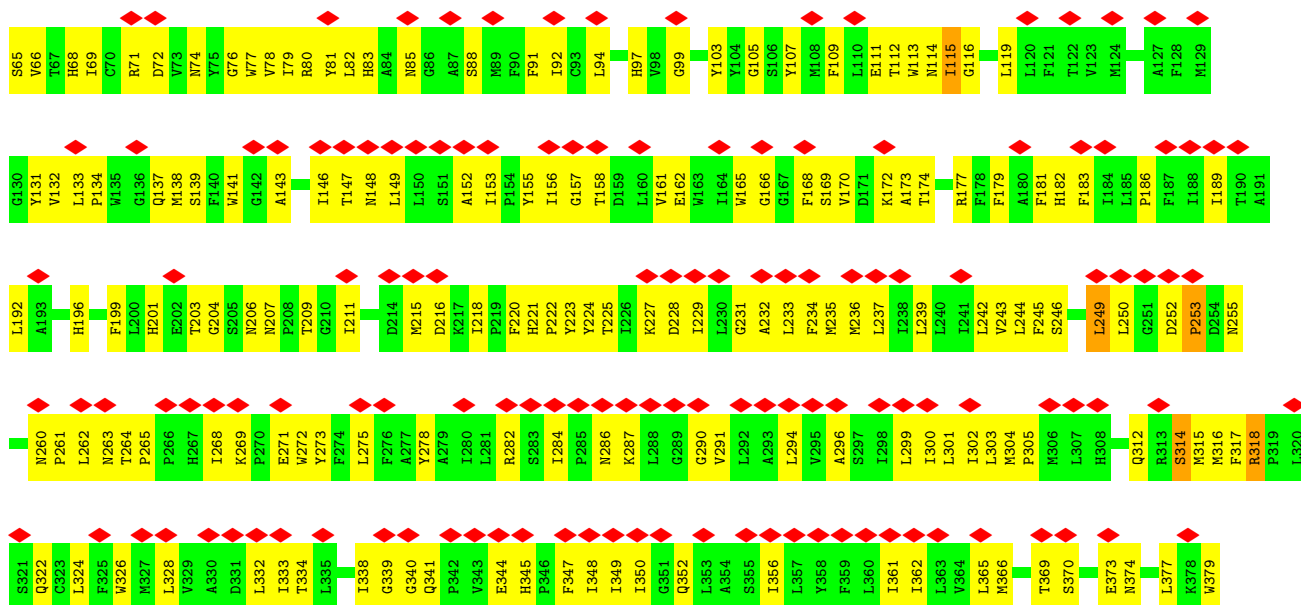


• Molecule 47: Cytochrome b

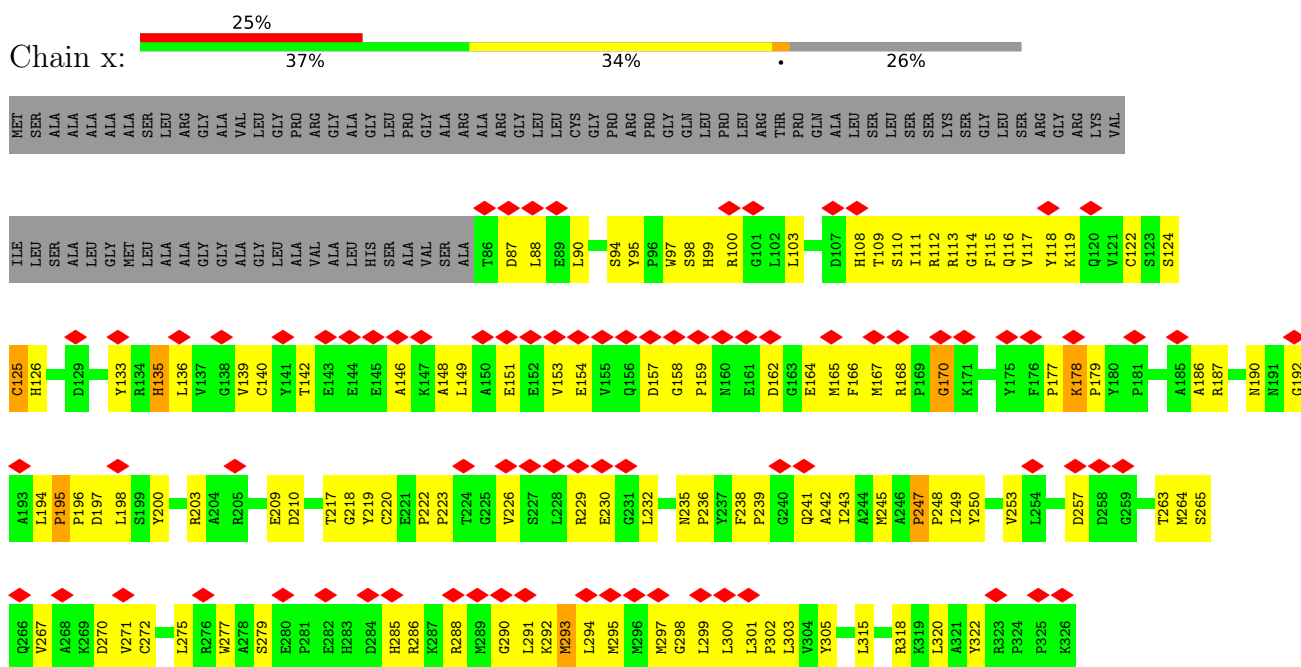


• Molecule 47: Cytochrome b

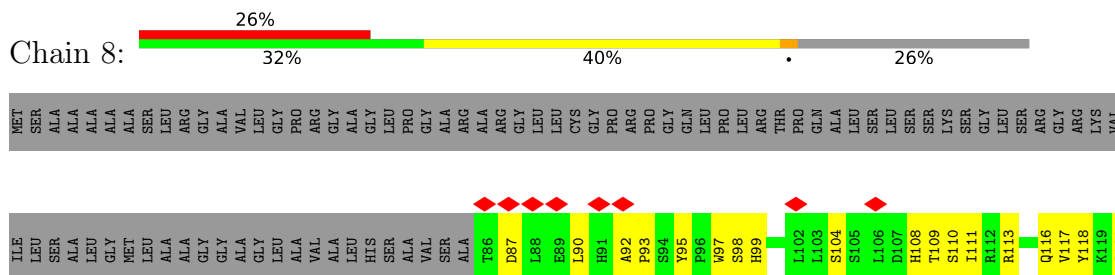


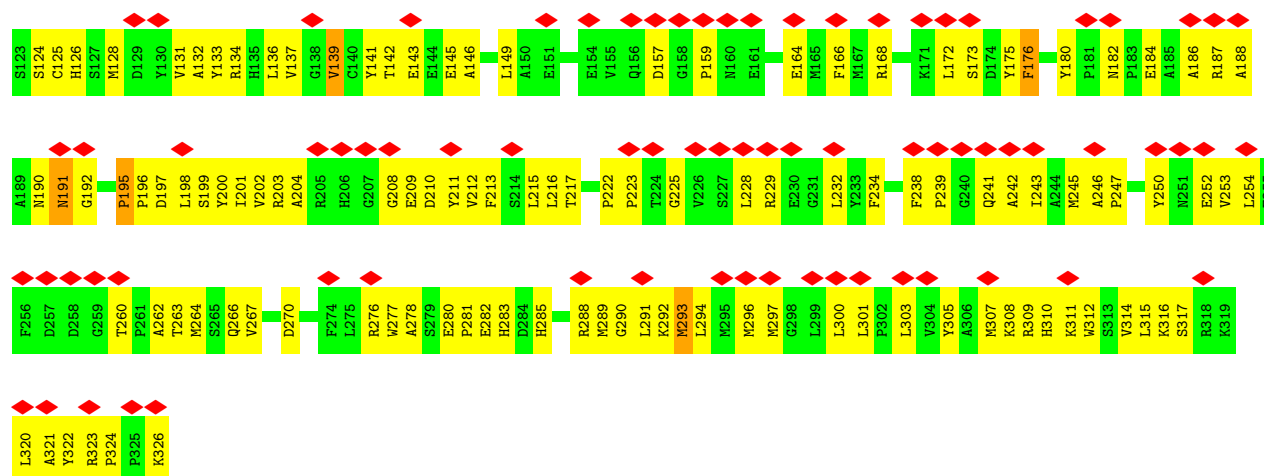


- Molecule 48: Cytochrome c1, heme protein, mitochondrial

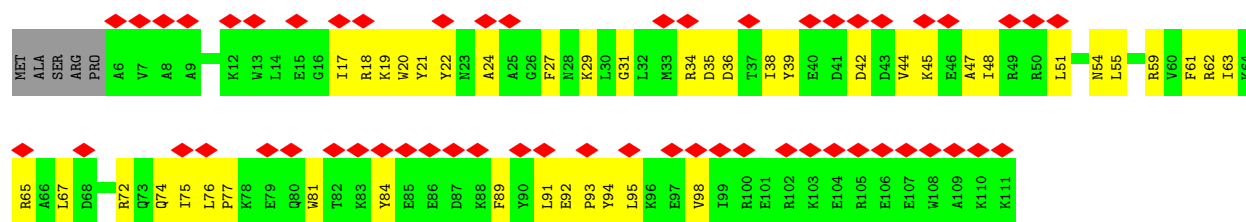


- Molecule 48: Cytochrome c1, heme protein, mitochondrial

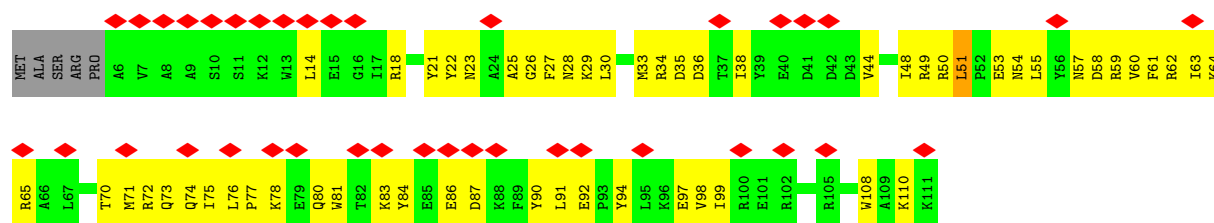
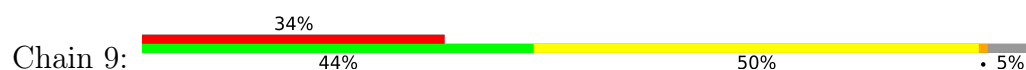




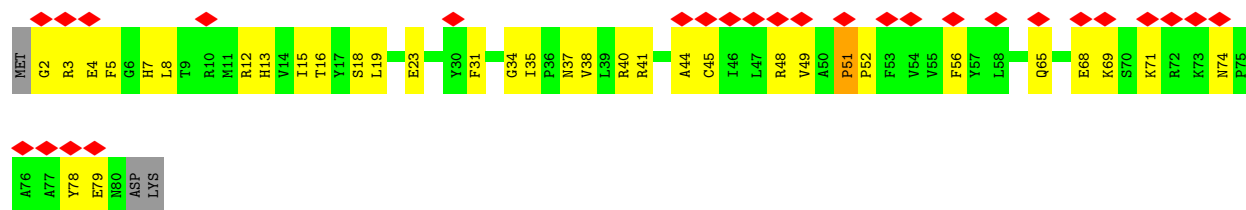
• Molecule 49: Cytochrome b-c1 complex subunit 7



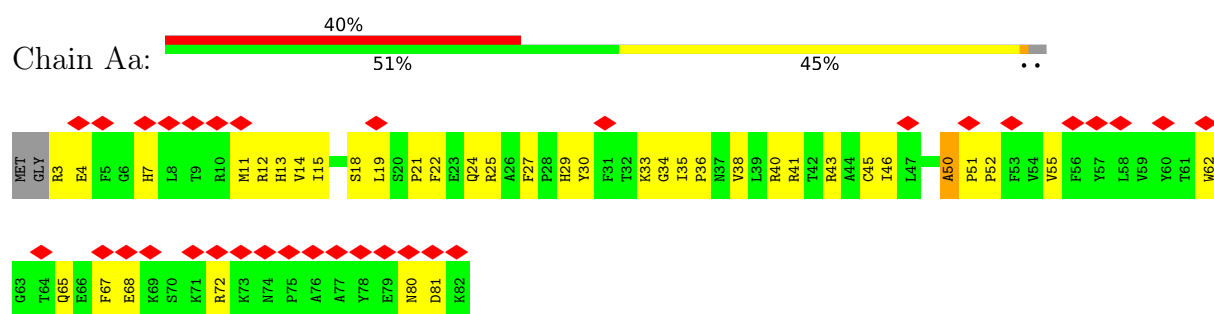
• Molecule 49: Cytochrome b-c1 complex subunit 7



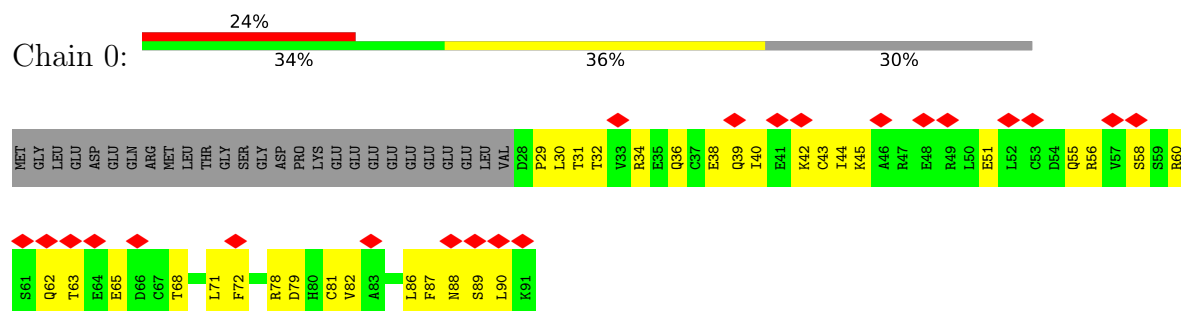
• Molecule 50: Cytochrome b-c1 complex subunit 8



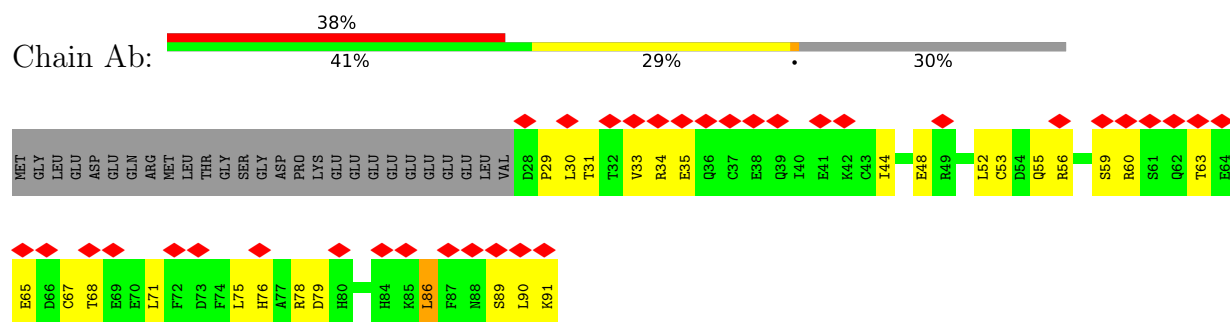
• Molecule 50: Cytochrome b-c1 complex subunit 8



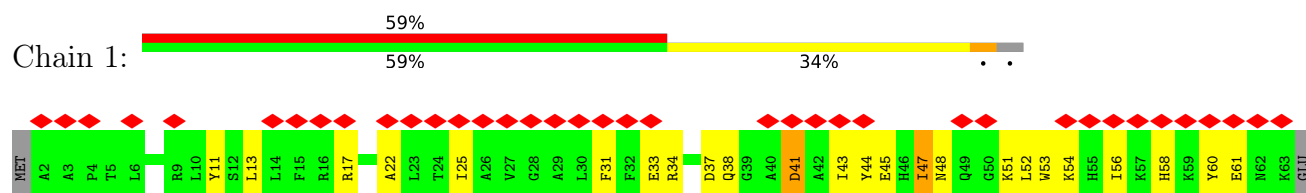
- Molecule 51: Cytochrome b-c1 complex subunit 6, mitochondrial



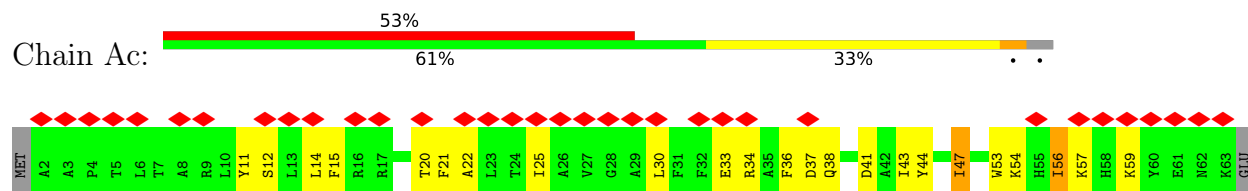
- Molecule 51: Cytochrome b-c1 complex subunit 6, mitochondrial



- Molecule 52: Cytochrome b-c1 complex subunit 9

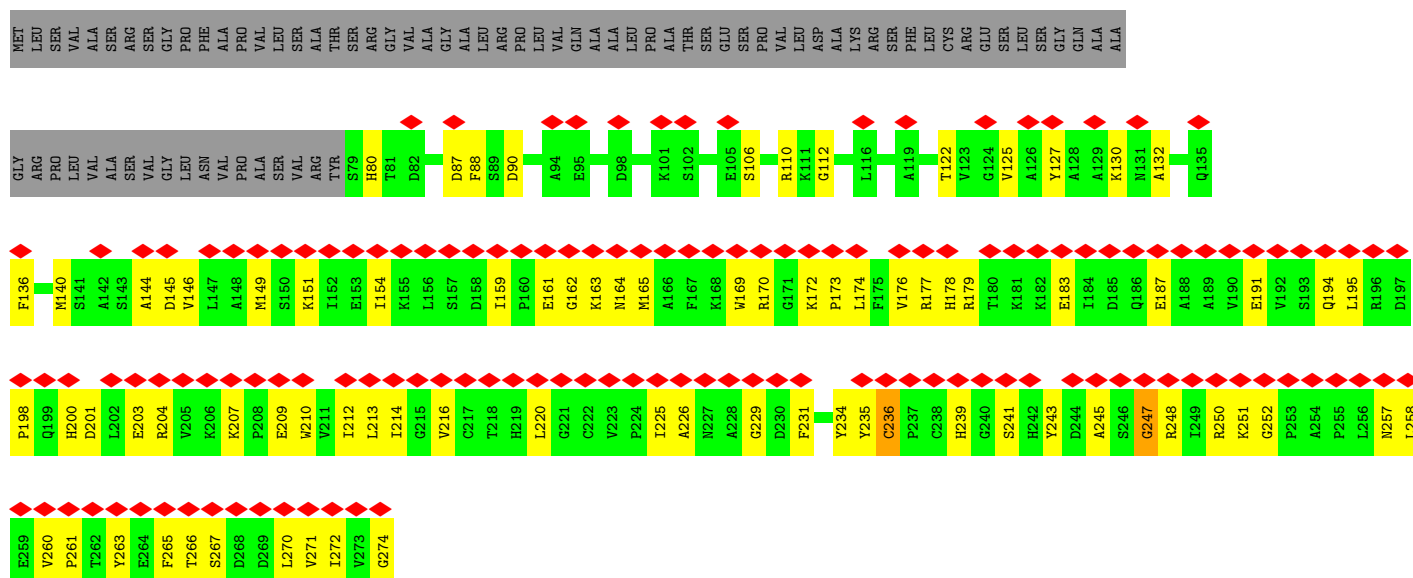


- Molecule 52: Cytochrome b-c1 complex subunit 9



- Molecule 53: Cytochrome b-c1 complex subunit Rieske, mitochondrial

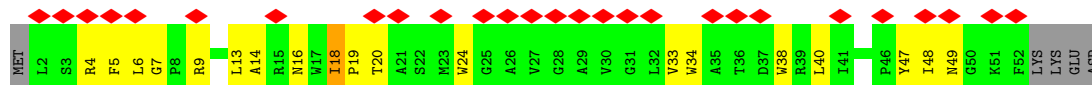




• Molecule 53: Cytochrome b-c1 complex subunit Rieske, mitochondrial

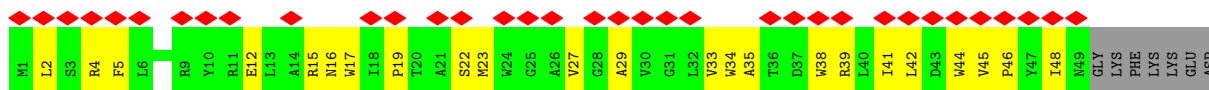


• Molecule 54: Cytochrome b-c1 complex subunit 10

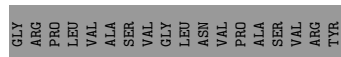
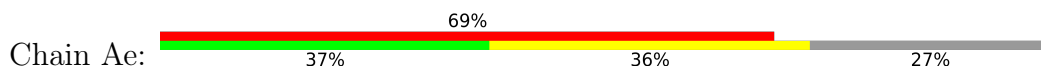


• Molecule 54: Cytochrome b-c1 complex subunit 10

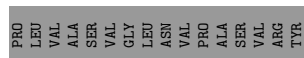
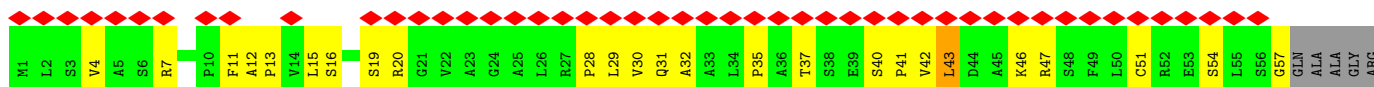
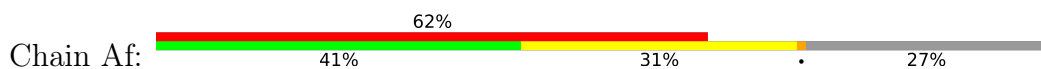




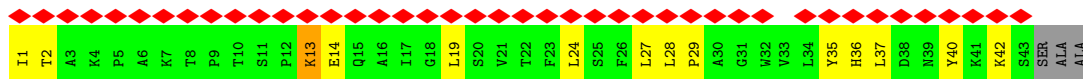
- Molecule 55: Cytochrome b-c1 complex subunit Rieske transit peptide, mitochondrial



- Molecule 55: Cytochrome b-c1 complex subunit Rieske transit peptide, mitochondrial



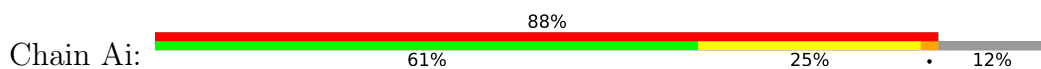
- Molecule 56: Cytochrome c oxidase subunit 8B, mitochondrial



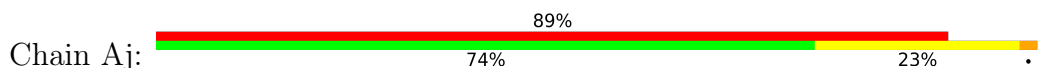
- Molecule 57: Cytochrome c oxidase subunit 7A1, mitochondrial

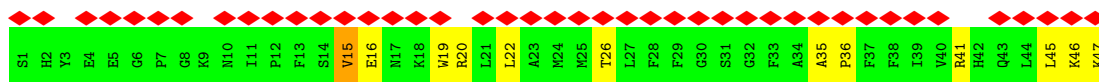


- Molecule 58: Cytochrome c oxidase subunit 7B, mitochondrial

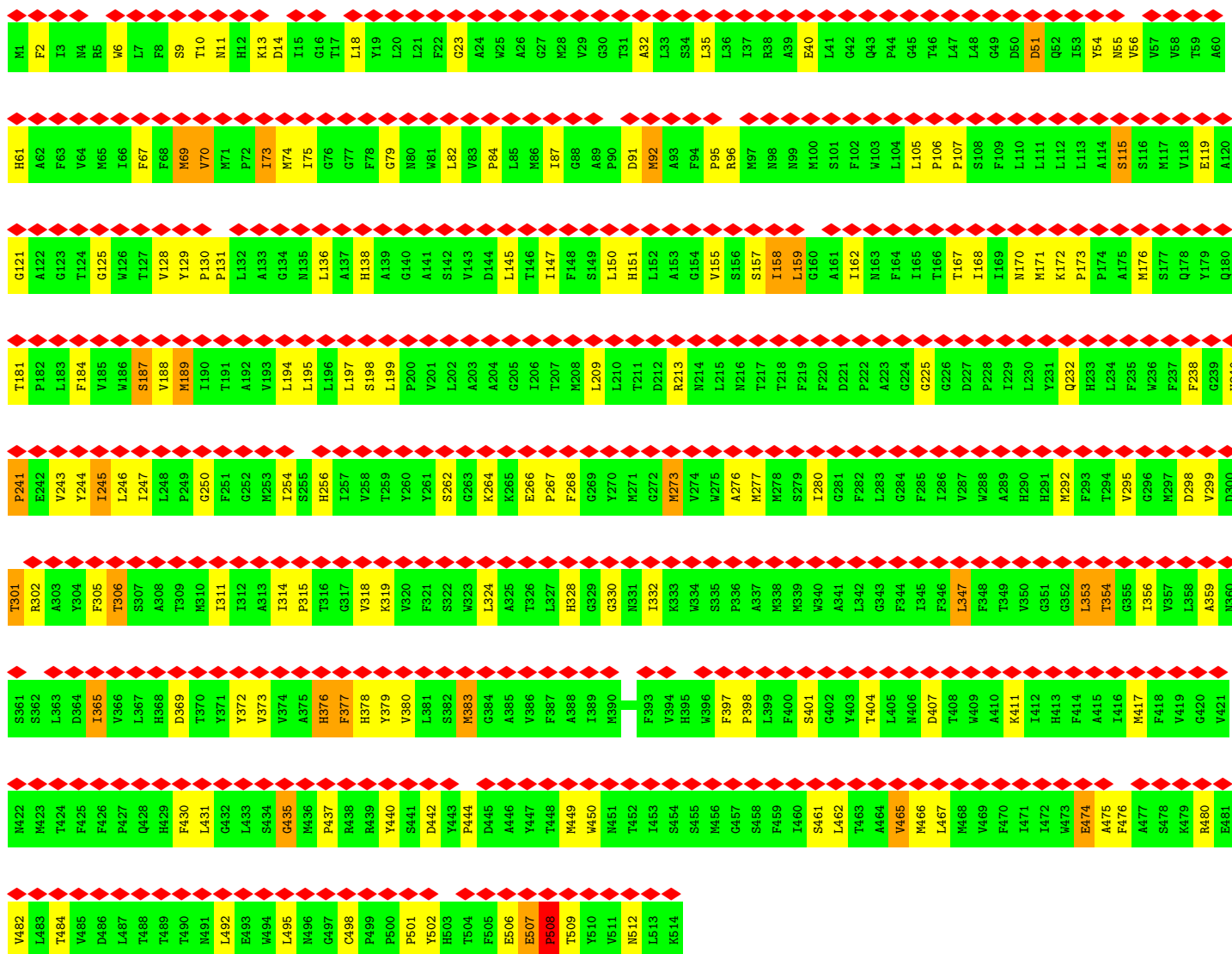


- Molecule 59: Cytochrome c oxidase subunit 7C, mitochondrial

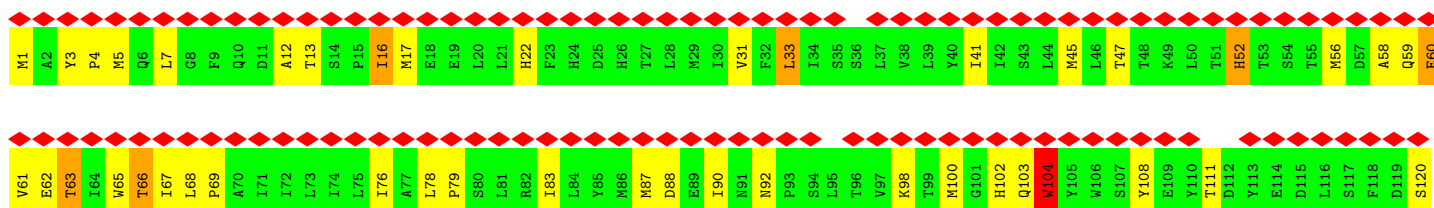


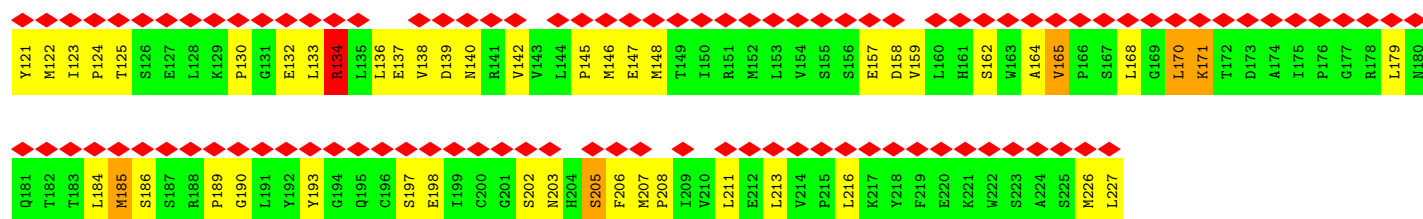


● Molecule 60: Cytochrome c oxidase subunit 1

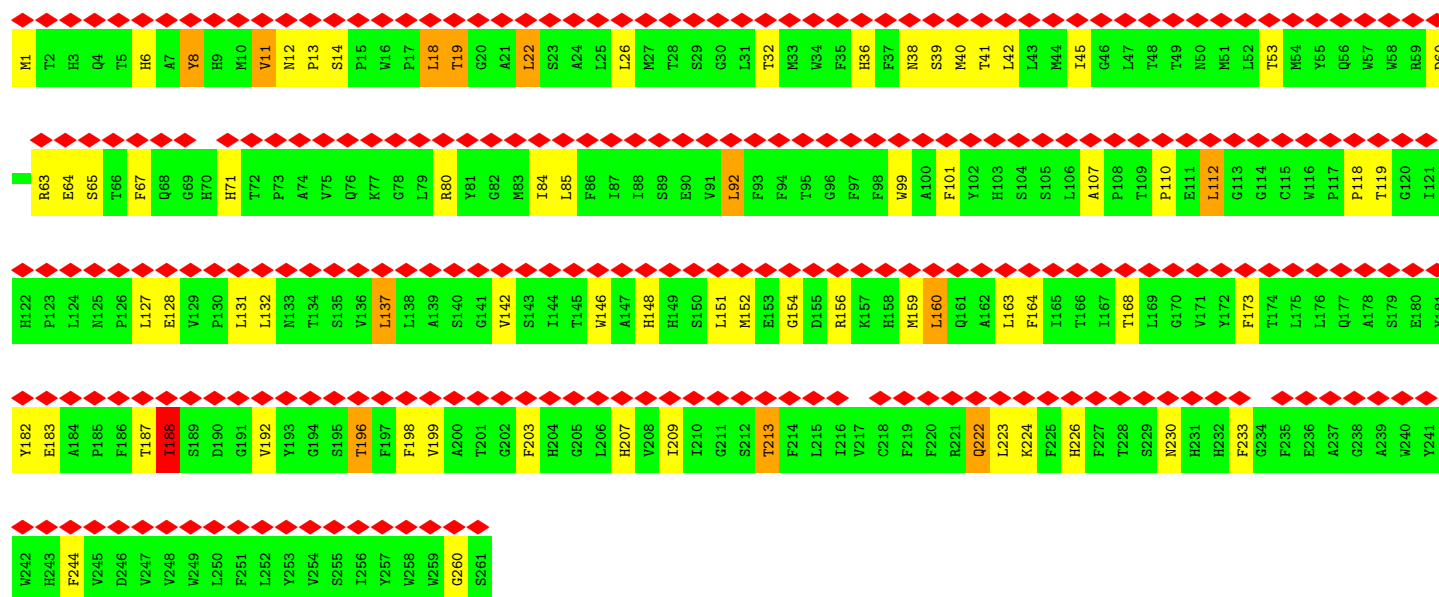
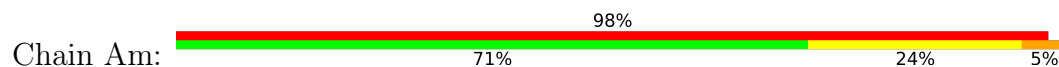


● Molecule 61: Cytochrome c oxidase subunit 2

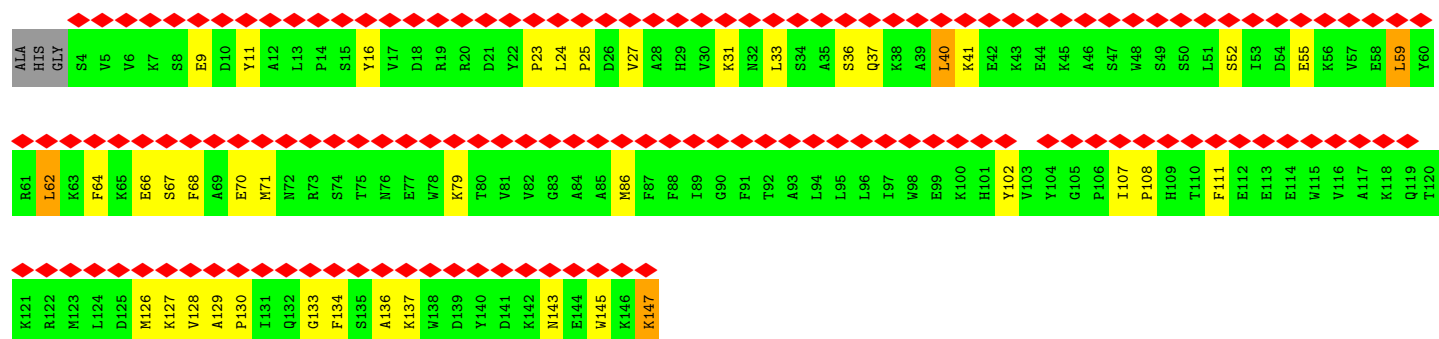
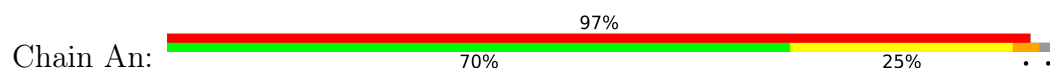




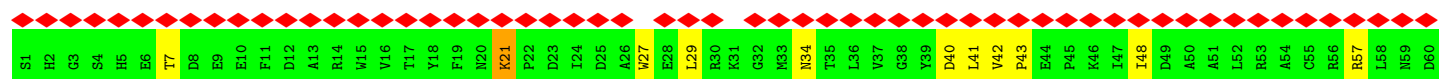
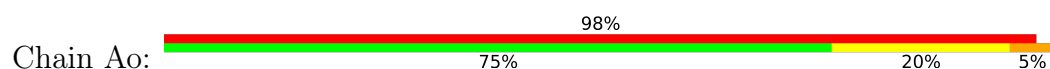
• Molecule 62: Cytochrome c oxidase subunit 3

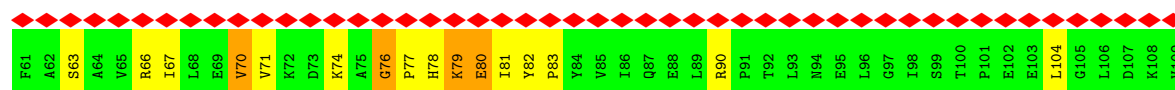


• Molecule 63: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



• Molecule 64: Cytochrome c oxidase subunit 5A, mitochondrial

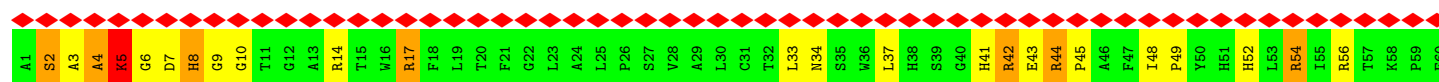




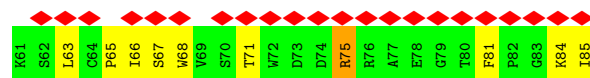
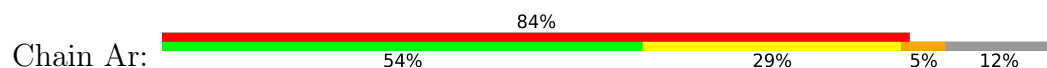
- Molecule 65: Cytochrome c oxidase subunit 5B, mitochondrial



- Molecule 66: Cytochrome c oxidase subunit 6A, mitochondrial



- Molecule 67: Cytochrome c oxidase subunit 6B1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	161912	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	0.519	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0504	Depositor
Map size ($\text{\AA}$)	518.4, 518.4, 518.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.71	0/611	0.94	2/810 (0.2%)
2	B	0.48	0/3199	0.94	10/4327 (0.2%)
3	C	0.75	0/3479	0.96	13/4718 (0.3%)
4	D	0.58	0/1727	1.02	5/2355 (0.2%)
5	E	0.51	0/1367	0.97	5/1860 (0.3%)
6	F	0.68	0/244	1.06	2/332 (0.6%)
7	G	0.56	0/5084	0.98	25/6898 (0.4%)
8	H	0.78	0/1439	1.03	7/1948 (0.4%)
9	I	0.81	0/1272	0.96	1/1721 (0.1%)
10	J	0.53	0/900	0.90	1/1218 (0.1%)
11	K	0.58	0/526	0.98	3/728 (0.4%)
11	R	0.40	0/89	1.34	0/123
12	L	0.50	0/2740	0.91	10/3721 (0.3%)
13	M	0.51	0/702	1.13	7/959 (0.7%)
14	N	0.50	0/914	0.95	4/1241 (0.3%)
15	O	0.44	0/656	0.87	1/890 (0.1%)
15	X	0.59	0/673	0.95	3/912 (0.3%)
16	P	0.42	0/684	0.93	0/922
17	Q	0.52	0/965	0.94	3/1301 (0.2%)
18	S	0.65	0/582	0.85	0/783
19	T	0.60	0/643	1.04	4/886 (0.5%)
20	U	0.57	0/1981	1.05	10/2711 (0.4%)
21	V	0.64	0/1030	0.92	1/1397 (0.1%)
22	W	0.58	0/1153	0.99	4/1561 (0.3%)
23	Y	0.63	0/412	0.97	3/567 (0.5%)
24	Z	0.53	0/567	0.84	2/777 (0.3%)
25	a	0.66	0/1157	0.94	4/1571 (0.3%)
26	b	0.67	1/756 (0.1%)	1.17	9/1042 (0.9%)
27	c	0.65	0/1115	1.07	7/1535 (0.5%)
28	d	0.66	0/1253	0.99	9/1697 (0.5%)
29	e	0.66	0/778	0.95	4/1059 (0.4%)
30	f	0.58	0/308	0.73	0/415

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	g	0.60	0/1027	0.92	1/1389 (0.1%)
32	h	0.65	0/812	0.96	2/1087 (0.2%)
33	i	0.85	0/2769	0.99	4/3764 (0.1%)
34	j	0.69	0/916	0.88	2/1253 (0.2%)
35	k	0.85	0/728	1.09	3/988 (0.3%)
36	l	0.67	0/4919	0.94	9/6693 (0.1%)
37	m	0.69	0/1312	0.90	1/1784 (0.1%)
38	n	0.58	0/368	0.92	0/499
39	o	0.64	0/1050	0.92	4/1430 (0.3%)
40	p	0.63	0/1463	1.05	12/1984 (0.6%)
41	q	0.80	0/3718	0.98	12/5070 (0.2%)
42	r	0.76	0/2581	1.03	7/3529 (0.2%)
43	s	0.55	0/1387	0.91	1/1876 (0.1%)
44	t	0.55	0/758	1.02	5/1032 (0.5%)
45	5	0.40	0/3531	0.87	10/4793 (0.2%)
45	u	0.50	0/3523	0.90	14/4782 (0.3%)
46	6	0.39	0/3179	0.82	1/4303 (0.0%)
46	v	0.43	0/3179	0.87	4/4303 (0.1%)
47	7	0.45	0/3115	0.87	8/4259 (0.2%)
47	w	0.53	0/3115	0.95	13/4259 (0.3%)
48	8	0.42	0/1976	0.91	7/2681 (0.3%)
48	x	0.44	0/1976	0.95	8/2681 (0.3%)
49	9	0.39	0/941	0.80	2/1262 (0.2%)
49	y	0.41	0/941	0.81	0/1262
50	Aa	0.43	0/701	0.90	2/948 (0.2%)
50	z	0.49	0/688	0.95	1/931 (0.1%)
51	0	0.42	0/534	0.82	1/714 (0.1%)
51	Ab	0.41	0/534	0.79	1/714 (0.1%)
52	1	0.39	0/520	0.78	0/701
52	Ac	0.35	0/520	0.77	1/701 (0.1%)
53	2	0.38	0/1549	0.85	3/2095 (0.1%)
53	4	0.37	0/1549	0.82	4/2095 (0.2%)
54	3	0.39	0/430	0.92	1/590 (0.2%)
54	Ad	0.41	0/410	0.93	0/564
55	Ae	0.40	0/399	0.89	0/542
55	Af	0.42	0/394	0.95	0/536
56	Ag	0.68	0/345	0.99	1/470 (0.2%)
57	Ah	0.71	0/440	1.04	3/596 (0.5%)
58	Ai	0.75	0/398	1.01	1/546 (0.2%)
59	Aj	0.77	0/399	0.97	2/534 (0.4%)
60	Ak	0.86	7/4164 (0.2%)	1.16	36/5688 (0.6%)
61	Al	0.77	0/1868	1.12	12/2544 (0.5%)
62	Am	0.74	0/2211	1.02	8/3023 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
63	An	0.68	0/1229	0.96	3/1658 (0.2%)
64	Ao	0.64	0/898	1.03	6/1218 (0.5%)
65	Ap	0.72	0/765	1.13	3/1038 (0.3%)
66	Aq	0.69	0/699	1.10	6/950 (0.6%)
67	Ar	0.68	0/648	1.17	5/877 (0.6%)
All	All	0.61	8/110582 (0.0%)	0.96	389/150221 (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
2	B	0	1
4	D	0	1
10	J	0	1
21	V	0	1
25	a	0	1
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	Ak	61	HIS	CG-CD2	7.48	1.44	1.35
60	Ak	378	HIS	ND1-CE1	7.33	1.39	1.32
60	Ak	378	HIS	CE1-NE2	-6.50	1.26	1.32
60	Ak	69	MET	SD-CE	-6.26	1.64	1.79
60	Ak	376	HIS	ND1-CE1	5.59	1.38	1.32
60	Ak	61	HIS	ND1-CE1	5.53	1.38	1.32
60	Ak	378	HIS	CG-CD2	5.38	1.41	1.35
26	b	77	ILE	CA-CB	5.30	1.57	1.54

All (389) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	p	155	PRO	N-CA-CB	14.65	110.84	103.22
22	W	10	MET	CA-C-N	-13.21	106.78	120.38
22	W	10	MET	C-N-CA	-13.21	106.78	120.38
13	M	38	PRO	CA-C-N	11.67	132.12	119.28
13	M	38	PRO	C-N-CA	11.67	132.12	119.28
12	L	134	TRP	N-CA-C	10.47	125.36	112.59
60	Ak	376	HIS	ND1-CE1-NE2	10.26	118.66	108.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	435	PRO	N-CA-CB	9.98	110.22	101.83
25	a	109	HIS	N-CA-C	-9.96	100.42	111.28
8	H	170	GLY	CA-C-N	9.58	129.82	119.28
8	H	170	GLY	C-N-CA	9.58	129.82	119.28
45	u	293	GLY	CA-C-N	9.57	129.51	119.85
45	u	293	GLY	C-N-CA	9.57	129.51	119.85
42	r	280	PHE	N-CA-C	9.34	122.66	111.82
20	U	201	LEU	CA-C-N	-9.23	110.87	120.38
20	U	201	LEU	C-N-CA	-9.23	110.87	120.38
67	Ar	52	VAL	N-CA-C	8.91	121.18	108.17
67	Ar	81	PHE	CA-C-N	8.78	128.43	119.56
67	Ar	81	PHE	C-N-CA	8.78	128.43	119.56
47	w	264	THR	CA-C-N	8.75	126.05	119.66
47	w	264	THR	C-N-CA	8.75	126.05	119.66
26	b	30	PRO	N-CA-CB	8.36	110.95	102.17
36	l	562	LEU	CA-C-N	-8.29	109.48	119.84
36	l	562	LEU	C-N-CA	-8.29	109.48	119.84
12	L	133	GLU	N-CA-C	8.24	120.34	111.36
2	B	227	PRO	CA-C-N	-8.16	111.38	119.78
2	B	227	PRO	C-N-CA	-8.16	111.38	119.78
4	D	159	VAL	N-CA-C	8.09	118.19	110.42
59	Aj	20	ARG	N-CA-C	-8.09	102.55	111.36
33	i	255	PRO	N-CA-C	8.08	120.56	110.70
2	B	327	ILE	CB-CA-C	-8.04	103.47	114.00
60	Ak	82	LEU	N-CA-C	8.03	122.35	112.23
60	Ak	378	HIS	ND1-CE1-NE2	7.96	116.36	108.40
27	c	180	PRO	N-CA-CB	7.91	110.72	103.20
13	M	44	GLY	CA-C-N	7.90	127.82	119.05
13	M	44	GLY	C-N-CA	7.90	127.82	119.05
5	E	218	PRO	N-CA-CB	7.86	110.67	103.20
26	b	36	PRO	N-CA-CB	7.72	110.57	103.08
60	Ak	435	GLY	N-CA-C	7.72	126.15	115.27
60	Ak	56	VAL	N-CA-C	-7.66	103.33	110.53
5	E	183	ALA	CA-C-N	-7.66	111.87	119.76
5	E	183	ALA	C-N-CA	-7.66	111.87	119.76
42	r	315	PRO	CA-C-N	7.65	127.54	119.05
42	r	315	PRO	C-N-CA	7.65	127.54	119.05
48	x	195	PRO	CA-C-N	7.64	127.65	119.78
48	x	195	PRO	C-N-CA	7.64	127.65	119.78
42	r	200	LEU	N-CA-C	7.62	120.47	111.71
7	G	166	GLY	CA-C-N	7.58	127.62	119.28
7	G	166	GLY	C-N-CA	7.58	127.62	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	s	89	ILE	N-CA-C	7.58	118.38	110.72
40	p	145	PRO	CA-C-N	-7.45	111.09	119.28
40	p	145	PRO	C-N-CA	-7.45	111.09	119.28
11	K	83	PRO	N-CA-C	7.44	119.78	110.70
44	t	26	PRO	N-CA-CB	7.41	110.27	103.08
53	4	236	CYS	CA-C-N	7.41	127.43	119.28
53	4	236	CYS	C-N-CA	7.41	127.43	119.28
56	Ag	27	LEU	N-CA-C	7.40	119.43	111.36
60	Ak	330	GLY	N-CA-C	7.31	120.37	112.33
26	b	124	PRO	N-CA-CB	7.24	110.85	103.25
60	Ak	9	SER	N-CA-C	7.23	119.90	110.43
45	5	278	ARG	N-CA-C	7.21	122.25	113.17
27	c	174	PRO	N-CA-CB	7.20	110.68	103.48
28	d	18	PRO	N-CA-CB	7.15	110.76	103.25
48	8	247	PRO	CA-C-N	7.15	127.14	119.28
48	8	247	PRO	C-N-CA	7.15	127.14	119.28
60	Ak	376	HIS	CE1-NE2-CD2	-7.14	101.86	109.00
64	Ao	76	GLY	CA-C-N	7.13	128.36	120.45
64	Ao	76	GLY	C-N-CA	7.13	128.36	120.45
60	Ak	332	ILE	N-CA-C	7.11	118.96	109.37
64	Ao	42	VAL	N-CA-C	-7.07	99.70	108.05
28	d	12	GLU	CA-C-N	-7.07	113.10	120.38
28	d	12	GLU	C-N-CA	-7.07	113.10	120.38
28	d	44	PRO	N-CA-CB	7.04	110.77	103.23
3	C	72	PRO	N-CA-CB	7.00	110.48	103.48
44	t	75	PRO	N-CA-CB	7.00	110.23	103.51
37	m	69	GLY	N-CA-C	-6.98	106.18	115.32
7	G	346	VAL	CA-C-N	6.96	134.24	121.70
7	G	346	VAL	C-N-CA	6.96	134.24	121.70
3	C	75	THR	N-CA-C	6.94	118.84	111.28
3	C	162	GLN	CA-C-N	6.93	124.72	119.66
3	C	162	GLN	C-N-CA	6.93	124.72	119.66
60	Ak	130	PRO	N-CA-C	-6.93	102.25	110.70
36	l	477	VAL	CA-C-N	6.92	126.89	119.76
36	l	477	VAL	C-N-CA	6.92	126.89	119.76
62	Am	36	HIS	N-CA-C	6.88	122.09	113.43
2	B	318	ILE	N-CA-C	6.84	114.67	107.76
64	Ao	21	LYS	CA-C-N	6.83	126.34	119.24
64	Ao	21	LYS	C-N-CA	6.83	126.34	119.24
60	Ak	125	GLY	N-CA-C	-6.82	104.23	112.48
15	X	72	PRO	N-CA-CB	6.82	110.50	103.00
47	7	264	THR	CA-C-N	6.81	124.63	119.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	7	264	THR	C-N-CA	6.81	124.63	119.66
19	T	55	VAL	CA-C-N	6.79	126.77	119.78
19	T	55	VAL	C-N-CA	6.79	126.77	119.78
27	c	178	PRO	N-CA-CB	6.78	110.37	103.25
6	F	75	PRO	N-CA-CB	6.77	110.45	103.00
26	b	37	PRO	N-CA-CB	6.76	110.44	103.00
63	An	133	GLY	N-CA-C	6.76	129.20	113.18
15	O	72	PRO	N-CA-CB	6.76	110.43	103.00
20	U	224	GLY	N-CA-C	6.75	120.82	112.73
17	Q	43	VAL	CB-CA-C	-6.74	107.29	113.70
3	C	71	PRO	N-CA-CB	6.74	109.62	103.08
66	Aq	5	LYS	N-CA-C	6.74	125.15	110.80
26	b	33	PRO	N-CA-CB	6.73	110.31	103.25
60	Ak	507	GLU	N-CA-C	-6.73	97.92	109.15
17	Q	76	PRO	N-CA-CB	6.71	110.30	103.25
23	Y	85	PRO	N-CA-CB	6.71	110.29	103.25
8	H	42	ASN	CB-CA-C	-6.67	108.87	116.54
48	8	195	PRO	CA-C-N	6.66	126.64	119.78
48	8	195	PRO	C-N-CA	6.66	126.64	119.78
8	H	162	CYS	CA-C-N	6.63	126.58	119.28
8	H	162	CYS	C-N-CA	6.63	126.58	119.28
27	c	158	PRO	N-CA-CB	6.62	110.20	103.25
47	w	265	PRO	CA-C-N	6.61	126.55	119.28
47	w	265	PRO	C-N-CA	6.61	126.55	119.28
27	c	162	PRO	N-CA-CB	6.60	110.18	103.25
7	G	449	PRO	N-CA-CB	6.58	110.49	103.39
33	i	115	VAL	CA-C-N	-6.57	112.06	119.28
33	i	115	VAL	C-N-CA	-6.57	112.06	119.28
60	Ak	74	MET	N-CA-C	6.56	118.09	111.07
64	Ao	81	ILE	N-CA-C	6.56	116.69	110.53
50	z	51	PRO	N-CA-C	6.55	118.69	110.70
60	Ak	506	GLU	N-CA-C	-6.54	104.15	111.28
53	2	236	CYS	CA-C-N	6.53	126.47	119.28
53	2	236	CYS	C-N-CA	6.53	126.47	119.28
13	M	41	LEU	CA-C-N	6.53	126.51	119.78
13	M	41	LEU	C-N-CA	6.53	126.51	119.78
60	Ak	61	HIS	CB-CG-CD2	-6.51	122.74	131.20
5	E	49	PRO	N-CA-CB	6.48	110.06	103.25
23	Y	89	PRO	N-CA-CB	6.48	110.06	103.25
40	p	156	PRO	N-CA-CB	6.44	110.01	103.25
44	t	27	PRO	N-CA-CB	6.43	110.64	103.44
14	N	106	GLU	CA-C-N	6.41	124.34	119.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	106	GLU	C-N-CA	6.41	124.34	119.66
4	D	224	VAL	N-CA-C	6.41	119.06	111.05
60	Ak	61	HIS	ND1-CE1-NE2	6.41	114.81	108.40
48	x	222	PRO	CA-C-N	6.40	126.37	120.03
48	x	222	PRO	C-N-CA	6.40	126.37	120.03
41	q	189	SER	CB-CA-C	-6.40	109.18	116.54
8	H	116	CYS	N-CA-C	-6.40	105.44	113.18
45	u	421	GLY	N-CA-C	-6.39	100.67	112.62
7	G	540	ASN	CA-C-N	6.39	126.96	120.38
7	G	540	ASN	C-N-CA	6.39	126.96	120.38
45	5	72	GLY	N-CA-C	6.36	120.10	110.18
44	t	23	PRO	N-CA-CB	6.35	110.32	103.33
28	d	20	PRO	N-CA-CB	6.35	109.92	103.25
45	5	339	GLN	N-CA-C	-6.32	104.44	111.71
20	U	304	LEU	N-CA-C	-6.32	104.39	111.28
7	G	406	ASN	CA-C-N	6.31	126.22	119.28
7	G	406	ASN	C-N-CA	6.31	126.22	119.28
28	d	22	PRO	N-CA-CB	6.30	109.86	103.25
11	K	97	PRO	N-CA-CB	6.29	109.92	103.00
7	G	179	CYS	N-CA-C	-6.29	100.35	109.59
66	Aq	2	SER	N-CA-C	6.26	119.56	109.79
60	Ak	10	THR	N-CA-C	-6.25	103.84	112.03
26	b	118	PRO	N-CA-CB	6.22	109.78	103.25
41	q	207	MET	N-CA-C	-6.22	100.60	109.24
20	U	249	PRO	N-CA-CB	6.20	110.09	103.39
47	w	272	TRP	N-CA-C	6.20	118.04	111.28
45	u	424	ILE	CA-C-N	6.18	126.15	119.78
45	u	424	ILE	C-N-CA	6.18	126.15	119.78
67	Ar	63	LEU	N-CA-C	6.14	119.24	111.69
53	4	247	GLY	N-CA-C	-6.12	106.79	115.30
46	v	364	GLY	N-CA-C	-6.12	106.88	115.32
26	b	56	PRO	N-CA-CB	6.11	110.00	103.52
26	b	106	PRO	N-CA-CB	6.09	109.97	103.52
60	Ak	157	SER	N-CA-C	6.08	118.88	111.82
28	d	122	ARG	N-CA-C	-6.08	104.46	112.24
44	t	41	ALA	N-CA-C	6.07	117.90	111.28
42	r	196	ALA	CA-C-N	-6.06	112.62	119.28
42	r	196	ALA	C-N-CA	-6.06	112.62	119.28
27	c	65	TYR	N-CA-C	6.05	123.18	109.81
60	Ak	170	ASN	N-CA-C	6.04	120.72	113.23
20	U	160	VAL	N-CA-C	6.04	116.30	107.37
52	Ac	56	ILE	N-CA-C	-6.03	107.11	112.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	94	GLY	N-CA-C	6.02	118.95	112.33
34	j	98	LEU	N-CA-C	-6.01	104.64	111.07
62	Am	8	TYR	N-CA-C	6.01	118.28	110.53
12	L	55	VAL	N-CA-C	-6.00	96.87	109.34
23	Y	87	PRO	N-CA-CB	6.00	109.86	103.39
24	Z	43	ASP	CA-C-N	5.99	125.87	119.28
24	Z	43	ASP	C-N-CA	5.99	125.87	119.28
7	G	612	PRO	CA-C-N	5.98	125.86	119.28
7	G	612	PRO	C-N-CA	5.98	125.86	119.28
66	Aq	44	ARG	CA-C-N	5.98	126.00	119.90
66	Aq	44	ARG	C-N-CA	5.98	126.00	119.90
45	u	339	GLN	N-CA-C	-5.97	104.69	111.07
41	q	278	ARG	N-CA-C	5.95	118.56	110.06
60	Ak	171	MET	N-CA-C	5.95	120.25	111.87
47	7	284	ILE	CA-C-N	5.95	125.90	119.78
47	7	284	ILE	C-N-CA	5.95	125.90	119.78
61	Al	47	THR	N-CA-C	5.93	119.83	112.59
36	l	588	PHE	N-CA-C	-5.93	104.73	111.14
27	c	155	PRO	N-CA-CB	5.91	109.46	103.25
39	o	83	THR	CA-C-N	5.90	125.77	119.28
39	o	83	THR	C-N-CA	5.90	125.77	119.28
3	C	236	LEU	CA-C-N	5.88	125.83	119.78
3	C	236	LEU	C-N-CA	5.88	125.83	119.78
61	Al	207	MET	CA-C-N	5.87	127.17	119.84
61	Al	207	MET	C-N-CA	5.87	127.17	119.84
39	o	81	ARG	CA-C-N	5.86	125.73	119.28
39	o	81	ARG	C-N-CA	5.86	125.73	119.28
60	Ak	119	GLU	CB-CA-C	-5.86	109.80	116.54
29	e	66	LEU	N-CA-C	-5.86	105.03	111.82
60	Ak	67	PHE	N-CA-C	5.85	119.60	112.23
61	Al	134	ARG	N-CA-C	5.84	123.25	110.80
61	Al	202	SER	N-CA-C	5.84	118.11	111.11
62	Am	198	PHE	N-CA-C	5.83	117.64	111.28
6	F	111	CYS	N-CA-C	-5.83	106.08	113.43
26	b	30	PRO	N-CA-C	-5.83	107.98	114.92
4	D	85	GLU	N-CA-C	5.82	117.10	107.20
54	3	18	ILE	CB-CA-C	-5.82	108.18	114.35
40	p	5	ALA	CA-C-N	5.82	125.75	119.76
40	p	5	ALA	C-N-CA	5.82	125.75	119.76
46	6	134	MET	N-CA-C	-5.78	104.89	111.07
61	Al	190	GLY	N-CA-C	5.78	117.78	110.38
57	Ah	25	GLY	N-CA-C	5.76	119.02	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	Ak	129	TYR	CB-CA-C	-5.75	100.39	109.42
12	L	265	PHE	N-CA-C	5.74	117.88	108.52
14	N	8	THR	CB-CA-C	-5.73	108.32	115.89
36	l	438	PRO	CA-C-N	5.73	125.66	119.76
36	l	438	PRO	C-N-CA	5.73	125.66	119.76
40	p	149	PRO	N-CA-CB	5.73	109.58	103.39
41	q	112	ALA	CA-C-N	5.72	132.00	121.70
41	q	112	ALA	C-N-CA	5.72	132.00	121.70
4	D	216	VAL	N-CA-C	-5.71	107.42	112.90
45	5	298	ASN	CA-C-N	5.70	125.37	119.56
45	5	298	ASN	C-N-CA	5.70	125.37	119.56
36	l	111	ASP	CA-C-N	5.69	125.60	119.85
36	l	111	ASP	C-N-CA	5.69	125.60	119.85
47	w	318	ARG	CA-C-N	5.68	125.53	119.28
47	w	318	ARG	C-N-CA	5.68	125.53	119.28
12	L	269	ASN	N-CA-C	5.67	118.21	110.55
32	h	46	GLY	N-CA-C	-5.67	108.43	114.67
2	B	150	GLY	N-CA-C	-5.67	106.36	115.08
47	w	218	ILE	N-CA-C	5.66	113.83	109.19
29	e	62	GLU	CA-C-N	-5.64	112.70	120.71
29	e	62	GLU	C-N-CA	-5.64	112.70	120.71
10	J	121	LEU	N-CA-C	5.63	117.65	110.61
33	i	165	GLY	N-CA-C	-5.62	107.96	115.32
8	H	178	GLU	N-CA-C	5.61	117.40	111.28
61	Al	104	TRP	N-CA-C	5.61	122.75	110.80
20	U	314	VAL	N-CA-C	-5.61	108.38	113.71
40	p	78	GLN	CA-C-N	5.61	125.58	120.03
40	p	78	GLN	C-N-CA	5.61	125.58	120.03
45	u	45	VAL	CA-C-N	5.61	125.51	119.85
45	u	45	VAL	C-N-CA	5.61	125.51	119.85
3	C	365	PRO	CA-C-N	5.61	125.56	119.78
3	C	365	PRO	C-N-CA	5.61	125.56	119.78
12	L	203	PRO	N-CA-C	5.60	119.87	111.14
46	v	182	TYR	N-CA-C	5.60	117.91	109.23
63	An	129	ALA	CA-C-N	5.59	126.83	119.84
63	An	129	ALA	C-N-CA	5.59	126.83	119.84
20	U	204	HIS	N-CA-C	5.58	116.26	108.00
1	A	20	HIS	N-CA-C	5.58	118.12	111.71
40	p	133	TRP	N-CA-C	5.57	117.35	111.28
7	G	471	LYS	CA-C-N	5.56	125.50	119.78
7	G	471	LYS	C-N-CA	5.56	125.50	119.78
34	j	28	ASN	N-CA-C	5.56	117.77	107.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	q	72	LEU	N-CA-C	5.56	118.27	111.82
35	k	87	THR	N-CA-C	5.55	117.90	110.35
45	u	460	GLY	N-CA-C	5.55	123.66	112.34
15	X	130	ILE	N-CA-C	5.55	113.98	107.77
40	p	144	THR	CA-C-N	5.55	126.09	120.38
40	p	144	THR	C-N-CA	5.55	126.09	120.38
59	Aj	16	GLU	N-CA-C	5.53	117.39	111.36
65	Ap	82	CYS	CA-C-N	5.53	125.37	119.28
65	Ap	82	CYS	C-N-CA	5.53	125.37	119.28
20	U	165	ILE	N-CA-C	5.52	116.25	110.62
47	7	8	HIS	CA-C-N	5.50	125.33	119.28
47	7	8	HIS	C-N-CA	5.50	125.33	119.28
12	L	195	PHE	CA-C-N	5.50	125.33	119.28
12	L	195	PHE	C-N-CA	5.50	125.33	119.28
48	x	235	ASN	CA-C-N	5.49	125.32	119.28
48	x	235	ASN	C-N-CA	5.49	125.32	119.28
62	Am	188	ILE	CB-CA-C	-5.49	104.74	112.14
45	u	453	CYS	CA-C-N	5.47	125.38	119.85
45	u	453	CYS	C-N-CA	5.47	125.38	119.85
15	X	154	VAL	N-CA-C	5.46	117.92	111.09
28	d	27	PRO	N-CA-CB	5.46	109.29	103.39
66	Aq	72	ASN	CA-C-N	5.45	125.79	119.47
66	Aq	72	ASN	C-N-CA	5.45	125.79	119.47
7	G	364	ASP	N-CA-C	5.45	117.12	108.79
7	G	685	VAL	N-CA-C	5.44	113.94	107.73
46	v	197	ILE	N-CA-C	5.44	116.08	110.36
3	C	64	PRO	CA-C-N	5.44	125.38	119.78
3	C	64	PRO	C-N-CA	5.44	125.38	119.78
22	W	30	LEU	N-CA-C	5.43	115.19	108.19
47	w	284	ILE	CA-C-N	5.43	125.37	119.78
47	w	284	ILE	C-N-CA	5.43	125.37	119.78
20	U	93	ILE	N-CA-C	5.42	116.14	110.62
57	Ah	2	GLU	N-CA-C	5.42	122.33	110.80
4	D	104	THR	N-CA-C	-5.41	99.29	110.80
41	q	168	GLN	N-CA-C	-5.41	106.64	113.18
32	h	94	PRO	N-CA-C	5.40	117.29	110.70
45	5	293	GLY	CA-C-N	5.40	125.34	119.78
45	5	293	GLY	C-N-CA	5.40	125.34	119.78
46	v	174	LEU	N-CA-C	5.40	117.98	111.40
51	0	88	ASN	N-CA-C	-5.39	106.65	113.18
22	W	11	PRO	N-CA-C	5.39	117.28	110.70
60	Ak	372	TYR	N-CA-C	-5.38	105.31	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	Ak	245	ILE	N-CA-C	-5.38	104.33	111.05
48	8	285	HIS	N-CA-C	5.36	117.21	111.36
29	e	76	TYR	CB-CA-C	-5.36	108.83	116.34
21	V	93	GLY	N-CA-C	-5.35	105.92	112.77
47	w	203	THR	N-CA-C	-5.35	107.76	114.56
60	Ak	159	LEU	N-CA-C	-5.34	105.54	111.36
25	a	166	GLY	CA-C-N	5.34	125.15	119.28
25	a	166	GLY	C-N-CA	5.34	125.15	119.28
50	Aa	50	ALA	CA-C-N	-5.34	114.88	120.38
50	Aa	50	ALA	C-N-CA	-5.34	114.88	120.38
45	5	358	PHE	N-CA-C	5.30	116.90	108.79
41	q	456	GLY	CA-C-N	5.29	125.10	119.28
41	q	456	GLY	C-N-CA	5.29	125.10	119.28
14	N	107	PRO	O-C-N	5.29	123.74	121.31
53	4	223	VAL	N-CA-C	5.29	113.10	107.76
31	g	25	PRO	O-C-N	5.28	123.63	121.15
41	q	44	GLN	CB-CA-C	-5.28	109.51	115.79
60	Ak	305	PHE	N-CA-C	5.28	118.81	112.38
7	G	184	ARG	N-CA-C	-5.27	106.11	112.54
35	k	54	THR	N-CA-C	5.27	117.77	111.71
65	Ap	38	ALA	N-CA-C	5.27	117.93	110.50
45	u	319	GLY	N-CA-C	-5.25	107.47	115.66
12	L	308	SER	CA-C-N	5.23	125.04	119.28
12	L	308	SER	C-N-CA	5.23	125.04	119.28
5	E	91	GLY	N-CA-C	-5.23	108.03	115.30
35	k	24	SER	CB-CA-C	-5.22	109.57	115.79
13	M	95	VAL	N-CA-C	5.22	115.24	108.35
60	Ak	262	SER	N-CA-C	-5.22	106.60	113.17
47	7	318	ARG	CA-C-N	5.21	124.83	119.05
47	7	318	ARG	C-N-CA	5.21	124.83	119.05
7	G	547	LEU	N-CA-C	-5.20	106.09	112.90
60	Ak	401	SER	N-CA-C	5.18	119.73	113.41
60	Ak	353	LEU	N-CA-C	-5.17	105.72	111.36
60	Ak	377	PHE	N-CA-C	5.17	119.44	113.18
62	Am	99	TRP	N-CA-C	-5.17	105.53	111.07
7	G	124	HIS	CA-C-N	5.17	125.10	119.78
7	G	124	HIS	C-N-CA	5.17	125.10	119.78
9	I	86	THR	N-CA-C	5.16	116.82	108.26
41	q	346	ARG	CB-CA-C	-5.16	110.22	117.23
2	B	412	LEU	N-CA-C	-5.14	105.57	111.07
42	r	28	LEU	N-CA-C	-5.14	106.11	112.38
45	u	465	LEU	CA-C-N	5.13	125.07	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	u	465	LEU	C-N-CA	5.13	125.07	119.78
47	w	156	ILE	N-CA-C	5.13	115.85	110.62
1	A	2	THR	N-CA-C	5.12	116.20	108.46
61	Al	165	VAL	CA-C-N	5.12	126.25	119.84
61	Al	165	VAL	C-N-CA	5.12	126.25	119.84
7	G	686	PRO	CA-C-N	5.12	124.91	119.28
7	G	686	PRO	C-N-CA	5.12	124.91	119.28
11	K	82	VAL	CB-CA-C	-5.11	107.30	114.00
57	Ah	9	GLN	N-CA-C	-5.11	105.60	111.07
49	9	51	LEU	CA-C-N	5.10	125.04	119.78
49	9	51	LEU	C-N-CA	5.10	125.04	119.78
67	Ar	22	ASN	N-CA-C	5.10	117.61	109.81
47	w	133	LEU	N-CA-C	5.09	120.39	113.16
2	B	222	LYS	CA-C-N	5.09	125.00	119.76
2	B	222	LYS	C-N-CA	5.09	125.00	119.76
17	Q	97	TRP	N-CA-C	-5.09	103.82	110.53
60	Ak	73	ILE	N-CA-C	5.08	115.23	110.30
19	T	16	GLU	CA-C-N	5.08	124.69	119.05
19	T	16	GLU	C-N-CA	5.08	124.69	119.05
2	B	104	LYS	CA-C-N	5.08	126.19	119.84
2	B	104	LYS	C-N-CA	5.08	126.19	119.84
62	Am	244	PHE	N-CA-C	-5.07	105.19	111.33
3	C	175	GLY	N-CA-C	-5.06	106.65	112.73
41	q	370	PRO	O-C-N	5.06	123.64	121.31
60	Ak	6	TRP	N-CA-C	5.06	119.72	113.50
61	Al	66	THR	N-CA-C	-5.06	107.77	114.04
51	Ab	86	LEU	N-CA-C	5.05	116.78	111.28
60	Ak	2	PHE	N-CA-C	-5.04	105.67	111.07
61	Al	12	ALA	N-CA-C	5.04	117.47	109.96
62	Am	107	ALA	CA-C-N	5.04	125.82	119.98
62	Am	107	ALA	C-N-CA	5.04	125.82	119.98
48	8	176	PHE	CA-C-N	5.03	124.97	119.78
48	8	176	PHE	C-N-CA	5.03	124.97	119.78
28	d	62	TYR	N-CA-C	5.02	116.71	109.07
45	5	465	LEU	CA-C-N	5.02	124.95	119.78
45	5	465	LEU	C-N-CA	5.02	124.95	119.78
60	Ak	378	HIS	N-CA-C	-5.02	106.33	112.90
61	Al	65	TRP	N-CA-C	5.02	119.12	113.15
60	Ak	70	VAL	N-CA-C	5.01	115.44	110.23
53	2	247	GLY	N-CA-C	-5.01	107.36	115.08
48	x	178	LYS	CA-C-N	5.01	124.61	119.05
48	x	178	LYS	C-N-CA	5.01	124.61	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	Ai	35	GLN	N-CA-C	5.01	119.15	113.19
7	G	411	ALA	CA-C-N	5.00	124.61	119.05
7	G	411	ALA	C-N-CA	5.00	124.61	119.05
3	C	144	MET	N-CA-C	5.00	117.62	111.82

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	327	ILE	Peptide
4	D	223	PRO	Peptide
10	J	98	LYS	Peptide
21	V	12	ILE	Peptide
25	a	109	HIS	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	598	0	612	14	0
2	B	3128	0	3089	195	0
3	C	3391	0	3271	218	0
4	D	1679	0	1611	130	0
5	E	1463	0	1373	88	0
6	F	242	0	156	8	0
7	G	5005	0	4900	392	0
8	H	1408	0	1356	75	0
9	I	1241	0	1249	101	0
10	J	877	0	854	63	0
11	K	520	0	276	10	0
11	R	90	0	32	28	0
12	L	2665	0	2631	205	0
13	M	685	0	646	41	0
14	N	895	0	915	65	0
15	O	647	0	602	43	0
15	X	663	0	634	34	0
16	P	673	0	685	47	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	942	0	925	89	0
18	S	567	0	565	27	0
19	T	622	0	602	24	0
20	U	1941	0	1585	132	0
21	V	1009	0	1006	40	0
22	W	1122	0	1088	57	0
23	Y	400	0	290	14	0
24	Z	550	0	475	20	0
25	a	1124	0	1107	74	0
26	b	741	0	573	28	0
27	c	1073	0	872	54	0
28	d	1233	0	1038	67	0
29	e	757	0	686	53	0
30	f	300	0	310	6	0
31	g	996	0	990	53	0
32	h	798	0	746	57	0
33	i	2706	0	2863	158	0
34	j	893	0	927	57	0
35	k	718	0	753	51	0
36	l	4790	0	4919	249	0
37	m	1280	0	1251	80	0
38	n	359	0	321	12	0
39	o	1021	0	1006	42	0
40	p	1415	0	1294	75	0
41	q	3627	0	3830	196	0
42	r	2508	0	2607	139	0
43	s	1350	0	1310	97	0
44	t	749	0	547	47	0
45	5	3459	0	3349	271	0
45	u	3452	0	3339	204	0
46	6	3127	0	3105	199	0
46	v	3127	0	3105	185	0
47	7	3017	0	3078	202	0
47	w	3017	0	3078	238	0
48	8	1918	0	1862	147	0
48	x	1918	0	1862	155	0
49	9	921	0	917	65	0
49	y	921	0	917	37	0
50	Aa	679	0	677	53	0
50	z	666	0	663	30	0
51	0	528	0	510	32	0
51	Ab	528	0	510	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	1	507	0	509	28	0
52	Ac	507	0	509	28	0
53	2	1517	0	1496	91	0
53	4	1517	0	1496	112	0
54	3	414	0	407	24	0
54	Ad	395	0	385	26	0
55	Ae	394	0	406	34	0
55	Af	389	0	398	22	0
56	Ag	335	0	352	13	0
57	Ah	431	0	428	17	0
58	Ai	384	0	366	12	0
59	Aj	386	0	388	8	0
60	Ak	4025	0	4003	87	0
61	Al	1822	0	1834	73	0
62	Am	2124	0	2044	50	0
63	An	1195	0	1183	33	0
64	Ao	878	0	868	21	0
65	Ap	748	0	728	27	0
66	Aq	672	0	645	29	0
67	Ar	628	0	582	21	0
68	B	8	0	0	4	0
68	G	16	0	0	5	0
68	H	16	0	0	4	0
68	I	8	0	0	0	0
69	B	31	0	19	25	0
70	2	4	0	0	2	0
70	4	4	0	0	1	0
70	E	4	0	0	1	0
70	G	4	0	0	0	0
71	2	52	0	88	25	0
71	4	52	0	88	5	0
71	H	52	0	88	7	0
71	V	52	0	88	2	0
71	i	52	0	88	6	0
72	L	48	0	26	12	0
73	Q	34	0	40	22	0
73	X	34	0	40	7	0
74	5	64	0	72	7	0
74	8	64	0	72	7	0
74	Aa	64	0	72	17	0
74	V	63	0	68	5	0
74	i	64	0	72	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
74	l	64	0	72	7	0
74	s	64	0	72	2	0
74	u	64	0	72	17	0
74	x	64	0	72	7	0
74	z	64	0	72	6	0
75	2	49	0	75	46	0
75	5	49	0	75	18	0
75	7	90	0	131	45	0
75	W	49	0	75	8	0
75	i	49	0	75	19	0
75	l	49	0	75	6	0
75	q	49	0	75	9	0
75	u	49	0	75	50	0
75	w	49	0	75	31	0
76	7	86	0	60	35	0
76	w	86	0	60	36	0
77	8	43	0	32	9	0
77	x	43	0	32	10	0
78	Ak	120	0	108	4	0
79	Ak	1	0	0	0	0
79	Al	2	0	0	0	0
80	Ak	1	0	0	0	0
81	Ap	1	0	0	0	0
All	All	109982	0	107681	5573	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 26.

All (5573) 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)
76:w:402:HEM:CHA	76:w:402:HEM:C1A	1.74	1.68
76:7:403:HEM:CHB	76:7:403:HEM:C4A	1.77	1.67
76:w:401:HEM:CHB	76:w:401:HEM:C4A	1.76	1.67
76:7:404:HEM:CHA	76:7:404:HEM:C1A	1.75	1.65
76:w:401:HEM:CHA	76:w:401:HEM:C1A	1.75	1.63
76:w:402:HEM:CHB	76:w:402:HEM:C4A	1.75	1.63
76:7:403:HEM:CHA	76:7:403:HEM:C1A	1.74	1.62
76:7:404:HEM:CHB	76:7:404:HEM:C4A	1.76	1.62
7:G:314:LEU:CB	11:R:139:PRO:CB	1.77	1.56
47:w:234:PHE:CE1	48:x:301:LEU:HD22	1.38	1.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:314:LEU:HB2	11:R:139:PRO:CB	1.21	1.56
20:U:85:LEU:CB	20:U:159:VAL:HA	1.13	1.55
20:U:150:GLU:HB2	20:U:300:VAL:CG1	1.24	1.54
44:t:111:ARG:NH1	44:t:115:ARG:HH12	1.08	1.49
71:2:301:PLX:H182	75:2:302:PEE:C39	1.40	1.46
43:s:46:CYS:SG	43:s:56:CYS:SG	1.47	1.45
12:L:201:ILE:HG22	12:L:203:PRO:CD	1.46	1.44
47:w:234:PHE:CZ	48:x:301:LEU:HD22	1.51	1.43
20:U:150:GLU:CB	20:U:300:VAL:HG11	1.48	1.42
7:G:314:LEU:CD1	11:R:139:PRO:CB	1.95	1.42
74:u:501:CDL:C36	75:u:502:PEE:H28	1.49	1.42
7:G:371:VAL:HG23	7:G:482:GLN:CG	1.51	1.40
7:G:371:VAL:CG2	7:G:482:GLN:CG	1.98	1.39
45:5:278:ARG:HH12	45:5:463:GLU:N	1.13	1.39
45:5:278:ARG:NH1	45:5:463:GLU:N	1.72	1.37
74:u:501:CDL:H361	75:u:502:PEE:C18	1.53	1.37
23:Y:88:ASP:CB	44:t:100:LYS:NZ	1.88	1.36
17:Q:82:LEU:HD21	73:Q:201:ZMP:C11	1.55	1.35
20:U:85:LEU:CB	20:U:159:VAL:CA	2.02	1.35
44:t:111:ARG:NH1	44:t:115:ARG:NH1	1.74	1.32
7:G:371:VAL:CG2	7:G:482:GLN:HG3	1.52	1.32
10:J:63:THR:HG22	17:Q:70:ASN:ND2	1.40	1.32
7:G:314:LEU:HD12	11:R:139:PRO:CB	1.54	1.31
3:C:286:TYR:CA	4:D:162:ALA:HB2	1.61	1.28
71:2:301:PLX:C18	75:2:302:PEE:H65	1.62	1.28
45:5:478:LEU:CD1	75:5:502:PEE:H12	1.65	1.27
75:7:402:PEE:H12	74:Aa:101:CDL:PA1	1.72	1.27
76:7:404:HEM:C4A	76:7:404:HEM:C1B	2.02	1.26
76:7:403:HEM:CHA	76:7:403:HEM:C2A	2.18	1.25
76:w:402:HEM:CHA	76:w:402:HEM:C2A	2.20	1.25
76:7:404:HEM:CHB	76:7:404:HEM:C3A	2.20	1.25
76:w:402:HEM:CHB	76:w:402:HEM:C3A	2.19	1.24
47:w:316:MET:HB2	75:w:403:PEE:O2P	1.31	1.24
47:w:234:PHE:CE1	48:x:301:LEU:CD2	2.20	1.24
76:w:401:HEM:CHB	76:w:401:HEM:C3A	2.20	1.24
44:t:111:ARG:CD	44:t:115:ARG:HH11	1.50	1.24
76:w:402:HEM:C4A	76:w:402:HEM:C1B	2.07	1.24
12:L:206:ILE:CG2	12:L:245:VAL:HG21	1.67	1.23
76:7:403:HEM:C4A	76:7:403:HEM:C1B	2.08	1.23
7:G:314:LEU:HD12	11:R:139:PRO:CA	1.68	1.22
53:2:136:PHE:CD2	75:2:302:PEE:H34	1.73	1.21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:265:PHE:CD1	12:L:335:LEU:HB2	1.58	1.21
76:w:401:HEM:C1A	76:w:401:HEM:C4D	2.14	1.20
7:G:314:LEU:CG	11:R:139:PRO:CB	2.18	1.20
76:w:401:HEM:CHA	76:w:401:HEM:C2A	2.22	1.20
76:7:404:HEM:CHA	76:7:404:HEM:C2A	2.24	1.20
76:w:402:HEM:C1A	76:w:402:HEM:C4D	2.14	1.19
12:L:128:ASN:O	12:L:167:ILE:HD12	1.42	1.19
44:t:111:ARG:HH11	44:t:115:ARG:NH1	1.34	1.18
12:L:201:ILE:CG2	12:L:203:PRO:HD3	1.72	1.18
76:w:401:HEM:C4A	76:w:401:HEM:C1B	2.11	1.18
76:7:403:HEM:C1A	76:7:403:HEM:C4D	2.21	1.18
5:E:63:ILE:O	5:E:67:VAL:HG23	1.40	1.17
76:7:403:HEM:CHB	76:7:403:HEM:C3A	2.26	1.17
2:B:118:ASP:HB3	69:B:502:FMN:HM72	1.27	1.17
76:7:404:HEM:C1A	76:7:404:HEM:C4D	2.21	1.17
74:u:501:CDL:C14	75:u:502:PEE:H54	1.72	1.17
17:Q:82:LEU:CD2	73:Q:201:ZMP:C11	2.22	1.16
44:t:111:ARG:HD3	44:t:115:ARG:NH1	1.58	1.16
47:w:30:TRP:CZ3	75:w:403:PEE:H21	1.81	1.16
7:G:371:VAL:HG22	7:G:482:GLN:HG2	1.25	1.16
7:G:313:LEU:CD2	11:R:141:SER:O	1.95	1.15
10:J:63:THR:CG2	17:Q:70:ASN:ND2	2.08	1.15
12:L:201:ILE:CG2	12:L:203:PRO:CD	2.23	1.15
41:q:191:SER:OG	75:q:501:PEE:H3	1.43	1.15
54:Ad:4:ARG:NH2	54:Ad:5:PHE:CE2	2.15	1.15
7:G:472:PRO:HG3	7:G:500:ILE:HG21	1.21	1.14
75:u:502:PEE:H17	71:2:301:PLX:H72	1.19	1.14
53:2:136:PHE:CE2	75:2:302:PEE:H34	1.82	1.14
27:c:168:LEU:CA	44:t:98:ARG:HB3	1.78	1.13
75:7:402:PEE:C5	74:Aa:101:CDL:OA4	1.97	1.13
47:w:244:LEU:HD23	48:x:290:GLY:HA2	1.26	1.13
43:s:46:CYS:SG	43:s:56:CYS:CB	2.35	1.12
33:i:291:TYR:CE2	75:i:501:PEE:H48	1.83	1.12
12:L:129:LEU:HD12	12:L:167:ILE:HD11	1.31	1.11
12:L:206:ILE:HG21	12:L:245:VAL:HG21	1.28	1.11
17:Q:82:LEU:CD2	73:Q:201:ZMP:H11	1.81	1.11
47:w:316:MET:CB	75:w:403:PEE:O2P	1.99	1.11
43:s:47:ARG:HH12	43:s:53:PRO:CA	1.63	1.11
47:w:244:LEU:HD23	48:x:290:GLY:CA	1.79	1.11
27:c:168:LEU:HA	44:t:98:ARG:CB	1.81	1.10
45:5:478:LEU:HD11	75:5:502:PEE:H12	1.30	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:286:TYR:HA	4:D:162:ALA:CB	1.81	1.10
75:u:502:PEE:H49	75:u:502:PEE:H19	1.11	1.10
75:7:402:PEE:H12	74:Aa:101:CDL:OA3	1.49	1.10
54:Ad:4:ARG:CZ	54:Ad:5:PHE:CE2	2.35	1.10
20:U:150:GLU:CB	20:U:300:VAL:CG1	2.14	1.10
26:b:126:GLN:HA	44:t:85:HIS:CE1	1.87	1.10
43:s:47:ARG:NH1	43:s:53:PRO:CA	2.15	1.10
12:L:201:ILE:HG22	12:L:203:PRO:HD3	1.20	1.09
12:L:265:PHE:CD1	12:L:335:LEU:CB	2.32	1.08
54:Ad:4:ARG:NH2	54:Ad:5:PHE:HE2	1.50	1.08
12:L:211:ASP:OD2	12:L:214:LEU:N	1.86	1.07
12:L:211:ASP:OD1	12:L:213:PHE:N	1.87	1.07
12:L:201:ILE:HG22	12:L:203:PRO:HD2	1.33	1.07
17:Q:71:ALA:HA	73:Q:201:ZMP:H15A	1.37	1.07
12:L:128:ASN:HD21	12:L:152:ILE:HG21	1.13	1.06
75:W:401:PEE:C45	42:r:73:ILE:CG1	2.34	1.06
23:Y:88:ASP:CB	44:t:100:LYS:HZ1	1.54	1.05
17:Q:82:LEU:CD2	73:Q:201:ZMP:H11A	1.84	1.05
73:X:201:ZMP:H4A	40:p:44:MET:HE1	1.38	1.04
3:C:80:LEU:HD13	3:C:81:THR:N	1.72	1.03
12:L:204:SER:OG	12:L:266:VAL:HA	1.58	1.03
45:5:278:ARG:NH2	45:5:461:PRO:HB2	1.73	1.03
7:G:479:SER:OG	7:G:687:PRO:HD3	1.58	1.03
44:t:111:ARG:HD3	44:t:115:ARG:HH11	0.93	1.03
47:7:30:TRP:CH2	75:7:402:PEE:H21	1.94	1.02
17:Q:63:VAL:HG22	73:Q:201:ZMP:H4	1.38	1.02
20:U:87:HIS:HA	20:U:160:VAL:HG13	1.38	1.02
20:U:150:GLU:HB2	20:U:300:VAL:HG13	1.39	1.02
20:U:85:LEU:O	20:U:160:VAL:HG12	1.58	1.01
74:u:501:CDL:H142	75:u:502:PEE:H54	1.36	1.01
75:u:502:PEE:C13	71:2:301:PLX:H72	1.91	1.01
12:L:129:LEU:HD12	12:L:167:ILE:CD1	1.91	1.01
74:u:501:CDL:H141	75:u:502:PEE:H54	1.42	1.00
75:2:302:PEE:H73	75:2:302:PEE:H64	1.42	1.00
17:Q:71:ALA:HA	73:Q:201:ZMP:C15	1.91	0.99
20:U:304:LEU:H	20:U:304:LEU:HD12	1.24	0.99
7:G:370:GLU:OE1	7:G:482:GLN:NE2	1.96	0.98
47:w:316:MET:HE3	75:w:403:PEE:O1P	1.62	0.98
75:u:502:PEE:H50	75:u:502:PEE:H16	1.45	0.98
2:B:118:ASP:CB	69:B:502:FMN:HM72	1.94	0.98
75:7:402:PEE:N	74:Aa:101:CDL:OA4	1.97	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:i:291:TYR:CZ	75:i:501:PEE:H48	1.99	0.98
9:I:123:MET:HB2	9:I:144:MET:HE1	1.44	0.97
23:Y:88:ASP:CB	44:t:100:LYS:HZ3	1.59	0.97
48:x:118:TYR:HA	48:x:122:CYS:HB2	1.45	0.97
75:u:502:PEE:H16	75:u:502:PEE:C32	1.95	0.97
7:G:403:VAL:HG11	7:G:476:LEU:CD1	1.95	0.96
48:8:288:ARG:HH12	52:Ac:41:ASP:CG	1.72	0.96
7:G:314:LEU:HD12	11:R:139:PRO:HA	1.43	0.96
75:W:401:PEE:C45	42:r:73:ILE:HG13	1.95	0.96
47:7:30:TRP:CZ3	75:7:402:PEE:H21	2.01	0.96
43:s:47:ARG:HH12	43:s:53:PRO:N	1.63	0.96
75:u:502:PEE:H49	75:u:502:PEE:C14	1.95	0.96
47:w:25:SER:HB3	47:w:218:ILE:HD12	1.48	0.96
76:w:401:HEM:CHA	76:w:401:HEM:HAA1	1.96	0.95
43:s:47:ARG:NH1	43:s:53:PRO:HA	1.80	0.95
45:5:276:ARG:HD3	45:5:462:ILE:HD12	1.47	0.95
75:u:502:PEE:H17	71:2:301:PLX:C7	1.96	0.95
48:8:280:GLU:CD	48:8:283:HIS:HD2	1.73	0.95
75:u:502:PEE:H19	75:u:502:PEE:C31	1.96	0.95
48:8:280:GLU:OE2	48:8:283:HIS:HD2	1.49	0.95
7:G:371:VAL:HG22	7:G:482:GLN:CG	1.80	0.95
45:5:278:ARG:NH1	45:5:462:ILE:C	2.23	0.95
7:G:371:VAL:CG2	7:G:482:GLN:HG2	1.81	0.95
12:L:265:PHE:HD1	12:L:335:LEU:HB2	1.26	0.94
12:L:207:PHE:CZ	12:L:345:LEU:HA	2.02	0.94
12:L:238:GLN:HG3	12:L:269:ASN:O	1.68	0.94
20:U:88:PHE:CB	20:U:162:GLU:N	2.31	0.94
43:s:47:ARG:NH1	43:s:53:PRO:HB3	1.82	0.94
60:Ak:365:ILE:HD12	61:Al:87:MET:HE1	1.48	0.94
12:L:204:SER:CB	12:L:265:PHE:O	2.15	0.94
26:b:126:GLN:HA	44:t:85:HIS:HE1	1.32	0.94
43:s:47:ARG:NH1	43:s:53:PRO:CB	2.31	0.94
75:2:302:PEE:H66	75:2:302:PEE:H28	1.49	0.93
75:u:502:PEE:C31	75:u:502:PEE:H26	1.97	0.93
44:t:111:ARG:CZ	44:t:115:ARG:NH1	2.30	0.93
2:B:119:GLU:H	69:B:502:FMN:C7M	1.80	0.93
71:2:301:PLX:H181	75:2:302:PEE:H70	1.49	0.93
27:c:39:GLY:O	27:c:74:ASP:CB	2.17	0.92
75:7:402:PEE:C5	74:Aa:101:CDL:PA1	2.57	0.92
43:s:47:ARG:HH11	43:s:53:PRO:HB3	1.34	0.92
45:5:278:ARG:HH21	45:5:461:PRO:HB2	1.31	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:w:244:LEU:CD2	48:x:290:GLY:HA2	2.00	0.92
20:U:299:LEU:HD21	20:U:306:VAL:HG12	1.51	0.92
60:Ak:449:MET:SD	61:Al:5:MET:HE2	2.09	0.92
41:q:261:PHE:HE1	75:q:501:PEE:H44	1.33	0.92
12:L:265:PHE:CE1	12:L:335:LEU:HA	2.05	0.92
3:C:182:ASN:HD22	3:C:403:PRO:HB2	1.32	0.92
66:Aq:5:LYS:HZ3	66:Aq:6:GLY:H	0.93	0.92
48:8:291:LEU:HD23	52:Ac:44:TYR:HB2	1.52	0.91
2:B:125:CYS:HB3	5:E:181:VAL:HG23	1.49	0.91
47:w:103:TYR:CE2	75:w:403:PEE:H13	2.04	0.91
75:w:403:PEE:H8	74:z:101:CDL:HA32	1.48	0.91
7:G:314:LEU:HB3	11:R:139:PRO:CB	1.97	0.91
47:w:30:TRP:HZ3	75:w:403:PEE:H21	1.33	0.91
7:G:560:LEU:HD11	7:G:566:ILE:HD11	1.52	0.90
76:w:401:HEM:CHA	76:w:401:HEM:CAA	2.48	0.90
12:L:129:LEU:HA	12:L:167:ILE:HD13	1.49	0.90
53:2:132:ALA:HB1	75:2:302:PEE:H24	1.54	0.90
48:x:122:CYS:HA	77:x:401:HEC:HAB	1.51	0.90
47:w:234:PHE:CZ	48:x:301:LEU:CD2	2.46	0.90
7:G:472:PRO:CG	7:G:500:ILE:HG21	2.00	0.90
53:2:132:ALA:CB	75:2:302:PEE:H24	2.02	0.89
71:2:301:PLX:H182	75:2:302:PEE:H64	1.52	0.89
45:u:480:PHE:CD1	54:3:20:THR:OG1	2.25	0.89
7:G:136:GLU:O	10:J:88:GLN:NE2	2.06	0.89
20:U:91:ALA:HB2	20:U:144:GLN:NE2	1.86	0.89
53:2:136:PHE:HE2	75:2:302:PEE:H30	1.37	0.89
9:I:211:ARG:NH1	9:I:211:ARG:HB3	1.88	0.89
41:q:191:SER:OG	75:q:501:PEE:C1	2.20	0.89
22:W:71:LEU:HB3	22:W:75:PHE:HE2	1.36	0.89
47:w:234:PHE:CD1	48:x:301:LEU:HD22	2.06	0.89
46:v:246:LEU:HD23	46:v:248:GLY:H	1.37	0.88
47:7:237:LEU:HD13	48:8:297:MET:HG2	1.55	0.88
24:Z:29:LEU:HD22	24:Z:50:ALA:HB2	1.55	0.88
62:Am:112:LEU:HG	62:Am:118:PRO:HB3	1.55	0.88
7:G:652:ASN:HB2	7:G:655:ARG:HH21	1.39	0.88
45:5:278:ARG:HH12	45:5:463:GLU:H	0.94	0.88
3:C:399:ALA:HB3	4:D:140:ARG:HH12	1.38	0.88
45:5:52:GLN:HE22	45:5:58:ARG:HE	1.18	0.88
7:G:481:LEU:O	7:G:486:GLY:HA3	1.74	0.87
45:5:268:CYS:HG	45:5:351:THR:HG1	1.09	0.87
45:u:44:SER:HB2	46:v:55:TYR:CB	2.04	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:ASN:N	69:B:502:FMN:O2P	2.06	0.87
20:U:91:ALA:HB1	20:U:95:TYR:CG	2.09	0.87
75:u:502:PEE:H1	71:2:301:PLX:H4	1.53	0.87
20:U:150:GLU:CA	20:U:300:VAL:HG11	2.05	0.87
47:7:326:TRP:HH2	75:7:402:PEE:O5	1.55	0.87
12:L:128:ASN:O	12:L:167:ILE:CD1	2.22	0.87
47:7:326:TRP:CH2	75:7:402:PEE:O5	2.28	0.86
42:r:41:GLY:HA3	42:r:44:GLY:H	1.37	0.86
32:h:95:PRO:CB	32:h:99:LEU:CB	2.52	0.86
66:Aq:5:LYS:HZ3	66:Aq:6:GLY:N	1.73	0.86
3:C:166:ARG:NH1	22:W:10:MET:SD	2.48	0.86
12:L:175:LYS:O	12:L:182:ARG:NH1	2.09	0.86
47:w:234:PHE:CD1	48:x:301:LEU:CD2	2.57	0.86
7:G:300:GLN:HB2	11:R:137:TRP:CB	2.06	0.86
12:L:206:ILE:CG2	12:L:245:VAL:CG2	2.52	0.86
33:i:291:TYR:CZ	75:i:501:PEE:C31	2.59	0.86
44:t:38:GLU:O	44:t:58:TYR:CD1	2.28	0.86
46:v:78:GLY:HA3	46:v:192:CYS:HB3	1.57	0.86
75:5:502:PEE:H17	47:7:229:ILE:HD11	1.56	0.86
7:G:479:SER:OG	7:G:687:PRO:CD	2.24	0.86
17:Q:82:LEU:HD21	73:Q:201:ZMP:H11	0.88	0.85
17:Q:82:LEU:HD23	73:Q:201:ZMP:H11A	1.57	0.85
53:2:136:PHE:HD2	75:2:302:PEE:H34	1.38	0.85
53:4:234:TYR:HB2	53:4:243:TYR:HB2	1.58	0.85
10:J:63:THR:HG22	17:Q:70:ASN:HD21	1.08	0.85
20:U:91:ALA:HB1	20:U:95:TYR:CD2	2.11	0.85
46:v:288:VAL:HG22	46:v:378:LEU:HD11	1.58	0.85
47:7:103:TYR:OH	47:7:322:GLN:NE2	2.10	0.85
46:v:290:GLN:HB2	46:v:325:ALA:HB1	1.58	0.85
12:L:265:PHE:CE1	12:L:335:LEU:CA	2.60	0.85
71:2:301:PLX:C18	75:2:302:PEE:C39	2.37	0.85
15:O:123:GLU:OE2	17:Q:37:ARG:NH2	2.09	0.85
16:P:25:GLN:HG3	16:P:26:ARG:HG2	1.58	0.84
20:U:91:ALA:HA	20:U:95:TYR:HB2	1.59	0.84
61:Al:78:LEU:HB2	61:Al:79:PRO:HD3	1.58	0.84
20:U:150:GLU:HB2	20:U:300:VAL:HG11	0.85	0.84
48:8:288:ARG:NH1	52:Ac:41:ASP:OD1	2.09	0.84
43:s:96:LEU:HD11	43:s:99:HIS:HB2	1.59	0.84
7:G:124:HIS:NE2	68:G:801:SF4:S1	2.49	0.84
73:X:201:ZMP:H4A	40:p:44:MET:CE	2.06	0.84
36:l:226:GLN:NE2	36:l:314:MET:SD	2.51	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:t:56:ARG:HG3	44:t:57:ASP:H	1.40	0.84
26:b:86:LEU:HA	26:b:89:HIS:CE1	2.12	0.84
36:l:27:TYR:O	36:l:115:ASN:ND2	2.11	0.84
7:G:313:LEU:HD23	11:R:141:SER:O	1.78	0.84
48:x:125:CYS:HB3	48:x:179:PRO:HB3	1.57	0.84
54:Ad:4:ARG:CZ	54:Ad:5:PHE:HE2	1.83	0.84
20:U:88:PHE:CB	20:U:162:GLU:CB	2.54	0.84
34:j:25:PRO:HG2	42:r:60:PRO:HD3	1.58	0.83
60:Ak:187:SER:HB2	60:Ak:277:MET:HE1	1.60	0.83
48:x:297:MET:HE1	75:2:302:PEE:H55	1.58	0.83
12:L:211:ASP:CG	12:L:213:PHE:H	1.85	0.83
46:v:227:HIS:HE1	46:v:231:LYS:HE2	1.43	0.83
53:2:136:PHE:CE2	75:2:302:PEE:C21	2.60	0.83
12:L:204:SER:HB3	12:L:265:PHE:O	1.76	0.83
20:U:138:TYR:CD2	20:U:189:TYR:CE1	2.65	0.83
12:L:201:ILE:HG23	12:L:203:PRO:HD3	1.60	0.83
45:5:278:ARG:HH12	45:5:463:GLU:CA	1.92	0.83
20:U:143:LEU:HD11	33:i:317:PHE:HE2	1.44	0.83
75:u:502:PEE:H16	75:u:502:PEE:C31	2.08	0.83
41:q:418:LYS:NZ	41:q:419:TYR:O	2.12	0.83
44:t:13:ALA:HA	44:t:22:MET:CB	2.09	0.83
76:w:401:HEM:CHB	76:w:401:HEM:CMA	2.57	0.83
48:8:223:PRO:HB3	51:Ab:67:CYS:HB2	1.61	0.83
2:B:119:GLU:N	69:B:502:FMN:C7M	2.41	0.82
2:B:297:LYS:HG2	2:B:332:CYS:HB3	1.59	0.82
21:V:141:VAL:HG22	25:a:157:ARG:HD3	1.59	0.82
20:U:111:SER:O	20:U:136:TRP:CH2	2.32	0.82
75:2:302:PEE:H64	75:2:302:PEE:C43	2.08	0.82
47:w:241:ILE:HG13	48:x:293:MET:HE1	1.62	0.82
48:x:157:ASP:HB2	48:x:168:ARG:HG3	1.58	0.82
7:G:472:PRO:HG3	7:G:500:ILE:CG2	2.05	0.82
7:G:643:ARG:NH1	7:G:656:TYR:OH	2.12	0.82
47:7:138:MET:HG2	47:7:255:ASN:HB2	1.59	0.82
7:G:371:VAL:HG23	7:G:482:GLN:HG3	0.83	0.82
20:U:111:SER:O	20:U:136:TRP:CZ2	2.31	0.82
39:o:24:ASP:HB3	45:u:264:ALA:HB3	1.60	0.82
41:q:261:PHE:CE1	75:q:501:PEE:H44	2.14	0.82
46:6:116:ARG:HH12	46:6:178:HIS:HB3	1.43	0.82
10:J:61:ILE:HG22	10:J:64:LEU:HB2	1.62	0.82
53:2:136:PHE:CE2	75:2:302:PEE:H30	2.14	0.82
46:6:116:ARG:NH1	46:6:186:LEU:O	2.12	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:7:245:PHE:CE1	48:8:290:GLY:HA3	2.14	0.82
4:D:168:ARG:HH11	4:D:185:ARG:HG3	1.45	0.82
4:D:149:GLU:OE1	10:J:61:ILE:HD13	1.80	0.81
12:L:129:LEU:CD1	12:L:167:ILE:HD11	2.10	0.81
45:5:276:ARG:O	50:Aa:15:ILE:HA	1.78	0.81
74:u:501:CDL:H142	75:u:502:PEE:C34	2.09	0.81
45:5:273:SER:OG	50:Aa:18:SER:O	1.98	0.81
2:B:120:GLY:O	2:B:121:GLU:O	1.97	0.81
36:l:305:SER:OG	36:l:336:LYS:NZ	2.13	0.81
10:J:111:LEU:HG	10:J:112:MET:HG2	1.62	0.81
12:L:128:ASN:ND2	12:L:152:ILE:HG21	1.95	0.81
36:l:477:VAL:HG12	44:t:87:TRP:HZ2	1.44	0.81
71:2:301:PLX:H182	75:2:302:PEE:H65	0.81	0.81
75:7:402:PEE:H12	74:Aa:101:CDL:OA4	1.69	0.81
47:w:316:MET:CE	75:w:403:PEE:O1P	2.28	0.81
66:Aq:5:LYS:NZ	66:Aq:6:GLY:H	1.78	0.81
46:v:84:ARG:HD2	55:Af:15:LEU:HD12	1.63	0.81
46:v:113:THR:HB	46:v:120:ALA:HB3	1.61	0.81
8:H:68:ARG:HH12	22:W:28:ARG:HB3	1.45	0.80
12:L:363:THR:HG22	17:Q:51:GLN:HE21	1.45	0.80
46:6:183:ARG:NH2	46:6:253:TYR:O	2.14	0.80
53:2:136:PHE:HE2	75:2:302:PEE:C19	1.93	0.80
10:J:65:THR:OG1	10:J:67:VAL:HG22	1.79	0.80
45:5:277:HIS:HA	50:Aa:14:VAL:O	1.81	0.80
45:5:469:ASN:ND2	47:7:223:TYR:OH	2.15	0.80
54:Ad:41:ILE:HA	54:Ad:44:TRP:HD1	1.44	0.80
20:U:296:LEU:HD23	20:U:296:LEU:O	1.82	0.80
48:8:291:LEU:HD12	48:8:291:LEU:O	1.80	0.80
43:s:46:CYS:SG	43:s:56:CYS:HB2	2.21	0.80
67:Ar:39:CYS:SG	67:Ar:53:CYS:HB3	2.22	0.80
45:u:278:ARG:HH12	45:u:463:GLU:HB2	1.47	0.80
12:L:206:ILE:HG22	12:L:245:VAL:HG21	1.63	0.80
20:U:88:PHE:CB	20:U:162:GLU:H	1.93	0.80
47:7:245:PHE:HE1	48:8:290:GLY:HA3	1.47	0.80
7:G:598:ASN:N	7:G:602:ARG:O	2.15	0.79
14:N:38:ILE:HB	14:N:45:ARG:HD2	1.65	0.79
25:a:187:PRO:HB3	43:s:47:ARG:HG2	1.61	0.79
28:d:110:LEU:HD11	36:l:203:MET:HG2	1.63	0.79
36:l:477:VAL:HG13	44:t:55:GLN:HE21	1.47	0.79
36:l:566:THR:HG22	75:q:501:PEE:H75	1.64	0.79
67:Ar:39:CYS:SG	67:Ar:53:CYS:CB	2.70	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:60:GLY:O	72:L:401:NDP:H4B	1.81	0.79
75:W:401:PEE:C45	42:r:73:ILE:HD11	2.11	0.79
45:5:286:HIS:HB2	55:Ae:43:LEU:HD21	1.65	0.79
47:7:30:TRP:CZ3	75:7:402:PEE:C15	2.64	0.79
55:Ae:11:PHE:HA	55:Ae:24:GLY:HA2	1.62	0.79
8:H:153:ILE:HG21	9:I:162:TYR:HD1	1.47	0.79
28:d:141:ASP:O	28:d:158:LYS:NZ	2.15	0.79
35:k:37:MET:HE3	37:m:60:TYR:HE1	1.45	0.79
74:u:501:CDL:C14	75:u:502:PEE:C34	2.59	0.79
76:7:404:HEM:CHA	76:7:404:HEM:CAA	2.60	0.79
3:C:286:TYR:C	4:D:162:ALA:HB2	2.08	0.79
48:x:298:GLY:O	48:x:302:PRO:CD	2.31	0.79
47:7:300:ILE:HG13	47:7:303:LEU:HD12	1.62	0.79
7:G:403:VAL:CG1	7:G:476:LEU:HD12	2.13	0.79
45:5:278:ARG:CZ	45:5:462:ILE:H	1.94	0.79
7:G:405:THR:HA	7:G:686:PRO:HB3	1.64	0.79
28:d:160:LYS:NZ	31:g:114:ILE:O	2.16	0.79
33:i:25:HIS:CD2	33:i:84:TRP:HB3	2.18	0.79
45:5:278:ARG:HH21	45:5:461:PRO:CB	1.94	0.79
17:Q:56:VAL:HG12	17:Q:60:ARG:HH12	1.47	0.79
3:C:286:TYR:HA	4:D:162:ALA:HB2	0.84	0.79
36:l:145:GLU:OE2	36:l:176:ARG:NH2	2.15	0.79
50:z:68:GLU:HA	50:z:71:LYS:HE3	1.63	0.79
7:G:314:LEU:HD13	11:R:139:PRO:CB	2.12	0.78
12:L:48:ARG:NH1	12:L:96:PRO:O	2.15	0.78
73:X:201:ZMP:C4	40:p:44:MET:HE1	2.13	0.78
53:4:84:ARG:HH21	45:5:204:PRO:HG2	1.48	0.78
35:k:80:MET:SD	37:m:175:ASN:ND2	2.57	0.78
74:u:501:CDL:H141	75:u:502:PEE:H58	1.65	0.78
48:8:109:THR:HG22	48:8:113:ARG:HE	1.48	0.78
75:i:501:PEE:H37	41:q:155:ALA:HB3	1.63	0.78
53:2:267:SER:HB3	53:2:270:LEU:HB2	1.64	0.78
46:6:272:VAL:HG22	46:6:337:GLY:HA2	1.66	0.78
48:8:252:GLU:HA	48:8:262:ALA:HB3	1.63	0.78
53:4:163:LYS:HA	53:4:227:ASN:HD21	1.46	0.78
54:Ad:4:ARG:NH2	54:Ad:5:PHE:CZ	2.51	0.78
7:G:371:VAL:HG23	7:G:482:GLN:CB	2.12	0.78
20:U:303:LYS:O	20:U:306:VAL:HG22	1.83	0.78
3:C:423:LYS:HG2	4:D:115:THR:HG22	1.65	0.78
8:H:135:ARG:HG3	8:H:137:ASP:H	1.49	0.78
75:2:302:PEE:H49	75:2:302:PEE:H14	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:5:51:SER:HB2	45:5:59:VAL:HB	1.65	0.78
21:V:90:TYR:CD2	21:V:126:LYS:HB2	2.19	0.78
47:7:23:ALA:O	47:7:218:ILE:N	2.16	0.78
75:5:502:PEE:H17	47:7:229:ILE:CD1	2.12	0.78
33:i:95:MET:HE2	33:i:149:ILE:HA	1.65	0.78
4:D:168:ARG:NH1	4:D:185:ARG:HE	1.80	0.77
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.48	0.77
15:O:132:ASP:OD1	17:Q:37:ARG:NH1	2.17	0.77
44:t:111:ARG:CD	44:t:115:ARG:NH1	2.32	0.77
5:E:27:UNK:CB	5:E:66:ILE:HD11	2.13	0.77
9:I:211:ARG:HB3	9:I:211:ARG:HH11	1.47	0.77
41:q:204:MET:HG2	41:q:298:ILE:HD11	1.66	0.77
48:x:298:GLY:O	48:x:302:PRO:HD2	1.85	0.77
3:C:208:GLU:OE1	9:I:103:ARG:NH2	2.17	0.77
5:E:63:ILE:O	5:E:67:VAL:CG2	2.29	0.77
47:w:30:TRP:CZ3	75:w:403:PEE:H18	2.19	0.77
47:w:316:MET:HE3	75:w:403:PEE:P	2.24	0.77
47:7:328:LEU:HB2	47:7:361:ILE:HG21	1.67	0.77
12:L:192:ARG:NH1	12:L:196:PRO:O	2.18	0.77
7:G:403:VAL:CB	7:G:476:LEU:HD12	2.14	0.77
42:r:109:SER:OG	42:r:192:GLU:OE2	2.02	0.77
45:u:44:SER:CB	46:v:55:TYR:CB	2.62	0.77
46:v:65:ILE:HG22	46:v:67:ALA:H	1.49	0.77
46:v:287:SER:OG	55:Af:7:ARG:NH1	2.18	0.77
7:G:403:VAL:HG11	7:G:476:LEU:HD12	1.64	0.77
9:I:115:ALA:O	9:I:116:SER:OG	2.03	0.77
46:6:328:ALA:HB3	46:6:335:LEU:H	1.50	0.77
47:7:30:TRP:CH2	75:7:402:PEE:H17	2.19	0.77
15:O:83:VAL:HG21	15:O:145:VAL:HG22	1.66	0.77
28:d:97:LYS:NZ	29:e:113:ARG:O	2.18	0.77
43:s:115:LEU:HD22	43:s:117:TRP:HE1	1.50	0.77
75:7:402:PEE:H6	50:Aa:41:ARG:HH21	1.32	0.77
16:P:67:ALA:HB3	16:P:75:LYS:HB2	1.65	0.77
22:W:57:ARG:HH12	42:r:168:THR:HA	1.50	0.77
75:W:401:PEE:C45	42:r:73:ILE:CD1	2.63	0.77
46:v:214:THR:HG22	46:v:216:ALA:H	1.48	0.77
45:5:125:THR:HG22	45:5:127:GLU:H	1.49	0.77
3:C:211:PHE:CE2	9:I:98:HIS:HE1	2.03	0.77
41:q:16:TRP:HA	41:q:93:LYS:HD3	1.67	0.77
45:5:149:ASP:HA	45:5:153:ASN:HD22	1.48	0.77
7:G:181:ARG:HD3	7:G:225:ILE:HG12	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:5:501:CDL:H342	75:5:502:PEE:H27	1.66	0.76
69:B:502:FMN:H9	69:B:502:FMN:O4'	1.85	0.76
28:d:153:ARG:NH1	41:q:183:SER:O	2.16	0.76
31:g:77:LEU:HD11	71:i:502:PLX:H312	1.68	0.76
45:u:285:ALA:HA	45:u:460:GLY:HA2	1.66	0.76
45:5:276:ARG:CD	45:5:462:ILE:HD12	2.15	0.76
75:5:502:PEE:H75	54:Ad:35:ALA:HB1	1.67	0.76
67:Ar:75:ARG:HG2	67:Ar:75:ARG:HH11	1.48	0.76
2:B:378:SER:O	2:B:380:GLY:N	2.18	0.76
15:X:122:MET:HE1	15:X:144:ILE:HD13	1.66	0.76
75:u:502:PEE:H26	75:u:502:PEE:H48	1.66	0.76
3:C:286:TYR:C	4:D:162:ALA:CB	2.59	0.76
16:P:31:GLN:HB3	16:P:34:ARG:HH21	1.50	0.76
48:x:95:TYR:HB3	51:0:87:PHE:HE2	1.50	0.76
7:G:305:PRO:HG2	7:G:319:TRP:HA	1.67	0.76
44:t:111:ARG:NE	44:t:115:ARG:HH11	1.83	0.76
45:5:478:LEU:HD11	75:5:502:PEE:C5	2.14	0.76
10:J:99:MET:HB2	10:J:128:PHE:HE2	1.50	0.76
25:a:78:THR:HG21	29:e:100:VAL:HG21	1.68	0.76
45:u:247:GLN:NE2	45:u:251:SER:OG	2.18	0.76
25:a:126:TYR:OH	41:q:40:SER:O	2.03	0.76
48:8:280:GLU:OE2	48:8:283:HIS:CD2	2.37	0.76
7:G:374:THR:HG21	7:G:532:PRO:HA	1.67	0.76
48:x:111:ILE:HD13	48:x:277:TRP:HD1	1.49	0.76
53:2:164:ASN:ND2	53:2:234:TYR:OH	2.18	0.76
76:7:403:HEM:CHB	76:7:403:HEM:C2A	2.68	0.76
3:C:358:VAL:HG12	3:C:360:ASP:H	1.50	0.76
4:D:149:GLU:OE1	10:J:61:ILE:CD1	2.33	0.76
15:O:123:GLU:OE1	15:O:130:ILE:N	2.18	0.76
33:i:112:HIS:HB2	33:i:184:ILE:HD11	1.67	0.76
20:U:289:ASP:O	20:U:293:PHE:CD1	2.38	0.76
12:L:236:VAL:CG2	12:L:271:TYR:O	2.34	0.75
33:i:291:TYR:CE2	75:i:501:PEE:C31	2.67	0.75
47:w:30:TRP:CE3	75:w:403:PEE:H18	2.21	0.75
71:2:301:PLX:C18	75:2:302:PEE:H70	2.16	0.75
54:3:14:ALA:O	54:3:18:ILE:HG13	1.87	0.75
58:Ai:42:PRO:HA	61:Al:5:MET:HE3	1.68	0.75
12:L:45:LYS:O	12:L:50:SER:OG	2.02	0.75
12:L:59:PHE:CE1	12:L:126:VAL:HG13	2.21	0.75
47:w:77:TRP:CZ3	48:x:286:ARG:HD3	2.20	0.75
12:L:65:LEU:HD13	12:L:242:ILE:HD11	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:51:ASP:O	18:S:53:ARG:N	2.18	0.75
48:x:291:LEU:HD21	48:x:295:MET:HE3	1.67	0.75
4:D:146:TYR:HD1	14:N:112:TRP:HZ2	1.35	0.75
17:Q:62:LYS:HE3	17:Q:66:MET:HE2	1.67	0.75
47:w:234:PHE:CE2	48:x:301:LEU:HD13	2.21	0.75
61:Al:59:GLN:H	61:Al:62:GLU:HG3	1.51	0.75
5:E:92:TRP:NE1	5:E:124:ARG:O	2.19	0.75
12:L:201:ILE:CG2	12:L:203:PRO:CG	2.65	0.75
20:U:299:LEU:O	20:U:299:LEU:HD23	1.86	0.75
47:7:344:GLU:HG3	50:Aa:67:PHE:HE1	1.51	0.75
2:B:422:HIS:O	7:G:76:ARG:NE	2.20	0.75
29:e:92:PHE:O	29:e:96:SER:OG	2.03	0.75
43:s:77:HIS:HB3	43:s:114:LYS:HE3	1.67	0.75
45:5:278:ARG:CZ	45:5:462:ILE:N	2.50	0.75
3:C:141:TYR:CG	9:I:91:CYS:HB3	2.21	0.74
20:U:304:LEU:H	20:U:304:LEU:CD1	1.98	0.74
33:i:172:GLN:HG2	33:i:177:LYS:HD2	1.67	0.74
54:3:33:VAL:HG13	54:3:38:TRP:HB3	1.66	0.74
46:v:278:THR:HG22	46:v:331:SER:HA	1.68	0.74
76:w:402:HEM:CHB	76:w:402:HEM:CMA	2.65	0.74
47:7:326:TRP:CH2	75:7:402:PEE:H13	2.21	0.74
7:G:615:LEU:O	7:G:617:ARG:NH1	2.21	0.74
25:a:57:ILE:HG23	25:a:58:LYS:H	1.51	0.74
45:5:278:ARG:NH2	45:5:461:PRO:CB	2.50	0.74
73:X:201:ZMP:H19A	40:p:13:GLN:HE21	1.52	0.74
28:d:69:ARG:NH2	38:n:43:LEU:O	2.20	0.74
41:q:59:ASP:HB3	41:q:245:ARG:HH22	1.52	0.74
7:G:36:VAL:O	7:G:38:GLY:N	2.21	0.74
75:7:402:PEE:P	74:Aa:101:CDL:HA21	2.27	0.74
3:C:211:PHE:HE2	9:I:98:HIS:HE1	1.33	0.74
19:T:53:TYR:HA	22:W:69:ILE:HD11	1.69	0.74
53:2:234:TYR:HB2	53:2:243:TYR:HB2	1.68	0.74
3:C:286:TYR:CA	4:D:162:ALA:CB	2.53	0.74
4:D:209:GLU:OE2	9:I:175:ARG:NH1	2.21	0.74
12:L:236:VAL:HG22	12:L:271:TYR:O	1.87	0.74
62:Am:187:THR:HG21	66:Aq:68:THR:HG21	1.68	0.74
3:C:311:TYR:HA	3:C:314:VAL:HG22	1.68	0.74
25:a:187:PRO:HA	43:s:48:TRP:CE2	2.22	0.74
29:e:106:VAL:HA	29:e:109:LEU:HD13	1.70	0.74
36:l:361:GLY:H	36:l:435:PRO:HA	1.50	0.74
47:w:103:TYR:CZ	75:w:403:PEE:H13	2.22	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:52:GLN:HE21	45:u:56:GLY:HA2	1.52	0.73
46:6:66:LYS:H	46:6:217:ARG:HB3	1.53	0.73
76:7:404:HEM:CHA	76:7:404:HEM:HAA1	2.17	0.73
20:U:91:ALA:CB	20:U:95:TYR:CG	2.71	0.73
75:u:502:PEE:H50	75:u:502:PEE:C12	2.18	0.73
45:5:278:ARG:O	45:5:280:ASP:N	2.21	0.73
47:7:207:ASN:ND2	47:7:211:ILE:O	2.21	0.73
7:G:481:LEU:O	7:G:486:GLY:CA	2.34	0.73
7:G:697:THR:O	7:G:702:ARG:NH1	2.17	0.73
20:U:85:LEU:O	20:U:160:VAL:CG1	2.36	0.73
43:s:26:LYS:HE2	43:s:97:PHE:HE1	1.52	0.73
2:B:423:THR:OG1	68:B:501:SF4:S3	2.46	0.73
3:C:259:GLU:OE2	22:W:23:ARG:NH1	2.21	0.73
7:G:160:VAL:H	7:G:174:THR:HG22	1.52	0.73
25:a:127:ASP:O	29:e:112:TYR:OH	2.05	0.73
45:u:176:ASP:OD1	53:2:80:HIS:ND1	2.21	0.73
12:L:59:PHE:CE1	12:L:126:VAL:CG1	2.71	0.73
45:5:304:LEU:HD13	45:5:354:LEU:HD11	1.70	0.73
48:8:280:GLU:CD	48:8:283:HIS:CD2	2.62	0.73
45:u:125:THR:HG22	45:u:126:ARG:H	1.54	0.73
45:5:91:TYR:CZ	45:5:202:GLU:HG3	2.23	0.73
3:C:80:LEU:HD13	3:C:80:LEU:C	2.14	0.73
3:C:136:PHE:HE2	3:C:151:TYR:CD1	2.06	0.73
7:G:277:MET:HA	7:G:284:GLU:H	1.53	0.73
12:L:128:ASN:OD1	12:L:152:ILE:HD13	1.89	0.73
46:v:41:THR:HG21	46:v:49:ILE:HG22	1.70	0.73
76:w:402:HEM:CHA	76:w:402:HEM:CAA	2.67	0.73
45:5:277:HIS:HE1	45:5:279:ASP:OD2	1.69	0.73
7:G:140:GLN:NE2	68:G:801:SF4:S3	2.61	0.73
12:L:59:PHE:HD1	12:L:127:ILE:O	1.72	0.73
25:a:167:PRO:HG2	25:a:168:TRP:HD1	1.54	0.73
45:u:294:PRO:HB2	45:u:301:ASN:HD21	1.52	0.73
47:w:30:TRP:CZ3	75:w:403:PEE:C15	2.69	0.73
47:w:312:GLN:HE22	47:w:317:PHE:H	1.37	0.73
6:F:108:THR:CB	6:F:109:GLY:CA	2.66	0.73
47:w:316:MET:HB2	75:w:403:PEE:P	2.28	0.73
50:z:2:GLY:O	50:z:7:HIS:NE2	2.20	0.73
10:J:75:ARG:NH1	10:J:102:ASP:O	2.21	0.72
29:e:149:LEU:HD12	29:e:150:PRO:HD2	1.68	0.72
43:s:140:ASN:ND2	43:s:143:HIS:O	2.22	0.72
46:v:227:HIS:CE1	46:v:231:LYS:HE2	2.24	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:132:ALA:HB1	75:2:302:PEE:C16	2.17	0.72
46:6:71:TYR:OH	46:6:217:ARG:NH1	2.21	0.72
75:7:402:PEE:H5	50:Aa:41:ARG:HH21	1.37	0.72
48:8:113:ARG:NH1	48:8:270:ASP:OD2	2.22	0.72
2:B:296:LEU:HB3	2:B:332:CYS:HB2	1.70	0.72
12:L:238:GLN:OE1	12:L:266:VAL:CG1	2.37	0.72
16:P:24:CYS:SG	16:P:30:SER:OG	2.47	0.72
42:r:24:GLU:HG3	42:r:271:LEU:HD22	1.71	0.72
48:x:291:LEU:HD23	48:x:291:LEU:C	2.14	0.72
14:N:28:TYR:HA	14:N:31:ILE:HD12	1.69	0.72
16:P:24:CYS:SG	16:P:27:SER:OG	2.45	0.72
17:Q:51:GLN:HB2	17:Q:100:ARG:HH22	1.54	0.72
36:l:477:VAL:HG12	44:t:87:TRP:CZ2	2.25	0.72
45:u:274:GLU:HG2	50:z:18:SER:HB2	1.71	0.72
45:u:278:ARG:NH1	45:u:462:ILE:O	2.23	0.72
48:x:318:ARG:HH12	48:x:320:LEU:HD23	1.53	0.72
46:6:183:ARG:HD2	46:6:252:LYS:HE2	1.70	0.72
61:Al:184:LEU:HD11	61:Al:211:LEU:HD21	1.69	0.72
2:B:149:MET:HE3	2:B:241:THR:HG21	1.69	0.72
10:J:95:LYS:HG3	10:J:96:LYS:HG3	1.72	0.72
31:g:3:MET:O	31:g:5:SER:N	2.22	0.72
33:i:12:THR:HG21	37:m:163:ILE:HD13	1.72	0.72
42:r:149:ILE:HD11	42:r:185:TRP:HE3	1.53	0.72
48:x:297:MET:CE	75:2:302:PEE:H55	2.18	0.72
48:8:202:VAL:HG11	48:8:276:ARG:HD3	1.71	0.72
66:Aq:54:ARG:HD3	66:Aq:54:ARG:N	2.04	0.72
2:B:118:ASP:HB3	69:B:502:FMN:C7M	2.15	0.72
45:u:70:THR:HG1	45:u:410:CYS:HG	1.33	0.72
45:u:296:TRP:HE3	45:u:347:CYS:HB2	1.55	0.72
53:4:142:ALA:O	47:7:74:ASN:ND2	2.22	0.72
47:7:131:TYR:HA	76:7:403:HEM:HAA2	1.72	0.72
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.70	0.72
7:G:611:THR:HG21	10:J:105:GLU:HA	1.70	0.72
7:G:645:ARG:NH2	7:G:648:GLU:OE2	2.23	0.72
13:M:46:SER:O	13:M:52:ASN:ND2	2.22	0.72
47:w:244:LEU:HD23	48:x:290:GLY:N	2.03	0.72
52:1:52:LEU:HD13	52:1:54:LYS:HE3	1.70	0.72
47:7:112:THR:O	47:7:196:HIS:NE2	2.22	0.72
75:7:401:PEE:H61	75:7:401:PEE:H27	1.69	0.72
75:7:401:PEE:O4	48:8:289:MET:CB	2.37	0.72
2:B:112:TYR:HB2	2:B:240:THR:HG22	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:w:168:PHE:HB3	53:4:170:ARG:HG3	1.70	0.72
47:w:237:LEU:HD13	48:x:301:LEU:HD11	1.72	0.72
48:x:223:PRO:HG2	51:0:68:THR:HA	1.71	0.72
20:U:87:HIS:CA	20:U:160:VAL:HG13	2.17	0.72
2:B:118:ASP:OD1	69:B:502:FMN:HM71	1.89	0.72
3:C:399:ALA:CB	4:D:140:ARG:HH12	2.03	0.72
47:w:234:PHE:CE2	48:x:301:LEU:HD22	2.22	0.72
2:B:119:GLU:H	69:B:502:FMN:HM73	1.53	0.72
7:G:474:VAL:HG11	7:G:493:VAL:CG2	2.19	0.72
20:U:138:TYR:CD2	20:U:189:TYR:OH	2.42	0.72
36:l:267:MET:O	36:l:274:GLN:NE2	2.23	0.72
42:r:145:THR:HG23	42:r:297:THR:HG21	1.72	0.72
46:v:259:ARG:HE	46:v:444:LEU:HD22	1.55	0.72
60:Ak:176:MET:HE3	60:Ak:181:THR:HG22	1.71	0.72
17:Q:99:GLN:H	17:Q:102:HIS:HB2	1.55	0.71
22:W:54:ASN:ND2	42:r:313:SER:O	2.23	0.71
27:c:168:LEU:HA	44:t:98:ARG:HB3	0.85	0.71
36:l:173:LEU:HD13	41:q:405:LEU:HD11	1.69	0.71
41:q:290:SER:HA	41:q:319:HIS:HE2	1.54	0.71
46:v:127:ARG:NH1	46:v:224:GLY:O	2.23	0.71
48:x:87:ASP:OD2	48:x:241:GLN:NE2	2.22	0.71
63:An:23:PRO:O	64:Ao:66:ARG:HD3	1.89	0.71
20:U:89:PRO:O	20:U:90:GLU:CB	2.38	0.71
20:U:299:LEU:HD23	20:U:299:LEU:C	2.14	0.71
20:U:304:LEU:HD12	20:U:304:LEU:N	2.02	0.71
45:u:195:THR:HG22	45:u:197:LEU:H	1.52	0.71
48:x:88:LEU:HD21	50:z:71:LYS:HD2	1.73	0.71
52:Ac:11:TYR:HA	52:Ac:15:PHE:HB2	1.72	0.71
7:G:224:ASP:OD2	10:J:86:ASN:ND2	2.24	0.71
46:v:66:LYS:NZ	46:v:401:LEU:O	2.22	0.71
48:8:321:ALA:HB3	50:Aa:15:ILE:HB	1.72	0.71
7:G:403:VAL:HB	7:G:476:LEU:HD12	1.72	0.71
27:c:94:HIS:O	27:c:98:ARG:N	2.23	0.71
48:x:162:ASP:H	48:8:184:GLU:HB2	1.55	0.71
53:2:136:PHE:HD2	75:2:302:PEE:H37	1.56	0.71
53:4:173:PRO:HB2	53:4:215:GLY:HA3	1.71	0.71
48:8:116:GLN:NE2	48:8:141:TYR:OH	2.23	0.71
63:An:147:LYS:HA	63:An:147:LYS:HE3	1.71	0.71
10:J:63:THR:HG21	17:Q:70:ASN:ND2	2.05	0.71
12:L:131:GLY:HA3	72:L:401:NDP:O3D	1.91	0.71
22:W:144:THR:O	75:W:401:PEE:N	2.15	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:g:20:ALA:O	31:g:22:SER:N	2.21	0.71
53:4:177:ARG:NH2	53:4:183:GLU:OE2	2.24	0.71
12:L:242:ILE:HD12	12:L:242:ILE:O	1.90	0.71
28:d:117:GLU:OE1	28:d:120:SER:OG	2.08	0.71
36:l:483:PRO:HD2	36:l:486:MET:HB2	1.71	0.71
40:p:16:VAL:HG12	40:p:64:LEU:HD21	1.72	0.71
46:6:177:LEU:HB2	46:6:439:ALA:HB2	1.71	0.71
50:Aa:80:ASN:HB2	51:Ab:65:GLU:HB2	1.72	0.71
4:D:68:ILE:HG22	4:D:69:LEU:HG	1.72	0.71
47:w:15:ASN:HA	47:w:19:ILE:HB	1.73	0.71
75:2:302:PEE:H28	75:2:302:PEE:C40	2.21	0.71
4:D:111:LEU:HG	4:D:160:TYR:CB	2.21	0.71
17:Q:29:LYS:HE3	73:Q:201:ZMP:P1	2.30	0.71
17:Q:42:GLU:OE1	17:Q:46:THR:OG1	2.09	0.71
2:B:214:GLU:OE2	2:B:224:ARG:NH1	2.24	0.70
7:G:313:LEU:HD22	11:R:141:SER:O	1.89	0.70
9:I:99:MET:HG2	9:I:106:MET:HB3	1.73	0.70
28:d:140:GLN:HB2	39:o:127:ILE:HG22	1.73	0.70
47:w:272:TRP:HA	47:w:275:LEU:HG	1.73	0.70
45:u:165:ARG:NH2	45:u:211:LEU:O	2.24	0.70
8:H:43:MET:HE1	14:N:8:THR:HG21	1.72	0.70
22:W:113:THR:HG22	22:W:115:ARG:H	1.57	0.70
46:6:173:VAL:HG21	46:6:268:HIS:HB2	1.74	0.70
60:Ak:11:ASN:HD22	60:Ak:14:ASP:H	1.39	0.70
5:E:163:THR:HG22	5:E:170:THR:HG22	1.72	0.70
46:6:121:TYR:HB3	46:6:137:LEU:HD11	1.74	0.70
22:W:86:MET:O	22:W:90:ASN:ND2	2.24	0.70
44:t:13:ALA:CB	44:t:22:MET:CB	2.69	0.70
47:7:318:ARG:NH1	47:7:370:SER:OG	2.24	0.70
2:B:120:GLY:O	2:B:121:GLU:C	2.34	0.70
7:G:287:SER:HB3	7:G:290:THR:HG22	1.74	0.70
10:J:109:ASN:ND2	10:J:111:LEU:O	2.25	0.70
44:t:38:GLU:O	44:t:58:TYR:HD1	1.72	0.70
5:E:133:GLN:HB2	5:E:174:VAL:HG21	1.74	0.70
12:L:206:ILE:HG22	12:L:245:VAL:CG2	2.19	0.70
75:i:501:PEE:H7	36:l:567:SER:OG	1.92	0.70
41:q:23:ILE:HA	41:q:26:ASN:HD22	1.55	0.70
46:v:362:ALA:O	46:v:429:LYS:NZ	2.24	0.70
48:x:111:ILE:HD13	48:x:277:TRP:CD1	2.25	0.70
48:x:299:LEU:C	48:x:299:LEU:HD23	2.16	0.70
16:P:20:ARG:HG2	16:P:54:LEU:HB2	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:i:241:THR:OG1	33:i:300:SER:OG	2.08	0.70
34:j:56:PHE:HE1	37:m:70:TYR:HB3	1.57	0.70
42:r:156:MET:HE1	42:r:177:THR:HG21	1.74	0.70
46:v:158:LEU:HD12	46:v:197:ILE:HG23	1.72	0.70
53:4:133:VAL:HG11	75:5:502:PEE:H72	1.73	0.70
47:7:30:TRP:CZ3	75:7:402:PEE:H17	2.27	0.70
5:E:153:GLN:HE21	5:E:159:LYS:HE3	1.55	0.70
13:M:41:LEU:HD12	13:M:42:PRO:HD2	1.72	0.70
16:P:20:ARG:NH1	16:P:74:GLU:OE2	2.25	0.70
32:h:18:MET:HE1	35:k:56:ALA:HA	1.73	0.70
35:k:23:ARG:NH2	37:m:23:LYS:O	2.25	0.70
62:Am:156:ARG:HH11	62:Am:156:ARG:HG3	1.56	0.70
12:L:204:SER:N	12:L:265:PHE:O	2.23	0.70
21:V:134:GLN:O	21:V:136:PHE:N	2.25	0.70
46:6:182:TYR:HB2	46:6:187:ALA:HB2	1.74	0.70
20:U:138:TYR:CD2	20:U:189:TYR:HE1	2.08	0.69
20:U:299:LEU:CD2	20:U:306:VAL:HG12	2.22	0.69
46:v:116:ARG:NH1	46:v:188:ASN:O	2.25	0.69
46:6:112:VAL:N	55:Ae:15:LEU:O	2.22	0.69
20:U:310:THR:OG1	33:i:310:ASN:ND2	2.26	0.69
36:l:355:ASP:OD2	36:l:357:ARG:NH1	2.26	0.69
53:2:204:ARG:HH12	53:2:248:ARG:HA	1.57	0.69
50:Aa:43:ARG:HA	50:Aa:46:ILE:HG22	1.74	0.69
2:B:378:SER:OG	68:B:501:SF4:S4	2.48	0.69
7:G:490:LEU:HD23	7:G:490:LEU:O	1.92	0.69
15:O:134:ASP:HA	15:O:137:LYS:HG2	1.74	0.69
25:a:143:GLU:OE1	41:q:175:ASN:ND2	2.25	0.69
45:5:388:VAL:HG12	45:5:392:LYS:HE3	1.73	0.69
57:Ah:20:VAL:H	62:Am:12:ASN:HD22	1.38	0.69
7:G:265:THR:HG22	7:G:270:VAL:HA	1.74	0.69
20:U:91:ALA:CA	20:U:95:TYR:HB2	2.23	0.69
29:e:100:VAL:HG23	29:e:101:LEU:H	1.56	0.69
61:Al:13:THR:HB	61:Al:168:LEU:HD23	1.73	0.69
75:i:501:PEE:H37	41:q:155:ALA:CB	2.23	0.69
36:l:270:ASN:OD1	36:l:271:LYS:N	2.25	0.69
47:w:217:LYS:HE2	50:z:3:ARG:HH12	1.57	0.69
4:D:76:VAL:HG23	13:M:69:VAL:HB	1.74	0.69
4:D:93:VAL:HG11	4:D:153:ILE:HD11	1.74	0.69
6:F:113:TYR:O	6:F:115:GLY:N	2.26	0.69
22:W:71:LEU:HB3	22:W:75:PHE:CE2	2.25	0.69
23:Y:94:ASP:O	44:t:108:LEU:HD21	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:166:LEU:O	44:t:98:ARG:O	2.09	0.69
41:q:208:PRO:HD3	41:q:236:LEU:HD22	1.73	0.69
43:s:47:ARG:HH21	43:s:47:ARG:HG3	1.58	0.69
76:w:401:HEM:HAA1	76:w:401:HEM:HHA	1.75	0.69
53:2:177:ARG:NH2	53:2:183:GLU:OE2	2.25	0.69
47:7:57:SER:HA	47:7:61:THR:HB	1.75	0.69
48:8:280:GLU:HG3	48:8:283:HIS:HB2	1.75	0.69
7:G:299:ARG:O	11:R:134:ILE:O	2.09	0.69
36:l:69:MET:HE1	41:q:376:ILE:HD11	1.74	0.69
45:u:332:ALA:HA	45:u:337:LEU:HB2	1.75	0.69
22:W:121:MET:HE2	22:W:137:THR:HG22	1.73	0.69
35:k:59:MET:HG3	35:k:60:PRO:N	2.08	0.69
37:m:76:THR:HG23	37:m:77:GLU:H	1.58	0.69
45:u:120:LEU:HD11	46:v:299:VAL:HG13	1.75	0.69
48:x:243:ILE:HG12	48:x:245:MET:H	1.58	0.69
76:7:404:HEM:CHB	76:7:404:HEM:CMA	2.71	0.69
36:l:505:ASN:O	36:l:508:THR:OG1	2.10	0.68
53:2:191:GLU:HB3	53:2:194:GLN:HG2	1.74	0.68
55:Ae:43:LEU:H	55:Ae:46:LYS:HE2	1.58	0.68
7:G:356:ASP:OD1	7:G:645:ARG:NH1	2.26	0.68
8:H:86:TYR:O	9:I:108:ARG:NH1	2.27	0.68
14:N:21:HIS:NE2	14:N:63:PRO:O	2.26	0.68
14:N:24:LEU:HD23	14:N:27:LEU:HD12	1.74	0.68
53:2:136:PHE:HE2	75:2:302:PEE:C21	2.06	0.68
61:Al:186:SER:HB3	61:Al:213:LEU:HD22	1.76	0.68
12:L:58:VAL:O	12:L:83:PRO:HD2	1.93	0.68
13:M:48:LYS:O	13:M:52:ASN:ND2	2.27	0.68
36:l:26:ILE:HD11	36:l:31:LEU:HD22	1.76	0.68
41:q:336:ARG:NH1	41:q:433:GLU:OE1	2.27	0.68
15:O:110:LEU:HD13	15:O:114:ASP:HB3	1.73	0.68
20:U:138:TYR:HD2	20:U:189:TYR:CE1	2.09	0.68
75:W:401:PEE:C45	42:r:73:ILE:HG12	2.23	0.68
45:u:63:GLN:HE22	45:u:238:GLU:HA	1.58	0.68
4:D:124:ASN:OD1	14:N:111:GLN:NE2	2.20	0.68
25:a:96:ALA:HB1	28:d:62:TYR:HA	1.73	0.68
60:Ak:69:MET:HE2	60:Ak:70:VAL:HG23	1.74	0.68
7:G:313:LEU:HD21	11:R:141:SER:O	1.91	0.68
12:L:240:VAL:HG22	12:L:267:GLY:N	2.08	0.68
40:p:107:TRP:O	40:p:108:HIS:ND1	2.25	0.68
45:u:104:ARG:NH1	45:u:149:ASP:OD2	2.26	0.68
46:6:376:ASN:HA	46:6:379:LYS:HD3	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:228:VAL:HG23	7:G:230:ALA:H	1.57	0.68
32:h:20:ILE:HG22	32:h:22:SER:H	1.58	0.68
45:5:274:GLU:HA	45:5:456:VAL:HB	1.75	0.68
45:5:276:ARG:CD	45:5:462:ILE:CD1	2.72	0.68
49:9:34:ARG:NH2	49:9:92:GLU:OE2	2.26	0.68
2:B:382:CYS:SG	2:B:423:THR:OG1	2.52	0.68
8:H:76:TYR:HD1	42:r:33:LEU:HD11	1.59	0.68
33:i:72:MET:HE3	33:i:76:ILE:HD11	1.76	0.68
46:v:145:GLU:HG3	46:v:147:ARG:HE	1.59	0.68
46:6:70:ARG:HH22	46:6:332:ASP:HB2	1.57	0.68
7:G:63:PHE:O	7:G:181:ARG:NH2	2.26	0.68
14:N:92:ARG:O	14:N:96:ARG:NH1	2.26	0.68
25:a:127:ASP:OD1	25:a:128:GLY:N	2.26	0.68
30:f:72:ARG:HE	31:g:22:SER:HB2	1.57	0.68
48:x:126:HIS:NE2	77:x:401:HEC:ND	2.42	0.68
45:5:301:ASN:ND2	55:Ae:57:GLY:O	2.27	0.68
45:5:378:ARG:HA	45:5:382:SER:HB3	1.76	0.68
22:W:143:TYR:O	75:W:401:PEE:N	2.26	0.68
28:d:78:GLU:HG3	31:g:108:LYS:HD2	1.74	0.68
45:u:266:THR:OG1	45:u:268:CYS:SG	2.50	0.68
47:7:153:ILE:HG21	47:7:156:ILE:HG13	1.76	0.68
3:C:135:TYR:CZ	9:I:162:TYR:HE2	2.11	0.67
3:C:305:THR:HG22	3:C:306:GLN:HG3	1.76	0.67
12:L:241:TYR:CD2	12:L:243:VAL:HB	2.28	0.67
34:j:80:GLN:NE2	42:r:317:GLN:O	2.26	0.67
74:u:501:CDL:H152	75:u:502:PEE:H58	1.74	0.67
46:v:41:THR:HB	46:v:49:ILE:H	1.59	0.67
53:4:130:LYS:NZ	54:Ad:34:TRP:O	2.25	0.67
2:B:224:ARG:NH2	2:B:233:VAL:O	2.28	0.67
34:j:46:SER:HB3	37:m:78:MET:HE2	1.77	0.67
36:l:302:VAL:O	36:l:305:SER:OG	2.08	0.67
45:u:192:PHE:HB3	45:u:195:THR:HB	1.75	0.67
45:u:451:ASP:OD1	45:u:472:ARG:NH2	2.28	0.67
48:8:217:THR:HG22	51:Ab:34:ARG:HH22	1.59	0.67
2:B:127:ASP:HA	2:B:130:ILE:HD12	1.76	0.67
7:G:346:VAL:O	7:G:521:SER:OG	2.12	0.67
27:c:116:ARG:HA	75:l:701:PEE:O5	1.94	0.67
33:i:5:ILE:HD11	37:m:166:VAL:HG13	1.77	0.67
2:B:378:SER:OG	2:B:385:CYS:SG	2.53	0.67
3:C:80:LEU:HD22	3:C:81:THR:H	1.60	0.67
7:G:309:ASN:OD1	7:G:313:LEU:N	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:210:LEU:HD22	13:M:39:PRO:HD2	1.75	0.67
16:P:23:LEU:HD21	16:P:34:ARG:HG2	1.75	0.67
75:w:403:PEE:H25	75:w:403:PEE:H61	1.77	0.67
46:6:179:ALA:HA	46:6:187:ALA:HB1	1.77	0.67
48:8:117:VAL:HG21	48:8:267:VAL:HG23	1.77	0.67
60:Ak:151:HIS:O	60:Ak:155:VAL:HG23	1.95	0.67
12:L:83:PRO:HB2	12:L:108:TRP:CD1	2.29	0.67
73:X:201:ZMP:H6A	40:p:48:PHE:HE1	1.58	0.67
27:c:120:SER:O	36:l:535:ARG:NH1	2.28	0.67
53:2:179:ARG:N	53:2:209:GLU:O	2.27	0.67
46:6:81:HIS:HA	46:6:84:ARG:HH21	1.59	0.67
48:8:202:VAL:HA	48:8:212:VAL:HG21	1.75	0.67
7:G:543:LYS:N	7:G:563:ASP:OD2	2.26	0.67
12:L:129:LEU:HA	12:L:167:ILE:CD1	2.24	0.67
14:N:23:ARG:O	14:N:27:LEU:HG	1.95	0.67
75:u:502:PEE:H3	71:2:301:PLX:H32	1.76	0.67
51:0:56:ARG:NH2	51:0:65:GLU:OE2	2.28	0.67
45:5:278:ARG:O	45:5:279:ASP:C	2.35	0.67
62:Am:154:GLY:HA2	65:Ap:6:VAL:HG22	1.75	0.67
67:Ar:38:ARG:HG2	67:Ar:85:ILE:HG23	1.77	0.67
28:d:162:ARG:NH1	29:e:139:SER:O	2.28	0.67
46:v:259:ARG:NH2	46:v:447:THR:OG1	2.27	0.67
46:v:309:LEU:HD23	46:v:354:ALA:HB1	1.76	0.67
46:6:110:LEU:HA	46:6:123:VAL:HA	1.76	0.67
48:8:209:GLU:HB3	48:8:276:ARG:HD3	1.77	0.67
62:Am:209:ILE:O	62:Am:213:THR:HG23	1.95	0.67
2:B:296:LEU:N	2:B:332:CYS:SG	2.67	0.67
4:D:218:ARG:HD2	17:Q:101:THR:HA	1.75	0.67
9:I:202:ARG:O	9:I:206:ARG:NH2	2.28	0.67
34:j:98:LEU:HD22	42:r:298:LEU:HD21	1.75	0.67
45:u:101:THR:HA	45:u:154:CYS:HA	1.75	0.67
75:7:402:PEE:C4	74:Aa:101:CDL:OA4	2.42	0.67
76:7:404:HEM:CHB	76:7:404:HEM:C2A	2.78	0.67
76:7:404:HEM:HAA1	76:7:404:HEM:HHA	1.76	0.67
48:8:266:GLN:NE2	51:Ab:91:LYS:OXT	2.27	0.67
12:L:59:PHE:HE1	12:L:126:VAL:CG1	2.06	0.67
12:L:206:ILE:HG21	12:L:245:VAL:CG2	2.15	0.67
20:U:303:LYS:O	20:U:306:VAL:CG2	2.43	0.67
15:X:89:LEU:HD23	24:Z:48:ASN:HA	1.76	0.67
24:Z:22:TRP:HB3	24:Z:51:TRP:CB	2.25	0.67
42:r:134:ARG:NH1	42:r:206:GLU:OE2	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:s:47:ARG:CZ	43:s:53:PRO:HA	2.24	0.67
47:w:72:ASP:HA	53:2:144:ALA:HB3	1.77	0.67
51:0:60:ARG:HB2	51:0:63:THR:HG23	1.76	0.67
53:4:118:THR:HG21	71:4:301:PLX:H11	1.77	0.67
7:G:650:SER:OG	7:G:652:ASN:OD1	2.13	0.66
17:Q:19:PRO:HA	17:Q:77:ARG:HD3	1.77	0.66
43:s:47:ARG:HG3	43:s:47:ARG:NH2	2.07	0.66
3:C:300:TRP:CH2	3:C:305:THR:HG21	2.30	0.66
7:G:97:MET:HG3	7:G:98:LYS:HG2	1.76	0.66
72:L:401:NDP:O2X	72:L:401:NDP:H1B	1.94	0.66
17:Q:63:VAL:HG22	73:Q:201:ZMP:C4	2.23	0.66
42:r:138:GLN:NE2	42:r:194:ASN:OD1	2.27	0.66
3:C:266:ARG:O	3:C:270:ASN:ND2	2.28	0.66
34:j:71:LEU:O	37:m:147:TYR:OH	2.13	0.66
47:w:136:GLY:H	47:w:139:SER:HB2	1.60	0.66
47:w:262:LEU:HA	53:4:173:PRO:HG3	1.77	0.66
45:5:53:LEU:HD12	45:5:57:LEU:HD22	1.76	0.66
46:6:196:ARG:HH22	46:6:204:GLN:HE22	1.42	0.66
56:Ag:14:GLU:HG2	59:Aj:19:TRP:HZ2	1.59	0.66
12:L:123:SER:OG	12:L:125:VAL:O	2.12	0.66
21:V:9:TYR:CZ	21:V:21:LYS:HE2	2.29	0.66
21:V:12:ILE:HG23	21:V:21:LYS:HD3	1.78	0.66
15:X:84:LEU:HD11	15:X:100:VAL:HG22	1.78	0.66
51:0:55:GLN:HA	51:0:58:SER:HB2	1.77	0.66
53:4:79:SER:OG	49:9:57:ASN:ND2	2.27	0.66
45:5:186:TYR:O	45:5:275:ILE:HD12	1.94	0.66
48:8:243:ILE:HG12	48:8:245:MET:H	1.60	0.66
7:G:371:VAL:CG2	7:G:482:GLN:CB	2.71	0.66
9:I:100:ALA:HB2	9:I:113:PHE:HE2	1.60	0.66
12:L:124:ASN:OD1	12:L:125:VAL:N	2.29	0.66
21:V:44:LYS:NZ	74:V:201:CDL:OA3	2.28	0.66
31:g:12:PRO:HG2	32:h:9:ARG:HB2	1.77	0.66
42:r:228:TYR:HA	42:r:231:ILE:HG22	1.78	0.66
54:3:20:THR:O	54:3:24:TRP:CD1	2.49	0.66
64:Ao:43:PRO:HB2	64:Ao:48:ILE:HD11	1.76	0.66
18:S:6:LEU:HA	18:S:9:ILE:HG22	1.76	0.66
23:Y:47:PHE:O	23:Y:49:GLN:N	2.29	0.66
25:a:174:ILE:HG21	32:h:20:ILE:HD11	1.77	0.66
46:v:183:ARG:HG2	46:6:449:PHE:HE2	1.60	0.66
60:Ak:298:ASP:HB2	60:Ak:301:THR:HG23	1.77	0.66
3:C:372:LYS:NZ	8:H:163:PRO:O	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:65:LEU:CD1	12:L:242:ILE:HD11	2.26	0.66
28:d:139:PHE:HB2	29:e:137:MET:HE3	1.77	0.66
62:Am:160:LEU:HD13	62:Am:222:GLN:HG2	1.78	0.66
7:G:194:ASP:OD2	7:G:212:LYS:NZ	2.29	0.66
7:G:281:ILE:O	7:G:417:ARG:NH1	2.29	0.66
20:U:337:PRO:O	20:U:346:ASN:ND2	2.27	0.66
22:W:73:PRO:HG3	43:s:40:ASN:HD21	1.60	0.66
47:7:30:TRP:HZ3	75:7:402:PEE:C15	2.08	0.66
75:7:402:PEE:C5	74:Aa:101:CDL:OA3	2.37	0.66
63:An:24:LEU:H	64:Ao:34:ASN:HD21	1.44	0.66
15:X:111:ASP:OD1	15:X:112:SER:N	2.28	0.66
46:v:48:VAL:HB	46:v:219:ALA:HB1	1.78	0.66
7:G:466:LEU:HD21	7:G:496:ILE:CG2	2.25	0.66
13:M:39:PRO:O	13:M:41:LEU:N	2.29	0.66
17:Q:63:VAL:HA	73:Q:201:ZMP:C4	2.25	0.66
47:w:23:ALA:O	47:w:218:ILE:N	2.25	0.66
53:4:161:GLU:HA	53:4:178:HIS:HB3	1.77	0.66
49:9:23:ASN:HA	49:9:28:ASN:HD22	1.61	0.66
3:C:205:GLU:OE2	3:C:209:LYS:NZ	2.28	0.65
5:E:133:GLN:HE21	5:E:187:GLN:HE21	1.41	0.65
7:G:63:PHE:HB2	7:G:75:CYS:SG	2.36	0.65
16:P:89:ARG:O	16:P:93:ASN:ND2	2.29	0.65
19:T:45:ILE:HG22	22:W:58:ARG:HH21	1.61	0.65
45:u:465:LEU:HD12	45:u:466:PRO:HD2	1.77	0.65
47:w:51:LEU:HD12	47:w:83:HIS:CD2	2.32	0.65
45:5:342:GLN:HE21	45:5:357:HIS:HD2	1.44	0.65
49:9:70:THR:O	49:9:73:GLN:NE2	2.30	0.65
2:B:418:GLN:O	2:B:422:HIS:ND1	2.29	0.65
4:D:83:GLU:OE1	4:D:142:ARG:NH1	2.29	0.65
5:E:182:ASN:OD1	5:E:183:ALA:N	2.28	0.65
12:L:48:ARG:NH1	12:L:98:GLY:O	2.28	0.65
12:L:171:ASN:C	12:L:181:LEU:HD22	2.21	0.65
29:e:113:ARG:NH1	41:q:452:LYS:O	2.29	0.65
41:q:170:THR:HG23	41:q:171:THR:HG23	1.78	0.65
45:u:79:SER:N	45:u:126:ARG:O	2.30	0.65
45:u:478:LEU:HG	75:u:502:PEE:H12	1.77	0.65
47:w:103:TYR:CD2	75:w:403:PEE:H16	2.31	0.65
45:5:327:THR:OG1	45:5:375:GLN:NE2	2.30	0.65
55:Ae:42:VAL:HG13	55:Ae:46:LYS:HZ1	1.62	0.65
7:G:597:VAL:HA	7:G:603:ALA:HA	1.76	0.65
45:u:238:GLU:OE1	45:u:241:GLN:N	2.22	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:v:299:VAL:O	55:Af:31:GLN:NE2	2.29	0.65
47:w:14:ILE:HG22	47:w:19:ILE:HG13	1.78	0.65
46:6:43:LEU:HD13	46:6:238:LEU:HD21	1.76	0.65
47:7:206:ASN:OD1	47:7:207:ASN:N	2.28	0.65
71:H:303:PLX:H4	71:H:303:PLX:H1B3	1.79	0.65
20:U:91:ALA:CB	20:U:144:GLN:NE2	2.58	0.65
27:c:175:THR:O	27:c:179:GLU:N	2.27	0.65
34:j:73:LEU:O	42:r:160:TYR:OH	2.15	0.65
35:k:41:PHE:CE1	35:k:60:PRO:HB2	2.31	0.65
48:x:305:TYR:OH	74:x:402:CDL:OA3	2.08	0.65
50:Aa:65:GLN:HA	50:Aa:68:GLU:HG2	1.76	0.65
5:E:129:LYS:HB3	5:E:168:LEU:HG	1.78	0.65
7:G:301:ARG:O	11:R:136:GLU:CB	2.44	0.65
11:K:60:ARG:O	11:K:67:GLU:O	2.15	0.65
25:a:70:LEU:HD13	29:e:87:MET:HE1	1.77	0.65
43:s:28:ALA:HB2	43:s:82:PHE:HE1	1.61	0.65
45:u:85:LYS:NZ	45:u:215:ASP:OD2	2.29	0.65
47:w:149:LEU:HD21	47:w:281:LEU:HD21	1.79	0.65
47:w:282:ARG:HH22	47:w:347:PHE:HB2	1.62	0.65
48:x:117:VAL:HG11	48:x:271:VAL:HG22	1.78	0.65
46:6:82:LEU:HA	46:6:158:LEU:HD21	1.77	0.65
48:8:322:TYR:HB2	49:9:61:PHE:CE2	2.31	0.65
4:D:146:TYR:CD1	14:N:112:TRP:HZ2	2.14	0.65
7:G:275:PRO:HB3	7:G:286:ILE:HB	1.79	0.65
34:j:9:THR:HG21	42:r:6:ILE:HG21	1.78	0.65
41:q:32:LEU:O	41:q:35:SER:OG	2.10	0.65
53:2:154:ILE:HD12	53:2:270:LEU:HD22	1.78	0.65
46:6:379:LYS:HG2	46:6:413:LEU:HG	1.78	0.65
8:H:101:HIS:ND1	8:H:149:MET:HE1	2.12	0.65
12:L:66:GLY:HA3	12:L:69:VAL:HG22	1.78	0.65
18:S:56:GLY:H	18:S:64:LYS:HZ3	1.43	0.65
47:w:160:LEU:HD23	47:w:164:ILE:HD11	1.77	0.65
48:x:187:ARG:NH1	48:x:192:GLY:O	2.28	0.65
45:5:278:ARG:NH1	45:5:463:GLU:CA	2.54	0.65
76:7:403:HEM:CHA	76:7:403:HEM:CAA	2.74	0.65
48:8:159:PRO:HB3	48:8:164:GLU:HG3	1.78	0.65
49:9:50:ARG:HD2	49:9:94:TYR:HB3	1.79	0.65
31:g:54:PRO:HG2	31:g:58:ALA:HB2	1.77	0.65
45:u:296:TRP:HB3	45:u:349:ALA:HA	1.78	0.65
46:v:183:ARG:NH2	46:v:253:TYR:O	2.30	0.65
7:G:466:LEU:HD11	7:G:500:ILE:HD11	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:q:112:ALA:CB	41:q:113:THR:HA	2.26	0.65
45:u:326:SER:O	45:u:330:SER:N	2.29	0.65
48:x:113:ARG:NH1	48:x:270:ASP:OD2	2.29	0.65
75:7:401:PEE:H64	75:7:401:PEE:C19	2.27	0.65
75:7:402:PEE:O3P	74:Aa:101:CDL:HA21	1.97	0.65
60:Ak:172:LYS:HB2	60:Ak:172:LYS:NZ	2.12	0.65
4:D:148:ASP:HB2	4:D:151:THR:HG22	1.79	0.65
7:G:36:VAL:HG11	7:G:56:VAL:HG11	1.79	0.65
20:U:150:GLU:CG	20:U:300:VAL:CG1	2.75	0.65
25:a:133:TYR:OH	28:d:87:GLU:OE1	2.11	0.65
33:i:106:LEU:HD21	33:i:139:LEU:HD21	1.77	0.65
33:i:106:LEU:O	33:i:135:LYS:NZ	2.30	0.65
34:j:68:GLU:HG2	34:j:98:LEU:HD12	1.79	0.65
47:w:182:HIS:HE1	76:w:401:HEM:C1B	2.15	0.65
47:w:230:LEU:HD21	48:x:305:TYR:HD1	1.62	0.65
45:5:478:LEU:HD12	75:5:502:PEE:H12	1.74	0.65
61:Al:120:SER:OG	61:Al:138:VAL:HG21	1.97	0.65
7:G:68:ARG:CZ	7:G:283:GLU:HB2	2.27	0.64
7:G:595:THR:OG1	7:G:603:ALA:O	2.15	0.64
17:Q:127:ASP:HB3	17:Q:128:PRO:HD2	1.79	0.64
36:l:106:TRP:HB2	36:l:449:LEU:HD11	1.79	0.64
40:p:145:PRO:HB2	40:p:146:PRO:HD2	1.78	0.64
47:7:68:HIS:HD2	47:7:72:ASP:HB2	1.62	0.64
55:Ae:50:LEU:HD22	55:Ae:52:ARG:HG2	1.78	0.64
8:H:116:CYS:N	68:H:301:SF4:S4	2.70	0.64
15:O:111:ASP:OD2	17:Q:64:ARG:NH2	2.30	0.64
36:l:481:THR:HG22	44:t:92:HIS:ND1	2.12	0.64
39:o:25:ILE:HG23	45:u:262:VAL:H	1.62	0.64
45:u:279:ASP:HA	50:z:12:ARG:HG3	1.79	0.64
45:5:180:ARG:HH21	55:Ae:52:ARG:HD2	1.63	0.64
56:Ag:40:TYR:HA	59:Aj:45:LEU:HD21	1.78	0.64
3:C:361:ALA:HB3	7:G:149:ASP:HB2	1.78	0.64
42:r:199:ASP:OD2	42:r:279:ARG:NH2	2.28	0.64
45:u:478:LEU:HG	75:u:502:PEE:C5	2.28	0.64
76:w:402:HEM:CHA	76:w:402:HEM:HAA1	2.27	0.64
45:5:363:MET:SD	45:5:464:GLN:NE2	2.71	0.64
48:8:253:VAL:HG12	48:8:254:LEU:HG	1.80	0.64
5:E:57:PRO:HA	5:E:60:TYR:HD2	1.62	0.64
7:G:173:MET:O	7:G:175:ARG:N	2.26	0.64
7:G:221:ASN:ND2	7:G:286:ILE:O	2.21	0.64
7:G:368:THR:N	7:G:533:GLY:O	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:v:93:GLY:HA3	46:v:139:ASN:HD21	1.62	0.64
75:2:302:PEE:H49	75:2:302:PEE:C11	2.27	0.64
45:5:273:SER:O	45:5:456:VAL:N	2.29	0.64
7:G:262:VAL:HG23	7:G:276:ARG:HB2	1.80	0.64
43:s:45:LEU:O	43:s:49:GLU:HG2	1.96	0.64
44:t:13:ALA:CA	44:t:22:MET:CB	2.74	0.64
60:Ak:195:LEU:HD23	60:Ak:245:ILE:HD13	1.79	0.64
67:Ar:39:CYS:HG	67:Ar:53:CYS:HG	0.66	0.64
2:B:312:ASP:HA	2:B:315:LEU:HD12	1.78	0.64
3:C:362:LYS:HE3	7:G:149:ASP:HB3	1.80	0.64
3:C:427:PRO:O	3:C:431:HIS:ND1	2.30	0.64
5:E:131:HIS:H	5:E:189:ASN:HD21	1.44	0.64
7:G:37:ASP:OD1	7:G:38:GLY:N	2.30	0.64
15:O:102:SER:HB2	15:O:107:ASP:OD2	1.96	0.64
20:U:138:TYR:HD2	20:U:189:TYR:HH	1.39	0.64
45:u:387:GLU:OE2	45:u:390:ARG:NH2	2.24	0.64
46:v:136:PHE:O	46:v:140:VAL:N	2.28	0.64
45:5:211:LEU:HD21	45:5:216:LEU:HD21	1.79	0.64
46:6:376:ASN:HD22	46:6:379:LYS:HD3	1.63	0.64
12:L:150:HIS:ND1	12:L:190:GLU:OE2	2.23	0.64
48:x:151:GLU:HA	48:x:170:GLY:HA3	1.79	0.64
46:6:171:ALA:HA	55:Ae:11:PHE:CZ	2.32	0.64
2:B:229:PHE:O	2:B:233:VAL:N	2.29	0.64
3:C:40:ASP:OD1	3:C:41:VAL:N	2.27	0.64
4:D:124:ASN:H	14:N:111:GLN:NE2	1.96	0.64
5:E:78:ALA:HB3	5:E:105:LEU:HD21	1.79	0.64
8:H:151:LYS:HA	9:I:161:GLY:HA2	1.79	0.64
9:I:216:ARG:HG3	9:I:216:ARG:O	1.97	0.64
25:a:168:TRP:HB2	31:g:4:MET:H	1.63	0.64
27:c:55:TYR:OH	27:c:74:ASP:O	2.14	0.64
45:u:70:THR:OG1	45:u:410:CYS:SG	2.47	0.64
49:y:27:PHE:O	49:y:31:GLY:N	2.30	0.64
60:Ak:273:MET:HG3	60:Ak:319:LYS:HZ1	1.61	0.64
25:a:163:ARG:NH2	31:g:102:ASP:OD2	2.27	0.64
39:o:42:ARG:NH1	40:p:146:PRO:O	2.24	0.64
41:q:94:LEU:O	41:q:97:THR:OG1	2.16	0.64
53:2:204:ARG:HE	53:2:260:VAL:HG21	1.62	0.64
47:7:30:TRP:HH2	75:7:402:PEE:H21	1.58	0.64
7:G:210:ILE:HG22	7:G:212:LYS:H	1.62	0.64
18:S:70:ASP:OD1	43:s:75:LYS:NZ	2.31	0.64
26:b:87:LYS:O	26:b:91:THR:OG1	2.12	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:i:291:TYR:CZ	75:i:501:PEE:H49	2.33	0.64
47:w:278:TYR:HA	47:w:281:LEU:HD13	1.80	0.64
47:w:378:LYS:NZ	49:y:92:GLU:OE2	2.30	0.64
53:2:241:SER:HA	53:2:251:LYS:HB2	1.79	0.64
53:4:177:ARG:NH2	53:4:227:ASN:OD1	2.30	0.64
47:7:282:ARG:NH1	47:7:338:ILE:O	2.30	0.64
49:9:83:LYS:HB2	49:9:86:GLU:HG2	1.79	0.64
12:L:236:VAL:HG23	12:L:272:LEU:HA	1.80	0.63
20:U:138:TYR:HD2	20:U:189:TYR:OH	1.80	0.63
25:a:119:ARG:HH22	28:d:63:TYR:HB3	1.63	0.63
47:w:8:HIS:CD2	47:w:10:LEU:HB3	2.33	0.63
53:2:239:HIS:ND1	70:2:303:FES:S2	2.70	0.63
46:6:183:ARG:HB2	46:6:252:LYS:HG3	1.79	0.63
47:7:147:THR:HG22	47:7:161:VAL:HG13	1.79	0.63
52:Ac:22:ALA:HA	52:Ac:25:ILE:HD12	1.80	0.63
62:Am:101:PHE:HZ	62:Am:260:GLY:HA3	1.61	0.63
2:B:297:LYS:N	2:B:332:CYS:SG	2.66	0.63
3:C:335:GLU:OE2	8:H:39:LYS:NZ	2.30	0.63
7:G:298:LYS:O	11:R:134:ILE:O	2.17	0.63
7:G:624:ARG:NE	7:G:636:TYR:O	2.30	0.63
20:U:138:TYR:CD2	20:U:189:TYR:CZ	2.85	0.63
20:U:150:GLU:HB2	20:U:300:VAL:HG12	1.64	0.63
29:e:113:ARG:HH22	41:q:452:LYS:HB2	1.62	0.63
44:t:13:ALA:HB2	44:t:22:MET:CB	2.27	0.63
45:u:406:THR:OG1	46:v:387:GLU:OE2	2.13	0.63
45:5:468:TYR:HA	45:5:471:ILE:HD12	1.80	0.63
46:6:111:SER:HA	55:Ae:16:SER:HB3	1.81	0.63
36:l:70:THR:HA	36:l:75:GLU:HG3	1.79	0.63
47:w:106:SER:OG	76:w:402:HEM:O2D	2.16	0.63
71:2:301:PLX:C19	75:2:302:PEE:H65	2.25	0.63
45:5:75:ILE:HG22	45:5:77:ALA:H	1.61	0.63
10:J:77:VAL:HG21	10:J:99:MET:HG2	1.81	0.63
27:c:93:ASP:OD1	39:o:44:LYS:NZ	2.31	0.63
41:q:6:ILE:O	41:q:9:THR:OG1	2.13	0.63
43:s:96:LEU:CD1	43:s:99:HIS:HB2	2.27	0.63
45:u:437:ASP:OD1	45:u:438:ALA:N	2.32	0.63
47:w:173:ALA:O	47:w:177:ARG:HG2	1.98	0.63
75:w:403:PEE:H61	75:w:403:PEE:H28	1.81	0.63
53:4:164:ASN:HB2	53:4:177:ARG:HD2	1.80	0.63
45:5:179:MET:HE2	55:Ae:43:LEU:HD22	1.79	0.63
45:5:383:ALA:O	45:5:442:ARG:NH2	2.27	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:464:GLN:HA	7:G:467:LYS:HD3	1.80	0.63
12:L:170:LEU:HD21	12:L:264:ALA:HB1	1.79	0.63
18:S:31:ASN:HA	18:S:61:HIS:ND1	2.13	0.63
43:s:96:LEU:HD12	43:s:99:HIS:H	1.61	0.63
61:Al:122:MET:HB2	61:Al:208:PRO:HD2	1.81	0.63
63:An:16:TYR:CE1	63:An:25:PRO:HG3	2.34	0.63
2:B:146:GLY:O	2:B:151:ALA:N	2.31	0.63
3:C:94:VAL:HG11	3:C:116:LEU:HD12	1.81	0.63
7:G:391:ILE:N	7:G:600:GLU:OE2	2.23	0.63
12:L:195:PHE:CD1	12:L:198:ALA:HB2	2.34	0.63
26:b:86:LEU:O	26:b:90:VAL:HG12	1.98	0.63
36:l:128:MET:HE1	36:l:255:ALA:HB2	1.80	0.63
53:4:236:CYS:HB3	53:4:241:SER:HB2	1.81	0.63
45:5:391:GLY:HA2	45:5:394:ILE:HD12	1.80	0.63
49:9:14:LEU:O	49:9:18:ARG:HG2	1.98	0.63
67:Ar:57:ARG:HB3	67:Ar:57:ARG:HH11	1.64	0.63
7:G:479:SER:HG	7:G:687:PRO:HD3	1.61	0.63
7:G:662:ALA:H	16:P:57:GLU:HB3	1.64	0.63
9:I:155:SER:N	9:I:185:GLY:O	2.31	0.63
13:M:93:LYS:HA	14:N:50:GLN:HE22	1.64	0.63
16:P:44:LEU:O	16:P:48:ASN:N	2.31	0.63
17:Q:63:VAL:CG2	73:Q:201:ZMP:H4	2.21	0.63
47:w:37:LEU:HB3	76:w:402:HEM:HBB2	1.79	0.63
48:x:292:LYS:HD2	75:2:302:PEE:H8	1.81	0.63
52:1:34:ARG:HB2	54:3:48:ILE:HG23	1.80	0.63
2:B:176:ALA:HA	2:B:181:LEU:HD12	1.79	0.63
33:i:190:MET:HE2	33:i:205:LEU:HA	1.79	0.63
33:i:211:MET:SD	33:i:333:SER:HB2	2.39	0.63
41:q:336:ARG:HH12	41:q:429:SER:HA	1.63	0.63
75:u:502:PEE:H49	75:u:502:PEE:H26	1.78	0.63
46:v:253:TYR:OH	46:v:437:SER:N	2.32	0.63
49:y:61:PHE:HE2	49:y:65:ARG:HH21	1.47	0.63
50:z:51:PRO:HG2	50:z:52:PRO:HD3	1.81	0.63
75:7:402:PEE:N	50:Aa:41:ARG:NH2	2.42	0.63
7:G:341:ILE:HB	7:G:546:PHE:HD1	1.64	0.63
9:I:89:LEU:HD21	9:I:133:MET:HE2	1.79	0.63
11:K:88:ARG:HB2	11:K:90:LEU:HD13	1.81	0.63
36:l:73:THR:HG21	36:l:194:ASN:HD21	1.64	0.63
45:u:452:GLN:N	45:u:472:ARG:HH12	1.97	0.63
2:B:301:GLU:HA	2:B:306:GLY:HA2	1.80	0.62
2:B:331:VAL:HG23	2:B:332:CYS:H	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:124:ASP:OD1	36:l:358:LYS:NZ	2.22	0.62
36:l:14:ILE:HD11	36:l:43:ALA:HB2	1.81	0.62
41:q:35:SER:O	41:q:38:SER:OG	2.13	0.62
41:q:403:THR:HA	41:q:406:TYR:CE2	2.34	0.62
45:5:100:GLY:HA3	45:5:106:GLY:HA2	1.81	0.62
45:5:277:HIS:CE1	45:5:279:ASP:CG	2.76	0.62
2:B:51:TRP:HB3	2:B:133:HIS:HA	1.79	0.62
3:C:166:ARG:HH22	22:W:11:PRO:HD2	1.65	0.62
16:P:65:LEU:HB3	16:P:77:VAL:HB	1.81	0.62
21:V:24:ALA:O	21:V:27:SER:OG	2.11	0.62
45:u:113:VAL:HG11	45:u:120:LEU:HD23	1.81	0.62
45:u:289:ILE:HG13	45:u:456:VAL:HG22	1.79	0.62
46:v:319:GLN:O	46:v:321:PHE:N	2.32	0.62
45:5:276:ARG:HD3	45:5:462:ILE:CD1	2.28	0.62
47:7:377:LEU:HB3	49:9:34:ARG:HD2	1.81	0.62
3:C:171:ARG:NH1	3:C:231:GLY:O	2.32	0.62
7:G:192:VAL:HG12	7:G:194:ASP:H	1.63	0.62
7:G:481:LEU:O	7:G:482:GLN:O	2.17	0.62
7:G:550:ALA:HA	7:G:575:VAL:HB	1.81	0.62
8:H:153:ILE:HG21	9:I:162:TYR:CD1	2.33	0.62
41:q:225:ILE:HB	41:q:331:ASN:HD22	1.63	0.62
41:q:407:SER:O	41:q:410:MET:HG2	1.99	0.62
45:u:460:GLY:HA3	45:u:461:PRO:C	2.23	0.62
48:8:309:ARG:HG3	50:Aa:27:PHE:HE1	1.63	0.62
3:C:286:TYR:O	4:D:162:ALA:CB	2.47	0.62
7:G:275:PRO:HG2	10:J:86:ASN:HD22	1.62	0.62
17:Q:36:TYR:HD1	17:Q:67:PHE:CE2	2.18	0.62
43:s:47:ARG:O	43:s:50:GLU:O	2.18	0.62
45:5:165:ARG:HH12	45:5:211:LEU:HB3	1.63	0.62
46:6:392:PHE:HD2	46:6:393:LEU:HD12	1.64	0.62
47:7:71:ARG:NH2	48:8:278:ALA:O	2.32	0.62
4:D:154:GLU:HA	4:D:179:ALA:HB3	1.81	0.62
7:G:298:LYS:O	11:R:134:ILE:HA	1.99	0.62
7:G:607:LYS:NZ	10:J:148:GLU:OE2	2.31	0.62
12:L:168:SER:O	12:L:202:LYS:HA	1.99	0.62
13:M:92:LYS:N	14:N:46:LYS:HZ1	1.98	0.62
22:W:60:LEU:HD22	43:s:98:ARG:HH21	1.63	0.62
26:b:100:ARG:HG2	28:d:118:GLY:HA2	1.82	0.62
29:e:65:ASN:HB2	29:e:68:GLU:HB2	1.81	0.62
34:j:69:ILE:HD12	42:r:148:ILE:HG13	1.82	0.62
45:5:231:LEU:HD21	45:5:242:LEU:HG	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:Ak:84:PRO:HG3	60:Ak:92:MET:HE3	1.80	0.62
60:Ak:187:SER:CB	60:Ak:277:MET:HE1	2.28	0.62
2:B:86:ARG:NE	2:B:92:GLY:O	2.29	0.62
3:C:36:GLN:HG3	3:C:37:TRP:H	1.64	0.62
7:G:391:ILE:HA	7:G:394:VAL:HG23	1.82	0.62
17:Q:56:VAL:HG12	17:Q:60:ARG:NH1	2.13	0.62
17:Q:71:ALA:HA	73:Q:201:ZMP:H15	1.78	0.62
33:i:42:PRO:HG3	37:m:167:VAL:HG22	1.82	0.62
3:C:279:THR:HG23	14:N:13:GLY:HA3	1.82	0.62
10:J:97:TRP:CE2	10:J:131:LYS:HB2	2.34	0.62
14:N:97:TRP:HB3	14:N:100:TRP:CH2	2.34	0.62
20:U:134:GLN:HG2	20:U:172:LEU:HD12	1.82	0.62
24:Z:36:LEU:O	24:Z:40:GLY:N	2.33	0.62
29:e:71:PRO:HB3	40:p:108:HIS:HB2	1.82	0.62
33:i:34:GLU:HG2	35:k:66:PHE:HB3	1.82	0.62
33:i:159:MET:HB2	33:i:278:MET:HE1	1.82	0.62
47:w:241:ILE:HG13	48:x:293:MET:CE	2.29	0.62
53:4:234:TYR:N	53:4:243:TYR:O	2.22	0.62
3:C:345:SER:O	3:C:349:ASN:ND2	2.33	0.62
3:C:397:TYR:HE2	4:D:140:ARG:NH1	1.98	0.62
9:I:170:VAL:HG11	9:I:176:ILE:HD11	1.80	0.62
12:L:265:PHE:HZ	12:L:338:LEU:HD12	1.63	0.62
32:h:86:LEU:O	32:h:90:GLY:N	2.32	0.62
36:l:332:HIS:CE1	36:l:336:LYS:HG3	2.34	0.62
41:q:175:ASN:OD1	41:q:176:PHE:N	2.32	0.62
48:x:194:LEU:HD12	48:x:195:PRO:HD2	1.81	0.62
46:6:355:TYR:HE1	46:6:436:LYS:HE2	1.65	0.62
61:Al:16:ILE:HD12	61:Al:17:MET:N	2.15	0.62
5:E:177:LEU:N	70:E:301:FES:S1	2.67	0.62
7:G:64:CYS:O	7:G:184:ARG:NH2	2.33	0.62
7:G:615:LEU:HD12	7:G:617:ARG:HH12	1.65	0.62
34:j:105:GLU:HG2	34:j:111:LEU:HB2	1.82	0.62
36:l:159:HIS:NE2	40:p:96:CYS:SG	2.68	0.62
45:u:473:SER:HB3	75:u:502:PEE:H10	1.81	0.62
53:4:153:GLU:HB3	53:4:273:VAL:HB	1.82	0.62
45:5:170:GLN:HE21	45:5:174:GLU:HG3	1.64	0.62
48:8:288:ARG:NH1	52:Ac:41:ASP:CG	2.52	0.62
3:C:292:MET:HG3	3:C:431:HIS:HD2	1.64	0.62
7:G:179:CYS:SG	7:G:227:PRO:HG3	2.39	0.62
12:L:188:GLU:OE2	12:L:202:LYS:NZ	2.29	0.62
21:V:139:PRO:O	21:V:141:VAL:N	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:l:8:THR:O	36:l:11:THR:HG22	2.00	0.62
45:u:273:SER:HB3	50:z:19:LEU:HD23	1.82	0.62
45:5:171:GLU:O	45:5:175:ASN:ND2	2.32	0.62
46:6:162:LYS:NZ	46:6:194:ASP:OD1	2.27	0.62
60:Ak:11:ASN:HD21	60:Ak:13:LYS:HB2	1.64	0.62
4:D:186:ARG:NH1	17:Q:92:GLU:OE2	2.33	0.61
12:L:354:ARG:HG3	12:L:357:ARG:HD2	1.82	0.61
41:q:225:ILE:HD11	41:q:328:CYS:HA	1.82	0.61
46:v:436:LYS:HB2	46:v:450:VAL:HG21	1.82	0.61
48:x:217:THR:HG21	51:0:30:LEU:HD21	1.82	0.61
45:5:479:ARG:NH2	74:5:501:CDL:OB2	2.33	0.61
60:Ak:92:MET:HE2	60:Ak:167:THR:HG21	1.82	0.61
14:N:55:LYS:HA	14:N:58:MET:HE2	1.82	0.61
33:i:210:THR:HG22	33:i:333:SER:HB3	1.81	0.61
74:u:501:CDL:C14	75:u:502:PEE:H58	2.30	0.61
46:v:155:GLN:NE2	46:v:200:VAL:O	2.34	0.61
46:v:322:ASP:HB3	46:v:341:ILE:HB	1.82	0.61
47:w:345:HIS:HA	47:w:348:ILE:HD12	1.82	0.61
47:7:27:ILE:HG23	47:7:31:TRP:HB2	1.81	0.61
47:7:269:LYS:NZ	47:7:340:GLY:O	2.33	0.61
49:9:36:ASP:OD2	49:9:62:ARG:NH1	2.32	0.61
64:Ao:82:TYR:HB3	64:Ao:83:PRO:HD3	1.82	0.61
28:d:147:GLY:HA3	31:g:121:VAL:HG21	1.81	0.61
36:l:421:ALA:O	36:l:424:THR:HG22	2.00	0.61
40:p:108:HIS:CE1	40:p:110:SER:HB3	2.36	0.61
40:p:108:HIS:H	40:p:112:LYS:HE2	1.65	0.61
48:x:94:SER:HB2	48:x:100:ARG:HH12	1.64	0.61
49:y:18:ARG:O	49:y:22:TYR:N	2.31	0.61
45:5:413:ILE:HG12	45:5:423:ARG:HD2	1.81	0.61
48:8:99:HIS:NE2	48:8:209:GLU:OE1	2.24	0.61
11:K:84:PRO:HA	11:K:87:HIS:HB3	1.83	0.61
12:L:203:PRO:HB2	72:L:401:NDP:C5N	2.30	0.61
43:s:26:LYS:NZ	43:s:95:GLN:O	2.34	0.61
47:w:319:PRO:HA	47:w:322:GLN:HB3	1.83	0.61
45:5:100:GLY:HA2	45:5:109:LEU:HD13	1.82	0.61
45:5:222:GLN:O	45:5:225:LYS:NZ	2.33	0.61
45:5:277:HIS:HE1	45:5:279:ASP:CG	2.08	0.61
48:8:186:ALA:HB1	48:8:195:PRO:HD2	1.81	0.61
49:9:78:LYS:HA	49:9:81:TRP:CD1	2.34	0.61
2:B:285:PRO:HG3	5:E:143:ARG:HH22	1.65	0.61
41:q:336:ARG:NH1	41:q:429:SER:HA	2.16	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:v:283:ALA:HA	46:v:286:PHE:HD2	1.64	0.61
47:w:58:ASP:HA	47:w:172:LYS:HG3	1.83	0.61
45:5:296:TRP:N	45:5:348:TYR:O	2.33	0.61
46:6:133:LEU:HA	46:6:136:PHE:HB2	1.80	0.61
7:G:165:ILE:HD12	7:G:171:THR:HG21	1.81	0.61
27:c:110:ASP:OD1	41:q:278:ARG:NH1	2.33	0.61
32:h:21:GLN:O	32:h:25:GLN:NE2	2.33	0.61
42:r:85:MET:HB3	42:r:233:MET:SD	2.40	0.61
47:7:77:TRP:HB2	47:7:81:TYR:CE2	2.36	0.61
75:7:402:PEE:H8	50:Aa:45:CYS:SG	2.40	0.61
52:Ac:53:TRP:O	52:Ac:57:LYS:N	2.33	0.61
56:Ag:13:LYS:H	56:Ag:13:LYS:HD3	1.64	0.61
57:Ah:3:ASN:C	57:Ah:3:ASN:HD22	2.08	0.61
60:Ak:128:VAL:HG22	60:Ak:128:VAL:O	1.99	0.61
62:Am:148:HIS:O	62:Am:152:MET:HG3	2.01	0.61
62:Am:154:GLY:HA2	65:Ap:6:VAL:CG2	2.30	0.61
2:B:79:GLU:OE2	2:B:259:GLY:N	2.34	0.61
7:G:254:MET:HE3	7:G:289:LYS:HE3	1.82	0.61
12:L:315:THR:HG23	12:L:318:LYS:H	1.65	0.61
19:T:25:ILE:HD11	42:r:300:LEU:HD12	1.83	0.61
20:U:150:GLU:CG	20:U:300:VAL:HG11	2.26	0.61
21:V:141:VAL:HB	33:i:273:ASN:HD21	1.65	0.61
33:i:173:THR:O	33:i:227:THR:OG1	2.19	0.61
47:w:8:HIS:HE1	47:7:199:PHE:HE1	1.46	0.61
4:D:76:VAL:HG12	4:D:86:ILE:HG22	1.83	0.61
7:G:313:LEU:HD22	11:R:141:SER:HA	1.82	0.61
26:b:72:VAL:O	26:b:76:LEU:HB2	2.01	0.61
35:k:88:ASP:HB3	35:k:90:VAL:HG12	1.82	0.61
36:l:270:ASN:OD1	36:l:272:LEU:N	2.33	0.61
43:s:47:ARG:HH21	43:s:47:ARG:CG	2.13	0.61
45:u:280:ASP:HA	45:u:461:PRO:HB3	1.81	0.61
48:x:116:GLN:HA	48:x:119:LYS:HE2	1.83	0.61
45:5:56:GLY:HA3	45:5:227:PRO:HB3	1.83	0.61
47:7:132:VAL:HA	47:7:139:SER:HB3	1.82	0.61
60:Ak:92:MET:CE	60:Ak:167:THR:HG21	2.31	0.61
2:B:98:LYS:NZ	69:B:502:FMN:O3P	2.34	0.61
7:G:133:GLN:HG3	7:G:137:CYS:HB2	1.81	0.61
12:L:195:PHE:HD1	12:L:198:ALA:HB2	1.66	0.61
28:d:114:GLN:HG2	36:l:199:GLN:HA	1.81	0.61
32:h:100:GLY:O	32:h:104:PRO:N	2.34	0.61
41:q:270:ILE:HD13	41:q:398:MET:HE3	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:z:12:ARG:HG2	50:z:13:HIS:ND1	2.15	0.61
46:6:351:ILE:HD11	46:6:448:PRO:HG2	1.82	0.61
47:7:65:SER:O	47:7:68:HIS:HB3	2.00	0.61
47:7:312:GLN:HG2	49:9:38:ILE:HA	1.83	0.61
12:L:59:PHE:CZ	12:L:126:VAL:HG13	2.35	0.61
12:L:355:ARG:HB3	34:j:31:SER:HB2	1.83	0.61
38:n:11:HIS:HA	38:n:14:HIS:HD2	1.66	0.61
41:q:286:ILE:O	41:q:289:SER:OG	2.14	0.61
42:r:173:TRP:NE1	42:r:244:GLY:O	2.34	0.61
45:5:149:ASP:HA	45:5:153:ASN:ND2	2.16	0.61
3:C:161:ILE:HD11	3:C:358:VAL:HG11	1.82	0.60
12:L:141:PHE:HZ	12:L:180:TYR:HB3	1.65	0.60
12:L:204:SER:OG	12:L:265:PHE:O	2.18	0.60
48:x:88:LEU:HD11	50:z:71:LYS:HG2	1.83	0.60
48:x:301:LEU:O	74:x:402:CDL:H362	2.01	0.60
53:2:179:ARG:NH2	53:2:201:ASP:OD2	2.29	0.60
2:B:275:LEU:HA	2:B:289:GLU:HA	1.82	0.60
7:G:138:ASP:OD2	10:J:89:SER:OG	2.20	0.60
21:V:137:ALA:HB3	33:i:275:SER:HB3	1.83	0.60
27:c:63:GLU:O	27:c:77:LYS:HB3	2.01	0.60
33:i:181:TYR:HA	33:i:184:ILE:HG22	1.84	0.60
36:l:119:LYS:NZ	74:l:702:CDL:OB5	2.33	0.60
36:l:362:LEU:HB2	36:l:365:ALA:HB3	1.83	0.60
41:q:204:MET:HE2	41:q:209:LEU:HD22	1.82	0.60
42:r:24:GLU:HA	42:r:271:LEU:HD13	1.83	0.60
45:u:112:GLU:HG3	45:u:116:MET:HE2	1.82	0.60
45:u:397:ASN:ND2	46:v:107:GLY:O	2.23	0.60
47:w:240:LEU:HA	47:w:243:VAL:HG12	1.83	0.60
45:5:465:LEU:HD12	45:5:466:PRO:HD2	1.83	0.60
2:B:427:LEU:HB3	68:B:501:SF4:S4	2.41	0.60
4:D:196:HIS:HB2	4:D:199:ARG:HD3	1.82	0.60
12:L:88:PRO:O	12:L:91:THR:OG1	2.15	0.60
18:S:23:THR:HG23	42:r:5:ASN:HD21	1.65	0.60
23:Y:94:ASP:C	44:t:108:LEU:HD21	2.25	0.60
45:u:469:ASN:O	45:u:473:SER:N	2.34	0.60
53:2:125:VAL:HG11	71:2:301:PLX:H122	1.83	0.60
53:2:176:VAL:HG12	53:2:212:ILE:HG22	1.82	0.60
53:4:83:ILE:HG22	48:8:323:ARG:HH22	1.66	0.60
62:Am:119:THR:O	66:Aq:52:HIS:HE1	1.84	0.60
2:B:179:ALA:HB3	2:B:181:LEU:HG	1.82	0.60
4:D:97:LEU:HA	4:D:100:LEU:HD12	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:211:ASP:OD1	12:L:212:ARG:N	2.34	0.60
12:L:217:PHE:HA	12:L:220:MET:HG2	1.84	0.60
14:N:77:ILE:O	14:N:81:ILE:HG23	2.01	0.60
41:q:59:ASP:OD1	41:q:60:SER:N	2.34	0.60
52:1:45:GLU:HG2	52:1:54:LYS:HE2	1.83	0.60
49:9:64:LYS:HE2	50:Aa:14:VAL:HG11	1.83	0.60
52:Ac:54:LYS:HA	52:Ac:57:LYS:HD3	1.83	0.60
4:D:186:ARG:NE	4:D:191:TYR:O	2.35	0.60
6:F:99:TYR:HE2	7:G:157:LYS:H	1.50	0.60
14:N:44:TYR:CD2	14:N:94:MET:HE2	2.36	0.60
43:s:29:ALA:HA	43:s:32:TYR:HB3	1.83	0.60
62:Am:192:VAL:O	62:Am:196:THR:HB	2.01	0.60
5:E:152:ILE:HD11	5:E:201:ILE:HG21	1.84	0.60
7:G:47:THR:OG1	7:G:51:GLN:OE1	2.19	0.60
27:c:82:SER:H	27:c:119:THR:HG22	1.66	0.60
46:v:235:GLU:HA	46:v:238:LEU:HB2	1.84	0.60
47:w:30:TRP:CZ3	75:w:403:PEE:C13	2.84	0.60
45:5:77:ALA:HA	45:5:81:TYR:CE2	2.37	0.60
45:5:278:ARG:HH11	45:5:462:ILE:C	2.09	0.60
65:Ap:13:ALA:O	65:Ap:18:ARG:HD2	2.00	0.60
4:D:102:ASP:HB3	14:N:90:LEU:HD22	1.83	0.60
8:H:41:VAL:HG12	13:M:113:LEU:HD23	1.83	0.60
16:P:31:GLN:HA	16:P:34:ARG:HE	1.66	0.60
20:U:91:ALA:CB	20:U:95:TYR:CD1	2.84	0.60
20:U:164:SER:O	20:U:167:SER:OG	2.19	0.60
36:l:409:LEU:O	36:l:412:THR:OG1	2.14	0.60
45:u:39:ALA:HA	45:u:42:LEU:HD12	1.84	0.60
46:v:320:PRO:HB2	46:v:343:GLN:HE21	1.67	0.60
53:2:136:PHE:CD2	75:2:302:PEE:H37	2.37	0.60
47:7:282:ARG:NH1	47:7:341:GLN:O	2.35	0.60
49:9:51:LEU:HD23	49:9:94:TYR:CE2	2.37	0.60
4:D:101:ARG:HH12	4:D:159:VAL:HA	1.67	0.60
5:E:182:ASN:ND2	5:E:194:GLU:OE1	2.34	0.60
20:U:85:LEU:CB	20:U:159:VAL:N	2.65	0.60
21:V:90:TYR:HD2	21:V:126:LYS:HB2	1.67	0.60
24:Z:48:ASN:OD1	24:Z:52:ARG:NH1	2.32	0.60
36:l:132:VAL:O	36:l:262:ARG:NH1	2.34	0.60
75:u:502:PEE:H13	71:2:301:PLX:H6	1.84	0.60
46:v:69:SER:O	46:v:188:ASN:ND2	2.31	0.60
45:5:48:THR:OG1	45:5:423:ARG:NH1	2.32	0.60
46:6:359:LYS:O	46:6:363:GLN:N	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:235:ASP:OD1	3:C:236:LEU:N	2.35	0.60
7:G:476:LEU:HD22	7:G:493:VAL:HG11	1.83	0.60
10:J:68:PRO:HG2	10:J:71:HIS:HD2	1.67	0.60
12:L:65:LEU:HD13	12:L:242:ILE:CD1	2.31	0.60
17:Q:26:ASN:HA	17:Q:29:LYS:HD3	1.83	0.60
15:X:90:TYR:HD2	15:X:93:ILE:HD12	1.66	0.60
43:s:70:PHE:CE2	43:s:74:ILE:HD11	2.37	0.60
46:v:81:HIS:O	46:v:84:ARG:HG2	2.02	0.60
47:7:115:ILE:HG22	47:7:196:HIS:HD2	1.67	0.60
56:Ag:28:LEU:HB2	56:Ag:29:PRO:HD3	1.83	0.60
65:Ap:62:CYS:SG	65:Ap:84:SER:OG	2.60	0.60
2:B:244:ASN:OD1	2:B:245:VAL:N	2.35	0.60
3:C:316:PHE:HA	3:C:342:ARG:HH11	1.66	0.60
9:I:200:LEU:O	9:I:204:ILE:HD12	2.02	0.60
31:g:15:PHE:O	31:g:80:ARG:NH1	2.34	0.60
33:i:255:PRO:HB2	41:q:120:ILE:HG13	1.82	0.60
41:q:106:LEU:HA	41:q:109:THR:HG22	1.84	0.60
41:q:205:VAL:HG22	41:q:212:LEU:HD23	1.84	0.60
47:w:247:PRO:HG3	48:x:286:ARG:NH2	2.17	0.60
53:4:92:ARG:HA	50:Aa:24:GLN:HA	1.84	0.60
53:4:267:SER:OG	53:4:269:ASP:OD1	2.19	0.60
46:6:185:ALA:HA	46:6:188:ASN:HD22	1.67	0.60
55:Ae:16:SER:OG	55:Ae:19:SER:N	2.34	0.60
3:C:375:MET:HE2	7:G:124:HIS:HD2	1.67	0.59
14:N:77:ILE:HA	14:N:80:VAL:HG12	1.84	0.59
20:U:91:ALA:HB2	20:U:144:GLN:HE22	1.63	0.59
36:l:342:CYS:O	36:l:345:SER:OG	2.16	0.59
36:l:467:ILE:O	36:l:471:ASN:ND2	2.35	0.59
45:u:121:ASN:ND2	45:u:132:TYR:OH	2.30	0.59
53:2:243:TYR:OH	70:2:303:FES:S1	2.60	0.59
47:7:316:MET:HA	47:7:322:GLN:NE2	2.17	0.59
59:Aj:46:LYS:O	59:Aj:47:LYS:HB2	2.02	0.59
64:Ao:80:GLU:H	64:Ao:80:GLU:CD	2.10	0.59
4:D:247:GLN:NE2	14:N:115:PRO:HG2	2.17	0.59
7:G:650:SER:OG	7:G:652:ASN:N	2.32	0.59
9:I:157:ALA:HB1	9:I:173:CYS:HB2	1.83	0.59
45:u:78:GLY:HA3	45:u:127:GLU:HA	1.84	0.59
47:w:119:LEU:HD22	76:w:402:HEM:HHC	1.84	0.59
48:x:187:ARG:HB3	48:x:192:GLY:HA2	1.84	0.59
45:5:79:SER:HB2	45:5:201:VAL:HG22	1.85	0.59
7:G:219:SER:O	7:G:222:ILE:HG12	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:17:ARG:NH1	16:P:18:GLU:OE2	2.35	0.59
17:Q:62:LYS:HG2	17:Q:107:PHE:CE1	2.37	0.59
26:b:83:HIS:ND1	36:l:6:SER:OG	2.27	0.59
27:c:123:PRO:HB3	40:p:75:GLN:NE2	2.18	0.59
45:u:270:PHE:CD2	45:u:292:GLU:HB2	2.38	0.59
46:v:70:ARG:HB2	46:v:185:ALA:HB1	1.83	0.59
46:v:420:ALA:HB3	46:v:423:ASP:HB2	1.84	0.59
47:w:8:HIS:ND1	47:w:9:PRO:HD2	2.17	0.59
53:4:217:CYS:SG	53:4:222:CYS:N	2.75	0.59
48:8:87:ASP:OD2	48:8:241:GLN:NE2	2.35	0.59
48:8:217:THR:O	51:Ab:34:ARG:NH2	2.35	0.59
2:B:424:ILE:HG23	7:G:76:ARG:HD2	1.83	0.59
17:Q:59:GLY:O	17:Q:63:VAL:HG23	2.03	0.59
36:l:80:PHE:HB3	36:l:82:MET:HE2	1.83	0.59
36:l:391:SER:O	36:l:395:ILE:HG12	2.02	0.59
46:v:272:VAL:HG11	46:v:335:LEU:HB3	1.83	0.59
61:Al:145:PRO:CG	61:Al:148:MET:HE2	2.33	0.59
61:Al:226:MET:O	61:Al:227:LEU:HB2	2.01	0.59
3:C:330:TYR:HD2	3:C:331:LEU:HD12	1.65	0.59
4:D:118:ASP:OD1	4:D:119:VAL:N	2.36	0.59
12:L:167:ILE:HG13	12:L:201:ILE:HD13	1.83	0.59
36:l:72:GLN:O	36:l:74:VAL:N	2.34	0.59
36:l:244:SER:HA	36:l:248:HIS:HD2	1.67	0.59
75:l:701:PEE:H21	75:l:701:PEE:H62	1.85	0.59
46:v:259:ARG:HH21	46:v:444:LEU:HD22	1.68	0.59
47:w:326:TRP:HB3	50:z:52:PRO:HG2	1.84	0.59
62:Am:6:HIS:HD2	62:Am:8:TYR:H	1.49	0.59
2:B:104:LYS:O	2:B:106:SER:N	2.36	0.59
3:C:317:ASP:H	3:C:339:GLN:HE21	1.49	0.59
7:G:32:ILE:HG21	7:G:98:LYS:H	1.67	0.59
26:b:71:ALA:O	26:b:75:VAL:HG22	2.02	0.59
35:k:75:LEU:HD22	37:m:71:THR:HG21	1.83	0.59
37:m:64:MET:O	37:m:67:VAL:N	2.35	0.59
46:v:101:ARG:HB3	49:9:108:TRP:CZ2	2.38	0.59
47:w:206:ASN:OD1	47:w:207:ASN:N	2.34	0.59
75:7:402:PEE:H8	50:Aa:45:CYS:HB3	1.82	0.59
48:8:92:ALA:HB2	48:8:211:TYR:HB2	1.85	0.59
7:G:421:SER:O	7:G:425:ASN:N	2.28	0.59
20:U:307:LEU:O	20:U:310:THR:HG22	2.03	0.59
21:V:12:ILE:HG12	21:V:21:LYS:HE3	1.84	0.59
22:W:97:ILE:HG23	32:h:86:LEU:HD12	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:44:THR:O	27:c:48:ARG:N	2.36	0.59
40:p:31:CYS:O	40:p:33:HIS:N	2.36	0.59
71:4:301:PLX:H1C3	71:4:301:PLX:H32	1.85	0.59
12:L:170:LEU:HD23	12:L:202:LYS:HB3	1.84	0.59
12:L:202:LYS:N	12:L:203:PRO:HD3	2.18	0.59
16:P:63:PRO:HB2	16:P:79:LEU:HD11	1.84	0.59
46:v:286:PHE:HZ	46:v:430:LYS:HD3	1.67	0.59
48:8:108:HIS:HA	48:8:111:ILE:HD12	1.85	0.59
61:Al:179:LEU:HD21	67:Ar:65:PRO:HD3	1.85	0.59
22:W:60:LEU:CD2	43:s:98:ARG:HH21	2.15	0.59
37:m:115:ILE:O	37:m:117:PHE:N	2.35	0.59
46:6:50:ALA:HB3	46:6:221:ILE:HG13	1.83	0.59
46:6:287:SER:HB3	55:Ae:7:ARG:HH12	1.67	0.59
22:W:144:THR:OG1	34:j:2:ASN:ND2	2.36	0.59
36:l:357:ARG:HD2	40:p:80:TYR:HB2	1.84	0.59
46:v:91:THR:OG1	46:v:94:ALA:N	2.36	0.59
47:w:207:ASN:ND2	47:w:211:ILE:O	2.26	0.59
75:w:403:PEE:H8	74:z:101:CDL:CA3	2.28	0.59
48:x:135:HIS:HB3	48:x:277:TRP:HH2	1.67	0.59
53:4:103:SER:O	53:4:107:SER:N	2.36	0.59
53:4:195:LEU:HD13	53:4:248:ARG:HD2	1.84	0.59
45:5:66:GLN:O	45:5:236:GLY:N	2.35	0.59
48:8:132:ALA:HB2	48:8:175:TYR:CD1	2.38	0.59
48:8:305:TYR:OH	74:8:401:CDL:OA3	2.13	0.59
2:B:320:GLY:HA3	2:B:350:GLY:HA3	1.85	0.58
3:C:375:MET:HE2	7:G:124:HIS:CD2	2.38	0.58
7:G:326:VAL:HG11	7:G:582:VAL:HG11	1.84	0.58
7:G:549:GLY:H	7:G:568:TYR:HE1	1.51	0.58
7:G:652:ASN:HD21	16:P:56:ARG:HD2	1.68	0.58
8:H:76:TYR:CD1	42:r:33:LEU:HD11	2.38	0.58
12:L:293:LEU:HD12	12:L:294:PRO:HD2	1.84	0.58
18:S:51:ASP:CG	18:S:52:ARG:H	2.11	0.58
41:q:404:ALA:O	41:q:407:SER:OG	2.19	0.58
47:w:137:GLN:HE21	47:w:141:TRP:CD1	2.21	0.58
47:w:352:GLN:O	47:w:356:ILE:HD12	2.03	0.58
53:4:162:GLY:N	53:4:178:HIS:O	2.36	0.58
45:5:157:GLU:O	45:5:161:ILE:HG12	2.03	0.58
67:Ar:57:ARG:HG3	67:Ar:60:TYR:CE2	2.38	0.58
7:G:466:LEU:HD21	7:G:496:ILE:HG22	1.85	0.58
10:J:119:ASP:OD2	10:J:122:SER:HB3	2.04	0.58
14:N:21:HIS:HA	14:N:24:LEU:HD12	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:136:GLU:OE2	17:Q:33:ARG:NH2	2.36	0.58
37:m:22:SER:O	37:m:24:PRO:HD3	2.03	0.58
41:q:102:LEU:HD21	41:q:230:VAL:HG11	1.85	0.58
46:v:64:PHE:CE2	46:v:397:GLY:HA3	2.37	0.58
46:v:85:LEU:HD12	46:v:158:LEU:HD23	1.85	0.58
46:v:203:ASP:HA	46:v:206:HIS:HD2	1.68	0.58
46:v:313:VAL:HG22	46:v:353:SER:HB2	1.85	0.58
53:4:89:SER:HB3	53:4:97:LEU:HD12	1.85	0.58
53:4:266:THR:HG21	53:4:272:ILE:HD12	1.85	0.58
45:5:274:GLU:CA	45:5:456:VAL:HB	2.33	0.58
58:Ai:43:SER:OG	58:Ai:45:VAL:HG12	2.03	0.58
2:B:392:MET:HE3	2:B:419:ILE:HD12	1.85	0.58
2:B:423:THR:HG21	2:B:428:GLY:HA3	1.84	0.58
7:G:403:VAL:HG11	7:G:476:LEU:HD11	1.80	0.58
31:g:77:LEU:HD21	33:i:342:ALA:HB1	1.85	0.58
33:i:78:LEU:HD21	35:k:47:ILE:HG21	1.85	0.58
33:i:280:THR:HG22	41:q:162:VAL:HG11	1.83	0.58
36:l:34:ASN:HA	36:l:105:MET:HE1	1.85	0.58
41:q:189:SER:OG	41:q:190:TRP:N	2.37	0.58
45:u:134:LYS:HD3	46:v:384:MET:HE2	1.85	0.58
45:u:335:ARG:HH21	45:u:337:LEU:HD21	1.69	0.58
54:3:4:ARG:HG3	54:3:5:PHE:N	2.18	0.58
2:B:89:GLY:HA3	69:B:502:FMN:H4'	1.85	0.58
2:B:424:ILE:HG22	7:G:76:ARG:NH1	2.18	0.58
19:T:41:TYR:O	19:T:45:ILE:HD12	2.03	0.58
31:g:13:LEU:HD23	71:i:502:PLX:H31	1.84	0.58
34:j:83:ASN:O	34:j:86:THR:OG1	2.20	0.58
36:l:112:PRO:HG2	40:p:179:MET:HB3	1.84	0.58
36:l:342:CYS:O	36:l:346:ILE:HD12	2.02	0.58
40:p:11:THR:H	40:p:14:GLN:HE21	1.51	0.58
41:q:373:ILE:HA	41:q:376:ILE:HG22	1.84	0.58
43:s:83:THR:HA	43:s:86:TRP:NE1	2.18	0.58
47:w:105:GLY:HA3	47:w:313:ARG:O	2.03	0.58
76:7:403:HEM:CHB	76:7:403:HEM:CMA	2.81	0.58
4:D:115:THR:OG1	4:D:129:VAL:HB	2.04	0.58
25:a:56:ILE:HB	40:p:179:MET:HE1	1.84	0.58
33:i:10:ILE:HD11	33:i:129:LEU:HD11	1.86	0.58
43:s:31:HIS:CE1	43:s:119:ARG:HB2	2.38	0.58
43:s:111:VAL:O	43:s:116:GLY:N	2.34	0.58
44:t:56:ARG:CG	44:t:57:ASP:H	2.14	0.58
45:u:174:GLU:O	45:u:177:SER:OG	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:v:56:ALA:O	46:v:127:ARG:NH2	2.37	0.58
45:5:397:ASN:HD21	46:6:125:CYS:HA	1.68	0.58
45:5:397:ASN:HA	45:5:400:VAL:HB	1.85	0.58
61:A:59:GLN:HA	61:A:62:GLU:HB2	1.83	0.58
2:B:244:ASN:HB2	69:B:502:FMN:O2P	2.04	0.58
12:L:206:ILE:HA	12:L:240:VAL:O	2.04	0.58
15:O:115:GLN:NE2	15:O:135:ALA:O	2.32	0.58
18:S:12:MET:HE1	42:r:20:LEU:HB2	1.85	0.58
22:W:90:ASN:OD1	22:W:128:ARG:NH2	2.26	0.58
29:e:74:HIS:ND1	29:e:87:MET:SD	2.77	0.58
36:l:10:THR:HA	36:l:13:ILE:HG22	1.84	0.58
36:l:144:TRP:NE1	36:l:179:ASP:OD1	2.34	0.58
41:q:243:MET:HE1	41:q:298:ILE:HG13	1.85	0.58
43:s:83:THR:HA	43:s:86:TRP:CD1	2.38	0.58
45:u:166:ASP:OD1	45:u:167:VAL:N	2.37	0.58
46:v:394:ASP:OD1	46:v:395:GLU:N	2.37	0.58
48:x:250:TYR:CE2	48:x:253:VAL:HA	2.37	0.58
46:6:217:ARG:NH2	46:6:246:LEU:O	2.36	0.58
47:7:119:LEU:HD11	47:7:192:LEU:HB3	1.86	0.58
3:C:385:TYR:HD1	8:H:122:VAL:HG21	1.68	0.58
8:H:60:THR:HG23	71:H:303:PLX:H12	1.86	0.58
9:I:121:ASP:OD1	9:I:121:ASP:N	2.36	0.58
10:J:75:ARG:HD2	10:J:104:ARG:HE	1.68	0.58
25:a:78:THR:HG21	29:e:96:SER:HA	1.83	0.58
25:a:160:MET:HE2	25:a:166:GLY:HA3	1.84	0.58
26:b:73:THR:O	26:b:77:ILE:HG22	2.03	0.58
36:l:288:THR:HG21	36:l:307:SER:OG	2.04	0.58
41:q:269:MET:HE1	41:q:296:LEU:HD21	1.86	0.58
45:u:296:TRP:NE1	45:u:419:THR:OG1	2.36	0.58
48:x:103:LEU:HD21	52:1:47:ILE:HG21	1.86	0.58
53:4:99:SER:HA	45:5:269:ARG:HE	1.68	0.58
45:5:64:SER:N	45:5:235:GLY:O	2.27	0.58
47:7:44:GLN:HE21	76:7:403:HEM:HBB2	1.69	0.58
50:Aa:68:GLU:O	50:Aa:72:ARG:HG2	2.02	0.58
4:D:232:LYS:HD3	10:J:123:ASN:HB3	1.85	0.58
7:G:138:ASP:O	7:G:142:GLN:HG2	2.04	0.58
10:J:97:TRP:HB2	10:J:128:PHE:HB2	1.86	0.58
12:L:59:PHE:HE1	12:L:126:VAL:HG13	1.66	0.58
20:U:138:TYR:HD2	20:U:189:TYR:CZ	2.22	0.58
33:i:25:HIS:HD2	33:i:84:TRP:HB3	1.68	0.58
36:l:120:TYR:HB3	36:l:154:LEU:HD11	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:5:96:LEU:HA	45:5:99:LYS:HG2	1.84	0.58
45:5:142:LYS:O	45:5:145:GLU:HG2	2.03	0.58
45:5:373:GLN:NE2	45:5:471:ILE:O	2.36	0.58
60:Ak:172:LYS:HB2	60:Ak:172:LYS:HZ2	1.68	0.58
4:D:153:ILE:O	4:D:178:PHE:HA	2.04	0.58
7:G:299:ARG:HD2	7:G:705:GLN:HE21	1.69	0.58
33:i:2:ASN:O	33:i:5:ILE:HG22	2.03	0.58
33:i:254:LEU:HD11	33:i:290:LEU:HD11	1.85	0.58
42:r:134:ARG:HD3	42:r:200:LEU:HD23	1.85	0.58
45:u:308:ASN:HD21	45:u:345:ASN:HB2	1.69	0.58
47:w:312:GLN:OE1	47:w:318:ARG:NE	2.37	0.58
45:5:125:THR:HB	45:5:128:HIS:H	1.69	0.58
55:Af:16:SER:OG	55:Af:19:SER:O	2.22	0.58
60:Ak:404:THR:O	60:Ak:480:ARG:NH1	2.37	0.58
7:G:371:VAL:HA	7:G:534:VAL:HG12	1.84	0.58
9:I:99:MET:CE	9:I:113:PHE:HZ	2.16	0.58
33:i:268:GLN:HA	41:q:165:VAL:HG11	1.85	0.58
33:i:318:GLU:OE1	33:i:318:GLU:N	2.37	0.58
74:i:503:CDL:OB4	41:q:90:THR:OG1	2.12	0.58
41:q:229:MET:HE2	41:q:328:CYS:HB3	1.85	0.58
43:s:26:LYS:NZ	43:s:97:PHE:CE1	2.71	0.58
52:1:43:ILE:HG22	52:1:47:ILE:HD11	1.86	0.58
45:5:270:PHE:CG	45:5:292:GLU:HB2	2.38	0.58
45:5:277:HIS:HB3	45:5:459:LEU:HD13	1.85	0.58
75:5:502:PEE:H19	75:5:502:PEE:O4	2.04	0.58
47:7:366:MET:O	47:7:369:THR:OG1	2.18	0.58
48:8:316:LYS:HD3	49:9:72:ARG:HG2	1.84	0.58
5:E:183:ALA:HB3	5:E:195:ASP:HA	1.86	0.57
9:I:78:ARG:HH11	42:r:57:THR:HG22	1.68	0.57
22:W:10:MET:HG3	22:W:12:PRO:HD3	1.85	0.57
23:Y:94:ASP:O	44:t:108:LEU:CD2	2.52	0.57
36:l:34:ASN:HA	36:l:37:LYS:HG2	1.85	0.57
42:r:199:ASP:HB3	42:r:279:ARG:HE	1.69	0.57
45:5:244:ASP:OD1	45:5:245:LEU:N	2.37	0.57
47:7:141:TRP:NE1	47:7:263:ASN:O	2.36	0.57
61:Al:193:TYR:HE1	63:An:126:MET:HE1	1.68	0.57
62:Am:203:PHE:O	62:Am:207:HIS:HD2	1.87	0.57
33:i:112:HIS:CB	33:i:184:ILE:HD11	2.33	0.57
33:i:291:TYR:HE1	41:q:147:LEU:HD21	1.69	0.57
43:s:26:LYS:CE	43:s:97:PHE:HE1	2.17	0.57
46:v:49:ILE:HD11	46:v:230:LEU:HB3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:w:30:TRP:CH2	75:w:403:PEE:H18	2.39	0.57
47:w:315:MET:SD	47:w:318:ARG:NH2	2.77	0.57
48:8:128:MET:HE2	48:8:131:VAL:HG21	1.85	0.57
3:C:266:ARG:HD2	71:H:303:PLX:H1A2	1.86	0.57
14:N:22:GLU:O	14:N:26:ILE:HD12	2.04	0.57
15:X:115:GLN:O	15:X:118:ILE:HG13	2.04	0.57
47:w:24:PRO:O	47:w:224:TYR:OH	2.16	0.57
4:D:212:TYR:HA	4:D:219:VAL:HA	1.86	0.57
7:G:472:PRO:CG	7:G:500:ILE:HD13	2.35	0.57
12:L:211:ASP:O	12:L:215:ASN:ND2	2.30	0.57
24:Z:27:THR:HG21	24:Z:50:ALA:HB1	1.87	0.57
25:a:187:PRO:CB	43:s:47:ARG:HG2	2.32	0.57
34:j:56:PHE:HZ	37:m:71:THR:HA	1.69	0.57
45:u:374:GLY:O	45:u:378:ARG:N	2.34	0.57
45:5:121:ASN:ND2	45:5:132:TYR:OH	2.36	0.57
45:5:296:TRP:HE3	45:5:347:CYS:HB2	1.69	0.57
49:9:73:GLN:OE1	50:Aa:41:ARG:NH1	2.37	0.57
51:Ab:55:GLN:O	51:Ab:59:SER:N	2.37	0.57
52:Ac:14:LEU:O	52:Ac:20:THR:OG1	2.22	0.57
2:B:270:ASN:HD21	2:B:340:ASP:HB2	1.70	0.57
7:G:260:ASN:HD22	7:G:278:HIS:HB2	1.70	0.57
7:G:474:VAL:CG1	7:G:493:VAL:CG2	2.82	0.57
10:J:74:THR:O	10:J:104:ARG:NH2	2.38	0.57
13:M:40:LYS:HG2	22:W:8:GLN:HA	1.86	0.57
36:l:161:ARG:NH1	36:l:238:GLU:OE2	2.37	0.57
36:l:371:THR:O	36:l:375:ILE:HD12	2.05	0.57
47:w:105:GLY:HA2	47:w:107:TYR:CE2	2.39	0.57
52:1:34:ARG:HG2	54:3:48:ILE:HA	1.87	0.57
53:4:164:ASN:HD21	53:4:175:PHE:HB3	1.68	0.57
45:5:274:GLU:CB	45:5:456:VAL:HB	2.34	0.57
46:6:70:ARG:HD2	46:6:186:LEU:HD12	1.87	0.57
56:Ag:40:TYR:CE2	59:Aj:41:ARG:HG3	2.40	0.57
7:G:621:LYS:HG2	17:Q:122:PHE:CE1	2.39	0.57
8:H:100:GLU:OE2	8:H:193:ASN:ND2	2.37	0.57
9:I:211:ARG:HH11	9:I:211:ARG:CB	2.16	0.57
25:a:160:MET:HG3	25:a:166:GLY:HA3	1.86	0.57
27:c:167:TYR:O	27:c:169:GLU:N	2.31	0.57
45:u:114:GLU:OE2	46:v:305:ALA:N	2.37	0.57
46:6:70:ARG:NH1	46:6:331:SER:OG	2.37	0.57
47:7:326:TRP:CZ2	75:7:402:PEE:H13	2.39	0.57
47:7:345:HIS:HA	47:7:348:ILE:HD12	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:9:44:VAL:O	49:9:48:ILE:HG12	2.04	0.57
52:Ac:30:LEU:HA	54:Ad:34:TRP:CD1	2.40	0.57
1:A:54:TYR:OH	61:Al:189:PRO:HD2	2.05	0.57
16:P:20:ARG:HH22	16:P:68:ARG:HG2	1.69	0.57
20:U:145:TYR:CE2	20:U:149:LEU:HD13	2.40	0.57
22:W:73:PRO:HB3	43:s:44:MET:SD	2.44	0.57
27:c:42:PRO:O	27:c:44:THR:N	2.37	0.57
46:v:254:ARG:NH2	46:6:257:GLU:OE1	2.38	0.57
46:v:402:VAL:HG23	46:v:403:ALA:H	1.70	0.57
47:w:171:ASP:OD1	47:w:172:LYS:N	2.30	0.57
53:2:127:TYR:HA	54:3:34:TRP:HH2	1.69	0.57
45:5:128:HIS:CE1	45:5:415:ARG:HG3	2.38	0.57
45:5:183:VAL:HG21	45:5:286:HIS:HD2	1.69	0.57
45:5:278:ARG:NH1	45:5:463:GLU:H	1.67	0.57
45:5:400:VAL:HA	46:6:57:PRO:HB2	1.86	0.57
46:6:90:THR:HB	46:6:96:SER:HB2	1.85	0.57
46:6:359:LYS:HG2	46:6:432:VAL:HG22	1.86	0.57
55:Ae:14:VAL:O	55:Ae:21:GLY:HA2	2.04	0.57
67:Ar:71:THR:O	67:Ar:75:ARG:HD3	2.05	0.57
2:B:118:ASP:OD1	69:B:502:FMN:C7M	2.52	0.57
3:C:135:TYR:CE1	9:I:162:TYR:HE2	2.22	0.57
4:D:111:LEU:CD1	4:D:163:ALA:HB2	2.34	0.57
5:E:179:ALA:HB3	5:E:185:MET:SD	2.44	0.57
7:G:319:TRP:HZ3	7:G:585:PRO:HG2	1.70	0.57
8:H:135:ARG:NH1	8:H:141:ARG:HG3	2.20	0.57
17:Q:80:ASP:OD1	17:Q:81:LEU:N	2.37	0.57
43:s:121:ASP:OD1	43:s:122:LEU:N	2.37	0.57
47:w:100:ARG:NH1	76:w:402:HEM:O1D	2.37	0.57
75:2:302:PEE:H66	75:2:302:PEE:C18	2.30	0.57
46:6:305:ALA:HA	46:6:311:GLN:HE21	1.69	0.57
46:6:343:GLN:HB2	46:6:346:SER:HB3	1.86	0.57
67:Ar:75:ARG:HG2	67:Ar:75:ARG:NH1	2.19	0.57
2:B:119:GLU:N	69:B:502:FMN:HM71	2.19	0.57
3:C:294:ARG:HH21	3:C:301:ASP:CG	2.13	0.57
4:D:168:ARG:NH1	4:D:185:ARG:NE	2.51	0.57
7:G:605:GLN:OE1	7:G:643:ARG:NH2	2.38	0.57
7:G:637:ASP:N	7:G:641:GLN:OE1	2.37	0.57
16:P:36:PHE:CZ	16:P:44:LEU:HD11	2.40	0.57
17:Q:63:VAL:HA	73:Q:201:ZMP:H4A	1.85	0.57
33:i:235:ASN:OD1	33:i:236:LYS:N	2.38	0.57
45:u:134:LYS:NZ	45:u:407:THR:OG1	2.24	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:402:HIS:ND1	55:Af:54:SER:HB2	2.20	0.57
47:w:254:ASP:O	47:w:257:THR:OG1	2.21	0.57
48:x:157:ASP:N	48:x:166:PHE:O	2.31	0.57
45:5:383:ALA:HB3	45:5:442:ARG:HE	1.70	0.57
46:6:380:ALA:O	46:6:384:MET:HG2	2.05	0.57
5:E:205:ILE:HA	5:E:208:LEU:HD12	1.86	0.57
7:G:287:SER:OG	7:G:288:ASP:N	2.38	0.57
20:U:91:ALA:C	20:U:95:TYR:HB2	2.30	0.57
26:b:100:ARG:O	26:b:101:LYS:HG2	2.05	0.57
29:e:79:ASP:HB2	29:e:82:VAL:HG12	1.86	0.57
33:i:172:GLN:N	33:i:172:GLN:OE1	2.37	0.57
34:j:73:LEU:HD23	42:r:151:LEU:HD12	1.87	0.57
36:l:72:GLN:OE1	36:l:72:GLN:N	2.36	0.57
45:u:92:PHE:HE2	45:u:211:LEU:HD22	1.70	0.57
46:6:116:ARG:HA	46:6:190:LEU:HD21	1.86	0.57
2:B:88:ARG:O	2:B:244:ASN:ND2	2.36	0.56
4:D:94:ILE:HD11	4:D:154:GLU:HB2	1.86	0.56
10:J:145:PHE:HD2	10:J:147:VAL:HG23	1.69	0.56
12:L:207:PHE:HZ	12:L:345:LEU:HA	1.67	0.56
17:Q:33:ARG:O	17:Q:37:ARG:HG3	2.04	0.56
32:h:14:LEU:HD13	37:m:152:TRP:CD2	2.40	0.56
33:i:255:PRO:HG3	41:q:123:GLU:HB3	1.87	0.56
34:j:6:THR:O	34:j:10:ASN:ND2	2.34	0.56
34:j:78:ALA:HA	37:m:144:ALA:HB1	1.87	0.56
47:w:59:THR:OG1	47:w:172:LYS:N	2.37	0.56
47:w:88:SER:O	47:w:92:ILE:HG12	2.04	0.56
45:5:290:ALA:HB2	45:5:344:PHE:HZ	1.69	0.56
45:5:460:GLY:HA3	45:5:461:PRO:C	2.28	0.56
49:9:54:ASN:OD1	49:9:55:LEU:N	2.38	0.56
61:Al:132:GLU:HB3	61:Al:137:GLU:HG3	1.87	0.56
2:B:74:ASP:O	2:B:78:GLY:N	2.34	0.56
2:B:236:PHE:CE1	5:E:74:HIS:HB2	2.40	0.56
13:M:7:VAL:HG13	13:M:8:ILE:HG13	1.86	0.56
20:U:170:VAL:HG21	20:U:243:TYR:HB2	1.86	0.56
74:l:702:CDL:H722	74:l:702:CDL:H531	1.87	0.56
46:v:288:VAL:O	46:v:292:VAL:HG23	2.05	0.56
53:2:136:PHE:HE2	75:2:302:PEE:C20	2.17	0.56
45:5:119:HIS:HB3	45:5:134:LYS:HB2	1.85	0.56
45:5:424:ILE:O	45:5:429:TRP:NE1	2.37	0.56
48:8:320:LEU:HD22	49:9:64:LYS:HG2	1.87	0.56
2:B:88:ARG:N	69:B:502:FMN:O1P	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:96:ARG:HB2	3:C:115:LEU:HD11	1.86	0.56
3:C:117:HIS:HA	3:C:462:ASP:HB3	1.88	0.56
4:D:107:GLN:HE22	4:D:136:ARG:HB3	1.70	0.56
9:I:153:MET:HA	9:I:183:VAL:HG23	1.86	0.56
10:J:74:THR:HG23	10:J:104:ARG:HH22	1.70	0.56
12:L:238:GLN:CG	12:L:269:ASN:O	2.49	0.56
15:O:79:ILE:HG22	15:O:145:VAL:HG13	1.88	0.56
17:Q:39:TRP:O	17:Q:43:VAL:HG23	2.05	0.56
20:U:123:PRO:HB2	20:U:180:PHE:CE1	2.41	0.56
71:V:202:PLX:H82	71:V:202:PLX:H252	1.86	0.56
15:X:137:LYS:O	15:X:139:MET:HG2	2.05	0.56
34:j:75:LEU:HD21	42:r:305:ILE:HG12	1.88	0.56
41:q:14:MET:HE1	41:q:30:HIS:NE2	2.21	0.56
42:r:287:HIS:CE1	42:r:291:LYS:HG3	2.40	0.56
46:v:65:ILE:HG13	46:v:218:MET:HG2	1.88	0.56
46:v:196:ARG:O	46:v:200:VAL:N	2.39	0.56
47:w:30:TRP:CD2	75:w:403:PEE:H18	2.40	0.56
48:x:99:HIS:NE2	48:x:209:GLU:OE2	2.33	0.56
48:x:124:SER:HB2	77:x:401:HEC:HBB3	1.88	0.56
52:1:34:ARG:NH1	52:1:38:GLN:OE1	2.38	0.56
52:1:34:ARG:NH2	54:3:49:ASN:O	2.37	0.56
45:5:35:THR:N	46:6:226:SER:HB3	2.21	0.56
45:5:95:HIS:CD2	46:6:301:ARG:HG3	2.40	0.56
45:5:338:CYS:SG	45:5:368:MET:HG2	2.44	0.56
46:6:261:GLN:NE2	46:6:442:GLY:O	2.38	0.56
46:6:291:HIS:CG	46:6:378:LEU:HD21	2.40	0.56
47:7:24:PRO:O	47:7:224:TYR:OH	2.19	0.56
47:7:173:ALA:O	47:7:177:ARG:HG2	2.05	0.56
47:7:296:ALA:HA	47:7:299:LEU:HB3	1.87	0.56
60:Ak:184:PHE:H	60:Ak:256:HIS:HE1	1.52	0.56
4:D:243:PRO:HB3	7:G:58:MET:HE1	1.87	0.56
12:L:59:PHE:CZ	12:L:126:VAL:CG1	2.88	0.56
23:Y:47:PHE:HE2	24:Z:57:PHE:CG	2.23	0.56
33:i:288:LEU:HD11	36:l:570:GLN:NE2	2.19	0.56
43:s:96:LEU:CD1	43:s:99:HIS:H	2.19	0.56
46:v:65:ILE:HG21	46:v:213:PHE:CD1	2.40	0.56
46:v:250:LYS:NZ	46:v:332:ASP:O	2.38	0.56
57:Ah:45:TYR:CD2	62:Am:42:LEU:HD13	2.41	0.56
7:G:180:THR:OG1	7:G:184:ARG:NH1	2.38	0.56
29:e:112:TYR:O	41:q:46:GLY:N	2.36	0.56
36:l:123:LEU:HD21	74:l:702:CDL:H511	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:l:155:ILE:HD11	36:l:248:HIS:NE2	2.21	0.56
45:u:478:LEU:HD11	75:u:502:PEE:O4P	2.05	0.56
46:v:38:LEU:HD22	46:v:50:ALA:HB1	1.88	0.56
53:4:206:LYS:HB2	53:4:265:PHE:CD2	2.40	0.56
46:6:84:ARG:HB3	55:Ae:15:LEU:HD12	1.87	0.56
46:6:386:VAL:HG13	46:6:392:PHE:HD1	1.70	0.56
48:8:276:ARG:NH2	48:8:280:GLU:OE2	2.38	0.56
1:A:12:LEU:HD22	64:Ao:78:HIS:ND1	2.20	0.56
4:D:230:PHE:O	10:J:123:ASN:ND2	2.39	0.56
5:E:207:GLU:HG2	5:E:212:LYS:O	2.06	0.56
7:G:48:THR:HA	7:G:95:PRO:HA	1.88	0.56
7:G:180:THR:O	7:G:182:CYS:N	2.39	0.56
7:G:278:HIS:NE2	7:G:280:ASP:HB2	2.20	0.56
8:H:49:ASP:O	8:H:52:SER:OG	2.20	0.56
8:H:115:ALA:O	8:H:140:ARG:NH2	2.37	0.56
14:N:69:GLU:HB3	14:N:77:ILE:HG23	1.87	0.56
22:W:90:ASN:HD21	22:W:128:ARG:HH12	1.54	0.56
25:a:67:PHE:HD2	25:a:68:LEU:HD12	1.69	0.56
36:l:150:MET:HE1	36:l:153:LEU:HD22	1.86	0.56
45:u:337:LEU:C	45:u:368:MET:HE2	2.30	0.56
53:2:136:PHE:HE2	75:2:302:PEE:H34	1.56	0.56
45:5:91:TYR:CG	45:5:202:GLU:HA	2.41	0.56
46:6:60:ARG:HD2	46:6:393:LEU:HD22	1.88	0.56
48:8:108:HIS:HD2	52:Ac:56:ILE:HD12	1.70	0.56
3:C:333:ARG:NH2	3:C:455:ASP:OD2	2.38	0.56
7:G:540:ASN:HD21	7:G:559:ASP:HA	1.71	0.56
42:r:75:PRO:HA	42:r:223:PHE:CE1	2.39	0.56
46:v:305:ALA:HA	46:v:311:GLN:NE2	2.20	0.56
46:v:378:LEU:HD13	46:v:416:ILE:HG13	1.87	0.56
47:w:155:TYR:HD2	47:w:156:ILE:HG13	1.71	0.56
53:2:163:LYS:O	53:2:177:ARG:HG3	2.05	0.56
53:4:126:ALA:HA	75:5:502:PEE:H61	1.86	0.56
45:5:367:ASP:OD1	47:7:6:LYS:NZ	2.35	0.56
48:8:291:LEU:CD2	52:Ac:44:TYR:HB2	2.31	0.56
48:8:322:TYR:OH	49:9:58:ASP:OD1	2.17	0.56
60:Ak:95:PRO:HB2	62:Am:11:VAL:HG13	1.87	0.56
7:G:266:ARG:H	7:G:271:MET:HG2	1.71	0.56
7:G:340:ALA:HA	7:G:545:LEU:HB3	1.86	0.56
7:G:366:LEU:HD13	7:G:530:TYR:HA	1.87	0.56
9:I:100:ALA:HB2	9:I:113:PHE:CE2	2.40	0.56
36:l:400:ASN:HA	36:l:409:LEU:HD11	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:m:45:LEU:HD23	37:m:50:SER:HA	1.87	0.56
40:p:108:HIS:NE2	40:p:110:SER:HB3	2.21	0.56
45:u:179:MET:HG3	55:Af:43:LEU:HD13	1.88	0.56
47:w:138:MET:HB2	47:w:255:ASN:ND2	2.21	0.56
46:6:163:ALA:O	46:6:167:GLN:HG3	2.06	0.56
47:7:25:SER:HA	47:7:218:ILE:HD12	1.88	0.56
66:Aq:5:LYS:HD2	66:Aq:6:GLY:N	2.21	0.56
3:C:87:GLN:HA	9:I:87:PHE:HE1	1.69	0.56
3:C:396:THR:O	3:C:410:TYR:HA	2.06	0.56
9:I:82:LEU:HD13	9:I:122:VAL:HG11	1.88	0.56
9:I:150:VAL:CG2	9:I:179:VAL:HA	2.36	0.56
13:M:109:ASP:OD1	13:M:110:GLN:N	2.39	0.56
15:O:117:GLU:O	15:O:120:MET:HG2	2.06	0.56
17:Q:62:LYS:HG2	17:Q:107:PHE:HE1	1.70	0.56
73:X:201:ZMP:H19A	40:p:13:GLN:NE2	2.17	0.56
27:c:172:GLY:HA3	44:t:56:ARG:HE	1.71	0.56
74:u:501:CDL:H361	75:u:502:PEE:H28	0.65	0.56
74:u:501:CDL:C15	75:u:502:PEE:H58	2.36	0.56
46:6:83:LEU:HD13	46:6:208:TYR:CD2	2.40	0.56
2:B:126:LYS:HZ1	2:B:274:LYS:HE2	1.71	0.56
5:E:56:THR:OG1	5:E:59:ASN:ND2	2.39	0.56
7:G:209:TYR:CD2	7:G:210:ILE:HG13	2.40	0.56
9:I:99:MET:HE3	9:I:113:PHE:HZ	1.71	0.56
12:L:203:PRO:HB2	72:L:401:NDP:H5N	1.87	0.56
14:N:38:ILE:HG21	14:N:45:ARG:HB2	1.87	0.56
17:Q:36:TYR:HD1	17:Q:67:PHE:HE2	1.52	0.56
25:a:176:LYS:HE2	32:h:45:HIS:HE1	1.71	0.56
42:r:157:ASN:OD1	42:r:158:GLY:N	2.39	0.56
47:w:374:ASN:HA	47:w:379:TRP:HB2	1.86	0.56
46:6:171:ALA:HA	55:Ae:11:PHE:HZ	1.70	0.56
47:7:314:SER:HB3	47:7:316:MET:HG2	1.88	0.56
61:Al:145:PRO:HG3	61:Al:148:MET:HE2	1.87	0.56
5:E:186:VAL:HG23	5:E:196:LEU:HD21	1.88	0.55
17:Q:54:ILE:HG21	17:Q:107:PHE:HE2	1.71	0.55
17:Q:102:HIS:HA	17:Q:105:ARG:NH2	2.21	0.55
25:a:97:GLU:O	28:d:62:TYR:HB2	2.06	0.55
47:w:103:TYR:CD2	75:w:403:PEE:H13	2.40	0.55
45:5:39:ALA:HA	45:5:42:LEU:HD12	1.87	0.55
45:5:365:ILE:HD12	45:5:464:GLN:HB3	1.87	0.55
49:9:72:ARG:HH12	49:9:74:GLN:NE2	2.04	0.55
54:Ad:2:LEU:HD23	54:Ad:4:ARG:HH12	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:Ak:69:MET:HE2	60:Ak:70:VAL:CG2	2.36	0.55
4:D:168:ARG:HH11	4:D:185:ARG:CG	2.17	0.55
4:D:192:GLY:O	4:D:194:GLU:N	2.37	0.55
5:E:95:ILE:HG22	5:E:99:ASN:HD21	1.70	0.55
5:E:201:ILE:O	5:E:205:ILE:HD12	2.06	0.55
7:G:32:ILE:HG21	7:G:98:LYS:N	2.22	0.55
7:G:68:ARG:NH1	7:G:279:GLU:OE2	2.38	0.55
7:G:377:ALA:HB3	16:P:45:LYS:HZ1	1.71	0.55
12:L:65:LEU:O	72:L:401:NDP:O1N	2.24	0.55
12:L:206:ILE:HG12	72:L:401:NDP:N7N	2.21	0.55
12:L:241:TYR:CE2	12:L:243:VAL:HB	2.40	0.55
12:L:369:VAL:O	12:L:370:LYS:CB	2.54	0.55
25:a:137:MET:HB3	38:n:38:PHE:CE2	2.41	0.55
29:e:86:ASN:HD21	41:q:81:GLN:HE22	1.54	0.55
31:g:30:ASP:OD1	31:g:31:PRO:HD2	2.06	0.55
45:u:58:ARG:HH11	45:u:230:VAL:HG22	1.71	0.55
48:x:153:VAL:HG11	48:x:177:PRO:HG3	1.88	0.55
45:5:52:GLN:HE22	45:5:58:ARG:NE	1.98	0.55
45:5:120:LEU:HD11	46:6:299:VAL:HA	1.89	0.55
49:9:23:ASN:HA	49:9:28:ASN:ND2	2.21	0.55
61:Al:193:TYR:CE1	63:An:126:MET:HE1	2.39	0.55
3:C:223:HIS:HD2	9:I:187:PRO:HD3	1.70	0.55
3:C:335:GLU:O	3:C:339:GLN:HG2	2.05	0.55
5:E:53:PHE:HE1	5:E:90:ASN:HD21	1.53	0.55
5:E:140:CYS:SG	5:E:185:MET:HE3	2.46	0.55
12:L:113:LYS:HE3	12:L:154:GLN:HE21	1.71	0.55
20:U:131:TYR:CD1	20:U:185:CYS:HB3	2.41	0.55
22:W:56:GLU:OE1	22:W:59:ARG:NH1	2.28	0.55
25:a:168:TRP:HE3	31:g:3:MET:HB2	1.70	0.55
32:h:29:ILE:HD11	37:m:136:PHE:HE2	1.71	0.55
32:h:95:PRO:C	32:h:97:HIS:N	2.63	0.55
42:r:32:GLN:HB2	42:r:34:ARG:HG2	1.89	0.55
43:s:24:VAL:HG22	43:s:86:TRP:CD2	2.42	0.55
43:s:82:PHE:HD1	43:s:107:PHE:CE1	2.25	0.55
45:5:87:ASN:HD22	45:5:199:GLN:HE21	1.53	0.55
45:5:310:ILE:HD11	45:5:388:VAL:HA	1.88	0.55
45:5:361:ASP:OD1	45:5:362:ASN:N	2.38	0.55
46:6:372:GLN:HA	46:6:375:LYS:HD3	1.86	0.55
48:8:182:ASN:ND2	48:8:184:GLU:OE2	2.38	0.55
3:C:116:LEU:O	3:C:116:LEU:HD23	2.05	0.55
4:D:114:LEU:HD23	4:D:166:TYR:HB3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:35:PHE:O	7:G:101:ASN:HA	2.07	0.55
7:G:585:PRO:HB2	7:G:616:ALA:HB2	1.88	0.55
8:H:42:ASN:C	8:H:44:ARG:H	2.14	0.55
14:N:28:TYR:HB3	14:N:56:LEU:HD22	1.88	0.55
21:V:47:ALA:O	21:V:48:SER:OG	2.25	0.55
32:h:14:LEU:O	32:h:17:TRP:NE1	2.35	0.55
33:i:93:VAL:HG11	37:m:117:PHE:CD2	2.41	0.55
36:l:149:ILE:HG12	41:q:364:LEU:HD11	1.88	0.55
36:l:297:ASP:OD1	36:l:298:ILE:N	2.38	0.55
38:n:13:VAL:HB	41:q:14:MET:HG3	1.87	0.55
45:u:180:ARG:CZ	45:u:342:GLN:HE22	2.18	0.55
45:u:276:ARG:HB3	50:z:16:THR:HB	1.88	0.55
75:u:502:PEE:H17	71:2:301:PLX:C6	2.36	0.55
48:x:159:PRO:HA	48:x:164:GLU:HA	1.88	0.55
53:2:173:PRO:HG2	47:7:262:LEU:HG	1.88	0.55
45:5:280:ASP:HA	45:5:461:PRO:HB3	1.87	0.55
46:6:157:GLN:HA	46:6:160:ILE:HD12	1.87	0.55
2:B:55:GLY:O	2:B:58:SER:OG	2.16	0.55
12:L:238:GLN:NE2	12:L:269:ASN:O	2.39	0.55
14:N:101:GLU:N	14:N:101:GLU:OE1	2.38	0.55
16:P:25:GLN:O	16:P:34:ARG:NH1	2.39	0.55
31:g:51:ARG:NH1	33:i:221:HIS:HE1	2.04	0.55
36:l:247:LEU:HB2	36:l:252:MET:HB2	1.88	0.55
53:2:87:ASP:OD1	53:2:88:PHE:N	2.40	0.55
54:Ad:33:VAL:HA	54:Ad:38:TRP:HB3	1.88	0.55
3:C:368:ARG:HA	3:C:371:MET:HG2	1.89	0.55
10:J:63:THR:CG2	17:Q:70:ASN:HD22	2.15	0.55
12:L:145:PHE:HB2	12:L:183:SER:OG	2.06	0.55
12:L:298:TYR:CD2	12:L:319:VAL:HG13	2.42	0.55
21:V:21:LYS:HG2	21:V:75:CYS:SG	2.47	0.55
33:i:84:TRP:HE1	35:k:53:PHE:HE2	1.53	0.55
34:j:102:LEU:HD22	42:r:294:LEU:HD22	1.87	0.55
36:l:159:HIS:CE1	40:p:96:CYS:HG	2.24	0.55
45:u:93:VAL:HG11	45:u:224:TYR:HE2	1.71	0.55
47:w:304:MET:O	47:w:308:HIS:N	2.35	0.55
48:8:142:THR:O	48:8:146:ALA:N	2.33	0.55
48:8:250:TYR:CZ	48:8:253:VAL:HA	2.41	0.55
48:8:291:LEU:HD12	48:8:291:LEU:C	2.29	0.55
2:B:199:ARG:NH2	5:E:84:ASP:OD2	2.40	0.55
20:U:299:LEU:CD2	20:U:306:VAL:CG1	2.85	0.55
21:V:135:VAL:HG13	21:V:136:PHE:H	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:q:196:TRP:HE3	41:q:197:LEU:HD23	1.72	0.55
45:u:49:GLN:HB2	45:u:239:HIS:CE1	2.41	0.55
45:u:114:GLU:HB3	46:v:306:THR:HB	1.88	0.55
46:v:167:GLN:HE21	55:Af:41:PRO:HB3	1.70	0.55
46:v:173:VAL:O	46:v:177:LEU:N	2.38	0.55
47:w:76:GLY:HA2	47:w:79:ILE:HD12	1.88	0.55
53:2:170:ARG:HE	47:7:168:PHE:HB3	1.71	0.55
45:5:122:ALA:O	46:6:300:LYS:HE3	2.07	0.55
7:G:292:PHE:HB3	7:G:706:THR:HG21	1.88	0.55
12:L:86:CYS:SG	12:L:87:GLU:N	2.80	0.55
33:i:167:TRP:CE3	36:l:573:MET:HB3	2.42	0.55
75:l:701:PEE:H12	75:l:701:PEE:O3P	2.06	0.55
41:q:10:MET:O	41:q:13:PRO:HD2	2.06	0.55
45:u:126:ARG:NH1	45:u:199:GLN:O	2.39	0.55
46:v:71:TYR:HB3	46:v:212:HIS:CE1	2.42	0.55
47:w:366:MET:HB3	47:w:367:PRO:HD3	1.89	0.55
48:x:229:ARG:HB3	48:x:232:LEU:HG	1.88	0.55
53:2:214:ILE:HG13	53:2:216:VAL:H	1.71	0.55
54:3:47:TYR:HD2	54:3:48:ILE:HG13	1.71	0.55
63:An:108:PRO:HG2	63:An:111:PHE:CE2	2.42	0.55
2:B:88:ARG:C	2:B:244:ASN:HD22	2.15	0.55
7:G:365:SER:OG	7:G:367:CYS:SG	2.58	0.55
12:L:59:PHE:CD1	12:L:127:ILE:O	2.56	0.55
20:U:304:LEU:O	20:U:308:ASN:N	2.40	0.55
23:Y:53:SER:HA	23:Y:56:ILE:HD12	1.89	0.55
36:l:4:PHE:HE2	36:l:61:MET:HB3	1.71	0.55
41:q:305:THR:O	41:q:308:SER:OG	2.14	0.55
46:v:145:GLU:HG3	46:v:147:ARG:NE	2.21	0.55
47:w:30:TRP:CH2	75:w:403:PEE:C13	2.89	0.55
47:w:256:TYR:HB3	48:x:200:TYR:CD1	2.42	0.55
51:0:36:GLN:HA	51:0:39:GLN:HG2	1.88	0.55
46:6:66:LYS:HD2	46:6:118:SER:HB3	1.89	0.55
46:6:177:LEU:HD21	46:6:272:VAL:HG21	1.87	0.55
62:Am:151:LEU:HB2	62:Am:159:MET:HG3	1.89	0.55
62:Am:222:GLN:HE21	62:Am:222:GLN:HA	1.71	0.55
1:A:63:MET:HB3	1:A:68:ILE:HD11	1.89	0.55
2:B:116:ASN:ND2	69:B:502:FMN:C9	2.70	0.55
2:B:383:THR:HG23	2:B:384:PRO:HD3	1.89	0.55
3:C:80:LEU:HD13	3:C:81:THR:CA	2.37	0.55
3:C:271:ARG:NH2	42:r:281:ARG:HB2	2.22	0.55
3:C:438:MET:HG2	3:C:450:ILE:HD11	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:652:ASN:HA	7:G:655:ARG:HE	1.71	0.55
9:I:164:HIS:CE1	9:I:171:ARG:HD2	2.42	0.55
12:L:238:GLN:OE1	12:L:266:VAL:HG11	2.06	0.55
23:Y:88:ASP:CB	44:t:100:LYS:CE	2.81	0.55
33:i:112:HIS:CE1	33:i:164:ILE:HG21	2.42	0.55
75:i:501:PEE:C23	41:q:155:ALA:HB3	2.33	0.55
46:v:60:ARG:HG3	46:v:124:GLU:HG2	1.88	0.55
47:7:221:HIS:O	47:7:225:THR:OG1	2.16	0.55
54:Ad:39:ARG:HA	54:Ad:42:LEU:HB2	1.88	0.55
2:B:288:VAL:HG21	2:B:303:HIS:HB3	1.88	0.54
3:C:293:LEU:HB3	3:C:298:ILE:HD11	1.88	0.54
7:G:319:TRP:HE1	17:Q:122:PHE:HE2	1.54	0.54
12:L:238:GLN:NE2	12:L:267:GLY:O	2.40	0.54
18:S:56:GLY:H	18:S:64:LYS:NZ	2.05	0.54
25:a:108:GLU:HG2	25:a:111:GLU:HA	1.89	0.54
33:i:217:MET:CB	33:i:326:LEU:HD13	2.36	0.54
33:i:291:TYR:CE1	75:i:501:PEE:H49	2.42	0.54
40:p:132:SER:OG	40:p:136:GLU:OE2	2.24	0.54
41:q:82:SER:HB2	41:q:432:ARG:NH1	2.22	0.54
47:w:184:ILE:HG23	47:w:185:LEU:HD12	1.89	0.54
47:7:146:ILE:HA	47:7:149:LEU:HD13	1.88	0.54
75:7:401:PEE:C19	75:7:401:PEE:C39	2.86	0.54
75:7:402:PEE:H6	50:Aa:41:ARG:NH2	2.04	0.54
2:B:184:LYS:O	2:B:186:ALA:N	2.39	0.54
3:C:53:TYR:HE1	75:i:501:PEE:O1P	1.90	0.54
3:C:324:GLY:O	3:C:329:ARG:NH2	2.40	0.54
5:E:137:THR:OG1	5:E:176:CYS:N	2.39	0.54
8:H:63:TRP:NE1	71:H:303:PLX:O7	2.37	0.54
12:L:239:PRO:CG	12:L:345:LEU:HD13	2.37	0.54
25:a:133:TYR:HD2	38:n:41:LYS:HD2	1.73	0.54
29:e:113:ARG:HH12	41:q:452:LYS:HB2	1.71	0.54
33:i:112:HIS:HB2	33:i:184:ILE:CD1	2.37	0.54
33:i:238:PRO:HB2	74:i:503:CDL:HB32	1.87	0.54
36:l:303:ALA:O	36:l:306:THR:HG22	2.07	0.54
36:l:410:LEU:O	36:l:414:ILE:HD12	2.07	0.54
42:r:293:PHE:O	42:r:297:THR:HG23	2.07	0.54
44:t:111:ARG:HH11	44:t:115:ARG:HH12	0.96	0.54
46:v:359:LYS:O	46:v:363:GLN:HG2	2.07	0.54
51:0:38:GLU:HA	51:0:43:CYS:HB2	1.90	0.54
45:5:67:PRO:HB2	46:6:383:LEU:HD23	1.89	0.54
48:8:216:LEU:HD11	77:8:402:HEC:HBB	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Aq:5:LYS:HD2	66:Aq:5:LYS:C	2.32	0.54
4:D:64:TYR:HE1	13:M:94:ALA:HA	1.71	0.54
5:E:133:GLN:NE2	5:E:187:GLN:HE21	2.06	0.54
7:G:382:ARG:HA	7:G:385:TYR:CE2	2.42	0.54
7:G:523:VAL:HG13	7:G:597:VAL:HB	1.89	0.54
20:U:91:ALA:HA	20:U:95:TYR:CB	2.35	0.54
22:W:117:VAL:O	22:W:118:THR:OG1	2.23	0.54
37:m:31:LEU:HD13	42:r:118:TRP:HH2	1.72	0.54
45:u:38:TYR:OH	45:u:430:GLU:OE1	2.24	0.54
46:v:54:ASN:O	46:v:127:ARG:NH2	2.39	0.54
47:w:165:TRP:CE3	47:w:169:SER:HA	2.42	0.54
53:4:248:ARG:HA	53:4:257:ASN:CG	2.32	0.54
46:6:48:VAL:HB	46:6:219:ALA:HA	1.89	0.54
55:Ae:9:GLY:H	55:Ae:25:ALA:HB3	1.72	0.54
4:D:109:LYS:O	4:D:110:SER:OG	2.22	0.54
7:G:349:GLU:HG3	7:G:620:TRP:CG	2.42	0.54
20:U:138:TYR:CD1	20:U:138:TYR:C	2.85	0.54
20:U:296:LEU:HD23	20:U:296:LEU:C	2.31	0.54
22:W:60:LEU:CD2	43:s:98:ARG:NH2	2.71	0.54
25:a:82:VAL:HG11	29:e:104:THR:HG21	1.89	0.54
28:d:84:CYS:SG	28:d:85:MET:N	2.80	0.54
39:o:56:ARG:NH2	39:o:58:GLY:O	2.40	0.54
41:q:106:LEU:HD13	41:q:234:VAL:HG11	1.88	0.54
41:q:244:MET:HG2	41:q:301:ILE:HD12	1.89	0.54
45:u:60:ALA:O	45:u:232:ALA:HA	2.07	0.54
53:4:153:GLU:HB2	53:4:169:TRP:CD1	2.42	0.54
45:5:51:SER:OG	45:5:239:HIS:NE2	2.28	0.54
45:5:404:ASP:OD2	46:6:389:SER:HB3	2.08	0.54
61:Al:111:THR:HG21	67:Ar:66:ILE:HD11	1.88	0.54
2:B:328:PRO:HB2	2:B:330:SER:C	2.33	0.54
3:C:178:THR:OG1	3:C:214:TYR:OH	2.23	0.54
7:G:124:HIS:NE2	68:G:801:SF4:S4	2.80	0.54
7:G:472:PRO:CB	7:G:500:ILE:HD13	2.37	0.54
19:T:49:THR:HA	22:W:62:ILE:HD13	1.89	0.54
21:V:53:VAL:HA	21:V:56:THR:HG22	1.90	0.54
27:c:125:SER:O	27:c:128:THR:OG1	2.22	0.54
28:d:145:ASP:HB3	31:g:121:VAL:H	1.72	0.54
32:h:12:LEU:HD23	32:h:14:LEU:HD23	1.89	0.54
35:k:32:CYS:HA	37:m:20:PHE:CZ	2.42	0.54
37:m:64:MET:O	37:m:67:VAL:HG12	2.07	0.54
46:v:375:LYS:HA	46:v:378:LEU:HD12	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:w:8:HIS:CE1	47:7:199:PHE:HE1	2.25	0.54
47:w:304:MET:HA	47:w:307:LEU:HB2	1.89	0.54
47:w:314:SER:OG	47:w:315:MET:N	2.33	0.54
53:2:213:LEU:HD11	53:2:247:GLY:HA3	1.88	0.54
45:5:71:VAL:HA	45:5:233:ALA:HB2	1.89	0.54
46:6:40:PHE:HB2	46:6:406:TYR:HB2	1.89	0.54
47:7:80:ARG:HH12	48:8:203:ARG:HH22	1.56	0.54
3:C:100:GLU:O	3:C:100:GLU:HG2	2.08	0.54
3:C:241:LEU:HD12	22:W:11:PRO:O	2.08	0.54
9:I:146:GLU:OE1	12:L:89:TYR:OH	2.16	0.54
20:U:136:TRP:CD1	20:U:136:TRP:C	2.85	0.54
25:a:137:MET:HE3	38:n:38:PHE:HE2	1.73	0.54
27:c:58:ARG:O	27:c:60:GLU:N	2.34	0.54
34:j:52:SER:H	37:m:74:MET:HE1	1.73	0.54
36:l:150:MET:HE3	74:l:702:CDL:H541	1.89	0.54
45:u:296:TRP:HZ3	55:Af:57:GLY:C	2.14	0.54
47:w:97:HIS:CE1	47:w:100:ARG:HH21	2.26	0.54
49:y:17:ILE:O	49:y:21:TYR:N	2.34	0.54
49:y:51:LEU:HD22	49:y:55:LEU:HD22	1.90	0.54
3:C:217:VAL:HG12	3:C:237:PRO:HD2	1.89	0.54
3:C:233:HIS:CD2	3:C:234:GLN:HG3	2.42	0.54
5:E:200:ASP:O	5:E:204:ILE:HG12	2.08	0.54
9:I:131:ASN:ND2	9:I:168:SER:HA	2.23	0.54
10:J:81:VAL:HG21	10:J:150:ARG:NH1	2.23	0.54
22:W:60:LEU:CD1	43:s:98:ARG:HH22	2.20	0.54
15:X:117:GLU:HB3	24:Z:45:TRP:HE1	1.72	0.54
25:a:167:PRO:HG2	25:a:168:TRP:CD1	2.40	0.54
36:l:541:ASN:HD22	75:l:701:PEE:H59	1.73	0.54
41:q:138:ASN:O	41:q:139:GLN:HG2	2.08	0.54
41:q:360:LEU:O	41:q:364:LEU:HB2	2.08	0.54
45:u:75:ILE:HG12	45:u:229:MET:HG2	1.90	0.54
45:5:424:ILE:HB	45:5:429:TRP:CE2	2.42	0.54
2:B:229:PHE:H	2:B:232:ASP:HB3	1.73	0.54
2:B:262:PHE:CZ	2:B:272:GLY:HA3	2.42	0.54
2:B:339:PHE:HB3	2:B:349:LEU:HB2	1.89	0.54
29:e:76:TYR:HE2	29:e:87:MET:HB3	1.73	0.54
42:r:41:GLY:HA3	42:r:44:GLY:N	2.15	0.54
74:u:501:CDL:HB62	74:u:501:CDL:H111	1.88	0.54
46:v:46:GLY:O	46:v:216:ALA:HA	2.06	0.54
53:4:92:ARG:HH22	45:5:193:GLN:HE21	1.55	0.54
46:6:67:ALA:HA	46:6:71:TYR:CE2	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Ab:86:LEU:O	51:Ab:89:SER:OG	2.25	0.54
65:Ap:48:LEU:O	65:Ap:50:PRO:HD3	2.08	0.54
2:B:94:PRO:HB2	2:B:97:LEU:HB3	1.90	0.54
7:G:239:THR:O	7:G:266:ARG:NH1	2.40	0.54
7:G:566:ILE:O	7:G:580:ALA:HB1	2.08	0.54
7:G:607:LYS:HZ3	10:J:78:ARG:HH21	1.55	0.54
9:I:71:ASP:OD2	9:I:211:ARG:HD2	2.07	0.54
16:P:35:ASP:O	16:P:39:LYS:NZ	2.34	0.54
28:d:10:TYR:O	28:d:14:PRO:HD2	2.07	0.54
36:l:26:ILE:O	36:l:29:THR:OG1	2.18	0.54
36:l:79:SER:OG	36:l:135:ASN:HB3	2.08	0.54
42:r:20:LEU:HD23	42:r:228:TYR:HB3	1.90	0.54
42:r:186:PHE:O	42:r:189:THR:OG1	2.20	0.54
46:v:234:ALA:O	46:v:238:LEU:HD13	2.08	0.54
46:v:253:TYR:HE2	46:v:435:ARG:HB3	1.73	0.54
53:4:228:ALA:O	53:4:235:TYR:N	2.36	0.54
46:6:76:ASN:HA	46:6:196:ARG:NH2	2.22	0.54
46:6:394:ASP:OD1	46:6:395:GLU:N	2.41	0.54
61:Al:165:VAL:HB	61:Al:170:LEU:HD12	1.90	0.54
2:B:76:ILE:HA	2:B:79:GLU:HB3	1.89	0.54
9:I:160:GLY:N	9:I:171:ARG:O	2.40	0.54
12:L:207:PHE:CD1	12:L:345:LEU:HD12	2.43	0.54
36:l:288:THR:HG23	36:l:304:PHE:HD1	1.73	0.54
41:q:451:PRO:O	41:q:454:ILE:HG22	2.08	0.54
43:s:12:ASP:OD1	43:s:13:LEU:N	2.40	0.54
47:w:236:MET:HE3	71:2:301:PLX:H192	1.89	0.54
47:w:286:ASN:HD21	47:w:288:LEU:HB3	1.73	0.54
47:7:91:PHE:HA	47:7:94:LEU:HB3	1.88	0.54
55:Ae:20:ARG:HD2	55:Ae:51:CYS:HA	1.89	0.54
65:Ap:82:CYS:N	65:Ap:86:GLY:O	2.41	0.54
2:B:369:ARG:HE	5:E:136:THR:HG22	1.73	0.53
3:C:80:LEU:CD1	3:C:81:THR:N	2.61	0.53
3:C:138:ARG:HH12	3:C:223:HIS:HB3	1.73	0.53
7:G:136:GLU:HB2	10:J:88:GLN:HE21	1.73	0.53
7:G:337:ASP:HA	7:G:542:PRO:HD2	1.90	0.53
10:J:64:LEU:HD11	17:Q:81:LEU:HD23	1.89	0.53
10:J:125:VAL:C	10:J:126:LEU:HD12	2.33	0.53
14:N:87:GLU:HA	14:N:90:LEU:HB3	1.89	0.53
17:Q:50:PHE:HB3	17:Q:52:LEU:HD13	1.88	0.53
33:i:277:ILE:O	33:i:280:THR:OG1	2.24	0.53
34:j:24:LEU:HB3	34:j:25:PRO:HD3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:r:1:MET:O	42:r:4:ILE:HG22	2.08	0.53
46:v:196:ARG:O	46:v:200:VAL:HG23	2.08	0.53
65:Ap:55:LYS:HA	65:Ap:74:LEU:O	2.08	0.53
7:G:258:GLY:O	7:G:604:GLN:NE2	2.42	0.53
8:H:211:TYR:CZ	13:M:39:PRO:HG3	2.43	0.53
12:L:172:ALA:O	12:L:185:ALA:HB2	2.08	0.53
12:L:239:PRO:HG3	12:L:345:LEU:HD13	1.90	0.53
13:M:106:LEU:O	13:M:108:LYS:N	2.41	0.53
21:V:78:ALA:HA	21:V:89:ASN:HD21	1.72	0.53
42:r:60:PRO:HB3	42:r:217:ALA:HB3	1.89	0.53
45:u:72:GLY:N	45:u:232:ALA:O	2.40	0.53
45:u:294:PRO:HB2	45:u:301:ASN:ND2	2.22	0.53
47:w:8:HIS:HE1	47:7:199:PHE:CE1	2.27	0.53
45:5:83:ASN:O	45:5:87:ASN:N	2.41	0.53
46:6:138:LEU:O	46:6:142:ALA:N	2.40	0.53
47:7:30:TRP:HZ3	75:7:402:PEE:H22	1.71	0.53
49:9:51:LEU:HD23	49:9:94:TYR:HE2	1.73	0.53
64:Ao:41:LEU:HD12	64:Ao:41:LEU:O	2.08	0.53
2:B:235:VAL:O	2:B:237:GLY:N	2.42	0.53
2:B:327:ILE:HD11	2:B:441:HIS:CD2	2.43	0.53
6:F:90:GLY:O	6:F:94:GLY:N	2.36	0.53
7:G:241:ARG:HG2	7:G:243:TRP:CZ2	2.43	0.53
10:J:84:ARG:NH2	10:J:86:ASN:OD1	2.42	0.53
36:l:68:TRP:HE3	36:l:76:LEU:HD11	1.73	0.53
36:l:482:MET:HE3	36:l:483:PRO:HB3	1.90	0.53
36:l:560:THR:O	36:l:565:THR:HG23	2.08	0.53
41:q:127:VAL:HB	41:q:128:PRO:HD3	1.90	0.53
47:w:183:PHE:O	47:w:186:PRO:HD2	2.08	0.53
47:w:185:LEU:HA	47:w:188:ILE:HD12	1.91	0.53
48:x:301:LEU:C	74:x:402:CDL:H362	2.33	0.53
45:5:44:SER:HB2	46:6:55:TYR:CB	2.38	0.53
45:5:128:HIS:HD2	45:5:418:LEU:HD22	1.74	0.53
47:7:3:ASN:O	47:7:7:SER:OG	2.17	0.53
48:8:252:GLU:N	48:8:262:ALA:O	2.39	0.53
60:Ak:407:ASP:O	60:Ak:411:LYS:HG3	2.07	0.53
3:C:380:HIS:ND1	7:G:144:MET:SD	2.77	0.53
7:G:136:GLU:OE1	7:G:136:GLU:N	2.41	0.53
7:G:319:TRP:HD1	17:Q:123:TYR:CD1	2.27	0.53
7:G:569:GLN:HE21	7:G:622:ILE:HD12	1.72	0.53
9:I:123:MET:HB3	9:I:150:VAL:HG12	1.91	0.53
9:I:159:GLY:O	9:I:161:GLY:N	2.32	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:123:GLU:OE1	15:X:130:ILE:N	2.41	0.53
41:q:103:GLN:O	41:q:107:ILE:HD12	2.09	0.53
41:q:204:MET:HE1	41:q:261:PHE:HB3	1.90	0.53
47:w:282:ARG:NH2	47:w:344:GLU:H	2.07	0.53
53:2:151:LYS:HA	53:2:169:TRP:HE1	1.72	0.53
75:2:302:PEE:C40	75:2:302:PEE:C18	2.85	0.53
46:6:61:ILE:HD13	46:6:134:MET:SD	2.49	0.53
46:6:116:ARG:NH2	46:6:175:GLU:OE1	2.42	0.53
47:7:111:GLU:HA	47:7:114:ASN:HD22	1.74	0.53
2:B:89:GLY:HA3	69:B:502:FMN:O5'	2.08	0.53
5:E:158:ILE:HD11	5:E:164:THR:HB	1.91	0.53
7:G:39:GLN:HE21	7:G:56:VAL:HG21	1.73	0.53
8:H:153:ILE:HD13	9:I:162:TYR:CD1	2.42	0.53
8:H:196:LYS:HD2	8:H:197:TRP:NE1	2.23	0.53
20:U:313:PRO:HB3	33:i:232:HIS:CE1	2.43	0.53
15:X:88:LYS:HB3	24:Z:19:TYR:CD1	2.43	0.53
25:a:184:LYS:O	25:a:186:THR:N	2.41	0.53
32:h:21:GLN:HA	35:k:53:PHE:CD1	2.43	0.53
34:j:106:TRP:CZ3	42:r:291:LYS:HA	2.43	0.53
36:l:38:THR:O	36:l:41:SER:OG	2.19	0.53
36:l:363:TYR:HB2	36:l:431:PHE:HB3	1.90	0.53
75:w:403:PEE:C3	74:z:101:CDL:HA32	2.30	0.53
49:y:76:LEU:O	49:y:81:TRP:NE1	2.32	0.53
47:7:242:LEU:HD21	47:7:250:LEU:HB3	1.89	0.53
51:Ab:78:ARG:NH1	51:Ab:79:ASP:OD1	2.41	0.53
62:Am:156:ARG:HG3	62:Am:156:ARG:NH1	2.22	0.53
2:B:267:ARG:HH21	2:B:336:LEU:HD22	1.74	0.53
2:B:273:THR:HG22	2:B:291:GLU:HA	1.90	0.53
3:C:391:VAL:O	3:C:415:GLY:HA2	2.09	0.53
4:D:231:ARG:NH2	8:H:128:ILE:O	2.42	0.53
10:J:145:PHE:CD2	10:J:147:VAL:HG23	2.43	0.53
15:O:93:ILE:HG12	15:O:108:LEU:HD23	1.90	0.53
20:U:345:TYR:HB3	31:g:54:PRO:HD3	1.91	0.53
33:i:174:GLN:OE1	33:i:174:GLN:N	2.30	0.53
34:j:71:LEU:HD11	35:k:65:VAL:HG21	1.91	0.53
41:q:337:VAL:HG13	41:q:339:SER:H	1.73	0.53
42:r:72:ILE:O	42:r:75:PRO:HD2	2.08	0.53
46:v:185:ALA:H	46:v:251:ALA:HB2	1.73	0.53
47:w:311:LYS:HD2	49:y:38:ILE:HG13	1.90	0.53
45:5:332:ALA:O	45:5:336:LYS:HA	2.08	0.53
61:Al:68:LEU:HB3	61:Al:69:PRO:HD3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:GLY:HA3	69:B:502:FMN:N5	2.23	0.53
2:B:288:VAL:HG11	2:B:303:HIS:CD2	2.44	0.53
20:U:85:LEU:CB	20:U:158:GLY:O	2.56	0.53
26:b:82:ILE:HG21	36:l:10:THR:HG23	1.91	0.53
28:d:145:ASP:HB3	31:g:121:VAL:N	2.24	0.53
31:g:93:PHE:O	31:g:96:VAL:HG22	2.08	0.53
32:h:95:PRO:O	32:h:97:HIS:N	2.42	0.53
41:q:355:MET:HA	41:q:358:TRP:HD1	1.73	0.53
46:v:169:PRO:HB2	46:v:268:HIS:CD2	2.43	0.53
47:w:26:ASN:O	47:w:208:PRO:HG2	2.09	0.53
53:4:156:LEU:HB2	53:4:271:VAL:H	1.74	0.53
45:5:77:ALA:HA	45:5:81:TYR:HE2	1.74	0.53
46:6:399:GLN:O	46:6:403:ALA:N	2.41	0.53
48:8:217:THR:HG22	51:Ab:34:ARG:NH2	2.23	0.53
48:8:222:PRO:HG2	48:8:228:LEU:HD11	1.90	0.53
66:Aq:42:ARG:HH11	66:Aq:42:ARG:HG3	1.74	0.53
7:G:465:ILE:HA	7:G:468:GLU:OE1	2.09	0.53
7:G:604:GLN:HA	7:G:656:TYR:HD1	1.74	0.53
16:P:91:LEU:O	16:P:94:VAL:HB	2.09	0.53
28:d:144:SER:O	28:d:146:LEU:N	2.40	0.53
33:i:248:LEU:HD21	33:i:296:LEU:HD22	1.91	0.53
33:i:331:VAL:HG13	33:i:335:LEU:HD12	1.91	0.53
41:q:329:LEU:HD21	41:q:359:TRP:CD2	2.42	0.53
45:u:274:GLU:HB3	45:u:468:TYR:HD1	1.73	0.53
45:u:294:PRO:HB3	45:u:298:ASN:ND2	2.24	0.53
47:w:196:HIS:NE2	76:w:402:HEM:ND	2.56	0.53
46:6:81:HIS:CD2	46:6:158:LEU:HD22	2.44	0.53
63:An:67:SER:OG	63:An:70:GLU:HG3	2.08	0.53
66:Aq:2:SER:OG	66:Aq:3:ALA:N	2.41	0.53
66:Aq:8:HIS:O	66:Aq:10:GLY:N	2.42	0.53
2:B:62:TRP:CE2	2:B:140:GLU:HG2	2.43	0.53
3:C:427:PRO:HD2	3:C:460:GLU:OE2	2.08	0.53
7:G:222:ILE:HA	7:G:225:ILE:HG22	1.91	0.53
8:H:37:THR:N	13:M:105:GLU:O	2.42	0.53
9:I:159:GLY:HA2	9:I:172:GLY:HA2	1.90	0.53
12:L:109:ASN:O	12:L:115:SER:OG	2.27	0.53
12:L:299:ARG:HE	12:L:316:ARG:HH11	1.56	0.53
34:j:31:SER:HA	34:j:34:THR:HG22	1.90	0.53
36:l:97:THR:O	36:l:101:MET:HG2	2.09	0.53
40:p:65:ARG:O	40:p:69:GLU:HG2	2.08	0.53
41:q:61:LEU:HD22	41:q:241:TYR:HD1	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:t:56:ARG:HG3	44:t:57:ASP:N	2.19	0.53
45:u:48:THR:HG23	45:u:423:ARG:HD2	1.91	0.53
45:u:63:GLN:NE2	45:u:238:GLU:HA	2.23	0.53
47:w:232:ALA:HA	47:w:235:MET:HG2	1.90	0.53
45:5:469:ASN:HD22	47:7:223:TYR:HH	1.52	0.53
48:8:132:ALA:HB2	48:8:175:TYR:HD1	1.73	0.53
48:8:134:ARG:HA	48:8:137:VAL:HG23	1.89	0.53
60:Ak:302:ARG:O	60:Ak:306:THR:HG23	2.09	0.53
61:Al:136:LEU:HB3	61:Al:193:TYR:HD2	1.73	0.53
63:An:128:VAL:O	63:An:134:PHE:HB3	2.09	0.53
3:C:406:GLU:OE1	4:D:140:ARG:NH2	2.42	0.53
4:D:124:ASN:CG	14:N:111:GLN:HE22	2.15	0.53
4:D:225:GLU:O	12:L:49:SER:OG	2.19	0.53
7:G:462:PHE:O	7:G:465:ILE:HG13	2.09	0.53
12:L:148:ILE:HB	12:L:149:PRO:HD3	1.91	0.53
12:L:243:VAL:HG12	12:L:247:LYS:HE2	1.90	0.53
12:L:265:PHE:CZ	12:L:338:LEU:HD12	2.43	0.53
17:Q:63:VAL:HA	73:Q:201:ZMP:H4	1.91	0.53
22:W:66:GLU:OE2	43:s:124:GLU:N	2.42	0.53
28:d:78:GLU:OE2	28:d:81:ASP:HB2	2.09	0.53
30:f:61:GLN:OE1	31:g:76:TYR:OH	2.27	0.53
33:i:175:LEU:HG	33:i:296:LEU:HD11	1.91	0.53
34:j:6:THR:HA	34:j:9:THR:HG22	1.90	0.53
41:q:76:MET:SD	41:q:230:VAL:HG23	2.50	0.53
41:q:373:ILE:HG23	41:q:448:THR:HG22	1.90	0.53
43:s:103:GLN:OE1	43:s:103:GLN:N	2.41	0.53
45:u:424:ILE:HG23	45:u:429:TRP:HE1	1.73	0.53
46:v:358:VAL:HG11	46:v:431:PHE:CD2	2.44	0.53
47:w:68:HIS:O	47:w:72:ASP:HB2	2.09	0.53
48:x:265:SER:HB2	51:0:30:LEU:HB2	1.90	0.53
48:x:298:GLY:O	48:x:302:PRO:HD3	2.08	0.53
47:7:26:ASN:HD21	47:7:207:ASN:HB2	1.73	0.53
75:7:402:PEE:H8	50:Aa:45:CYS:CB	2.39	0.53
63:An:23:PRO:HD2	64:Ao:34:ASN:HD22	1.74	0.53
2:B:157:TYR:HB3	2:B:212:LEU:HD11	1.90	0.52
4:D:50:ARG:NH2	13:M:64:MET:SD	2.71	0.52
6:F:108:THR:CB	6:F:109:GLY:HA2	2.37	0.52
7:G:161:GLU:OE1	7:G:161:GLU:N	2.36	0.52
33:i:231:SER:HB2	33:i:305:PHE:HB2	1.90	0.52
42:r:287:HIS:ND1	42:r:291:LYS:HG3	2.24	0.52
44:t:24:THR:O	44:t:28:ASP:N	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:75:ILE:HG21	45:u:224:TYR:CD1	2.43	0.52
53:4:156:LEU:HD12	53:4:271:VAL:HB	1.90	0.52
53:4:179:ARG:HD3	53:4:245:ALA:O	2.09	0.52
47:7:233:LEU:HD23	48:8:301:LEU:HD12	1.91	0.52
61:Al:203:ASN:HD22	61:Al:206:PHE:HD2	1.55	0.52
63:An:40:LEU:HD13	63:An:59:LEU:HD13	1.90	0.52
63:An:52:SER:OG	63:An:55:GLU:HG3	2.08	0.52
2:B:318:ILE:HG13	2:B:357:MET:HE1	1.91	0.52
3:C:131:GLN:HE21	8:H:122:VAL:HA	1.74	0.52
3:C:141:TYR:CD2	9:I:91:CYS:HB3	2.44	0.52
12:L:82:VAL:O	12:L:105:PHE:HA	2.10	0.52
12:L:180:TYR:CZ	12:L:321:ARG:HG2	2.45	0.52
18:S:53:ARG:HD2	32:h:102:GLU:HA	1.92	0.52
20:U:91:ALA:CB	20:U:144:GLN:HE21	2.20	0.52
20:U:145:TYR:OH	20:U:202:PRO:O	2.27	0.52
15:X:115:GLN:HE21	15:X:138:LEU:HD23	1.75	0.52
36:l:504:LEU:O	36:l:507:THR:OG1	2.23	0.52
40:p:30:TRP:NE1	40:p:76:HIS:HB2	2.24	0.52
45:u:365:ILE:HB	45:u:464:GLN:HB3	1.91	0.52
46:v:257:GLU:OE2	46:v:449:PHE:HB3	2.10	0.52
47:w:330:ALA:HB2	50:z:52:PRO:HB3	1.89	0.52
48:x:116:GLN:HE22	48:x:257:ASP:HB3	1.74	0.52
52:1:48:ASN:HB2	52:1:51:LYS:HD2	1.90	0.52
45:5:402:HIS:CE1	55:Ae:54:SER:HB2	2.44	0.52
47:7:147:THR:HG21	47:7:165:TRP:NE1	2.25	0.52
4:D:111:LEU:HD12	4:D:163:ALA:HB2	1.92	0.52
4:D:152:PRO:HG3	17:Q:20:ILE:HA	1.91	0.52
4:D:238:PRO:HA	10:J:92:ASN:HB3	1.91	0.52
6:F:106:THR:HA	6:F:117:GLN:HA	1.90	0.52
7:G:169:VAL:HG11	7:G:222:ILE:HD11	1.91	0.52
7:G:250:SER:HB2	7:G:606:THR:HG23	1.91	0.52
20:U:95:TYR:OH	20:U:144:GLN:HA	2.09	0.52
22:W:73:PRO:HG3	43:s:40:ASN:ND2	2.25	0.52
23:Y:73:PHE:HA	36:l:385:TYR:HE2	1.73	0.52
33:i:336:VAL:HG21	71:i:502:PLX:H362	1.90	0.52
45:u:71:VAL:HA	45:u:233:ALA:HB2	1.90	0.52
47:w:6:LYS:HE3	47:w:15:ASN:ND2	2.24	0.52
48:x:243:ILE:HD11	77:x:401:HEC:HHA	1.91	0.52
45:5:319:GLY:HA3	46:6:88:SER:HB3	1.90	0.52
47:7:148:ASN:O	47:7:287:LYS:NZ	2.43	0.52
49:9:61:PHE:HD2	49:9:65:ARG:HH21	1.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:Ak:225:GLY:HA3	62:Am:112:LEU:HD13	1.92	0.52
65:Ap:8:THR:OG1	65:Ap:11:GLU:HG2	2.09	0.52
65:Ap:51:SER:HB2	65:Ap:91:LEU:HD11	1.90	0.52
2:B:413:TRP:HB2	2:B:439:ILE:HD13	1.92	0.52
4:D:88:ILE:HB	4:D:145:THR:HG22	1.92	0.52
7:G:525:ALA:HB1	7:G:530:TYR:HB2	1.91	0.52
9:I:106:MET:HE3	9:I:111:VAL:HG23	1.92	0.52
11:K:79:GLY:O	11:K:83:PRO:HG2	2.08	0.52
14:N:24:LEU:HA	14:N:27:LEU:HD12	1.91	0.52
74:V:201:CDL:OA7	74:V:201:CDL:O1	2.26	0.52
25:a:136:THR:OG1	41:q:51:ASN:ND2	2.43	0.52
43:s:68:LEU:O	43:s:72:ARG:HG2	2.09	0.52
46:v:64:PHE:HE2	46:v:397:GLY:HA3	1.73	0.52
46:v:195:TYR:HE1	46:v:196:ARG:NH2	2.07	0.52
47:w:68:HIS:ND1	47:w:72:ASP:OD2	2.34	0.52
53:4:222:CYS:O	53:4:224:PRO:HD3	2.09	0.52
45:5:81:TYR:HE1	45:5:265:PHE:HD2	1.57	0.52
46:6:91:THR:OG1	46:6:139:ASN:OD1	2.26	0.52
47:7:116:GLY:C	76:7:404:HEM:HBC2	2.34	0.52
61:Al:102:HIS:O	61:Al:104:TRP:N	2.42	0.52
2:B:379:CYS:SG	2:B:381:GLN:HG2	2.50	0.52
26:b:100:ARG:CG	28:d:118:GLY:HA2	2.39	0.52
31:g:121:VAL:O	39:o:129:TYR:OH	2.25	0.52
36:l:199:GLN:OE1	36:l:199:GLN:N	2.42	0.52
40:p:129:ARG:HD2	40:p:168:TRP:CD2	2.45	0.52
43:s:31:HIS:HE1	43:s:119:ARG:HB2	1.73	0.52
45:u:214:ALA:O	45:u:217:THR:OG1	2.19	0.52
53:4:147:LEU:O	53:4:151:LYS:HB2	2.09	0.52
48:8:215:LEU:HD21	77:8:402:HEC:HBA1	1.92	0.52
61:Al:104:TRP:CG	61:Al:203:ASN:HB2	2.44	0.52
3:C:66:TRP:CE2	20:U:312:ILE:HD11	2.45	0.52
15:O:76:LEU:HD21	15:O:155:TYR:HA	1.92	0.52
21:V:94:GLY:HA3	21:V:119:GLY:HA2	1.92	0.52
32:h:7:GLN:HE21	32:h:16:ARG:NH2	2.07	0.52
33:i:113:PHE:HD1	35:k:97:GLN:C	2.18	0.52
33:i:338:PRO:HA	43:s:170:TRP:HZ2	1.75	0.52
36:l:306:THR:HB	36:l:336:LYS:HE2	1.91	0.52
43:s:96:LEU:CD1	43:s:99:HIS:CB	2.88	0.52
45:u:305:GLN:HE22	45:u:345:ASN:HB3	1.73	0.52
46:v:82:LEU:HD13	46:v:158:LEU:HD11	1.92	0.52
46:v:113:THR:O	46:v:120:ALA:N	2.37	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:5:101:THR:HG21	45:5:149:ASP:OD1	2.10	0.52
45:5:274:GLU:HG3	45:5:456:VAL:CG1	2.39	0.52
48:8:180:TYR:HD2	48:8:186:ALA:HB2	1.74	0.52
52:Ac:43:ILE:O	52:Ac:47:ILE:HD12	2.09	0.52
2:B:118:ASP:CB	69:B:502:FMN:C7M	2.80	0.52
2:B:174:ARG:O	2:B:178:GLU:HG2	2.09	0.52
2:B:220:GLN:NE2	5:E:114:GLU:HB3	2.24	0.52
2:B:328:PRO:O	2:B:331:VAL:HG13	2.09	0.52
7:G:195:LEU:HA	7:G:208:THR:HB	1.91	0.52
7:G:543:LYS:HD2	7:G:563:ASP:OD2	2.09	0.52
7:G:641:GLN:O	7:G:644:SER:HB2	2.09	0.52
27:c:69:GLY:HA3	39:o:83:THR:OG1	2.10	0.52
29:e:93:PHE:HA	29:e:97:ILE:HG22	1.90	0.52
33:i:112:HIS:O	33:i:115:VAL:HG12	2.09	0.52
41:q:220:HIS:CE1	41:q:232:ALA:HB2	2.45	0.52
41:q:273:SER:O	41:q:276:CYS:HB3	2.10	0.52
46:v:214:THR:HG22	46:v:216:ALA:N	2.20	0.52
49:y:20:TRP:O	49:y:24:ALA:N	2.42	0.52
45:5:405:GLY:C	45:5:408:PRO:HD2	2.34	0.52
47:7:252:ASP:N	47:7:253:PRO:HD3	2.25	0.52
4:D:75:GLN:HB3	13:M:71:SER:HA	1.92	0.52
7:G:650:SER:HB3	7:G:651:PRO:HA	1.92	0.52
12:L:261:LYS:HB3	12:L:333:PRO:HG3	1.92	0.52
14:N:11:LEU:HB2	14:N:14:LEU:HB2	1.91	0.52
19:T:11:ASN:O	19:T:15:LYS:HG2	2.10	0.52
34:j:106:TRP:HZ3	42:r:291:LYS:HA	1.75	0.52
36:l:559:GLU:O	36:l:563:PRO:HD2	2.10	0.52
41:q:447:LEU:HD21	41:q:454:ILE:HD12	1.91	0.52
43:s:26:LYS:HE2	43:s:97:PHE:CE1	2.40	0.52
60:Ak:240:HIS:HB3	60:Ak:241:PRO:HD3	1.92	0.52
2:B:119:GLU:CB	2:B:127:ASP:HB2	2.40	0.52
2:B:222:LYS:HB3	2:B:381:GLN:OE1	2.10	0.52
4:D:114:LEU:O	4:D:170:ILE:HD11	2.10	0.52
7:G:387:LEU:HD23	7:G:389:THR:O	2.09	0.52
20:U:289:ASP:O	20:U:293:PHE:HD1	1.88	0.52
34:j:87:MET:HG3	37:m:147:TYR:HB3	1.91	0.52
36:l:258:PHE:HA	36:l:261:ILE:HD12	1.90	0.52
36:l:342:CYS:HB2	36:l:369:THR:HG23	1.91	0.52
41:q:196:TRP:CD1	41:q:250:LEU:HD22	2.45	0.52
41:q:325:MET:HE2	41:q:362:ALA:HB2	1.91	0.52
47:w:65:SER:O	47:w:68:HIS:HB3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:w:312:GLN:HB3	47:w:314:SER:H	1.75	0.52
48:x:95:TYR:HB3	51:0:87:PHE:CE2	2.38	0.52
48:x:219:TYR:OH	48:x:245:MET:HE3	2.10	0.52
53:4:191:GLU:OE1	53:4:194:GLN:HG2	2.08	0.52
46:6:177:LEU:HD11	46:6:272:VAL:HG21	1.92	0.52
48:8:229:ARG:HB3	48:8:232:LEU:HD12	1.92	0.52
48:8:266:GLN:HE22	51:Ab:91:LYS:C	2.17	0.52
1:A:28:SER:HB2	61:Al:33:LEU:HD23	1.91	0.52
2:B:244:ASN:CB	69:B:502:FMN:O2P	2.58	0.52
3:C:80:LEU:HD12	3:C:101:LEU:CD1	2.40	0.52
3:C:81:THR:HG22	34:j:44:MET:HE1	1.90	0.52
7:G:121:LEU:HD21	7:G:139:LEU:HD21	1.92	0.52
7:G:408:ARG:HG3	7:G:409:PHE:CD1	2.44	0.52
7:G:591:GLU:OE1	7:G:591:GLU:N	2.43	0.52
10:J:135:VAL:O	10:J:139:GLU:HG2	2.10	0.52
12:L:128:ASN:OD1	12:L:152:ILE:CD1	2.57	0.52
16:P:90:THR:HA	16:P:93:ASN:HD22	1.75	0.52
22:W:108:GLU:O	32:h:75:ARG:NH1	2.42	0.52
22:W:113:THR:HG22	22:W:115:ARG:N	2.25	0.52
41:q:251:ASN:OD1	41:q:304:GLN:NE2	2.37	0.52
45:u:87:ASN:HD21	45:u:199:GLN:HB2	1.75	0.52
45:u:112:GLU:O	45:u:115:SER:OG	2.16	0.52
45:u:462:ILE:HG23	45:u:465:LEU:HB3	1.92	0.52
48:x:275:LEU:O	48:x:279:SER:N	2.37	0.52
45:5:442:ARG:O	45:5:446:SER:OG	2.20	0.52
46:6:52:LEU:HD22	46:6:54:ASN:ND2	2.24	0.52
46:6:95:SER:O	46:6:99:ILE:HD12	2.10	0.52
46:6:116:ARG:NH1	46:6:178:HIS:HB3	2.19	0.52
46:6:290:GLN:O	46:6:294:GLY:N	2.42	0.52
47:7:165:TRP:O	47:7:174:THR:OG1	2.25	0.52
61:Al:186:SER:CB	61:Al:213:LEU:HD22	2.40	0.52
4:D:124:ASN:HB3	4:D:148:ASP:OD1	2.10	0.51
4:D:172:ASP:O	4:D:173:MET:HE2	2.10	0.51
7:G:581:ASP:OD1	7:G:582:VAL:N	2.43	0.51
8:H:148:ASP:N	8:H:148:ASP:OD1	2.41	0.51
12:L:263:PHE:HA	12:L:333:PRO:O	2.09	0.51
20:U:85:LEU:CB	20:U:159:VAL:C	2.79	0.51
36:l:67:HIS:HA	36:l:77:SER:CB	2.40	0.51
36:l:383:MET:O	36:l:389:PHE:HB2	2.10	0.51
41:q:269:MET:HE2	41:q:399:ASN:HB2	1.92	0.51
45:u:366:ASP:O	45:u:370:PHE:N	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:v:70:ARG:NH2	46:v:332:ASP:OD2	2.43	0.51
47:w:83:HIS:CD2	76:w:401:HEM:C1A	2.98	0.51
48:x:203:ARG:HG3	48:x:279:SER:OG	2.09	0.51
53:2:179:ARG:HH22	53:2:201:ASP:CG	2.18	0.51
46:6:63:LEU:HD11	46:6:121:TYR:HD2	1.75	0.51
48:8:108:HIS:CD2	52:Ac:56:ILE:HD12	2.45	0.51
60:Ak:398:PRO:O	60:Ak:498:CYS:HB3	2.09	0.51
61:Al:1:MET:SD	61:Al:133:LEU:CD1	2.98	0.51
64:Ao:63:SER:O	64:Ao:67:ILE:HG13	2.10	0.51
5:E:131:HIS:NE2	5:E:172:ILE:HD13	2.25	0.51
9:I:84:PRO:HA	9:I:122:VAL:O	2.11	0.51
9:I:203:LYS:HG3	9:I:206:ARG:NH1	2.25	0.51
21:V:107:SER:HB3	21:V:110:ILE:HG22	1.92	0.51
33:i:217:MET:HB2	33:i:326:LEU:HD13	1.91	0.51
36:l:14:ILE:O	36:l:17:ILE:HG22	2.10	0.51
48:x:135:HIS:HB3	48:x:277:TRP:CH2	2.44	0.51
53:4:170:ARG:NH2	53:4:262:THR:OG1	2.44	0.51
48:8:125:CYS:HB2	48:8:195:PRO:HG3	1.92	0.51
48:8:145:GLU:O	48:8:149:LEU:HG	2.10	0.51
60:Ak:268:PHE:CZ	61:Al:58:ALA:HA	2.44	0.51
2:B:149:MET:HB2	2:B:151:ALA:HB2	1.92	0.51
3:C:87:GLN:HE22	9:I:117:PRO:HD3	1.75	0.51
4:D:155:SER:HB3	4:D:181:HIS:HB2	1.92	0.51
7:G:648:GLU:HG3	7:G:649:VAL:N	2.25	0.51
8:H:158:CYS:N	68:H:302:SF4:S2	2.73	0.51
9:I:208:LYS:HG3	9:I:212:ILE:CD1	2.40	0.51
12:L:239:PRO:O	12:L:267:GLY:HA3	2.11	0.51
16:P:20:ARG:O	16:P:65:LEU:HD12	2.09	0.51
18:S:59:ARG:O	18:S:61:HIS:N	2.43	0.51
20:U:178:GLN:HG3	20:U:235:TYR:HB2	1.92	0.51
23:Y:73:PHE:HA	36:l:385:TYR:CE2	2.46	0.51
29:e:122:ALA:O	29:e:126:VAL:HG23	2.10	0.51
33:i:9:LEU:O	33:i:12:THR:HG22	2.10	0.51
36:l:439:PRO:O	36:l:440:LEU:HB2	2.10	0.51
39:o:8:PRO:HB3	39:o:14:LEU:HB3	1.91	0.51
46:6:290:GLN:HB2	46:6:325:ALA:HB1	1.91	0.51
46:6:355:TYR:CE1	46:6:436:LYS:HE2	2.43	0.51
48:8:293:MET:HE2	48:8:293:MET:C	2.36	0.51
61:Al:100:MET:CE	61:Al:157:GLU:HG3	2.40	0.51
4:D:85:GLU:HB2	4:D:144:LYS:NZ	2.25	0.51
7:G:173:MET:C	7:G:174:THR:HG1	2.17	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:70:LEU:HG	42:r:272:TRP:CZ2	2.45	0.51
31:g:122:ARG:C	39:o:109:ARG:HH12	2.19	0.51
40:p:79:PRO:HG2	40:p:81:ILE:HD11	1.91	0.51
41:q:207:MET:HE1	41:q:240:GLY:HA2	1.92	0.51
42:r:120:GLY:HA3	42:r:132:ALA:HB2	1.92	0.51
45:u:315:ASP:OD1	45:u:316:SER:N	2.42	0.51
46:v:66:LYS:HB3	46:v:217:ARG:HB3	1.93	0.51
47:w:27:ILE:HG23	47:w:31:TRP:HB2	1.93	0.51
53:2:236:CYS:HB2	53:2:243:TYR:HE2	1.76	0.51
54:3:4:ARG:O	54:3:5:PHE:C	2.51	0.51
54:3:9:ARG:O	54:3:13:LEU:N	2.39	0.51
53:4:213:LEU:HA	53:4:261:PRO:HD3	1.93	0.51
71:4:301:PLX:H252	75:5:502:PEE:O5	2.11	0.51
45:5:337:LEU:HB2	45:5:368:MET:HE2	1.92	0.51
48:8:293:MET:HE2	48:8:294:LEU:HA	1.93	0.51
61:A1:59:GLN:N	61:A1:62:GLU:HG3	2.24	0.51
5:E:104:ILE:HG22	5:E:105:LEU:HD12	1.92	0.51
15:O:80:LYS:HE2	15:O:142:GLN:HE22	1.75	0.51
35:k:67:ALA:O	35:k:70:GLU:HG2	2.09	0.51
39:o:25:ILE:O	45:u:262:VAL:N	2.42	0.51
40:p:20:TYR:HD1	40:p:48:PHE:HE2	1.57	0.51
41:q:152:TYR:O	41:q:205:VAL:HG11	2.11	0.51
43:s:79:ALA:H	43:s:81:PRO:HD2	1.75	0.51
46:v:95:SER:O	46:v:99:ILE:HD12	2.09	0.51
47:w:9:PRO:O	47:w:13:ILE:HG12	2.10	0.51
45:5:80:ARG:NE	45:5:350:GLU:OE2	2.44	0.51
45:5:276:ARG:HD2	45:5:462:ILE:CD1	2.41	0.51
45:5:285:ALA:HA	45:5:460:GLY:HA2	1.91	0.51
45:5:314:TYR:HA	45:5:318:TYR:HE2	1.75	0.51
47:7:243:VAL:HG13	47:7:244:LEU:HD12	1.92	0.51
2:B:137:LYS:NZ	2:B:256:ARG:HH22	2.08	0.51
3:C:108:LYS:HG3	3:C:436:ASP:OD1	2.11	0.51
5:E:134:VAL:O	5:E:174:VAL:N	2.43	0.51
7:G:98:LYS:NZ	7:G:100:TRP:HE1	2.08	0.51
7:G:335:GLY:C	7:G:363:SER:HB2	2.35	0.51
7:G:341:ILE:HB	7:G:546:PHE:CD1	2.45	0.51
7:G:557:ARG:HB3	7:G:560:LEU:HD22	1.91	0.51
10:J:64:LEU:CD1	17:Q:81:LEU:HD23	2.40	0.51
20:U:154:SER:OG	20:U:155:THR:N	2.43	0.51
27:c:140:MET:SD	36:l:407:TRP:HH2	2.33	0.51
28:d:85:MET:O	28:d:89:GLU:HB2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:f:41:TRP:CD1	30:f:43:LYS:H	2.27	0.51
36:l:346:ILE:HA	36:l:366:MET:HE1	1.93	0.51
45:u:126:ARG:HG2	45:u:201:VAL:HG22	1.93	0.51
45:u:195:THR:HG23	45:u:268:CYS:SG	2.50	0.51
48:x:243:ILE:HD13	48:x:245:MET:HE2	1.92	0.51
53:4:220:LEU:HD12	53:4:239:HIS:CE1	2.46	0.51
46:6:326:PHE:CE1	55:Ae:9:GLY:HA3	2.46	0.51
49:9:33:MET:H	49:9:62:ARG:HH12	1.57	0.51
49:9:36:ASP:O	49:9:59:ARG:NH2	2.44	0.51
62:Am:18:LEU:HD22	62:Am:22:LEU:HD22	1.92	0.51
67:Ar:60:TYR:C	67:Ar:60:TYR:CD1	2.88	0.51
3:C:118:ARG:HD3	9:I:163:TYR:CZ	2.45	0.51
4:D:122:ARG:HB3	14:N:111:GLN:HE21	1.76	0.51
7:G:44:GLU:HG3	7:G:45:PRO:HD2	1.91	0.51
7:G:474:VAL:HG11	7:G:493:VAL:HG22	1.92	0.51
15:O:79:ILE:O	15:O:83:VAL:HG23	2.10	0.51
16:P:66:TRP:HA	16:P:75:LYS:O	2.10	0.51
32:h:71:LYS:O	32:h:74:LYS:HG2	2.10	0.51
33:i:298:TYR:O	33:i:303:THR:OG1	2.29	0.51
36:l:396:ILE:HD11	36:l:413:LEU:HD23	1.93	0.51
37:m:93:PHE:CE2	37:m:97:LEU:HD11	2.46	0.51
43:s:169:PHE:HE1	74:s:201:CDL:H531	1.75	0.51
45:u:160:GLN:O	45:u:164:GLU:HG2	2.11	0.51
48:x:293:MET:SD	48:x:293:MET:C	2.94	0.51
53:4:214:ILE:HG22	53:4:259:GLU:HB3	1.92	0.51
46:6:65:ILE:HG22	46:6:67:ALA:H	1.75	0.51
46:6:67:ALA:HA	46:6:71:TYR:HE2	1.75	0.51
2:B:77:LEU:HG	2:B:81:LYS:HE3	1.93	0.51
7:G:655:ARG:HB3	7:G:658:ASP:HB2	1.91	0.51
12:L:202:LYS:N	12:L:203:PRO:CD	2.73	0.51
25:a:135:LYS:O	25:a:139:ILE:HG12	2.10	0.51
28:d:11:PRO:O	28:d:15:ARG:N	2.44	0.51
33:i:30:TRP:CG	33:i:71:MET:HE2	2.46	0.51
33:i:303:THR:HG21	41:q:143:LEU:HD21	1.92	0.51
41:q:296:LEU:HB3	41:q:381:ILE:HD11	1.91	0.51
45:u:164:GLU:O	45:u:168:ILE:HG12	2.10	0.51
45:u:318:TYR:HE1	55:Af:20:ARG:HA	1.74	0.51
48:x:97:TRP:CZ2	48:x:210:ASP:HA	2.46	0.51
48:x:229:ARG:NH1	48:x:230:GLU:HB3	2.25	0.51
49:y:29:LYS:HB3	49:y:75:ILE:HD11	1.93	0.51
53:4:136:PHE:HE1	47:7:79:ILE:HG12	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:7:333:ILE:CD1	75:7:402:PEE:H62	2.40	0.51
60:Ak:250:GLY:O	60:Ak:254:ILE:HG12	2.11	0.51
61:Al:78:LEU:HB2	61:Al:79:PRO:CD	2.38	0.51
2:B:73:PRO:O	2:B:76:ILE:HG12	2.11	0.51
7:G:298:LYS:O	11:R:134:ILE:C	2.54	0.51
7:G:337:ASP:O	7:G:541:PRO:HB2	2.10	0.51
7:G:383:SER:HA	7:G:386:LEU:HD12	1.93	0.51
12:L:241:TYR:CB	12:L:343:THR:OG1	2.59	0.51
14:N:64:ASP:O	14:N:68:LEU:HB2	2.11	0.51
31:g:16:LEU:HD12	31:g:17:PRO:HD2	1.93	0.51
36:l:33:PRO:HB2	36:l:105:MET:HE2	1.93	0.51
41:q:112:ALA:HB3	41:q:113:THR:HA	1.92	0.51
41:q:319:HIS:HA	41:q:322:THR:HG22	1.92	0.51
43:s:112:LEU:O	43:s:116:GLY:HA2	2.11	0.51
46:v:312:ALA:HA	46:v:315:LYS:HE3	1.92	0.51
46:v:440:ALA:O	46:v:444:LEU:HD21	2.10	0.51
49:y:54:ASN:OD1	49:y:55:LEU:N	2.43	0.51
47:7:153:ILE:HB	47:7:157:GLY:HA3	1.92	0.51
48:8:190:ASN:HD21	77:8:402:HEC:HBC3	1.75	0.51
48:8:245:MET:HG2	48:8:246:ALA:O	2.11	0.51
48:8:314:VAL:HG23	50:Aa:21:PRO:HG3	1.92	0.51
2:B:118:ASP:CA	69:B:502:FMN:HM72	2.40	0.51
3:C:41:VAL:O	3:C:45:GLU:HG2	2.11	0.51
7:G:560:LEU:HA	7:G:563:ASP:O	2.11	0.51
8:H:64:THR:O	8:H:67:VAL:HG12	2.11	0.51
9:I:159:GLY:C	9:I:161:GLY:H	2.19	0.51
18:S:50:ARG:O	18:S:54:ILE:HG12	2.11	0.51
21:V:103:ALA:O	21:V:106:ARG:NH1	2.40	0.51
27:c:90:TYR:OH	39:o:44:LYS:HE3	2.11	0.51
27:c:97:LEU:HD22	27:c:113:ILE:HD11	1.92	0.51
28:d:120:SER:OG	28:d:121:TYR:N	2.43	0.51
36:l:106:TRP:O	36:l:109:HIS:ND1	2.33	0.51
36:l:452:ASN:HA	36:l:455:LYS:HD3	1.93	0.51
47:7:246:SER:HB2	47:7:249:LEU:HB2	1.93	0.51
76:7:404:HEM:HBB2	76:7:404:HEM:HMB1	1.92	0.51
3:C:271:ARG:HH22	42:r:281:ARG:HB2	1.75	0.50
3:C:272:THR:O	3:C:327:TYR:HB2	2.11	0.50
5:E:132:ILE:HD11	5:E:169:PHE:HD1	1.76	0.50
7:G:50:LEU:O	7:G:54:GLU:HG2	2.11	0.50
9:I:78:ARG:NH1	42:r:57:THR:HG22	2.26	0.50
12:L:350:ILE:HG13	12:L:357:ARG:NH2	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:71:SER:O	13:M:73:GLN:N	2.44	0.50
20:U:318:GLU:CD	20:U:318:GLU:H	2.19	0.50
31:g:32:ARG:HB3	33:i:339:MET:HE1	1.93	0.50
33:i:24:SER:HA	33:i:86:ILE:HD11	1.94	0.50
33:i:40:MET:O	33:i:43:VAL:HG12	2.10	0.50
33:i:337:LEU:C	33:i:339:MET:H	2.19	0.50
35:k:26:LEU:HD11	35:k:78:LEU:HD13	1.93	0.50
37:m:31:LEU:HD13	42:r:118:TRP:CH2	2.46	0.50
45:u:165:ARG:HH12	45:u:210:LYS:N	2.08	0.50
46:v:161:ASP:OD2	55:Af:15:LEU:HD13	2.11	0.50
46:v:261:GLN:OE1	46:v:444:LEU:HB2	2.12	0.50
47:w:312:GLN:HB2	47:w:318:ARG:HE	1.76	0.50
46:6:62:GLY:HA2	46:6:122:THR:HA	1.93	0.50
47:7:28:SER:C	47:7:227:LYS:HZ1	2.19	0.50
48:8:200:TYR:O	48:8:204:ALA:N	2.44	0.50
63:An:64:PHE:CE1	64:Ao:66:ARG:HD2	2.46	0.50
3:C:36:GLN:HG3	3:C:37:TRP:N	2.26	0.50
4:D:108:PHE:HB3	4:D:132:LEU:HB3	1.93	0.50
7:G:607:LYS:NZ	10:J:78:ARG:HH21	2.09	0.50
9:I:179:VAL:HG21	9:I:182:TYR:OH	2.11	0.50
12:L:154:GLN:HA	12:L:157:LYS:HG2	1.93	0.50
14:N:96:ARG:CZ	14:N:96:ARG:HB2	2.41	0.50
15:O:99:SER:HB3	15:O:102:SER:OG	2.11	0.50
17:Q:29:LYS:NZ	73:Q:201:ZMP:O3	2.45	0.50
18:S:66:LEU:HB3	43:s:75:LYS:HE2	1.92	0.50
33:i:33:PHE:HE1	33:i:137:ALA:HB1	1.75	0.50
37:m:8:ILE:O	37:m:11:THR:OG1	2.21	0.50
44:t:51:LEU:HD12	44:t:51:LEU:N	2.26	0.50
45:u:53:LEU:HD12	45:u:57:LEU:HB3	1.93	0.50
45:u:274:GLU:CD	45:u:468:TYR:HB2	2.36	0.50
53:2:159:ILE:HG12	53:2:165:MET:HB2	1.93	0.50
54:3:38:TRP:HE1	54:3:40:LEU:HG	1.75	0.50
71:4:301:PLX:C25	75:5:502:PEE:O5	2.60	0.50
60:Ak:184:PHE:H	60:Ak:256:HIS:CE1	2.29	0.50
2:B:379:CYS:O	7:G:201:GLY:N	2.40	0.50
7:G:544:VAL:HG23	7:G:566:ILE:HG23	1.93	0.50
7:G:645:ARG:HA	7:G:648:GLU:HG2	1.93	0.50
8:H:178:GLU:OE2	9:I:203:LYS:HD2	2.11	0.50
12:L:277:VAL:HA	12:L:280:ILE:HD12	1.93	0.50
15:O:120:MET:HA	15:O:123:GLU:OE2	2.11	0.50
26:b:85:TYR:O	26:b:89:HIS:ND1	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:69:GLY:C	39:o:86:THR:HG21	2.36	0.50
27:c:92:TRP:CD1	27:c:98:ARG:HG3	2.47	0.50
34:j:71:LEU:O	34:j:74:PRO:HD2	2.11	0.50
36:l:21:MET:O	36:l:24:SER:OG	2.23	0.50
41:q:12:LEU:HB2	41:q:13:PRO:HD3	1.93	0.50
43:s:85:TYR:HE1	43:s:104:GLN:HB2	1.76	0.50
47:w:35:SER:O	47:w:39:ILE:HG12	2.11	0.50
48:8:126:HIS:ND1	48:8:195:PRO:HB2	2.25	0.50
48:8:292:LYS:O	52:Ac:36:PHE:HZ	1.94	0.50
3:C:393:PRO:HD2	4:D:245:TYR:CD2	2.47	0.50
7:G:35:PHE:N	7:G:100:TRP:O	2.41	0.50
7:G:51:GLN:NE2	10:J:156:LYS:O	2.43	0.50
7:G:53:CYS:HA	7:G:56:VAL:HG12	1.93	0.50
21:V:71:GLY:O	21:V:74:SER:OG	2.27	0.50
24:Z:28:PRO:O	24:Z:31:THR:OG1	2.21	0.50
25:a:69:LYS:HD3	25:a:72:ARG:HH12	1.76	0.50
31:g:2:THR:O	31:g:3:MET:HG2	2.11	0.50
31:g:32:ARG:NH2	43:s:172:MET:HG3	2.26	0.50
33:i:7:THR:HA	33:i:10:ILE:HG22	1.93	0.50
41:q:237:LYS:HZ1	41:q:319:HIS:CE1	2.29	0.50
45:u:195:THR:HG22	45:u:197:LEU:N	2.23	0.50
45:u:296:TRP:N	45:u:348:TYR:O	2.43	0.50
46:v:70:ARG:HA	46:v:185:ALA:O	2.11	0.50
46:v:136:PHE:O	46:v:140:VAL:HG23	2.11	0.50
47:w:103:TYR:CD2	75:w:403:PEE:C12	2.95	0.50
47:w:182:HIS:CE1	76:w:401:HEM:C1B	2.98	0.50
48:8:280:GLU:O	48:8:283:HIS:HB2	2.11	0.50
60:Ak:40:GLU:HG2	60:Ak:54:TYR:CD1	2.47	0.50
60:Ak:347:LEU:HG	60:Ak:383:MET:HE3	1.93	0.50
2:B:330:SER:HA	2:B:333:GLU:HB2	1.94	0.50
4:D:56:LYS:O	4:D:59:SER:OG	2.18	0.50
5:E:213:ILE:HG22	5:E:214:PRO:O	2.12	0.50
12:L:213:PHE:O	12:L:216:TYR:HB3	2.12	0.50
32:h:37:GLU:HB2	32:h:63:PHE:CE1	2.45	0.50
34:j:104:TYR:HE2	37:m:169:MET:HG3	1.76	0.50
35:k:52:HIS:ND1	37:m:138:GLU:OE1	2.45	0.50
40:p:91:TYR:CD2	40:p:92:GLU:HG3	2.46	0.50
45:u:89:ALA:HA	45:u:92:PHE:CD2	2.46	0.50
46:v:147:ARG:HD2	46:v:149:TRP:CH2	2.47	0.50
46:v:309:LEU:HG	46:v:357:GLN:HB3	1.94	0.50
50:z:31:PHE:O	50:z:35:ILE:HD12	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:220:LEU:HD22	47:7:268:ILE:HG12	1.93	0.50
53:4:92:ARG:HH22	45:5:193:GLN:NE2	2.10	0.50
53:4:156:LEU:HB2	53:4:271:VAL:HG12	1.92	0.50
45:5:313:HIS:HB2	55:Ae:20:ARG:HH22	1.76	0.50
45:5:381:THR:HB	54:Ad:17:TRP:CH2	2.47	0.50
46:6:155:GLN:HE21	46:6:198:GLY:HA2	1.77	0.50
49:9:29:LYS:HG2	49:9:81:TRP:CZ2	2.46	0.50
49:9:62:ARG:O	49:9:65:ARG:HG2	2.11	0.50
50:Aa:62:TRP:HA	50:Aa:65:GLN:HG2	1.94	0.50
51:Ab:30:LEU:O	51:Ab:34:ARG:HG3	2.10	0.50
60:Ak:75:ILE:O	60:Ak:79:GLY:HA3	2.11	0.50
61:Al:136:LEU:HB3	61:Al:193:TYR:CD2	2.46	0.50
63:An:40:LEU:HD22	63:An:59:LEU:HD13	1.92	0.50
66:Aq:5:LYS:NZ	66:Aq:5:LYS:HB3	2.27	0.50
2:B:125:CYS:HB2	5:E:180:CYS:N	2.26	0.50
3:C:196:ALA:O	3:C:198:THR:N	2.41	0.50
7:G:34:VAL:HG21	7:G:96:VAL:HB	1.93	0.50
7:G:299:ARG:HG2	7:G:300:GLN:H	1.77	0.50
21:V:84:PRO:O	21:V:89:ASN:ND2	2.43	0.50
36:l:74:VAL:HG21	36:l:190:LEU:HD11	1.93	0.50
36:l:173:LEU:HD23	75:l:701:PEE:H18	1.94	0.50
42:r:135:ALA:HB1	42:r:201:THR:HG22	1.93	0.50
45:u:206:GLU:HA	45:u:209:ARG:HG2	1.93	0.50
46:v:137:LEU:HA	46:v:140:VAL:HB	1.93	0.50
47:w:234:PHE:CD1	48:x:301:LEU:HD21	2.45	0.50
76:w:401:HEM:HBC2	76:w:401:HEM:HMC1	1.92	0.50
48:x:322:TYR:HB2	49:y:61:PHE:CD1	2.47	0.50
48:x:322:TYR:HB2	49:y:61:PHE:CE1	2.46	0.50
53:4:80:HIS:CE1	53:4:81:THR:HG23	2.47	0.50
45:5:306:VAL:O	45:5:310:ILE:HD12	2.12	0.50
60:Ak:11:ASN:ND2	60:Ak:14:ASP:H	2.07	0.50
60:Ak:232:GLN:HB2	60:Ak:292:MET:HE3	1.93	0.50
61:Al:139:ASP:OD1	61:Al:140:ASN:N	2.44	0.50
2:B:125:CYS:SG	5:E:179:ALA:HA	2.52	0.50
2:B:406:PRO:O	2:B:409:ILE:HG12	2.12	0.50
5:E:214:PRO:HG2	5:E:216:PRO:HG3	1.94	0.50
15:O:138:LEU:O	15:O:140:CYS:N	2.45	0.50
18:S:9:ILE:O	18:S:12:MET:HB3	2.11	0.50
32:h:73:MET:HE3	37:m:126:VAL:HG11	1.93	0.50
36:l:139:GLN:HA	36:l:142:ILE:HG22	1.93	0.50
36:l:347:ILE:HG23	36:l:352:ASP:HA	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:m:116:ILE:HG22	37:m:117:PHE:CD2	2.46	0.50
41:q:18:SER:HB2	41:q:23:ILE:HG22	1.93	0.50
46:v:305:ALA:HA	46:v:311:GLN:HE21	1.77	0.50
47:w:32:ASN:O	47:w:35:SER:OG	2.19	0.50
47:w:316:MET:HB3	75:w:403:PEE:O2P	2.03	0.50
48:x:142:THR:O	48:x:146:ALA:N	2.44	0.50
48:x:263:THR:HG21	51:0:29:PRO:HD2	1.92	0.50
49:y:91:LEU:HA	49:y:94:TYR:HD2	1.77	0.50
51:0:38:GLU:HA	51:0:43:CYS:CB	2.42	0.50
45:5:182:VAL:HG12	45:5:186:TYR:CE2	2.46	0.50
47:7:6:LYS:O	47:7:12:LYS:HD3	2.11	0.50
47:7:88:SER:HB3	47:7:272:TRP:HZ2	1.77	0.50
47:7:287:LYS:O	47:7:291:VAL:HG23	2.12	0.50
2:B:132:ARG:HA	2:B:165:GLU:CD	2.37	0.50
2:B:371:ILE:HD12	2:B:396:MET:HG3	1.94	0.50
2:B:387:GLU:OE2	7:G:123:ASN:ND2	2.27	0.50
7:G:595:THR:HA	7:G:605:GLN:HA	1.94	0.50
14:N:88:LEU:O	14:N:92:ARG:HG2	2.11	0.50
19:T:30:ILE:HG12	34:j:92:LEU:HD13	1.92	0.50
26:b:73:THR:OG1	26:b:74:HIS:N	2.45	0.50
28:d:35:LYS:O	28:d:39:LEU:N	2.44	0.50
29:e:93:PHE:O	29:e:98:VAL:HG22	2.12	0.50
33:i:34:GLU:OE2	35:k:70:GLU:HB3	2.12	0.50
33:i:163:LEU:HD23	33:i:285:THR:HG21	1.93	0.50
34:j:65:PHE:CE2	42:r:290:TRP:HZ3	2.29	0.50
36:l:297:ASP:CG	36:l:300:LYS:H	2.19	0.50
36:l:313:MET:HB3	36:l:328:HIS:HD2	1.76	0.50
46:v:114:SER:HA	46:v:119:MET:HA	1.94	0.50
46:v:328:ALA:HB3	46:v:335:LEU:HB2	1.94	0.50
47:w:264:THR:HB	53:4:222:CYS:HA	1.94	0.50
47:w:338:ILE:HD11	47:w:350:ILE:HG22	1.94	0.50
49:y:44:VAL:HG22	49:y:95:LEU:HD13	1.93	0.50
53:4:226:ALA:C	53:4:228:ALA:H	2.19	0.50
45:5:278:ARG:NE	45:5:462:ILE:H	2.10	0.50
54:Ad:39:ARG:HA	54:Ad:42:LEU:HD12	1.94	0.50
60:Ak:145:LEU:HD21	62:Am:32:THR:HG21	1.93	0.50
2:B:320:GLY:HA2	2:B:353:ALA:HB3	1.92	0.50
2:B:446:LEU:O	2:B:450:MET:HG3	2.11	0.50
3:C:181:LEU:HD21	3:C:211:PHE:HE1	1.75	0.50
3:C:447:VAL:O	3:C:450:ILE:HG22	2.12	0.50
4:D:55:HIS:HD2	4:D:78:VAL:HG11	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:158:ARG:HH22	7:G:178:GLN:HE22	1.60	0.50
7:G:607:LYS:HD3	10:J:78:ARG:HD2	1.93	0.50
12:L:75:ARG:NH2	17:Q:110:THR:O	2.45	0.50
15:O:80:LYS:HG2	15:O:145:VAL:HG11	1.93	0.50
15:O:114:ASP:O	15:O:118:ILE:HG13	2.12	0.50
15:X:104:PHE:HZ	15:X:118:ILE:HG12	1.77	0.50
25:a:156:VAL:HG21	31:g:92:MET:HG3	1.94	0.50
25:a:176:LYS:HB2	32:h:45:HIS:CE1	2.47	0.50
32:h:95:PRO:O	32:h:99:LEU:N	2.44	0.50
33:i:71:MET:HG3	35:k:40:LEU:HD23	1.94	0.50
37:m:125:TRP:HA	37:m:128:TYR:CE2	2.47	0.50
46:v:173:VAL:O	46:v:176:ASN:HB3	2.12	0.50
47:w:92:ILE:O	47:w:96:ILE:HD12	2.11	0.50
47:w:312:GLN:NE2	47:w:317:PHE:H	2.06	0.50
48:x:236:PRO:HB3	51:0:72:PHE:CE1	2.46	0.50
45:5:323:HIS:HB3	46:6:97:PHE:HD1	1.77	0.50
45:5:404:ASP:OD1	45:5:405:GLY:N	2.44	0.50
46:6:82:LEU:HD13	46:6:158:LEU:HD11	1.93	0.50
47:7:99:GLY:HA3	75:7:402:PEE:H29	1.94	0.50
48:8:293:MET:C	48:8:293:MET:CE	2.85	0.50
49:9:51:LEU:HD21	49:9:91:LEU:HD23	1.93	0.50
50:Aa:34:GLY:O	50:Aa:38:VAL:HG23	2.12	0.50
9:I:154:GLY:O	9:I:158:ASN:ND2	2.45	0.49
12:L:167:ILE:HG21	72:L:401:NDP:O4D	2.12	0.49
14:N:31:ILE:O	14:N:35:LEU:HG	2.12	0.49
14:N:104:VAL:HG22	14:N:105:GLU:HG2	1.93	0.49
15:O:123:GLU:HB2	15:O:128:PHE:O	2.12	0.49
16:P:40:ARG:O	16:P:44:LEU:HG	2.12	0.49
21:V:13:PRO:O	21:V:15:GLY:N	2.45	0.49
22:W:66:GLU:O	22:W:69:ILE:HG22	2.12	0.49
36:l:416:THR:O	36:l:419:THR:OG1	2.29	0.49
41:q:252:PRO:O	41:q:255:ASN:ND2	2.41	0.49
43:s:103:GLN:O	43:s:106:LYS:N	2.45	0.49
45:u:75:ILE:HG22	45:u:77:ALA:H	1.77	0.49
46:v:259:ARG:NE	46:v:444:LEU:HD22	2.26	0.49
47:w:152:ALA:HB1	47:w:288:LEU:HA	1.93	0.49
49:y:19:LYS:HA	49:y:22:TYR:HB3	1.94	0.49
53:2:132:ALA:HB2	75:2:302:PEE:H24	1.89	0.49
53:2:151:LYS:HG3	53:2:274:GLY:HA3	1.94	0.49
46:6:261:GLN:HA	46:6:444:LEU:HD12	1.94	0.49
66:Aq:44:ARG:HD2	66:Aq:74:ARG:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:308:ARG:HG2	7:G:581:ASP:HA	1.94	0.49
20:U:145:TYR:HB2	20:U:165:ILE:HD11	1.92	0.49
26:b:94:PRO:HG3	28:d:11:PRO:HG3	1.94	0.49
26:b:100:ARG:NE	28:d:118:GLY:O	2.40	0.49
35:k:10:MET:HE1	37:m:103:MET:SD	2.53	0.49
36:l:296:ASN:HA	36:l:356:ILE:HG12	1.94	0.49
75:l:701:PEE:H11	75:l:701:PEE:O2P	2.12	0.49
40:p:58:VAL:HG11	45:u:228:ARG:HH22	1.77	0.49
45:u:96:LEU:HD13	45:u:156:LEU:HD21	1.94	0.49
46:v:49:ILE:HG13	46:v:220:LEU:HD22	1.93	0.49
47:w:361:ILE:HG12	47:w:365:LEU:HD12	1.93	0.49
45:5:278:ARG:NH1	45:5:462:ILE:N	2.60	0.49
45:5:388:VAL:O	45:5:392:LYS:HG3	2.11	0.49
46:6:64:PHE:CD2	46:6:397:GLY:HA3	2.47	0.49
47:7:30:TRP:HA	47:7:33:PHE:CD2	2.47	0.49
47:7:113:TRP:NE1	47:7:301:LEU:O	2.38	0.49
47:7:265:PRO:HG2	47:7:268:ILE:HD13	1.94	0.49
5:E:129:LYS:H	5:E:168:LEU:HA	1.77	0.49
7:G:299:ARG:HD2	7:G:705:GLN:NE2	2.26	0.49
7:G:341:ILE:HD11	7:G:538:ARG:HH12	1.77	0.49
10:J:77:VAL:HG23	10:J:101:PHE:CD1	2.46	0.49
14:N:114:TRP:CG	14:N:115:PRO:HA	2.48	0.49
33:i:31:ILE:HG23	35:k:66:PHE:HE2	1.76	0.49
42:r:87:VAL:HG23	42:r:95:LEU:HD22	1.94	0.49
46:v:320:PRO:HB2	46:v:343:GLN:NE2	2.27	0.49
75:w:403:PEE:H61	75:w:403:PEE:C17	2.42	0.49
48:x:112:ARG:NH2	48:x:140:CYS:O	2.45	0.49
53:4:80:HIS:CD2	45:5:182:VAL:HG22	2.48	0.49
53:4:99:SER:HA	45:5:269:ARG:NE	2.27	0.49
46:6:346:SER:O	46:6:350:VAL:HG23	2.12	0.49
47:7:137:GLN:HE22	47:7:260:ASN:H	1.59	0.49
48:8:116:GLN:O	48:8:120:GLN:HG2	2.12	0.49
54:Ad:29:ALA:O	54:Ad:33:VAL:HG23	2.12	0.49
60:Ak:508:PRO:HG3	62:Am:6:HIS:HB3	1.94	0.49
3:C:375:MET:HA	7:G:126:LEU:HD21	1.95	0.49
12:L:329:LEU:HB2	12:L:331:HIS:CE1	2.47	0.49
32:h:2:PRO:O	32:h:4:PHE:N	2.45	0.49
32:h:21:GLN:HA	35:k:53:PHE:CE1	2.47	0.49
36:l:527:GLY:C	36:l:529:TYR:H	2.20	0.49
41:q:25:ILE:O	41:q:29:VAL:HG12	2.13	0.49
41:q:208:PRO:HG3	41:q:216:LEU:HD13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:x:232:LEU:HB3	48:x:242:ALA:HB1	1.95	0.49
71:4:301:PLX:O7	75:5:502:PEE:H50	2.13	0.49
45:5:274:GLU:HB2	45:5:456:VAL:HB	1.95	0.49
45:5:292:GLU:OE2	45:5:351:THR:HB	2.12	0.49
47:7:324:LEU:HD13	47:7:365:LEU:HB3	1.95	0.49
55:Ae:32:ALA:O	55:Ae:35:PRO:HD2	2.13	0.49
2:B:79:GLU:HG3	2:B:254:ILE:HG22	1.93	0.49
7:G:83:GLU:HB2	7:G:101:ASN:O	2.12	0.49
7:G:136:GLU:OE1	7:G:242:PRO:HG2	2.13	0.49
7:G:333:PHE:HB3	7:G:337:ASP:HB2	1.95	0.49
12:L:98:GLY:HA3	12:L:103:ILE:HG12	1.94	0.49
31:g:35:TYR:OH	33:i:335:LEU:O	2.31	0.49
33:i:311:MET:HG3	33:i:315:TRP:HE1	1.78	0.49
42:r:70:MET:HA	42:r:73:ILE:HG22	1.94	0.49
42:r:257:ILE:O	42:r:261:LEU:HD13	2.13	0.49
46:v:423:ASP:O	46:v:426:ASN:HB3	2.12	0.49
47:w:186:PRO:HA	47:w:189:ILE:HD12	1.95	0.49
48:x:217:THR:HG23	48:x:264:MET:HE2	1.93	0.49
45:5:478:LEU:HD13	75:5:502:PEE:H12	1.81	0.49
46:6:174:LEU:HD22	55:Ae:11:PHE:CE1	2.47	0.49
47:7:32:ASN:ND2	47:7:227:LYS:O	2.45	0.49
48:8:136:LEU:HD23	48:8:176:PHE:HZ	1.77	0.49
6:F:108:THR:CB	6:F:109:GLY:HA3	2.43	0.49
7:G:525:ALA:O	7:G:529:GLY:N	2.45	0.49
12:L:145:PHE:CD2	12:L:184:LYS:HG3	2.47	0.49
15:X:118:ILE:HA	24:Z:45:TRP:HZ2	1.77	0.49
15:X:140:CYS:HB2	15:X:143:GLU:HG3	1.93	0.49
33:i:159:MET:HB2	33:i:278:MET:CE	2.41	0.49
36:l:15:LEU:O	36:l:18:PRO:HD2	2.13	0.49
36:l:282:ALA:O	36:l:285:THR:OG1	2.19	0.49
42:r:105:MET:HG3	42:r:237:PHE:CE1	2.48	0.49
45:u:87:ASN:H	45:u:207:ASN:HD21	1.61	0.49
45:u:339:GLN:HB2	45:u:359:VAL:HB	1.95	0.49
46:v:407:MET:HG2	46:v:408:GLN:O	2.13	0.49
47:w:282:ARG:HH21	47:w:348:ILE:HG13	1.78	0.49
48:x:126:HIS:ND1	48:x:196:PRO:O	2.34	0.49
48:x:238:PHE:CD1	48:x:239:PRO:HD2	2.47	0.49
45:5:149:ASP:O	45:5:153:ASN:HB2	2.12	0.49
45:5:373:GLN:OE1	45:5:474:GLY:HA3	2.13	0.49
46:6:116:ARG:HH12	46:6:178:HIS:CB	2.21	0.49
47:7:302:ILE:O	47:7:305:PRO:HD2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:8:134:ARG:HB3	48:8:173:SER:HA	1.95	0.49
55:Ae:26:LEU:HA	55:Ae:27:ARG:O	2.12	0.49
2:B:62:TRP:NE1	2:B:140:GLU:HG2	2.28	0.49
8:H:83:THR:OG1	42:r:35:LYS:HE2	2.11	0.49
12:L:66:GLY:N	12:L:129:LEU:HD23	2.28	0.49
20:U:91:ALA:HB2	20:U:95:TYR:CD1	2.48	0.49
26:b:84:TYR:O	26:b:87:LYS:HG2	2.12	0.49
27:c:123:PRO:HB3	40:p:75:GLN:HE21	1.76	0.49
31:g:43:SER:HA	33:i:331:VAL:HG21	1.93	0.49
32:h:10:LEU:HB3	32:h:12:LEU:HD13	1.94	0.49
33:i:312:LYS:HA	33:i:315:TRP:CE2	2.48	0.49
34:j:38:GLU:OE2	42:r:126:LYS:HD2	2.12	0.49
36:l:51:LEU:O	36:l:55:MET:HG2	2.13	0.49
41:q:7:PRO:HA	41:q:10:MET:HB2	1.94	0.49
41:q:297:VAL:O	41:q:301:ILE:HG12	2.13	0.49
45:u:75:ILE:HD13	45:u:224:TYR:CD1	2.47	0.49
47:w:77:TRP:CH2	48:x:286:ARG:HD3	2.48	0.49
52:1:53:TRP:HA	52:1:56:ILE:HB	1.94	0.49
46:6:85:LEU:HD12	46:6:158:LEU:HD23	1.93	0.49
48:8:122:CYS:HA	77:8:402:HEC:HAB	1.94	0.49
48:8:196:PRO:HG2	77:8:402:HEC:HAA1	1.94	0.49
48:8:300:LEU:HD23	48:8:303:LEU:HD12	1.94	0.49
52:Ac:56:ILE:HG22	52:Ac:59:LYS:HE3	1.93	0.49
3:C:298:ILE:HG22	14:N:11:LEU:HD22	1.95	0.49
7:G:131:CYS:SG	7:G:229:GLY:HA3	2.52	0.49
7:G:172:ILE:HG13	7:G:175:ARG:HH22	1.76	0.49
7:G:236:TYR:CE2	7:G:272:ARG:HD3	2.48	0.49
7:G:652:ASN:ND2	16:P:56:ARG:HD2	2.28	0.49
8:H:83:THR:HG22	9:I:102:PRO:O	2.13	0.49
8:H:159:GLN:HE21	8:H:212:ARG:NH1	2.11	0.49
9:I:102:PRO:HA	42:r:34:ARG:HB3	1.94	0.49
33:i:125:GLN:O	33:i:128:LEU:HG	2.13	0.49
38:n:17:VAL:HG13	38:n:18:PRO:HD3	1.94	0.49
39:o:25:ILE:HG23	45:u:262:VAL:N	2.26	0.49
41:q:418:LYS:HG2	41:q:419:TYR:O	2.12	0.49
47:w:62:ALA:O	47:w:65:SER:OG	2.18	0.49
49:y:35:ASP:O	49:y:38:ILE:HG22	2.13	0.49
45:5:362:ASN:OD1	45:5:461:PRO:HG2	2.12	0.49
46:6:184:ASN:OD1	46:6:252:LYS:HG2	2.12	0.49
46:6:359:LYS:HE2	46:6:432:VAL:HG22	1.94	0.49
47:7:155:TYR:HD2	47:7:156:ILE:HG23	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:8:139:VAL:HG21	48:8:277:TRP:HZ2	1.77	0.49
48:8:213:PHE:O	48:8:217:THR:OG1	2.17	0.49
60:Ak:168:ILE:HG21	60:Ak:189:MET:HG3	1.94	0.49
61:Al:90:ILE:HD12	61:Al:90:ILE:H	1.77	0.49
65:Ap:37:LYS:HD3	65:Ap:37:LYS:N	2.27	0.49
7:G:308:ARG:HH12	11:R:144:TYR:H	1.60	0.49
7:G:358:LEU:HB3	7:G:364:ASP:CB	2.42	0.49
7:G:377:ALA:HB3	16:P:45:LYS:NZ	2.27	0.49
7:G:479:SER:OG	7:G:687:PRO:CG	2.59	0.49
7:G:546:PHE:CD2	7:G:549:GLY:HA3	2.48	0.49
9:I:150:VAL:HG23	9:I:179:VAL:HA	1.95	0.49
9:I:190:ALA:O	9:I:193:LEU:HB3	2.12	0.49
13:M:71:SER:C	13:M:73:GLN:N	2.69	0.49
18:S:27:HIS:ND1	18:S:36:LYS:HD3	2.28	0.49
19:T:78:LEU:HA	19:T:80:TRP:NE1	2.28	0.49
20:U:113:ASN:O	20:U:132:ARG:NH2	2.41	0.49
20:U:150:GLU:CG	20:U:300:VAL:HG12	2.43	0.49
20:U:332:LYS:HA	20:U:335:GLU:CD	2.38	0.49
26:b:83:HIS:O	26:b:86:LEU:HB3	2.13	0.49
28:d:109:ARG:HH12	28:d:131:GLN:HE22	1.61	0.49
30:f:47:THR:HB	31:g:61:HIS:CE1	2.47	0.49
32:h:60:PHE:O	32:h:64:VAL:HG23	2.13	0.49
36:l:338:MET:SD	36:l:457:LEU:HB3	2.53	0.49
39:o:73:SER:OG	39:o:74:ALA:N	2.45	0.49
43:s:77:HIS:HD2	43:s:114:LYS:HG2	1.77	0.49
44:t:96:VAL:O	44:t:100:LYS:HG2	2.13	0.49
47:w:160:LEU:O	47:w:164:ILE:HD12	2.12	0.49
52:1:31:PHE:CD1	54:3:48:ILE:HD11	2.48	0.49
53:4:127:TYR:HE1	52:Ac:33:GLU:HG3	1.76	0.49
45:5:384:THR:HG22	45:5:386:SER:H	1.77	0.49
48:8:314:VAL:HG13	50:Aa:18:SER:HB3	1.95	0.49
62:Am:119:THR:O	66:Aq:52:HIS:CE1	2.63	0.49
2:B:118:ASP:O	2:B:162:PHE:HE2	1.96	0.49
3:C:43:TRP:O	3:C:46:GLN:HG2	2.13	0.49
7:G:213:MET:HG2	7:G:215:MET:HG3	1.95	0.49
7:G:610:VAL:O	7:G:611:THR:OG1	2.30	0.49
8:H:37:THR:OG1	8:H:38:TYR:N	2.45	0.49
12:L:93:HIS:O	12:L:96:PRO:HD2	2.13	0.49
13:M:96:THR:OG1	13:M:98:ALA:O	2.26	0.49
25:a:178:LEU:O	32:h:23:ALA:HA	2.13	0.49
25:a:185:THR:OG1	25:a:186:THR:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:l:178:GLY:HA2	36:l:218:LEU:HD23	1.95	0.49
36:l:449:LEU:HD12	36:l:450:LEU:N	2.27	0.49
42:r:28:LEU:O	42:r:32:GLN:HG2	2.13	0.49
47:w:241:ILE:CG1	48:x:293:MET:HE1	2.38	0.49
48:x:299:LEU:HD23	48:x:299:LEU:O	2.12	0.49
45:5:335:ARG:NH1	45:5:367:ASP:OD2	2.45	0.49
45:5:467:ASP:CG	47:7:223:TYR:HH	2.11	0.49
46:6:66:LYS:HB3	46:6:217:ARG:HH11	1.78	0.49
46:6:359:LYS:HE2	46:6:432:VAL:HG13	1.93	0.49
61:Al:13:THR:HG22	61:Al:13:THR:O	2.12	0.49
66:Aq:42:ARG:NH1	66:Aq:74:ARG:HH21	2.10	0.49
4:D:88:ILE:HG22	4:D:89:HIS:O	2.12	0.48
5:E:183:ALA:HB1	5:E:184:PRO:HD2	1.93	0.48
5:E:197:THR:O	5:E:201:ILE:HD12	2.13	0.48
7:G:173:MET:C	7:G:175:ARG:H	2.18	0.48
14:N:27:LEU:O	14:N:31:ILE:HG13	2.13	0.48
20:U:196:THR:HG22	20:U:200:TYR:HE2	1.77	0.48
25:a:78:THR:CG2	29:e:100:VAL:HG21	2.41	0.48
28:d:142:ARG:HD2	29:e:138:GLU:O	2.13	0.48
32:h:44:ALA:HA	32:h:47:ILE:HD11	1.95	0.48
33:i:59:TYR:OH	33:i:134:GLN:NE2	2.46	0.48
75:u:502:PEE:H17	71:2:301:PLX:H6	1.94	0.48
47:w:83:HIS:NE2	76:w:401:HEM:NA	2.61	0.48
47:w:367:PRO:O	47:w:371:ILE:HG12	2.13	0.48
50:z:37:ASN:O	50:z:40:ARG:HG2	2.13	0.48
53:2:204:ARG:NH2	53:2:257:ASN:HB3	2.28	0.48
53:4:93:ARG:HA	50:Aa:25:ARG:HB3	1.94	0.48
53:4:156:LEU:HB3	53:4:269:ASP:O	2.13	0.48
45:5:273:SER:H	45:5:455:ALA:HA	1.77	0.48
46:6:186:LEU:HD11	46:6:330:TYR:CG	2.48	0.48
46:6:293:LEU:HD22	46:6:361:ILE:HD11	1.93	0.48
46:6:320:PRO:HA	55:Ae:35:PRO:HB3	1.94	0.48
76:7:403:HEM:CHA	76:7:403:HEM:HAA1	2.42	0.48
76:7:404:HEM:C1A	76:7:404:HEM:CHB	2.96	0.48
48:8:209:GLU:HB3	48:8:276:ARG:CD	2.43	0.48
49:9:36:ASP:OD1	49:9:59:ARG:HG3	2.13	0.48
2:B:147:ARG:C	2:B:150:GLY:H	2.22	0.48
3:C:211:PHE:CE2	9:I:98:HIS:CE1	2.93	0.48
7:G:234:LYS:N	7:G:235:PRO:HD2	2.28	0.48
12:L:58:VAL:O	12:L:83:PRO:CD	2.61	0.48
12:L:265:PHE:HZ	12:L:338:LEU:CD1	2.25	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:e:100:VAL:HG23	29:e:101:LEU:N	2.26	0.48
33:i:111:PHE:HA	36:l:591:PHE:CE1	2.48	0.48
34:j:67:LEU:HD21	35:k:68:ALA:HB3	1.94	0.48
37:m:34:ILE:HG12	37:m:61:LEU:CD1	2.43	0.48
41:q:71:TRP:O	41:q:74:PRO:HD2	2.12	0.48
42:r:280:PHE:O	42:r:281:ARG:HB3	2.12	0.48
45:u:141:PRO:HA	45:u:245:LEU:HD21	1.94	0.48
46:v:195:TYR:O	46:v:199:LYS:NZ	2.24	0.48
48:x:186:ALA:O	48:x:190:ASN:ND2	2.44	0.48
52:1:33:GLU:O	52:1:37:ASP:HB2	2.12	0.48
53:4:89:SER:OG	53:4:92:ARG:NH1	2.46	0.48
45:5:110:GLU:OE1	46:6:299:VAL:HG21	2.13	0.48
46:6:51:SER:OG	46:6:225:VAL:O	2.31	0.48
46:6:85:LEU:HD13	46:6:157:GLN:HG3	1.94	0.48
46:6:212:HIS:O	46:6:217:ARG:HD2	2.14	0.48
47:7:69:ILE:O	47:7:76:GLY:HA3	2.12	0.48
47:7:186:PRO:HA	47:7:189:ILE:HD12	1.96	0.48
47:7:332:LEU:CD1	75:7:402:PEE:H37	2.43	0.48
48:8:157:ASP:OD2	48:8:168:ARG:N	2.46	0.48
50:Aa:29:HIS:HB2	50:Aa:33:LYS:HE2	1.95	0.48
50:Aa:29:HIS:O	50:Aa:33:LYS:HB3	2.12	0.48
57:Ah:8:LYS:NZ	57:Ah:8:LYS:HB3	2.28	0.48
60:Ak:115:SER:O	60:Ak:121:GLY:HA2	2.14	0.48
61:Al:16:ILE:HD12	61:Al:17:MET:H	1.78	0.48
62:Am:65:SER:HB3	62:Am:71:HIS:CE1	2.48	0.48
3:C:182:ASN:ND2	3:C:403:PRO:HB2	2.14	0.48
12:L:127:ILE:HG22	12:L:129:LEU:HD13	1.96	0.48
14:N:38:ILE:HG22	14:N:39:PRO:O	2.13	0.48
19:T:25:ILE:HG13	42:r:299:ALA:HB1	1.94	0.48
20:U:108:VAL:HG21	20:U:115:SER:HB3	1.95	0.48
20:U:235:TYR:CZ	20:U:239:ILE:HD11	2.46	0.48
32:h:95:PRO:O	32:h:96:PRO:C	2.54	0.48
36:l:109:HIS:HE1	36:l:348:HIS:HE1	1.60	0.48
39:o:125:PHE:O	39:o:127:ILE:N	2.41	0.48
40:p:26:HIS:O	40:p:29:SER:OG	2.19	0.48
49:y:47:ALA:HB2	49:y:98:VAL:HG21	1.95	0.48
45:5:442:ARG:HH22	54:Ad:16:ASN:CG	2.21	0.48
46:6:182:TYR:CD1	46:6:251:ALA:HB1	2.49	0.48
60:Ak:377:PHE:HA	60:Ak:380:VAL:HG22	1.93	0.48
2:B:105:PRO:O	2:B:107:ASP:N	2.38	0.48
3:C:444:LEU:O	3:C:447:VAL:HG12	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:71:LYS:HB3	4:D:72:TYR:CD2	2.48	0.48
7:G:408:ARG:HB3	7:G:415:ASN:ND2	2.29	0.48
17:Q:40:TYR:CE1	17:Q:60:ARG:HD3	2.49	0.48
27:c:89:TRP:CZ2	40:p:86:PRO:HD3	2.48	0.48
28:d:60:ARG:O	28:d:62:TYR:HD2	1.96	0.48
33:i:120:GLN:HE21	33:i:177:LYS:HE2	1.79	0.48
45:u:126:ARG:HD2	45:u:348:TYR:OH	2.13	0.48
53:4:154:ILE:HG12	53:4:272:ILE:HA	1.96	0.48
45:5:136:LEU:HD21	46:6:380:ALA:HA	1.95	0.48
45:5:473:SER:HB3	75:5:502:PEE:H10	1.95	0.48
74:5:501:CDL:H732	47:7:4:ILE:HG12	1.96	0.48
46:6:126:LEU:HD12	46:6:129:ASP:OD2	2.13	0.48
46:6:181:ALA:HB3	46:6:335:LEU:HD11	1.94	0.48
46:6:230:LEU:HA	46:6:233:VAL:HG22	1.95	0.48
47:7:61:THR:HG22	47:7:65:SER:HB3	1.95	0.48
47:7:138:MET:SD	47:7:255:ASN:ND2	2.85	0.48
47:7:275:LEU:HA	47:7:278:TYR:HB3	1.95	0.48
48:8:133:TYR:O	48:8:136:LEU:HG	2.13	0.48
1:A:39:VAL:O	1:A:42:LYS:HE2	2.14	0.48
2:B:53:LEU:O	2:B:57:GLN:HG3	2.13	0.48
2:B:137:LYS:HZ1	2:B:256:ARG:HH22	1.61	0.48
2:B:324:THR:OG1	2:B:437:GLY:HA3	2.14	0.48
3:C:346:GLN:O	3:C:350:LYS:HG2	2.13	0.48
7:G:320:GLU:HA	17:Q:123:TYR:CE1	2.47	0.48
7:G:336:ASN:N	7:G:363:SER:HB2	2.28	0.48
7:G:454:ASP:O	7:G:459:ASN:N	2.41	0.48
9:I:79:ARG:O	9:I:201:GLN:NE2	2.46	0.48
9:I:106:MET:HE1	9:I:113:PHE:CE1	2.48	0.48
9:I:136:ALA:HB2	34:j:41:PHE:CE1	2.48	0.48
17:Q:79:VAL:O	17:Q:82:LEU:HB3	2.12	0.48
19:T:50:PRO:HD3	22:W:62:ILE:CD1	2.43	0.48
21:V:55:ARG:HG2	21:V:59:TYR:HE2	1.78	0.48
22:W:126:GLY:C	22:W:127:LEU:HD12	2.38	0.48
25:a:133:TYR:O	25:a:137:MET:HG2	2.13	0.48
33:i:244:MET:O	33:i:248:LEU:HD13	2.12	0.48
34:j:81:THR:HG21	37:m:148:SER:HB3	1.95	0.48
36:l:223:LYS:HB2	36:l:256:GLY:HA3	1.94	0.48
46:v:51:SER:HB3	46:v:227:HIS:HB2	1.95	0.48
47:w:241:ILE:CG1	48:x:293:MET:CE	2.92	0.48
47:w:286:ASN:ND2	47:w:288:LEU:HB3	2.28	0.48
47:w:330:ALA:HA	47:w:333:ILE:HD12	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:y:94:TYR:O	49:y:98:VAL:HG23	2.13	0.48
53:4:93:ARG:HD3	53:4:95:GLU:OE2	2.13	0.48
53:4:103:SER:OG	45:5:269:ARG:HB2	2.13	0.48
45:5:74:TRP:CZ3	45:5:232:ALA:HB3	2.48	0.48
45:5:134:LYS:NZ	45:5:407:THR:OG1	2.47	0.48
45:5:192:PHE:O	45:5:198:ALA:HB2	2.12	0.48
45:5:425:PRO:HG2	45:5:428:GLU:HB2	1.95	0.48
47:7:152:ALA:HB2	47:7:287:LYS:HE3	1.94	0.48
61:Al:186:SER:HB3	61:Al:213:LEU:CD2	2.42	0.48
2:B:183:GLY:O	2:B:192:ASP:HA	2.12	0.48
3:C:230:GLY:O	3:C:358:VAL:HG23	2.12	0.48
5:E:110:MET:O	5:E:114:GLU:HG3	2.14	0.48
12:L:238:GLN:CD	12:L:266:VAL:CG1	2.87	0.48
12:L:281:PHE:CD2	12:L:288:PHE:HD1	2.32	0.48
20:U:85:LEU:CB	20:U:158:GLY:C	2.87	0.48
21:V:55:ARG:HG2	21:V:59:TYR:CE2	2.49	0.48
29:e:97:ILE:HG23	29:e:98:VAL:HG13	1.94	0.48
36:l:96:VAL:O	36:l:100:ILE:HG12	2.14	0.48
36:l:489:THR:HA	36:l:492:ILE:HG22	1.95	0.48
41:q:221:VAL:HG13	41:q:340:ARG:HH11	1.77	0.48
42:r:172:ILE:O	42:r:173:TRP:HB2	2.14	0.48
45:u:212:SER:O	45:u:216:LEU:HG	2.13	0.48
46:v:156:SER:HA	46:v:159:ARG:CZ	2.43	0.48
47:w:89:MET:HE2	47:w:235:MET:HB2	1.95	0.48
51:0:31:THR:HA	51:0:34:ARG:HD2	1.95	0.48
53:2:213:LEU:HD12	53:2:234:TYR:HE2	1.79	0.48
47:7:137:GLN:HB3	47:7:255:ASN:HB3	1.96	0.48
47:7:275:LEU:HB3	47:7:339:GLY:HA3	1.95	0.48
48:8:310:HIS:CE1	50:Aa:21:PRO:HB2	2.48	0.48
50:Aa:51:PRO:O	50:Aa:55:VAL:HG23	2.13	0.48
60:Ak:11:ASN:ND2	60:Ak:13:LYS:HB2	2.28	0.48
60:Ak:266:GLU:HB2	60:Ak:267:PRO:HD2	1.94	0.48
61:Al:59:GLN:O	61:Al:62:GLU:HB2	2.13	0.48
4:D:218:ARG:HG3	17:Q:101:THR:HG22	1.94	0.48
8:H:45:GLU:OE1	8:H:45:GLU:N	2.47	0.48
9:I:159:GLY:HA2	9:I:172:GLY:CA	2.44	0.48
22:W:60:LEU:HD11	43:s:98:ARG:HH22	1.79	0.48
32:h:27:HIS:NE2	37:m:141:MET:HE2	2.28	0.48
36:l:124:PHE:HE1	36:l:147:VAL:HG13	1.78	0.48
43:s:169:PHE:CE1	74:s:201:CDL:H531	2.48	0.48
45:u:467:ASP:OD1	45:u:468:TYR:N	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:u:502:PEE:H26	75:u:502:PEE:C33	2.44	0.48
48:x:122:CYS:HA	77:x:401:HEC:CAB	2.35	0.48
51:0:40:ILE:O	51:0:44:ILE:HD12	2.13	0.48
52:1:44:TYR:HA	52:1:47:ILE:HD12	1.96	0.48
48:8:128:MET:HE3	48:8:199:SER:HA	1.94	0.48
48:8:292:LYS:NZ	52:Ac:37:ASP:HA	2.29	0.48
59:Aj:15:VAL:HG21	60:Ak:476:PHE:CD1	2.48	0.48
61:Al:83:ILE:O	61:Al:87:MET:HG3	2.14	0.48
67:Ar:24:ASN:ND2	67:Ar:26:THR:H	2.11	0.48
1:A:44:LYS:HD3	61:Al:22:HIS:CE1	2.49	0.48
2:B:225:LEU:HD21	7:G:93:ALA:HB2	1.96	0.48
2:B:295:PRO:O	2:B:298:GLU:HB3	2.14	0.48
3:C:126:TYR:CE1	4:D:204:LEU:HD23	2.49	0.48
3:C:252:SER:HA	3:C:255:ILE:HG22	1.95	0.48
7:G:173:MET:C	7:G:175:ARG:N	2.72	0.48
7:G:421:SER:HA	7:G:424:HIS:HB2	1.95	0.48
7:G:543:LYS:HG3	7:G:565:PHE:CD2	2.49	0.48
12:L:174:ILE:HG13	12:L:182:ARG:HG2	1.96	0.48
12:L:204:SER:OG	12:L:204:SER:O	2.31	0.48
33:i:106:LEU:HD12	33:i:138:PRO:HB2	1.96	0.48
33:i:174:GLN:HE21	33:i:177:LYS:HE2	1.79	0.48
33:i:228:LEU:O	33:i:231:SER:OG	2.12	0.48
35:k:27:MET:HE2	37:m:71:THR:OG1	2.14	0.48
37:m:8:ILE:O	37:m:12:ILE:HD12	2.14	0.48
46:v:253:TYR:CE2	46:v:435:ARG:HB3	2.49	0.48
47:w:9:PRO:HA	47:w:12:LYS:HD2	1.96	0.48
53:4:80:HIS:ND1	45:5:185:ASP:OD2	2.47	0.48
45:5:93:VAL:HG21	45:5:219:TYR:HD2	1.79	0.48
47:7:43:LEU:HD13	75:7:401:PEE:C19	2.44	0.48
48:8:126:HIS:NE2	77:8:402:HEC:NB	2.61	0.48
2:B:317:VAL:HG22	2:B:356:VAL:HA	1.95	0.48
3:C:95:LEU:HD22	3:C:458:PHE:HZ	1.79	0.48
3:C:139:LEU:O	3:C:141:TYR:N	2.46	0.48
3:C:426:ALA:HB1	3:C:460:GLU:HG2	1.96	0.48
7:G:348:ALA:HA	7:G:351:LEU:HG	1.96	0.48
12:L:261:LYS:HE2	12:L:333:PRO:HB3	1.95	0.48
12:L:318:LYS:O	12:L:322:VAL:HG23	2.13	0.48
14:N:58:MET:SD	14:N:71:GLN:HG3	2.54	0.48
17:Q:82:LEU:CG	73:Q:201:ZMP:C11	2.89	0.48
20:U:150:GLU:HA	20:U:300:VAL:HG11	1.91	0.48
21:V:98:GLY:O	21:V:102:GLY:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:99:SER:HB3	15:X:102:SER:HB3	1.95	0.48
15:X:141:PRO:HA	15:X:144:ILE:HD12	1.95	0.48
25:a:115:HIS:CG	25:a:116:PRO:HD2	2.49	0.48
33:i:174:GLN:HA	33:i:226:THR:HA	1.96	0.48
33:i:175:LEU:HD21	33:i:230:LEU:HD22	1.95	0.48
35:k:7:ASN:HD22	37:m:10:SER:CB	2.27	0.48
45:u:347:CYS:HA	45:u:352:GLY:HA2	1.95	0.48
46:v:91:THR:HA	46:v:144:PRO:HA	1.95	0.48
48:x:148:ALA:HA	48:x:151:GLU:OE1	2.13	0.48
48:x:250:TYR:CZ	48:x:253:VAL:HA	2.49	0.48
53:4:131:ASN:ND2	75:7:401:PEE:H7	2.29	0.48
46:6:74:SER:HA	46:6:77:LEU:HG	1.96	0.48
46:6:84:ARG:HD3	46:6:114:SER:HB3	1.95	0.48
46:6:382:TYR:O	46:6:385:SER:OG	2.24	0.48
47:7:158:THR:O	47:7:161:VAL:HB	2.14	0.48
74:8:401:CDL:HB22	49:9:73:GLN:HB2	1.96	0.48
57:Ah:45:TYR:HD2	62:Am:42:LEU:HD13	1.77	0.48
63:An:68:PHE:HA	63:An:71:MET:HG2	1.96	0.48
2:B:331:VAL:O	2:B:335:VAL:HG22	2.14	0.48
3:C:242:ASP:OD1	3:C:243:ASP:N	2.47	0.48
3:C:288:PHE:CE1	3:C:431:HIS:HA	2.48	0.48
3:C:329:ARG:O	3:C:333:ARG:HG2	2.14	0.48
4:D:94:ILE:HB	4:D:95:PRO:HD3	1.93	0.48
7:G:153:PHE:C	7:G:154:LEU:HD12	2.39	0.48
20:U:197:ALA:HA	20:U:200:TYR:CD2	2.49	0.48
27:c:65:TYR:CG	27:c:72:TYR:HE1	2.32	0.48
32:h:95:PRO:C	32:h:97:HIS:H	2.21	0.48
33:i:124:LEU:HB2	33:i:220:ILE:HD11	1.95	0.48
33:i:172:GLN:NE2	36:l:578:SER:OG	2.46	0.48
43:s:24:VAL:HG22	43:s:86:TRP:CE3	2.49	0.48
45:u:96:LEU:HB3	45:u:164:GLU:CD	2.38	0.48
46:v:106:VAL:HG21	46:v:133:LEU:HD11	1.96	0.48
46:v:121:TYR:HB3	46:v:137:LEU:HD11	1.94	0.48
47:w:97:HIS:NE2	76:w:402:HEM:NA	2.62	0.48
47:w:147:THR:HG21	47:w:165:TRP:HE1	1.78	0.48
47:w:183:PHE:CG	47:7:183:PHE:CE2	3.02	0.48
51:0:32:THR:O	51:0:36:GLN:HG3	2.14	0.48
45:5:460:GLY:HA3	45:5:462:ILE:HG23	1.96	0.48
46:6:148:ARG:HA	46:6:202:PRO:HG2	1.95	0.48
55:Ae:26:LEU:HA	55:Ae:27:ARG:C	2.38	0.48
57:Ah:16:ASN:ND2	57:Ah:16:ASN:H	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Aq:42:ARG:HD2	66:Aq:42:ARG:O	2.13	0.48
2:B:357:MET:HG2	5:E:142:LEU:HD21	1.96	0.47
7:G:223:ILE:HD13	7:G:233:SER:HB3	1.95	0.47
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.21	0.47
7:G:308:ARG:NE	7:G:312:GLY:O	2.47	0.47
7:G:574:ASP:O	7:G:576:GLY:N	2.46	0.47
7:G:621:LYS:HG2	17:Q:122:PHE:HE1	1.77	0.47
8:H:92:PRO:HB3	13:M:34:ARG:HH22	1.79	0.47
8:H:117:LYS:N	68:H:301:SF4:S4	2.83	0.47
17:Q:64:ARG:O	17:Q:68:MET:HG2	2.13	0.47
18:S:4:GLU:O	18:S:7:PRO:HD2	2.14	0.47
20:U:95:TYR:O	20:U:98:SER:OG	2.25	0.47
25:a:165:ASP:HA	43:s:151:ASN:HD21	1.79	0.47
27:c:122:THR:HG21	27:c:129:MET:HE1	1.95	0.47
32:h:20:ILE:O	35:k:53:PHE:HE1	1.97	0.47
36:l:270:ASN:O	36:l:274:GLN:NE2	2.43	0.47
45:u:296:TRP:HB2	45:u:347:CYS:O	2.14	0.47
47:w:33:PHE:HA	47:w:36:LEU:HD12	1.96	0.47
47:w:158:THR:O	47:w:162:GLU:HG2	2.14	0.47
47:w:379:TRP:NE1	49:y:34:ARG:HH11	2.12	0.47
51:0:42:LYS:HD2	51:0:45:LYS:HD2	1.96	0.47
53:2:90:ASP:OD1	53:2:90:ASP:N	2.46	0.47
75:2:302:PEE:C11	75:2:302:PEE:C30	2.92	0.47
45:5:95:HIS:HB3	45:5:164:GLU:OE2	2.14	0.47
45:5:196:PRO:HA	45:5:199:GLN:HE22	1.78	0.47
47:7:231:GLY:O	47:7:235:MET:HG2	2.14	0.47
47:7:344:GLU:O	47:7:348:ILE:HG13	2.14	0.47
54:Ad:41:ILE:HA	54:Ad:44:TRP:CD1	2.36	0.47
60:Ak:197:LEU:O	62:Am:92:LEU:HD22	2.13	0.47
62:Am:80:ARG:O	62:Am:84:ILE:HG12	2.14	0.47
3:C:113:ILE:HD11	4:D:187:ILE:HD12	1.96	0.47
4:D:147:THR:HG22	4:D:148:ASP:O	2.14	0.47
5:E:183:ALA:HB1	5:E:184:PRO:CD	2.45	0.47
7:G:302:LEU:HD22	7:G:570:GLY:O	2.14	0.47
9:I:129:LEU:HD23	9:I:130:THR:N	2.29	0.47
12:L:125:VAL:HG12	12:L:163:LYS:HB2	1.95	0.47
12:L:241:TYR:CE2	12:L:243:VAL:CG2	2.97	0.47
16:P:44:LEU:O	16:P:48:ASN:ND2	2.46	0.47
32:h:47:ILE:HA	32:h:51:ARG:HD3	1.95	0.47
37:m:7:PHE:O	37:m:10:SER:OG	2.19	0.47
40:p:62:GLN:O	40:p:66:GLN:HG2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:u:55:ASN:ND2	45:u:253:LEU:HB3	2.28	0.47
45:u:61:SER:OG	45:u:233:ALA:O	2.32	0.47
45:u:92:PHE:O	45:u:96:LEU:HG	2.14	0.47
75:u:502:PEE:H16	75:u:502:PEE:C30	2.44	0.47
46:v:82:LEU:HD21	46:v:151:VAL:HG13	1.95	0.47
46:v:116:ARG:NH1	46:v:186:LEU:O	2.47	0.47
46:v:179:ALA:HA	46:v:187:ALA:HB1	1.96	0.47
47:w:322:GLN:O	47:w:325:PHE:HB3	2.14	0.47
48:x:267:VAL:O	48:x:271:VAL:HG23	2.13	0.47
49:y:59:ARG:HA	49:y:62:ARG:NH2	2.30	0.47
46:6:65:ILE:HG12	46:6:218:MET:HG2	1.95	0.47
46:6:259:ARG:HG3	46:6:440:ALA:HB3	1.95	0.47
46:6:359:LYS:O	46:6:363:GLN:HG3	2.13	0.47
76:7:403:HEM:CHB	76:7:403:HEM:C1A	2.96	0.47
48:8:124:SER:HB2	77:8:402:HEC:HMC3	1.96	0.47
52:Ac:53:TRP:HA	52:Ac:56:ILE:HB	1.96	0.47
54:Ad:4:ARG:HH21	54:Ad:5:PHE:HZ	1.61	0.47
54:Ad:45:VAL:HG23	54:Ad:48:ILE:HG12	1.94	0.47
60:Ak:87:ILE:O	60:Ak:173:PRO:HD3	2.13	0.47
3:C:270:ASN:C	42:r:284:GLN:HE22	2.21	0.47
7:G:49:VAL:HG23	7:G:94:MET:O	2.15	0.47
7:G:170:LYS:HB3	7:G:232:THR:O	2.14	0.47
13:M:93:LYS:HA	14:N:50:GLN:NE2	2.29	0.47
15:O:104:PHE:HB3	15:O:138:LEU:HD21	1.96	0.47
18:S:51:ASP:OD2	18:S:60:TYR:HB2	2.14	0.47
19:T:4:ARG:O	19:T:7:SER:OG	2.18	0.47
25:a:112:TYR:HD1	28:d:64:TYR:O	1.96	0.47
28:d:163:MET:SD	29:e:147:ILE:HD11	2.55	0.47
34:j:73:LEU:O	34:j:76:PRO:HD2	2.13	0.47
43:s:47:ARG:HH12	43:s:53:PRO:CD	2.24	0.47
45:u:454:PRO:O	45:u:468:TYR:OH	2.30	0.47
47:w:59:THR:HG23	47:w:135:TRP:CZ2	2.49	0.47
47:w:146:ILE:HA	47:w:149:LEU:HD13	1.95	0.47
53:4:196:ARG:NH1	53:4:250:ARG:O	2.46	0.47
53:4:220:LEU:HD12	53:4:239:HIS:HE1	1.79	0.47
45:5:53:LEU:HD22	45:5:248:LYS:NZ	2.28	0.47
45:5:316:SER:O	46:6:157:GLN:NE2	2.45	0.47
45:5:424:ILE:HB	45:5:429:TRP:CZ2	2.49	0.47
46:6:35:PRO:C	46:6:37:ASP:H	2.22	0.47
46:6:216:ALA:HB3	46:6:244:LEU:HA	1.97	0.47
46:6:234:ALA:O	46:6:238:LEU:HD13	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:An:41:LYS:HD3	63:An:62:LEU:HD23	1.97	0.47
65:Ap:31:TYR:HE1	65:Ap:98:HIS:HE1	1.62	0.47
2:B:250:VAL:O	2:B:253:THR:OG1	2.23	0.47
7:G:133:GLN:HB3	68:G:801:SF4:S2	2.54	0.47
7:G:308:ARG:NH1	11:R:144:TYR:H	2.11	0.47
7:G:557:ARG:O	7:G:560:LEU:HB2	2.14	0.47
8:H:76:TYR:HA	8:H:79:ARG:HH21	1.79	0.47
9:I:202:ARG:NH1	11:K:74:PHE:HA	2.29	0.47
10:J:77:VAL:HG22	10:J:78:ARG:H	1.80	0.47
18:S:66:LEU:O	18:S:69:ILE:HG13	2.14	0.47
29:e:65:ASN:ND2	41:q:427:LYS:HE2	2.30	0.47
36:l:158:TRP:CZ2	36:l:240:PRO:HB3	2.50	0.47
36:l:233:LEU:HB3	36:l:234:PRO:HD3	1.96	0.47
41:q:339:SER:OG	41:q:344:LEU:HB2	2.14	0.47
45:u:55:ASN:ND2	45:u:253:LEU:O	2.42	0.47
45:u:74:TRP:CE3	45:u:414:GLY:HA3	2.49	0.47
47:w:31:TRP:CH2	47:w:208:PRO:HA	2.50	0.47
47:w:240:LEU:HD21	75:2:302:PEE:H18	1.97	0.47
54:3:7:GLY:HA3	49:9:110:LYS:HB2	1.94	0.47
53:4:254:ALA:HB2	70:4:302:FES:S1	2.55	0.47
53:4:268:ASP:OD1	53:4:269:ASP:N	2.48	0.47
45:5:165:ARG:NH1	45:5:211:LEU:HB3	2.28	0.47
47:7:48:GLY:HA2	47:7:51:LEU:HD12	1.95	0.47
47:7:315:MET:HE2	47:7:318:ARG:HH22	1.78	0.47
51:Ab:48:GLU:O	51:Ab:52:LEU:HG	2.14	0.47
62:Am:164:PHE:O	62:Am:168:THR:HG23	2.14	0.47
4:D:114:LEU:HG	4:D:170:ILE:HD11	1.96	0.47
4:D:181:HIS:HD2	4:D:184:LEU:N	2.12	0.47
8:H:37:THR:N	13:M:107:SER:H	2.12	0.47
9:I:131:ASN:N	9:I:168:SER:O	2.47	0.47
12:L:59:PHE:HE1	12:L:126:VAL:HG12	1.78	0.47
12:L:110:GLY:HA2	12:L:116:ILE:HD11	1.97	0.47
17:Q:55:SER:OG	17:Q:58:GLN:HB2	2.15	0.47
21:V:124:LEU:HD21	75:q:501:PEE:H54	1.96	0.47
28:d:115:GLN:HG2	36:l:62:ILE:HG22	1.96	0.47
33:i:124:LEU:HD21	33:i:176:ARG:HG2	1.96	0.47
36:l:109:HIS:HE1	36:l:348:HIS:CE1	2.32	0.47
36:l:227:PHE:O	36:l:230:HIS:ND1	2.46	0.47
36:l:312:LEU:O	36:l:315:VAL:HG22	2.14	0.47
41:q:282:LEU:HD11	41:q:410:MET:HE3	1.97	0.47
41:q:325:MET:HA	41:q:440:HIS:ND1	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:x:197:ASP:OD1	48:x:198:LEU:N	2.47	0.47
48:x:250:TYR:O	48:x:253:VAL:HG23	2.14	0.47
53:2:162:GLY:O	53:2:177:ARG:NH2	2.47	0.47
53:4:127:TYR:CE1	52:Ac:33:GLU:HG3	2.49	0.47
45:5:314:TYR:HB3	45:5:341:PHE:CE2	2.48	0.47
45:5:389:VAL:HA	45:5:392:LYS:HD2	1.97	0.47
46:6:283:ALA:HA	46:6:286:PHE:HD2	1.80	0.47
47:7:260:ASN:HB2	47:7:263:ASN:HB2	1.97	0.47
47:7:271:GLU:HB2	47:7:273:TYR:CE2	2.49	0.47
55:Ae:29:LEU:O	55:Ae:31:GLN:N	2.45	0.47
65:Ap:49:VAL:HG21	65:Ap:74:LEU:HD12	1.95	0.47
3:C:102:SER:OG	3:C:103:GLY:N	2.46	0.47
3:C:156:GLU:OE2	3:C:163:PRO:HG3	2.14	0.47
4:D:55:HIS:CD2	4:D:78:VAL:HG11	2.49	0.47
7:G:39:GLN:NE2	7:G:56:VAL:HG21	2.29	0.47
7:G:472:PRO:HG3	7:G:500:ILE:HD13	1.96	0.47
7:G:624:ARG:HH21	7:G:637:ASP:HB2	1.80	0.47
12:L:112:ASP:O	12:L:115:SER:OG	2.31	0.47
16:P:31:GLN:HB3	16:P:34:ARG:NH2	2.24	0.47
34:j:74:PRO:HB2	37:m:147:TYR:HE2	1.79	0.47
36:l:176:ARG:HD2	41:q:400:MET:HG2	1.96	0.47
36:l:399:VAL:HG12	36:l:409:LEU:HD12	1.97	0.47
36:l:562:LEU:HG	36:l:563:PRO:HD3	1.97	0.47
37:m:61:LEU:HD21	42:r:111:LEU:HD21	1.96	0.47
37:m:81:GLU:HB2	37:m:85:SER:HB3	1.96	0.47
46:v:60:ARG:HH12	46:v:389:SER:C	2.23	0.47
48:x:98:SER:OG	52:1:51:LYS:NZ	2.35	0.47
48:x:288:ARG:NH2	52:1:44:TYR:CD2	2.83	0.47
49:y:44:VAL:O	49:y:48:ILE:HG12	2.14	0.47
53:4:179:ARG:HH12	53:4:201:ASP:CG	2.22	0.47
45:5:94:GLU:OE1	45:5:124:SER:OG	2.28	0.47
45:5:234:ALA:N	45:5:410:CYS:SG	2.87	0.47
46:6:49:ILE:HA	46:6:220:LEU:HB3	1.96	0.47
48:8:243:ILE:HD13	48:8:245:MET:HE2	1.97	0.47
49:9:94:TYR:O	49:9:98:VAL:HG23	2.15	0.47
5:E:70:TYR:HE2	5:E:78:ALA:HA	1.79	0.47
7:G:86:PRO:O	7:G:108:LYS:NZ	2.29	0.47
7:G:466:LEU:CD2	7:G:496:ILE:CG2	2.92	0.47
7:G:568:TYR:CE1	7:G:576:GLY:HA3	2.50	0.47
10:J:97:TRP:CZ2	10:J:131:LYS:HB2	2.50	0.47
15:O:121:ALA:O	15:O:124:ASP:HB3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:49:GLU:CB	20:U:294:HIS:CE1	2.98	0.47
20:U:128:GLY:O	20:U:132:ARG:HG3	2.14	0.47
21:V:90:TYR:CE2	21:V:126:LYS:HD3	2.49	0.47
24:Z:75:PHE:O	24:Z:79:VAL:HG23	2.14	0.47
28:d:99:ASP:OD1	29:e:137:MET:HE1	2.15	0.47
33:i:276:ILE:HG21	75:q:501:PEE:H7	1.97	0.47
75:i:501:PEE:H27	75:i:501:PEE:H33	1.62	0.47
35:k:10:MET:SD	37:m:103:MET:HG3	2.55	0.47
36:l:67:HIS:HA	36:l:77:SER:HB2	1.96	0.47
36:l:477:VAL:HG11	44:t:55:GLN:HG2	1.97	0.47
36:l:511:LEU:HA	40:p:36:LYS:HG3	1.97	0.47
39:o:53:ASP:HB3	40:p:133:TRP:CZ2	2.50	0.47
41:q:355:MET:HE2	41:q:358:TRP:CD1	2.49	0.47
42:r:135:ALA:CB	42:r:201:THR:HG22	2.44	0.47
42:r:196:ALA:O	42:r:199:ASP:HB2	2.15	0.47
47:w:218:ILE:HG23	47:w:219:PRO:HD2	1.97	0.47
51:0:34:ARG:HD3	51:0:78:ARG:HH22	1.79	0.47
51:0:68:THR:O	51:0:71:LEU:HB3	2.15	0.47
46:6:82:LEU:HB2	46:6:158:LEU:HD11	1.96	0.47
46:6:181:ALA:HA	46:6:254:ARG:O	2.14	0.47
47:7:211:ILE:HG21	49:9:63:ILE:HD13	1.97	0.47
74:8:401:CDL:H521	74:8:401:CDL:H552	1.68	0.47
49:9:75:ILE:HG21	50:Aa:40:ARG:NH2	2.30	0.47
50:Aa:81:ASP:HA	51:Ab:63:THR:HG22	1.97	0.47
2:B:75:TRP:O	2:B:79:GLU:N	2.43	0.47
3:C:53:TYR:CE1	75:i:501:PEE:O1P	2.67	0.47
7:G:335:GLY:HA2	7:G:362:ASP:HB2	1.96	0.47
8:H:59:GLN:HG3	8:H:64:THR:OG1	2.14	0.47
10:J:91:VAL:O	10:J:94:THR:OG1	2.30	0.47
12:L:147:LYS:O	12:L:150:HIS:HB3	2.15	0.47
15:O:90:TYR:HE2	15:O:92:LYS:HB2	1.79	0.47
19:T:69:HIS:HA	19:T:70:PRO:C	2.40	0.47
22:W:46:GLY:HA2	42:r:172:ILE:CD1	2.45	0.47
33:i:88:LYS:HG2	33:i:89:MET:O	2.14	0.47
41:q:50:LEU:HD23	41:q:51:ASN:N	2.30	0.47
45:u:196:PRO:O	45:u:199:GLN:NE2	2.48	0.47
47:w:206:ASN:HA	47:w:313:ARG:HH12	1.80	0.47
48:x:135:HIS:CB	48:x:277:TRP:HH2	2.28	0.47
49:y:42:ASP:HA	49:y:45:LYS:HD2	1.96	0.47
50:z:74:ASN:HB3	50:z:78:TYR:CE2	2.49	0.47
51:0:34:ARG:NH1	51:0:78:ARG:HH12	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:170:ARG:HG3	47:7:168:PHE:HB3	1.97	0.47
53:4:206:LYS:HB2	53:4:265:PHE:CE2	2.50	0.47
53:4:266:THR:OG1	53:4:270:LEU:O	2.33	0.47
45:5:88:GLY:H	45:5:207:ASN:ND2	2.13	0.47
45:5:438:ALA:O	45:5:442:ARG:HG3	2.14	0.47
47:7:316:MET:HE2	47:7:317:PHE:CE1	2.50	0.47
48:8:312:TRP:O	48:8:316:LYS:HG2	2.15	0.47
54:Ad:19:PRO:O	54:Ad:22:SER:OG	2.25	0.47
60:Ak:172:LYS:HB3	60:Ak:176:MET:HE2	1.96	0.47
61:Al:63:THR:O	61:Al:66:THR:HG22	2.15	0.47
62:Am:173:PHE:C	62:Am:173:PHE:CD1	2.92	0.47
2:B:398:ARG:O	2:B:402:GLY:N	2.47	0.47
7:G:342:ALA:HA	7:G:547:LEU:HB2	1.96	0.47
12:L:219:SER:HA	12:L:221:ARG:NH1	2.30	0.47
16:P:31:GLN:HA	16:P:34:ARG:HB2	1.97	0.47
17:Q:88:MET:O	17:Q:91:GLU:HB3	2.15	0.47
19:T:84:LEU:O	22:W:59:ARG:NH2	2.48	0.47
22:W:57:ARG:NE	42:r:316:PRO:HG3	2.29	0.47
24:Z:32:VAL:HG21	40:p:35:ASP:OD1	2.14	0.47
36:l:246:LEU:HD23	36:l:247:LEU:HD23	1.96	0.47
36:l:419:THR:HA	36:l:422:TYR:CE2	2.49	0.47
43:s:106:LYS:O	43:s:109:GLU:HG2	2.15	0.47
45:u:74:TRP:CZ2	45:u:411:GLU:HA	2.50	0.47
45:u:470:ARG:HH22	74:u:501:CDL:HA32	1.80	0.47
46:v:138:LEU:HA	46:v:141:THR:HG22	1.97	0.47
47:w:56:THR:HG22	47:w:58:ASP:H	1.80	0.47
45:5:82:GLU:HG2	45:5:90:GLY:HA3	1.97	0.47
45:5:164:GLU:O	45:5:168:ILE:HG12	2.14	0.47
48:8:118:TYR:HA	48:8:122:CYS:HB2	1.97	0.47
48:8:278:ALA:O	48:8:281:PRO:HD3	2.14	0.47
48:8:308:LYS:HE3	74:8:401:CDL:OA6	2.13	0.47
60:Ak:507:GLU:O	60:Ak:508:PRO:O	2.32	0.47
63:An:33:LEU:HD13	63:An:41:LYS:HG3	1.97	0.47
3:C:266:ARG:HG2	3:C:270:ASN:HD21	1.80	0.47
14:N:9:THR:O	14:N:14:LEU:HD23	2.14	0.47
33:i:181:TYR:O	33:i:184:ILE:HG22	2.14	0.47
33:i:189:TRP:CZ2	33:i:282:MET:HG2	2.50	0.47
36:l:281:GLY:O	36:l:285:THR:HG23	2.14	0.47
43:s:85:TYR:CE1	43:s:104:GLN:HB2	2.50	0.47
46:v:65:ILE:HG21	46:v:213:PHE:HD1	1.78	0.47
46:v:174:LEU:HD22	55:Af:11:PHE:CE1	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:w:24:PRO:HD3	47:w:217:LYS:NZ	2.30	0.47
47:w:72:ASP:O	53:2:144:ALA:N	2.44	0.47
48:x:90:LEU:HD13	51:0:72:PHE:HB3	1.96	0.47
51:0:40:ILE:HD12	51:0:81:CYS:SG	2.54	0.47
52:1:11:TYR:HB2	53:2:112:GLY:HA3	1.97	0.47
53:4:154:ILE:HG22	53:4:270:LEU:HD22	1.97	0.47
53:4:233:GLY:HA3	53:4:244:ASP:HA	1.96	0.47
45:5:104:ARG:HH21	45:5:146:LEU:HA	1.80	0.47
47:7:5:ARG:HA	47:7:11:MET:SD	2.55	0.47
47:7:207:ASN:ND2	47:7:209:THR:HB	2.30	0.47
49:9:35:ASP:HB3	49:9:91:LEU:HD12	1.97	0.47
52:Ac:21:PHE:O	52:Ac:25:ILE:HG13	2.15	0.47
56:Ag:35:TYR:HE1	63:An:102:TYR:CD2	2.33	0.47
60:Ak:397:PHE:HB3	60:Ak:398:PRO:HD3	1.95	0.47
63:An:108:PRO:HG2	63:An:111:PHE:CD2	2.50	0.47
2:B:278:ILE:HG13	2:B:282:VAL:HG11	1.96	0.46
11:K:60:ARG:HA	11:K:67:GLU:O	2.14	0.46
12:L:109:ASN:OD1	12:L:110:GLY:N	2.48	0.46
15:O:104:PHE:O	15:O:108:LEU:HB2	2.16	0.46
20:U:196:THR:HG22	20:U:200:TYR:CE2	2.50	0.46
22:W:10:MET:CG	22:W:12:PRO:HD3	2.44	0.46
36:l:126:ILE:O	36:l:130:ILE:HG12	2.14	0.46
45:u:73:VAL:HG11	45:u:229:MET:HE3	1.96	0.46
46:v:413:LEU:HA	46:v:416:ILE:HG22	1.96	0.46
47:w:49:LEU:HG	47:w:53:MET:HE3	1.97	0.46
47:w:138:MET:SD	47:w:268:ILE:HD12	2.55	0.46
45:5:274:GLU:HG3	45:5:456:VAL:HG11	1.97	0.46
46:6:65:ILE:HG21	46:6:213:PHE:CD1	2.50	0.46
47:7:30:TRP:CZ3	75:7:402:PEE:C13	2.98	0.46
56:Ag:1:ILE:O	56:Ag:1:ILE:HG23	2.15	0.46
58:Al:43:SER:HA	61:Al:4:PRO:HB2	1.96	0.46
3:C:325:ASP:OD1	3:C:325:ASP:N	2.46	0.46
3:C:395:ALA:CB	3:C:412:VAL:HG12	2.45	0.46
3:C:447:VAL:O	3:C:451:ILE:HG13	2.16	0.46
4:D:124:ASN:ND2	4:D:146:TYR:HD2	2.12	0.46
7:G:226:CYS:SG	7:G:227:PRO:HD2	2.55	0.46
12:L:167:ILE:HA	12:L:201:ILE:HB	1.97	0.46
15:O:104:PHE:HB3	15:O:138:LEU:HD11	1.95	0.46
20:U:98:SER:O	20:U:103:GLY:HA2	2.16	0.46
25:a:176:LYS:HE2	32:h:45:HIS:CE1	2.51	0.46
35:k:75:LEU:HD11	37:m:68:PHE:HE1	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:l:124:PHE:CE1	36:l:147:VAL:HG13	2.51	0.46
36:l:572:LYS:O	36:l:575:ILE:HG13	2.15	0.46
37:m:132:ASP:N	37:m:132:ASP:OD1	2.46	0.46
41:q:235:LEU:O	41:q:238:LEU:HG	2.16	0.46
47:w:108:MET:HG3	47:w:313:ARG:HG3	1.96	0.46
48:x:115:PHE:CZ	48:x:149:LEU:HD21	2.50	0.46
48:x:301:LEU:HD23	48:x:301:LEU:HA	1.72	0.46
46:6:78:GLY:HA3	46:6:192:CYS:HA	1.96	0.46
46:6:343:GLN:HB2	46:6:346:SER:CB	2.45	0.46
2:B:70:LEU:HD12	2:B:75:TRP:CE2	2.50	0.46
2:B:274:LYS:HD2	2:B:275:LEU:H	1.80	0.46
4:D:124:ASN:HD21	4:D:146:TYR:HD2	1.62	0.46
5:E:132:ILE:HA	5:E:188:ILE:HG12	1.97	0.46
7:G:32:ILE:HG22	7:G:33:GLU:O	2.15	0.46
7:G:319:TRP:HD1	17:Q:123:TYR:CE1	2.33	0.46
8:H:46:PRO:HB2	8:H:56:ARG:NH2	2.31	0.46
16:P:89:ARG:O	16:P:92:GLU:HG2	2.16	0.46
25:a:146:LYS:O	25:a:150:ARG:HG3	2.15	0.46
27:c:42:PRO:HG3	27:c:67:ASP:N	2.30	0.46
27:c:83:GLN:HG2	27:c:112:TYR:O	2.15	0.46
27:c:121:PRO:HB3	39:o:13:THR:O	2.15	0.46
29:e:76:TYR:CE1	41:q:432:ARG:HB3	2.50	0.46
33:i:337:LEU:HD21	41:q:120:ILE:HD11	1.97	0.46
34:j:52:SER:HB3	34:j:55:PHE:CD2	2.51	0.46
36:l:276:MET:HA	36:l:279:CYS:SG	2.56	0.46
37:m:130:THR:HG22	37:m:132:ASP:H	1.79	0.46
40:p:104:LEU:O	40:p:106:ASP:N	2.48	0.46
41:q:42:LEU:HD21	41:q:453:MET:HB3	1.98	0.46
51:0:60:ARG:HB3	51:0:62:GLN:OE1	2.15	0.46
53:4:138:SER:HA	53:4:141:SER:HB3	1.96	0.46
53:4:249:ILE:N	53:4:257:ASN:OD1	2.33	0.46
45:5:88:GLY:H	45:5:207:ASN:HD22	1.63	0.46
45:5:137:SER:O	45:5:140:LEU:HB3	2.16	0.46
47:7:88:SER:O	47:7:92:ILE:HG12	2.16	0.46
49:9:25:ALA:HB1	49:9:27:PHE:CE2	2.50	0.46
74:Aa:101:CDL:H312	74:Aa:101:CDL:H341	1.68	0.46
1:A:21:ILE:HD12	1:A:21:ILE:HA	1.81	0.46
7:G:252:ASP:OD2	7:G:259:SER:OG	2.28	0.46
8:H:66:LEU:O	42:r:277:TYR:OH	2.34	0.46
12:L:303:ARG:HB2	12:L:316:ARG:HD2	1.96	0.46
12:L:318:LYS:HD2	12:L:321:ARG:HD2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:83:VAL:HG22	15:O:122:MET:SD	2.55	0.46
71:V:202:PLX:H191	71:V:202:PLX:H161	1.60	0.46
28:d:121:TYR:O	28:d:123:GLN:HG2	2.16	0.46
36:l:446:ASN:O	36:l:447:ASN:HB2	2.14	0.46
36:l:503:GLU:O	36:l:507:THR:HG23	2.16	0.46
36:l:511:LEU:HB3	36:l:512:LYS:H	1.48	0.46
74:l:702:CDL:H742	41:q:364:LEU:HD23	1.98	0.46
39:o:53:ASP:HB3	40:p:133:TRP:CE2	2.51	0.46
40:p:86:PRO:HA	40:p:91:TYR:CD1	2.50	0.46
41:q:211:GLY:C	41:q:212:LEU:HD12	2.41	0.46
44:t:35:LYS:O	44:t:36:GLU:C	2.57	0.46
46:v:130:ILE:HG21	46:v:225:VAL:HG22	1.97	0.46
46:v:244:LEU:HB3	46:v:245:GLY:H	1.60	0.46
46:v:293:LEU:HD21	46:v:309:LEU:HD22	1.97	0.46
47:w:97:HIS:HE1	47:w:100:ARG:NH2	2.13	0.46
47:w:265:PRO:HA	47:w:266:PRO:HD3	1.74	0.46
47:w:312:GLN:NE2	47:w:317:PHE:HB2	2.29	0.46
49:y:22:TYR:CD1	49:y:84:TYR:HD1	2.33	0.46
49:y:36:ASP:OD2	49:y:62:ARG:NH1	2.39	0.46
53:4:87:ASP:OD1	53:4:88:PHE:N	2.49	0.46
45:5:172:LEU:HD21	45:5:202:GLU:HB3	1.96	0.46
45:5:280:ASP:HB3	50:Aa:12:ARG:HD2	1.96	0.46
47:7:83:HIS:NE2	76:7:403:HEM:NB	2.62	0.46
47:7:153:ILE:HG22	47:7:155:TYR:H	1.80	0.46
47:7:204:GLY:HA3	50:Aa:3:ARG:HH21	1.79	0.46
63:An:23:PRO:HB3	64:Ao:70:VAL:CG2	2.45	0.46
3:C:298:ILE:HD12	3:C:300:TRP:H	1.81	0.46
4:D:105:ASN:HB3	13:M:97:PRO:HD3	1.96	0.46
7:G:32:ILE:HD12	7:G:45:PRO:HA	1.97	0.46
7:G:598:ASN:HB3	7:G:602:ARG:HB3	1.96	0.46
9:I:78:ARG:CZ	9:I:147:PRO:HG3	2.45	0.46
16:P:19:ILE:HD11	16:P:65:LEU:HD11	1.97	0.46
19:T:53:TYR:OH	43:s:41:LYS:NZ	2.31	0.46
27:c:84:GLN:NE2	27:c:114:ARG:HG3	2.30	0.46
37:m:55:MET:O	37:m:59:ILE:N	2.38	0.46
40:p:94:TYR:CD2	40:p:177:ARG:HG2	2.51	0.46
42:r:146:LEU:O	42:r:149:ILE:HG13	2.15	0.46
42:r:303:TRP:CE2	42:r:307:LEU:HD11	2.50	0.46
45:u:37:THR:HB	45:u:40:GLN:OE1	2.15	0.46
47:w:57:SER:HB2	47:w:176:THR:HA	1.97	0.46
47:w:182:HIS:CE1	76:w:401:HEM:NB	2.83	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:w:200:LEU:HD13	76:w:402:HEM:HAD2	1.97	0.46
74:x:402:CDL:H561	74:x:402:CDL:H532	1.66	0.46
53:2:213:LEU:HD23	53:2:260:VAL:HG22	1.97	0.46
53:4:141:SER:OG	53:4:142:ALA:N	2.48	0.46
61:Al:108:TYR:N	61:Al:108:TYR:CD1	2.82	0.46
65:Ap:40:SER:OG	65:Ap:45:ASP:HB3	2.16	0.46
66:Aq:67:HIS:CD2	66:Aq:78:LEU:HD11	2.50	0.46
2:B:424:ILE:HG22	7:G:76:ARG:HH11	1.78	0.46
4:D:64:TYR:O	4:D:68:ILE:HG13	2.15	0.46
4:D:191:TYR:HB3	17:Q:98:LYS:HG2	1.96	0.46
9:I:199:GLN:HA	9:I:202:ARG:HE	1.81	0.46
12:L:178:SER:HB2	12:L:180:TYR:CD1	2.51	0.46
15:O:119:ILE:O	15:O:123:GLU:HG2	2.14	0.46
20:U:138:TYR:C	20:U:138:TYR:HD1	2.23	0.46
15:X:120:MET:SD	40:p:24:LEU:HD23	2.56	0.46
27:c:167:TYR:CB	44:t:102:PHE:HB2	2.45	0.46
31:g:30:ASP:OD2	31:g:32:ARG:NH1	2.48	0.46
39:o:75:ASN:OD1	39:o:79:ASN:ND2	2.47	0.46
41:q:296:LEU:HB3	41:q:381:ILE:CD1	2.46	0.46
46:v:83:LEU:HD22	46:v:119:MET:HE1	1.98	0.46
47:w:17:ALA:HA	47:w:21:LEU:HD23	1.97	0.46
48:x:299:LEU:C	48:x:299:LEU:CD2	2.85	0.46
45:5:80:ARG:HA	45:5:196:PRO:HB2	1.97	0.46
45:5:311:ILE:HD11	45:5:379:LEU:HD11	1.98	0.46
45:5:451:ASP:HA	45:5:472:ARG:HH12	1.81	0.46
47:7:23:ALA:N	47:7:218:ILE:O	2.47	0.46
75:7:402:PEE:H5	50:Aa:41:ARG:NH2	2.07	0.46
48:8:260:THR:HG21	48:8:266:GLN:HE21	1.81	0.46
48:8:326:LYS:NZ	49:9:54:ASN:HB3	2.30	0.46
2:B:320:GLY:N	2:B:353:ALA:O	2.48	0.46
3:C:135:TYR:CZ	9:I:162:TYR:CE2	2.99	0.46
3:C:223:HIS:CD2	9:I:187:PRO:HD3	2.50	0.46
4:D:215:GLU:CB	12:L:71:ASN:ND2	2.79	0.46
7:G:235:PRO:HG3	7:G:292:PHE:CE1	2.50	0.46
7:G:566:ILE:HD12	7:G:579:MET:O	2.16	0.46
8:H:68:ARG:NH1	22:W:28:ARG:HB3	2.22	0.46
9:I:117:PRO:HA	9:I:120:SER:OG	2.15	0.46
22:W:54:ASN:HD21	42:r:315:PRO:N	2.13	0.46
47:w:40:CYS:SG	47:w:235:MET:HE1	2.56	0.46
47:w:139:SER:N	47:w:255:ASN:HD21	2.14	0.46
48:x:125:CYS:HA	48:x:126:HIS:HB2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:140:MET:O	47:7:166:GLY:HA2	2.15	0.46
53:4:169:TRP:HB3	53:4:174:LEU:HD22	1.97	0.46
53:4:204:ARG:NH1	53:4:246:SER:OG	2.49	0.46
45:5:126:ARG:HH22	45:5:200:SER:HA	1.81	0.46
47:7:26:ASN:ND2	47:7:207:ASN:HB2	2.30	0.46
47:7:260:ASN:HB2	47:7:263:ASN:CB	2.46	0.46
49:9:36:ASP:HA	49:9:59:ARG:NE	2.30	0.46
50:Aa:41:ARG:HD3	74:Aa:101:CDL:H111	1.97	0.46
52:Ac:21:PHE:CE2	52:Ac:25:ILE:HD11	2.51	0.46
61:Al:1:MET:SD	61:Al:133:LEU:HD11	2.56	0.46
2:B:85:LEU:HD21	2:B:247:THR:HG23	1.98	0.46
2:B:120:GLY:C	2:B:121:GLU:O	2.58	0.46
3:C:387:GLU:HA	4:D:235:LEU:HD22	1.98	0.46
7:G:65:TYR:OH	7:G:67:GLU:HB3	2.16	0.46
7:G:639:LEU:O	7:G:643:ARG:HG3	2.16	0.46
8:H:200:GLU:OE1	11:K:85:GLU:HB2	2.16	0.46
14:N:95:LEU:C	14:N:98:LYS:H	2.23	0.46
20:U:150:GLU:HG3	20:U:300:VAL:HG12	1.98	0.46
22:W:43:LEU:HD12	42:r:179:TRP:HE1	1.80	0.46
15:X:114:ASP:OD1	40:p:45:ARG:NE	2.48	0.46
26:b:68:SER:O	26:b:72:VAL:HG23	2.16	0.46
27:c:144:PHE:HZ	36:l:279:CYS:HG	1.60	0.46
31:g:45:LEU:HD22	74:i:503:CDL:H341	1.97	0.46
33:i:91:ASN:OD1	33:i:93:VAL:HG12	2.16	0.46
34:j:73:LEU:HD13	37:m:55:MET:HE1	1.98	0.46
36:l:313:MET:HE3	36:l:313:MET:HB2	1.80	0.46
36:l:491:LEU:O	36:l:495:ILE:HG12	2.16	0.46
37:m:17:PHE:HA	37:m:20:PHE:HB3	1.98	0.46
40:p:58:VAL:HG21	45:u:228:ARG:HH21	1.81	0.46
40:p:121:LYS:O	40:p:124:GLN:HB2	2.15	0.46
45:u:384:THR:HG21	54:3:9:ARG:HE	1.80	0.46
45:u:480:PHE:CE1	54:3:20:THR:OG1	2.66	0.46
46:v:67:ALA:HB1	46:v:208:TYR:OH	2.16	0.46
47:w:112:THR:HG22	47:w:196:HIS:CE1	2.50	0.46
47:w:311:LYS:HG3	47:w:379:TRP:CG	2.51	0.46
48:x:272:CYS:HA	48:x:275:LEU:HD12	1.98	0.46
51:0:40:ILE:HG22	51:0:42:LYS:H	1.80	0.46
53:4:143:SER:OG	53:4:145:ASP:OD1	2.28	0.46
53:4:176:VAL:HG12	53:4:212:ILE:HG22	1.97	0.46
45:5:91:TYR:HD1	45:5:201:VAL:HG12	1.80	0.46
45:5:417:LEU:HA	45:5:421:GLY:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:6:326:PHE:HE1	55:Ae:9:GLY:HA3	1.81	0.46
47:7:182:HIS:NE2	76:7:403:HEM:NA	2.64	0.46
48:8:324:PRO:HB2	48:8:326:LYS:OXT	2.16	0.46
49:9:75:ILE:HD13	50:Aa:40:ARG:HH22	1.81	0.46
57:Ah:11:LEU:HD23	57:Ah:11:LEU:O	2.15	0.46
65:Ap:98:HIS:ND1	65:Ap:98:HIS:N	2.64	0.46
3:C:330:TYR:CD2	3:C:331:LEU:HD12	2.50	0.46
4:D:222:GLU:HG2	4:D:223:PRO:HD2	1.98	0.46
7:G:206:VAL:HG11	68:G:802:SF4:S2	2.55	0.46
9:I:132:LYS:O	9:I:135:PRO:HD2	2.16	0.46
9:I:152:SER:HB3	9:I:182:TYR:CD1	2.51	0.46
9:I:163:TYR:O	9:I:169:VAL:HG21	2.16	0.46
12:L:350:ILE:HG21	12:L:366:MET:HE2	1.97	0.46
35:k:79:VAL:O	35:k:83:ASN:N	2.49	0.46
41:q:148:TYR:HE2	41:q:218:LYS:NZ	2.14	0.46
41:q:225:ILE:HB	41:q:331:ASN:ND2	2.28	0.46
42:r:186:PHE:CE1	42:r:270:PHE:HE1	2.34	0.46
43:s:38:LYS:N	43:s:39:PRO:HD2	2.31	0.46
45:u:226:ALA:H	45:u:253:LEU:HD21	1.79	0.46
45:u:286:HIS:CE1	45:u:359:VAL:HG22	2.51	0.46
48:x:248:PRO:HB3	77:x:401:HEC:HMC2	1.97	0.46
75:2:302:PEE:C30	75:2:302:PEE:C10	2.93	0.46
74:5:501:CDL:HA32	47:7:5:ARG:HD3	1.98	0.46
46:6:196:ARG:HH22	46:6:204:GLN:NE2	2.12	0.46
47:7:216:ASP:OD2	49:9:64:LYS:HG3	2.16	0.46
47:7:290:GLY:O	47:7:294:LEU:HB2	2.15	0.46
51:Ab:31:THR:O	51:Ab:35:GLU:HG3	2.16	0.46
52:Ac:34:ARG:O	52:Ac:38:GLN:HG2	2.16	0.46
60:Ak:195:LEU:CD2	60:Ak:245:ILE:HD13	2.45	0.46
61:Al:76:ILE:O	61:Al:79:PRO:HD2	2.16	0.46
66:Aq:5:LYS:HZ3	66:Aq:5:LYS:HB3	1.81	0.46
3:C:55:THR:O	3:C:59:ALA:N	2.48	0.46
3:C:393:PRO:HG3	3:C:415:GLY:HA3	1.98	0.46
4:D:113:ASP:CG	4:D:131:ASN:HD22	2.20	0.46
4:D:126:PHE:HZ	4:D:199:ARG:HE	1.64	0.46
5:E:110:MET:HE1	7:G:209:TYR:H	1.81	0.46
15:O:84:LEU:HD11	15:O:100:VAL:HG22	1.97	0.46
16:P:67:ALA:O	16:P:74:GLU:HA	2.16	0.46
19:T:80:TRP:CH2	19:T:81:LEU:HD12	2.51	0.46
25:a:55:PHE:HB2	26:b:28:LEU:HD23	1.97	0.46
29:e:113:ARG:HH12	41:q:452:LYS:C	2.24	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:h:95:PRO:O	32:h:98:HIS:N	2.43	0.46
35:k:7:ASN:HD22	37:m:10:SER:HB2	1.81	0.46
37:m:123:GLY:HA3	37:m:125:TRP:CZ3	2.51	0.46
42:r:204:GLU:O	42:r:208:VAL:N	2.49	0.46
45:u:70:THR:HG22	45:u:134:LYS:HA	1.98	0.46
45:u:87:ASN:ND2	45:u:199:GLN:HG3	2.30	0.46
46:v:291:HIS:CD2	46:v:378:LEU:HD23	2.50	0.46
47:w:207:ASN:HD22	47:w:213:SER:HB3	1.81	0.46
47:w:312:GLN:HE22	47:w:317:PHE:N	2.09	0.46
75:w:403:PEE:O5	74:z:101:CDL:OA7	2.33	0.46
48:x:299:LEU:CD2	48:x:303:LEU:HD12	2.46	0.46
45:5:101:THR:OG1	45:5:102:LYS:N	2.43	0.46
45:5:104:ARG:HB2	45:5:105:PRO:O	2.16	0.46
45:5:347:CYS:HA	45:5:352:GLY:HA2	1.98	0.46
46:6:186:LEU:HD21	46:6:330:TYR:CD2	2.51	0.46
46:6:277:ALA:HB3	46:6:333:SER:C	2.40	0.46
56:Ag:2:THR:OG1	60:Ak:484:THR:HB	2.15	0.46
60:Ak:306:THR:HB	60:Ak:359:ALA:O	2.15	0.46
61:Al:41:ILE:O	61:Al:45:MET:HG2	2.16	0.46
3:C:177:ILE:HG23	3:C:210:MET:HE2	1.97	0.45
5:E:143:ARG:HB3	5:E:184:PRO:HD3	1.97	0.45
7:G:49:VAL:HA	7:G:96:VAL:HG13	1.98	0.45
21:V:9:TYR:CE1	21:V:21:LYS:HE2	2.51	0.45
25:a:78:THR:HB	29:e:96:SER:HB2	1.98	0.45
27:c:145:TRP:CH2	27:c:149:ILE:HD11	2.51	0.45
28:d:124:ASN:O	28:d:127:LYS:HB3	2.15	0.45
33:i:256:PRO:HD3	41:q:124:ALA:HA	1.98	0.45
36:l:132:VAL:HG23	36:l:133:THR:HG23	1.97	0.45
38:n:11:HIS:HA	38:n:14:HIS:CD2	2.49	0.45
41:q:59:ASP:CB	41:q:245:ARG:HH22	2.26	0.45
41:q:406:TYR:O	41:q:409:TYR:HB3	2.16	0.45
42:r:77:LEU:HD22	42:r:115:SER:HB3	1.97	0.45
42:r:228:TYR:O	42:r:231:ILE:HG22	2.16	0.45
45:u:79:SER:HB2	45:u:201:VAL:HG13	1.97	0.45
47:w:206:ASN:OD1	47:w:313:ARG:NH2	2.48	0.45
50:z:3:ARG:O	50:z:8:LEU:HD21	2.16	0.45
51:0:82:VAL:HG12	51:0:86:LEU:HB2	1.98	0.45
53:2:106:SER:CB	53:2:110:ARG:HE	2.28	0.45
53:4:80:HIS:HB3	45:5:182:VAL:HG13	1.98	0.45
46:6:56:ALA:O	46:6:127:ARG:NH2	2.49	0.45
46:6:289:LEU:HD11	46:6:428:ALA:HB2	1.96	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:6:300:LYS:HG2	46:6:301:ARG:HG2	1.97	0.45
47:7:239:LEU:O	47:7:243:VAL:HG12	2.16	0.45
60:Ak:435:GLY:O	60:Ak:437:PRO:HD3	2.16	0.45
61:Al:58:ALA:O	61:Al:60:GLU:HG3	2.16	0.45
61:Al:185:MET:SD	61:Al:185:MET:C	2.99	0.45
3:C:316:PHE:HB3	3:C:343:ILE:HD11	1.98	0.45
5:E:72:GLU:HA	5:E:75:LYS:HZ1	1.80	0.45
5:E:92:TRP:CZ3	5:E:94:PRO:HB3	2.51	0.45
8:H:42:ASN:O	8:H:44:ARG:N	2.41	0.45
10:J:75:ARG:HH11	10:J:101:PHE:HB3	1.80	0.45
22:W:120:MET:C	22:W:122:GLY:H	2.24	0.45
15:X:85:TYR:O	15:X:89:LEU:HD13	2.15	0.45
15:X:112:SER:HA	15:X:115:GLN:HB3	1.97	0.45
25:a:182:SER:O	25:a:184:LYS:HG3	2.16	0.45
26:b:72:VAL:HA	26:b:76:LEU:HD12	1.97	0.45
33:i:279:PRO:HA	33:i:282:MET:HE2	1.97	0.45
36:l:12:LEU:HD22	36:l:129:MET:HB3	1.99	0.45
36:l:124:PHE:HA	36:l:150:MET:HG3	1.97	0.45
36:l:159:HIS:CE1	40:p:96:CYS:SG	3.09	0.45
36:l:584:ILE:O	36:l:588:PHE:HB2	2.15	0.45
41:q:112:ALA:HB1	41:q:113:THR:HA	1.98	0.45
41:q:346:ARG:HG3	41:q:420:THR:OG1	2.15	0.45
45:u:54:ASP:OD1	45:u:55:ASN:N	2.49	0.45
75:u:502:PEE:H49	75:u:502:PEE:C17	2.44	0.45
46:v:61:ILE:HD13	46:v:134:MET:HG3	1.98	0.45
47:w:47:THR:HG22	47:w:83:HIS:HB2	1.97	0.45
47:w:344:GLU:O	47:w:348:ILE:HG13	2.15	0.45
47:w:379:TRP:HE1	49:y:34:ARG:HH11	1.64	0.45
54:3:16:ASN:O	54:3:19:PRO:HD2	2.16	0.45
53:4:197:ASP:HB3	53:4:257:ASN:OD1	2.17	0.45
45:5:61:SER:HA	45:5:233:ALA:O	2.16	0.45
45:5:377:MET:HE2	45:5:477:TRP:H	1.81	0.45
47:7:51:LEU:HB3	76:7:403:HEM:HMD2	1.97	0.45
48:8:238:PHE:HB3	48:8:241:GLN:O	2.16	0.45
48:8:317:SER:OG	50:Aa:24:GLN:NE2	2.49	0.45
58:Ai:9:PHE:HD1	58:Ai:10:HIS:HD2	1.63	0.45
60:Ak:299:VAL:HA	60:Ak:302:ARG:NH1	2.31	0.45
2:B:412:LEU:HD22	2:B:439:ILE:HD11	1.98	0.45
3:C:162:GLN:N	4:D:46:THR:O	2.46	0.45
3:C:300:TRP:CZ3	3:C:305:THR:HG21	2.51	0.45
3:C:431:HIS:HB3	3:C:454:GLN:NE2	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:245:TYR:HE1	13:M:65:PRO:N	2.15	0.45
5:E:148:ILE:O	5:E:152:ILE:HD12	2.16	0.45
10:J:109:ASN:OD1	10:J:110:PRO:HD2	2.15	0.45
12:L:242:ILE:HG23	12:L:243:VAL:N	2.32	0.45
12:L:288:PHE:CE2	12:L:290:PRO:HG3	2.52	0.45
14:N:28:TYR:CD1	14:N:56:LEU:HB2	2.51	0.45
20:U:143:LEU:HD11	33:i:317:PHE:CE2	2.36	0.45
21:V:12:ILE:HG12	21:V:21:LYS:CE	2.46	0.45
25:a:147:ALA:HB1	41:q:172:GLY:HA3	1.98	0.45
25:a:179:ILE:HD11	32:h:41:ILE:HG21	1.98	0.45
27:c:58:ARG:C	27:c:60:GLU:H	2.23	0.45
27:c:110:ASP:OD1	27:c:111:MET:N	2.49	0.45
75:i:501:PEE:H36	41:q:155:ALA:HB1	1.97	0.45
35:k:4:VAL:O	35:k:8:ILE:HD12	2.16	0.45
36:l:211:MET:O	36:l:214:ILE:HG13	2.16	0.45
36:l:316:THR:O	36:l:319:ILE:HG22	2.16	0.45
36:l:360:GLY:HA3	36:l:437:PHE:HD1	1.81	0.45
39:o:32:ALA:O	39:o:36:ARG:HG3	2.16	0.45
40:p:11:THR:H	40:p:14:GLN:NE2	2.14	0.45
41:q:229:MET:CE	41:q:328:CYS:HB3	2.46	0.45
42:r:307:LEU:HA	42:r:310:MET:HG2	1.99	0.45
45:u:277:HIS:HD2	50:z:15:ILE:HD12	1.82	0.45
75:u:502:PEE:H13	71:2:301:PLX:H4	1.98	0.45
46:v:52:LEU:HD22	46:v:392:PHE:CZ	2.51	0.45
46:v:324:SER:HB2	55:Af:28:PRO:HG2	1.98	0.45
47:w:50:PHE:CE2	53:2:136:PHE:HB3	2.51	0.45
47:w:130:GLY:HA2	47:w:133:LEU:HD12	1.98	0.45
53:2:170:ARG:NE	47:7:168:PHE:HB3	2.30	0.45
53:4:187:GLU:OE1	53:4:248:ARG:NH2	2.49	0.45
45:5:192:PHE:HE2	45:5:353:LEU:HD11	1.80	0.45
45:5:214:ALA:O	45:5:218:GLU:HG2	2.17	0.45
45:5:325:SER:O	45:5:390:ARG:NH1	2.50	0.45
45:5:451:ASP:OD1	45:5:472:ARG:NH2	2.47	0.45
46:6:212:HIS:HE1	46:6:246:LEU:HD23	1.82	0.45
48:8:157:ASP:HB3	48:8:166:PHE:CZ	2.51	0.45
63:An:66:GLU:O	64:Ao:66:ARG:NH2	2.49	0.45
1:A:12:LEU:HD22	64:Ao:78:HIS:CE1	2.52	0.45
4:D:74:GLN:HE22	4:D:89:HIS:HB2	1.81	0.45
9:I:108:ARG:HA	42:r:37:PRO:HA	1.98	0.45
12:L:250:ILE:O	12:L:254:LYS:HG2	2.15	0.45
13:M:41:LEU:CD1	13:M:42:PRO:HD2	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:197:ALA:HA	20:U:200:TYR:HD2	1.81	0.45
29:e:65:ASN:OD1	41:q:427:LYS:HG3	2.17	0.45
31:g:13:LEU:HA	71:i:502:PLX:H31	1.99	0.45
31:g:85:TYR:CE1	43:s:165:SER:HA	2.52	0.45
33:i:17:THR:HG23	33:i:137:ALA:HB2	1.99	0.45
33:i:68:MET:HB3	35:k:36:MET:SD	2.56	0.45
42:r:105:MET:HG3	42:r:237:PHE:HE1	1.80	0.45
43:s:15:VAL:HG21	43:s:61:LYS:HG2	1.97	0.45
53:2:243:TYR:HB3	53:2:247:GLY:HA2	1.98	0.45
75:2:302:PEE:C11	75:2:302:PEE:C31	2.93	0.45
46:6:212:HIS:CE1	46:6:246:LEU:HD23	2.52	0.45
48:8:197:ASP:O	48:8:201:ILE:HB	2.17	0.45
49:9:60:VAL:HG11	50:Aa:11:MET:HG3	1.99	0.45
64:Ao:76:GLY:HA3	64:Ao:77:PRO:HD2	1.85	0.45
3:C:266:ARG:HD2	71:H:303:PLX:H11	1.99	0.45
7:G:301:ARG:H	11:R:137:TRP:H	1.64	0.45
7:G:348:ALA:O	7:G:351:LEU:HG	2.16	0.45
7:G:355:LYS:HD2	7:G:530:TYR:OH	2.16	0.45
7:G:697:THR:OG1	7:G:698:ASP:N	2.50	0.45
8:H:38:TYR:OH	13:M:106:LEU:HD12	2.17	0.45
8:H:86:TYR:CD1	8:H:90:LYS:HG2	2.51	0.45
9:I:76:TRP:HA	9:I:79:ARG:HG2	1.97	0.45
12:L:91:THR:O	12:L:94:LEU:HB2	2.16	0.45
14:N:44:TYR:O	14:N:48:THR:HG22	2.17	0.45
33:i:287:LEU:HD23	75:i:501:PEE:H62	1.99	0.45
42:r:73:ILE:HA	42:r:76:ILE:HD12	1.98	0.45
44:t:111:ARG:HD3	44:t:115:ARG:CZ	2.37	0.45
46:v:63:LEU:HD11	46:v:218:MET:HE2	1.99	0.45
53:4:122:THR:HG23	75:5:502:PEE:H54	1.97	0.45
53:4:156:LEU:HD23	53:4:157:SER:HB3	1.98	0.45
53:4:214:ILE:CG2	53:4:259:GLU:HB3	2.47	0.45
45:5:374:GLY:O	45:5:378:ARG:HG3	2.16	0.45
3:C:322:SER:OG	3:C:323:ARG:N	2.49	0.45
4:D:228:GLN:O	4:D:229:GLU:HG2	2.17	0.45
5:E:95:ILE:HG22	5:E:99:ASN:ND2	2.32	0.45
7:G:101:ASN:OD1	7:G:102:ILE:N	2.49	0.45
15:O:80:LYS:HE2	15:O:142:GLN:NE2	2.31	0.45
20:U:138:TYR:CE2	20:U:189:TYR:CZ	3.04	0.45
15:X:131:PRO:HG2	15:X:134:ASP:HB2	1.97	0.45
25:a:114:LYS:HA	28:d:63:TYR:CD1	2.52	0.45
28:d:135:VAL:HG13	29:e:137:MET:HE2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:e:74:HIS:CE1	29:e:87:MET:SD	3.10	0.45
74:i:503:CDL:H141	41:q:17:MET:HE2	1.98	0.45
41:q:201:MET:O	41:q:205:VAL:HG23	2.17	0.45
47:w:312:GLN:HE21	47:w:317:PHE:HB2	1.82	0.45
48:x:133:TYR:HA	48:x:136:LEU:HD12	1.99	0.45
47:7:32:ASN:OD1	47:7:228:ASP:HA	2.17	0.45
47:7:33:PHE:HA	47:7:36:LEU:HD12	1.97	0.45
48:8:263:THR:HG21	51:Ab:29:PRO:HD2	1.97	0.45
49:9:78:LYS:HA	49:9:81:TRP:NE1	2.32	0.45
60:Ak:495:LEU:HA	60:Ak:495:LEU:HD23	1.68	0.45
61:Al:60:GLU:CD	61:Al:61:VAL:H	2.25	0.45
61:Al:162:SER:HB2	61:Al:198:GLU:HB2	1.99	0.45
63:An:33:LEU:HD22	63:An:37:GLN:HB3	1.97	0.45
2:B:88:ARG:HD2	2:B:274:LYS:HD3	1.99	0.45
2:B:299:LEU:HD21	2:B:337:MET:HG3	1.98	0.45
3:C:172:VAL:O	3:C:176:GLU:HG2	2.17	0.45
3:C:194:ILE:HD11	3:C:268:TRP:NE1	2.32	0.45
3:C:197:MET:HE3	42:r:32:GLN:NE2	2.31	0.45
3:C:280:ALA:HB2	14:N:12:VAL:HG12	1.99	0.45
4:D:92:GLY:O	4:D:96:VAL:HG23	2.17	0.45
7:G:490:LEU:HD23	7:G:490:LEU:C	2.41	0.45
12:L:242:ILE:HD12	12:L:242:ILE:C	2.41	0.45
14:N:87:GLU:O	14:N:90:LEU:HB3	2.17	0.45
15:X:88:LYS:HE3	15:X:98:LEU:HD23	1.99	0.45
15:X:155:TYR:HA	26:b:20:ARG:HG2	1.99	0.45
27:c:42:PRO:HB3	27:c:64:PRO:HB2	1.98	0.45
31:g:85:TYR:HD1	31:g:88:ARG:HE	1.63	0.45
36:l:35:TYR:O	36:l:39:THR:OG1	2.28	0.45
39:o:60:ILE:HD12	39:o:60:ILE:O	2.17	0.45
41:q:203:PHE:HB3	41:q:243:MET:HB2	1.98	0.45
41:q:440:HIS:O	41:q:443:PRO:HD2	2.17	0.45
45:u:220:VAL:HG13	45:u:224:TYR:HD2	1.82	0.45
46:v:47:LEU:HD13	46:v:238:LEU:HG	1.99	0.45
46:v:63:LEU:HA	46:v:220:LEU:HA	1.98	0.45
46:v:156:SER:HA	46:v:159:ARG:NH1	2.31	0.45
46:v:186:LEU:HD13	46:v:330:TYR:CD2	2.52	0.45
47:w:240:LEU:CD2	75:2:302:PEE:H18	2.46	0.45
47:w:300:ILE:HG13	47:w:303:LEU:HD12	1.99	0.45
47:7:17:ALA:C	47:7:21:LEU:HD23	2.42	0.45
47:7:269:LYS:HB2	47:7:275:LEU:HD21	1.98	0.45
49:9:51:LEU:HD11	49:9:91:LEU:HD21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:Af:32:ALA:O	55:Af:35:PRO:HD2	2.17	0.45
2:B:412:LEU:HD21	2:B:435:VAL:HG11	1.98	0.45
3:C:80:LEU:C	3:C:80:LEU:CD1	2.86	0.45
3:C:292:MET:HG3	3:C:431:HIS:CD2	2.47	0.45
4:D:75:GLN:CD	13:M:68:ILE:HD11	2.42	0.45
4:D:122:ARG:HB3	14:N:111:GLN:HG2	1.99	0.45
4:D:204:LEU:HD12	4:D:205:SER:N	2.31	0.45
7:G:422:TRP:HE3	7:G:423:LEU:HD12	1.81	0.45
14:N:38:ILE:HB	14:N:45:ARG:CD	2.42	0.45
25:a:140:LEU:HA	25:a:143:GLU:OE2	2.17	0.45
32:h:17:TRP:CD1	32:h:17:TRP:H	2.35	0.45
75:i:501:PEE:H21	41:q:148:TYR:CE1	2.51	0.45
36:l:150:MET:HA	36:l:150:MET:HE2	1.99	0.45
36:l:156:GLY:HA3	41:q:416:ARG:HH21	1.82	0.45
37:m:34:ILE:HG12	37:m:61:LEU:HD11	1.98	0.45
39:o:56:ARG:O	39:o:58:GLY:N	2.48	0.45
41:q:130:LEU:HD22	41:q:150:LEU:HD12	1.98	0.45
41:q:318:ALA:HB2	41:q:373:ILE:HG13	1.99	0.45
42:r:82:ALA:HB1	42:r:229:ALA:HB3	1.99	0.45
42:r:181:LEU:HG	42:r:300:LEU:HD23	1.98	0.45
46:v:272:VAL:HG13	46:v:336:PHE:O	2.17	0.45
47:w:180:ALA:HB3	47:7:53:MET:SD	2.57	0.45
50:z:45:CYS:SG	50:z:48:ARG:NH1	2.89	0.45
46:6:45:ASN:HB3	46:6:238:LEU:HG	1.99	0.45
46:6:234:ALA:HA	46:6:237:PHE:CE2	2.52	0.45
47:7:253:PRO:C	47:7:255:ASN:H	2.25	0.45
49:9:30:LEU:HA	49:9:76:LEU:HD13	1.98	0.45
49:9:50:ARG:NH1	49:9:97:GLU:OE1	2.50	0.45
57:Ah:2:GLU:CG	57:Ah:3:ASN:H	2.30	0.45
60:Ak:147:ILE:HD11	60:Ak:209:LEU:HD23	1.98	0.45
60:Ak:273:MET:HG3	60:Ak:319:LYS:NZ	2.30	0.45
60:Ak:431:LEU:HD21	60:Ak:450:TRP:HB2	1.98	0.45
78:Ak:602:HEA:HHC	78:Ak:602:HEA:O11	2.17	0.45
62:Am:183:GLU:O	66:Aq:42:ARG:NH2	2.50	0.45
2:B:114:VAL:HA	2:B:155:TYR:O	2.16	0.45
2:B:208:GLU:HA	69:B:502:FMN:O2'	2.16	0.45
2:B:235:VAL:HG22	2:B:240:THR:HG21	1.99	0.45
3:C:188:THR:HG23	3:C:200:PHE:HA	1.99	0.45
3:C:400:ILE:O	3:C:406:GLU:HA	2.17	0.45
5:E:60:TYR:O	5:E:63:ILE:HG13	2.17	0.45
5:E:102:ALA:HB2	5:E:112:VAL:HG21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:164:THR:HG22	5:E:169:PHE:H	1.82	0.45
7:G:346:VAL:HA	7:G:347:ASP:HB2	1.98	0.45
8:H:77:LEU:HD12	42:r:31:MET:HE2	1.98	0.45
12:L:145:PHE:HD2	12:L:183:SER:HB3	1.80	0.45
12:L:204:SER:CA	12:L:265:PHE:O	2.64	0.45
12:L:305:PHE:O	12:L:312:PRO:HB3	2.17	0.45
17:Q:37:ARG:O	17:Q:41:ARG:HG2	2.16	0.45
18:S:69:ILE:HD13	43:s:72:ARG:HE	1.81	0.45
25:a:91:VAL:HG23	25:a:92:PHE:CD1	2.52	0.45
28:d:159:GLN:NE2	29:e:142:PHE:O	2.43	0.45
33:i:28:LEU:HA	33:i:28:LEU:HD23	1.76	0.45
35:k:54:THR:HA	35:k:57:ASN:ND2	2.31	0.45
37:m:76:THR:HG23	37:m:77:GLU:N	2.27	0.45
39:o:62:ASP:HA	39:o:63:PRO:HD3	1.88	0.45
45:u:47:GLU:OE1	45:u:47:GLU:N	2.49	0.45
45:u:156:LEU:HB2	45:u:213:ARG:NE	2.32	0.45
45:u:324:MET:O	45:u:325:SER:OG	2.34	0.45
46:v:49:ILE:HA	46:v:220:LEU:O	2.17	0.45
75:w:403:PEE:H61	75:w:403:PEE:C18	2.45	0.45
49:y:92:GLU:HB2	49:y:93:PRO:HD3	1.99	0.45
53:2:183:GLU:O	53:2:187:GLU:HG2	2.16	0.45
45:5:190:THR:O	45:5:271:THR:OG1	2.35	0.45
45:5:305:GLN:HG3	55:Ae:57:GLY:HA2	1.97	0.45
46:6:336:PHE:CE2	46:6:338:ILE:HD11	2.51	0.45
46:6:352:LYS:O	46:6:356:ASP:N	2.45	0.45
47:7:234:PHE:CZ	74:8:401:CDL:H321	2.51	0.45
58:Ai:15:ASN:HD21	63:An:79:LYS:NZ	2.15	0.45
60:Ak:240:HIS:O	60:Ak:243:VAL:HG22	2.16	0.45
66:Aq:3:ALA:O	66:Aq:4:ALA:HB2	2.17	0.45
2:B:220:GLN:NE2	5:E:118:PHE:HB2	2.32	0.45
3:C:159:LEU:HD11	13:M:60:ARG:HD3	1.99	0.45
3:C:320:ILE:O	8:H:41:VAL:HG22	2.17	0.45
7:G:313:LEU:HD22	11:R:141:SER:CA	2.47	0.45
7:G:397:ALA:O	7:G:427:LEU:HD22	2.17	0.45
12:L:72:HIS:HB2	12:L:250:ILE:HD12	1.99	0.45
15:O:119:ILE:HD11	15:O:130:ILE:HG21	1.97	0.45
21:V:39:TYR:CZ	36:l:593:ILE:HD11	2.52	0.45
27:c:144:PHE:CZ	36:l:279:CYS:SG	3.10	0.45
29:e:87:MET:HG3	29:e:88:ARG:N	2.32	0.45
29:e:94:GLY:O	29:e:99:LEU:HD13	2.17	0.45
33:i:263:LYS:O	33:i:267:ILE:HG12	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:l:552:LEU:HA	36:l:556:ILE:HG22	1.98	0.45
41:q:201:MET:SD	75:q:501:PEE:H37	2.56	0.45
45:u:125:THR:HG22	45:u:126:ARG:N	2.26	0.45
47:w:231:GLY:HA2	74:x:402:CDL:H111	1.98	0.45
53:2:200:HIS:O	53:2:203:GLU:HG2	2.17	0.45
53:4:236:CYS:N	53:4:241:SER:O	2.44	0.45
45:5:205:SER:O	45:5:209:ARG:HG3	2.16	0.45
45:5:424:ILE:HG12	45:5:432:ARG:HE	1.81	0.45
47:7:47:THR:HG23	47:7:79:ILE:HG23	1.99	0.45
47:7:107:TYR:CE2	47:7:304:MET:HG3	2.52	0.45
49:9:22:TYR:CD2	49:9:84:TYR:HD1	2.35	0.45
49:9:53:GLU:OE2	50:Aa:12:ARG:NH1	2.49	0.45
65:Ap:31:TYR:HE1	65:Ap:98:HIS:CE1	2.34	0.45
2:B:75:TRP:CE2	2:B:76:ILE:HG23	2.51	0.44
2:B:266:GLY:HA2	2:B:293:SER:HB3	1.99	0.44
2:B:316:ALA:HB1	2:B:325:PRO:HB2	1.99	0.44
3:C:129:TYR:CZ	3:C:419:PRO:HB3	2.53	0.44
3:C:386:THR:OG1	3:C:387:GLU:N	2.49	0.44
12:L:178:SER:HB2	12:L:180:TYR:CE1	2.53	0.44
12:L:271:TYR:OH	12:L:346:GLU:HG3	2.17	0.44
14:N:111:GLN:HB2	14:N:112:TRP:CD1	2.51	0.44
26:b:118:PRO:O	26:b:120:MET:N	2.51	0.44
27:c:72:TYR:CD1	27:c:72:TYR:O	2.70	0.44
32:h:48:GLY:O	32:h:50:ILE:N	2.48	0.44
33:i:233:THR:HG23	33:i:241:THR:HB	1.99	0.44
33:i:241:THR:C	33:i:243:LEU:H	2.25	0.44
41:q:297:VAL:HG23	41:q:315:LEU:HD22	1.99	0.44
46:v:297:PRO:HA	46:v:304:ASN:ND2	2.32	0.44
46:v:320:PRO:O	46:v:343:GLN:HG2	2.17	0.44
47:w:6:LYS:HE3	47:w:15:ASN:HD22	1.81	0.44
48:x:97:TRP:CD1	48:x:97:TRP:N	2.83	0.44
74:x:402:CDL:OB4	50:z:41:ARG:NH1	2.50	0.44
53:2:177:ARG:O	53:2:210:TRP:HA	2.17	0.44
71:2:301:PLX:H162	75:2:302:PEE:H73	2.00	0.44
53:4:170:ARG:O	53:4:170:ARG:HG2	2.18	0.44
46:6:49:ILE:HG13	46:6:220:LEU:HD22	1.98	0.44
48:8:184:GLU:HA	48:8:187:ARG:HB2	1.99	0.44
48:8:296:MET:HG2	52:Ac:36:PHE:CZ	2.52	0.44
57:Ah:30:ILE:HG13	57:Ah:31:LEU:N	2.33	0.44
58:Ai:40:TRP:HB3	60:Ak:449:MET:HE3	1.98	0.44
60:Ak:158:ILE:O	60:Ak:162:ILE:HG13	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:89:HIS:CG	4:D:90:PRO:HD2	2.51	0.44
7:G:651:PRO:HD3	16:P:22:HIS:CE1	2.51	0.44
9:I:99:MET:HE3	9:I:113:PHE:CZ	2.50	0.44
17:Q:80:ASP:O	17:Q:83:VAL:HG12	2.17	0.44
18:S:51:ASP:OD1	18:S:52:ARG:N	2.50	0.44
19:T:70:PRO:O	19:T:72:ASP:N	2.50	0.44
20:U:299:LEU:C	20:U:299:LEU:CD2	2.85	0.44
75:i:501:PEE:C23	41:q:155:ALA:CB	2.94	0.44
36:l:190:LEU:HD23	41:q:383:THR:HG21	1.98	0.44
37:m:24:PRO:HB3	37:m:89:VAL:HG11	1.99	0.44
41:q:201:MET:HE2	41:q:201:MET:HA	1.99	0.44
42:r:230:ASN:HA	42:r:233:MET:HE2	1.99	0.44
45:u:275:ILE:N	45:u:456:VAL:O	2.44	0.44
45:u:308:ASN:HA	45:u:343:THR:HG21	1.98	0.44
46:v:84:ARG:CZ	46:v:191:TYR:HE1	2.31	0.44
46:v:300:LYS:HG2	46:v:301:ARG:HG2	2.00	0.44
53:2:145:ASP:OD1	53:2:146:VAL:N	2.49	0.44
53:4:88:PHE:O	53:4:92:ARG:N	2.50	0.44
46:6:138:LEU:HA	46:6:141:THR:HG22	1.99	0.44
47:7:116:GLY:O	76:7:404:HEM:HMC3	2.17	0.44
48:8:143:GLU:HA	48:8:146:ALA:HB3	1.99	0.44
60:Ak:131:PRO:HB2	61:Al:159:VAL:HA	1.99	0.44
67:Ar:58:ARG:HD2	67:Ar:58:ARG:HA	1.74	0.44
3:C:232:VAL:CG1	3:C:356:ILE:HB	2.47	0.44
3:C:279:THR:HG22	3:C:281:GLU:HG2	1.99	0.44
4:D:124:ASN:H	14:N:111:GLN:HE21	1.61	0.44
7:G:691:ILE:O	7:G:694:PHE:HB3	2.17	0.44
11:K:60:ARG:C	11:K:67:GLU:O	2.61	0.44
14:N:55:LYS:HD3	14:N:58:MET:HE2	1.99	0.44
15:O:111:ASP:OD1	15:O:114:ASP:HB2	2.17	0.44
18:S:59:ARG:HB3	18:S:61:HIS:CD2	2.53	0.44
20:U:97:ASP:HB3	20:U:104:LYS:O	2.17	0.44
25:a:170:GLN:NE2	31:g:8:PRO:HD3	2.32	0.44
27:c:63:GLU:O	27:c:77:LYS:CB	2.65	0.44
33:i:102:LEU:HD23	33:i:102:LEU:HA	1.75	0.44
33:i:201:THR:OG1	33:i:202:ILE:N	2.50	0.44
36:l:49:VAL:N	36:l:50:PRO:HD2	2.32	0.44
36:l:108:MET:HE1	36:l:240:PRO:HB2	1.98	0.44
36:l:156:GLY:HA3	41:q:416:ARG:NH2	2.33	0.44
36:l:281:GLY:O	36:l:284:THR:HG22	2.18	0.44
36:l:516:PRO:HB3	40:p:30:TRP:HH2	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:m:109:LYS:C	37:m:111:GLU:H	2.25	0.44
40:p:145:PRO:HB2	40:p:146:PRO:CD	2.46	0.44
41:q:237:LYS:N	41:q:237:LYS:HD2	2.33	0.44
42:r:165:LEU:HD23	42:r:240:ILE:HD12	1.99	0.44
45:u:296:TRP:CZ3	55:Af:57:GLY:C	2.94	0.44
46:v:84:ARG:HH12	55:Af:13:PRO:HB2	1.81	0.44
48:x:178:LYS:HA	48:x:179:PRO:HD3	1.83	0.44
53:2:170:ARG:C	53:2:172:LYS:H	2.24	0.44
45:5:158:ASP:O	45:5:162:GLU:HG2	2.16	0.44
48:8:201:ILE:HA	48:8:204:ALA:HB3	1.99	0.44
74:8:401:CDL:H311	74:8:401:CDL:H742	1.98	0.44
59:Aj:35:ALA:HB3	59:Aj:36:PRO:HD3	1.99	0.44
61:Al:1:MET:SD	61:Al:133:LEU:HD13	2.58	0.44
61:Al:121:TYR:C	61:Al:138:VAL:HG23	2.42	0.44
2:B:114:VAL:O	2:B:242:VAL:HA	2.18	0.44
2:B:123:GLY:N	5:E:180:CYS:SG	2.90	0.44
2:B:220:GLN:O	2:B:222:LYS:N	2.46	0.44
3:C:181:LEU:HD21	3:C:211:PHE:CE1	2.52	0.44
4:D:100:LEU:HD11	4:D:143:VAL:HG11	1.99	0.44
4:D:124:ASN:HB2	4:D:147:THR:C	2.42	0.44
4:D:247:GLN:HG2	14:N:113:LYS:NZ	2.32	0.44
7:G:173:MET:O	7:G:174:THR:OG1	2.28	0.44
7:G:320:GLU:HA	17:Q:123:TYR:HE1	1.82	0.44
7:G:339:ALA:HB3	7:G:544:VAL:HG12	1.99	0.44
8:H:153:ILE:HD13	9:I:162:TYR:CE1	2.51	0.44
9:I:86:THR:HB	9:I:96:MET:HE1	2.00	0.44
9:I:125:VAL:HG11	9:I:173:CYS:SG	2.58	0.44
25:a:112:TYR:CD1	28:d:66:ARG:HB2	2.53	0.44
31:g:40:GLY:HA2	31:g:70:PHE:CD2	2.52	0.44
36:l:270:ASN:ND2	36:l:273:VAL:HG23	2.32	0.44
36:l:297:ASP:OD1	36:l:299:LYS:N	2.45	0.44
40:p:13:GLN:O	40:p:16:VAL:HG22	2.17	0.44
41:q:24:TRP:CH2	41:q:84:LEU:HD11	2.53	0.44
42:r:74:ALA:HB3	42:r:75:PRO:HD3	1.99	0.44
43:s:40:ASN:O	43:s:43:PHE:HB3	2.17	0.44
43:s:142:TYR:O	43:s:144:SER:N	2.50	0.44
46:v:207:TYR:O	46:v:210:GLN:HG2	2.16	0.44
46:v:326:PHE:HB2	46:v:339:TYR:HB2	1.99	0.44
47:w:19:ILE:O	47:w:221:HIS:HB2	2.18	0.44
47:w:53:MET:HE2	47:7:181:PHE:CE1	2.53	0.44
47:w:137:GLN:HE21	47:w:265:PRO:HD3	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:5:101:THR:OG1	45:5:153:ASN:HB3	2.18	0.44
45:5:479:ARG:NE	74:5:501:CDL:H762	2.32	0.44
46:6:111:SER:OG	46:6:122:THR:O	2.35	0.44
59:Aj:36:PRO:HG2	60:Ak:32:ALA:HB3	1.98	0.44
60:Ak:379:TYR:CE2	60:Ak:383:MET:HE2	2.52	0.44
61:Al:122:MET:HB2	61:Al:208:PRO:CD	2.47	0.44
62:Am:19:THR:CG2	62:Am:53:THR:OG1	2.66	0.44
62:Am:42:LEU:HA	62:Am:42:LEU:HD12	1.66	0.44
62:Am:63:ARG:HA	62:Am:67:PHE:CD2	2.53	0.44
65:Ap:33:ILE:HG22	65:Ap:34:LEU:HD12	1.98	0.44
66:Aq:42:ARG:HG3	66:Aq:42:ARG:NH1	2.32	0.44
2:B:106:SER:C	2:B:108:GLY:H	2.25	0.44
3:C:320:ILE:HG22	3:C:321:GLY:O	2.18	0.44
4:D:225:GLU:CD	12:L:47:GLY:HA3	2.42	0.44
7:G:163:LYS:HD2	7:G:207:GLY:HA3	1.99	0.44
7:G:333:PHE:HE2	7:G:543:LYS:HD3	1.83	0.44
7:G:597:VAL:HG12	7:G:598:ASN:O	2.17	0.44
12:L:63:GLY:HA3	72:L:401:NDP:O2A	2.18	0.44
13:M:71:SER:C	13:M:73:GLN:H	2.26	0.44
19:T:30:ILE:O	19:T:33:PRO:HD2	2.18	0.44
22:W:103:ASP:OD1	22:W:103:ASP:N	2.51	0.44
15:X:130:ILE:HA	15:X:131:PRO:HD2	1.85	0.44
28:d:91:GLN:HA	28:d:94:ARG:CZ	2.47	0.44
34:j:92:LEU:O	34:j:96:ILE:HD12	2.17	0.44
36:l:151:SER:O	36:l:155:ILE:HG12	2.18	0.44
36:l:514:LYS:O	36:l:515:TYR:HB2	2.18	0.44
39:o:124:THR:C	39:o:126:ASN:H	2.25	0.44
41:q:167:ILE:HA	41:q:170:THR:HG22	1.98	0.44
41:q:295:ALA:O	41:q:298:ILE:HG22	2.17	0.44
42:r:248:ASP:OD2	42:r:250:HIS:HB2	2.18	0.44
43:s:26:LYS:CE	43:s:97:PHE:CE1	2.99	0.44
47:w:304:MET:HB2	47:w:305:PRO:HD3	2.00	0.44
45:5:200:SER:OG	45:5:202:GLU:OE1	2.35	0.44
49:9:22:TYR:CE2	49:9:84:TYR:HA	2.52	0.44
57:Ah:31:LEU:HD23	57:Ah:31:LEU:HA	1.83	0.44
11:K:80:SER:O	11:K:83:PRO:HD2	2.17	0.44
12:L:329:LEU:HD12	12:L:329:LEU:O	2.17	0.44
15:O:85:TYR:O	15:O:89:LEU:HD13	2.18	0.44
16:P:93:ASN:O	16:P:95:LEU:HG	2.18	0.44
19:T:29:ALA:HB2	42:r:303:TRP:HE3	1.82	0.44
20:U:154:SER:HG	20:U:155:THR:H	1.63	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:60:SER:HB2	40:p:107:TRP:CD1	2.52	0.44
34:j:104:TYR:O	34:j:108:GLN:HG2	2.18	0.44
37:m:12:ILE:HG22	37:m:39:VAL:HG21	2.00	0.44
40:p:107:TRP:HE3	40:p:111:GLU:HB3	1.82	0.44
41:q:11:LEU:HB2	41:q:100:ILE:CD1	2.48	0.44
42:r:286:MET:HE3	42:r:286:MET:HB2	1.85	0.44
45:u:48:THR:HG22	45:u:62:GLU:N	2.32	0.44
45:u:68:THR:HG21	46:v:384:MET:SD	2.58	0.44
45:u:308:ASN:HD21	45:u:345:ASN:CB	2.30	0.44
45:u:465:LEU:HA	45:u:466:PRO:HD3	1.81	0.44
46:v:81:HIS:HB2	46:v:190:LEU:O	2.18	0.44
46:v:425:ILE:O	46:v:429:LYS:HG2	2.18	0.44
52:1:58:HIS:HA	52:1:61:GLU:HG2	1.99	0.44
47:7:97:HIS:NE2	76:7:404:HEM:NA	2.66	0.44
47:7:149:LEU:HD23	47:7:294:LEU:HD22	1.99	0.44
47:7:333:ILE:HD11	75:7:402:PEE:H62	1.99	0.44
51:Ab:86:LEU:HD21	51:Ab:90:LEU:HD12	1.99	0.44
61:Al:59:GLN:CA	61:Al:62:GLU:HB2	2.46	0.44
61:Al:98:LYS:HB2	61:Al:98:LYS:HE3	1.80	0.44
64:Ao:70:VAL:HG12	64:Ao:71:VAL:N	2.32	0.44
1:A:19:PHE:CD1	1:A:19:PHE:C	2.94	0.44
1:A:61:GLU:OE1	1:A:64:ARG:NH1	2.51	0.44
69:B:502:FMN:H9	69:B:502:FMN:HO4'	1.83	0.44
3:C:275:ILE:HA	3:C:276:GLY:HA2	1.67	0.44
5:E:153:GLN:HG3	5:E:158:ILE:O	2.17	0.44
7:G:202:ASN:O	7:G:203:ASP:HB2	2.17	0.44
7:G:356:ASP:HB3	7:G:634:LEU:HD22	1.99	0.44
7:G:379:THR:HA	7:G:385:TYR:CE2	2.53	0.44
10:J:138:ALA:HB1	10:J:143:TRP:HB2	1.99	0.44
20:U:129:ASN:HA	20:U:132:ARG:HB2	2.00	0.44
20:U:141:ARG:O	20:U:144:GLN:HB3	2.18	0.44
21:V:92:ILE:O	21:V:96:ALA:N	2.48	0.44
33:i:230:LEU:O	33:i:233:THR:HG22	2.18	0.44
35:k:11:ALA:HB1	37:m:17:PHE:HD2	1.83	0.44
36:l:182:PHE:HE1	36:l:259:LEU:HD11	1.82	0.44
41:q:10:MET:C	41:q:13:PRO:HD2	2.43	0.44
45:u:152:GLN:HE22	45:u:249:HIS:C	2.25	0.44
45:u:281:ALA:HB3	50:z:12:ARG:NH1	2.33	0.44
48:x:285:HIS:CD2	48:x:285:HIS:O	2.70	0.44
52:1:38:GLN:O	52:1:41:ASP:HB2	2.18	0.44
47:7:107:TYR:HB3	47:7:113:TRP:CE3	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:9:55:LEU:HB3	49:9:90:TYR:CE1	2.53	0.44
50:Aa:81:ASP:O	51:Ab:60:ARG:NH1	2.51	0.44
57:Ah:3:ASN:ND2	57:Ah:5:VAL:HG13	2.33	0.44
60:Ak:51:ASP:O	60:Ak:55:ASN:HB2	2.18	0.44
61:Al:63:THR:HA	61:Al:66:THR:HG22	2.00	0.44
66:Aq:44:ARG:HA	66:Aq:45:PRO:HD2	1.76	0.44
2:B:76:ILE:O	2:B:80:VAL:HG23	2.18	0.44
2:B:276:PHE:CD1	2:B:352:ALA:HB1	2.53	0.44
7:G:283:GLU:C	7:G:285:TRP:H	2.25	0.44
16:P:36:PHE:O	16:P:40:ARG:HB2	2.18	0.44
17:Q:101:THR:OG1	17:Q:102:HIS:N	2.50	0.44
19:T:56:PRO:HG3	43:s:41:LYS:HD2	1.98	0.44
22:W:127:LEU:HG	32:h:83:ARG:NH1	2.33	0.44
36:l:414:ILE:O	36:l:418:LEU:HG	2.18	0.44
37:m:28:TYR:HB3	37:m:83:TRP:CH2	2.52	0.44
47:w:237:LEU:HD13	48:x:301:LEU:CD1	2.44	0.44
48:x:140:CYS:HA	52:1:53:TRP:CE2	2.53	0.44
48:x:142:THR:OG1	52:1:60:TYR:HE2	2.01	0.44
74:z:101:CDL:H311	74:z:101:CDL:H532	2.00	0.44
45:5:385:GLU:OE2	45:5:438:ALA:HB3	2.17	0.44
45:5:400:VAL:HG13	46:6:57:PRO:C	2.43	0.44
46:6:59:SER:HB2	46:6:127:ARG:HA	2.00	0.44
46:6:72:GLU:OE1	46:6:79:THR:HB	2.17	0.44
46:6:81:HIS:HA	46:6:84:ARG:HE	1.82	0.44
48:8:108:HIS:CE1	52:Ac:53:TRP:HB2	2.53	0.44
48:8:320:LEU:HD22	49:9:64:LYS:HE3	2.00	0.44
49:9:61:PHE:CD1	50:Aa:14:VAL:HG22	2.53	0.44
60:Ak:240:HIS:NE2	60:Ak:244:TYR:CE2	2.81	0.44
1:A:26:MET:N	1:A:26:MET:SD	2.91	0.44
2:B:61:ASP:HB3	2:B:62:TRP:H	1.47	0.44
2:B:73:PRO:HB2	2:B:74:ASP:H	1.59	0.44
3:C:66:TRP:NE1	20:U:312:ILE:HD11	2.32	0.44
3:C:399:ALA:HA	3:C:407:PHE:O	2.17	0.44
4:D:155:SER:N	4:D:179:ALA:O	2.27	0.44
5:E:160:VAL:HG12	5:E:161:GLY:N	2.32	0.44
5:E:164:THR:HG23	5:E:167:LYS:N	2.33	0.44
7:G:246:ARG:HH12	7:G:267:THR:HG22	1.82	0.44
7:G:319:TRP:CZ3	7:G:585:PRO:HG2	2.49	0.44
7:G:405:THR:OG1	7:G:479:SER:HB3	2.18	0.44
9:I:148:ARG:NH1	34:j:30:TYR:OH	2.51	0.44
12:L:64:PHE:CD1	12:L:210:GLU:HB2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:123:GLU:OE1	15:O:130:ILE:HG12	2.18	0.44
17:Q:119:LEU:HD21	17:Q:123:TYR:HE2	1.83	0.44
33:i:298:TYR:CE1	41:q:134:THR:HG21	2.53	0.44
36:l:19:ILE:O	36:l:22:SER:HB3	2.17	0.44
36:l:54:PHE:O	36:l:58:GLY:HA2	2.17	0.44
42:r:144:VAL:HG23	42:r:145:THR:H	1.83	0.44
42:r:152:SER:OG	42:r:301:CYS:SG	2.76	0.44
42:r:284:GLN:HA	42:r:287:HIS:HB3	2.00	0.44
45:u:120:LEU:HD21	46:v:299:VAL:HG22	2.00	0.44
45:u:206:GLU:OE1	45:u:209:ARG:HD2	2.18	0.44
45:u:478:LEU:CG	75:u:502:PEE:H12	2.45	0.44
47:w:137:GLN:NE2	47:w:265:PRO:HD3	2.33	0.44
50:z:49:VAL:O	50:z:52:PRO:HD2	2.18	0.44
53:2:127:TYR:HA	54:3:34:TRP:CH2	2.50	0.44
53:2:170:ARG:HG2	53:2:170:ARG:O	2.18	0.44
53:4:127:TYR:HD2	48:8:296:MET:HE2	1.82	0.44
46:6:37:ASP:C	46:6:52:LEU:HG	2.43	0.44
46:6:180:ALA:HA	46:6:258:ILE:HD12	1.99	0.44
47:7:81:TYR:OH	48:8:282:GLU:OE2	2.19	0.44
47:7:347:PHE:HD1	47:7:350:ILE:HD12	1.83	0.44
50:Aa:51:PRO:HG2	50:Aa:52:PRO:HD3	1.99	0.44
62:Am:223:LEU:HA	62:Am:223:LEU:HD23	1.78	0.44
63:An:40:LEU:HD22	63:An:59:LEU:CD1	2.47	0.44
2:B:375:LYS:HD3	2:B:393:ASN:HD22	1.83	0.43
4:D:64:TYR:CE1	13:M:94:ALA:HA	2.52	0.43
5:E:108:PRO:HA	5:E:109:PRO:HD3	1.93	0.43
5:E:188:ILE:HG22	5:E:189:ASN:HD22	1.83	0.43
8:H:73:THR:HG23	42:r:272:TRP:HE1	1.83	0.43
9:I:87:PHE:HD1	9:I:87:PHE:HA	1.68	0.43
19:T:49:THR:HA	19:T:50:PRO:HD3	1.65	0.43
74:V:201:CDL:H532	33:i:110:PRO:HB3	2.00	0.43
24:Z:57:PHE:CZ	36:l:435:PRO:HG3	2.52	0.43
25:a:134:GLU:OE1	38:n:39:ARG:HG2	2.18	0.43
25:a:178:LEU:HD21	32:h:16:ARG:HG3	2.00	0.43
26:b:97:VAL:HG22	36:l:63:ILE:HG22	1.99	0.43
31:g:26:PRO:HG2	31:g:75:TYR:CE1	2.52	0.43
35:k:7:ASN:OD1	37:m:14:VAL:HG21	2.18	0.43
36:l:226:GLN:HB3	36:l:280:LEU:CD2	2.48	0.43
36:l:313:MET:O	36:l:317:ILE:HD12	2.17	0.43
36:l:355:ASP:OD2	40:p:80:TYR:HD1	2.00	0.43
39:o:97:PRO:O	39:o:100:PHE:HB3	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:o:112:LYS:O	39:o:116:ILE:HG12	2.18	0.43
75:u:502:PEE:H1	75:u:502:PEE:H13	1.73	0.43
46:v:39:GLU:HB2	46:v:227:HIS:CG	2.53	0.43
46:v:285:ALA:HB2	46:v:423:ASP:OD2	2.17	0.43
47:w:103:TYR:CE2	75:w:403:PEE:C11	2.91	0.43
48:x:217:THR:CG2	51:0:30:LEU:HD21	2.48	0.43
48:x:294:LEU:HD23	48:x:294:LEU:HA	1.82	0.43
53:2:229:GLY:HA2	53:2:235:TYR:HB2	1.99	0.43
45:5:58:ARG:HG3	45:5:230:VAL:HG13	2.00	0.43
45:5:170:GLN:HE21	45:5:174:GLU:CG	2.31	0.43
47:7:55:TYR:HB2	47:7:69:ILE:HD11	2.00	0.43
47:7:237:LEU:HA	48:8:297:MET:HE3	2.00	0.43
50:Aa:38:VAL:HA	74:Aa:101:CDL:H112	1.99	0.43
51:Ab:53:CYS:HA	51:Ab:56:ARG:HD3	1.99	0.43
60:Ak:70:VAL:HG11	60:Ak:246:LEU:HD22	1.99	0.43
3:C:133:LEU:HB3	3:C:134:PRO:HD3	1.99	0.43
3:C:154:ALA:HA	3:C:398:THR:HG21	2.00	0.43
3:C:317:ASP:H	3:C:339:GLN:NE2	2.13	0.43
5:E:164:THR:HG23	5:E:167:LYS:H	1.82	0.43
7:G:298:LYS:O	11:R:134:ILE:CA	2.65	0.43
12:L:47:GLY:N	12:L:50:SER:OG	2.52	0.43
12:L:297:ALA:O	12:L:301:VAL:HG23	2.18	0.43
16:P:54:LEU:HB3	16:P:56:ARG:NH1	2.33	0.43
18:S:53:ARG:HB3	32:h:102:GLU:O	2.19	0.43
20:U:134:GLN:HE22	20:U:171:PHE:HB2	1.83	0.43
28:d:103:VAL:HA	28:d:106:ILE:HG22	2.00	0.43
36:l:367:PRO:O	36:l:370:THR:HB	2.18	0.43
36:l:546:GLN:HB2	41:q:278:ARG:HE	1.83	0.43
41:q:159:PRO:O	41:q:162:VAL:HG12	2.18	0.43
42:r:46:LEU:O	42:r:46:LEU:HD23	2.18	0.43
45:u:341:PHE:HB3	45:u:358:PHE:HB3	2.00	0.43
74:u:501:CDL:H361	75:u:502:PEE:C19	2.38	0.43
47:w:97:HIS:CE1	47:w:100:ARG:NH2	2.85	0.43
47:w:105:GLY:HA2	47:w:107:TYR:CD2	2.54	0.43
47:w:278:TYR:O	47:w:281:LEU:HB2	2.18	0.43
48:x:223:PRO:O	48:x:226:VAL:HG12	2.18	0.43
48:x:249:ILE:HD12	48:x:264:MET:HE3	2.00	0.43
51:0:42:LYS:HA	51:0:45:LYS:HE3	1.99	0.43
53:2:154:ILE:HA	53:2:271:VAL:O	2.18	0.43
53:2:195:LEU:HD13	53:2:248:ARG:HD2	2.00	0.43
53:4:99:SER:HA	45:5:269:ARG:CD	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:4:180:THR:O	53:4:184:ILE:HD12	2.17	0.43
53:4:183:GLU:O	53:4:186:GLN:HB3	2.18	0.43
45:5:279:ASP:OD1	50:Aa:13:HIS:HB3	2.18	0.43
46:6:183:ARG:HH12	46:6:435:ARG:HH22	1.66	0.43
62:Am:148:HIS:CE1	62:Am:152:MET:HE3	2.54	0.43
4:D:231:ARG:NE	8:H:120:GLU:OE2	2.50	0.43
7:G:83:GLU:HB2	7:G:101:ASN:HB3	2.01	0.43
7:G:241:ARG:HA	7:G:242:PRO:HD3	1.90	0.43
7:G:532:PRO:C	7:G:534:VAL:H	2.26	0.43
9:I:179:VAL:HG21	9:I:182:TYR:CE1	2.53	0.43
12:L:265:PHE:CZ	12:L:335:LEU:HA	2.53	0.43
20:U:303:LYS:HA	20:U:306:VAL:HG22	2.00	0.43
25:a:187:PRO:HA	43:s:48:TRP:CZ2	2.52	0.43
36:l:286:LEU:HD22	36:l:411:MET:SD	2.58	0.43
37:m:61:LEU:HD13	37:m:65:LEU:HD12	1.99	0.43
39:o:30:ARG:NH1	40:p:10:LEU:O	2.51	0.43
42:r:114:TYR:HE2	42:r:118:TRP:CZ2	2.36	0.43
46:v:297:PRO:HA	46:v:304:ASN:HD22	1.84	0.43
47:w:264:THR:HG21	53:4:221:GLY:C	2.42	0.43
48:x:291:LEU:HD23	48:x:291:LEU:O	2.18	0.43
45:5:146:LEU:O	45:5:150:ILE:N	2.46	0.43
45:5:414:GLY:O	45:5:418:LEU:HD13	2.17	0.43
46:6:227:HIS:NE2	46:6:231:LYS:HD2	2.32	0.43
46:6:259:ARG:HD2	46:6:444:LEU:HD22	2.00	0.43
47:7:169:SER:OG	47:7:170:VAL:N	2.50	0.43
48:8:250:TYR:O	48:8:253:VAL:HG23	2.18	0.43
57:Ah:11:LEU:HD23	57:Ah:11:LEU:C	2.44	0.43
2:B:135:PRO:O	2:B:139:VAL:HG23	2.17	0.43
2:B:226:LYS:HB3	2:B:227:PRO:HA	1.99	0.43
2:B:370:LEU:O	2:B:373:PHE:HB3	2.19	0.43
2:B:403:ASP:HA	2:B:453:PHE:CD2	2.54	0.43
3:C:123:LEU:HB3	3:C:135:TYR:OH	2.18	0.43
3:C:447:VAL:HA	3:C:450:ILE:HG22	2.00	0.43
6:F:86:CYS:HG	6:F:95:HIS:CE1	2.35	0.43
7:G:203:ASP:O	7:G:205:GLN:HG3	2.18	0.43
7:G:301:ARG:HH22	7:G:588:ALA:HB2	1.84	0.43
7:G:306:MET:HB2	7:G:583:ILE:HD12	2.00	0.43
8:H:86:TYR:CE1	8:H:90:LYS:HG2	2.53	0.43
9:I:118:ARG:NE	42:r:214:GLU:OE1	2.51	0.43
9:I:154:GLY:HA2	9:I:188:PRO:HD3	2.00	0.43
10:J:96:LYS:HE2	14:N:116:ILE:HG21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:88:PHE:CB	20:U:162:GLU:CA	2.93	0.43
25:a:75:ILE:HD13	74:l:702:CDL:H161	2.01	0.43
25:a:176:LYS:NZ	32:h:42:GLU:HG2	2.34	0.43
36:l:37:LYS:HG3	36:l:38:THR:N	2.33	0.43
36:l:275:THR:HG22	36:l:279:CYS:SG	2.58	0.43
41:q:14:MET:HE2	41:q:26:ASN:HB3	2.01	0.43
42:r:22:LEU:HD12	42:r:47:GLN:HB3	1.99	0.43
42:r:169:GLN:HB3	42:r:244:GLY:HA3	2.00	0.43
45:u:480:PHE:HD1	54:3:20:THR:OG1	1.94	0.43
47:w:223:TYR:O	47:w:226:ILE:HG22	2.18	0.43
47:w:223:TYR:CE2	48:x:315:LEU:HD11	2.53	0.43
50:z:23:GLU:OE2	53:2:110:ARG:NH1	2.51	0.43
47:7:40:CYS:O	47:7:44:GLN:HG2	2.18	0.43
47:7:66:VAL:HG21	47:7:134:PRO:HA	1.99	0.43
54:Ad:23:MET:O	54:Ad:27:VAL:HG23	2.17	0.43
60:Ak:247:ILE:HB	78:Ak:602:HEA:HBC1	2.01	0.43
2:B:159:ARG:HB3	2:B:161:GLU:OE1	2.18	0.43
2:B:208:GLU:OE1	2:B:210:THR:N	2.52	0.43
3:C:35:ARG:NH2	29:e:59:PRO:HA	2.34	0.43
9:I:115:ALA:O	9:I:116:SER:CB	2.65	0.43
12:L:65:LEU:HA	12:L:66:GLY:HA2	1.51	0.43
12:L:182:ARG:O	12:L:186:VAL:HG23	2.18	0.43
12:L:272:LEU:HA	12:L:272:LEU:HD12	1.75	0.43
18:S:36:LYS:HG3	18:S:37:ARG:N	2.33	0.43
31:g:31:PRO:O	31:g:34:VAL:HG22	2.18	0.43
33:i:189:TRP:CZ3	33:i:282:MET:HE3	2.53	0.43
41:q:221:VAL:HA	41:q:340:ARG:NH1	2.33	0.43
47:w:64:SER:O	47:w:67:THR:OG1	2.28	0.43
48:x:219:TYR:CE1	48:x:247:PRO:HG3	2.54	0.43
51:0:79:ASP:HA	51:0:82:VAL:HB	1.99	0.43
54:3:20:THR:O	54:3:24:TRP:HD1	1.97	0.43
45:5:58:ARG:HG2	45:5:230:VAL:HG22	1.99	0.43
47:7:362:ILE:HA	47:7:366:MET:HE2	1.99	0.43
49:9:26:GLY:HA2	49:9:29:LYS:NZ	2.34	0.43
55:Af:46:LYS:HG2	55:Af:47:ARG:O	2.18	0.43
2:B:277:ASN:OD1	2:B:278:ILE:N	2.51	0.43
3:C:365:PRO:HA	3:C:366:PRO:HD3	1.75	0.43
3:C:412:VAL:HG23	3:C:420:TYR:HB3	2.00	0.43
4:D:83:GLU:HB3	4:D:142:ARG:HH12	1.82	0.43
7:G:103:LEU:HB2	7:G:106:SER:HB2	2.00	0.43
7:G:403:VAL:HB	7:G:476:LEU:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:560:LEU:O	7:G:564:CYS:N	2.51	0.43
12:L:298:TYR:HD2	12:L:319:VAL:HG13	1.82	0.43
16:P:28:PRO:O	16:P:31:GLN:HG2	2.17	0.43
17:Q:40:TYR:HE1	17:Q:60:ARG:HD3	1.83	0.43
73:Q:201:ZMP:H15	73:Q:201:ZMP:H17	1.72	0.43
19:T:78:LEU:HD12	43:s:123:GLY:O	2.19	0.43
22:W:60:LEU:HD21	43:s:98:ARG:NH2	2.33	0.43
33:i:86:ILE:HB	33:i:87:THR:H	1.66	0.43
75:i:501:PEE:H65	75:i:501:PEE:H71	1.79	0.43
37:m:5:ILE:HA	37:m:8:ILE:HG12	2.00	0.43
40:p:79:PRO:O	40:p:81:ILE:HD12	2.19	0.43
47:w:119:LEU:HD22	76:w:402:HEM:CHC	2.48	0.43
47:w:132:VAL:HG11	47:w:178:PHE:HD2	1.82	0.43
48:x:109:THR:OG1	48:x:110:SER:N	2.51	0.43
48:x:297:MET:HE1	75:2:302:PEE:C34	2.41	0.43
51:0:87:PHE:HD1	51:0:90:LEU:HD21	1.83	0.43
52:1:11:TYR:HB2	53:2:112:GLY:CA	2.49	0.43
53:2:174:LEU:HD21	53:2:212:ILE:HD12	2.01	0.43
53:4:145:ASP:OD1	53:4:146:VAL:N	2.52	0.43
45:5:400:VAL:HG13	46:6:57:PRO:O	2.18	0.43
46:6:186:LEU:HD21	46:6:330:TYR:CE2	2.54	0.43
2:B:188:GLY:C	2:B:190:GLY:H	2.26	0.43
2:B:285:PRO:HB3	5:E:143:ARG:HH12	1.84	0.43
3:C:254:ARG:HD3	3:C:254:ARG:HA	1.76	0.43
5:E:48:ASN:O	5:E:50:ASP:N	2.52	0.43
5:E:132:ILE:HD11	5:E:169:PHE:CD1	2.52	0.43
7:G:237:ALA:C	7:G:239:THR:H	2.26	0.43
7:G:358:LEU:HB3	7:G:364:ASP:HB2	2.01	0.43
7:G:379:THR:HG21	7:G:531:LYS:HD3	1.99	0.43
8:H:148:ASP:OD2	8:H:151:LYS:HE2	2.19	0.43
8:H:162:CYS:SG	8:H:165:ASP:N	2.91	0.43
8:H:175:PHE:O	8:H:177:THR:HG23	2.17	0.43
12:L:65:LEU:HA	12:L:65:LEU:HD12	1.73	0.43
12:L:136:THR:OG1	12:L:139:PHE:HB2	2.18	0.43
17:Q:39:TRP:CE2	17:Q:90:LEU:HB2	2.54	0.43
23:Y:60:PHE:O	23:Y:64:THR:OG1	2.28	0.43
33:i:238:PRO:O	33:i:241:THR:HG22	2.17	0.43
37:m:57:PHE:HD2	42:r:107:ALA:HB1	1.83	0.43
43:s:27:ALA:HB1	43:s:85:TYR:CD2	2.53	0.43
46:v:112:VAL:HG22	46:v:121:TYR:HD1	1.84	0.43
46:v:364:GLY:HA2	46:v:425:ILE:HD12	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:x:95:TYR:HB2	48:x:97:TRP:HE1	1.83	0.43
48:x:263:THR:O	48:x:267:VAL:HG12	2.19	0.43
53:2:178:HIS:HB2	53:2:210:TRP:CH2	2.54	0.43
53:4:183:GLU:HB3	53:4:245:ALA:CB	2.49	0.43
45:5:278:ARG:HB2	50:Aa:12:ARG:O	2.19	0.43
45:5:428:GLU:O	45:5:431:SER:OG	2.26	0.43
46:6:38:LEU:HD13	46:6:406:TYR:CE2	2.53	0.43
46:6:71:TYR:HB3	46:6:212:HIS:CE1	2.53	0.43
46:6:90:THR:OG1	46:6:94:ALA:O	2.36	0.43
46:6:217:ARG:HE	46:6:245:GLY:HA3	1.84	0.43
47:7:30:TRP:HE1	74:Aa:101:CDL:HB31	1.83	0.43
47:7:379:TRP:CZ3	49:9:38:ILE:HD12	2.54	0.43
62:Am:19:THR:HG22	62:Am:53:THR:OG1	2.18	0.43
2:B:272:GLY:O	2:B:292:MET:HG2	2.18	0.43
2:B:280:GLY:O	2:B:282:VAL:N	2.51	0.43
2:B:395:VAL:HG11	2:B:412:LEU:HD12	2.00	0.43
3:C:395:ALA:HB2	3:C:412:VAL:HG12	2.00	0.43
4:D:191:TYR:CB	17:Q:98:LYS:HG2	2.49	0.43
7:G:299:ARG:HG2	7:G:300:GLN:N	2.34	0.43
7:G:390:THR:OG1	7:G:393:GLY:N	2.51	0.43
15:O:104:PHE:CB	15:O:138:LEU:HD11	2.49	0.43
17:Q:82:LEU:CG	73:Q:201:ZMP:H11A	2.48	0.43
20:U:91:ALA:HA	20:U:95:TYR:CG	2.54	0.43
21:V:39:TYR:HB2	74:V:201:CDL:H712	1.99	0.43
15:X:138:LEU:HD12	15:X:144:ILE:HG12	2.00	0.43
24:Z:24:ILE:O	24:Z:27:THR:OG1	2.30	0.43
28:d:114:GLN:NE2	36:l:203:MET:HE2	2.33	0.43
28:d:167:ARG:HH12	29:e:150:PRO:C	2.26	0.43
33:i:198:THR:O	33:i:201:THR:OG1	2.22	0.43
33:i:261:MET:SD	33:i:340:THR:HG22	2.58	0.43
36:l:197:ASP:OD1	36:l:198:LEU:N	2.52	0.43
36:l:249:SER:O	36:l:332:HIS:HE1	2.01	0.43
36:l:313:MET:O	36:l:316:THR:HB	2.19	0.43
37:m:54:LEU:HA	37:m:54:LEU:HD23	1.67	0.43
39:o:64:ALA:HA	39:o:67:ARG:HH11	1.84	0.43
39:o:81:ARG:HA	39:o:82:PRO:HD3	1.83	0.43
41:q:14:MET:O	41:q:18:SER:OG	2.18	0.43
41:q:450:ASN:OD1	41:q:452:LYS:HG2	2.19	0.43
42:r:14:LEU:O	42:r:17:VAL:HG22	2.18	0.43
46:v:176:ASN:ND2	46:v:260:ASP:OD2	2.51	0.43
46:v:268:HIS:CE1	46:v:341:ILE:HG23	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:w:30:TRP:CH2	75:w:403:PEE:H17	2.53	0.43
47:w:237:LEU:HD12	48:x:297:MET:CG	2.49	0.43
48:x:154:GLU:CD	48:x:167:MET:HB3	2.43	0.43
49:y:76:LEU:HD12	49:y:77:PRO:HD2	2.01	0.43
50:z:34:GLY:O	50:z:38:VAL:HG23	2.18	0.43
53:2:161:GLU:HB2	53:2:178:HIS:CE1	2.54	0.43
53:4:190:VAL:HG11	53:4:195:LEU:HD21	2.00	0.43
45:5:175:ASN:O	45:5:178:SER:OG	2.27	0.43
45:5:282:LEU:HA	45:5:283:PRO:HD3	1.90	0.43
45:5:335:ARG:HD2	45:5:337:LEU:HD21	2.00	0.43
47:7:29:SER:HA	47:7:227:LYS:NZ	2.34	0.43
48:8:97:TRP:CZ3	48:8:209:GLU:HB2	2.53	0.43
48:8:110:SER:OG	48:8:270:ASP:HA	2.19	0.43
48:8:234:PHE:HA	48:8:242:ALA:HA	2.01	0.43
54:Ad:4:ARG:NE	54:Ad:5:PHE:CE2	2.82	0.43
57:Ah:36:MET:O	57:Ah:40:LEU:HG	2.18	0.43
60:Ak:377:PHE:CD2	78:Ak:602:HEA:HAD1	2.54	0.43
61:Al:3:TYR:CD1	61:Al:3:TYR:N	2.86	0.43
63:An:126:MET:HG3	63:An:128:VAL:HG23	2.00	0.43
64:Ao:27:TRP:CH2	65:Ap:86:GLY:HA2	2.54	0.43
66:Aq:5:LYS:HB3	66:Aq:6:GLY:H	1.67	0.43
2:B:93:PHE:HD2	2:B:98:LYS:HB2	1.84	0.43
2:B:294:VAL:HA	2:B:295:PRO:HD2	1.87	0.43
3:C:153:LEU:HD12	3:C:171:ARG:HH21	1.83	0.43
3:C:408:GLY:O	3:C:425:LYS:N	2.46	0.43
3:C:438:MET:HE1	3:C:454:GLN:CD	2.43	0.43
7:G:266:ARG:O	7:G:267:THR:OG1	2.34	0.43
7:G:422:TRP:CE2	7:G:440:TYR:HB2	2.54	0.43
12:L:299:ARG:NE	12:L:316:ARG:HH11	2.15	0.43
17:Q:30:ARG:O	17:Q:34:GLU:HG3	2.19	0.43
18:S:43:TYR:HD2	37:m:135:PHE:HE1	1.67	0.43
20:U:141:ARG:HD2	20:U:168:ASP:OD2	2.19	0.43
26:b:95:TYR:HE2	28:d:109:ARG:HG2	1.83	0.43
29:e:113:ARG:HH12	41:q:452:LYS:CB	2.31	0.43
31:g:40:GLY:HA2	31:g:70:PHE:HD2	1.83	0.43
35:k:31:LEU:HB3	37:m:20:PHE:HE1	1.83	0.43
36:l:407:TRP:O	36:l:411:MET:HG2	2.19	0.43
37:m:57:PHE:CD2	42:r:107:ALA:HB1	2.54	0.43
43:s:109:GLU:HA	43:s:112:LEU:HG	2.01	0.43
43:s:121:ASP:H	43:s:124:GLU:CD	2.26	0.43
47:w:378:LYS:HZ3	49:y:89:PHE:HD2	1.65	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2:241:SER:OG	53:2:252:GLY:O	2.35	0.43
53:4:96:VAL:HG21	53:4:110:ARG:HD3	2.00	0.43
45:5:125:THR:HB	45:5:128:HIS:N	2.34	0.43
45:5:154:CYS:SG	45:5:220:VAL:HG11	2.59	0.43
74:5:501:CDL:H711	74:5:501:CDL:HB61	1.91	0.43
1:A:21:ILE:O	1:A:25:PHE:HD2	2.02	0.43
1:A:68:ILE:HG13	1:A:69:PHE:N	2.33	0.43
3:C:198:THR:OG1	42:r:275:ALA:O	2.26	0.43
3:C:219:GLY:O	8:H:97:PHE:HA	2.19	0.43
3:C:356:ILE:H	3:C:356:ILE:HG13	1.63	0.43
3:C:412:VAL:HG23	3:C:412:VAL:O	2.19	0.43
4:D:70:PRO:HA	4:D:73:VAL:HG22	2.01	0.43
5:E:111:ARG:NH1	5:E:114:GLU:OE1	2.52	0.43
7:G:379:THR:HG22	7:G:526:LEU:HD22	2.01	0.43
7:G:381:LEU:O	7:G:383:SER:N	2.42	0.43
9:I:91:CYS:O	9:I:94:VAL:HG22	2.19	0.43
9:I:214:TYR:CD1	9:I:214:TYR:C	2.97	0.43
15:X:115:GLN:O	15:X:119:ILE:HG22	2.19	0.43
28:d:164:LEU:HD21	29:e:149:LEU:HD11	2.01	0.43
31:g:55:VAL:HG12	31:g:56:VAL:HG23	2.00	0.43
32:h:22:SER:OG	32:h:23:ALA:N	2.52	0.43
36:l:27:TYR:OH	36:l:116:ARG:HG2	2.18	0.43
36:l:71:LEU:HG	41:q:310:MET:HE1	2.00	0.43
36:l:231:PRO:C	36:l:234:PRO:HD2	2.44	0.43
37:m:10:SER:O	37:m:13:PHE:HB3	2.19	0.43
37:m:30:GLY:O	37:m:34:ILE:HG13	2.19	0.43
41:q:106:LEU:HA	41:q:106:LEU:HD23	1.73	0.43
41:q:352:LEU:CD1	41:q:355:MET:HB2	2.49	0.43
42:r:288:LEU:O	42:r:292:SER:HB2	2.19	0.43
45:u:87:ASN:H	45:u:207:ASN:ND2	2.17	0.43
45:u:109:LEU:HG	45:u:146:LEU:HD11	2.01	0.43
47:w:30:TRP:HA	47:w:33:PHE:HD2	1.84	0.43
48:x:195:PRO:HA	48:x:196:PRO:HD3	1.79	0.43
53:4:98:ASP:OD2	53:4:101:LYS:HD3	2.19	0.43
45:5:81:TYR:CE1	45:5:265:PHE:HD2	2.36	0.43
45:5:396:ARG:O	45:5:400:VAL:HG23	2.19	0.43
46:6:85:LEU:HD21	55:Ae:15:LEU:HD22	2.00	0.43
47:7:109:PHE:CE1	47:7:203:THR:HB	2.53	0.43
62:Am:60:ASP:O	62:Am:64:GLU:HG3	2.18	0.43
65:Ap:53:THR:HG22	65:Ap:54:ASN:OD1	2.19	0.43
2:B:297:LYS:HG2	2:B:332:CYS:CB	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ILE:N	2:B:328:PRO:HD3	2.34	0.42
2:B:425:CYS:N	68:B:501:SF4:S3	2.84	0.42
3:C:148:GLU:HB3	3:C:227:ILE:HB	2.01	0.42
7:G:97:MET:HE3	7:G:100:TRP:CH2	2.54	0.42
7:G:224:ASP:HA	10:J:87:MET:SD	2.59	0.42
7:G:382:ARG:HA	7:G:385:TYR:CZ	2.54	0.42
7:G:382:ARG:HG2	7:G:386:LEU:HD11	2.01	0.42
7:G:540:ASN:ND2	7:G:562:LYS:HG3	2.34	0.42
9:I:118:ARG:HD2	42:r:214:GLU:HA	2.00	0.42
12:L:207:PHE:CZ	12:L:345:LEU:CA	2.90	0.42
13:M:38:PRO:HA	13:M:39:PRO:HD3	1.56	0.42
20:U:170:VAL:HG13	20:U:171:PHE:CD1	2.54	0.42
15:X:113:LEU:HD11	73:X:201:ZMP:H20A	2.01	0.42
24:Z:18:ASP:OD1	24:Z:19:TYR:N	2.51	0.42
33:i:170:LEU:O	33:i:295:ARG:NH1	2.48	0.42
33:i:262:PRO:O	33:i:266:ILE:HG12	2.19	0.42
33:i:288:LEU:HD11	36:l:570:GLN:HE21	1.83	0.42
33:i:337:LEU:O	33:i:340:THR:HG23	2.19	0.42
35:k:9:ILE:O	35:k:12:PHE:HB3	2.19	0.42
74:l:702:CDL:H762	41:q:445:LEU:HD22	2.01	0.42
41:q:225:ILE:CD1	41:q:328:CYS:HA	2.47	0.42
45:u:140:LEU:HB3	45:u:141:PRO:HD3	2.00	0.42
45:u:285:ALA:HA	45:u:460:GLY:CA	2.44	0.42
75:u:502:PEE:C33	75:u:502:PEE:C17	2.97	0.42
46:v:347:ALA:HB3	46:v:447:THR:HG22	2.01	0.42
47:w:161:VAL:HA	47:w:164:ILE:HD12	2.00	0.42
47:w:233:LEU:HD11	48:x:300:LEU:HD13	2.01	0.42
47:w:234:PHE:HZ	74:x:402:CDL:H361	1.84	0.42
47:w:333:ILE:HG22	50:z:56:PHE:CE1	2.54	0.42
54:3:4:ARG:C	54:3:6:LEU:N	2.76	0.42
45:5:300:ASP:OD2	45:5:448:TYR:OH	2.28	0.42
45:5:323:HIS:HB3	46:6:97:PHE:HA	2.01	0.42
45:5:332:ALA:HB1	45:5:338:CYS:O	2.18	0.42
47:7:25:SER:HB2	49:9:71:MET:SD	2.59	0.42
47:7:334:THR:O	47:7:338:ILE:HG12	2.19	0.42
48:8:133:TYR:HB2	48:8:172:LEU:O	2.18	0.42
48:8:326:LYS:HZ1	49:9:54:ASN:HB3	1.85	0.42
2:B:316:ALA:HA	2:B:326:LEU:O	2.18	0.42
3:C:83:ASN:HB3	3:C:98:VAL:HG22	2.01	0.42
3:C:172:VAL:HG23	3:C:311:TYR:CZ	2.54	0.42
3:C:383:LYS:HD2	3:C:383:LYS:HA	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:439:SER:O	3:C:439:SER:OG	2.30	0.42
7:G:44:GLU:CG	7:G:45:PRO:HD2	2.49	0.42
7:G:223:ILE:HG21	7:G:233:SER:HB3	2.01	0.42
10:J:63:THR:CG2	17:Q:70:ASN:CG	2.88	0.42
11:K:86:TRP:CD1	11:K:92:CYS:HA	2.54	0.42
16:P:30:SER:HA	16:P:63:PRO:HG2	2.00	0.42
21:V:87:PRO:HA	21:V:126:LYS:HG2	2.00	0.42
28:d:72:PRO:HB3	28:d:76:GLU:OE2	2.20	0.42
28:d:115:GLN:HG2	36:l:62:ILE:CG2	2.49	0.42
32:h:15:ASP:CG	33:i:28:LEU:HD12	2.44	0.42
33:i:58:LYS:NZ	33:i:117:GLU:OE1	2.51	0.42
33:i:255:PRO:HA	33:i:260:PHE:CG	2.54	0.42
35:k:57:ASN:O	35:k:60:PRO:HD2	2.19	0.42
36:l:216:LEU:HD11	36:l:263:PHE:CE2	2.54	0.42
36:l:418:LEU:HA	36:l:418:LEU:HD23	1.84	0.42
39:o:80:PHE:CZ	39:o:82:PRO:HA	2.55	0.42
45:u:66:GLN:OE1	45:u:67:PRO:HD2	2.19	0.42
45:u:152:GLN:NE2	45:u:250:PHE:HA	2.33	0.42
45:u:274:GLU:HB3	45:u:468:TYR:CD1	2.52	0.42
46:v:359:LYS:O	46:v:363:GLN:N	2.52	0.42
47:w:47:THR:HG23	47:w:79:ILE:HG23	2.01	0.42
47:w:97:HIS:CE1	76:w:402:HEM:C1A	3.08	0.42
48:x:116:GLN:HG2	48:x:119:LYS:HE2	2.01	0.42
53:2:265:PHE:CD1	53:2:271:VAL:HG23	2.54	0.42
53:4:172:LYS:HB2	53:4:214:ILE:HD11	2.00	0.42
46:6:66:LYS:HA	46:6:118:SER:HB2	2.00	0.42
46:6:209:VAL:HG13	46:6:213:PHE:CD2	2.55	0.42
47:7:105:GLY:HA2	47:7:107:TYR:CE1	2.54	0.42
48:8:238:PHE:CD1	48:8:239:PRO:HD2	2.54	0.42
49:9:29:LYS:HG2	49:9:81:TRP:CE2	2.54	0.42
62:Am:137:LEU:HA	62:Am:137:LEU:HD12	1.69	0.42
66:Aq:5:LYS:CD	66:Aq:6:GLY:N	2.82	0.42
2:B:62:TRP:CZ2	2:B:181:LEU:HD13	2.53	0.42
3:C:80:LEU:HD22	3:C:81:THR:N	2.31	0.42
3:C:84:PHE:HB3	3:C:85:GLY:H	1.63	0.42
3:C:241:LEU:HD23	3:C:241:LEU:HA	1.75	0.42
4:D:114:LEU:HD13	4:D:130:TYR:CE2	2.55	0.42
18:S:17:PHE:HE1	42:r:257:ILE:HG12	1.84	0.42
21:V:59:TYR:CD1	74:V:201:CDL:H222	2.54	0.42
28:d:159:GLN:NE2	29:e:140:ASN:HB3	2.35	0.42
31:g:42:CYS:HB3	74:i:503:CDL:H371	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:h:7:GLN:HE21	32:h:16:ARG:HH21	1.64	0.42
33:i:113:PHE:O	33:i:116:PRO:HD2	2.19	0.42
36:l:2:ASN:N	36:l:3:PRO:HD2	2.34	0.42
36:l:65:ASN:OD1	36:l:66:TRP:N	2.52	0.42
37:m:139:GLU:OE2	37:m:143:ILE:HD12	2.19	0.42
42:r:28:LEU:HD12	42:r:275:ALA:HB2	2.01	0.42
45:u:64:SER:HB3	45:u:235:GLY:HA2	2.02	0.42
46:v:259:ARG:NH2	46:v:444:LEU:HD22	2.34	0.42
47:w:28:SER:HB2	74:z:101:CDL:HB21	2.02	0.42
48:x:219:TYR:CD1	48:x:247:PRO:HG3	2.54	0.42
48:x:243:ILE:HD11	77:x:401:HEC:CHA	2.49	0.42
71:2:301:PLX:H181	75:2:302:PEE:C42	2.36	0.42
45:5:42:LEU:HD11	45:5:430:GLU:HG3	2.00	0.42
45:5:284:LEU:HD21	55:Ae:45:ALA:HA	2.01	0.42
47:7:27:ILE:HD12	47:7:224:TYR:CZ	2.55	0.42
47:7:271:GLU:O	47:7:275:LEU:HG	2.18	0.42
75:7:402:PEE:H71	75:7:402:PEE:H65	1.48	0.42
55:Af:4:VAL:HG21	55:Af:12:ALA:HB2	2.01	0.42
58:Ai:15:ASN:HD21	63:An:79:LYS:HZ3	1.66	0.42
58:Ai:44:PRO:HA	58:Ai:47:ARG:NH1	2.34	0.42
60:Ak:462:LEU:O	60:Ak:466:MET:HG3	2.20	0.42
62:Am:41:THR:O	62:Am:45:ILE:HG13	2.18	0.42
67:Ar:57:ARG:HB3	67:Ar:57:ARG:NH1	2.31	0.42
2:B:236:PHE:HE1	5:E:74:HIS:HB2	1.80	0.42
3:C:52:MET:HG3	33:i:173:THR:HG22	2.01	0.42
3:C:383:LYS:HA	3:C:386:THR:OG1	2.20	0.42
7:G:252:ASP:OD1	7:G:259:SER:N	2.52	0.42
7:G:396:GLU:OE1	7:G:396:GLU:N	2.52	0.42
7:G:708:ALA:HA	7:G:711:VAL:HG12	2.02	0.42
8:H:95:PRO:HA	8:H:204:ASN:OD1	2.19	0.42
10:J:81:VAL:HG21	10:J:150:ARG:HH12	1.85	0.42
10:J:107:TRP:CH2	10:J:118:ALA:HB2	2.54	0.42
12:L:169:HIS:HB2	12:L:184:LYS:HZ3	1.85	0.42
15:O:116:VAL:CG2	17:Q:33:ARG:HD2	2.49	0.42
20:U:90:GLU:O	20:U:141:ARG:NH1	2.53	0.42
20:U:145:TYR:HB2	20:U:165:ILE:CD1	2.49	0.42
27:c:91:ASP:OD1	27:c:91:ASP:N	2.36	0.42
31:g:64:LEU:O	31:g:68:THR:HG23	2.19	0.42
33:i:181:TYR:HA	33:i:184:ILE:CG2	2.49	0.42
33:i:298:TYR:HE1	41:q:134:THR:HG21	1.84	0.42
34:j:52:SER:HB3	34:j:55:PHE:CE2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:q:406:TYR:HA	41:q:409:TYR:HB3	2.00	0.42
42:r:22:LEU:HB2	42:r:48:PRO:HG3	2.01	0.42
46:v:277:ALA:HA	46:v:278:THR:HA	1.67	0.42
47:w:39:ILE:HG23	71:2:301:PLX:H233	2.01	0.42
47:w:378:LYS:NZ	49:y:89:PHE:HD2	2.17	0.42
48:x:115:PHE:CE2	48:x:149:LEU:HD11	2.53	0.42
51:0:86:LEU:O	51:0:89:SER:OG	2.19	0.42
46:6:123:VAL:CG2	46:6:133:LEU:HD23	2.49	0.42
46:6:154:LEU:O	46:6:157:GLN:HB3	2.19	0.42
46:6:204:GLN:HA	46:6:207:TYR:CD2	2.54	0.42
47:7:51:LEU:HD22	76:7:403:HEM:HBD1	2.01	0.42
48:8:98:SER:O	48:8:104:SER:HB2	2.19	0.42
48:8:126:HIS:HB3	48:8:198:LEU:HG	2.02	0.42
56:Ag:35:TYR:HE1	63:An:102:TYR:HD2	1.68	0.42
60:Ak:365:ILE:HD12	61:Al:87:MET:CE	2.34	0.42
61:Al:52:HIS:CD2	64:Ao:40:ASP:HB2	2.54	0.42
63:An:37:GLN:O	63:An:41:LYS:HG2	2.18	0.42
2:B:381:GLN:NE2	2:B:424:ILE:HD11	2.33	0.42
3:C:450:ILE:O	3:C:453:THR:HG22	2.20	0.42
7:G:351:LEU:HD13	7:G:530:TYR:CE2	2.53	0.42
8:H:92:PRO:O	8:H:93:LEU:HD12	2.19	0.42
12:L:131:GLY:CA	72:L:401:NDP:O3D	2.66	0.42
12:L:236:VAL:HG23	12:L:271:TYR:O	2.15	0.42
14:N:18:GLU:OE1	14:N:18:GLU:N	2.40	0.42
14:N:30:LYS:O	14:N:34:VAL:HG12	2.20	0.42
15:O:79:ILE:CG2	15:O:145:VAL:HG13	2.48	0.42
20:U:304:LEU:HD21	33:i:317:PHE:O	2.20	0.42
22:W:90:ASN:HD21	22:W:128:ARG:NH1	2.15	0.42
25:a:57:ILE:CD1	40:p:104:LEU:HD23	2.49	0.42
28:d:13:PRO:HB2	28:d:14:PRO:HD3	2.00	0.42
31:g:92:MET:O	31:g:96:VAL:HG13	2.19	0.42
31:g:96:VAL:HG12	31:g:103:PHE:CE2	2.54	0.42
33:i:287:LEU:HD11	41:q:151:PHE:CD1	2.54	0.42
37:m:51:PHE:O	37:m:55:MET:HG2	2.20	0.42
40:p:44:MET:HE3	40:p:48:PHE:CZ	2.55	0.42
41:q:210:TYR:CG	41:q:268:GLY:HA3	2.54	0.42
42:r:144:VAL:HG23	42:r:145:THR:N	2.34	0.42
42:r:165:LEU:HD21	42:r:241:LEU:HA	2.00	0.42
45:u:79:SER:HB3	45:u:126:ARG:HA	2.02	0.42
45:u:478:LEU:CG	75:u:502:PEE:C5	2.97	0.42
46:v:254:ARG:HA	46:v:435:ARG:NH2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:v:277:ALA:HB1	46:v:278:THR:HB	2.02	0.42
50:z:65:GLN:O	50:z:69:LYS:HG3	2.19	0.42
52:1:56:ILE:O	52:1:56:ILE:HG22	2.19	0.42
71:2:301:PLX:H22	71:2:301:PLX:H1A2	1.65	0.42
45:5:270:PHE:HZ	45:5:455:ALA:H	1.65	0.42
45:5:377:MET:HE1	45:5:450:TYR:CD1	2.54	0.42
45:5:460:GLY:CA	45:5:462:ILE:HG23	2.49	0.42
46:6:83:LEU:HD12	46:6:205:LEU:HD22	2.01	0.42
51:Ab:33:VAL:HG11	51:Ab:86:LEU:HB2	2.01	0.42
62:Am:80:ARG:HG2	62:Am:233:PHE:CE1	2.54	0.42
64:Ao:21:LYS:O	64:Ao:57:ARG:NH1	2.53	0.42
67:Ar:24:ASN:HD22	67:Ar:25:GLN:N	2.18	0.42
4:D:75:GLN:OE1	13:M:68:ILE:HD11	2.20	0.42
5:E:138:THR:HA	5:E:141:MET:HB3	2.00	0.42
7:G:64:CYS:SG	7:G:65:TYR:N	2.92	0.42
7:G:182:CYS:O	7:G:185:PHE:HB3	2.20	0.42
7:G:301:ARG:HH22	7:G:588:ALA:N	2.18	0.42
7:G:540:ASN:HA	7:G:541:PRO:HD3	1.63	0.42
73:Q:201:ZMP:H3	73:Q:201:ZMP:H22	1.76	0.42
20:U:91:ALA:CA	20:U:95:TYR:CB	2.95	0.42
15:X:120:MET:HE3	40:p:25:ARG:NH2	2.34	0.42
25:a:53:ARG:O	25:a:53:ARG:HD3	2.20	0.42
25:a:119:ARG:NH2	28:d:63:TYR:HB3	2.30	0.42
33:i:137:ALA:HB3	33:i:138:PRO:HD3	2.01	0.42
33:i:184:ILE:HG21	33:i:184:ILE:HD13	1.64	0.42
33:i:207:ILE:O	33:i:211:MET:HG2	2.19	0.42
34:j:66:ASP:O	34:j:69:ILE:HG22	2.18	0.42
36:l:247:LEU:HB2	36:l:252:MET:CB	2.49	0.42
36:l:313:MET:HB3	36:l:328:HIS:CD2	2.54	0.42
40:p:104:LEU:HD11	40:p:122:ARG:NE	2.34	0.42
41:q:166:TYR:OH	75:q:501:PEE:O1P	2.30	0.42
43:s:50:GLU:OE1	43:s:50:GLU:N	2.51	0.42
43:s:71:PHE:HA	43:s:74:ILE:HD12	2.01	0.42
45:u:103:ASN:CG	45:u:153:ASN:HD21	2.28	0.42
45:u:182:VAL:HG13	53:2:80:HIS:HB3	2.01	0.42
45:u:437:ASP:O	45:u:441:VAL:HG23	2.20	0.42
45:u:478:LEU:CD1	75:u:502:PEE:H12	2.50	0.42
47:w:130:GLY:HA3	47:w:182:HIS:CE1	2.53	0.42
47:w:234:PHE:CE2	48:x:301:LEU:CD1	2.98	0.42
48:x:108:HIS:ND1	48:x:139:VAL:HG23	2.34	0.42
53:2:225:ILE:HG22	53:2:226:ALA:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:2:301:PLX:H182	75:2:302:PEE:C40	2.35	0.42
53:4:89:SER:HA	53:4:92:ARG:HB3	2.00	0.42
45:5:99:LYS:HB3	45:5:160:GLN:HG2	2.02	0.42
45:5:278:ARG:CB	50:Aa:12:ARG:O	2.68	0.42
46:6:130:ILE:O	46:6:134:MET:HG2	2.20	0.42
48:8:297:MET:O	48:8:301:LEU:HD13	2.20	0.42
74:Aa:101:CDL:HA31	74:Aa:101:CDL:HB22	2.00	0.42
51:Ab:68:THR:HA	51:Ab:71:LEU:HB3	2.01	0.42
78:Ak:601:HEA:HHC	78:Ak:601:HEA:H122	2.02	0.42
65:Ap:82:CYS:HA	65:Ap:83:PRO:HD3	1.90	0.42
3:C:81:THR:HA	3:C:100:GLU:HA	2.02	0.42
3:C:286:TYR:O	4:D:162:ALA:HB1	2.17	0.42
3:C:323:ARG:N	3:C:328:ASP:OD2	2.53	0.42
3:C:375:MET:HA	7:G:126:LEU:CD2	2.49	0.42
3:C:429:PHE:HD1	3:C:461:VAL:HG13	1.84	0.42
5:E:114:GLU:HG2	7:G:197:THR:O	2.20	0.42
7:G:644:SER:O	7:G:647:GLU:HB3	2.19	0.42
7:G:653:LEU:C	7:G:655:ARG:H	2.27	0.42
10:J:101:PHE:CD2	10:J:121:LEU:HD13	2.55	0.42
12:L:236:VAL:H	12:L:325:SER:HB3	1.84	0.42
13:M:69:VAL:O	13:M:71:SER:N	2.52	0.42
21:V:9:TYR:HE1	21:V:25:SER:HB3	1.84	0.42
75:W:401:PEE:O2P	42:r:99:ASN:HB2	2.19	0.42
28:d:96:TYR:HD1	28:d:143:TYR:CZ	2.38	0.42
30:f:46:LEU:O	30:f:50:THR:HG23	2.19	0.42
34:j:59:ALA:O	34:j:62:PHE:HB3	2.19	0.42
36:l:3:PRO:O	36:l:7:LEU:HB2	2.19	0.42
41:q:204:MET:HE3	41:q:298:ILE:HD11	2.02	0.42
44:t:111:ARG:NE	44:t:115:ARG:NH1	2.49	0.42
45:u:361:ASP:OD1	45:u:362:ASN:N	2.52	0.42
48:x:115:PHE:HE2	48:x:149:LEU:HD11	1.85	0.42
49:y:63:ILE:O	49:y:67:LEU:HG	2.20	0.42
53:4:131:ASN:O	53:4:135:GLN:HG2	2.20	0.42
45:5:213:ARG:HA	45:5:216:LEU:HD12	2.02	0.42
45:5:240:ARG:HA	45:5:243:LEU:HB3	2.01	0.42
46:6:65:ILE:HG21	46:6:213:PHE:HD1	1.85	0.42
48:8:264:MET:HA	48:8:267:VAL:HG12	2.01	0.42
50:Aa:46:ILE:HG12	50:Aa:50:ALA:HB2	2.01	0.42
74:Aa:101:CDL:H111	74:Aa:101:CDL:HA4	1.59	0.42
51:Ab:44:ILE:O	51:Ab:48:GLU:HG3	2.19	0.42
56:Ag:37:LEU:HD23	56:Ag:37:LEU:HA	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:Ai:42:PRO:HA	61:Al:5:MET:CE	2.45	0.42
62:Am:40:MET:O	62:Am:41:THR:C	2.62	0.42
62:Am:110:PRO:HB3	67:Ar:30:TRP:CD2	2.54	0.42
67:Ar:84:LYS:HD2	67:Ar:84:LYS:HA	1.83	0.42
2:B:258:GLY:O	2:B:261:TRP:HB3	2.19	0.42
2:B:378:SER:O	2:B:378:SER:OG	2.37	0.42
4:D:111:LEU:HD11	4:D:163:ALA:HB2	1.99	0.42
7:G:333:PHE:HB3	7:G:337:ASP:CB	2.49	0.42
12:L:69:VAL:O	12:L:250:ILE:HD11	2.20	0.42
12:L:141:PHE:HB3	12:L:179:ARG:HH12	1.84	0.42
17:Q:35:LEU:HD22	17:Q:83:VAL:HG23	2.02	0.42
11:R:134:ILE:O	11:R:135:GLN:C	2.60	0.42
20:U:85:LEU:C	20:U:160:VAL:HG12	2.36	0.42
20:U:95:TYR:OH	20:U:147:ASP:OD2	2.25	0.42
27:c:71:GLY:O	39:o:79:ASN:HB2	2.19	0.42
27:c:105:ILE:HG21	27:c:109:LEU:HD22	2.01	0.42
34:j:113:TRP:HB2	34:j:114:ALA:H	1.50	0.42
36:l:81:LYS:HB3	36:l:135:ASN:HB2	2.01	0.42
36:l:387:THR:OG1	36:l:461:SER:O	2.35	0.42
36:l:409:LEU:O	36:l:413:LEU:HG	2.19	0.42
36:l:566:THR:O	36:l:570:GLN:HG2	2.20	0.42
37:m:61:LEU:HG	42:r:111:LEU:HD11	2.01	0.42
38:n:17:VAL:HG11	41:q:30:HIS:ND1	2.35	0.42
39:o:80:PHE:CG	39:o:81:ARG:N	2.87	0.42
41:q:196:TRP:CE3	41:q:197:LEU:HD23	2.52	0.42
42:r:84:THR:O	42:r:87:VAL:HG12	2.20	0.42
43:s:31:HIS:HB3	43:s:117:TRP:CH2	2.54	0.42
45:u:64:SER:N	45:u:235:GLY:O	2.50	0.42
45:u:341:PHE:HA	45:u:357:HIS:O	2.20	0.42
47:w:214:ASP:O	47:w:217:LYS:HG2	2.20	0.42
49:y:76:LEU:HA	49:y:77:PRO:HD3	1.91	0.42
53:4:108:ASP:OD2	52:Ac:12:SER:OG	2.38	0.42
45:5:285:ALA:HB2	45:5:461:PRO:O	2.20	0.42
49:9:77:PRO:HD2	49:9:80:GLN:OE1	2.19	0.42
61:Al:162:SER:HB3	61:Al:197:SER:C	2.44	0.42
66:Aq:77:PRO:HA	66:Aq:82:TYR:HA	2.01	0.42
2:B:447:GLU:O	2:B:450:MET:HB2	2.19	0.42
7:G:198:THR:O	7:G:204:MET:HA	2.20	0.42
12:L:120:VAL:HG21	12:L:155:VAL:CG1	2.50	0.42
15:O:77:GLU:OE1	15:O:77:GLU:N	2.47	0.42
17:Q:19:PRO:HG3	17:Q:23:ARG:HD3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:e:97:ILE:HD12	29:e:101:LEU:HD22	2.01	0.42
32:h:19:THR:HG22	32:h:20:ILE:HG13	2.01	0.42
36:l:137:LEU:HD22	36:l:186:MET:HG3	2.01	0.42
36:l:404:THR:OG1	36:l:405:ASN:N	2.53	0.42
36:l:508:THR:O	40:p:36:LYS:NZ	2.36	0.42
40:p:30:TRP:O	40:p:32:VAL:HG23	2.19	0.42
40:p:97:TYR:HB3	40:p:179:MET:HG2	2.01	0.42
45:u:193:GLN:OE1	45:u:271:THR:HG21	2.20	0.42
75:u:502:PEE:H43	47:w:42:ILE:HG21	2.00	0.42
46:v:183:ARG:HG2	46:6:449:PHE:CE2	2.47	0.42
47:w:147:THR:HG21	47:w:165:TRP:NE1	2.35	0.42
48:x:195:PRO:HB3	77:x:401:HEC:C1D	2.49	0.42
53:2:151:LYS:O	53:2:272:ILE:HG23	2.20	0.42
53:4:226:ALA:O	53:4:228:ALA:N	2.51	0.42
45:5:479:ARG:HH12	74:5:501:CDL:HB21	1.85	0.42
46:6:201:THR:OG1	46:6:204:GLN:HG3	2.20	0.42
48:8:93:PRO:HB2	48:8:95:TYR:CZ	2.54	0.42
55:Ae:42:VAL:HA	55:Ae:46:LYS:NZ	2.35	0.42
58:Ai:9:PHE:C	58:Ai:9:PHE:CD1	2.97	0.42
67:Ar:57:ARG:HA	67:Ar:60:TYR:CD2	2.55	0.42
3:C:317:ASP:HB2	3:C:339:GLN:NE2	2.35	0.42
7:G:464:GLN:O	7:G:467:LYS:HB2	2.20	0.42
7:G:566:ILE:HB	7:G:580:ALA:HA	2.02	0.42
20:U:91:ALA:CA	20:U:95:TYR:CG	3.02	0.42
20:U:150:GLU:CB	20:U:300:VAL:HG12	2.35	0.42
22:W:128:ARG:HD2	22:W:132:GLU:OE1	2.20	0.42
28:d:157:ALA:O	28:d:161:GLN:HG2	2.19	0.42
30:f:66:VAL:O	30:f:69:TYR:HB3	2.20	0.42
36:l:579:ASN:O	36:l:581:LYS:N	2.48	0.42
41:q:66:LEU:HA	41:q:66:LEU:HD12	1.80	0.42
41:q:378:GLU:O	41:q:381:ILE:HG12	2.20	0.42
45:u:478:LEU:HG	75:u:502:PEE:H11	1.99	0.42
75:u:502:PEE:H25	75:u:502:PEE:H53	2.01	0.42
46:v:145:GLU:H	46:v:145:GLU:CD	2.28	0.42
48:x:194:LEU:HA	48:x:195:PRO:HD2	1.91	0.42
53:2:145:ASP:O	53:2:149:MET:HG2	2.20	0.42
71:2:301:PLX:H72	71:2:301:PLX:H101	1.92	0.42
75:2:302:PEE:C30	75:2:302:PEE:H13	2.50	0.42
53:4:234:TYR:CD2	53:4:247:GLY:HA2	2.55	0.42
45:5:328:LEU:HD22	45:5:368:MET:SD	2.60	0.42
45:5:413:ILE:O	45:5:417:LEU:HG	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:7:51:LEU:HB3	76:7:403:HEM:CMD	2.50	0.42
47:7:157:GLY:O	47:7:161:VAL:HG23	2.20	0.42
47:7:221:HIS:HB3	47:7:222:PRO:HD3	2.02	0.42
48:8:202:VAL:HG11	48:8:276:ARG:CD	2.45	0.42
52:Ac:53:TRP:O	52:Ac:57:LYS:HG3	2.20	0.42
61:Al:146:MET:SD	61:Al:189:PRO:HB3	2.60	0.42
61:Al:193:TYR:N	61:Al:193:TYR:CD1	2.88	0.42
65:Ap:35:ALA:HA	65:Ap:36:PRO:HD3	1.91	0.42
2:B:207:GLY:HA3	69:B:502:FMN:C5A	2.50	0.41
3:C:228:ARG:HH11	3:C:233:HIS:CE1	2.38	0.41
7:G:170:LYS:HG2	7:G:172:ILE:HD11	2.01	0.41
7:G:490:LEU:C	7:G:490:LEU:CD2	2.93	0.41
71:H:303:PLX:H222	71:H:303:PLX:H191	1.66	0.41
14:N:51:ILE:HA	14:N:54:GLU:OE1	2.19	0.41
19:T:67:PRO:CB	19:T:72:ASP:HB2	2.50	0.41
20:U:107:ASP:OD1	20:U:110:LEU:HG	2.20	0.41
25:a:108:GLU:HG2	25:a:111:GLU:CA	2.49	0.41
28:d:82:ILE:HD11	41:q:182:TRP:HZ2	1.84	0.41
28:d:149:HIS:CE1	41:q:248:THR:HG22	2.55	0.41
35:k:19:LEU:N	35:k:32:CYS:SG	2.93	0.41
35:k:68:ALA:HB1	37:m:64:MET:HE2	2.01	0.41
36:l:250:SER:O	36:l:254:VAL:HG22	2.20	0.41
36:l:353:GLU:OE1	36:l:353:GLU:N	2.53	0.41
39:o:125:PHE:C	39:o:127:ILE:H	2.25	0.41
41:q:196:TRP:CH2	41:q:200:ILE:HG13	2.55	0.41
42:r:94:PRO:HB2	42:r:96:ILE:O	2.20	0.41
43:s:41:LYS:HG3	43:s:129:THR:HG21	2.02	0.41
43:s:42:GLU:OE1	43:s:133:THR:OG1	2.32	0.41
43:s:124:GLU:O	43:s:127:LYS:HG2	2.19	0.41
46:v:137:LEU:O	46:v:141:THR:N	2.50	0.41
46:6:290:GLN:HG3	46:6:291:HIS:N	2.34	0.41
47:7:133:LEU:HB2	47:7:134:PRO:HD3	2.02	0.41
48:8:208:GLY:H	48:8:211:TYR:HB3	1.85	0.41
48:8:307:MET:O	48:8:311:LYS:HG2	2.20	0.41
49:9:48:ILE:HG22	49:9:49:ARG:NH1	2.35	0.41
51:Ab:75:LEU:HA	51:Ab:78:ARG:HG2	2.02	0.41
2:B:319:PRO:O	2:B:350:GLY:HA3	2.20	0.41
2:B:363:ILE:HG21	2:B:442:PHE:HD2	1.85	0.41
3:C:95:LEU:HD13	3:C:458:PHE:CE2	2.55	0.41
3:C:179:ARG:HH12	3:C:303:ARG:CZ	2.34	0.41
4:D:116:ALA:HB3	4:D:174:PHE:CE2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:85:ALA:HA	7:G:86:PRO:HD3	1.79	0.41
7:G:259:SER:CB	7:G:282:ASN:HB3	2.46	0.41
7:G:282:ASN:HB2	7:G:285:TRP:O	2.20	0.41
8:H:101:HIS:NE2	8:H:169:GLU:OE2	2.53	0.41
12:L:141:PHE:CZ	12:L:180:TYR:HB3	2.50	0.41
20:U:202:PRO:HA	20:U:203:PRO:HD3	1.87	0.41
21:V:5:LEU:O	21:V:8:LYS:HB3	2.20	0.41
15:X:104:PHE:CZ	15:X:118:ILE:HG12	2.55	0.41
15:X:118:ILE:HA	24:Z:45:TRP:CZ2	2.55	0.41
24:Z:61:VAL:HG21	36:l:364:LYS:HE3	2.02	0.41
25:a:70:LEU:HD13	29:e:87:MET:CE	2.49	0.41
25:a:157:ARG:NH2	31:g:3:MET:SD	2.92	0.41
28:d:5:TRP:O	28:d:9:VAL:N	2.53	0.41
33:i:54:GLU:OE1	35:k:92:ASN:HA	2.20	0.41
33:i:172:GLN:HG2	33:i:177:LYS:CD	2.44	0.41
33:i:216:PHE:O	33:i:220:ILE:HG12	2.20	0.41
34:j:73:LEU:HD23	34:j:73:LEU:HA	1.73	0.41
41:q:29:VAL:HG13	41:q:30:HIS:N	2.34	0.41
41:q:370:PRO:HA	41:q:371:PRO:HA	1.68	0.41
43:s:42:GLU:O	43:s:46:CYS:HB3	2.20	0.41
45:u:277:HIS:CD2	50:z:15:ILE:HD12	2.55	0.41
45:u:375:GLN:O	45:u:378:ARG:HB3	2.20	0.41
46:v:103:ILE:HG23	46:v:109:LYS:HA	2.00	0.41
48:x:195:PRO:HB3	77:x:401:HEC:C2D	2.51	0.41
52:1:22:ALA:HA	52:1:25:ILE:HD12	2.02	0.41
53:2:231:PHE:CE2	53:2:250:ARG:HG3	2.55	0.41
53:2:261:PRO:O	53:2:263:TYR:HD1	2.02	0.41
54:3:4:ARG:O	54:3:6:LEU:N	2.53	0.41
53:4:191:GLU:OE1	53:4:193:SER:N	2.53	0.41
46:6:183:ARG:HB2	46:6:252:LYS:CG	2.50	0.41
47:7:14:ILE:HA	47:7:17:ALA:HB3	2.02	0.41
47:7:18:PHE:O	47:7:220:PHE:HB3	2.20	0.41
47:7:352:GLN:O	47:7:356:ILE:HG12	2.19	0.41
56:Ag:40:TYR:CZ	59:Aj:41:ARG:HD2	2.54	0.41
60:Ak:106:PRO:HB2	60:Ak:107:PRO:HD3	2.01	0.41
65:Ap:86:GLY:O	65:Ap:87:THR:O	2.38	0.41
2:B:51:TRP:HB2	2:B:135:PRO:HD3	2.02	0.41
2:B:338:ASP:N	2:B:338:ASP:OD1	2.52	0.41
2:B:369:ARG:HH21	5:E:136:THR:HB	1.86	0.41
3:C:162:GLN:HA	3:C:163:PRO:HD3	1.83	0.41
4:D:218:ARG:CG	17:Q:101:THR:HG22	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:84:ASP:O	5:E:88:ARG:N	2.51	0.41
7:G:65:TYR:CG	7:G:66:HIS:N	2.88	0.41
7:G:128:CYS:N	7:G:129:PRO:HD2	2.35	0.41
12:L:370:LYS:HA	12:L:371:PRO:HD3	1.94	0.41
12:L:373:LYS:HE3	12:L:373:LYS:HB2	1.70	0.41
72:L:401:NDP:O2X	72:L:401:NDP:O3B	2.33	0.41
14:N:16:VAL:HA	14:N:78:GLU:OE2	2.19	0.41
14:N:24:LEU:O	14:N:27:LEU:HB2	2.20	0.41
16:P:63:PRO:O	16:P:79:LEU:HG	2.20	0.41
17:Q:96:VAL:O	17:Q:96:VAL:HG12	2.20	0.41
20:U:296:LEU:C	20:U:296:LEU:CD2	2.93	0.41
23:Y:47:PHE:O	23:Y:47:PHE:CD1	2.73	0.41
32:h:3:PHE:HB2	33:i:144:GLN:HG2	2.02	0.41
32:h:3:PHE:HD1	33:i:144:GLN:NE2	2.17	0.41
33:i:190:MET:CE	33:i:205:LEU:HA	2.48	0.41
75:i:501:PEE:H57	41:q:151:PHE:CE2	2.56	0.41
34:j:83:ASN:OD1	37:m:148:SER:HB2	2.19	0.41
35:k:80:MET:CE	37:m:172:THR:HA	2.49	0.41
36:l:1:MET:O	36:l:4:PHE:HB3	2.21	0.41
36:l:68:TRP:CE3	36:l:76:LEU:HD11	2.53	0.41
36:l:542:LEU:HD23	36:l:542:LEU:HA	1.84	0.41
38:n:27:LEU:HB3	41:q:2:LEU:HD23	2.02	0.41
39:o:15:PRO:HG2	39:o:18:LEU:HD13	2.01	0.41
40:p:167:TRP:CD1	40:p:167:TRP:H	2.38	0.41
42:r:260:VAL:HA	42:r:263:THR:HG22	2.02	0.41
45:u:305:GLN:NE2	45:u:345:ASN:HB3	2.35	0.41
74:u:501:CDL:H141	75:u:502:PEE:C34	2.30	0.41
46:v:79:THR:HG23	46:v:205:LEU:HD23	2.03	0.41
46:v:261:GLN:HA	46:v:442:GLY:O	2.20	0.41
47:w:130:GLY:O	47:w:134:PRO:HD3	2.21	0.41
48:x:157:ASP:OD1	48:x:158:GLY:N	2.53	0.41
48:x:271:VAL:O	48:x:275:LEU:HG	2.19	0.41
51:0:78:ARG:O	51:0:82:VAL:HG23	2.20	0.41
47:7:215:MET:HG3	47:7:216:ASP:CG	2.45	0.41
48:8:322:TYR:HB2	49:9:61:PHE:CD2	2.55	0.41
60:Ak:276:ALA:O	60:Ak:280:ILE:HG13	2.21	0.41
60:Ak:354:THR:HG21	60:Ak:376:HIS:HA	2.02	0.41
67:Ar:65:PRO:HG2	67:Ar:68:TRP:CG	2.56	0.41
2:B:135:PRO:O	2:B:138:LEU:HB3	2.21	0.41
3:C:169:TRP:CZ2	3:C:350:LYS:HE2	2.55	0.41
3:C:397:TYR:CE2	4:D:140:ARG:NH1	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:149:ASP:OD1	7:G:150:ARG:N	2.52	0.41
7:G:354:LEU:O	7:G:357:LEU:HB3	2.19	0.41
7:G:472:PRO:HB2	7:G:500:ILE:HD13	2.03	0.41
16:P:21:ILE:HG13	16:P:64:LYS:O	2.20	0.41
17:Q:61:ASP:O	17:Q:65:GLU:HG3	2.20	0.41
20:U:167:SER:O	20:U:170:VAL:HG12	2.20	0.41
20:U:230:LYS:O	20:U:231:ILE:C	2.63	0.41
22:W:69:ILE:HD12	22:W:69:ILE:HA	1.85	0.41
22:W:73:PRO:O	22:W:76:GLN:HB3	2.21	0.41
22:W:108:GLU:O	32:h:75:ARG:NH2	2.53	0.41
28:d:80:LYS:HA	41:q:182:TRP:CH2	2.55	0.41
32:h:2:PRO:HB3	71:i:502:PLX:H1B3	2.02	0.41
40:p:10:LEU:HD21	40:p:15:LYS:HB2	2.02	0.41
40:p:20:TYR:HD1	40:p:48:PHE:CE2	2.35	0.41
45:u:480:PHE:CE1	52:l:17:ARG:HG3	2.55	0.41
47:w:9:PRO:O	47:w:12:LYS:HB2	2.21	0.41
47:w:97:HIS:HE1	47:w:100:ARG:HH21	1.66	0.41
47:w:119:LEU:O	47:w:123:VAL:HG23	2.20	0.41
47:w:169:SER:OG	47:w:170:VAL:N	2.54	0.41
47:w:315:MET:CE	47:w:318:ARG:HH22	2.34	0.41
49:y:19:LYS:O	49:y:22:TYR:HB3	2.21	0.41
53:2:216:VAL:O	53:2:258:LEU:HD22	2.21	0.41
53:4:111:LYS:HG2	50:Aa:22:PHE:CD1	2.56	0.41
45:5:269:ARG:NH1	45:5:271:THR:HG22	2.36	0.41
46:6:38:LEU:HD22	46:6:406:TYR:CE2	2.56	0.41
46:6:396:VAL:HA	46:6:399:GLN:NE2	2.36	0.41
47:7:14:ILE:HG22	47:7:19:ILE:HG13	2.02	0.41
47:7:132:VAL:CG2	47:7:143:ALA:HB2	2.51	0.41
47:7:221:HIS:HA	47:7:225:THR:HG23	2.03	0.41
50:Aa:30:TYR:CD1	74:Aa:101:CDL:H172	2.55	0.41
55:Af:29:LEU:O	55:Af:31:GLN:N	2.54	0.41
55:Af:42:VAL:HG12	55:Af:43:LEU:HB2	2.02	0.41
60:Ak:311:ILE:HG21	60:Ak:311:ILE:HD13	1.74	0.41
60:Ak:474:GLU:HG3	60:Ak:475:ALA:N	2.35	0.41
61:Al:164:ALA:HB2	61:Al:171:LYS:HD3	2.03	0.41
62:Am:188:ILE:H	62:Am:188:ILE:HG13	1.62	0.41
63:An:130:PRO:O	63:An:136:ALA:HB2	2.20	0.41
65:Ap:10:GLU:HG2	65:Ap:25:ARG:HH22	1.86	0.41
1:A:35:TYR:O	1:A:39:VAL:HB	2.20	0.41
2:B:115:VAL:HB	2:B:156:ILE:HG12	2.02	0.41
3:C:122:LYS:NZ	4:D:202:PHE:O	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:ARG:NH2	22:W:11:PRO:HD2	2.31	0.41
3:C:356:ILE:HD12	3:C:357:LYS:N	2.36	0.41
7:G:177:ILE:O	7:G:179:CYS:N	2.54	0.41
7:G:236:TYR:O	7:G:236:TYR:CG	2.73	0.41
7:G:236:TYR:CZ	7:G:272:ARG:HD3	2.55	0.41
7:G:345:LEU:HD11	7:G:698:ASP:HB2	2.03	0.41
7:G:366:LEU:HD13	7:G:530:TYR:HD1	1.85	0.41
12:L:201:ILE:CG2	12:L:203:PRO:HG3	2.48	0.41
19:T:62:ASN:O	19:T:63:MET:HB2	2.20	0.41
36:l:361:GLY:HA3	36:l:433:GLY:O	2.21	0.41
39:o:6:TYR:HE2	39:o:14:LEU:HA	1.85	0.41
39:o:126:ASN:OD1	39:o:126:ASN:N	2.53	0.41
40:p:59:LYS:HG3	40:p:63:LEU:HD13	2.03	0.41
41:q:115:LEU:HA	41:q:118:PHE:HB3	2.02	0.41
42:r:269:THR:O	42:r:273:ILE:HG12	2.20	0.41
45:u:75:ILE:HG21	45:u:224:TYR:HD1	1.82	0.41
45:u:245:LEU:HA	45:u:248:LYS:NZ	2.34	0.41
46:v:253:TYR:HE2	46:v:435:ARG:HE	1.66	0.41
47:w:137:GLN:HB2	47:w:257:THR:OG1	2.20	0.41
47:w:156:ILE:H	47:w:156:ILE:HD12	1.85	0.41
48:x:125:CYS:H	77:x:401:HEC:CBB	2.34	0.41
50:z:4:GLU:HG2	50:z:5:PHE:H	1.85	0.41
51:0:51:GLU:O	51:0:55:GLN:HG2	2.19	0.41
45:5:75:ILE:HB	45:5:129:THR:O	2.20	0.41
45:5:126:ARG:NH2	45:5:200:SER:HA	2.36	0.41
45:5:146:LEU:O	45:5:150:ILE:HG13	2.19	0.41
45:5:377:MET:HE1	45:5:450:TYR:HD1	1.85	0.41
46:6:221:ILE:HG22	46:6:393:LEU:HG	2.01	0.41
47:7:82:LEU:HD23	47:7:243:VAL:HG11	2.02	0.41
47:7:333:ILE:HD13	75:7:402:PEE:H62	2.02	0.41
47:7:374:ASN:O	47:7:379:TRP:N	2.52	0.41
48:8:250:TYR:CE2	48:8:253:VAL:HA	2.55	0.41
56:Ag:19:LEU:HD23	56:Ag:19:LEU:C	2.45	0.41
57:Ah:5:VAL:O	57:Ah:9:GLN:HG3	2.21	0.41
60:Ak:198:SER:HB2	60:Ak:238:PHE:HA	2.03	0.41
62:Am:224:LYS:NZ	62:Am:226:HIS:HE2	2.18	0.41
2:B:116:ASN:HB2	2:B:242:VAL:CG1	2.51	0.41
2:B:390:ASP:OD2	7:G:202:ASN:ND2	2.52	0.41
3:C:188:THR:CG2	3:C:200:PHE:HA	2.51	0.41
5:E:78:ALA:O	5:E:82:VAL:HG23	2.21	0.41
7:G:531:LYS:HA	7:G:532:PRO:C	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:639:LEU:O	7:G:642:VAL:HG12	2.20	0.41
14:N:114:TRP:HA	14:N:115:PRO:C	2.46	0.41
16:P:41:TYR:OH	16:P:45:LYS:NZ	2.53	0.41
21:V:9:TYR:HD1	21:V:24:ALA:HB3	1.85	0.41
22:W:125:TYR:CD2	22:W:128:ARG:HG3	2.56	0.41
25:a:98:LEU:HD12	28:d:64:TYR:HA	2.03	0.41
25:a:174:ILE:CG2	32:h:20:ILE:HD11	2.47	0.41
27:c:115:ASN:HA	36:l:166:THR:HG22	2.02	0.41
32:h:40:TRP:NE1	32:h:60:PHE:HB2	2.36	0.41
33:i:117:GLU:OE2	35:k:97:GLN:HA	2.21	0.41
33:i:203:LEU:HD11	33:i:261:MET:HE3	2.03	0.41
34:j:34:THR:OG1	42:r:64:ALA:N	2.54	0.41
34:j:72:LEU:HA	34:j:72:LEU:HD23	1.81	0.41
36:l:102:GLU:O	36:l:449:LEU:HD13	2.20	0.41
36:l:226:GLN:CD	36:l:280:LEU:HD22	2.45	0.41
36:l:591:PHE:O	36:l:594:THR:HG22	2.19	0.41
40:p:53:ASN:N	40:p:53:ASN:OD1	2.53	0.41
40:p:101:GLU:O	40:p:104:LEU:HG	2.21	0.41
40:p:120:ALA:O	40:p:124:GLN:HG3	2.20	0.41
42:r:32:GLN:O	42:r:33:LEU:HB2	2.20	0.41
42:r:196:ALA:HB3	42:r:197:PRO:CD	2.51	0.41
45:u:39:ALA:O	45:u:42:LEU:HB2	2.21	0.41
45:u:432:ARG:O	45:u:435:GLU:HB3	2.20	0.41
75:u:502:PEE:H19	75:u:502:PEE:C30	2.47	0.41
47:w:8:HIS:CE1	47:7:199:PHE:CE1	3.06	0.41
47:w:361:ILE:HA	47:w:365:LEU:HD12	2.02	0.41
46:6:174:LEU:O	46:6:178:HIS:CD2	2.73	0.41
46:6:227:HIS:N	46:6:228:PRO:HD2	2.35	0.41
46:6:260:ASP:O	46:6:441:SER:HA	2.20	0.41
46:6:428:ALA:O	46:6:431:PHE:HB3	2.21	0.41
47:7:59:THR:OG1	47:7:172:LYS:HB3	2.21	0.41
47:7:260:ASN:HA	47:7:261:PRO:HD3	1.94	0.41
60:Ak:168:ILE:CG2	60:Ak:189:MET:HG3	2.51	0.41
60:Ak:356:ILE:HD13	60:Ak:356:ILE:HA	1.90	0.41
60:Ak:501:PRO:O	60:Ak:502:TYR:C	2.63	0.41
3:C:224:ALA:O	3:C:226:TYR:N	2.53	0.41
4:D:87:PHE:CE2	14:N:112:TRP:CE3	3.08	0.41
4:D:238:PRO:HB2	4:D:239:TRP:CD1	2.56	0.41
5:E:134:VAL:HG23	5:E:186:VAL:HG22	2.01	0.41
5:E:140:CYS:O	5:E:145:SER:N	2.54	0.41
7:G:355:LYS:HD2	7:G:530:TYR:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:38:TYR:HB3	13:M:104:TRP:HE3	1.86	0.41
8:H:129:THR:HB	8:H:146:ASP:OD1	2.20	0.41
12:L:241:TYR:HB2	12:L:343:THR:OG1	2.21	0.41
21:V:62:THR:HG22	21:V:104:ARG:HG3	2.01	0.41
27:c:63:GLU:O	27:c:77:LYS:N	2.54	0.41
31:g:51:ARG:O	31:g:53:ARG:HG2	2.21	0.41
32:h:71:LYS:HA	32:h:74:LYS:HE3	2.03	0.41
36:l:52:LEU:HA	36:l:55:MET:HG2	2.03	0.41
39:o:51:TYR:CD2	39:o:52:ASN:HB3	2.56	0.41
42:r:20:LEU:HD22	42:r:232:ILE:HG23	2.02	0.41
43:s:50:GLU:HG3	43:s:55:ARG:HG3	2.03	0.41
43:s:96:LEU:HD12	43:s:99:HIS:CB	2.50	0.41
45:u:63:GLN:NE2	45:u:237:VAL:O	2.53	0.41
47:w:313:ARG:HD2	49:y:39:TYR:CD1	2.56	0.41
48:x:95:TYR:N	48:x:210:ASP:OD2	2.54	0.41
48:x:203:ARG:HD2	48:x:279:SER:O	2.20	0.41
48:x:288:ARG:NH2	52:l:44:TYR:HD2	2.19	0.41
49:y:72:ARG:C	49:y:74:GLN:H	2.29	0.41
53:4:133:VAL:CG1	75:5:502:PEE:H72	2.47	0.41
45:5:144:VAL:HG11	45:5:245:LEU:HG	2.02	0.41
45:5:278:ARG:HH12	45:5:463:GLU:CB	2.33	0.41
46:6:173:VAL:HG11	46:6:268:HIS:O	2.20	0.41
46:6:286:PHE:HZ	46:6:430:LYS:HD3	1.85	0.41
46:6:326:PHE:CG	46:6:327:ASN:N	2.89	0.41
47:7:131:TYR:O	47:7:134:PRO:HD2	2.20	0.41
48:8:180:TYR:CD2	48:8:186:ALA:HB2	2.55	0.41
48:8:238:PHE:CD1	48:8:243:ILE:HD12	2.56	0.41
55:Af:43:LEU:HD12	55:Af:46:LYS:HE2	2.03	0.41
57:Ah:12:PHE:O	57:Ah:23:LYS:HE2	2.21	0.41
60:Ak:23:GLY:HA3	60:Ak:73:ILE:HG13	2.03	0.41
63:An:137:LYS:O	63:An:145:TRP:HE3	2.03	0.41
64:Ao:104:LEU:HA	64:Ao:104:LEU:HD23	1.88	0.41
65:Ap:49:VAL:O	65:Ap:91:LEU:HD12	2.21	0.41
67:Ar:20:PHE:N	67:Ar:21:PRO:HD3	2.35	0.41
3:C:97:LEU:HD21	3:C:109:CYS:CB	2.51	0.41
3:C:129:TYR:CE2	3:C:419:PRO:HB3	2.55	0.41
3:C:202:TRP:CZ3	3:C:261:MET:SD	3.14	0.41
4:D:242:PHE:HA	4:D:243:PRO:HD2	1.89	0.41
7:G:217:GLU:O	7:G:288:ASP:HB2	2.20	0.41
7:G:282:ASN:N	7:G:282:ASN:OD1	2.53	0.41
9:I:118:ARG:NH2	34:j:35:SER:O	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:119:ASP:HA	10:J:120:PRO:HD3	1.84	0.41
12:L:283:VAL:HG12	12:L:369:VAL:HG21	2.02	0.41
14:N:14:LEU:HD11	14:N:78:GLU:HG2	2.03	0.41
20:U:163:ARG:O	20:U:167:SER:OG	2.37	0.41
20:U:305:GLU:HA	20:U:308:ASN:HB2	2.03	0.41
25:a:65:ARG:O	25:a:69:LYS:HG2	2.20	0.41
27:c:65:TYR:CG	27:c:72:TYR:CE1	3.09	0.41
27:c:82:SER:HB2	27:c:119:THR:H	1.85	0.41
27:c:127:ASN:O	27:c:131:LYS:HG3	2.21	0.41
33:i:170:LEU:C	33:i:295:ARG:HH22	2.29	0.41
33:i:199:THR:HA	33:i:202:ILE:HG22	2.02	0.41
33:i:211:MET:HE1	33:i:250:SER:HB3	2.03	0.41
71:i:502:PLX:H1B2	71:i:502:PLX:H21	1.67	0.41
34:j:26:GLN:O	34:j:27:LEU:HD12	2.21	0.41
42:r:210:GLY:O	42:r:213:VAL:HG23	2.21	0.41
45:u:186:TYR:HB3	45:u:275:ILE:HG21	2.03	0.41
45:u:470:ARG:O	45:u:473:SER:HB2	2.21	0.41
46:v:162:LYS:HZ2	46:v:166:PHE:HE2	1.67	0.41
47:w:53:MET:SD	53:2:140:MET:HG2	2.61	0.41
47:w:160:LEU:HD23	47:w:164:ILE:CD1	2.48	0.41
49:y:18:ARG:HA	49:y:21:TYR:HB3	2.03	0.41
50:z:37:ASN:HA	50:z:40:ARG:HG2	2.03	0.41
53:4:234:TYR:HD2	53:4:247:GLY:HA2	1.85	0.41
45:5:66:GLN:HB2	45:5:235:GLY:HA2	2.02	0.41
45:5:91:TYR:CD1	45:5:202:GLU:HA	2.56	0.41
45:5:93:VAL:HG11	45:5:224:TYR:CE2	2.56	0.41
46:6:327:ASN:HA	46:6:335:LEU:O	2.21	0.41
46:6:425:ILE:O	46:6:429:LYS:HG3	2.21	0.41
47:7:158:THR:O	47:7:162:GLU:HG3	2.20	0.41
47:7:186:PRO:O	47:7:189:ILE:HB	2.21	0.41
58:Ai:25:CYS:HB2	63:An:86:MET:O	2.21	0.41
60:Ak:461:SER:O	60:Ak:465:VAL:HG13	2.21	0.41
62:Am:146:TRP:NE1	66:Aq:17:ARG:HB2	2.35	0.41
65:Ap:16:LEU:O	65:Ap:20:VAL:HG13	2.21	0.41
2:B:57:GLN:C	2:B:60:GLY:H	2.29	0.41
2:B:291:GLU:HB3	2:B:294:VAL:HG13	2.03	0.41
2:B:314:LEU:HA	2:B:329:LYS:HA	2.01	0.41
2:B:410:ASP:OD2	13:M:50:SER:HB2	2.20	0.41
3:C:80:LEU:HD12	3:C:101:LEU:HD11	2.02	0.41
3:C:97:LEU:HD21	3:C:109:CYS:HB2	2.02	0.41
3:C:229:PRO:HG3	3:C:389:TYR:OH	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:61:PHE:CE1	13:M:97:PRO:HG3	2.56	0.41
4:D:66:ALA:O	4:D:70:PRO:HB3	2.21	0.41
7:G:31:LEU:HD12	7:G:31:LEU:O	2.20	0.41
7:G:68:ARG:NH2	7:G:277:MET:HE3	2.36	0.41
7:G:278:HIS:CE1	7:G:280:ASP:HB2	2.56	0.41
7:G:313:LEU:HD22	11:R:141:SER:C	2.45	0.41
7:G:462:PHE:CE1	7:G:465:ILE:HD11	2.55	0.41
7:G:652:ASN:CA	7:G:655:ARG:HE	2.34	0.41
8:H:38:TYR:CZ	13:M:106:LEU:HD12	2.56	0.41
8:H:73:THR:HG23	42:r:272:TRP:NE1	2.36	0.41
9:I:95:GLU:HG3	9:I:187:PRO:HB2	2.01	0.41
10:J:84:ARG:NH1	10:J:88:GLN:O	2.54	0.41
10:J:137:PHE:HA	10:J:140:LYS:HE2	2.03	0.41
12:L:171:ASN:HA	12:L:327:MET:HE3	2.02	0.41
17:Q:97:TRP:CD1	17:Q:97:TRP:N	2.87	0.41
17:Q:97:TRP:O	17:Q:98:LYS:HB2	2.21	0.41
19:T:36:SER:HA	19:T:37:PRO:HD2	1.84	0.41
20:U:66:GLY:HA3	20:U:75:LEU:CB	2.50	0.41
21:V:135:VAL:HG13	21:V:136:PHE:N	2.36	0.41
15:X:132:ASP:HB3	40:p:18:ARG:HD3	2.03	0.41
27:c:42:PRO:HB3	27:c:64:PRO:CB	2.51	0.41
28:d:14:PRO:HB3	28:d:109:ARG:NH1	2.36	0.41
28:d:94:ARG:HG2	41:q:47:GLU:OE2	2.21	0.41
29:e:76:TYR:HD1	41:q:81:GLN:HE21	1.68	0.41
29:e:93:PHE:CD2	41:q:29:VAL:HG23	2.56	0.41
29:e:143:ASP:HA	29:e:144:PRO:HD3	1.86	0.41
33:i:207:ILE:HA	33:i:207:ILE:HD13	1.82	0.41
36:l:84:TYR:HE1	36:l:472:ILE:HD12	1.85	0.41
36:l:90:ILE:HB	36:l:91:PRO:HD3	2.03	0.41
36:l:108:MET:O	36:l:111:ASP:N	2.39	0.41
36:l:247:LEU:HD13	36:l:252:MET:SD	2.61	0.41
36:l:257:VAL:O	36:l:261:ILE:HG13	2.21	0.41
36:l:297:ASP:OD2	36:l:300:LYS:HG2	2.21	0.41
36:l:297:ASP:HB3	36:l:300:LYS:HB2	2.03	0.41
36:l:383:MET:HB3	36:l:384:PRO:HD2	2.02	0.41
36:l:513:PHE:HB2	40:p:40:PHE:CE2	2.56	0.41
36:l:552:LEU:HA	36:l:556:ILE:CG2	2.51	0.41
38:n:30:ARG:HD3	38:n:30:ARG:HA	1.85	0.41
40:p:120:ALA:HA	40:p:123:GLU:OE1	2.21	0.41
41:q:55:THR:HG23	41:q:56:PHE:CD2	2.56	0.41
41:q:196:TRP:CZ3	41:q:200:ILE:HG13	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:q:426:ILE:O	41:q:427:LYS:HD2	2.20	0.41
43:s:137:LEU:HA	43:s:138:PRO:HD3	1.89	0.41
45:u:296:TRP:CD1	45:u:419:THR:HG23	2.55	0.41
45:u:377:MET:HE2	45:u:477:TRP:H	1.86	0.41
46:v:84:ARG:NH1	55:Af:13:PRO:HB2	2.36	0.41
46:v:284:ASN:O	46:v:288:VAL:HG23	2.21	0.41
47:w:77:TRP:HZ3	48:x:286:ARG:HD3	1.78	0.41
47:w:183:PHE:CG	47:7:183:PHE:HE2	2.39	0.41
47:w:379:TRP:CD1	49:y:34:ARG:HH11	2.39	0.41
48:x:114:GLY:HA3	48:x:270:ASP:O	2.21	0.41
48:x:292:LYS:HE3	48:x:292:LYS:HB2	1.83	0.41
48:x:299:LEU:HD21	48:x:303:LEU:HD12	2.02	0.41
48:x:300:LEU:HD23	48:x:300:LEU:HA	1.78	0.41
48:x:318:ARG:NH1	48:x:320:LEU:HD23	2.28	0.41
50:z:44:ALA:O	50:z:48:ARG:NH1	2.54	0.41
53:2:165:MET:HB3	53:2:176:VAL:HG23	2.03	0.41
54:3:18:ILE:N	54:3:19:PRO:CD	2.84	0.41
53:4:164:ASN:HA	53:4:177:ARG:HB2	2.02	0.41
53:4:242:HIS:ND1	53:4:251:LYS:HD3	2.36	0.41
45:5:91:TYR:HB2	45:5:201:VAL:O	2.20	0.41
45:5:99:LYS:HD2	45:5:160:GLN:CD	2.46	0.41
45:5:140:LEU:O	45:5:144:VAL:HG23	2.21	0.41
45:5:143:ALA:O	45:5:146:LEU:HB3	2.21	0.41
45:5:417:LEU:HD23	45:5:421:GLY:O	2.20	0.41
45:5:453:CYS:HA	45:5:454:PRO:HD3	1.93	0.41
46:6:63:LEU:HA	46:6:220:LEU:HA	2.03	0.41
46:6:87:SER:HB3	46:6:112:VAL:HG21	2.02	0.41
46:6:219:ALA:O	46:6:221:ILE:HD12	2.20	0.41
47:7:15:ASN:HA	47:7:19:ILE:HB	2.01	0.41
47:7:80:ARG:HB2	76:7:403:HEM:O2D	2.21	0.41
47:7:85:ASN:HB3	47:7:242:LEU:HD22	2.02	0.41
48:8:95:TYR:HB2	48:8:210:ASP:OD1	2.20	0.41
48:8:245:MET:HG3	77:8:402:HEC:NC	2.36	0.41
48:8:294:LEU:HA	48:8:294:LEU:HD23	1.83	0.41
49:9:54:ASN:OD1	49:9:55:LEU:HG	2.21	0.41
50:Aa:4:GLU:HB2	50:Aa:7:HIS:CE1	2.56	0.41
50:Aa:35:ILE:N	50:Aa:36:PRO:HD2	2.36	0.41
54:Ad:12:GLU:HA	54:Ad:15:ARG:HE	1.86	0.41
54:Ad:12:GLU:HA	54:Ad:15:ARG:HH21	1.85	0.41
54:Ad:45:VAL:HA	54:Ad:46:PRO:HD3	1.88	0.41
55:Ae:43:LEU:HA	55:Ae:46:LYS:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:Ak:314:ILE:HB	60:Ak:315:PRO:CD	2.50	0.41
60:Ak:430:PHE:O	60:Ak:431:LEU:C	2.64	0.41
2:B:373:PHE:CD1	5:E:175:GLU:HB3	2.56	0.41
3:C:139:LEU:HD11	3:C:424:ILE:HD13	2.02	0.41
5:E:74:HIS:NE2	10:J:166:TRP:HB3	2.36	0.41
5:E:129:LYS:HE2	5:E:168:LEU:HD21	2.03	0.41
7:G:278:HIS:HB3	7:G:282:ASN:OD1	2.21	0.41
7:G:646:LEU:HD22	7:G:653:LEU:HD22	2.03	0.41
8:H:42:ASN:C	8:H:44:ARG:N	2.75	0.41
8:H:63:TRP:CZ2	71:H:303:PLX:H82	2.55	0.41
9:I:159:GLY:C	9:I:161:GLY:N	2.79	0.41
9:I:208:LYS:HB2	9:I:211:ARG:HG3	2.02	0.41
12:L:83:PRO:HG3	12:L:119:VAL:HG21	2.03	0.41
72:L:401:NDP:O3B	72:L:401:NDP:P2B	2.79	0.41
15:O:84:LEU:HD11	15:O:100:VAL:CG2	2.50	0.41
15:X:79:ILE:CG2	15:X:145:VAL:HG13	2.51	0.41
29:e:67:TYR:HA	29:e:70:ASN:O	2.21	0.41
31:g:84:MET:HE3	33:i:347:ASN:HB3	2.03	0.41
35:k:1:MET:O	37:m:120:ASN:N	2.39	0.41
36:l:373:LEU:HD23	36:l:431:PHE:CE2	2.56	0.41
39:o:72:ARG:HH22	41:q:278:ARG:HH21	1.68	0.41
41:q:354:LEU:HG	41:q:358:TRP:NE1	2.35	0.41
42:r:26:LYS:HA	42:r:26:LYS:HD2	1.91	0.41
44:t:56:ARG:O	44:t:60:ALA:HB2	2.22	0.41
46:v:65:ILE:HG13	46:v:218:MET:HE3	2.01	0.41
46:v:322:ASP:HB3	46:v:341:ILE:HD13	2.03	0.41
47:w:316:MET:HG3	47:w:317:PHE:CD1	2.55	0.41
52:1:33:GLU:HA	53:2:127:TYR:CE1	2.55	0.41
53:4:121:THR:OG1	48:8:303:LEU:HB3	2.20	0.41
45:5:277:HIS:CE1	45:5:279:ASP:OD2	2.59	0.41
45:5:332:ALA:HB2	45:5:338:CYS:HB2	2.02	0.41
47:7:77:TRP:CH2	47:7:78:VAL:HG22	2.56	0.41
47:7:232:ALA:HA	47:7:235:MET:HG2	2.03	0.41
47:7:235:MET:HG3	47:7:236:MET:N	2.36	0.41
48:8:90:LEU:HD11	51:Ab:76:HIS:CE1	2.55	0.41
52:Ac:44:TYR:HA	52:Ac:47:ILE:HD12	2.02	0.41
60:Ak:398:PRO:HB3	60:Ak:482:VAL:HG21	2.03	0.41
62:Am:146:TRP:CE2	66:Aq:17:ARG:HB2	2.56	0.41
63:An:11:TYR:CD1	63:An:11:TYR:C	2.99	0.41
2:B:380:GLY:O	2:B:386:ARG:HB2	2.20	0.40
3:C:86:PRO:HB2	9:I:133:MET:HE1	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:HIS:HA	3:C:89:PRO:HD3	1.86	0.40
3:C:302:LEU:HD21	4:D:140:ARG:HH22	1.86	0.40
3:C:414:ASP:OD1	3:C:416:SER:N	2.47	0.40
4:D:114:LEU:HB3	4:D:166:TYR:CD2	2.57	0.40
4:D:153:ILE:HG23	4:D:178:PHE:CD1	2.56	0.40
5:E:185:MET:HA	5:E:196:LEU:HD13	2.02	0.40
7:G:171:THR:HG22	7:G:231:LEU:CD2	2.51	0.40
7:G:306:MET:HA	7:G:315:THR:O	2.21	0.40
7:G:529:GLY:HA3	16:P:54:LEU:HD11	2.02	0.40
7:G:624:ARG:HD3	7:G:636:TYR:CE1	2.57	0.40
9:I:152:SER:HB3	9:I:182:TYR:HD1	1.85	0.40
12:L:69:VAL:HG12	12:L:246:SER:HA	2.02	0.40
12:L:99:ASP:O	12:L:102:GLN:HG2	2.21	0.40
12:L:207:PHE:HE2	12:L:348:LYS:HB2	1.87	0.40
18:S:1:MET:HB3	18:S:2:TRP:H	1.64	0.40
20:U:299:LEU:HD23	20:U:306:VAL:CG1	2.51	0.40
15:X:80:LYS:HD3	15:X:100:VAL:HG21	2.03	0.40
25:a:129:PRO:CD	28:d:66:ARG:HH12	2.34	0.40
28:d:81:ASP:OD1	28:d:83:LEU:N	2.54	0.40
33:i:72:MET:HE1	35:k:43:MET:SD	2.60	0.40
34:j:58:VAL:HG21	34:j:113:TRP:HA	2.03	0.40
35:k:62:ILE:O	35:k:63:LEU:C	2.64	0.40
36:l:19:ILE:O	36:l:22:SER:CB	2.69	0.40
36:l:347:ILE:HG22	36:l:352:ASP:OD1	2.21	0.40
36:l:356:ILE:HA	36:l:359:MET:HB2	2.02	0.40
41:q:296:LEU:HA	41:q:296:LEU:HD23	1.77	0.40
42:r:114:TYR:CE2	42:r:118:TRP:CE2	3.10	0.40
45:u:190:THR:HG21	45:u:275:ILE:HG13	0.87	0.40
45:u:275:ILE:O	45:u:457:ALA:HA	2.21	0.40
45:u:321:GLY:O	45:u:323:HIS:N	2.54	0.40
45:u:417:LEU:HA	45:u:421:GLY:HA2	2.03	0.40
46:v:274:GLU:HA	46:v:335:LEU:HD23	2.04	0.40
52:1:25:ILE:HD13	53:2:122:THR:HG21	2.02	0.40
53:2:207:LYS:HD2	53:2:265:PHE:HE2	1.86	0.40
45:5:273:SER:HG	50:Aa:19:LEU:HA	1.86	0.40
47:7:223:TYR:CE2	48:8:315:LEU:HD11	2.56	0.40
60:Ak:264:LYS:NZ	61:Al:56:MET:HE2	2.35	0.40
63:An:127:LYS:O	63:An:130:PRO:HD3	2.20	0.40
65:Ap:19:GLU:HB3	65:Ap:98:HIS:CE1	2.56	0.40
2:B:224:ARG:HD3	10:J:164:PHE:CE1	2.56	0.40
3:C:136:PHE:CE2	3:C:151:TYR:CD1	2.98	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:268:TRP:HZ3	3:C:327:TYR:HD1	1.68	0.40
3:C:326:CYS:SG	3:C:453:THR:HB	2.61	0.40
4:D:230:PHE:HD1	9:I:165:TYR:CD2	2.39	0.40
7:G:314:LEU:CD1	11:R:139:PRO:CA	2.57	0.40
7:G:351:LEU:HD13	7:G:530:TYR:HE2	1.86	0.40
7:G:588:ALA:O	7:G:592:LYS:HE3	2.21	0.40
15:O:120:MET:HA	15:O:123:GLU:HG2	2.03	0.40
24:Z:49:GLU:OE1	40:p:38:ARG:HB2	2.21	0.40
27:c:96:ASP:HB2	41:q:346:ARG:NH1	2.36	0.40
28:d:65:HIS:CD2	29:e:120:ARG:HD2	2.56	0.40
33:i:211:MET:HB3	33:i:251:MET:CE	2.52	0.40
34:j:106:TRP:CZ3	42:r:291:LYS:HD3	2.57	0.40
35:k:59:MET:HG3	35:k:60:PRO:CD	2.51	0.40
41:q:420:THR:HB	41:q:423:ILE:HD12	2.02	0.40
42:r:307:LEU:N	42:r:308:PRO:HD2	2.35	0.40
43:s:96:LEU:CD1	43:s:99:HIS:N	2.84	0.40
46:v:371:VAL:O	46:v:375:LYS:HG3	2.21	0.40
47:w:128:PHE:O	47:w:132:VAL:HG23	2.21	0.40
46:6:70:ARG:NH2	46:6:251:ALA:H	2.20	0.40
46:6:130:ILE:HG13	46:6:134:MET:HE2	2.03	0.40
46:6:279:GLY:HA2	55:Ae:2:LEU:HD13	2.03	0.40
48:8:187:ARG:O	48:8:192:GLY:N	2.34	0.40
48:8:188:ALA:O	48:8:191:ASN:ND2	2.54	0.40
48:8:316:LYS:HA	49:9:72:ARG:HD3	2.02	0.40
49:9:87:ASP:OD1	49:9:87:ASP:N	2.54	0.40
55:Af:15:LEU:HD23	55:Af:15:LEU:HA	1.92	0.40
56:Ag:35:TYR:HD2	56:Ag:36:HIS:CE1	2.39	0.40
57:Ah:20:VAL:H	62:Am:12:ASN:ND2	2.14	0.40
62:Am:182:TYR:O	66:Aq:72:ASN:HB2	2.21	0.40
2:B:177:TYR:CD2	2:B:182:ILE:HD11	2.57	0.40
3:C:179:ARG:CD	3:C:183:HIS:HE1	2.35	0.40
7:G:304:GLN:HB2	7:G:316:TYR:HD1	1.86	0.40
9:I:194:LEU:HD12	9:I:194:LEU:HA	1.71	0.40
12:L:152:ILE:O	12:L:156:SER:OG	2.27	0.40
12:L:176:SER:O	12:L:182:ARG:NH1	2.54	0.40
12:L:302:GLY:O	12:L:306:GLU:HG3	2.21	0.40
13:M:54:TYR:CE2	13:M:58:ASP:HB3	2.56	0.40
15:O:134:ASP:HA	15:O:137:LYS:CG	2.45	0.40
17:Q:22:SER:OG	17:Q:28:ALA:HB2	2.21	0.40
20:U:318:GLU:HG2	20:U:319:ILE:HD12	2.03	0.40
20:U:336:LEU:HA	20:U:337:PRO:HD3	1.91	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:168:TRP:CD1	31:g:91:ASP:HB3	2.56	0.40
31:g:16:LEU:HA	31:g:17:PRO:HD3	1.85	0.40
33:i:124:LEU:HA	33:i:124:LEU:HD23	1.86	0.40
33:i:171:ASN:HB2	36:l:574:SER:OG	2.21	0.40
35:k:25:HIS:HA	35:k:88:ASP:HA	2.03	0.40
35:k:31:LEU:O	37:m:20:PHE:HZ	2.04	0.40
36:l:157:TRP:HD1	36:l:158:TRP:CD1	2.38	0.40
36:l:369:THR:OG1	36:l:445:GLU:OE2	2.36	0.40
36:l:474:PRO:O	44:t:55:GLN:NE2	2.54	0.40
37:m:27:ILE:HG23	37:m:28:TYR:N	2.35	0.40
37:m:134:GLY:O	37:m:136:PHE:N	2.50	0.40
41:q:176:PHE:HA	41:q:179:ILE:HG22	2.02	0.40
45:u:229:MET:SD	45:u:253:LEU:HD11	2.61	0.40
74:u:501:CDL:H341	75:u:502:PEE:C18	2.52	0.40
46:v:268:HIS:ND1	46:v:341:ILE:HG23	2.36	0.40
47:w:72:ASP:C	53:2:144:ALA:H	2.29	0.40
48:x:218:GLY:O	48:x:220:CYS:N	2.53	0.40
45:5:59:VAL:HG21	45:5:243:LEU:HA	2.04	0.40
45:5:379:LEU:O	45:5:383:ALA:HB2	2.22	0.40
47:7:373:GLU:HG2	49:9:21:TYR:OH	2.22	0.40
75:7:402:PEE:H2	50:Aa:45:CYS:SG	2.61	0.40
48:8:195:PRO:HA	77:8:402:HEC:HBD2	2.04	0.40
60:Ak:442:ASP:OD2	61:Al:134:ARG:NH2	2.54	0.40
61:Al:100:MET:HE3	61:Al:157:GLU:HG3	2.02	0.40
2:B:236:PHE:CD1	5:E:74:HIS:HB2	2.57	0.40
2:B:408:GLU:O	2:B:411:SER:OG	2.37	0.40
69:B:502:FMN:H9	69:B:502:FMN:H1'2	1.83	0.40
3:C:228:ARG:HH22	8:H:157:PHE:HE1	1.69	0.40
3:C:279:THR:HB	3:C:282:ASP:CB	2.50	0.40
3:C:438:MET:HE3	3:C:450:ILE:HG12	2.04	0.40
5:E:53:PHE:CD2	5:E:97:ALA:HA	2.56	0.40
7:G:368:THR:H	7:G:533:GLY:HA2	1.86	0.40
7:G:549:GLY:N	7:G:568:TYR:HE1	2.16	0.40
7:G:557:ARG:HD2	7:G:560:LEU:HD22	2.02	0.40
7:G:663:ASN:H	16:P:57:GLU:HG2	1.86	0.40
8:H:41:VAL:HA	13:M:113:LEU:HB3	2.04	0.40
9:I:211:ARG:NH1	9:I:211:ARG:CB	2.73	0.40
15:O:82:ARG:HG2	15:O:125:GLU:CD	2.46	0.40
16:P:90:THR:O	16:P:94:VAL:HG23	2.21	0.40
17:Q:98:LYS:NZ	17:Q:102:HIS:HB3	2.36	0.40
26:b:77:ILE:HG22	26:b:78:PRO:HD3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:i:142:LEU:HB3	33:i:194:LEU:HD11	2.03	0.40
33:i:221:HIS:HD2	33:i:240:ILE:HG21	1.85	0.40
33:i:323:MET:H	33:i:323:MET:HG2	1.66	0.40
36:l:103:PHE:HE2	36:l:242:PRO:HG3	1.85	0.40
36:l:140:LEU:HD21	36:l:259:LEU:HD12	2.04	0.40
39:o:28:GLU:O	39:o:31:LYS:HB2	2.21	0.40
39:o:48:LEU:HA	39:o:48:LEU:HD23	1.82	0.40
39:o:50:GLN:O	39:o:56:ARG:HD2	2.21	0.40
40:p:38:ARG:HA	40:p:38:ARG:HD2	1.83	0.40
42:r:11:ILE:HB	42:r:12:PRO:HD3	2.03	0.40
47:w:35:SER:N	76:w:402:HEM:O2A	2.54	0.40
47:w:312:GLN:HB2	47:w:318:ARG:HH21	1.87	0.40
76:w:401:HEM:CHB	76:w:401:HEM:HMA3	2.49	0.40
48:x:111:ILE:HG21	48:x:277:TRP:CD1	2.56	0.40
53:2:183:GLU:HB3	53:2:245:ALA:CB	2.51	0.40
75:2:302:PEE:H27	75:2:302:PEE:H67	2.04	0.40
46:6:261:GLN:HE22	46:6:444:LEU:HB2	1.87	0.40
46:6:427:ALA:O	46:6:430:LYS:HB3	2.21	0.40
47:7:43:LEU:CD1	75:7:401:PEE:C19	2.99	0.40
48:8:225:GLY:HA3	51:Ab:65:GLU:O	2.21	0.40
74:8:401:CDL:H121	74:8:401:CDL:H151	1.96	0.40
57:Ah:21:HIS:CD2	57:Ah:22:LEU:HG	2.57	0.40
61:Al:123:ILE:HA	61:Al:124:PRO:HD3	1.96	0.40
62:Am:6:HIS:CD2	62:Am:8:TYR:HB2	2.56	0.40
64:Ao:74:LYS:HD2	64:Ao:74:LYS:HA	1.95	0.40
64:Ao:79:LYS:HD3	64:Ao:79:LYS:H	1.87	0.40
2:B:355:ILE:HG22	2:B:357:MET:HG3	2.04	0.40
3:C:84:PHE:HD1	3:C:84:PHE:HA	1.75	0.40
3:C:393:PRO:HD2	4:D:245:TYR:HD2	1.87	0.40
5:E:156:LEU:HD13	5:E:158:ILE:HD12	2.04	0.40
7:G:620:TRP:CG	7:G:621:LYS:N	2.89	0.40
8:H:85:ASN:O	8:H:89:GLU:N	2.49	0.40
8:H:101:HIS:NE2	68:H:302:SF4:S1	2.89	0.40
8:H:162:CYS:SG	8:H:166:ALA:N	2.78	0.40
9:I:116:SER:HB3	42:r:208:VAL:HG22	2.02	0.40
10:J:111:LEU:C	10:J:113:GLY:H	2.30	0.40
14:N:24:LEU:HD21	14:N:81:ILE:HG22	2.02	0.40
16:P:26:ARG:HA	16:P:26:ARG:HD3	1.93	0.40
17:Q:70:ASN:O	73:Q:201:ZMP:H15A	2.22	0.40
18:S:13:ALA:O	18:S:17:PHE:N	2.50	0.40
20:U:137:LEU:HA	20:U:137:LEU:HD12	1.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:45:TRP:H	40:p:38:ARG:NH1	2.20	0.40
26:b:7:ASP:O	26:b:10:LEU:HG	2.21	0.40
31:g:13:LEU:HD11	32:h:6:VAL:HB	2.03	0.40
34:j:42:ASP:HA	34:j:43:PRO:HD3	1.97	0.40
35:k:34:GLU:HA	35:k:37:MET:HE2	2.03	0.40
36:l:37:LYS:O	36:l:98:TRP:NE1	2.55	0.40
36:l:152:PHE:HB2	36:l:172:ILE:HD11	2.04	0.40
36:l:154:LEU:HB3	36:l:243:VAL:HG11	2.03	0.40
36:l:338:MET:HB3	36:l:338:MET:HE3	1.82	0.40
36:l:345:SER:O	36:l:349:SER:OG	2.34	0.40
41:q:217:PRO:O	41:q:221:VAL:HG23	2.22	0.40
41:q:373:ILE:HD13	41:q:447:LEU:HD23	2.02	0.40
42:r:169:GLN:HE21	42:r:174:MET:HB2	1.86	0.40
45:u:45:VAL:HA	45:u:46:PRO:HD2	1.85	0.40
45:u:119:HIS:CE1	46:v:298:HIS:HD1	2.40	0.40
45:u:156:LEU:O	45:u:213:ARG:NE	2.48	0.40
45:u:280:ASP:HA	45:u:461:PRO:CB	2.51	0.40
45:u:296:TRP:CE3	45:u:347:CYS:HB2	2.45	0.40
46:v:160:ILE:O	46:v:164:VAL:HG22	2.22	0.40
52:1:33:GLU:HG3	53:2:130:LYS:NZ	2.36	0.40
47:7:133:LEU:HD21	47:7:179:PHE:HA	2.03	0.40
47:7:345:HIS:O	47:7:349:ILE:HD12	2.21	0.40
54:Ad:4:ARG:CG	54:Ad:5:PHE:N	2.84	0.40
58:Ai:24:PHE:CE1	58:Ai:28:VAL:HG21	2.56	0.40
60:Ak:440:TYR:CG	61:Al:205:SER:HB3	2.57	0.40
65:Ap:77:GLY:O	65:Ap:90:LYS:NZ	2.54	0.40
65:Ap:91:LEU:HD12	65:Ap:91:LEU:HA	1.89	0.40
66:Aq:42:ARG:NH1	66:Aq:74:ARG:NH2	2.69	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	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
2	B	408/464 (88%)	365 (90%)	30 (7%)	13 (3%)	3	25
3	C	428/463 (92%)	388 (91%)	28 (6%)	12 (3%)	4	27
4	D	206/264 (78%)	164 (80%)	29 (14%)	13 (6%)	1	15
5	E	170/249 (68%)	154 (91%)	11 (6%)	5 (3%)	3	26
6	F	42/123 (34%)	29 (69%)	10 (24%)	3 (7%)	1	14
7	G	669/727 (92%)	574 (86%)	66 (10%)	29 (4%)	2	20
8	H	174/212 (82%)	166 (95%)	7 (4%)	1 (1%)	21	57
9	I	154/216 (71%)	134 (87%)	12 (8%)	8 (5%)	1	18
10	J	107/175 (61%)	94 (88%)	12 (11%)	1 (1%)	14	48
11	K	95/145 (66%)	74 (78%)	14 (15%)	7 (7%)	1	13
11	R	16/145 (11%)	13 (81%)	2 (12%)	1 (6%)	1	15
12	L	335/377 (89%)	308 (92%)	15 (4%)	12 (4%)	2	23
13	M	90/113 (80%)	76 (84%)	6 (7%)	8 (9%)	0	10
14	N	110/116 (95%)	99 (90%)	6 (6%)	5 (4%)	2	20
15	O	83/156 (53%)	77 (93%)	2 (2%)	4 (5%)	2	19
15	X	83/156 (53%)	76 (92%)	4 (5%)	3 (4%)	2	23
16	P	81/99 (82%)	74 (91%)	6 (7%)	1 (1%)	10	42
17	Q	110/128 (86%)	99 (90%)	7 (6%)	4 (4%)	2	23
18	S	68/70 (97%)	63 (93%)	2 (3%)	3 (4%)	2	20
19	T	80/84 (95%)	69 (86%)	8 (10%)	3 (4%)	2	22
20	U	277/357 (78%)	249 (90%)	22 (8%)	6 (2%)	5	31
21	V	138/141 (98%)	127 (92%)	3 (2%)	8 (6%)	1	16
22	W	136/144 (94%)	124 (91%)	9 (7%)	3 (2%)	5	31
23	Y	57/105 (54%)	42 (74%)	5 (9%)	10 (18%)	0	2
24	Z	76/98 (78%)	71 (93%)	3 (4%)	2 (3%)	4	29
25	a	136/189 (72%)	118 (87%)	14 (10%)	4 (3%)	3	26
26	b	109/128 (85%)	95 (87%)	4 (4%)	10 (9%)	0	10
27	c	146/186 (78%)	119 (82%)	14 (10%)	13 (9%)	0	10
28	d	167/176 (95%)	151 (90%)	6 (4%)	10 (6%)	1	16
29	e	95/154 (62%)	83 (87%)	6 (6%)	6 (6%)	1	15
30	f	34/76 (45%)	29 (85%)	5 (15%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	g	119/122 (98%)	106 (89%)	7 (6%)	6 (5%)	1	18
32	h	102/106 (96%)	89 (87%)	8 (8%)	5 (5%)	1	19
33	i	345/347 (99%)	325 (94%)	17 (5%)	3 (1%)	14	48
34	j	112/115 (97%)	101 (90%)	9 (8%)	2 (2%)	6	34
35	k	95/98 (97%)	88 (93%)	4 (4%)	3 (3%)	3	25
36	l	604/606 (100%)	545 (90%)	41 (7%)	18 (3%)	3	26
37	m	172/175 (98%)	156 (91%)	11 (6%)	5 (3%)	3	26
38	n	45/58 (78%)	41 (91%)	4 (9%)	0	100	100
39	o	126/129 (98%)	108 (86%)	11 (9%)	7 (6%)	1	17
40	p	167/179 (93%)	145 (87%)	13 (8%)	9 (5%)	1	18
41	q	457/459 (100%)	426 (93%)	21 (5%)	10 (2%)	5	31
42	r	316/318 (99%)	285 (90%)	27 (8%)	4 (1%)	9	41
43	s	167/172 (97%)	149 (89%)	14 (8%)	4 (2%)	4	30
44	t	111/137 (81%)	100 (90%)	8 (7%)	3 (3%)	4	28
45	5	444/480 (92%)	412 (93%)	29 (6%)	3 (1%)	18	54
45	u	444/480 (92%)	407 (92%)	28 (6%)	9 (2%)	6	33
46	6	416/453 (92%)	383 (92%)	30 (7%)	3 (1%)	18	54
46	v	416/453 (92%)	379 (91%)	30 (7%)	7 (2%)	7	36
47	7	376/379 (99%)	348 (93%)	22 (6%)	6 (2%)	7	37
47	w	376/379 (99%)	352 (94%)	19 (5%)	5 (1%)	9	41
48	8	239/326 (73%)	221 (92%)	16 (7%)	2 (1%)	16	52
48	x	239/326 (73%)	219 (92%)	15 (6%)	5 (2%)	5	32
49	9	104/111 (94%)	102 (98%)	2 (2%)	0	100	100
49	y	104/111 (94%)	100 (96%)	4 (4%)	0	100	100
50	Aa	78/82 (95%)	70 (90%)	8 (10%)	0	100	100
50	z	77/82 (94%)	70 (91%)	6 (8%)	1 (1%)	9	41
51	0	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
51	Ab	62/91 (68%)	60 (97%)	2 (3%)	0	100	100
52	1	60/64 (94%)	55 (92%)	2 (3%)	3 (5%)	1	18
52	Ac	60/64 (94%)	57 (95%)	2 (3%)	1 (2%)	7	36
53	2	194/274 (71%)	178 (92%)	14 (7%)	2 (1%)	12	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	4	194/274 (71%)	178 (92%)	14 (7%)	2 (1%)	12	45
54	3	49/56 (88%)	45 (92%)	4 (8%)	0	100	100
54	Ad	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
55	Ae	55/78 (70%)	41 (74%)	13 (24%)	1 (2%)	6	34
55	Af	55/78 (70%)	40 (73%)	10 (18%)	5 (9%)	0	10
56	Ag	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
57	Ah	54/59 (92%)	48 (89%)	4 (7%)	2 (4%)	2	22
58	Ai	47/56 (84%)	41 (87%)	6 (13%)	0	100	100
59	Aj	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
60	Ak	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	52
61	Al	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	41
62	Am	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
63	An	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
64	Ao	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
65	Ap	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	2	21
66	Aq	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	15
67	Ar	73/85 (86%)	64 (88%)	8 (11%)	1 (1%)	9	39
All	All	13723/15851 (87%)	12412 (90%)	950 (7%)	361 (3%)	6	29

All (361) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	73	PRO
2	B	105	PRO
2	B	121	GLU
2	B	379	CYS
3	C	84	PHE
4	D	50	ARG
4	D	229	GLU
5	E	183	ALA
6	F	114	CYS
7	G	37	ASP
7	G	47	THR
7	G	181	ARG
7	G	287	SER
7	G	347	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	448	SER
7	G	482	GLN
11	K	62	VAL
12	L	135	GLU
16	P	50	ASP
18	S	52	ARG
18	S	60	TYR
19	T	63	MET
19	T	71	GLN
20	U	201	LEU
21	V	135	VAL
21	V	140	LYS
23	Y	51	THR
23	Y	85	PRO
23	Y	88	ASP
23	Y	89	PRO
24	Z	17	PRO
26	b	29	SER
26	b	33	PRO
26	b	124	PRO
27	c	100	ASN
27	c	155	PRO
27	c	178	PRO
28	d	9	VAL
28	d	18	PRO
28	d	20	PRO
28	d	121	TYR
29	e	59	PRO
31	g	3	MET
31	g	10	ARG
31	g	20	ALA
36	l	562	LEU
36	l	581	LYS
37	m	76	THR
39	o	57	LEU
39	o	83	THR
40	p	156	PRO
40	p	175	ARG
41	q	429	SER
42	r	208	VAL
43	s	49	GLU
45	u	337	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	v	142	ALA
52	1	13	LEU
45	5	105	PRO
45	5	249	HIS
47	7	62	ALA
57	Ah	2	GLU
60	Ak	328	HIS
60	Ak	508	PRO
65	Ap	2	SER
65	Ap	87	THR
65	Ap	95	GLN
66	Aq	4	ALA
66	Aq	9	GLY
67	Ar	46	LYS
2	B	50	ASP
2	B	331	VAL
2	B	378	SER
3	C	104	GLU
3	C	265	ASN
3	C	273	VAL
3	C	386	THR
4	D	138	ASN
4	D	192	GLY
7	G	210	ILE
7	G	288	ASP
7	G	336	ASN
7	G	368	THR
7	G	450	LYS
7	G	541	PRO
7	G	555	ILE
11	K	32	ASP
11	K	37	THR
12	L	86	CYS
12	L	230	SER
12	L	239	PRO
12	L	310	PHE
13	M	40	LYS
13	M	72	SER
14	N	9	THR
14	N	41	ASN
15	O	137	LYS
15	O	139	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	Q	76	PRO
19	T	50	PRO
20	U	90	GLU
20	U	115	SER
20	U	203	PRO
21	V	14	GLU
21	V	47	ALA
22	W	11	PRO
22	W	16	TYR
23	Y	40	ILE
23	Y	45	ARG
23	Y	48	PRO
23	Y	49	GLN
25	a	185	THR
26	b	112	GLU
26	b	118	PRO
27	c	59	VAL
27	c	154	GLN
28	d	22	PRO
28	d	119	GLU
28	d	120	SER
29	e	58	ASP
31	g	12	PRO
32	h	20	ILE
32	h	24	GLU
32	h	48	GLY
32	h	49	GLY
33	i	86	ILE
34	j	113	TRP
35	k	22	TYR
36	l	73	THR
36	l	440	LEU
36	l	586	LEU
37	m	24	PRO
39	o	5	LYS
40	p	106	ASP
41	q	22	MET
41	q	139	GLN
41	q	188	ASN
45	u	297	ALA
45	u	312	GLY
45	u	380	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	w	7	SER
47	w	254	ASP
48	x	125	CYS
52	1	47	ILE
53	4	141	SER
53	4	255	PRO
45	5	279	ASP
47	7	201	HIS
48	8	139	VAL
66	Aq	5	LYS
2	B	236	PHE
3	C	102	SER
3	C	139	LEU
3	C	197	MET
3	C	233	HIS
4	D	194	GLU
4	D	246	ARG
5	E	176	CYS
6	F	110	THR
7	G	174	THR
7	G	283	GLU
7	G	377	ALA
7	G	663	ASN
7	G	665	PHE
7	G	677	GLN
7	G	689	LEU
9	I	105	ASP
9	I	116	SER
9	I	156	CYS
11	K	17	HIS
12	L	178	SER
12	L	205	ASP
12	L	259	LYS
13	M	107	SER
15	O	138	LEU
20	U	112	GLY
21	V	48	SER
15	X	108	LEU
23	Y	86	TYR
23	Y	95	GLU
24	Z	59	ASN
25	a	188	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	b	88	TYR
26	b	101	LYS
26	b	119	LEU
27	c	43	LYS
27	c	167	TYR
28	d	23	GLN
28	d	144	SER
28	d	145	ASP
29	e	62	GLU
29	e	136	LEU
31	g	4	MET
34	j	24	LEU
35	k	50	ASN
36	l	55	MET
36	l	447	ASN
37	m	77	GLU
37	m	116	ILE
39	o	80	PHE
39	o	126	ASN
40	p	8	ALA
40	p	51	HIS
41	q	251	ASN
41	q	353	PRO
42	r	60	PRO
44	t	56	ARG
45	u	322	THR
46	v	244	LEU
46	v	251	ALA
46	v	261	GLN
48	x	165	MET
48	x	247	PRO
46	6	118	SER
46	6	244	LEU
47	7	249	LEU
55	Af	40	SER
61	Al	104	TRP
66	Aq	61	SER
2	B	186	ALA
2	B	237	GLY
4	D	105	ASN
4	D	121	THR
4	D	202	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	160	VAL
7	G	69	LEU
7	G	337	ASP
7	G	575	VAL
7	G	650	SER
8	H	175	PHE
9	I	89	LEU
12	L	102	GLN
12	L	370	LYS
13	M	108	LYS
14	N	76	GLN
14	N	103	LEU
14	N	105	GLU
15	O	155	TYR
17	Q	72	HIS
11	R	130	THR
18	S	51	ASP
21	V	15	GLY
21	V	17	GLU
22	W	118	THR
15	X	155	TYR
25	a	58	LYS
27	c	41	TYR
27	c	66	PRO
27	c	114	ARG
27	c	162	PRO
27	c	166	LEU
29	e	72	ASP
33	i	48	PHE
33	i	81	SER
35	k	96	LEU
36	l	477	VAL
36	l	511	LEU
36	l	512	LYS
36	l	536	LEU
37	m	25	SER
39	o	81	ARG
40	p	32	VAL
40	p	145	PRO
42	r	196	ALA
43	s	37	ASP
43	s	139	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	42	THR
46	v	184	ASN
48	x	135	HIS
52	1	41	ASP
53	2	266	THR
47	7	286	ASN
48	8	191	ASN
55	Af	43	LEU
55	Af	51	CYS
60	Ak	51	ASP
5	E	214	PRO
6	F	81	SER
7	G	281	ILE
7	G	582	VAL
7	G	654	VAL
10	J	96	LYS
11	K	41	GLU
12	L	330	PRO
13	M	31	ILE
13	M	70	MET
17	Q	127	ASP
20	U	68	ILE
15	X	137	LYS
25	a	102	PRO
26	b	105	PHE
27	c	172	GLY
32	h	98	HIS
36	l	195	ALA
36	l	211	MET
36	l	441	VAL
40	p	76	HIS
40	p	87	GLY
41	q	85	SER
41	q	368	ALA
42	r	281	ARG
43	s	79	ALA
45	u	233	ALA
46	v	241	ARG
47	w	135	TRP
47	7	314	SER
52	Ac	47	ILE
55	Af	37	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	Ah	3	ASN
61	Al	103	GLN
2	B	74	ASP
3	C	94	VAL
4	D	122	ARG
4	D	191	TYR
4	D	239	TRP
7	G	267	THR
9	I	159	GLY
9	I	171	ARG
11	K	55	PHE
11	K	64	TYR
12	L	83	PRO
13	M	92	LYS
13	M	93	LYS
17	Q	96	VAL
26	b	115	GLU
36	l	275	THR
45	u	279	ASP
45	u	419	THR
47	w	173	ALA
47	w	262	LEU
50	z	79	GLU
60	Ak	91	ASP
61	Al	158	ASP
66	Aq	49	PRO
46	6	371	VAL
2	B	94	PRO
9	I	160	GLY
36	l	563	PRO
39	o	94	GLY
55	Af	30	VAL
3	C	85	GLY
3	C	319	PRO
4	D	44	ARG
9	I	147	PRO
31	g	56	VAL
36	l	515	TYR
41	q	172	GLY
41	q	249	ILE
45	u	424	ILE
53	2	198	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	7	253	PRO
65	Ap	15	GLY
2	B	221	GLY
21	V	45	PRO
44	t	74	PHE
48	x	170	GLY
55	Ae	40	SER
5	E	216	PRO
46	v	46	GLY
36	l	483	PRO
29	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	58/58 (100%)	51 (88%)	7 (12%)	5	21
2	B	322/368 (88%)	320 (99%)	2 (1%)	78	81
3	C	351/393 (89%)	349 (99%)	2 (1%)	78	81
4	D	176/228 (77%)	175 (99%)	1 (1%)	78	81
5	E	145/173 (84%)	145 (100%)	0	100	100
6	F	9/97 (9%)	9 (100%)	0	100	100
7	G	518/610 (85%)	516 (100%)	2 (0%)	84	84
8	H	150/176 (85%)	150 (100%)	0	100	100
9	I	129/177 (73%)	128 (99%)	1 (1%)	73	77
10	J	95/152 (62%)	95 (100%)	0	100	100
11	K	11/131 (8%)	11 (100%)	0	100	100
12	L	280/323 (87%)	278 (99%)	2 (1%)	76	79
13	M	65/98 (66%)	65 (100%)	0	100	100
14	N	95/101 (94%)	95 (100%)	0	100	100
15	O	66/132 (50%)	66 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	X	71/132 (54%)	70 (99%)	1 (1%)	59	71
16	P	75/82 (92%)	75 (100%)	0	100	100
17	Q	101/112 (90%)	101 (100%)	0	100	100
18	S	58/58 (100%)	58 (100%)	0	100	100
19	T	65/70 (93%)	65 (100%)	0	100	100
20	U	151/307 (49%)	148 (98%)	3 (2%)	48	66
21	V	98/102 (96%)	98 (100%)	0	100	100
22	W	114/124 (92%)	114 (100%)	0	100	100
23	Y	24/84 (29%)	24 (100%)	0	100	100
24	Z	41/76 (54%)	41 (100%)	0	100	100
25	a	114/158 (72%)	113 (99%)	1 (1%)	70	76
26	b	46/121 (38%)	46 (100%)	0	100	100
27	c	87/160 (54%)	87 (100%)	0	100	100
28	d	99/156 (64%)	99 (100%)	0	100	100
29	e	74/129 (57%)	74 (100%)	0	100	100
30	f	31/66 (47%)	31 (100%)	0	100	100
31	g	107/109 (98%)	107 (100%)	0	100	100
32	h	75/94 (80%)	75 (100%)	0	100	100
33	i	310/311 (100%)	310 (100%)	0	100	100
34	j	97/100 (97%)	96 (99%)	1 (1%)	68	76
35	k	78/85 (92%)	77 (99%)	1 (1%)	61	72
36	l	534/540 (99%)	530 (99%)	4 (1%)	76	79
37	m	129/141 (92%)	128 (99%)	1 (1%)	73	77
38	n	33/55 (60%)	33 (100%)	0	100	100
39	o	101/114 (89%)	99 (98%)	2 (2%)	48	66
40	p	134/160 (84%)	134 (100%)	0	100	100
41	q	408/409 (100%)	405 (99%)	3 (1%)	76	79
42	r	275/275 (100%)	273 (99%)	2 (1%)	76	79
43	s	142/154 (92%)	138 (97%)	4 (3%)	38	60
44	t	41/120 (34%)	40 (98%)	1 (2%)	43	63
45	5	372/397 (94%)	370 (100%)	2 (0%)	81	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	u	370/397 (93%)	369 (100%)	1 (0%)	86	85
46	6	326/354 (92%)	326 (100%)	0	100	100
46	v	326/354 (92%)	326 (100%)	0	100	100
47	7	331/332 (100%)	330 (100%)	1 (0%)	86	85
47	w	331/332 (100%)	331 (100%)	0	100	100
48	8	205/259 (79%)	204 (100%)	1 (0%)	81	82
48	x	205/259 (79%)	204 (100%)	1 (0%)	81	82
49	9	95/99 (96%)	94 (99%)	1 (1%)	65	74
49	y	95/99 (96%)	95 (100%)	0	100	100
50	Aa	72/73 (99%)	72 (100%)	0	100	100
50	z	70/73 (96%)	70 (100%)	0	100	100
51	0	61/85 (72%)	61 (100%)	0	100	100
51	Ab	61/85 (72%)	61 (100%)	0	100	100
52	1	50/52 (96%)	50 (100%)	0	100	100
52	Ac	50/52 (96%)	50 (100%)	0	100	100
53	2	165/225 (73%)	165 (100%)	0	100	100
53	4	165/225 (73%)	165 (100%)	0	100	100
54	3	39/46 (85%)	39 (100%)	0	100	100
54	Ad	37/46 (80%)	37 (100%)	0	100	100
55	Ae	41/59 (70%)	41 (100%)	0	100	100
55	Af	41/59 (70%)	41 (100%)	0	100	100
56	Ag	37/38 (97%)	34 (92%)	3 (8%)	11	34
57	Ah	45/50 (90%)	39 (87%)	6 (13%)	4	18
58	Ai	39/46 (85%)	36 (92%)	3 (8%)	12	35
59	Aj	40/40 (100%)	37 (92%)	3 (8%)	12	36
60	Ak	427/427 (100%)	387 (91%)	40 (9%)	8	29
61	Al	211/211 (100%)	191 (90%)	20 (10%)	8	28
62	Am	226/226 (100%)	199 (88%)	27 (12%)	5	21
63	An	128/129 (99%)	118 (92%)	10 (8%)	11	35
64	Ao	95/95 (100%)	89 (94%)	6 (6%)	16	41
65	Ap	81/81 (100%)	73 (90%)	8 (10%)	7	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
66	Aq	68/68 (100%)	52 (76%)	16 (24%)	1 5
67	Ar	67/75 (89%)	58 (87%)	9 (13%)	4 18
All	All	11155/13269 (84%)	10956 (98%)	199 (2%)	51 68

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	4	LEU
1	A	8	GLN
1	A	22	VAL
1	A	26	MET
1	A	44	LYS
1	A	64	ARG
2	B	118	ASP
2	B	331	VAL
3	C	84	PHE
3	C	356	ILE
4	D	157	VAL
7	G	478	SER
7	G	489	ILE
9	I	91	CYS
12	L	242	ILE
12	L	272	LEU
20	U	93	ILE
20	U	138	TYR
20	U	304	LEU
15	X	93	ILE
25	a	53	ARG
34	j	96	ILE
35	k	8	ILE
36	l	63	ILE
36	l	283	ILE
36	l	317	ILE
36	l	468	ILE
37	m	12	ILE
39	o	60	ILE
39	o	76	ILE
41	q	37	ILE
41	q	96	ILE
41	q	107	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	r	187	ILE
42	r	309	ILE
43	s	46	CYS
43	s	47	ARG
43	s	89	ILE
43	s	103	GLN
44	t	111	ARG
45	u	462	ILE
48	x	293	MET
45	5	310	ILE
45	5	433	ILE
47	7	115	ILE
48	8	293	MET
49	9	99	ILE
56	Ag	13	LYS
56	Ag	24	LEU
56	Ag	42	LYS
57	Ah	2	GLU
57	Ah	5	VAL
57	Ah	8	LYS
57	Ah	16	ASN
57	Ah	23	LYS
57	Ah	27	THR
58	Ai	45	VAL
58	Ai	48	VAL
58	Ai	49	THR
59	Aj	15	VAL
59	Aj	22	LEU
59	Aj	26	THR
60	Ak	18	LEU
60	Ak	35	LEU
60	Ak	92	MET
60	Ak	96	ARG
60	Ak	105	LEU
60	Ak	115	SER
60	Ak	136	LEU
60	Ak	138	HIS
60	Ak	150	LEU
60	Ak	158	ILE
60	Ak	159	LEU
60	Ak	187	SER
60	Ak	188	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
60	Ak	189	MET
60	Ak	194	LEU
60	Ak	199	LEU
60	Ak	213	ARG
60	Ak	241	PRO
60	Ak	273	MET
60	Ak	295	VAL
60	Ak	301	THR
60	Ak	306	THR
60	Ak	318	VAL
60	Ak	324	LEU
60	Ak	347	LEU
60	Ak	353	LEU
60	Ak	354	THR
60	Ak	365	ILE
60	Ak	369	ASP
60	Ak	373	VAL
60	Ak	383	MET
60	Ak	417	MET
60	Ak	444	PRO
60	Ak	465	VAL
60	Ak	467	LEU
60	Ak	474	GLU
60	Ak	492	LEU
60	Ak	508	PRO
60	Ak	509	THR
60	Ak	512	ASN
61	Al	7	LEU
61	Al	16	ILE
61	Al	31	VAL
61	Al	33	LEU
61	Al	52	HIS
61	Al	60	GLU
61	Al	63	THR
61	Al	67	ILE
61	Al	88	ASP
61	Al	92	ASN
61	Al	125	THR
61	Al	130	PRO
61	Al	134	ARG
61	Al	142	VAL
61	Al	147	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
61	Al	170	LEU
61	Al	171	LYS
61	Al	185	MET
61	Al	205	SER
61	Al	216	LEU
62	Am	1	MET
62	Am	11	VAL
62	Am	13	PRO
62	Am	14	SER
62	Am	18	LEU
62	Am	19	THR
62	Am	22	LEU
62	Am	26	LEU
62	Am	38	ASN
62	Am	39	SER
62	Am	85	LEU
62	Am	92	LEU
62	Am	112	LEU
62	Am	127	LEU
62	Am	128	GLU
62	Am	131	LEU
62	Am	132	LEU
62	Am	137	LEU
62	Am	142	VAL
62	Am	160	LEU
62	Am	163	LEU
62	Am	188	ILE
62	Am	196	THR
62	Am	199	VAL
62	Am	213	THR
62	Am	222	GLN
62	Am	230	ASN
63	An	9	GLU
63	An	27	VAL
63	An	31	LYS
63	An	36	SER
63	An	40	LEU
63	An	59	LEU
63	An	62	LEU
63	An	107	ILE
63	An	143	ASN
63	An	147	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
64	Ao	7	THR
64	Ao	29	LEU
64	Ao	70	VAL
64	Ao	79	LYS
64	Ao	80	GLU
64	Ao	90	ARG
65	Ap	6	VAL
65	Ap	20	VAL
65	Ap	37	LYS
65	Ap	52	ILE
65	Ap	53	THR
65	Ap	74	LEU
65	Ap	95	GLN
65	Ap	98	HIS
66	Aq	5	LYS
66	Aq	7	ASP
66	Aq	8	HIS
66	Aq	14	ARG
66	Aq	17	ARG
66	Aq	33	LEU
66	Aq	34	ASN
66	Aq	37	LEU
66	Aq	41	HIS
66	Aq	42	ARG
66	Aq	43	GLU
66	Aq	48	ILE
66	Aq	54	ARG
66	Aq	56	ARG
66	Aq	68	THR
66	Aq	78	LEU
67	Ar	19	ARG
67	Ar	29	CYS
67	Ar	41	LYS
67	Ar	51	SER
67	Ar	53	CYS
67	Ar	57	ARG
67	Ar	60	TYR
67	Ar	67	SER
67	Ar	75	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (268) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	220	GLN
2	B	376	HIS
2	B	393	ASN
2	B	418	GLN
2	B	441	HIS
3	C	36	GLN
3	C	38	GLN
3	C	88	HIS
3	C	92	HIS
3	C	250	ASN
3	C	270	ASN
3	C	339	GLN
3	C	381	HIS
3	C	442	HIS
4	D	55	HIS
4	D	181	HIS
5	E	59	ASN
5	E	69	ASN
5	E	90	ASN
5	E	99	ASN
5	E	153	GLN
5	E	187	GLN
5	E	189	ASN
5	E	191	ASN
7	G	522	GLN
7	G	569	GLN
7	G	571	HIS
7	G	705	GLN
8	H	159	GLN
8	H	186	ASN
9	I	75	ASN
9	I	98	HIS
9	I	119	GLN
9	I	164	HIS
9	I	201	GLN
10	J	71	HIS
10	J	88	GLN
12	L	71	ASN
12	L	72	HIS
12	L	102	GLN
12	L	122	HIS
12	L	154	GLN
12	L	171	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	278	GLN
14	N	50	GLN
14	N	71	GLN
14	N	111	GLN
16	P	25	GLN
16	P	62	GLN
16	P	93	ASN
17	Q	48	HIS
17	Q	70	ASN
17	Q	99	GLN
18	S	27	HIS
19	T	69	HIS
20	U	134	GLN
20	U	144	GLN
20	U	188	HIS
20	U	294	HIS
21	V	89	ASN
21	V	134	GLN
22	W	112	HIS
15	X	115	GLN
25	a	90	ASN
25	a	132	ASN
27	c	56	ASN
28	d	100	GLN
28	d	114	GLN
28	d	131	GLN
28	d	149	HIS
33	i	47	ASN
33	i	120	GLN
33	i	134	GLN
33	i	144	GLN
33	i	221	HIS
33	i	273	ASN
33	i	310	ASN
33	i	319	HIS
34	j	2	ASN
35	k	57	ASN
36	l	59	GLN
36	l	165	ASN
36	l	192	HIS
36	l	194	ASN
36	l	296	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	l	328	HIS
36	l	332	HIS
36	l	541	ASN
36	l	546	GLN
36	l	570	GLN
37	m	46	ASN
37	m	120	ASN
38	n	14	HIS
39	o	55	ASN
40	p	13	GLN
40	p	14	GLN
40	p	33	HIS
40	p	51	HIS
40	p	75	GLN
40	p	139	GLN
41	q	20	HIS
41	q	44	GLN
41	q	81	GLN
41	q	138	ASN
41	q	168	GLN
41	q	220	HIS
41	q	251	ASN
41	q	304	GLN
41	q	331	ASN
41	q	440	HIS
42	r	5	ASN
42	r	47	GLN
42	r	230	ASN
42	r	235	ASN
42	r	247	HIS
42	r	284	GLN
42	r	304	HIS
42	r	317	GLN
43	s	30	HIS
43	s	31	HIS
43	s	77	HIS
43	s	95	GLN
43	s	151	ASN
44	t	55	GLN
45	u	43	GLN
45	u	52	GLN
45	u	63	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	u	87	ASN
45	u	95	HIS
45	u	223	HIS
45	u	247	GLN
45	u	277	HIS
45	u	286	HIS
45	u	301	ASN
45	u	305	GLN
45	u	308	ASN
45	u	342	GLN
45	u	357	HIS
45	u	452	GLN
46	v	139	ASN
46	v	167	GLN
46	v	206	HIS
46	v	291	HIS
46	v	311	GLN
46	v	343	GLN
46	v	363	GLN
46	v	368	ASN
46	v	399	GLN
46	v	446	HIS
47	w	8	HIS
47	w	32	ASN
47	w	74	ASN
47	w	114	ASN
47	w	137	GLN
47	w	182	HIS
47	w	255	ASN
48	x	116	GLN
48	x	135	HIS
48	x	266	GLN
48	x	285	HIS
49	y	23	ASN
49	y	28	ASN
51	0	39	GLN
52	1	49	GLN
53	2	164	ASN
53	2	178	HIS
54	3	16	ASN
53	4	186	GLN
53	4	194	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	4	219	HIS
53	4	227	ASN
45	5	52	GLN
45	5	87	ASN
45	5	121	ASN
45	5	128	HIS
45	5	153	ASN
45	5	160	GLN
45	5	170	GLN
45	5	277	HIS
45	5	301	ASN
45	5	313	HIS
45	5	342	GLN
45	5	345	ASN
45	5	357	HIS
45	5	397	ASN
45	5	402	HIS
45	5	452	GLN
45	5	464	GLN
45	5	469	ASN
46	6	45	ASN
46	6	155	GLN
46	6	178	HIS
46	6	188	ASN
46	6	204	GLN
46	6	212	HIS
46	6	227	HIS
46	6	239	ASN
46	6	261	GLN
46	6	284	ASN
46	6	311	GLN
46	6	376	ASN
47	7	8	HIS
47	7	15	ASN
47	7	44	GLN
47	7	68	HIS
47	7	308	HIS
47	7	322	GLN
47	7	345	HIS
48	8	91	HIS
48	8	108	HIS
48	8	116	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	8	191	ASN
48	8	266	GLN
48	8	283	HIS
49	9	28	ASN
49	9	74	GLN
51	Ab	84	HIS
52	Ac	49	GLN
52	Ac	58	HIS
54	Ad	16	ASN
54	Ad	49	ASN
56	Ag	39	ASN
57	Ah	3	ASN
57	Ah	16	ASN
57	Ah	21	HIS
58	Ai	10	HIS
58	Ai	15	ASN
58	Ai	35	GLN
58	Ai	41	ASN
60	Ak	4	ASN
60	Ak	11	ASN
60	Ak	12	HIS
60	Ak	55	ASN
60	Ak	99	ASN
60	Ak	170	ASN
60	Ak	178	GLN
60	Ak	256	HIS
60	Ak	360	ASN
60	Ak	368	HIS
60	Ak	413	HIS
60	Ak	503	HIS
60	Ak	512	ASN
61	Al	52	HIS
61	Al	91	ASN
61	Al	102	HIS
61	Al	195	GLN
61	Al	203	ASN
62	Am	3	HIS
62	Am	6	HIS
62	Am	12	ASN
62	Am	133	ASN
62	Am	148	HIS
62	Am	158	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
62	Am	204	HIS
62	Am	207	HIS
62	Am	222	GLN
62	Am	232	HIS
63	An	109	HIS
64	Ao	34	ASN
65	Ap	66	ASN
66	Aq	51	HIS
66	Aq	52	HIS
67	Ar	23	GLN
67	Ar	24	ASN
67	Ar	25	GLN
67	Ar	28	ASN
67	Ar	32	ASN
67	Ar	37	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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 52 ligands modelled in this entry, 5 are monoatomic - leaving 47 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
75	PEE	7	402	-	48,48,50	1.34	4 (8%)	51,53,55	1.04	2 (3%)
75	PEE	u	502	-	48,48,50	1.38	4 (8%)	51,53,55	0.91	2 (3%)
75	PEE	7	401	-	40,40,50	1.46	4 (10%)	43,45,55	0.95	3 (6%)
76	HEM	7	404	-	50,50,50	6.18	17 (34%)	66,82,82	5.31	30 (45%)
68	SF4	G	802	7	0,12,12	-	-	-	-	-
71	PLX	i	502	-	51,51,51	0.75	1 (1%)	55,59,59	0.65	1 (1%)
71	PLX	2	301	-	51,51,51	0.77	1 (1%)	55,59,59	0.58	1 (1%)
75	PEE	i	501	-	48,48,50	1.34	4 (8%)	51,53,55	0.96	2 (3%)
70	FES	4	302	53	0,4,4	-	-	-	-	-
74	CDL	z	101	-	63,63,99	1.22	5 (7%)	69,75,111	1.08	6 (8%)
73	ZMP	X	201	15	27,33,36	1.96	6 (22%)	32,40,45	1.98	7 (21%)
75	PEE	W	401	-	48,48,50	1.35	4 (8%)	51,53,55	0.98	2 (3%)
69	FMN	B	502	-	33,33,33	1.42	6 (18%)	48,50,50	1.30	8 (16%)
74	CDL	8	401	-	63,63,99	1.24	6 (9%)	69,75,111	0.99	4 (5%)
76	HEM	w	402	47	50,50,50	6.14	19 (38%)	66,82,82	5.30	32 (48%)
68	SF4	G	801	7	0,12,12	-	-	-	-	-
68	SF4	I	301	9	0,12,12	-	-	-	-	-
71	PLX	H	303	-	51,51,51	0.78	1 (1%)	55,59,59	0.63	1 (1%)
75	PEE	l	701	-	48,48,50	1.36	4 (8%)	51,53,55	0.94	2 (3%)
74	CDL	u	501	-	63,63,99	1.25	5 (7%)	69,75,111	1.00	4 (5%)
75	PEE	w	403	-	48,48,50	1.33	4 (8%)	51,53,55	0.98	2 (3%)
70	FES	E	301	-	0,4,4	-	-	-	-	-
73	ZMP	Q	201	-	27,33,36	1.94	5 (18%)	32,40,45	1.89	6 (18%)
74	CDL	i	503	-	63,63,99	1.22	5 (7%)	69,75,111	1.07	4 (5%)
71	PLX	4	301	-	51,51,51	0.79	1 (1%)	55,59,59	0.61	1 (1%)
68	SF4	B	501	2	0,12,12	-	-	-	-	-
77	HEC	8	402	48	50,50,50	1.68	5 (10%)	68,82,82	1.38	7 (10%)
70	FES	G	803	7	0,4,4	-	-	-	-	-
74	CDL	5	501	-	63,63,99	1.24	5 (7%)	69,75,111	0.99	4 (5%)
77	HEC	x	401	48	50,50,50	1.97	6 (12%)	68,82,82	1.51	11 (16%)
74	CDL	s	201	-	63,63,99	1.23	5 (7%)	69,75,111	1.04	4 (5%)
70	FES	2	303	-	0,4,4	-	-	-	-	-
75	PEE	q	501	-	48,48,50	1.35	4 (8%)	51,53,55	0.92	2 (3%)
72	NDP	L	401	-	49,52,52	1.20	5 (10%)	66,80,80	1.76	11 (16%)
68	SF4	H	301	8	0,12,12	-	-	-	-	-
74	CDL	l	702	-	63,63,99	1.22	5 (7%)	69,75,111	1.06	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
78	HEA	Ak	601	60	66,67,67	1.10	3 (4%)	78,103,103	1.37	11 (14%)
76	HEM	w	401	47	50,50,50	6.17	18 (36%)	66,82,82	5.29	32 (48%)
74	CDL	Aa	101	-	63,63,99	1.27	5 (7%)	69,75,111	1.13	5 (7%)
75	PEE	5	502	-	48,48,50	1.39	4 (8%)	51,53,55	0.96	2 (3%)
74	CDL	V	201	-	61,61,99	1.18	5 (8%)	64,71,111	1.11	4 (6%)
74	CDL	x	402	-	63,63,99	1.26	5 (7%)	69,75,111	1.08	5 (7%)
75	PEE	2	302	-	48,48,50	1.35	4 (8%)	51,53,55	0.95	2 (3%)
71	PLX	V	202	-	51,51,51	0.77	1 (1%)	55,59,59	0.58	1 (1%)
76	HEM	7	403	47	50,50,50	6.18	19 (38%)	66,82,82	5.33	36 (54%)
68	SF4	H	302	8	0,12,12	-	-	-	-	-
78	HEA	Ak	602	60	66,67,67	1.23	7 (10%)	78,103,103	1.36	11 (14%)

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
75	PEE	7	402	-	-	30/52/52/54	-
75	PEE	u	502	-	-	22/52/52/54	-
75	PEE	7	401	-	-	17/44/44/54	-
76	HEM	7	404	-	-	7/14/54/54	-
68	SF4	G	802	7	-	-	0/6/5/5
71	PLX	i	502	-	-	25/55/55/55	-
71	PLX	2	301	-	-	27/55/55/55	-
75	PEE	i	501	-	-	32/52/52/54	-
74	CDL	z	101	-	-	44/74/74/110	-
70	FES	4	302	53	-	-	0/1/1/1
73	ZMP	X	201	15	-	7/38/40/43	-
75	PEE	W	401	-	-	21/52/52/54	-
69	FMN	B	502	-	-	4/18/18/18	0/3/3/3
74	CDL	8	401	-	-	37/74/74/110	-
76	HEM	w	402	47	-	7/14/54/54	-
71	PLX	H	303	-	-	33/55/55/55	-
75	PEE	l	701	-	-	30/52/52/54	-
68	SF4	G	801	7	-	-	0/6/5/5
68	SF4	I	301	9	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	CDL	u	501	-	-	38/74/74/110	-
75	PEE	w	403	-	-	20/52/52/54	-
70	FES	E	301	-	-	-	0/1/1/1
73	ZMP	Q	201	-	-	11/38/40/43	-
74	CDL	i	503	-	-	41/74/74/110	-
71	PLX	4	301	-	-	26/55/55/55	-
77	HEC	8	402	48	1/1/3/7	6/14/54/54	-
68	SF4	B	501	2	-	-	0/6/5/5
70	FES	G	803	7	-	-	0/1/1/1
74	CDL	5	501	-	-	40/74/74/110	-
77	HEC	x	401	48	1/1/3/7	6/14/54/54	-
74	CDL	s	201	-	-	40/74/74/110	-
70	FES	2	303	-	-	-	0/1/1/1
75	PEE	q	501	-	-	22/52/52/54	-
72	NDP	L	401	-	-	15/34/77/77	0/5/5/5
68	SF4	H	301	8	-	-	0/6/5/5
74	CDL	l	702	-	-	25/74/74/110	-
78	HEA	Ak	601	60	-	9/36/76/76	-
76	HEM	w	401	47	-	5/14/54/54	-
74	CDL	Aa	101	-	-	32/74/74/110	-
75	PEE	5	502	-	-	20/52/52/54	-
74	CDL	V	201	-	-	28/69/69/110	-
74	CDL	x	402	-	-	44/74/74/110	-
75	PEE	2	302	-	-	27/52/52/54	-
71	PLX	V	202	-	-	32/55/55/55	-
76	HEM	7	403	47	-	8/14/54/54	-
68	SF4	H	302	8	-	-	0/6/5/5
78	HEA	Ak	602	60	-	7/36/76/76	-

All (212) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	w	401	HEM	CHC-C1C	17.06	1.71	1.38
76	7	403	HEM	CHB-C4A	17.06	1.77	1.39
76	7	404	HEM	CHC-C1C	16.94	1.71	1.38
76	w	402	HEM	CHC-C1C	16.75	1.70	1.38
76	7	404	HEM	CHB-C4A	16.67	1.76	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	7	403	HEM	CHD-C4C	16.64	1.70	1.38
76	7	403	HEM	CHC-C1C	16.50	1.70	1.38
76	w	401	HEM	CHB-C4A	16.47	1.76	1.39
76	7	404	HEM	CHD-C4C	16.46	1.70	1.38
76	w	401	HEM	CHD-C4C	16.34	1.70	1.38
76	w	402	HEM	CHD-C4C	16.26	1.70	1.38
76	w	402	HEM	CHB-C4A	16.24	1.75	1.39
76	w	401	HEM	CHA-C1A	16.02	1.75	1.39
76	7	404	HEM	CHA-C1A	15.90	1.75	1.39
76	7	403	HEM	CHA-C1A	15.82	1.74	1.39
76	w	402	HEM	CHA-C1A	15.74	1.74	1.39
76	7	403	HEM	CHD-C1D	14.45	1.72	1.39
76	7	404	HEM	CHD-C1D	14.34	1.72	1.39
76	w	401	HEM	CHD-C1D	14.12	1.71	1.39
76	w	402	HEM	CHD-C1D	13.93	1.71	1.39
76	w	401	HEM	CHC-C4B	13.47	1.70	1.39
76	7	404	HEM	CHC-C4B	13.43	1.69	1.39
76	w	402	HEM	CHC-C4B	13.36	1.69	1.39
76	7	403	HEM	CHC-C4B	12.98	1.68	1.39
76	w	401	HEM	CHB-C1B	10.45	1.59	1.38
76	w	402	HEM	CHA-C4D	10.25	1.59	1.38
76	7	403	HEM	CHB-C1B	10.21	1.59	1.38
76	7	404	HEM	CHA-C4D	10.19	1.59	1.38
76	w	402	HEM	CHB-C1B	10.14	1.59	1.38
76	7	403	HEM	CHA-C4D	10.09	1.59	1.38
76	7	404	HEM	CHB-C1B	9.98	1.58	1.38
76	w	401	HEM	CHA-C4D	9.89	1.58	1.38
77	x	401	HEC	C3D-C2D	7.89	1.53	1.36
77	8	402	HEC	C3D-C2D	7.77	1.53	1.36
76	w	401	HEM	C4D-ND	-6.92	1.28	1.40
76	w	402	HEM	C4D-ND	-6.92	1.28	1.40
76	7	404	HEM	C4D-ND	-6.76	1.28	1.40
76	7	403	HEM	C1B-NB	-6.67	1.28	1.40
76	7	403	HEM	C4D-ND	-6.67	1.28	1.40
73	Q	201	ZMP	C16-N2	6.62	1.48	1.33
76	w	402	HEM	C1B-NB	-6.56	1.29	1.40
76	7	404	HEM	C1B-NB	-6.55	1.29	1.40
73	X	201	ZMP	C16-N2	6.34	1.47	1.33
76	w	401	HEM	C1B-NB	-6.13	1.29	1.40
77	x	401	HEC	FE-ND	5.71	2.12	1.94
76	w	402	HEM	FE-NC	-5.28	1.77	1.95
76	7	404	HEM	FE-NC	-5.27	1.77	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	7	403	HEM	FE-NC	-5.27	1.77	1.95
76	w	401	HEM	FE-NC	-5.22	1.77	1.95
76	w	402	HEM	FE-NB	-5.13	1.78	1.94
76	7	404	HEM	FE-NB	-5.00	1.79	1.94
76	w	401	HEM	FE-NB	-4.83	1.79	1.94
77	x	401	HEC	FE-NB	4.81	2.09	1.94
76	7	403	HEM	FE-NB	-4.77	1.80	1.94
76	7	404	HEM	FE-ND	-4.69	1.80	1.94
76	w	402	HEM	FE-ND	-4.61	1.80	1.94
76	7	403	HEM	FE-ND	-4.59	1.80	1.94
69	B	502	FMN	C9A-C5A	4.56	1.48	1.41
74	x	402	CDL	OB8-CB7	4.45	1.46	1.33
73	X	201	ZMP	C9-C10	4.39	1.55	1.50
74	x	402	CDL	OA6-CA5	4.37	1.46	1.34
74	8	401	CDL	OB8-CB7	4.36	1.46	1.33
74	Aa	101	CDL	OB8-CB7	4.34	1.46	1.33
75	5	502	PEE	C39-C38	4.30	1.56	1.31
76	w	401	HEM	FE-ND	-4.29	1.81	1.94
74	Aa	101	CDL	OA6-CA5	4.28	1.46	1.34
75	7	401	PEE	C39-C38	4.27	1.56	1.31
75	u	502	PEE	O3-C30	4.27	1.45	1.33
75	7	402	PEE	C39-C38	4.25	1.56	1.31
75	q	501	PEE	C39-C38	4.25	1.56	1.31
74	l	702	CDL	OB8-CB7	4.24	1.45	1.33
75	u	502	PEE	C39-C38	4.24	1.56	1.31
75	w	403	PEE	C39-C38	4.24	1.56	1.31
75	5	502	PEE	O3-C30	4.24	1.45	1.33
75	2	302	PEE	C39-C38	4.23	1.56	1.31
74	z	101	CDL	OB8-CB7	4.22	1.45	1.33
75	W	401	PEE	C18-C19	4.21	1.56	1.31
75	W	401	PEE	C39-C38	4.21	1.56	1.31
75	5	502	PEE	C18-C19	4.21	1.56	1.31
75	l	701	PEE	C18-C19	4.21	1.56	1.31
74	s	201	CDL	OA6-CA5	4.20	1.46	1.34
75	2	302	PEE	O3-C30	4.20	1.45	1.33
75	l	701	PEE	C39-C38	4.20	1.56	1.31
75	u	502	PEE	C18-C19	4.20	1.56	1.31
74	5	501	CDL	OB8-CB7	4.20	1.45	1.33
74	8	401	CDL	OA6-CA5	4.19	1.46	1.34
75	2	302	PEE	C18-C19	4.18	1.56	1.31
75	q	501	PEE	C18-C19	4.18	1.56	1.31
74	u	501	CDL	OB8-CB7	4.18	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	u	501	CDL	OA6-CA5	4.18	1.46	1.34
75	l	701	PEE	O3-C30	4.17	1.45	1.33
74	5	501	CDL	OA6-CA5	4.17	1.46	1.34
75	i	501	PEE	C39-C38	4.16	1.55	1.31
75	w	403	PEE	C18-C19	4.14	1.55	1.31
74	i	503	CDL	OA6-CA5	4.13	1.46	1.34
75	i	501	PEE	O3-C30	4.13	1.45	1.33
75	i	501	PEE	C18-C19	4.13	1.55	1.31
75	7	402	PEE	O3-C30	4.12	1.45	1.33
75	W	401	PEE	O3-C30	4.12	1.45	1.33
74	i	503	CDL	OB8-CB7	4.12	1.45	1.33
75	7	402	PEE	C18-C19	4.11	1.55	1.31
74	V	201	CDL	OB8-CB7	4.11	1.45	1.33
74	l	702	CDL	OA6-CA5	4.09	1.45	1.34
74	V	201	CDL	OA6-CA5	4.09	1.45	1.34
75	7	401	PEE	O3-C30	4.07	1.45	1.33
74	u	501	CDL	OA8-CA7	4.07	1.45	1.33
74	z	101	CDL	OA6-CA5	4.06	1.45	1.34
75	7	401	PEE	C19-C18	4.06	1.56	1.28
73	Q	201	ZMP	C13-N1	4.05	1.42	1.33
75	q	501	PEE	O3-C30	4.05	1.45	1.33
74	s	201	CDL	OB8-CB7	4.04	1.45	1.33
73	X	201	ZMP	C13-N1	4.02	1.42	1.33
73	Q	201	ZMP	C9-C10	4.02	1.54	1.50
74	Aa	101	CDL	OA8-CA7	4.01	1.45	1.33
75	w	403	PEE	O3-C30	3.99	1.45	1.33
74	8	401	CDL	OA8-CA7	3.98	1.45	1.33
74	x	402	CDL	OA8-CA7	3.96	1.44	1.33
74	5	501	CDL	OA8-CA7	3.94	1.44	1.33
72	L	401	NDP	C5A-C4A	3.93	1.46	1.39
77	8	402	HEC	FE-NB	3.92	2.07	1.94
74	s	201	CDL	OA8-CA7	3.87	1.44	1.33
74	l	702	CDL	OA8-CA7	3.86	1.44	1.33
74	i	503	CDL	OA8-CA7	3.82	1.44	1.33
74	z	101	CDL	OA8-CA7	3.76	1.44	1.33
78	Ak	602	HEA	CMA-C3A	-3.74	1.37	1.45
77	x	401	HEC	FE-NA	3.51	2.07	1.95
77	x	401	HEC	FE-NC	3.49	2.07	1.95
76	w	401	HEM	C1C-NC	-3.49	1.33	1.39
75	u	502	PEE	O2-C10	3.48	1.44	1.34
75	5	502	PEE	O2-C10	3.44	1.44	1.34
76	w	402	HEM	C1C-NC	-3.41	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	l	702	CDL	OB6-CB5	3.38	1.43	1.34
75	q	501	PEE	O2-C10	3.34	1.43	1.34
74	i	503	CDL	OB6-CB5	3.33	1.43	1.34
75	l	701	PEE	O2-C10	3.31	1.43	1.34
75	i	501	PEE	O2-C10	3.30	1.43	1.34
76	7	403	HEM	C1C-NC	-3.28	1.33	1.39
74	V	201	CDL	OB6-CB5	3.26	1.43	1.34
76	7	404	HEM	C1C-NC	-3.26	1.33	1.39
75	w	403	PEE	O2-C10	3.26	1.43	1.34
74	8	401	CDL	OB6-CB5	3.25	1.43	1.34
74	Aa	101	CDL	OB6-CB5	3.23	1.43	1.34
75	W	401	PEE	O2-C10	3.23	1.43	1.34
75	7	401	PEE	O2-C10	3.20	1.43	1.34
69	B	502	FMN	C8-C7	3.17	1.48	1.40
74	s	201	CDL	OB6-CB5	3.16	1.43	1.34
77	8	402	HEC	FE-NA	3.15	2.05	1.95
74	5	501	CDL	OB6-CB5	3.14	1.43	1.34
75	7	402	PEE	O2-C10	3.13	1.43	1.34
74	u	501	CDL	OB6-CB5	3.13	1.43	1.34
74	z	101	CDL	OB6-CB5	3.12	1.43	1.34
72	L	401	NDP	C6N-C5N	3.10	1.38	1.33
75	2	302	PEE	O2-C10	3.10	1.43	1.34
76	w	402	HEM	C3C-C4C	-3.08	1.40	1.46
76	w	401	HEM	C3C-C4C	-3.06	1.40	1.46
74	x	402	CDL	OB6-CB5	3.06	1.42	1.34
69	B	502	FMN	C4-N3	-3.03	1.33	1.38
74	V	201	CDL	OA8-CA7	3.01	1.44	1.33
76	7	403	HEM	C4C-NC	-3.00	1.33	1.39
78	Ak	602	HEA	FE-NA	2.89	2.04	1.95
71	H	303	PLX	O6-C4	-2.86	1.40	1.44
71	V	202	PLX	O6-C4	-2.84	1.40	1.44
76	w	402	HEM	C4C-NC	-2.83	1.34	1.39
72	L	401	NDP	C5A-N7A	-2.82	1.33	1.39
76	7	404	HEM	C4C-NC	-2.80	1.34	1.39
76	w	402	HEM	C1D-C2D	-2.80	1.39	1.44
71	4	301	PLX	O6-C4	-2.78	1.40	1.44
76	7	404	HEM	C3C-C4C	-2.76	1.41	1.46
76	w	401	HEM	C4C-NC	-2.70	1.34	1.39
76	7	403	HEM	C3C-C4C	-2.69	1.41	1.46
78	Ak	602	HEA	C1D-C2D	2.69	1.49	1.44
73	Q	201	ZMP	C10-S1	-2.68	1.69	1.76
77	8	402	HEC	FE-ND	2.68	2.03	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	s	201	CDL	OB6-CB4	-2.68	1.39	1.46
78	Ak	601	HEA	CMA-C3A	-2.67	1.39	1.45
74	x	402	CDL	OB6-CB4	-2.67	1.39	1.46
74	u	501	CDL	OB6-CB4	-2.67	1.39	1.46
74	5	501	CDL	OB6-CB4	-2.66	1.39	1.46
78	Ak	602	HEA	C1D-ND	-2.65	1.35	1.40
78	Ak	601	HEA	C1A-C2A	-2.64	1.40	1.45
74	z	101	CDL	OB6-CB4	-2.63	1.40	1.46
78	Ak	602	HEA	C3A-C2A	-2.62	1.31	1.36
73	X	201	ZMP	C10-S1	-2.61	1.69	1.76
74	i	503	CDL	OB6-CB4	-2.61	1.40	1.46
74	Aa	101	CDL	OB6-CB4	-2.59	1.40	1.46
71	i	502	PLX	O6-C4	-2.56	1.41	1.44
71	2	301	PLX	O6-C4	-2.47	1.41	1.44
74	8	401	CDL	OB6-CB4	-2.43	1.40	1.46
74	V	201	CDL	OB6-CB4	-2.40	1.40	1.46
76	7	403	HEM	C1C-C2C	-2.38	1.40	1.45
69	B	502	FMN	C5A-N5	-2.30	1.35	1.39
74	l	702	CDL	OB6-CB4	-2.29	1.40	1.46
78	Ak	601	HEA	C3A-C4A	-2.26	1.42	1.46
78	Ak	602	HEA	CMD-C2D	2.25	1.55	1.50
76	w	401	HEM	C1D-C2D	-2.25	1.40	1.44
76	7	403	HEM	C3B-C4B	-2.24	1.40	1.44
76	w	401	HEM	C3C-C2C	2.19	1.41	1.37
72	L	401	NDP	C5A-C6A	2.17	1.47	1.41
77	8	402	HEC	FE-NC	2.15	2.02	1.95
73	X	201	ZMP	O5-C21	-2.14	1.39	1.44
69	B	502	FMN	C4A-N5	2.14	1.34	1.30
69	B	502	FMN	C2-N3	-2.13	1.34	1.39
76	7	404	HEM	C1D-C2D	-2.12	1.40	1.44
72	L	401	NDP	C8A-N7A	2.09	1.35	1.31
77	x	401	HEC	C3B-C2B	-2.08	1.32	1.36
73	X	201	ZMP	O4-C17	-2.07	1.38	1.42
76	w	402	HEM	C3B-C4B	-2.07	1.40	1.44
78	Ak	602	HEA	FE-NC	2.04	2.02	1.95
76	7	403	HEM	C3C-C2C	2.03	1.41	1.37
73	Q	201	ZMP	O4-C17	-2.01	1.38	1.42
76	w	402	HEM	C3C-C2C	2.00	1.41	1.37
74	8	401	CDL	C11-CA5	2.00	1.56	1.50

All (272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	7	404	HEM	C4A-CHB-C1B	-21.99	74.18	126.34
76	w	402	HEM	C4A-CHB-C1B	-21.13	76.23	126.34
76	7	403	HEM	C4A-CHB-C1B	-21.08	76.35	126.34
76	w	401	HEM	C4A-CHB-C1B	-20.45	77.84	126.34
76	w	402	HEM	C1A-CHA-C4D	-19.69	79.63	126.34
76	w	401	HEM	C1A-CHA-C4D	-19.58	79.89	126.34
76	7	404	HEM	C1A-CHA-C4D	-18.40	82.71	126.34
76	7	403	HEM	C1A-CHA-C4D	-18.21	83.16	126.34
76	7	403	HEM	CHA-C1A-C2A	-18.07	85.87	125.36
76	w	402	HEM	CHA-C1A-C2A	-17.40	87.35	125.36
76	w	401	HEM	CHA-C1A-C2A	-17.08	88.05	125.36
76	7	404	HEM	CHA-C1A-C2A	-16.67	88.95	125.36
76	w	402	HEM	CHB-C4A-C3A	-14.45	86.43	127.24
76	w	401	HEM	CHB-C4A-C3A	-14.37	86.64	127.24
76	7	404	HEM	CHB-C4A-C3A	-14.31	86.83	127.24
76	7	403	HEM	CHB-C4A-C3A	-13.33	89.58	127.24
76	7	403	HEM	C4A-NA-C1A	-8.79	96.74	105.35
76	7	404	HEM	C4A-NA-C1A	-8.27	97.25	105.35
76	7	403	HEM	C1C-CHC-C4B	-7.97	108.87	126.06
76	w	402	HEM	C4C-CHD-C1D	-7.45	109.99	126.06
76	7	404	HEM	C1C-CHC-C4B	-7.38	110.14	126.06
76	w	401	HEM	C4C-CHD-C1D	-7.36	110.19	126.06
76	w	402	HEM	C1C-CHC-C4B	-7.34	110.22	126.06
76	w	401	HEM	C1C-CHC-C4B	-7.23	110.46	126.06
76	7	403	HEM	C4A-C3A-C2A	-7.17	98.44	106.83
76	w	401	HEM	C4A-NA-C1A	-7.17	98.33	105.35
76	7	404	HEM	C4C-CHD-C1D	-7.13	110.67	126.06
76	7	403	HEM	C4C-CHD-C1D	-6.84	111.31	126.06
76	7	404	HEM	C2B-C1B-NB	6.46	117.50	109.84
76	w	402	HEM	C4A-NA-C1A	-6.24	99.24	105.35
72	L	401	NDP	C5A-C4A-N3A	-6.21	118.65	126.75
77	8	402	HEC	C1D-ND-C4D	6.17	111.45	105.07
76	w	401	HEM	C3D-C4D-ND	6.08	116.94	110.17
76	7	403	HEM	C3D-C4D-ND	6.04	116.89	110.17
73	X	201	ZMP	C11-S1-C10	6.04	120.67	101.87
76	w	402	HEM	C2B-C1B-NB	6.02	116.97	109.84
76	7	404	HEM	C3D-C4D-ND	5.75	116.56	110.17
76	7	403	HEM	C2B-C1B-NB	5.75	116.65	109.84
73	Q	201	ZMP	C9-C10-S1	5.66	120.05	113.46
76	w	401	HEM	C2B-C1B-NB	5.56	116.42	109.84
76	7	404	HEM	C4A-C3A-C2A	-5.51	100.39	106.83
73	X	201	ZMP	C9-C10-S1	5.39	119.73	113.46
76	w	402	HEM	C3D-C4D-ND	5.36	116.14	110.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	L	401	NDP	PN-O3-PA	-5.21	114.94	132.83
77	x	401	HEC	C1D-ND-C4D	5.16	110.40	105.07
76	w	401	HEM	C2A-C1A-NA	5.11	115.86	110.15
73	Q	201	ZMP	C11-S1-C10	5.11	117.78	101.87
76	7	404	HEM	C3B-C2B-C1B	-5.10	102.70	106.49
72	L	401	NDP	N3A-C4A-N9A	4.98	135.28	127.08
76	w	402	HEM	C3B-C2B-C1B	-4.94	102.82	106.49
74	V	201	CDL	OA6-CA5-C11	4.93	122.12	111.50
76	7	403	HEM	C4B-C3B-C2B	-4.60	103.46	107.11
74	Aa	101	CDL	OB6-CB5-C51	4.53	121.27	111.50
76	w	401	HEM	C4B-C3B-C2B	-4.49	103.55	107.11
76	w	401	HEM	C4C-C3C-C2C	-4.49	103.07	106.75
74	x	402	CDL	OA6-CA5-C11	4.48	121.16	111.50
74	V	201	CDL	OB6-CB5-C51	4.44	121.07	111.50
76	7	404	HEM	C4B-C3B-C2B	-4.43	103.60	107.11
76	7	404	HEM	C2A-C1A-NA	4.43	115.10	110.15
76	w	402	HEM	CHD-C1D-C2D	-4.40	118.11	124.98
76	7	403	HEM	C3B-C2B-C1B	-4.39	103.23	106.49
76	w	401	HEM	C2D-C1D-ND	4.37	115.11	109.88
76	7	404	HEM	C3A-C4A-NA	4.35	116.70	110.08
76	w	402	HEM	C4A-C3A-C2A	-4.34	101.75	106.83
76	7	403	HEM	C2A-C1A-NA	4.34	115.00	110.15
74	Aa	101	CDL	OA6-CA5-C11	4.34	120.85	111.50
76	w	402	HEM	C4C-C3C-C2C	-4.30	103.22	106.75
75	5	502	PEE	O2-C10-C11	4.29	120.74	111.50
74	i	503	CDL	OA6-CA5-C11	4.27	120.71	111.50
74	8	401	CDL	OB6-CB5-C51	4.21	120.58	111.50
76	w	402	HEM	C2D-C1D-ND	4.20	114.92	109.88
75	W	401	PEE	O2-C10-C11	4.16	120.47	111.50
74	s	201	CDL	OA6-CA5-C11	4.11	120.35	111.50
72	L	401	NDP	C2A-N3A-C4A	4.04	121.31	111.75
75	w	403	PEE	O2-C10-C11	4.01	120.13	111.50
74	z	101	CDL	OA6-CA5-C11	4.00	120.13	111.50
75	i	501	PEE	O2-C10-C11	4.00	120.11	111.50
76	w	401	HEM	C4D-ND-C1D	-3.97	100.97	105.07
76	w	401	HEM	C3A-C4A-NA	3.97	116.12	110.08
74	i	503	CDL	OB6-CB5-C51	3.97	120.05	111.50
76	w	402	HEM	C3A-C4A-NA	3.96	116.12	110.08
78	Ak	601	HEA	C17-C18-C19	-3.96	118.13	127.66
76	7	403	HEM	CHB-C4A-NA	-3.92	116.62	123.85
75	7	402	PEE	O2-C10-C11	3.92	119.96	111.50
76	w	402	HEM	C2A-C1A-NA	3.92	114.53	110.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	z	101	CDL	OB6-CB5-C51	3.91	119.94	111.50
76	7	403	HEM	C1B-NB-C4B	-3.91	101.03	105.07
76	w	401	HEM	CHD-C1D-C2D	-3.91	118.88	124.98
74	8	401	CDL	OA6-CA5-C11	3.89	119.88	111.50
75	l	701	PEE	O2-C10-C11	3.88	119.86	111.50
75	q	501	PEE	O2-C10-C11	3.86	119.82	111.50
74	u	501	CDL	OA6-CA5-C11	3.86	119.82	111.50
74	x	402	CDL	OB6-CB5-C51	3.85	119.80	111.50
76	7	404	HEM	C1B-NB-C4B	-3.84	101.10	105.07
73	Q	201	ZMP	O1-C10-C9	-3.83	119.47	123.99
74	l	702	CDL	OA6-CA5-C11	3.80	119.69	111.50
74	s	201	CDL	OB6-CB5-C51	3.79	119.67	111.50
74	5	501	CDL	OB6-CB5-C51	3.78	119.64	111.50
76	w	401	HEM	C3B-C2B-C1B	-3.76	103.69	106.49
76	7	404	HEM	CHB-C4A-NA	-3.76	116.92	123.85
76	7	403	HEM	C3A-C4A-NA	3.76	115.80	110.08
74	l	702	CDL	OB6-CB5-C51	3.73	119.54	111.50
72	L	401	NDP	N3A-C2A-N1A	-3.73	122.77	128.60
76	7	403	HEM	C2D-C1D-ND	3.70	114.32	109.88
76	w	402	HEM	CHB-C4A-NA	-3.70	117.04	123.85
74	5	501	CDL	OA6-CA5-C11	3.70	119.47	111.50
76	7	404	HEM	C4C-C3C-C2C	-3.69	103.72	106.75
77	x	401	HEC	C1C-CHC-C4B	-3.69	117.59	126.34
76	7	404	HEM	C2D-C1D-ND	3.66	114.26	109.88
74	u	501	CDL	OB6-CB5-C51	3.61	119.29	111.50
76	w	401	HEM	C1B-NB-C4B	-3.58	101.38	105.07
76	7	403	HEM	CHC-C4B-C3B	-3.57	117.45	125.13
75	2	302	PEE	O2-C10-C11	3.55	119.15	111.50
73	Q	201	ZMP	C15-C14-C13	3.54	118.25	112.36
76	w	402	HEM	C4B-C3B-C2B	-3.54	104.31	107.11
73	X	201	ZMP	O1-C10-C9	-3.52	119.84	123.99
75	u	502	PEE	O2-C10-C11	3.47	118.98	111.50
76	w	401	HEM	C4A-C3A-C2A	-3.45	102.79	106.83
76	w	402	HEM	C1B-NB-C4B	-3.43	101.53	105.07
76	7	403	HEM	C4D-ND-C1D	-3.43	101.53	105.07
76	7	404	HEM	CHD-C1D-C2D	-3.36	119.73	124.98
76	w	401	HEM	CHB-C4A-NA	-3.36	117.66	123.85
77	x	401	HEC	C4A-CHB-C1B	-3.31	118.91	126.06
75	7	401	PEE	O2-C10-C11	3.26	118.53	111.50
78	Ak	602	HEA	CHA-C1A-NA	-3.21	120.96	124.44
76	w	401	HEM	C1D-C2D-C3D	-3.18	103.61	106.96
74	l	702	CDL	OB8-CB7-C71	3.16	121.83	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	Ak	601	HEA	C13-C14-C15	-3.14	120.10	127.66
72	L	401	NDP	C4A-C5A-N7A	-3.12	106.82	110.62
76	w	401	HEM	CHD-C4C-C3C	-3.11	119.94	125.26
76	7	403	HEM	C4C-C3C-C2C	-3.09	104.21	106.75
76	w	402	HEM	C4D-ND-C1D	-3.09	101.89	105.07
75	7	402	PEE	O3-C30-C31	3.07	121.54	111.91
76	7	403	HEM	CHD-C1D-C2D	-3.07	120.19	124.98
76	7	404	HEM	C4D-ND-C1D	-3.06	101.92	105.07
76	7	404	HEM	CHB-C1B-C2B	-3.01	118.37	126.73
76	7	404	HEM	CHC-C4B-C3B	-2.96	118.77	125.13
77	8	402	HEC	CHA-C4D-ND	2.95	127.63	124.42
76	w	402	HEM	CHD-C4C-C3C	-2.93	120.25	125.26
73	X	201	ZMP	C15-C14-C13	2.92	117.23	112.36
76	w	401	HEM	CHC-C4B-C3B	-2.89	118.91	125.13
74	u	501	CDL	OA8-CA7-C31	2.89	120.96	111.91
76	7	403	HEM	C3C-C2C-C1C	-2.88	104.32	107.08
76	w	402	HEM	CHB-C1B-C2B	-2.87	118.75	126.73
78	Ak	601	HEA	C1B-C2B-C3B	2.87	110.23	106.80
76	w	401	HEM	CHA-C4D-ND	-2.86	120.84	124.37
76	7	403	HEM	CMB-C2B-C1B	2.86	129.40	125.04
69	B	502	FMN	C4A-C10-N1	-2.86	118.09	124.73
76	w	402	HEM	CHC-C4B-C3B	-2.85	118.99	125.13
72	L	401	NDP	C5A-N7A-C8A	2.84	107.54	103.51
74	x	402	CDL	OB8-CB7-C71	2.83	120.79	111.91
74	Aa	101	CDL	OB8-CB7-C71	2.83	120.78	111.91
76	w	401	HEM	CAA-CBA-CGA	-2.80	107.58	113.60
77	x	401	HEC	C4C-CHD-C1D	-2.80	119.70	126.34
76	w	402	HEM	C1D-C2D-C3D	-2.80	104.02	106.96
76	w	402	HEM	CHA-C1A-NA	-2.78	118.73	123.85
76	7	404	HEM	C4D-C3D-C2D	-2.76	102.87	106.90
77	x	401	HEC	CAA-CBA-CGA	-2.75	107.67	113.60
72	L	401	NDP	C4A-N9A-C8A	2.71	108.67	105.73
74	s	201	CDL	OB8-CB7-C71	2.70	120.38	111.91
76	w	402	HEM	C4D-C3D-C2D	-2.69	102.97	106.90
69	B	502	FMN	C4-C4A-N5	2.68	122.05	118.23
76	7	403	HEM	CHC-C1C-C2C	-2.68	119.86	125.48
76	7	403	HEM	C1A-C2A-C3A	-2.68	102.68	106.89
76	7	403	HEM	C4D-C3D-C2D	-2.67	103.00	106.90
74	i	503	CDL	OB8-CB7-C71	2.67	120.27	111.91
78	Ak	602	HEA	C4A-C3A-C2A	2.66	108.94	106.75
76	w	401	HEM	CHA-C1A-NA	-2.65	118.97	123.85
76	w	401	HEM	CMB-C2B-C1B	2.65	129.07	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	s	201	CDL	OA8-CA7-C31	2.64	120.18	111.91
75	2	302	PEE	O3-C30-C31	2.63	120.17	111.91
76	7	404	HEM	CAD-C3D-C4D	2.63	129.25	124.66
76	7	403	HEM	C1D-C2D-C3D	-2.62	104.21	106.96
76	w	402	HEM	CHA-C4D-ND	-2.61	121.16	124.37
78	Ak	602	HEA	CMD-C2D-C1D	2.59	128.99	125.04
74	5	501	CDL	OA8-CA7-C31	2.59	120.04	111.91
77	x	401	HEC	CAA-C2A-C3A	-2.59	123.06	127.88
74	5	501	CDL	OB8-CB7-C71	2.58	120.02	111.91
74	V	201	CDL	OB8-CB7-C71	2.58	120.01	111.91
74	z	101	CDL	OB8-CB7-C71	2.58	120.01	111.91
75	l	701	PEE	O3-C30-C31	2.57	119.98	111.91
74	u	501	CDL	OB8-CB7-C71	2.56	119.95	111.91
74	x	402	CDL	OA8-CA7-C31	2.56	119.95	111.91
74	z	101	CDL	OA8-CA7-C31	2.56	119.94	111.91
76	w	401	HEM	CAA-C2A-C3A	-2.54	121.25	127.07
76	7	403	HEM	CHA-C4D-C3D	-2.54	120.56	125.33
75	W	401	PEE	O3-C30-C31	2.52	119.81	111.91
77	8	402	HEC	C4C-NC-C1C	2.49	107.79	105.35
74	i	503	CDL	OA8-CA7-C31	2.49	119.72	111.91
75	q	501	PEE	O3-C30-C31	2.49	119.71	111.91
74	l	702	CDL	OA8-CA7-C31	2.48	119.70	111.91
71	4	301	PLX	C1C-N1-C1	2.48	120.07	109.92
76	7	404	HEM	C1D-C2D-C3D	-2.48	104.35	106.96
74	Aa	101	CDL	OA8-CA7-C31	2.48	119.69	111.91
76	w	402	HEM	CMB-C2B-C1B	2.48	128.81	125.04
77	x	401	HEC	CAD-CBD-CGD	-2.47	108.28	113.60
75	u	502	PEE	O3-C30-C31	2.47	119.66	111.91
76	w	401	HEM	CHB-C1B-C2B	-2.47	119.88	126.73
76	w	401	HEM	C4D-C3D-C2D	-2.46	103.32	106.90
78	Ak	602	HEA	C1D-C2D-C3D	-2.45	104.38	106.96
74	Aa	101	CDL	CB4-OB6-CB5	-2.44	111.78	117.79
71	i	502	PLX	C1C-N1-C1	2.43	119.84	109.92
78	Ak	601	HEA	C17-C16-C15	-2.42	105.01	112.98
78	Ak	601	HEA	C20-C19-C18	2.41	125.99	121.12
73	X	201	ZMP	C15-N2-C16	-2.40	118.30	122.59
71	H	303	PLX	C1C-N1-C1	2.40	119.75	109.92
76	7	403	HEM	CHC-C4B-NB	2.40	127.03	124.42
78	Ak	601	HEA	C3C-C4C-NC	2.39	111.72	110.25
75	w	403	PEE	O3-C30-C31	2.38	119.36	111.91
78	Ak	602	HEA	C25-C23-C24	2.36	119.82	114.60
76	7	404	HEM	CHA-C4D-ND	-2.36	121.47	124.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	Ak	602	HEA	CMB-C2B-C3B	-2.36	125.85	130.34
77	8	402	HEC	CMD-C2D-C1D	2.35	128.62	125.04
74	z	101	CDL	CA4-OA6-CA5	-2.35	112.01	117.79
78	Ak	601	HEA	CAD-C3D-C4D	2.35	128.76	124.66
78	Ak	601	HEA	C16-C17-C18	-2.35	104.16	111.88
76	w	402	HEM	CHD-C1D-ND	2.34	126.96	124.42
78	Ak	602	HEA	CAA-C2A-C1A	2.33	129.29	124.89
73	X	201	ZMP	C20-C18-C17	2.33	112.86	108.82
76	w	401	HEM	CAD-C3D-C4D	2.32	128.72	124.66
77	x	401	HEC	CAA-C2A-C1A	2.32	129.27	124.89
75	i	501	PEE	O3-C30-C31	2.32	119.19	111.91
69	B	502	FMN	C4A-C4-N3	2.32	119.07	113.19
76	7	403	HEM	CAD-C3D-C4D	2.31	128.70	124.66
77	8	402	HEC	C4A-NA-C1A	2.31	107.61	105.35
75	7	401	PEE	O3-C30-C31	2.31	119.16	111.91
75	5	502	PEE	O3-C30-C31	2.30	119.12	111.91
71	2	301	PLX	C1C-N1-C1	2.30	119.31	109.92
74	8	401	CDL	OA8-CA7-C31	2.29	119.10	111.91
76	7	404	HEM	CHD-C4C-C3C	-2.29	121.35	125.26
78	Ak	602	HEA	C13-C14-C15	-2.27	122.19	127.66
76	7	404	HEM	CHA-C1A-NA	-2.26	119.68	123.85
76	7	403	HEM	CHB-C1B-NB	-2.26	121.58	124.37
76	7	404	HEM	C3C-C2C-C1C	-2.26	104.92	107.08
69	B	502	FMN	C4-N3-C2	-2.26	121.47	125.64
71	V	202	PLX	C1C-N1-C1	2.24	119.09	109.92
77	8	402	HEC	C3C-C4C-NC	-2.24	107.64	110.15
77	x	401	HEC	C2A-C1A-NA	-2.24	108.15	110.32
74	x	402	CDL	CB4-OB6-CB5	-2.23	112.29	117.79
76	7	403	HEM	CHA-C1A-NA	-2.23	119.74	123.85
69	B	502	FMN	C10-N1-C2	2.23	121.36	116.90
72	L	401	NDP	C3D-C2D-C1D	2.22	105.65	101.43
76	7	403	HEM	C2C-C1C-NC	2.22	113.78	109.69
76	w	402	HEM	CAD-C3D-C4D	2.22	128.53	124.66
69	B	502	FMN	O4-C4-C4A	-2.21	120.73	126.60
73	Q	201	ZMP	C14-C15-N2	-2.21	107.43	111.90
78	Ak	602	HEA	C26-C15-C16	2.21	118.99	115.27
73	X	201	ZMP	O3-C16-N2	-2.20	118.26	122.99
76	7	404	HEM	CAA-C2A-C1A	2.20	129.23	124.89
72	L	401	NDP	N9A-C8A-N7A	-2.20	110.90	113.91
74	8	401	CDL	OB8-CB7-C71	2.19	118.79	111.91
78	Ak	601	HEA	C4B-C3B-C2B	-2.18	103.68	107.41
78	Ak	601	HEA	C12-C13-C14	-2.16	106.53	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	L	401	NDP	C6A-C5A-N7A	2.15	136.03	132.02
75	7	401	PEE	C17-C18-C19	-2.15	112.23	126.84
77	8	402	HEC	C4B-NB-C1B	2.14	107.28	105.07
77	x	401	HEC	C4A-NA-C1A	2.14	107.44	105.35
76	7	403	HEM	CMD-C2D-C1D	2.11	128.26	125.04
73	Q	201	ZMP	C11-C12-N1	-2.11	107.98	112.42
76	7	403	HEM	O2D-CGD-CBD	2.10	120.79	114.03
76	w	401	HEM	C1A-C2A-C3A	-2.10	103.59	106.89
74	V	201	CDL	CA4-OA6-CA5	-2.10	112.62	117.79
76	w	402	HEM	CHC-C4B-NB	2.09	126.69	124.42
78	Ak	602	HEA	CBD-CAD-C3D	2.08	118.41	112.63
69	B	502	FMN	C4A-C10-N10	2.07	119.51	116.48
78	Ak	601	HEA	C27-C19-C18	-2.07	118.37	123.68
76	7	403	HEM	CHB-C1B-C2B	-2.06	121.00	126.73
77	x	401	HEC	C1D-C2D-C3D	-2.05	104.80	106.96
76	w	402	HEM	O2A-CGA-CBA	2.05	120.62	114.03
78	Ak	602	HEA	C3A-C2A-C1A	-2.03	105.14	107.08
74	z	101	CDL	CB4-OB6-CB5	-2.02	112.81	117.79
69	B	502	FMN	N3-C2-N1	2.00	123.31	119.38

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
77	x	401	HEC	NA
77	8	402	HEC	NA

All (845) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	B	502	FMN	C1'-C2'-C3'-C4'
69	B	502	FMN	C3'-C4'-C5'-O5'
69	B	502	FMN	O4'-C4'-C5'-O5'
71	H	303	PLX	O7-C6-O6-C4
71	H	303	PLX	O9-C24-O8-C5
71	H	303	PLX	O9-C24-C25-C26
71	V	202	PLX	O7-C6-O6-C4
71	V	202	PLX	N1-C1-C2-O1
71	V	202	PLX	C25-C24-O8-C5
71	V	202	PLX	O9-C24-C25-C26
71	i	502	PLX	O7-C6-O6-C4
71	i	502	PLX	C3-O4-P1-O2
71	i	502	PLX	C2-O1-P1-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	2	301	PLX	O7-C6-C7-C8
71	2	301	PLX	O7-C6-O6-C4
71	2	301	PLX	C3-O4-P1-O2
71	2	301	PLX	C3-O4-P1-O3
71	2	301	PLX	N1-C1-C2-O1
71	2	301	PLX	C25-C24-O8-C5
71	4	301	PLX	C7-C6-O6-C4
71	4	301	PLX	O7-C6-O6-C4
71	4	301	PLX	C3-O4-P1-O2
71	4	301	PLX	C3-O4-P1-O3
71	4	301	PLX	C2-O1-P1-O4
71	4	301	PLX	C2-O1-P1-O2
71	4	301	PLX	C2-O1-P1-O3
72	L	401	NDP	C5B-O5B-PA-O1A
72	L	401	NDP	C5D-O5D-PN-O1N
73	Q	201	ZMP	C17-C16-N2-C15
73	X	201	ZMP	O3-C16-C17-C18
73	X	201	ZMP	N2-C16-C17-C18
73	X	201	ZMP	O3-C16-C17-O4
73	X	201	ZMP	N2-C16-C17-O4
73	X	201	ZMP	S1-C11-C12-N1
74	V	201	CDL	CA3-OA5-PA1-OA2
74	V	201	CDL	OA5-CA3-CA4-OA6
74	V	201	CDL	CA4-CA6-OA8-CA7
74	V	201	CDL	CB2-OB2-PB2-OB3
74	V	201	CDL	CB2-OB2-PB2-OB4
74	V	201	CDL	OB7-CB5-OB6-CB4
74	V	201	CDL	OB9-CB7-OB8-CB6
74	V	201	CDL	C71-CB7-OB8-CB6
74	i	503	CDL	OA7-CA5-OA6-CA4
74	i	503	CDL	C11-CA5-OA6-CA4
74	i	503	CDL	CB2-OB2-PB2-OB3
74	i	503	CDL	CB3-OB5-PB2-OB3
74	i	503	CDL	CB3-OB5-PB2-OB4
74	l	702	CDL	CA3-OA5-PA1-OA4
74	l	702	CDL	CB2-OB2-PB2-OB3
74	l	702	CDL	CB3-OB5-PB2-OB3
74	l	702	CDL	CB3-OB5-PB2-OB4
74	s	201	CDL	CA3-OA5-PA1-OA3
74	s	201	CDL	OA7-CA5-OA6-CA4
74	s	201	CDL	C11-CA5-OA6-CA4
74	s	201	CDL	CB3-OB5-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
74	u	501	CDL	CB2-C1-CA2-OA2
74	u	501	CDL	OA5-CA3-CA4-OA6
74	u	501	CDL	OA7-CA5-OA6-CA4
74	u	501	CDL	C11-CA5-OA6-CA4
74	x	402	CDL	O1-C1-CA2-OA2
74	x	402	CDL	C11-CA5-OA6-CA4
74	x	402	CDL	CB3-OB5-PB2-OB2
74	x	402	CDL	CB3-OB5-PB2-OB4
74	x	402	CDL	OB7-CB5-OB6-CB4
74	x	402	CDL	C51-CB5-OB6-CB4
74	z	101	CDL	CB2-C1-CA2-OA2
74	z	101	CDL	CB3-OB5-PB2-OB3
74	z	101	CDL	CB3-OB5-PB2-OB4
74	z	101	CDL	C51-CB5-OB6-CB4
74	5	501	CDL	CA2-OA2-PA1-OA3
74	5	501	CDL	OA5-CA3-CA4-OA6
74	5	501	CDL	C11-CA5-OA6-CA4
74	5	501	CDL	CB3-OB5-PB2-OB4
74	8	401	CDL	O1-C1-CB2-OB2
74	8	401	CDL	CA2-OA2-PA1-OA3
74	8	401	CDL	CA2-OA2-PA1-OA4
74	8	401	CDL	CA3-OA5-PA1-OA2
74	8	401	CDL	CA3-OA5-PA1-OA3
74	8	401	CDL	C11-CA5-OA6-CA4
74	Aa	101	CDL	CA2-OA2-PA1-OA3
74	Aa	101	CDL	CA3-OA5-PA1-OA3
74	Aa	101	CDL	CA3-OA5-PA1-OA4
74	Aa	101	CDL	OA7-CA5-OA6-CA4
74	Aa	101	CDL	C11-CA5-OA6-CA4
74	Aa	101	CDL	CB2-OB2-PB2-OB4
75	W	401	PEE	C11-C10-O2-C2
75	W	401	PEE	C5-C4-O4P-P
75	W	401	PEE	O4P-C4-C5-N
75	i	501	PEE	C11-C10-O2-C2
75	i	501	PEE	C4-O4P-P-O2P
75	i	501	PEE	C4-O4P-P-O1P
75	l	701	PEE	C5-C4-O4P-P
75	u	502	PEE	C11-C10-O2-C2
75	u	502	PEE	O4-C10-O2-C2
75	w	403	PEE	C37-C38-C39-C40
75	2	302	PEE	C4-O4P-P-O2P
75	5	502	PEE	C1-O3P-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	5	502	PEE	C4-O4P-P-O3P
75	5	502	PEE	C4-O4P-P-O2P
75	5	502	PEE	C4-O4P-P-O1P
75	7	401	PEE	C11-C10-O2-C2
75	7	401	PEE	C1-O3P-P-O2P
75	7	401	PEE	C1-O3P-P-O1P
75	7	401	PEE	C4-O4P-P-O2P
75	7	402	PEE	O4P-C4-C5-N
75	7	402	PEE	C39-C40-C41-C42
76	w	401	HEM	C2B-C3B-CAB-CBB
76	w	401	HEM	C4B-C3B-CAB-CBB
76	w	402	HEM	C2B-C3B-CAB-CBB
76	w	402	HEM	C4B-C3B-CAB-CBB
76	w	402	HEM	C2C-C3C-CAC-CBC
76	w	402	HEM	C4C-C3C-CAC-CBC
76	7	403	HEM	C1A-C2A-CAA-CBA
76	7	404	HEM	C2C-C3C-CAC-CBC
78	Ak	601	HEA	C2A-C3A-CMA-OMA
78	Ak	601	HEA	C4A-C3A-CMA-OMA
78	Ak	601	HEA	C12-C11-C3B-C2B
78	Ak	602	HEA	C2A-C3A-CMA-OMA
78	Ak	602	HEA	C4A-C3A-CMA-OMA
74	x	402	CDL	OB9-CB7-OB8-CB6
74	5	501	CDL	OB9-CB7-OB8-CB6
74	x	402	CDL	C71-CB7-OB8-CB6
74	5	501	CDL	C71-CB7-OB8-CB6
74	Aa	101	CDL	C71-CB7-OB8-CB6
74	s	201	CDL	OA9-CA7-OA8-CA6
74	Aa	101	CDL	OA9-CA7-OA8-CA6
74	Aa	101	CDL	OB9-CB7-OB8-CB6
74	x	402	CDL	OA7-CA5-OA6-CA4
74	z	101	CDL	OB7-CB5-OB6-CB4
74	5	501	CDL	OA7-CA5-OA6-CA4
74	8	401	CDL	OA7-CA5-OA6-CA4
75	W	401	PEE	O4-C10-O2-C2
75	i	501	PEE	O4-C10-O2-C2
75	7	401	PEE	O4-C10-O2-C2
74	Aa	101	CDL	C31-CA7-OA8-CA6
74	V	201	CDL	C51-CB5-OB6-CB4
74	z	101	CDL	OB9-CB7-OB8-CB6
74	i	503	CDL	C31-CA7-OA8-CA6
74	s	201	CDL	C31-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
74	x	402	CDL	C31-CA7-OA8-CA6
75	i	501	PEE	C37-C38-C39-C40
74	u	501	CDL	OA9-CA7-OA8-CA6
74	x	402	CDL	OA9-CA7-OA8-CA6
74	u	501	CDL	O1-C1-CA2-OA2
74	5	501	CDL	O1-C1-CA2-OA2
73	Q	201	ZMP	O3-C16-N2-C15
74	i	503	CDL	C51-CB5-OB6-CB4
74	l	702	CDL	C11-CA5-OA6-CA4
75	q	501	PEE	C11-C10-O2-C2
74	8	401	CDL	CB4-CB6-OB8-CB7
74	x	402	CDL	C31-C32-C33-C34
75	7	401	PEE	C31-C32-C33-C34
75	i	501	PEE	C32-C33-C34-C35
72	L	401	NDP	O4B-C4B-C5B-O5B
72	L	401	NDP	C3B-C4B-C5B-O5B
74	u	501	CDL	C31-CA7-OA8-CA6
74	z	101	CDL	C71-CB7-OB8-CB6
76	w	402	HEM	C3D-CAD-CBD-CGD
74	l	702	CDL	C73-C74-C75-C76
74	i	503	CDL	OA9-CA7-OA8-CA6
78	Ak	601	HEA	C15-C16-C17-C18
72	L	401	NDP	C1B-C2B-O2B-P2B
74	x	402	CDL	C53-C54-C55-C56
74	z	101	CDL	CA2-C1-CB2-OB2
74	8	401	CDL	CA2-C1-CB2-OB2
74	i	503	CDL	OB7-CB5-OB6-CB4
74	l	702	CDL	OA7-CA5-OA6-CA4
74	5	501	CDL	C31-CA7-OA8-CA6
75	l	701	PEE	C31-C30-O3-C3
71	V	202	PLX	C16-C17-C18-C19
74	8	401	CDL	C12-C13-C14-C15
71	4	301	PLX	C30-C31-C32-C33
75	i	501	PEE	C34-C35-C36-C37
74	z	101	CDL	O1-C1-CA2-OA2
74	i	503	CDL	OB6-CB4-CB6-OB8
75	q	501	PEE	O4-C10-O2-C2
74	Aa	101	CDL	C51-CB5-OB6-CB4
74	8	401	CDL	CA7-C31-C32-C33
71	2	301	PLX	C7-C8-C9-C10
75	l	701	PEE	C17-C18-C19-C20
75	q	501	PEE	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	2	302	PEE	C37-C38-C39-C40
71	H	303	PLX	C19-C20-C21-C22
74	i	503	CDL	CA7-C31-C32-C33
74	s	201	CDL	CA5-C11-C12-C13
74	z	101	CDL	CA5-C11-C12-C13
74	Aa	101	CDL	CB7-C71-C72-C73
75	i	501	PEE	C30-C31-C32-C33
75	7	402	PEE	C10-C11-C12-C13
74	V	201	CDL	C1-CA2-OA2-PA1
71	4	301	PLX	C2-C1-N1-C1C
74	i	503	CDL	CB5-C51-C52-C53
75	l	701	PEE	C30-C31-C32-C33
77	8	402	HEC	C3D-CAD-CBD-CGD
74	z	101	CDL	C11-CA5-OA6-CA4
74	5	501	CDL	OA9-CA7-OA8-CA6
74	s	201	CDL	CB7-C71-C72-C73
75	u	502	PEE	C30-C31-C32-C33
74	s	201	CDL	O1-C1-CA2-OA2
72	L	401	NDP	C3B-C2B-O2B-P2B
75	l	701	PEE	O5-C30-O3-C3
75	i	501	PEE	C39-C40-C41-C42
75	i	501	PEE	C17-C18-C19-C20
77	x	401	HEC	C1A-C2A-CAA-CBA
77	x	401	HEC	C2D-C3D-CAD-CBD
71	2	301	PLX	C3-O4-P1-O1
71	4	301	PLX	C3-O4-P1-O1
74	V	201	CDL	CB2-OB2-PB2-OB5
74	i	503	CDL	CA3-OA5-PA1-OA2
74	i	503	CDL	CB2-OB2-PB2-OB5
74	i	503	CDL	CB3-OB5-PB2-OB2
74	l	702	CDL	CA3-OA5-PA1-OA2
74	l	702	CDL	CB2-OB2-PB2-OB5
74	l	702	CDL	CB3-OB5-PB2-OB2
74	s	201	CDL	CA3-OA5-PA1-OA2
74	u	501	CDL	CB2-OB2-PB2-OB5
74	z	101	CDL	CB3-OB5-PB2-OB2
74	5	501	CDL	CB2-OB2-PB2-OB5
74	5	501	CDL	CB3-OB5-PB2-OB2
74	8	401	CDL	CA2-OA2-PA1-OA5
74	Aa	101	CDL	CA2-OA2-PA1-OA5
74	Aa	101	CDL	CA3-OA5-PA1-OA2
74	Aa	101	CDL	CB2-OB2-PB2-OB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	i	501	PEE	C4-O4P-P-O3P
75	l	701	PEE	C1-O3P-P-O4P
75	2	302	PEE	C4-O4P-P-O3P
75	5	502	PEE	C1-O3P-P-O4P
75	7	401	PEE	C1-O3P-P-O4P
75	7	401	PEE	C4-O4P-P-O3P
74	x	402	CDL	CB2-C1-CA2-OA2
74	5	501	CDL	CB2-C1-CA2-OA2
74	z	101	CDL	OA7-CA5-OA6-CA4
74	Aa	101	CDL	OB7-CB5-OB6-CB4
71	H	303	PLX	C2-C1-N1-C1C
71	H	303	PLX	C2-C1-N1-C1A
71	V	202	PLX	O6-C6-C7-C8
71	2	301	PLX	O6-C6-C7-C8
71	4	301	PLX	C9-C10-C11-C12
74	i	503	CDL	C53-C54-C55-C56
74	s	201	CDL	C51-C52-C53-C54
74	z	101	CDL	C12-C13-C14-C15
74	z	101	CDL	C13-C14-C15-C16
75	i	501	PEE	C22-C23-C24-C25
75	l	701	PEE	C34-C35-C36-C37
77	x	401	HEC	C3A-C2A-CAA-CBA
71	H	303	PLX	C15-C16-C17-C18
71	V	202	PLX	C10-C11-C12-C13
74	V	201	CDL	C13-C14-C15-C16
74	s	201	CDL	C14-C15-C16-C17
74	u	501	CDL	C52-C53-C54-C55
75	l	701	PEE	C23-C24-C25-C26
75	l	701	PEE	C14-C15-C16-C17
75	w	403	PEE	C20-C21-C22-C23
75	5	502	PEE	C11-C12-C13-C14
74	5	501	CDL	CA6-CA4-OA6-CA5
74	8	401	CDL	CA6-CA4-OA6-CA5
75	W	401	PEE	C33-C34-C35-C36
74	Aa	101	CDL	CB4-CB3-OB5-PB2
71	i	502	PLX	C17-C18-C19-C20
71	i	502	PLX	C34-C35-C36-C37
74	z	101	CDL	C31-C32-C33-C34
75	i	501	PEE	C21-C22-C23-C24
74	i	503	CDL	O1-C1-CA2-OA2
74	l	702	CDL	O1-C1-CB2-OB2
74	z	101	CDL	O1-C1-CB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	i	502	PLX	C26-C27-C28-C29
74	z	101	CDL	C73-C74-C75-C76
74	V	201	CDL	CB5-C51-C52-C53
74	i	503	CDL	C12-C13-C14-C15
74	u	501	CDL	C53-C54-C55-C56
75	q	501	PEE	C41-C42-C43-C44
71	2	301	PLX	C12-C13-C14-C15
75	w	403	PEE	C13-C14-C15-C16
75	w	403	PEE	C11-C12-C13-C14
75	2	302	PEE	C21-C22-C23-C24
71	V	202	PLX	C30-C31-C32-C33
71	i	502	PLX	C10-C11-C12-C13
74	s	201	CDL	C71-C72-C73-C74
74	u	501	CDL	C13-C14-C15-C16
74	x	402	CDL	C73-C74-C75-C76
74	Aa	101	CDL	C33-C34-C35-C36
75	u	502	PEE	C32-C33-C34-C35
74	8	401	CDL	C73-C74-C75-C76
75	q	501	PEE	C20-C21-C22-C23
75	q	501	PEE	C13-C14-C15-C16
75	2	302	PEE	C11-C12-C13-C14
71	4	301	PLX	C12-C13-C14-C15
75	l	701	PEE	C33-C34-C35-C36
75	2	302	PEE	C22-C23-C24-C25
75	7	401	PEE	C11-C12-C13-C14
75	q	501	PEE	C35-C36-C37-C38
75	5	502	PEE	C19-C20-C21-C22
75	7	402	PEE	C35-C36-C37-C38
75	u	502	PEE	C11-C12-C13-C14
75	w	403	PEE	C22-C23-C24-C25
71	V	202	PLX	C27-C28-C29-C30
73	Q	201	ZMP	C6-C7-C8-C9
74	i	503	CDL	C31-C32-C33-C34
74	Aa	101	CDL	C32-C33-C34-C35
74	Aa	101	CDL	C34-C35-C36-C37
74	Aa	101	CDL	C71-C72-C73-C74
75	5	502	PEE	C22-C23-C24-C25
71	H	303	PLX	C13-C14-C15-C16
71	2	301	PLX	C32-C33-C34-C35
75	q	501	PEE	C11-C12-C13-C14
74	l	702	CDL	C32-C33-C34-C35
74	u	501	CDL	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	V	202	PLX	C12-C13-C14-C15
71	V	202	PLX	C26-C27-C28-C29
71	4	301	PLX	C7-C8-C9-C10
75	i	501	PEE	C20-C21-C22-C23
75	u	502	PEE	C34-C35-C36-C37
75	w	403	PEE	C32-C33-C34-C35
74	5	501	CDL	C71-C72-C73-C74
75	7	402	PEE	C32-C33-C34-C35
71	2	301	PLX	C17-C18-C19-C20
74	x	402	CDL	C33-C34-C35-C36
75	2	302	PEE	C32-C33-C34-C35
71	4	301	PLX	C28-C29-C30-C31
77	x	401	HEC	C4D-C3D-CAD-CBD
71	i	502	PLX	C7-C8-C9-C10
71	V	202	PLX	C17-C18-C19-C20
71	2	301	PLX	C26-C27-C28-C29
74	x	402	CDL	C13-C14-C15-C16
74	z	101	CDL	C71-C72-C73-C74
74	Aa	101	CDL	C31-C32-C33-C34
75	W	401	PEE	C35-C36-C37-C38
74	i	503	CDL	C73-C74-C75-C76
75	i	501	PEE	C41-C42-C43-C44
74	l	702	CDL	CA2-C1-CB2-OB2
75	i	501	PEE	C13-C14-C15-C16
75	l	701	PEE	C11-C12-C13-C14
75	l	701	PEE	C42-C43-C44-C45
74	5	501	CDL	C31-C32-C33-C34
75	7	402	PEE	C41-C42-C43-C44
71	H	303	PLX	C2-C1-N1-C1B
75	7	402	PEE	C30-C31-C32-C33
71	H	303	PLX	C25-C26-C27-C28
74	8	401	CDL	C71-CB7-OB8-CB6
75	2	302	PEE	C11-C10-O2-C2
71	i	502	PLX	C12-C13-C14-C15
74	z	101	CDL	C72-C73-C74-C75
74	s	201	CDL	CB5-C51-C52-C53
74	5	501	CDL	CA7-C31-C32-C33
75	u	502	PEE	C10-C11-C12-C13
71	4	301	PLX	C10-C11-C12-C13
75	7	402	PEE	C12-C13-C14-C15
74	i	503	CDL	C55-C56-C57-C58
75	7	401	PEE	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	u	502	PEE	C37-C38-C39-C40
71	2	301	PLX	C28-C29-C30-C31
74	z	101	CDL	C15-C16-C17-C18
75	i	501	PEE	C15-C16-C17-C18
75	l	701	PEE	C19-C20-C21-C22
75	q	501	PEE	C15-C16-C17-C18
74	l	702	CDL	OB7-CB5-OB6-CB4
75	7	402	PEE	O4-C10-O2-C2
74	u	501	CDL	CB7-C71-C72-C73
74	u	501	CDL	C71-CB7-OB8-CB6
71	i	502	PLX	C33-C34-C35-C36
74	s	201	CDL	C73-C74-C75-C76
74	x	402	CDL	CB7-C71-C72-C73
71	i	502	PLX	C30-C31-C32-C33
75	5	502	PEE	C20-C21-C22-C23
73	Q	201	ZMP	C4-C5-C6-C7
74	u	501	CDL	C51-C52-C53-C54
71	2	301	PLX	C9-C10-C11-C12
74	x	402	CDL	C34-C35-C36-C37
75	W	401	PEE	C12-C13-C14-C15
74	l	702	CDL	C51-CB5-OB6-CB4
75	7	402	PEE	C11-C10-O2-C2
76	7	404	HEM	C4C-C3C-CAC-CBC
74	8	401	CDL	OB9-CB7-OB8-CB6
71	H	303	PLX	C10-C11-C12-C13
71	V	202	PLX	C9-C10-C11-C12
74	i	503	CDL	C71-C72-C73-C74
74	8	401	CDL	C71-C72-C73-C74
75	q	501	PEE	C31-C32-C33-C34
75	7	402	PEE	C40-C41-C42-C43
75	2	302	PEE	O4-C10-O2-C2
75	W	401	PEE	C21-C22-C23-C24
71	V	202	PLX	O6-C4-C5-O8
74	8	401	CDL	C13-C14-C15-C16
75	u	502	PEE	C12-C13-C14-C15
71	4	301	PLX	C2-C1-N1-C1B
71	4	301	PLX	C2-C1-N1-C1A
75	q	501	PEE	C23-C24-C25-C26
75	7	401	PEE	C34-C35-C36-C37
75	7	402	PEE	C19-C20-C21-C22
74	u	501	CDL	C71-C72-C73-C74
74	x	402	CDL	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	W	401	PEE	C11-C12-C13-C14
71	H	303	PLX	C9-C10-C11-C12
71	V	202	PLX	C18-C19-C20-C21
73	Q	201	ZMP	C2-C3-C4-C5
74	u	501	CDL	C32-C33-C34-C35
71	H	303	PLX	C16-C17-C18-C19
71	2	301	PLX	C13-C14-C15-C16
74	5	501	CDL	C13-C14-C15-C16
75	W	401	PEE	C31-C32-C33-C34
75	i	501	PEE	C23-C24-C25-C26
75	i	501	PEE	C40-C41-C42-C43
75	i	501	PEE	C16-C17-C18-C19
71	H	303	PLX	C2-O1-P1-O4
74	s	201	CDL	CB3-OB5-PB2-OB2
74	5	501	CDL	CA2-OA2-PA1-OA5
75	7	402	PEE	C1-O3P-P-O4P
75	7	402	PEE	C33-C34-C35-C36
75	2	302	PEE	C2-C1-O3P-P
74	V	201	CDL	OA5-CA3-CA4-CA6
74	i	503	CDL	OB5-CB3-CB4-CB6
74	l	702	CDL	OB5-CB3-CB4-CB6
74	u	501	CDL	OB5-CB3-CB4-CB6
75	i	501	PEE	O3P-C1-C2-C3
75	l	701	PEE	O3P-C1-C2-C3
75	w	403	PEE	O3P-C1-C2-C3
74	z	101	CDL	CA7-C31-C32-C33
75	u	502	PEE	C21-C22-C23-C24
75	q	501	PEE	C39-C40-C41-C42
74	V	201	CDL	C22-C23-C24-C25
74	i	503	CDL	CB2-C1-CA2-OA2
76	7	404	HEM	C3A-C2A-CAA-CBA
74	Aa	101	CDL	C51-C52-C53-C54
71	H	303	PLX	C11-C12-C13-C14
71	4	301	PLX	C3-C4-C5-O8
74	u	501	CDL	CA3-CA4-CA6-OA8
74	z	101	CDL	CA3-CA4-CA6-OA8
74	z	101	CDL	CB3-CB4-CB6-OB8
74	8	401	CDL	CB3-CB4-CB6-OB8
75	7	402	PEE	C1-C2-C3-O3
74	u	501	CDL	OB9-CB7-OB8-CB6
74	s	201	CDL	C74-C75-C76-C77
75	l	701	PEE	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	5	502	PEE	C33-C34-C35-C36
74	l	702	CDL	C13-C14-C15-C16
75	w	403	PEE	C41-C42-C43-C44
75	q	501	PEE	C10-C11-C12-C13
71	i	502	PLX	O6-C6-C7-C8
73	Q	201	ZMP	O3-C16-C17-O4
71	4	301	PLX	C31-C32-C33-C34
75	w	403	PEE	C35-C36-C37-C38
75	w	403	PEE	C39-C40-C41-C42
75	7	401	PEE	C15-C16-C17-C18
75	7	402	PEE	C15-C16-C17-C18
74	x	402	CDL	C12-C13-C14-C15
74	Aa	101	CDL	C15-C16-C17-C18
75	5	502	PEE	C42-C43-C44-C45
71	V	202	PLX	C13-C14-C15-C16
74	u	501	CDL	CA6-CA4-OA6-CA5
75	i	501	PEE	C42-C43-C44-C45
75	i	501	PEE	C2-C1-O3P-P
71	H	303	PLX	C28-C29-C30-C31
74	z	101	CDL	C75-C76-C77-C78
76	7	404	HEM	C2A-CAA-CBA-CGA
74	x	402	CDL	C11-C12-C13-C14
74	i	503	CDL	OA6-CA4-CA6-OA8
73	X	201	ZMP	C5-C6-C7-C8
75	2	302	PEE	C34-C35-C36-C37
75	2	302	PEE	C30-C31-C32-C33
71	i	502	PLX	C11-C10-C9-C8
75	2	302	PEE	C24-C25-C26-C27
75	7	402	PEE	C13-C14-C15-C16
71	2	301	PLX	C11-C10-C9-C8
74	8	401	CDL	C52-C53-C54-C55
74	i	503	CDL	C11-C12-C13-C14
71	H	303	PLX	O4-C3-C4-C5
71	V	202	PLX	O4-C3-C4-C5
74	s	201	CDL	OB5-CB3-CB4-CB6
75	2	302	PEE	C20-C21-C22-C23
75	l	701	PEE	O4P-C4-C5-N
77	8	402	HEC	C2B-C3B-CAB-CBB
71	i	502	PLX	C20-C21-C22-C23
71	2	301	PLX	C14-C15-C16-C17
74	8	401	CDL	C1-CA2-OA2-PA1
71	V	202	PLX	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
74	u	501	CDL	C75-C76-C77-C78
74	z	101	CDL	C33-C34-C35-C36
75	w	403	PEE	C40-C41-C42-C43
71	H	303	PLX	C29-C30-C31-C32
76	7	403	HEM	C3D-CAD-CBD-CGD
74	l	702	CDL	C34-C35-C36-C37
71	V	202	PLX	C3-C4-C5-O8
71	2	301	PLX	C3-C4-C5-O8
74	V	201	CDL	CA3-CA4-CA6-OA8
74	i	503	CDL	CB3-CB4-CB6-OB8
74	x	402	CDL	CA3-CA4-CA6-OA8
75	l	701	PEE	C20-C21-C22-C23
75	7	402	PEE	C22-C23-C24-C25
74	l	702	CDL	C53-C54-C55-C56
71	H	303	PLX	C3-C4-O6-C6
71	V	202	PLX	C5-C4-O6-C6
74	s	201	CDL	CA2-OA2-PA1-OA5
74	Aa	101	CDL	CB3-OB5-PB2-OB2
75	7	402	PEE	C4-O4P-P-O3P
74	l	702	CDL	OB5-CB3-CB4-OB6
74	u	501	CDL	OB5-CB3-CB4-OB6
74	z	101	CDL	OB5-CB3-CB4-OB6
75	w	403	PEE	O3P-C1-C2-O2
71	V	202	PLX	C28-C29-C30-C31
74	z	101	CDL	C11-C12-C13-C14
75	q	501	PEE	C24-C25-C26-C27
74	u	501	CDL	OA6-CA4-CA6-OA8
74	x	402	CDL	OA6-CA4-CA6-OA8
74	z	101	CDL	OB6-CB4-CB6-OB8
74	5	501	CDL	C75-C76-C77-C78
75	u	502	PEE	C14-C15-C16-C17
74	5	501	CDL	C51-CB5-OB6-CB4
71	i	502	PLX	C29-C30-C31-C32
74	s	201	CDL	CB4-CB3-OB5-PB2
74	u	501	CDL	C1-CA2-OA2-PA1
74	z	101	CDL	CB4-CB3-OB5-PB2
74	Aa	101	CDL	C1-CA2-OA2-PA1
71	i	502	PLX	C35-C36-C37-C38
71	2	301	PLX	C19-C20-C21-C22
75	7	402	PEE	C34-C35-C36-C37
71	2	301	PLX	C25-C26-C27-C28
75	l	701	PEE	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
74	i	503	CDL	C13-C14-C15-C16
71	V	202	PLX	C36-C37-C38-C39
71	i	502	PLX	C9-C10-C11-C12
71	V	202	PLX	O8-C24-C25-C26
74	s	201	CDL	C31-C32-C33-C34
75	7	402	PEE	C20-C21-C22-C23
71	2	301	PLX	O4-C3-C4-C5
74	s	201	CDL	OA5-CA3-CA4-CA6
74	u	501	CDL	OA5-CA3-CA4-CA6
74	z	101	CDL	OB5-CB3-CB4-CB6
74	8	401	CDL	OB5-CB3-CB4-CB6
74	8	401	CDL	C32-C33-C34-C35
75	5	502	PEE	C14-C15-C16-C17
75	7	402	PEE	C16-C17-C18-C19
71	4	301	PLX	C27-C28-C29-C30
75	2	302	PEE	C39-C40-C41-C42
75	7	402	PEE	C11-C12-C13-C14
75	l	701	PEE	C22-C23-C24-C25
73	Q	201	ZMP	N2-C16-C17-O4
74	8	401	CDL	C75-C76-C77-C78
75	i	501	PEE	C31-C32-C33-C34
71	H	303	PLX	C27-C28-C29-C30
74	l	702	CDL	CB6-CB4-OB6-CB5
76	7	403	HEM	C2B-C3B-CAB-CBB
74	5	501	CDL	C72-C73-C74-C75
75	u	502	PEE	C31-C32-C33-C34
74	x	402	CDL	CA4-CA3-OA5-PA1
74	5	501	CDL	CB3-CB4-CB6-OB8
71	V	202	PLX	O4-C3-C4-O6
74	i	503	CDL	OB5-CB3-CB4-OB6
74	s	201	CDL	OA5-CA3-CA4-OA6
74	s	201	CDL	OB5-CB3-CB4-OB6
74	8	401	CDL	C72-C71-CB7-OB8
74	x	402	CDL	C14-C15-C16-C17
74	z	101	CDL	C74-C75-C76-C77
71	H	303	PLX	C6-C7-C8-C9
71	i	502	PLX	C6-C7-C8-C9
74	s	201	CDL	CB2-C1-CA2-OA2
74	5	501	CDL	OB7-CB5-OB6-CB4
74	V	201	CDL	OA6-CA4-CA6-OA8
74	5	501	CDL	OB6-CB4-CB6-OB8
72	L	401	NDP	C5B-O5B-PA-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
72	L	401	NDP	C5D-O5D-PN-O3
74	s	201	CDL	C13-C14-C15-C16
75	2	302	PEE	C15-C16-C17-C18
75	w	403	PEE	O4-C10-O2-C2
74	Aa	101	CDL	C14-C15-C16-C17
73	Q	201	ZMP	C2-C1-C22-C23
74	i	503	CDL	C52-C53-C54-C55
75	i	501	PEE	C24-C25-C26-C27
77	8	402	HEC	C1A-C2A-CAA-CBA
71	i	502	PLX	C18-C19-C20-C21
74	Aa	101	CDL	C13-C14-C15-C16
71	2	301	PLX	C34-C35-C36-C37
74	i	503	CDL	C35-C36-C37-C38
71	V	202	PLX	C11-C12-C13-C14
74	s	201	CDL	C33-C34-C35-C36
71	H	303	PLX	C24-C25-C26-C27
71	H	303	PLX	C3-O4-P1-O1
71	i	502	PLX	C3-O4-P1-O1
75	W	401	PEE	C1-O3P-P-O4P
75	q	501	PEE	C4-O4P-P-O3P
74	i	503	CDL	O1-C1-CB2-OB2
74	x	402	CDL	C1-CA2-OA2-PA1
74	z	101	CDL	C1-CA2-OA2-PA1
74	8	401	CDL	CA4-CA3-OA5-PA1
75	l	701	PEE	C2-C1-O3P-P
71	H	303	PLX	C3-O4-P1-O3
71	H	303	PLX	C2-O1-P1-O2
72	L	401	NDP	C5B-O5B-PA-O2A
72	L	401	NDP	C5D-O5D-PN-O2N
74	V	201	CDL	CA2-OA2-PA1-OA4
74	V	201	CDL	CA3-OA5-PA1-OA4
74	V	201	CDL	CB3-OB5-PB2-OB3
74	i	503	CDL	CA3-OA5-PA1-OA3
74	i	503	CDL	CA3-OA5-PA1-OA4
74	s	201	CDL	CB3-OB5-PB2-OB3
74	u	501	CDL	CB2-OB2-PB2-OB4
74	x	402	CDL	CA2-OA2-PA1-OA3
74	x	402	CDL	CB3-OB5-PB2-OB3
74	5	501	CDL	CB2-OB2-PB2-OB3
74	5	501	CDL	CB3-OB5-PB2-OB3
75	l	701	PEE	C1-O3P-P-O2P
75	q	501	PEE	C4-O4P-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	q	501	PEE	C4-O4P-P-O1P
75	2	302	PEE	C4-O4P-P-O1P
75	5	502	PEE	C1-O3P-P-O1P
75	7	401	PEE	C4-O4P-P-O1P
75	7	402	PEE	C1-O3P-P-O2P
75	7	402	PEE	C1-O3P-P-O1P
74	5	501	CDL	OA5-CA3-CA4-CA6
71	4	301	PLX	C18-C19-C20-C21
75	1	701	PEE	C38-C39-C40-C41
75	2	302	PEE	C17-C18-C19-C20
75	7	402	PEE	C17-C18-C19-C20
71	i	502	PLX	C36-C37-C38-C39
71	4	301	PLX	C25-C24-O8-C5
75	2	302	PEE	C5-C4-O4P-P
75	W	401	PEE	C13-C14-C15-C16
71	H	303	PLX	C12-C13-C14-C15
71	i	502	PLX	C27-C28-C29-C30
71	H	303	PLX	O4-C3-C4-O6
71	2	301	PLX	O4-C3-C4-O6
74	5	501	CDL	OB5-CB3-CB4-OB6
75	i	501	PEE	O3P-C1-C2-O2
74	s	201	CDL	C15-C16-C17-C18
74	l	702	CDL	C15-C16-C17-C18
75	w	403	PEE	C11-C10-O2-C2
75	2	302	PEE	C14-C15-C16-C17
74	l	702	CDL	CB5-C51-C52-C53
74	z	101	CDL	C12-C11-CA5-OA6
71	H	303	PLX	N1-C1-C2-O1
74	V	201	CDL	OA9-CA7-OA8-CA6
74	i	503	CDL	CA3-CA4-CA6-OA8
74	u	501	CDL	CB3-CB4-CB6-OB8
74	5	501	CDL	CA3-CA4-CA6-OA8
71	4	301	PLX	O6-C4-C5-O8
74	u	501	CDL	OB6-CB4-CB6-OB8
74	z	101	CDL	OA6-CA4-CA6-OA8
74	5	501	CDL	OA6-CA4-CA6-OA8
74	8	401	CDL	OB6-CB4-CB6-OB8
75	7	402	PEE	O2-C2-C3-O3
74	V	201	CDL	C15-C16-C17-C18
74	8	401	CDL	C32-C31-CA7-OA8
74	i	503	CDL	C33-C34-C35-C36
71	V	202	PLX	O7-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	i	502	PLX	O7-C6-C7-C8
74	x	402	CDL	C35-C36-C37-C38
72	L	401	NDP	O4D-C1D-N1N-C6N
75	u	502	PEE	C33-C34-C35-C36
71	4	301	PLX	C33-C34-C35-C36
75	l	701	PEE	C41-C42-C43-C44
74	V	201	CDL	C12-C11-CA5-OA6
74	x	402	CDL	CA3-CA4-OA6-CA5
75	i	501	PEE	C3-C2-O2-C10
74	8	401	CDL	OB5-CB3-CB4-OB6
75	l	701	PEE	O3P-C1-C2-O2
71	2	301	PLX	C29-C30-C31-C32
75	2	302	PEE	C31-C32-C33-C34
75	5	502	PEE	C38-C39-C40-C41
77	8	402	HEC	C4B-C3B-CAB-CBB
71	i	502	PLX	C2-O1-P1-O4
74	u	501	CDL	CA3-OA5-PA1-OA2
74	x	402	CDL	CA3-OA5-PA1-OA2
74	z	101	CDL	CA2-OA2-PA1-OA5
74	z	101	CDL	CB2-OB2-PB2-OB5
74	5	501	CDL	CA3-OA5-PA1-OA2
75	i	501	PEE	C1-O3P-P-O4P
75	u	502	PEE	C4-O4P-P-O3P
75	2	302	PEE	C1-O3P-P-O4P
73	Q	201	ZMP	C22-C1-C2-C3
74	x	402	CDL	C74-C75-C76-C77
74	8	401	CDL	C55-C56-C57-C58
76	w	401	HEM	C3A-C2A-CAA-CBA
75	5	502	PEE	C40-C41-C42-C43
75	7	402	PEE	C31-C32-C33-C34
74	x	402	CDL	C52-C53-C54-C55
71	4	301	PLX	C4-C3-O4-P1
74	i	503	CDL	C32-C31-CA7-OA8
71	V	202	PLX	C33-C34-C35-C36
74	s	201	CDL	C71-CB7-OB8-CB6
75	l	701	PEE	C15-C16-C17-C18
72	L	401	NDP	C2D-C1D-N1N-C6N
75	i	501	PEE	O4P-C4-C5-N
75	5	502	PEE	O4P-C4-C5-N
74	5	501	CDL	C55-C56-C57-C58
71	V	202	PLX	C7-C8-C9-C10
74	5	501	CDL	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	V	202	PLX	C32-C33-C34-C35
74	i	503	CDL	C74-C75-C76-C77
74	z	101	CDL	CB7-C71-C72-C73
74	s	201	CDL	OA6-CA4-CA6-OA8
73	Q	201	ZMP	C5-C6-C7-C8
74	i	503	CDL	CB4-CB3-OB5-PB2
75	q	501	PEE	C18-C19-C20-C21
74	8	401	CDL	C54-C55-C56-C57
71	H	303	PLX	C3-C4-C5-O8
74	Aa	101	CDL	CB2-C1-CA2-OA2
78	Ak	601	HEA	CAD-CBD-CGD-O1D
75	W	401	PEE	C41-C42-C43-C44
75	w	403	PEE	C15-C16-C17-C18
76	w	402	HEM	CAA-CBA-CGA-O1A
74	V	201	CDL	C54-C55-C56-C57
75	l	701	PEE	C31-C32-C33-C34
74	x	402	CDL	C55-C56-C57-C58
76	w	401	HEM	CAD-CBD-CGD-O1D
76	7	404	HEM	CAD-CBD-CGD-O1D
77	8	402	HEC	C3A-C2A-CAA-CBA
74	8	401	CDL	C31-CA7-OA8-CA6
71	i	502	PLX	C32-C33-C34-C35
74	5	501	CDL	OB5-CB3-CB4-CB6
74	x	402	CDL	C75-C76-C77-C78
76	7	403	HEM	CAA-CBA-CGA-O2A
76	7	404	HEM	CAD-CBD-CGD-O2D
78	Ak	602	HEA	CAD-CBD-CGD-O1D
78	Ak	602	HEA	CAD-CBD-CGD-O2D
74	5	501	CDL	CB5-C51-C52-C53
71	4	301	PLX	C13-C14-C15-C16
77	x	401	HEC	CAA-CBA-CGA-O2A
74	s	201	CDL	OB9-CB7-OB8-CB6
75	7	401	PEE	C30-C31-C32-C33
76	7	403	HEM	CAA-CBA-CGA-O1A
75	W	401	PEE	C39-C40-C41-C42
75	u	502	PEE	C19-C20-C21-C22
75	7	402	PEE	C14-C15-C16-C17
75	W	401	PEE	C37-C38-C39-C40
75	u	502	PEE	C40-C41-C42-C43
78	Ak	601	HEA	CAA-CBA-CGA-O1A
78	Ak	601	HEA	CAD-CBD-CGD-O2D
75	u	502	PEE	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
74	z	101	CDL	C32-C31-CA7-OA8
74	8	401	CDL	OA9-CA7-OA8-CA6
74	i	503	CDL	C1-CB2-OB2-PB2
75	q	501	PEE	O2-C10-C11-C12
74	5	501	CDL	C14-C15-C16-C17
75	l	701	PEE	C32-C33-C34-C35
75	q	501	PEE	C36-C37-C38-C39
75	w	403	PEE	C36-C37-C38-C39
76	w	402	HEM	CAA-CBA-CGA-O2A
71	H	303	PLX	O8-C24-C25-C26
77	x	401	HEC	CAA-CBA-CGA-O1A
69	B	502	FMN	O2'-C2'-C3'-C4'
76	7	403	HEM	CAD-CBD-CGD-O1D
76	7	403	HEM	CAD-CBD-CGD-O2D
71	2	301	PLX	O6-C4-C5-O8
75	u	502	PEE	C23-C24-C25-C26
75	5	502	PEE	C36-C37-C38-C39
71	V	202	PLX	C20-C21-C22-C23
74	Aa	101	CDL	CA5-C11-C12-C13
75	7	401	PEE	C14-C15-C16-C17
75	7	401	PEE	C42-C43-C44-C45
74	x	402	CDL	C72-C71-CB7-OB8
75	w	403	PEE	C19-C20-C21-C22
74	l	702	CDL	C35-C36-C37-C38
75	q	501	PEE	C38-C39-C40-C41
75	7	401	PEE	C38-C39-C40-C41
75	2	302	PEE	C40-C41-C42-C43
74	V	201	CDL	C72-C71-CB7-OB8
74	5	501	CDL	C72-C71-CB7-OB8
73	Q	201	ZMP	C3-C4-C5-C6
75	W	401	PEE	C18-C19-C20-C21
75	7	402	PEE	C36-C37-C38-C39
74	s	201	CDL	CA3-CA4-CA6-OA8
75	2	302	PEE	O3P-C1-C2-O2
74	x	402	CDL	C52-C51-CB5-OB6
74	V	201	CDL	CA5-C11-C12-C13
74	V	201	CDL	C20-C21-C22-C23
76	7	403	HEM	C4B-C3B-CAB-CBB
72	L	401	NDP	O4D-C4D-C5D-O5D
76	w	401	HEM	CAD-CBD-CGD-O2D
78	Ak	602	HEA	CAA-CBA-CGA-O2A
75	W	401	PEE	C38-C39-C40-C41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
72	L	401	NDP	O4D-C1D-N1N-C2N
78	Ak	602	HEA	CAA-CBA-CGA-O1A
74	x	402	CDL	C32-C31-CA7-OA8
74	z	101	CDL	C52-C51-CB5-OB6
74	s	201	CDL	C72-C73-C74-C75
74	5	501	CDL	C15-C16-C17-C18
71	H	303	PLX	O6-C4-C5-O8
74	l	702	CDL	OB6-CB4-CB6-OB8
75	2	302	PEE	C36-C37-C38-C39
74	u	501	CDL	C12-C11-CA5-OA6
74	s	201	CDL	C32-C31-CA7-OA8
75	l	701	PEE	O4-C10-O2-C2
75	W	401	PEE	C16-C17-C18-C19
75	i	501	PEE	C38-C39-C40-C41
74	u	501	CDL	C32-C31-CA7-OA8
75	W	401	PEE	O2-C10-C11-C12
74	5	501	CDL	C72-C71-CB7-OB9
75	u	502	PEE	O2-C10-C11-C12
74	V	201	CDL	C72-C71-CB7-OB9
74	x	402	CDL	C72-C71-CB7-OB9
74	8	401	CDL	C72-C71-CB7-OB9
74	s	201	CDL	C52-C51-CB5-OB6
75	u	502	PEE	C41-C42-C43-C44
75	5	502	PEE	C21-C22-C23-C24
78	Ak	601	HEA	CAA-CBA-CGA-O2A
71	H	303	PLX	C2-O1-P1-O3
74	u	501	CDL	CA3-OA5-PA1-OA3
74	u	501	CDL	CB2-OB2-PB2-OB3
74	x	402	CDL	CA3-OA5-PA1-OA3
74	x	402	CDL	CB2-OB2-PB2-OB4
74	z	101	CDL	CA2-OA2-PA1-OA3
74	z	101	CDL	CA3-OA5-PA1-OA4
74	z	101	CDL	CB2-OB2-PB2-OB3
74	Aa	101	CDL	CB3-OB5-PB2-OB4
75	W	401	PEE	C4-O4P-P-O1P
75	q	501	PEE	C1-O3P-P-O1P
75	w	403	PEE	C4-O4P-P-O2P
75	2	302	PEE	C1-O3P-P-O1P
74	x	402	CDL	C32-C31-CA7-OA9
75	i	501	PEE	C33-C34-C35-C36
75	w	403	PEE	O4P-C4-C5-N
75	l	701	PEE	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	W	401	PEE	O4-C10-C11-C12
78	Ak	602	HEA	C26-C15-C16-C17
71	V	202	PLX	C1-C2-O1-P1
71	2	301	PLX	C1-C2-O1-P1
75	w	403	PEE	C10-C11-C12-C13
74	s	201	CDL	C32-C31-CA7-OA9
74	x	402	CDL	C52-C51-CB5-OB7
74	z	101	CDL	C52-C51-CB5-OB7
72	L	401	NDP	C2D-C1D-N1N-C2N
75	5	502	PEE	O3-C30-C31-C32
71	H	303	PLX	C34-C35-C36-C37
71	V	202	PLX	C35-C36-C37-C38
74	8	401	CDL	C52-C51-CB5-OB6
74	Aa	101	CDL	C32-C31-CA7-OA8
75	u	502	PEE	O3-C30-C31-C32
74	u	501	CDL	CA2-C1-CB2-OB2
74	8	401	CDL	CB2-C1-CA2-OA2
74	s	201	CDL	C54-C55-C56-C57
74	u	501	CDL	C12-C11-CA5-OA7
74	u	501	CDL	C32-C31-CA7-OA9
75	u	502	PEE	O4-C10-C11-C12
78	Ak	601	HEA	O11-C11-C3B-C2B
74	s	201	CDL	C72-C71-CB7-OB8
74	u	501	CDL	C52-C51-CB5-OB6
75	2	302	PEE	O2-C10-C11-C12
75	i	501	PEE	C11-C12-C13-C14
75	5	502	PEE	O5-C30-C31-C32
73	X	201	ZMP	C6-C7-C8-C9
74	8	401	CDL	C52-C51-CB5-OB7
76	7	404	HEM	CAA-CBA-CGA-O2A
75	l	701	PEE	C36-C37-C38-C39
74	s	201	CDL	C72-C71-CB7-OB9
74	i	503	CDL	C52-C51-CB5-OB6
77	8	402	HEC	CAA-CBA-CGA-O2A

There are no ring outliers.

45 monomers are involved in 481 short contacts:

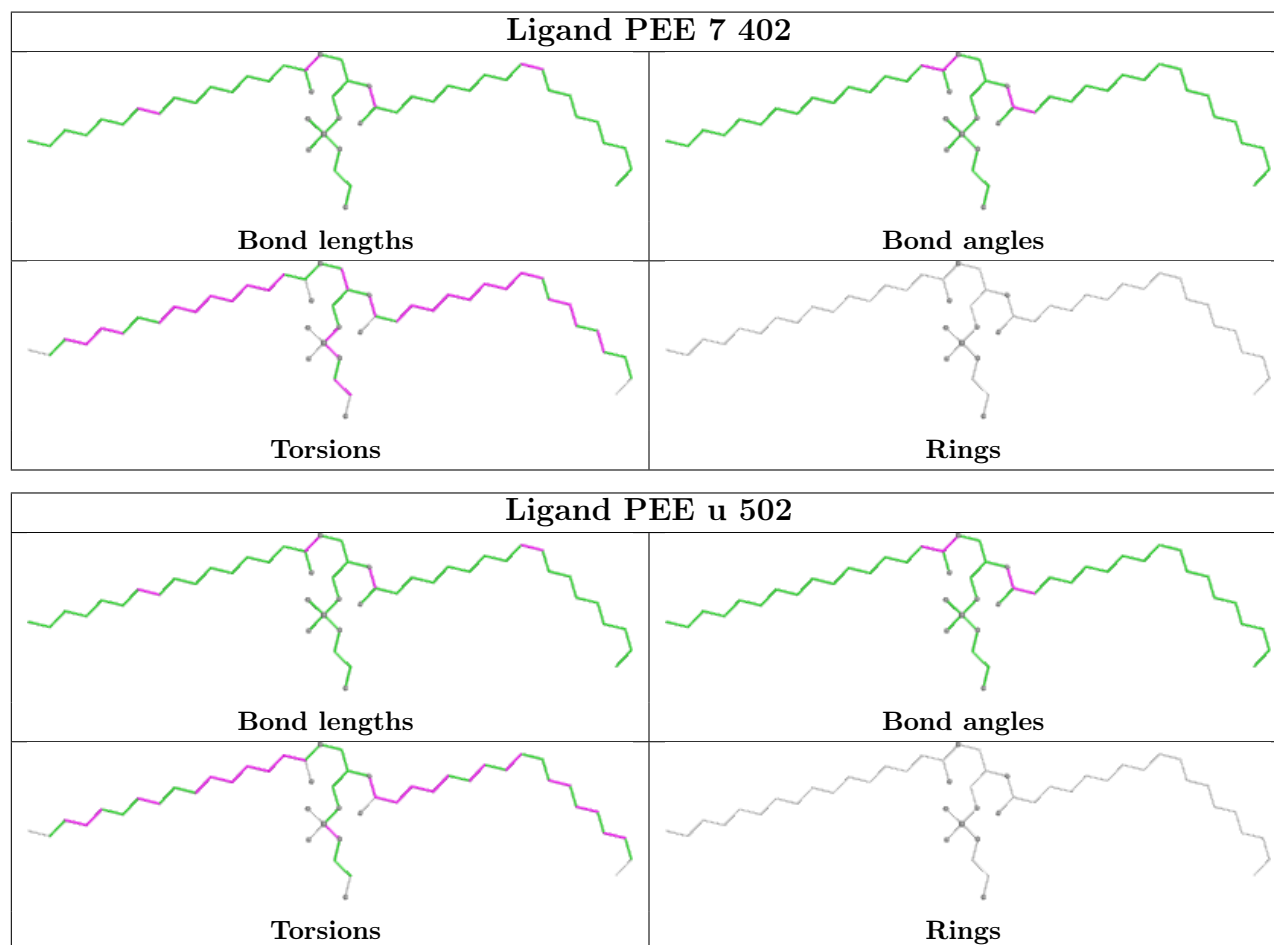
Mol	Chain	Res	Type	Clashes	Symm-Clashes
75	7	402	PEE	38	0
75	u	502	PEE	50	0
75	7	401	PEE	7	0

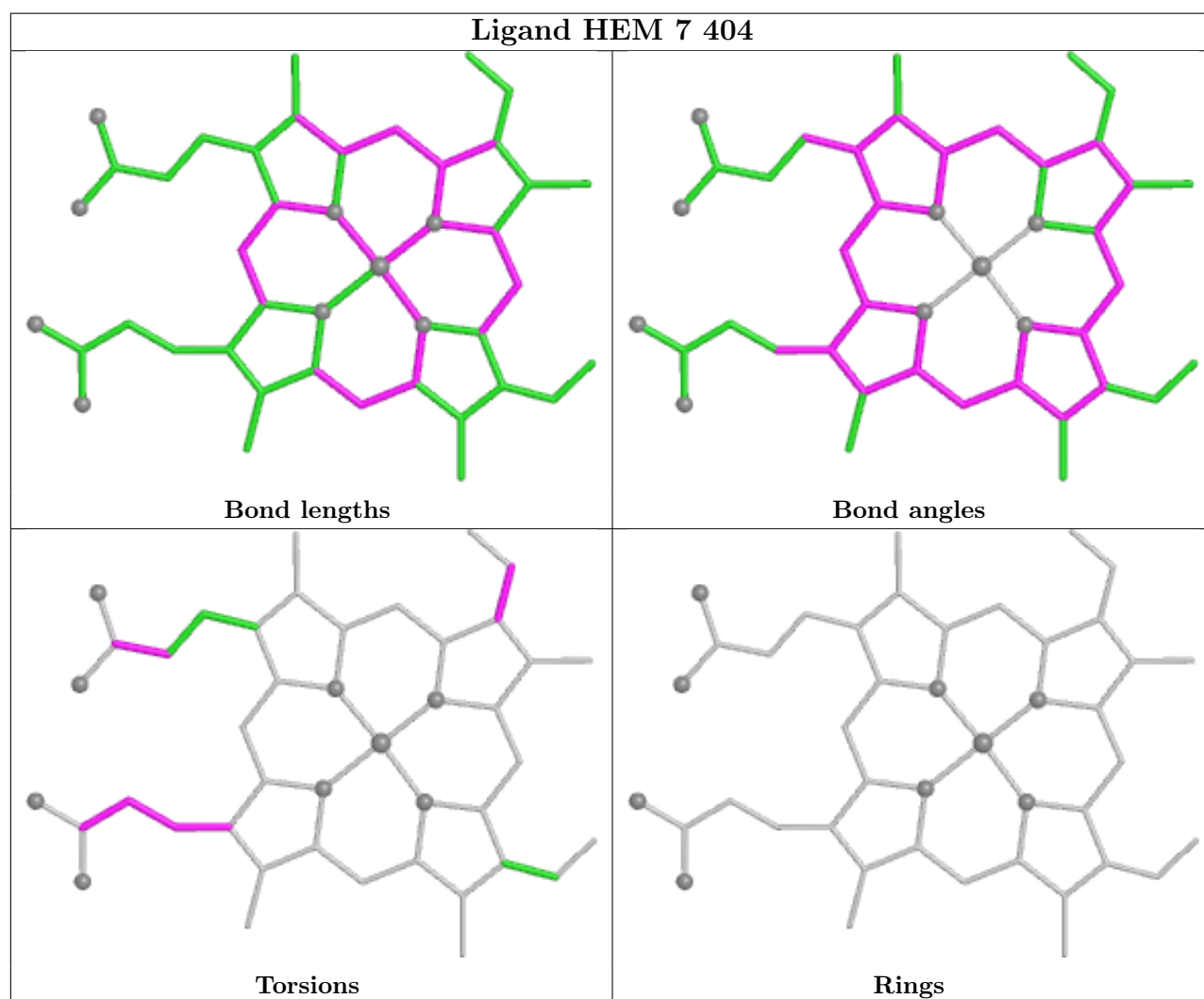
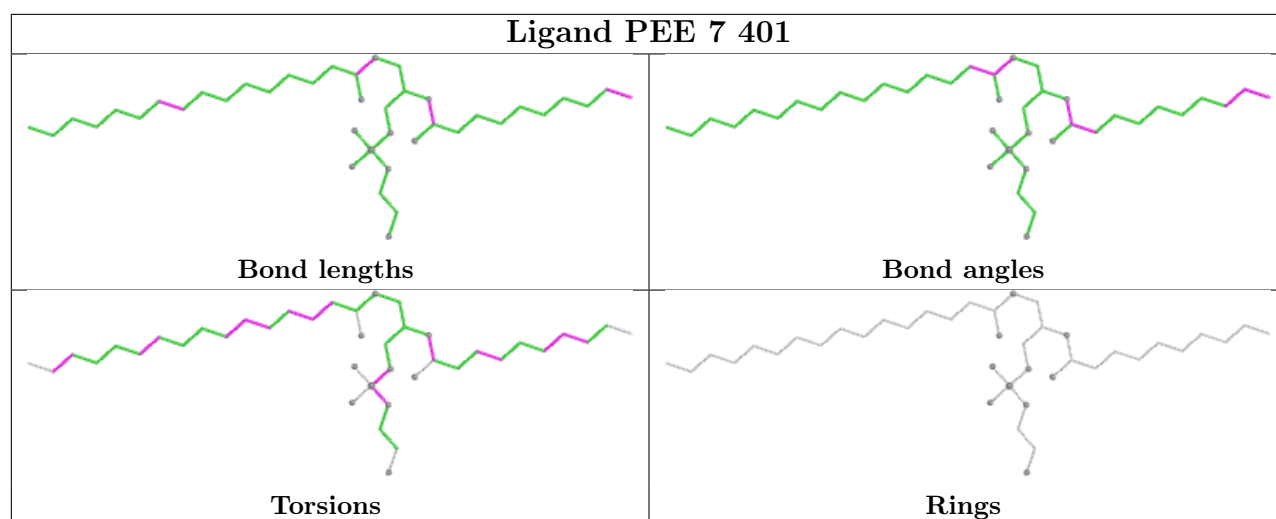
Continued on next page...

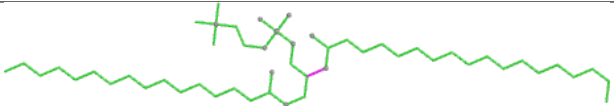
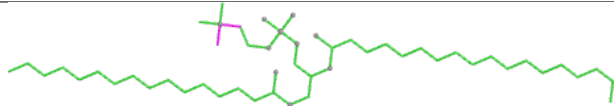
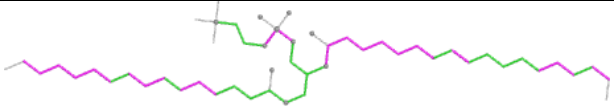
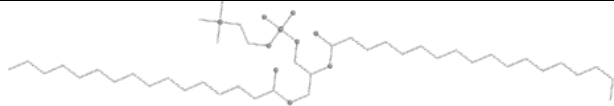
Continued from previous page...

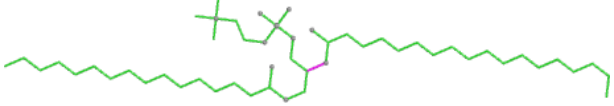
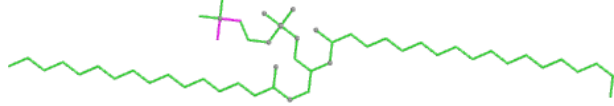
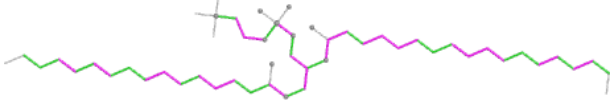
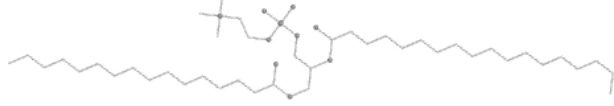
Mol	Chain	Res	Type	Clashes	Symm-Clashes
76	7	404	HEM	16	0
68	G	802	SF4	1	0
71	i	502	PLX	6	0
71	2	301	PLX	25	0
75	i	501	PEE	19	0
70	4	302	FES	1	0
74	z	101	CDL	6	0
73	X	201	ZMP	7	0
75	W	401	PEE	8	0
69	B	502	FMN	25	0
74	8	401	CDL	7	0
76	w	402	HEM	19	0
68	G	801	SF4	4	0
71	H	303	PLX	7	0
75	l	701	PEE	6	0
74	u	501	CDL	17	0
75	w	403	PEE	31	0
70	E	301	FES	1	0
73	Q	201	ZMP	22	0
74	i	503	CDL	5	0
71	4	301	PLX	5	0
68	B	501	SF4	4	0
77	8	402	HEC	9	0
74	5	501	CDL	7	0
77	x	401	HEC	10	0
74	s	201	CDL	2	0
70	2	303	FES	2	0
75	q	501	PEE	9	0
72	L	401	NDP	12	0
68	H	301	SF4	2	0
74	l	702	CDL	7	0
78	Ak	601	HEA	1	0
76	w	401	HEM	17	0
74	Aa	101	CDL	17	0
75	5	502	PEE	18	0
74	V	201	CDL	5	0
74	x	402	CDL	7	0
75	2	302	PEE	46	0
71	V	202	PLX	2	0
76	7	403	HEM	19	0
68	H	302	SF4	2	0
78	Ak	602	HEA	3	0

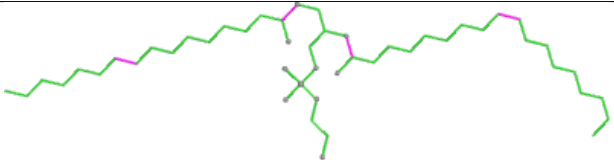
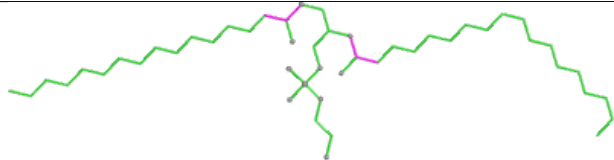
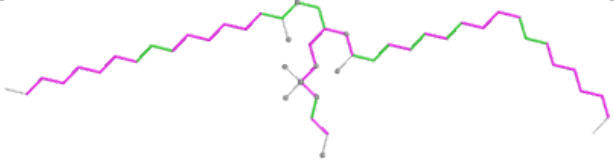
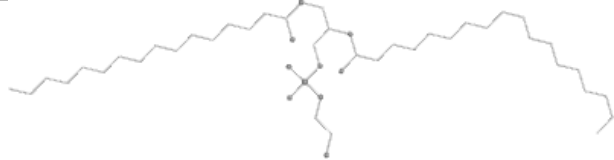
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

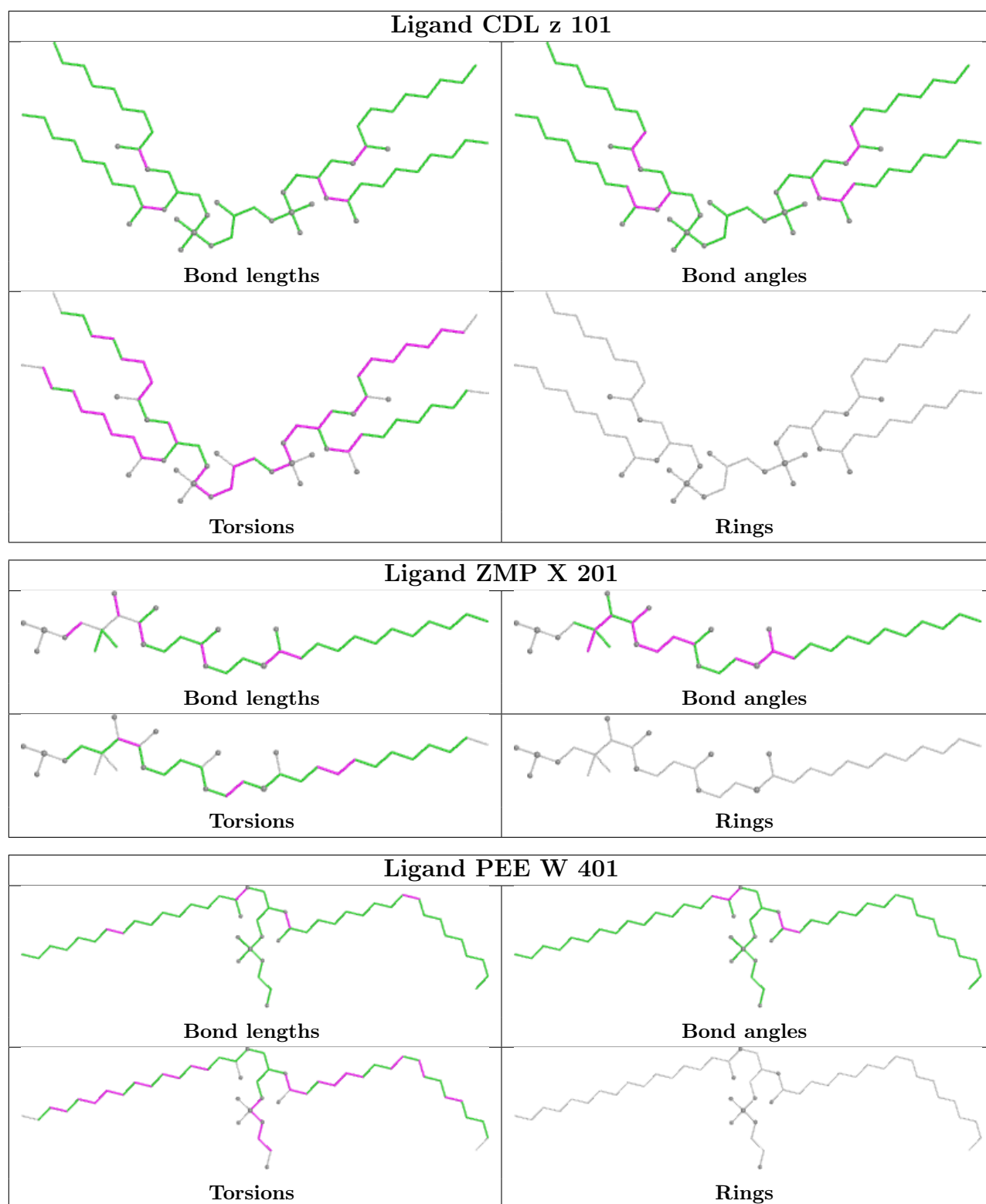


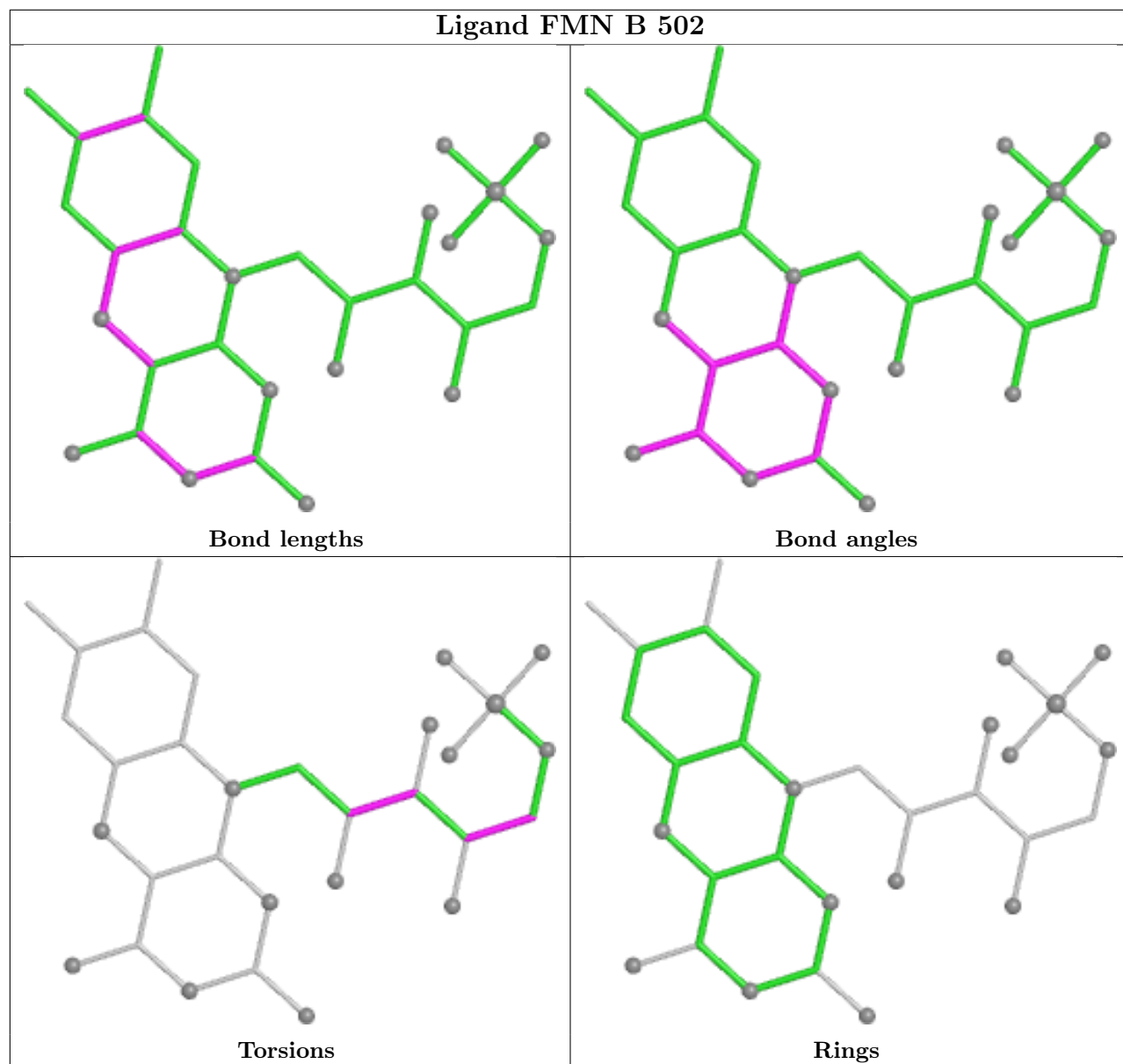


Ligand PLX i 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

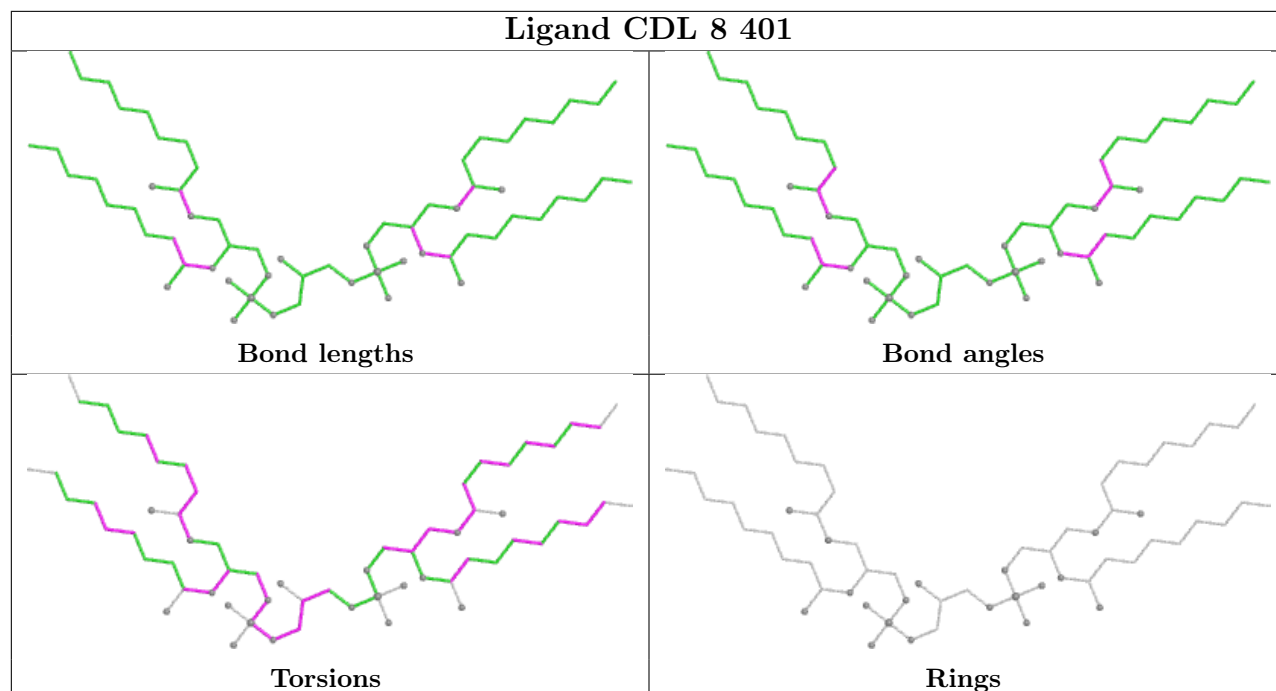
Ligand PLX 2 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEE i 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

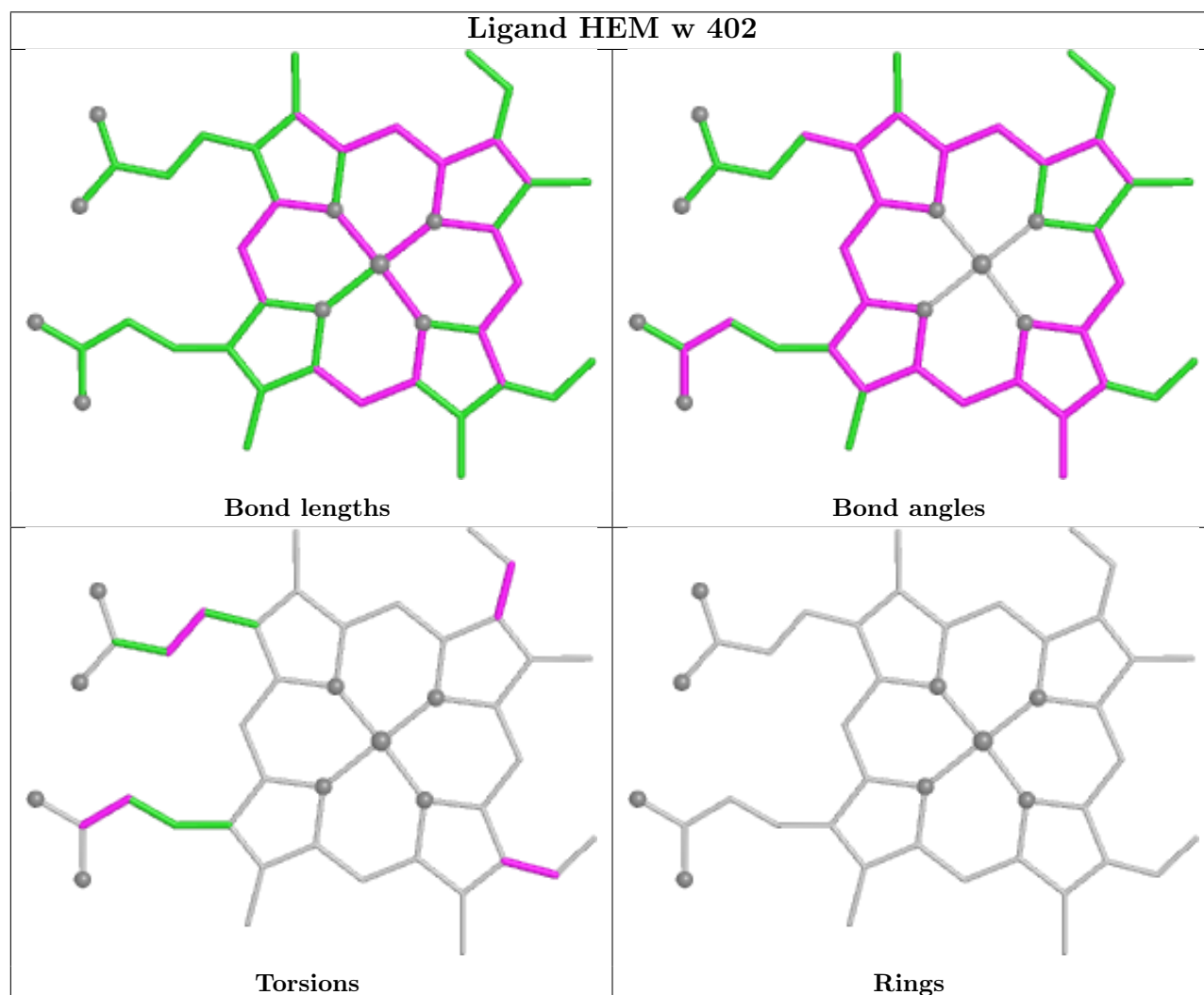


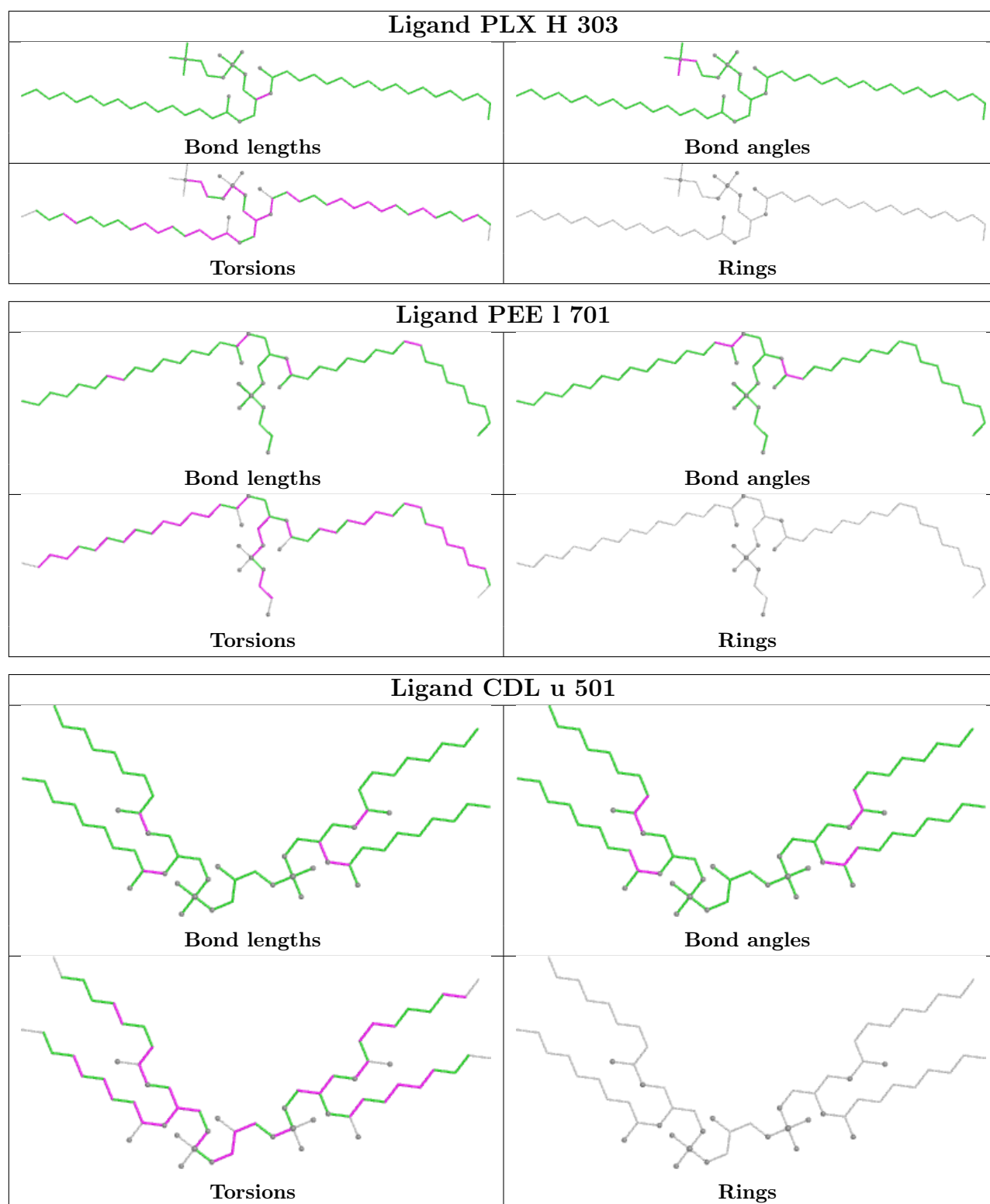


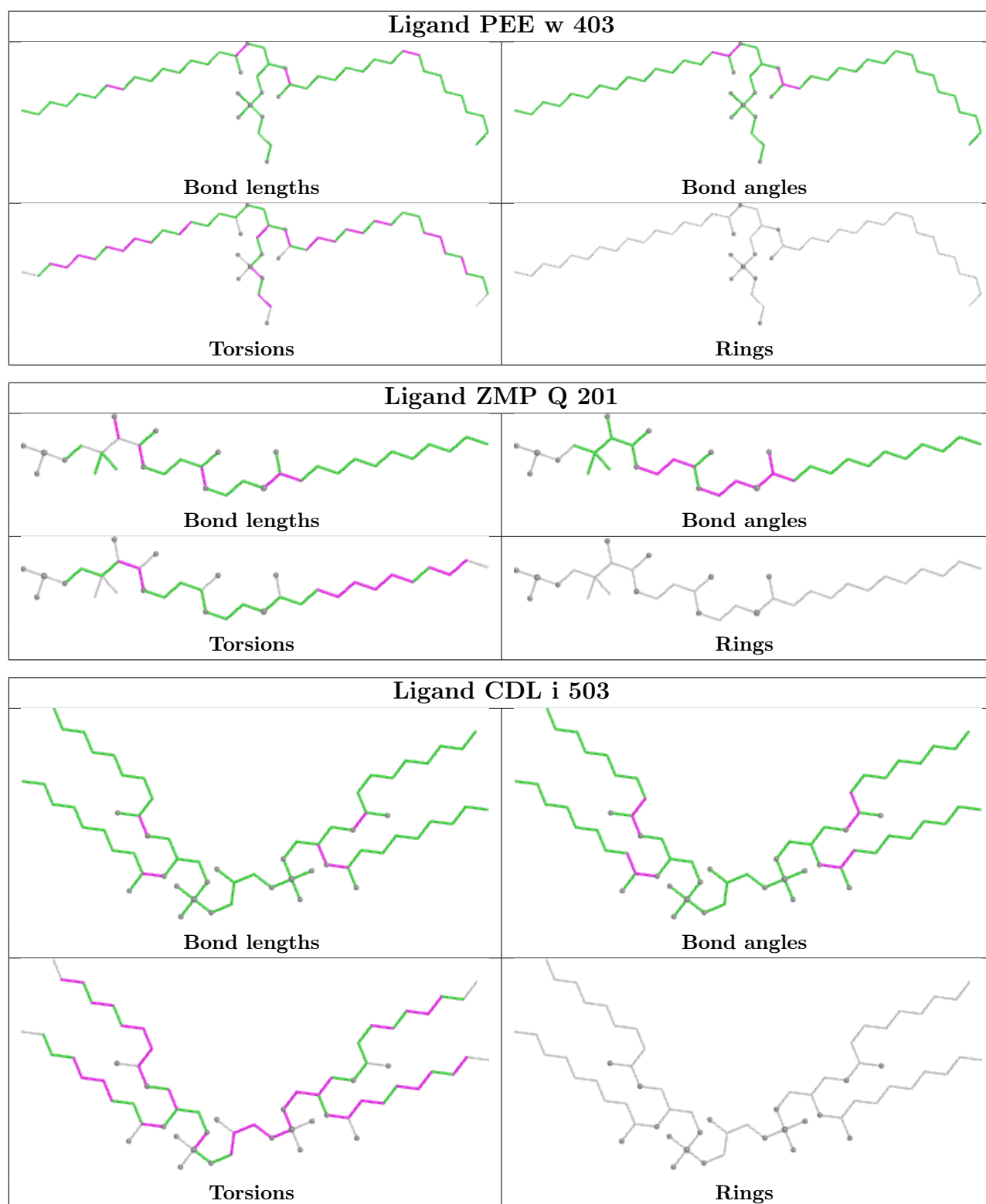
Ligand CDL 8 401



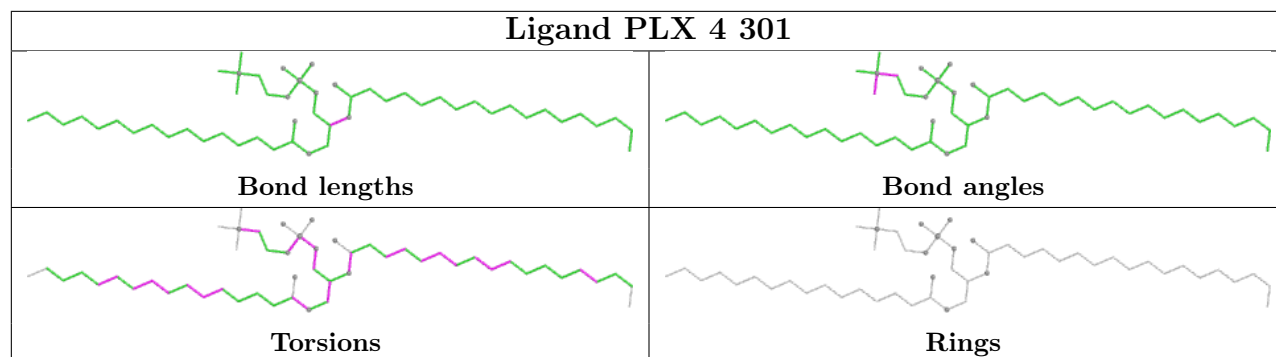
Ligand HEM w 402



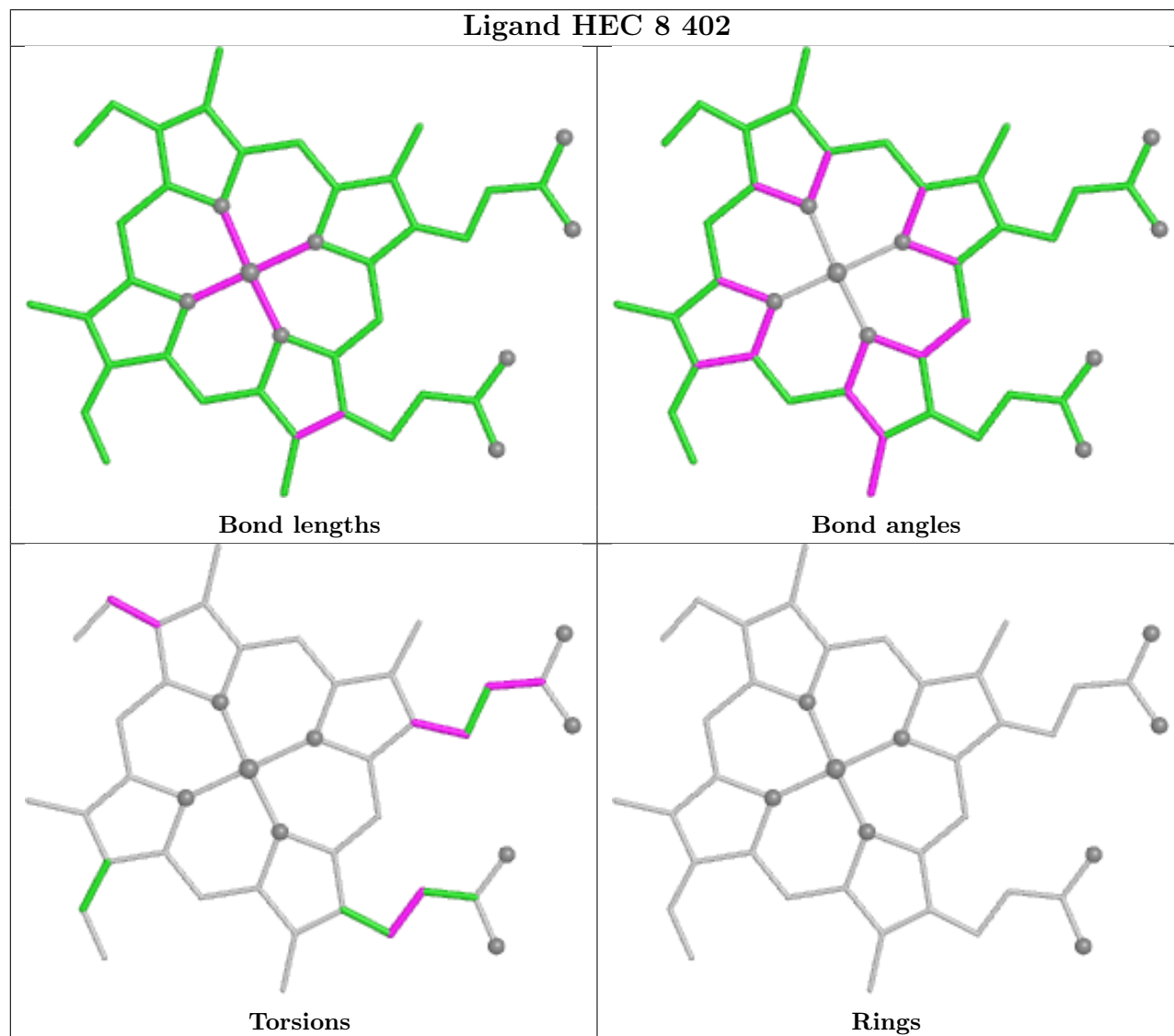


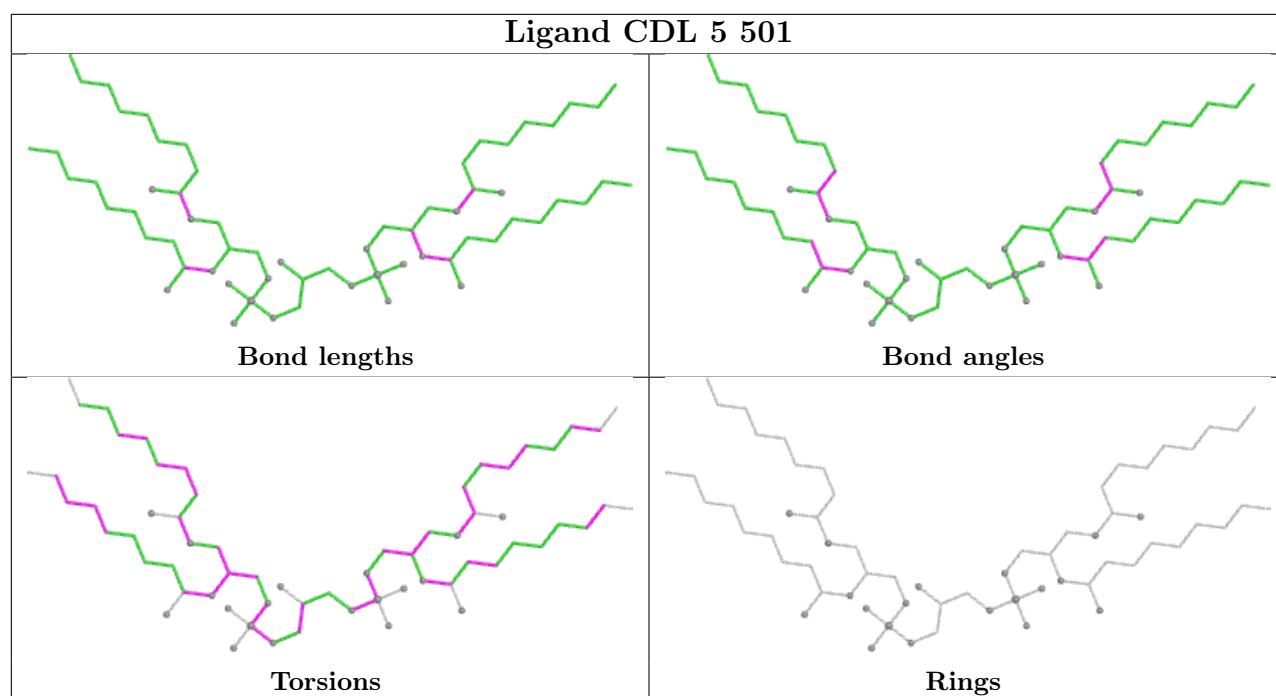


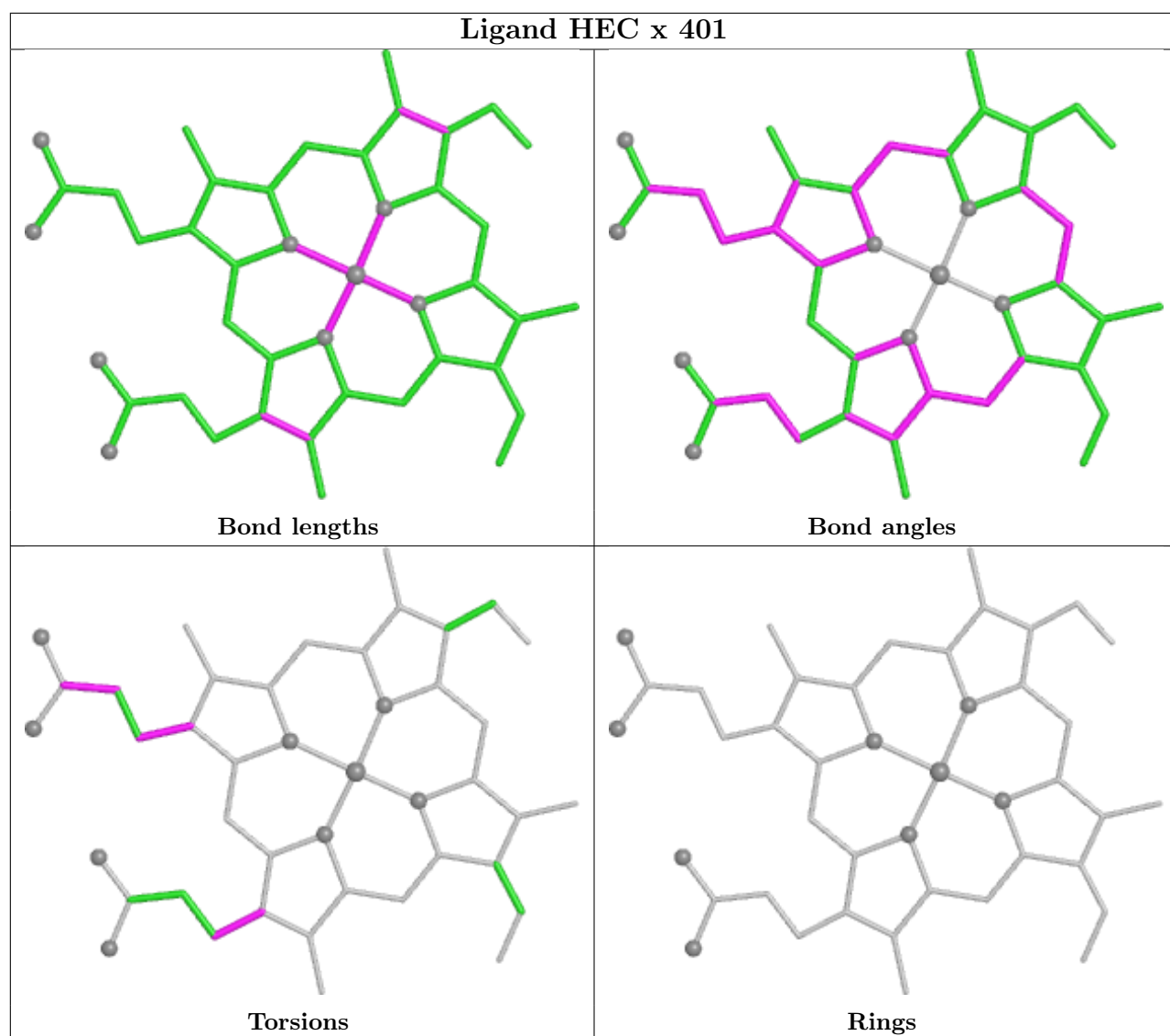
Ligand PLX 4 301

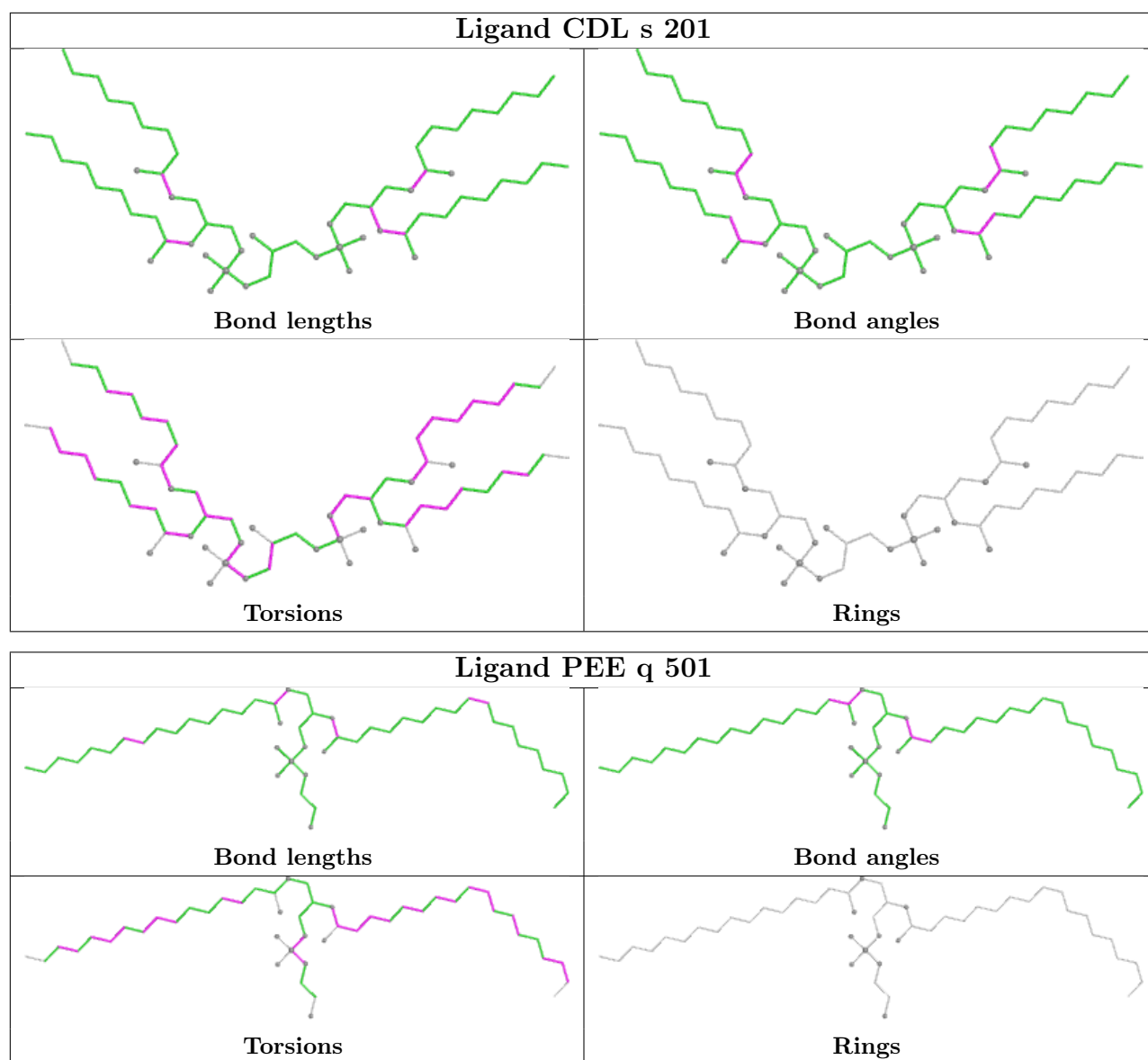


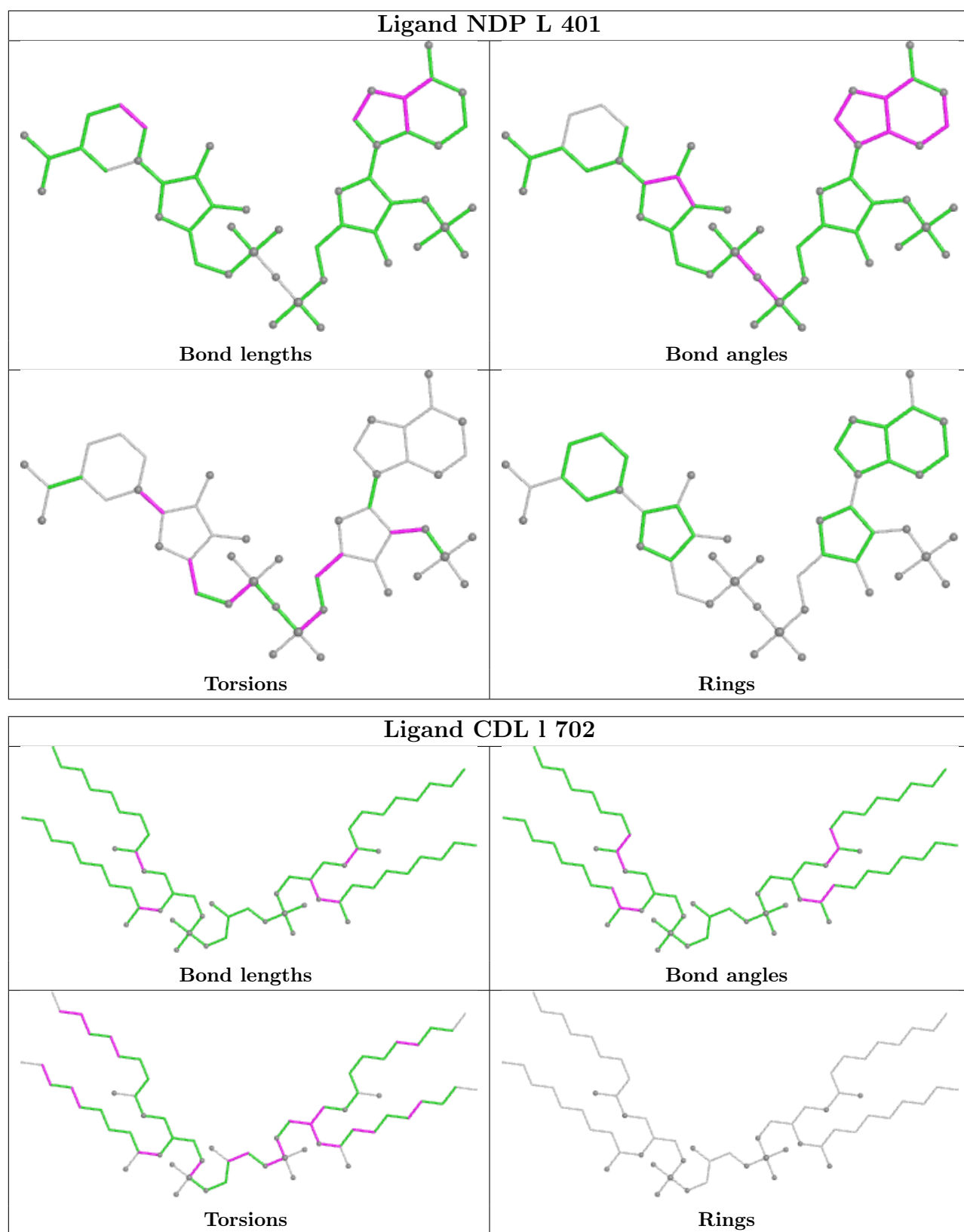
Ligand HEC 8 402

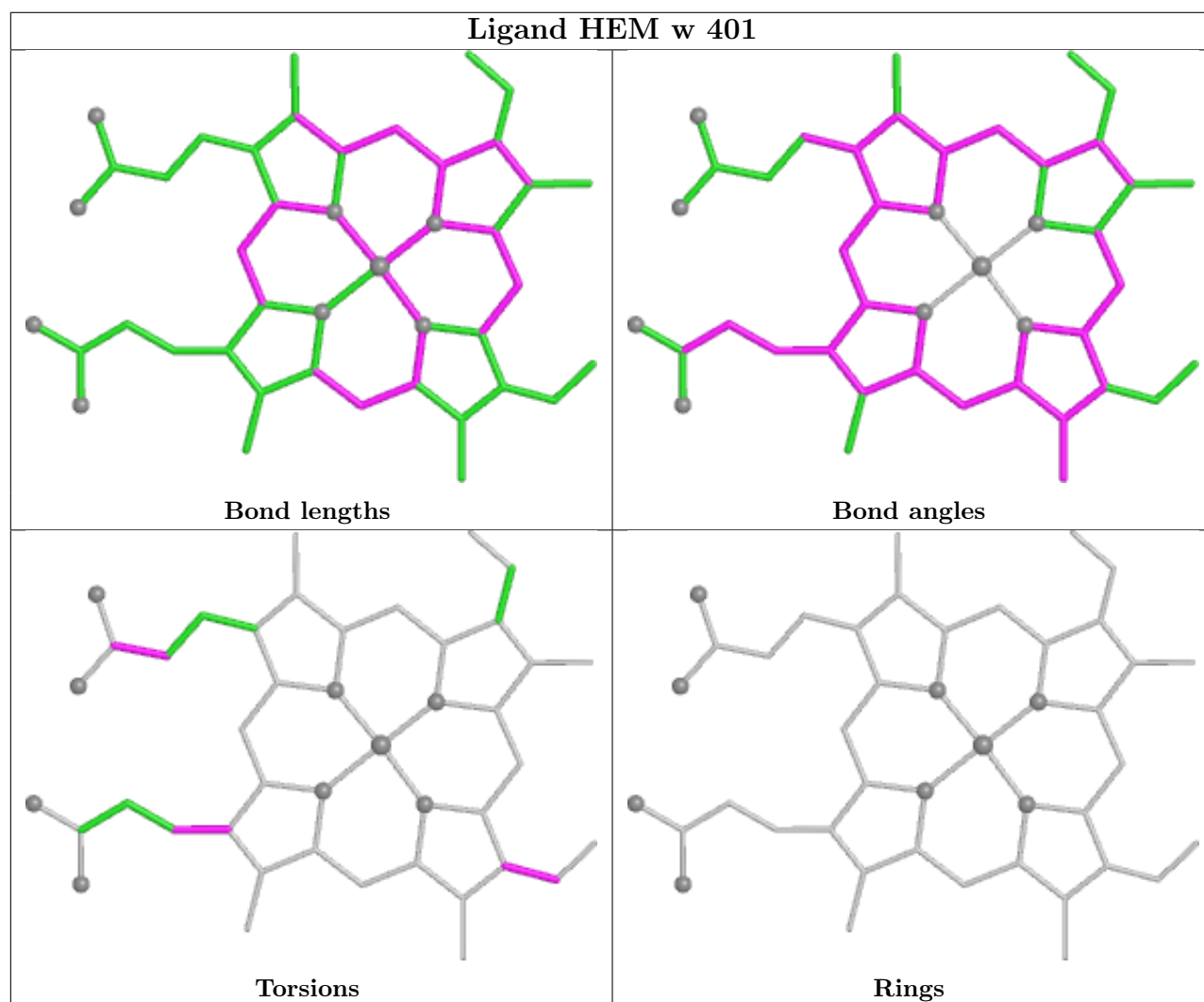
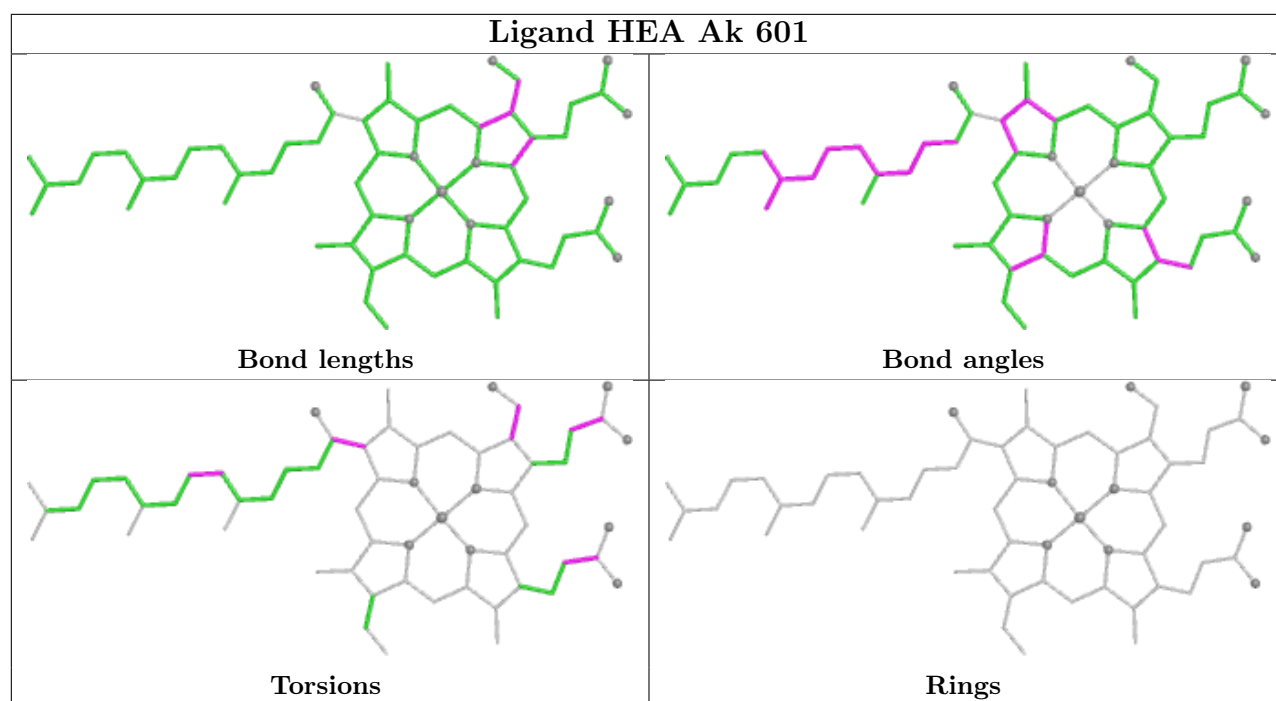


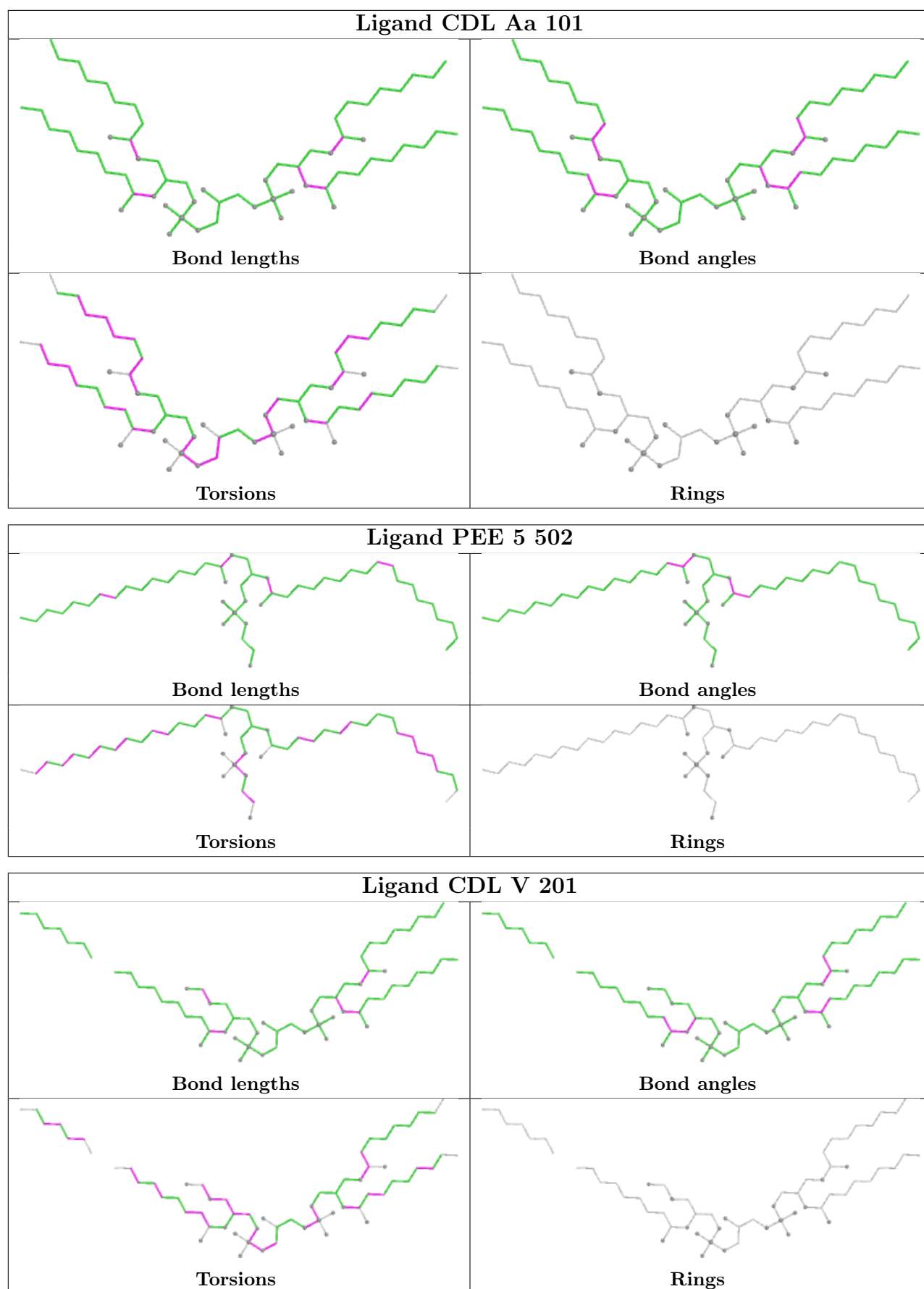


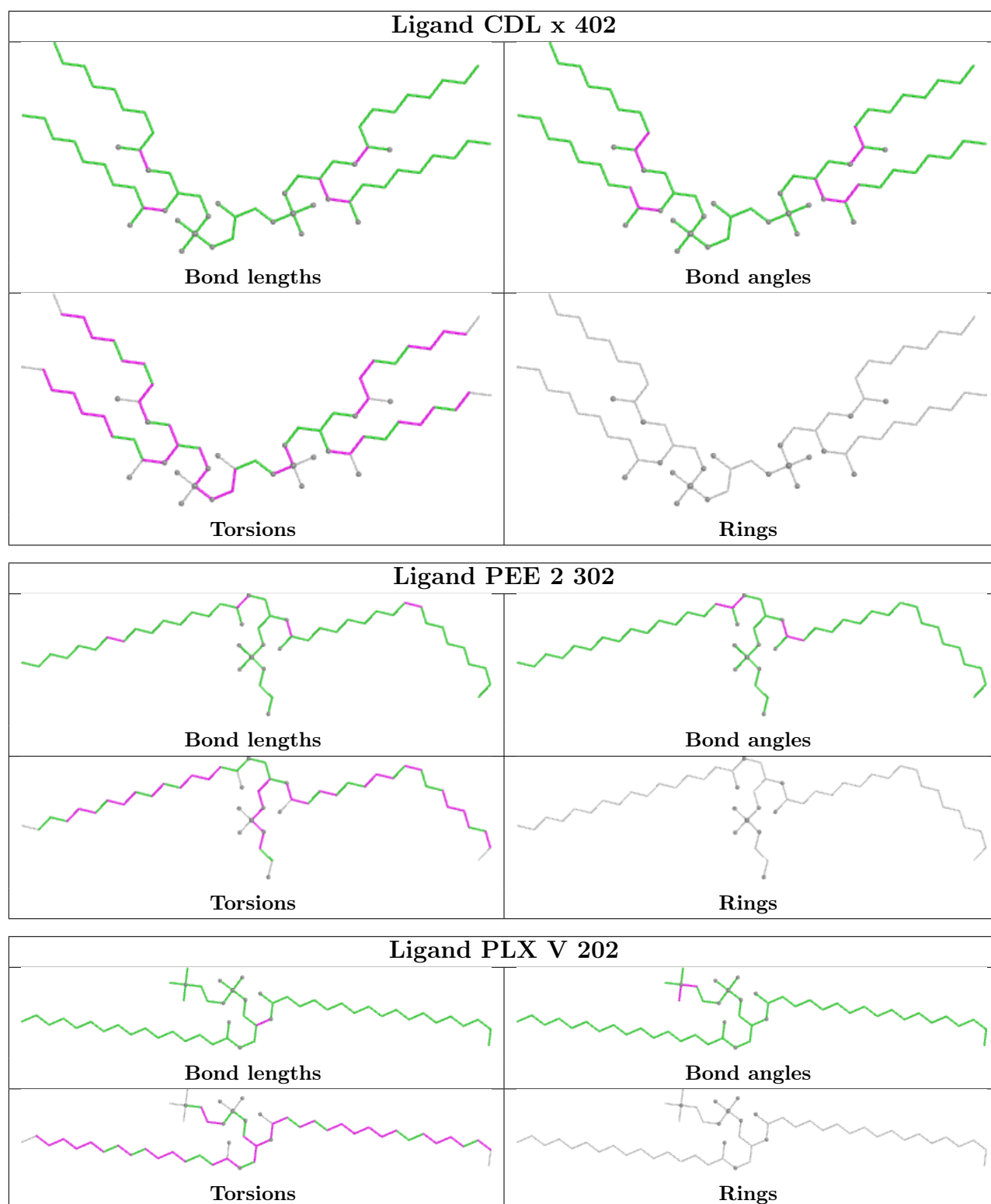


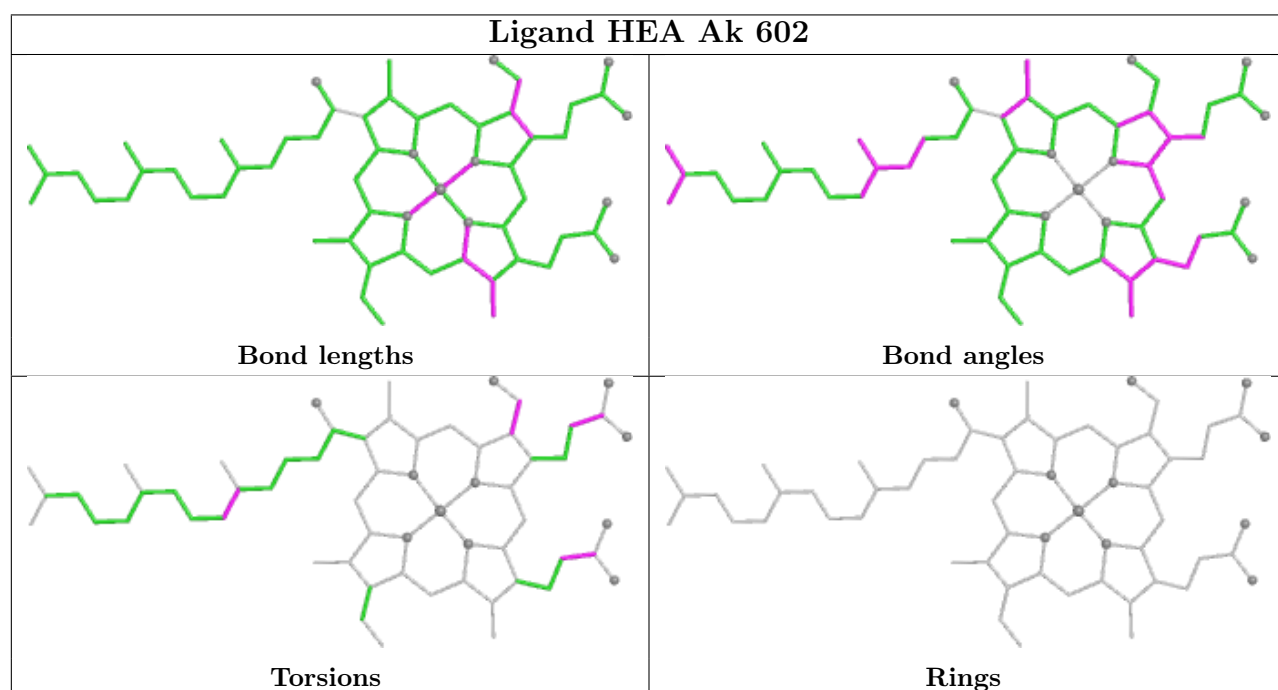
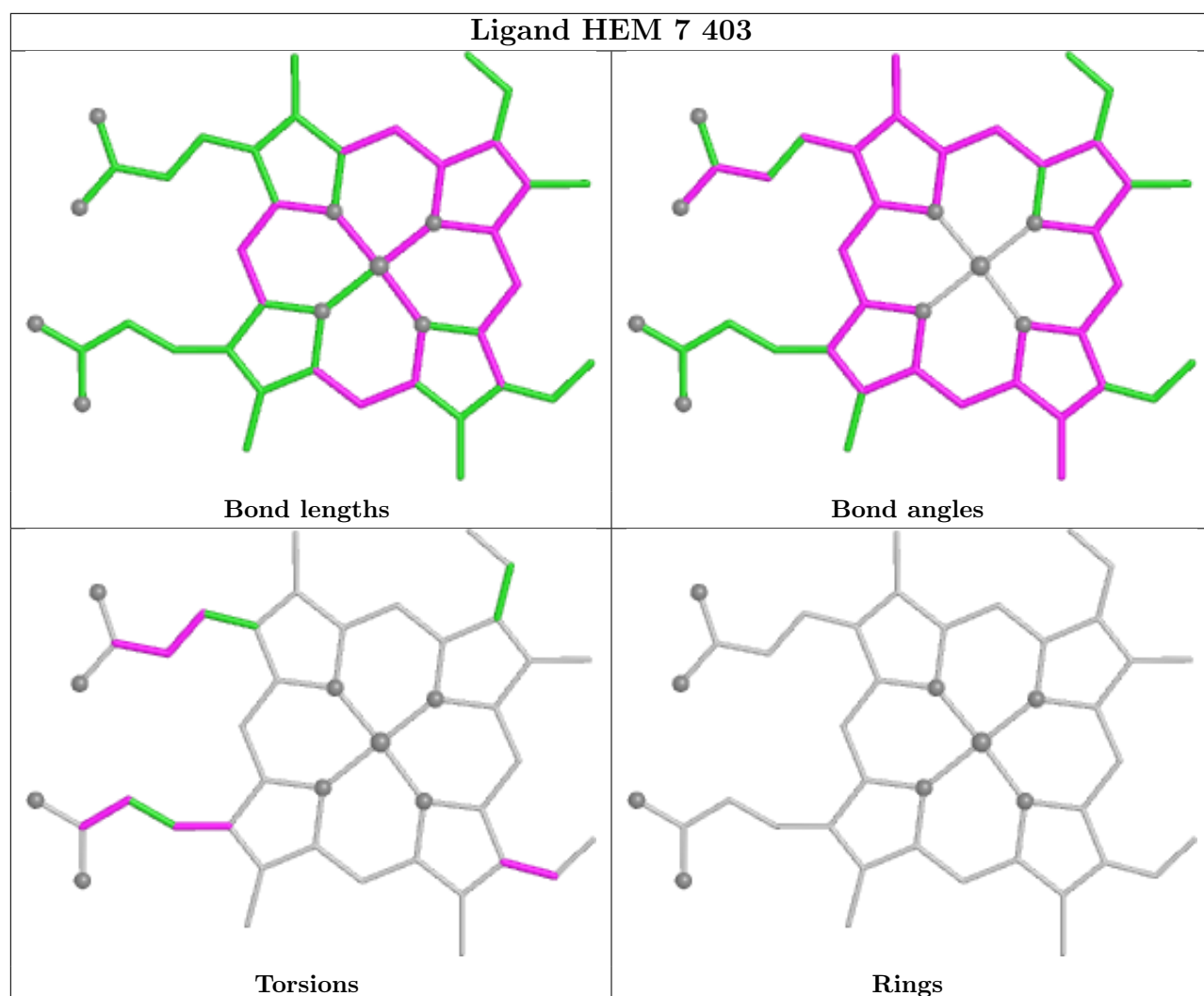












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

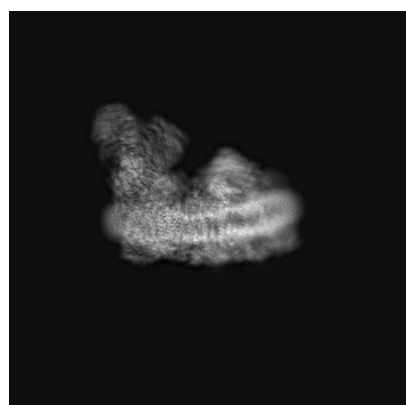
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9539. These allow visual inspection of the internal detail of the map and identification of artifacts.

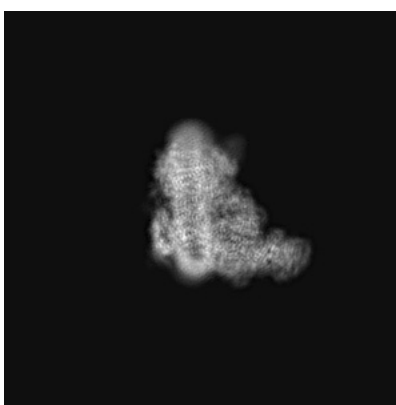
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

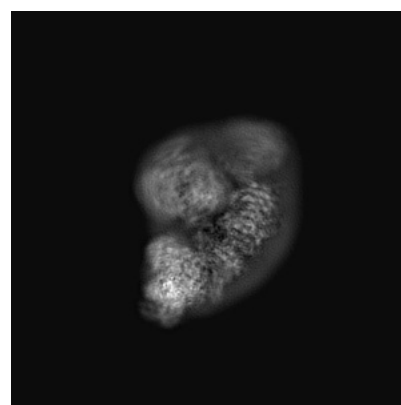
6.1.1 Primary map



X



Y



Z

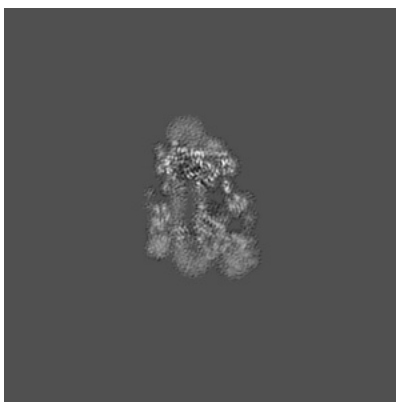
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

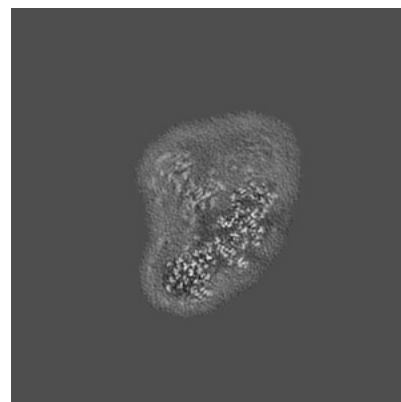
6.2.1 Primary map



X Index: 240



Y Index: 240

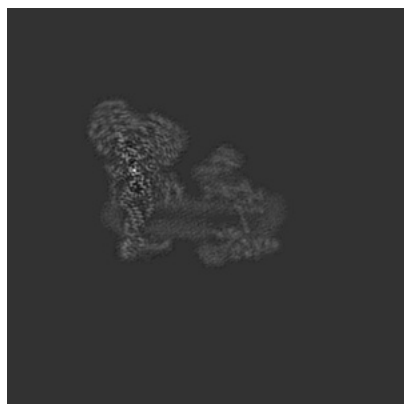


Z Index: 240

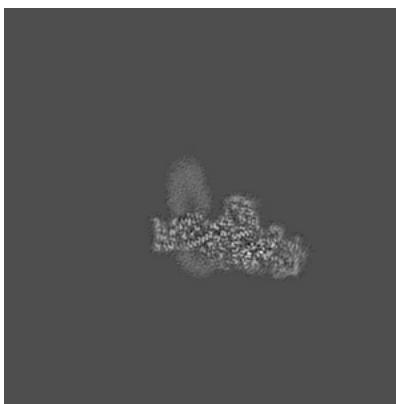
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

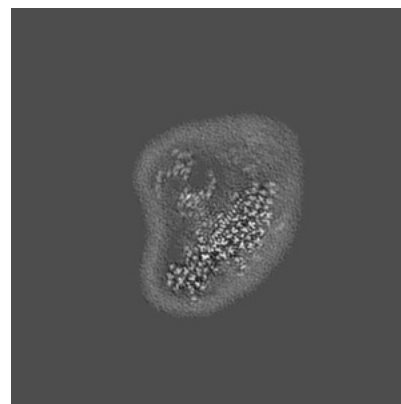
6.3.1 Primary map



X Index: 191



Y Index: 145

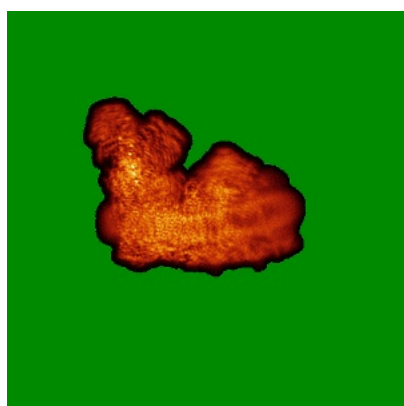


Z Index: 231

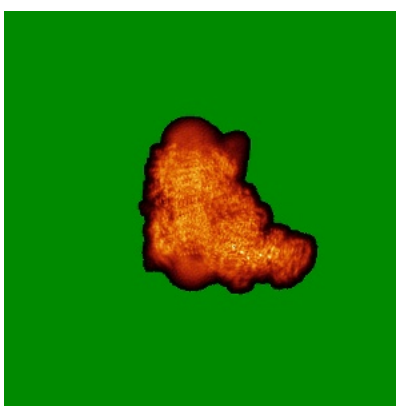
The images above show the largest variance slices of the map in three orthogonal directions.

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

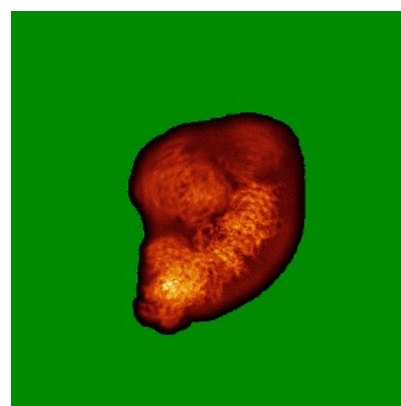
6.4.1 Primary map



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 0.0504. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

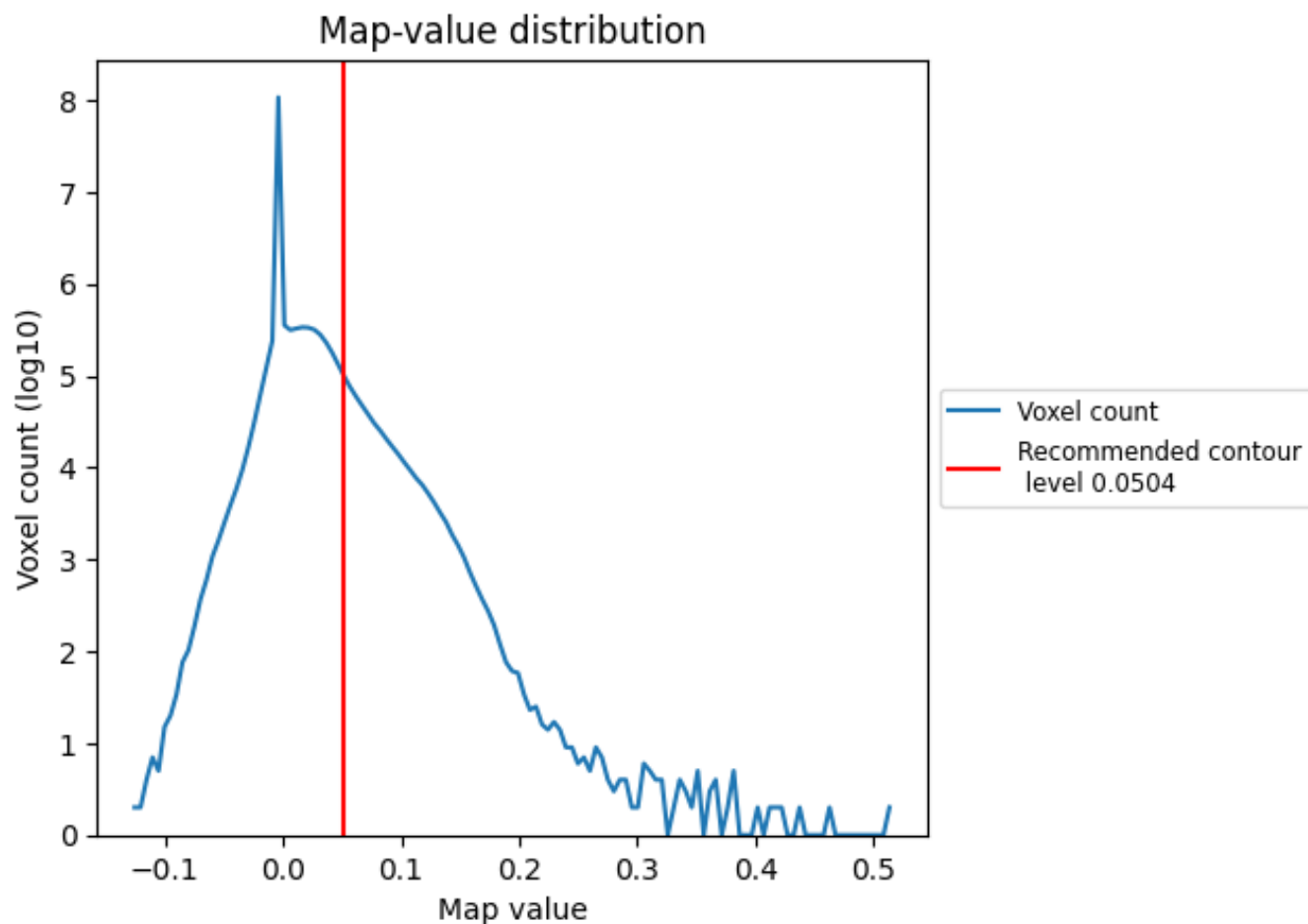
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

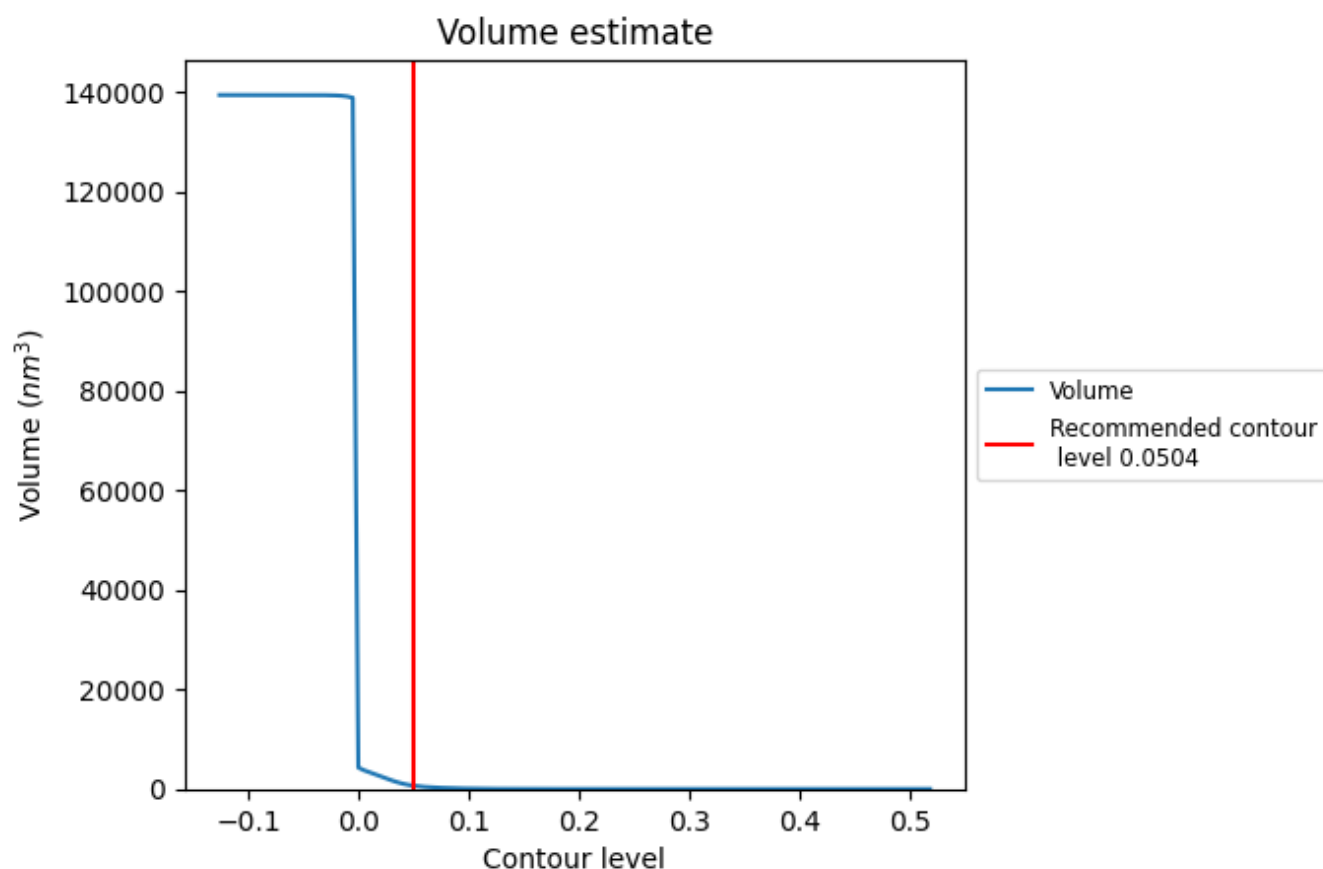
This section contains the results of statistical analysis of the map.

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.

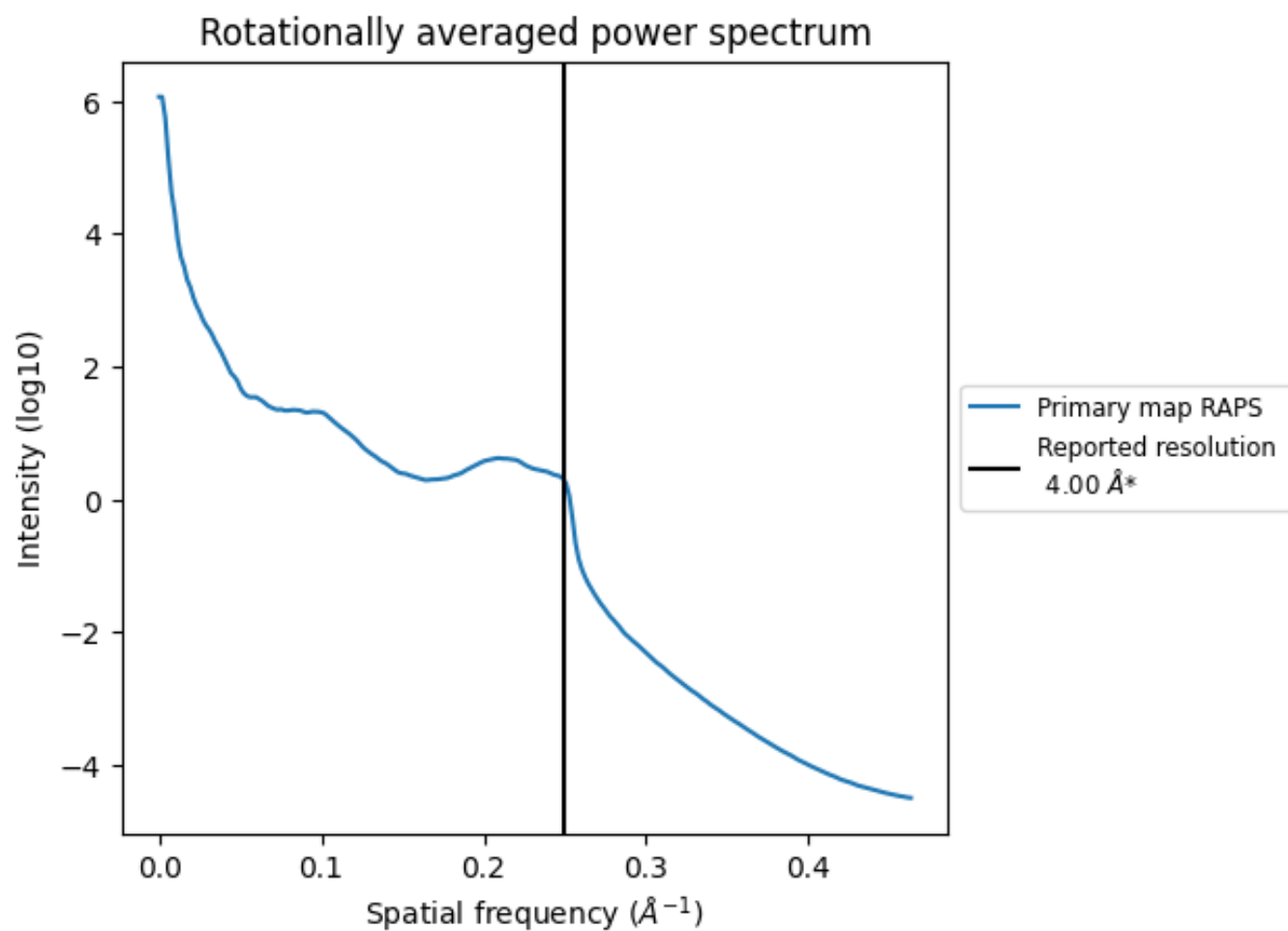
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 645 nm^3 ; this corresponds to an approximate mass of 583 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 0.250 Å⁻¹

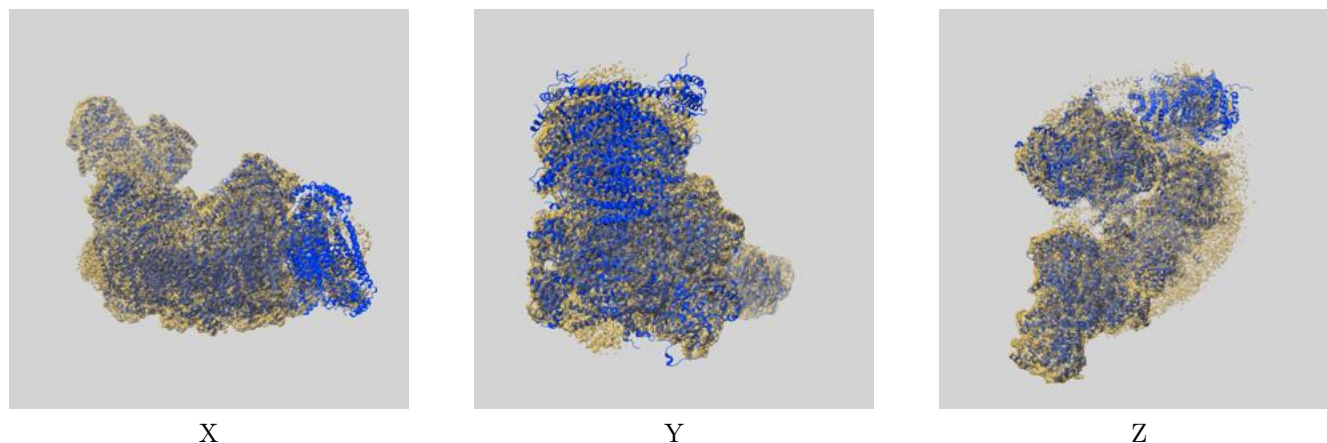
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

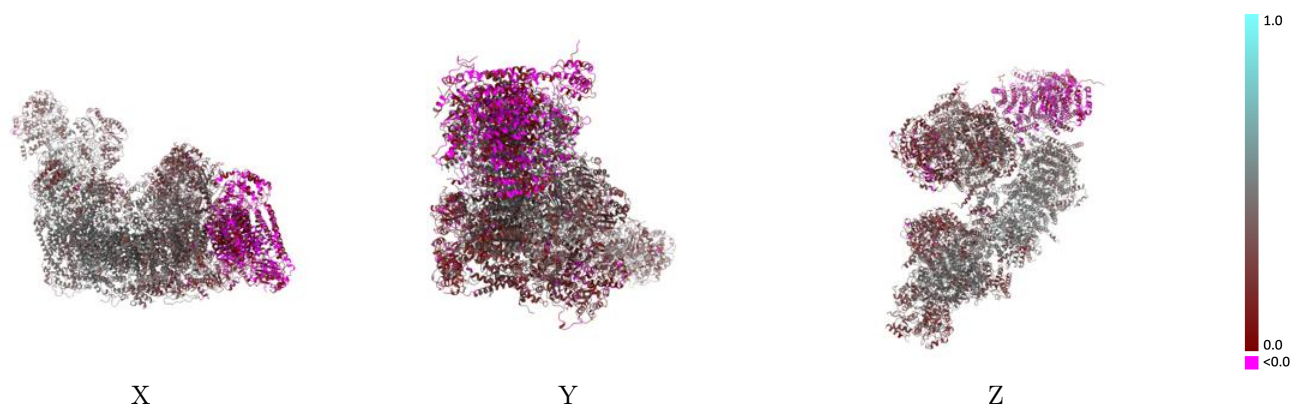
This section contains information regarding the fit between EMDB map EMD-9539 and PDB model 5GUP. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



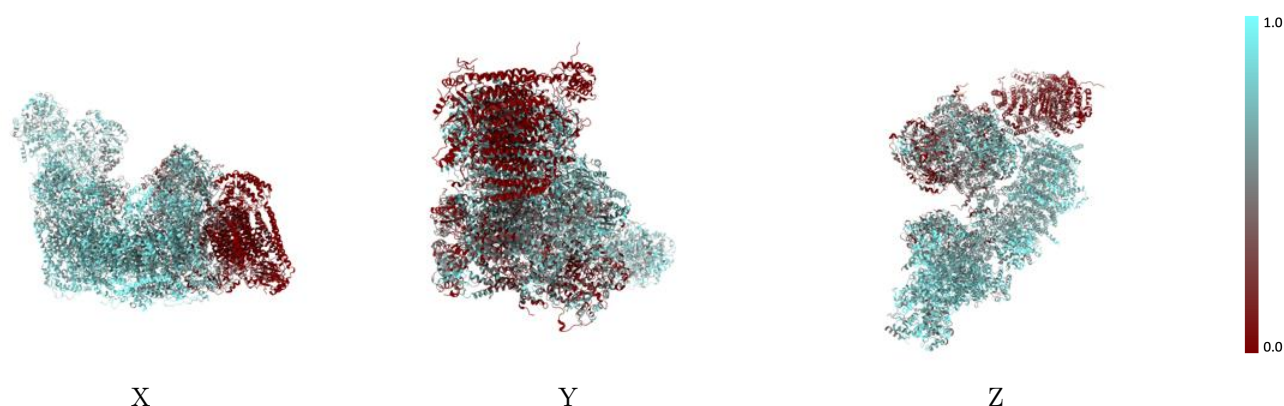
The images above show the 3D surface view of the map at the recommended contour level 0.0504 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



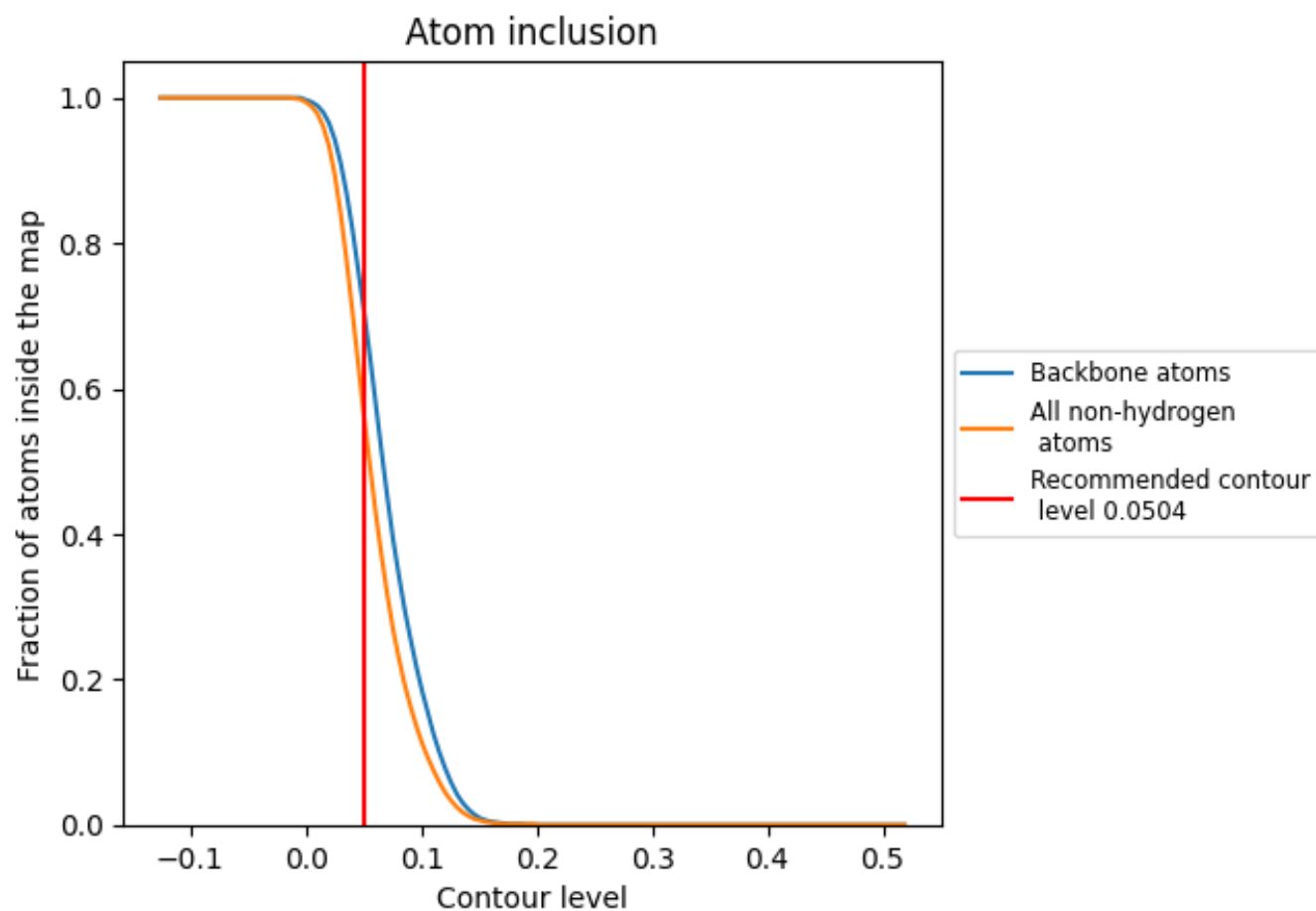
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0504).

9.4 Atom inclusion ⓘ



At the recommended contour level, 71% of all backbone atoms, 56% 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 (0.0504) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5630	 0.3210
0	 0.5190	 0.2820
1	 0.3490	 0.2500
2	 0.2290	 0.2380
3	 0.4180	 0.3100
4	 0.2310	 0.2150
5	 0.4020	 0.2360
6	 0.3350	 0.2240
7	 0.4720	 0.3060
8	 0.5010	 0.2670
9	 0.5120	 0.2880
A	 0.0090	 0.0280
Aa	 0.4200	 0.2560
Ab	 0.3860	 0.2050
Ac	 0.4020	 0.2340
Ad	 0.2830	 0.2220
Ae	 0.0550	 0.1380
Af	 0.1310	 0.2360
Ag	 0.0630	 0.0600
Ah	 0.0350	 -0.0050
Ai	 0.0080	 -0.0150
Aj	 0.1320	 0.0390
Ak	 0.0560	 0.0150
Al	 0.0760	 0.0170
Am	 0.0400	 0.0350
An	 0.0380	 0.0370
Ao	 0.0340	 0.0210
Ap	 0.0640	 0.0150
Aq	 0.0080	 -0.0050
Ar	 0.0480	 0.0160
B	 0.7030	 0.3330
C	 0.7990	 0.4620
D	 0.7920	 0.4200
E	 0.7200	 0.3530
F	 0.7660	 0.3820



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
G	 0.7160	 0.3650
H	 0.8140	 0.4740
I	 0.7820	 0.4530
J	 0.7020	 0.4110
K	 0.5310	 0.3890
L	 0.6070	 0.3330
M	 0.6570	 0.4030
N	 0.6690	 0.3080
O	 0.4760	 0.2630
P	 0.6540	 0.2970
Q	 0.6320	 0.3480
R	 0.4000	 0.3430
S	 0.7430	 0.4220
T	 0.7790	 0.4160
U	 0.8140	 0.4130
V	 0.6730	 0.4320
W	 0.7710	 0.4210
X	 0.7570	 0.4130
Y	 0.8420	 0.4200
Z	 0.7900	 0.3920
a	 0.8130	 0.4420
b	 0.8330	 0.4090
c	 0.8310	 0.4510
d	 0.8390	 0.4140
e	 0.7800	 0.4310
f	 0.7530	 0.3890
g	 0.8030	 0.4500
h	 0.7790	 0.4240
i	 0.7810	 0.4840
j	 0.6500	 0.4360
k	 0.7770	 0.4640
l	 0.7240	 0.4290
m	 0.6480	 0.4130
n	 0.7970	 0.4250
o	 0.7690	 0.4440
p	 0.8140	 0.4270
q	 0.7820	 0.4750
r	 0.7300	 0.4580
s	 0.8040	 0.4260
t	 0.7890	 0.3280
u	 0.6340	 0.3640
v	 0.5800	 0.3020

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
w	 0.5450	 0.3340
x	 0.5320	 0.2960
y	 0.4060	 0.2970
z	 0.5060	 0.3470