



Full wwPDB EM Validation Report ⓘ

Aug 13, 2026 – 02:00 AM JST

PDB ID : 8ZSQ / pdb_00008zsq
EMDB ID : EMD-60424
Title : Respirasome closed state 1 bound by metformin (SC-MetC1)
Authors : Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.
Deposited on : 2024-06-05
Resolution : 2.86 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

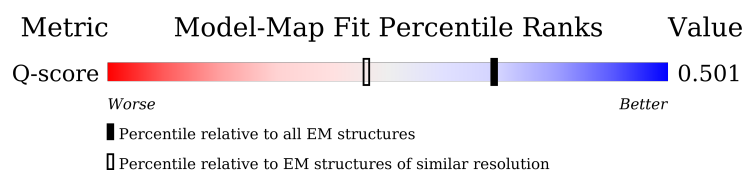
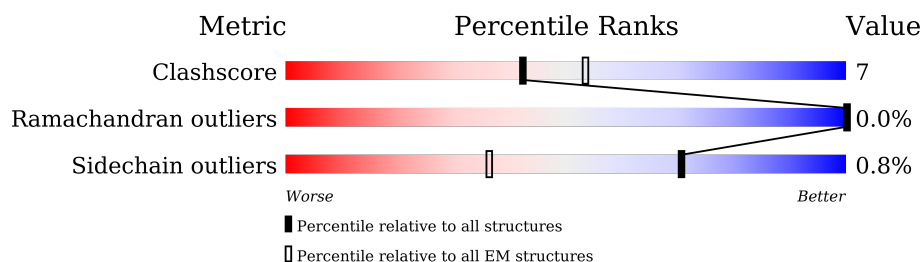
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 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.



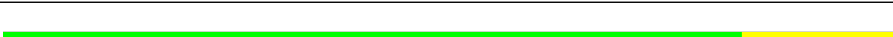
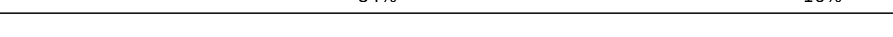
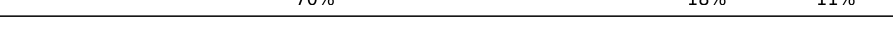
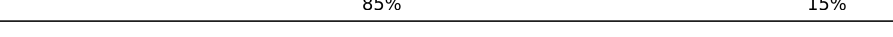
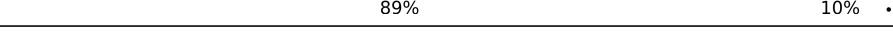
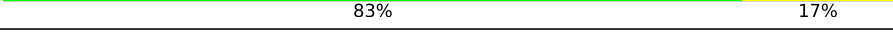
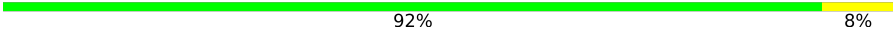
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12017 (2.36 - 3.36)

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	4L	98	 78% 22%
2	5A	102	 84% 15% .
3	5B	95	 80% 19% .
4	6A	75	 81% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	6B	82	 78%21%
6	6C	70	 87%13%
7	7A	57	 84%16%
8	7B	50	 88%12%
9	7C	47	 74%23%
10	8B	43	 86%14%
11	A1	70	 83%17%
12	A2	85	 86%13%
13	A3	83	 94%6%
14	A5	112	 88%12%
15	A6	114	 83%17%
16	A7	112	 74%12%13%
17	A8	171	 85%15%
18	A9	341	 84%16%
19	AB	87	 70%18%11%
19	AC	87	 86%13%
20	AK	321	 85%15%
21	AL	140	 90%10%
22	AM	144	 89%10%
23	AN	142	 83%17%
24	B1	56	 80%20%
25	B2	67	 82%18%
26	B3	80	 85%15%
27	B4	128	 92%8%
28	B5	138	 90%10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	B6	126	
30	B7	125	
31	B8	156	
32	B9	178	
33	BK	174	
34	BL	99	
35	C1	514	
36	C2	228	
37	C3	260	
38	C4	138	
39	CA	49	
40	CB	121	
41	N1	318	
42	N2	347	
43	N3	115	
44	N4	459	
45	N5	603	
46	N6	174	
47	QA	419	
47	Qa	419	
48	QB	446	
48	Qb	446	
49	QC	379	
49	Qc	379	
50	QD	241	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
50	Qd	241	 82% 17% .
51	QE	274	 57% 15% 28%
51	QK	274	 22% 5% 73%
51	Qe	274	 61% 11% 28%
52	QF	67	 87% 13%
52	Qf	67	 82% 13% .
53	QG	101	 88% 12%
53	Qg	101	 87% 12% .
54	QH	79	 80% 19% .
54	Qh	79	 87% 13%
55	QI	62	 90% 8% .
55	Qi	62	 89% 8% .
56	QJ	52	 81% 13% 6%
56	Qj	52	 83% 13% . .
57	S1	689	 79% 21%
58	S2	430	 78% 22%
59	S3	208	 86% 14%
60	S4	124	 85% 15% .
61	S5	105	 92% 8%
62	S6	96	 91% 9%
63	S7	156	 79% 19% .
64	S8	176	 80% 20%
65	V1	431	 78% 22%
66	V2	217	 86% 13% .
67	V3	42	 74% 26%

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
81	HEC	QD	401	X	-	-	-
81	HEC	Qd	401	X	-	-	-
82	FES	QE	303	-	-	X	-
82	FES	Qe	303	-	-	X	-

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 117589 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4L	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5A	102	Total	C	N	O	S	0	0
			825	528	139	156	2		

- Molecule 3 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5B	95	Total	C	N	O	S	0	0
			724	449	128	141	6		

- Molecule 4 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6A	75	Total	C	N	O	S	0	0
			620	401	118	100	1		

- Molecule 5 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6B	82	Total	C	N	O	S	0	0
			684	431	125	123	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6C	70	Total	C	N	O	S	0	0
			574	375	101	95	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7A	57	Total	C	N	O	S	0	0
			447	287	76	81	3		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7B	50	Total	C	N	O	S	0	0
			392	254	66	71	1		

- Molecule 9 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	7C	47	Total	C	N	O	S	0	0
			387	257	65	63	2		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	8B	43	Total	C	N	O	0	0
			338	222	57	59		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A1	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A2	85	Total	C	N	O	S	0	0
			686	431	128	125	2		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A3	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A5	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A6	114	Total	C	N	O	S	0	0
			967	617	178	167	5		

- Molecule 16 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A7	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A8	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A9	341	Total	C	N	O	S	0	0
			2743	1777	480	477	9		

- Molecule 19 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AB	77	Total	C	N	O	S	0	0
			624	402	93	124	5		
19	AC	87	Total	C	N	O	S	0	0
			702	452	103	142	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AK	321	Total	C	N	O	S	0	0
			2601	1655	444	492	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AL	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AM	144	Total	C	N	O	S	0	0
			1204	770	218	212	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AN	142	Total	C	N	O	S	0	0
			1173	755	203	206	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B1	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B2	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B3	80	Total	C	N	O	S	0	0
			641	418	108	114	1		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B4	128	Total	C	N	O	S	0	0
			1062	691	182	189			

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B5	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B6	103	Total	C	N	O	S	0	0
			882	577	156	148	1		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B7	125	Total	C	N	O	S	0	0
			1068	663	204	190	11		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B8	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B9	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BK	174	Total	C	N	O	S	0	0
			1456	913	264	271	8		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BL	99	Total	C	N	O	S	0	0
			828	531	137	156	4		

- Molecule 35 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	C1	514	Total	C	N	O	S	0	0
			4024	2692	625	675	32		

- Molecule 36 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	C2	228	Total	C	N	O	S	0	0
			1833	1193	282	340	18		

- Molecule 37 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	C3	260	Total	C	N	O	S	0	0
			2103	1403	337	353	10		

- Molecule 38 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	C4	138	Total	C	N	O	S	0	0
			1153	751	188	210	4		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	CA	49	Total	C	N	O	0	0
			417	276	71	70		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	CB	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	N1	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	N2	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 43 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	N3	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	N4	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	N5	603	Total	C	N	O	S	0	0
			4785	3173	741	820	51		

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	N6	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		

- Molecule 47 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	QA	419	Total	C	N	O	S	0	0
			3147	1971	557	611	8		
47	Qa	419	Total	C	N	O	S	0	0
			3147	1971	557	611	8		

- Molecule 48 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	QB	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		
48	Qb	433	Total	C	N	O	S	0	0
			3367	2103	592	653	19		

- Molecule 49 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	QC	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
49	Qc	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		

- Molecule 50 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	QD	241	Total	C	N	O	S	0	0
			1921	1225	330	350	16		
50	Qd	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	QE	196	Total	C	N	O	S	0	0
			1517	955	265	290	7		
51	QK	73	Total	C	N	O	S	0	0
			520	328	98	92	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Qe	196	Total	C	N	O	S	0	0
			1517	955	265	290	7		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	QF	67	Total	C	N	O	S	0	0
			552	336	100	111	5		
52	Qf	64	Total	C	N	O	S	0	0
			528	320	97	106	5		

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	QG	101	Total	C	N	O	S	0	0
			893	572	157	162	2		
53	Qg	101	Total	C	N	O	S	0	0
			893	572	157	162	2		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	QH	78	Total	C	N	O	S	0	0
			662	432	121	107	2		
54	Qh	79	Total	C	N	O	S	0	0
			666	434	122	108	2		

- Molecule 55 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	QI	62	Total	C	N	O	0	0
			507	331	90	86		
55	Qi	60	Total	C	N	O	0	0
			493	322	87	84		

- Molecule 56 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	QJ	49	Total	C	N	O	S	0	0
			405	269	71	63	2		
56	Qj	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 57 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	S1	689	Total	C	N	O	S	0	0
			5290	3317	922	1012	39		

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	S2	430	Total	C	N	O	S	0	0
			3459	2212	594	629	24		

- Molecule 59 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	S3	208	Total	C	N	O	S	0	0
			1738	1124	298	314	2		

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	S4	124	Total	C	N	O	S	0	0
			1007	637	179	188	3		

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	S5	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	S6	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	S7	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	S8	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	V1	431	Total	C	N	O	S	0	0
			3316	2092	592	612	20		

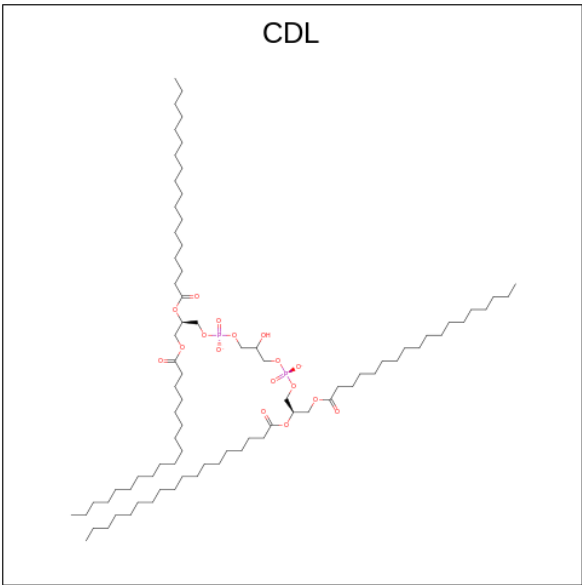
- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	V2	217	Total	C	N	O	S	0	0
			1671	1065	281	315	10		

- Molecule 67 is a protein called NADH:ubiquinone oxidoreductase subunit V3.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	V3	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

- Molecule 68 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
68	4L	1	Total	C	O	P	0
			92	73	17	2	
68	7A	1	Total	C	O	P	0
			91	72	17	2	
68	A7	1	Total	C	O	P	0
			51	32	17	2	
68	A8	1	Total	C	O	P	0
			83	64	17	2	
68	AK	1	Total	C	O	P	0
			68	49	17	2	
68	AL	1	Total	C	O	P	0
			94	75	17	2	
68	B4	1	Total	C	O	P	0
			80	61	17	2	
68	B5	1	Total	C	O	P	0
			100	81	17	2	
68	C3	1	Total	C	O	P	0
			87	68	17	2	
68	C3	1	Total	C	O	P	0
			83	64	17	2	
68	CB	1	Total	C	O	P	0
			100	81	17	2	
68	N1	1	Total	C	O	P	0
			78	59	17	2	
68	N4	1	Total	C	O	P	0
			62	43	17	2	
68	N5	1	Total	C	O	P	0
			89	70	17	2	

Continued on next page...

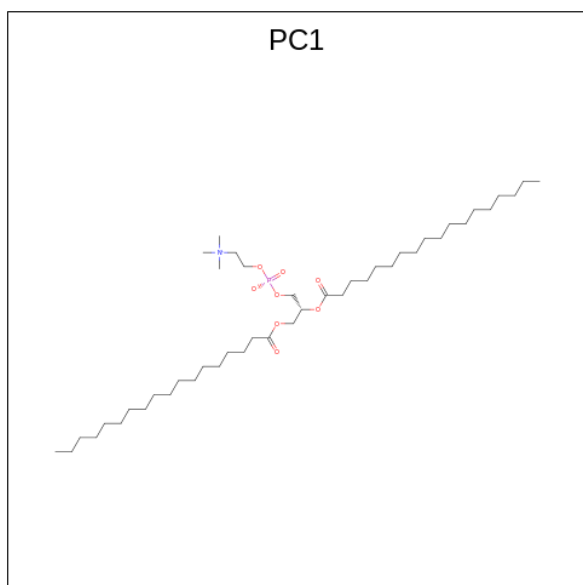
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
68	N5	1	Total	C	O	P	0
			100	81	17	2	
68	QB	1	Total	C	O	P	0
			64	45	17	2	
68	QC	1	Total	C	O	P	0
			55	36	17	2	
68	QD	1	Total	C	O	P	0
			64	45	17	2	
68	QH	1	Total	C	O	P	0
			61	42	17	2	
68	QH	1	Total	C	O	P	0
			64	45	17	2	
68	Qb	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 69 is ZINC ION (CCD ID: ZN) (formula: Zn).

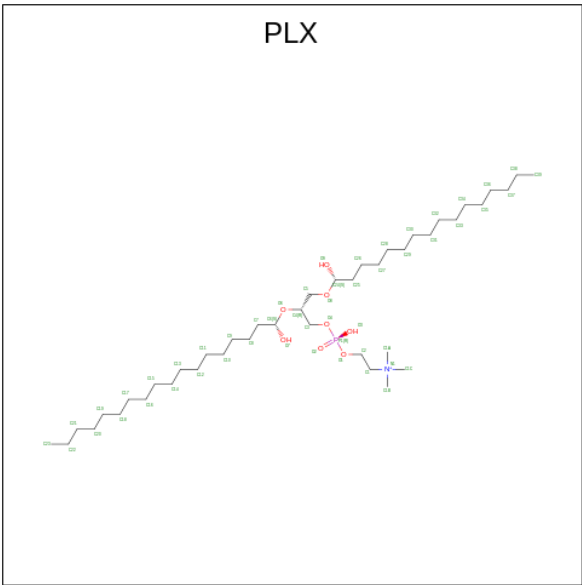
Mol	Chain	Residues	Atoms		AltConf
69	5B	1	Total	Zn	0
			1	1	
69	S6	1	Total	Zn	0
			1	1	

- Molecule 70 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



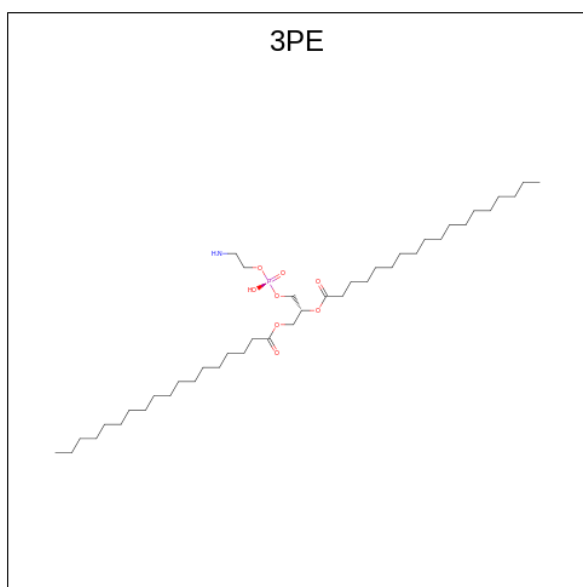
Mol	Chain	Residues	Atoms					AltConf
70	6A	1	Total	C	N	O	P	0
			45	35	1	8	1	
70	C1	1	Total	C	N	O	P	0
			33	23	1	8	1	
70	C1	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	C1	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	C1	1	Total	C	N	O	P	0
			50	40	1	8	1	
70	C3	1	Total	C	N	O	P	0
			44	34	1	8	1	
70	C3	1	Total	C	N	O	P	0
			49	39	1	8	1	
70	C3	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	C3	1	Total	C	N	O	P	0
			43	33	1	8	1	
70	N1	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	N3	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	QB	1	Total	C	N	O	P	0
			51	41	1	8	1	
70	Qb	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	Qc	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	Qh	1	Total	C	N	O	P	0
			54	44	1	8	1	

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



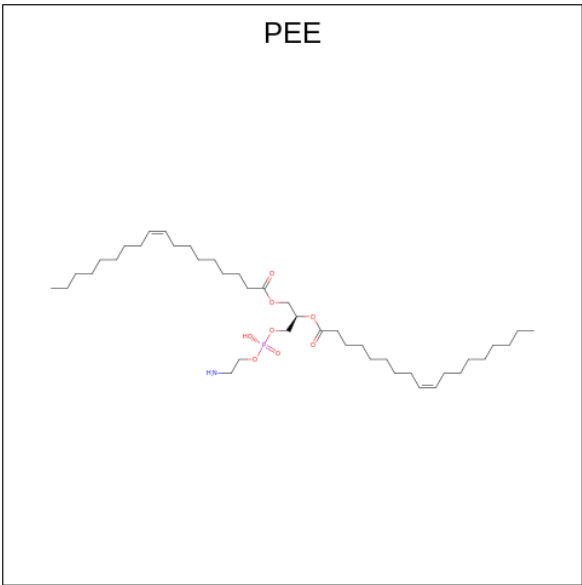
Mol	Chain	Residues	Atoms					AltConf
71	6C	1	Total	C	N	O	P	0
			43	33	1	8	1	
71	AL	1	Total	C	N	O	P	0
			47	37	1	8	1	
71	AM	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	B1	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	CB	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	N4	1	Total	C	N	O	P	0
			49	39	1	8	1	
71	N6	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	QI	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	Qi	1	Total	C	N	O	P	0
			46	36	1	8	1	
71	S7	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 72 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
72	7A	1	Total	C	N	O	P	0
			43	33	1	8	1	
72	B8	1	Total	C	N	O	P	0
			32	22	1	8	1	
72	C1	1	Total	C	N	O	P	0
			39	29	1	8	1	
72	C1	1	Total	C	N	O	P	0
			46	36	1	8	1	
72	CA	1	Total	C	N	O	P	0
			51	41	1	8	1	
72	CB	1	Total	C	N	O	P	0
			46	36	1	8	1	
72	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
72	QE	1	Total	C	N	O	P	0
			44	34	1	8	1	
72	QJ	1	Total	C	N	O	P	0
			34	24	1	8	1	
72	Qc	1	Total	C	N	O	P	0
			48	38	1	8	1	
72	Qj	1	Total	C	N	O	P	0
			29	19	1	8	1	
72	S7	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 73 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



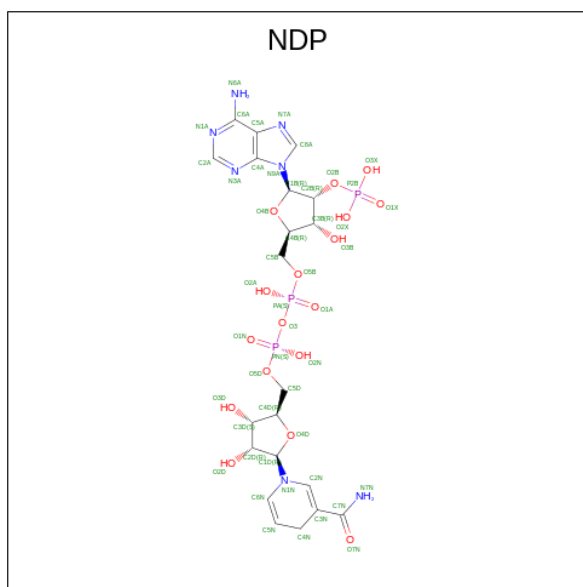
Mol	Chain	Residues	Atoms					AltConf
73	7C	1	Total	C	N	O	P	0
			51	41	1	8	1	
73	A9	1	Total	C	N	O	P	0
			39	29	1	8	1	
73	N1	1	Total	C	N	O	P	0
			31	21	1	8	1	
73	N3	1	Total	C	N	O	P	0
			51	41	1	8	1	
73	N4	1	Total	C	N	O	P	0
			49	39	1	8	1	
73	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
73	N5	1	Total	C	N	O	P	0
			40	30	1	8	1	
73	N5	1	Total	C	N	O	P	0
			51	41	1	8	1	
73	QB	1	Total	C	N	O	P	0
			34	24	1	8	1	
73	QC	1	Total	C	N	O	P	0
			40	30	1	8	1	
73	QE	1	Total	C	N	O	P	0
			47	37	1	8	1	
73	Qc	1	Total	C	N	O	P	0
			42	32	1	8	1	
73	Qe	1	Total	C	N	O	P	0
			51	41	1	8	1	
73	Qe	1	Total	C	N	O	P	0
			24	14	1	8	1	

Continued on next page...

Continued from previous page...

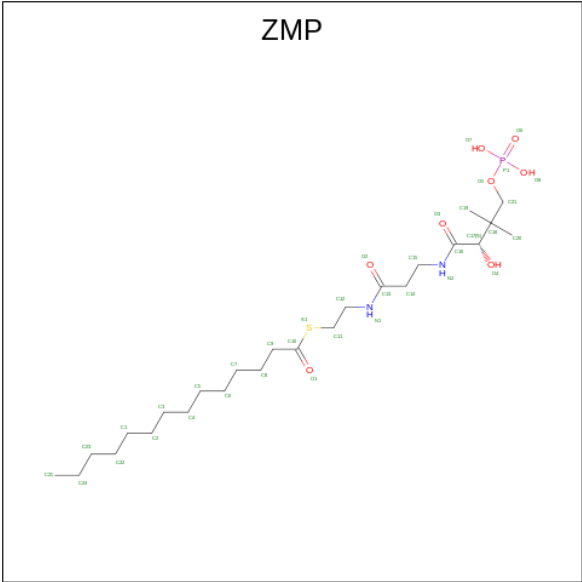
Mol	Chain	Residues	Atoms					AltConf
73	S2	1	Total	C	N	O	P	0
			48	38	1	8	1	
73	S8	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 74 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



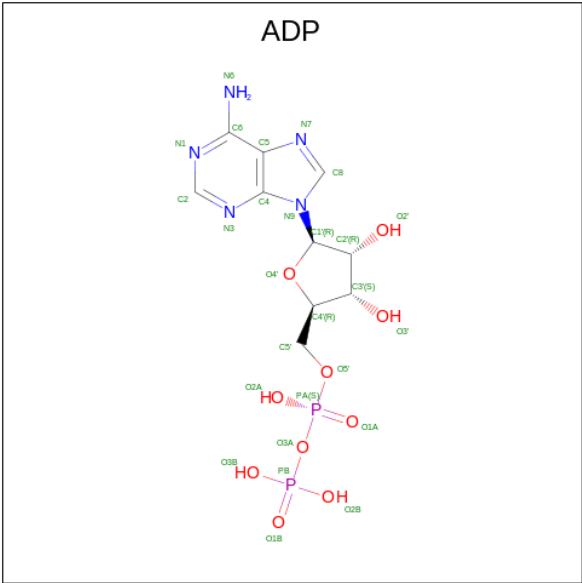
Mol	Chain	Residues	Atoms					AltConf
74	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 75 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



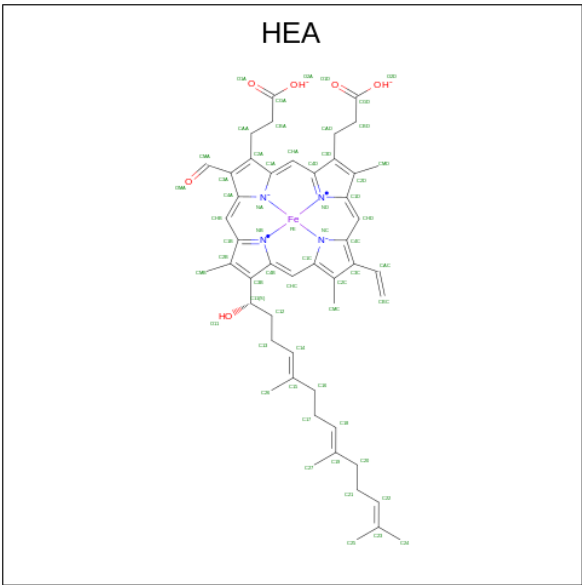
Mol	Chain	Residues	Atoms						AltConf
75	AB	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	
75	AC	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 76 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
76	AK	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 77 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
77	C1	1	Total 60	C 49	Fe 1	N 4	O 6	0
77	C1	1	Total 60	C 49	Fe 1	N 4	O 6	0

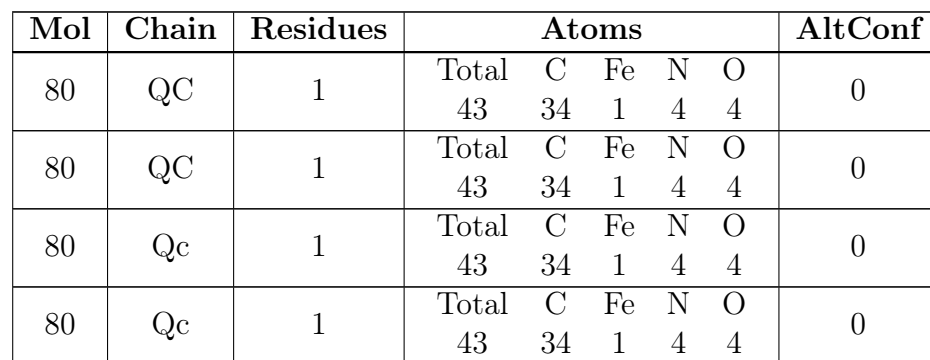
- Molecule 78 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
78	C1	1	Total	Cu	0
			1	1	
78	C2	2	Total	Cu	0
			2	2	

- Molecule 79 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
79	C1	1	Total	Mg	0
			1	1	
79	S1	1	Total	Mg	0
			1	1	

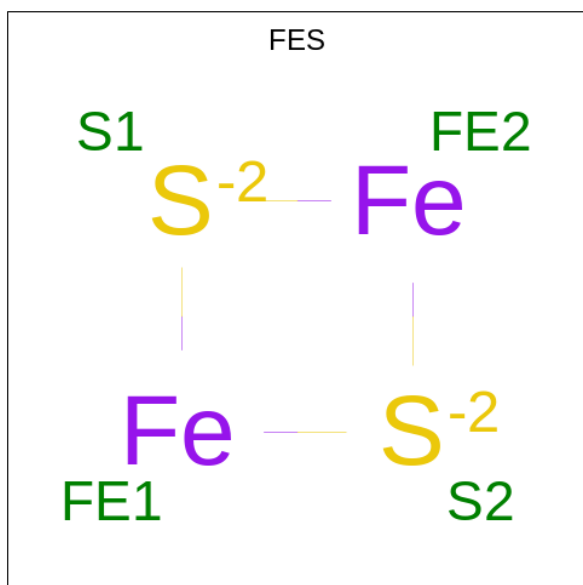
- Molecule 80 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



- # HEC
-
- The diagram illustrates the chemical structure of the HEC (Hexaethylcyclotriphosphazene) complex. It features a central Iron (Fe) atom coordinated by four Nitrogen (N) atoms in a square planar arrangement. The N atoms are part of a macrocyclic ligand with various substituents. The substituents are labeled as follows: CAC, CMC, CBB, CMB, CHB, CMA, CAA, CBA, CAD, CBD, CGD, O2D, O1D, O2A, and O1A. The structure is shown in a perspective view, with the central Fe atom and the four N atoms forming a square. The macrocyclic ligand is represented by a series of lines connecting the N atoms and their substituents.

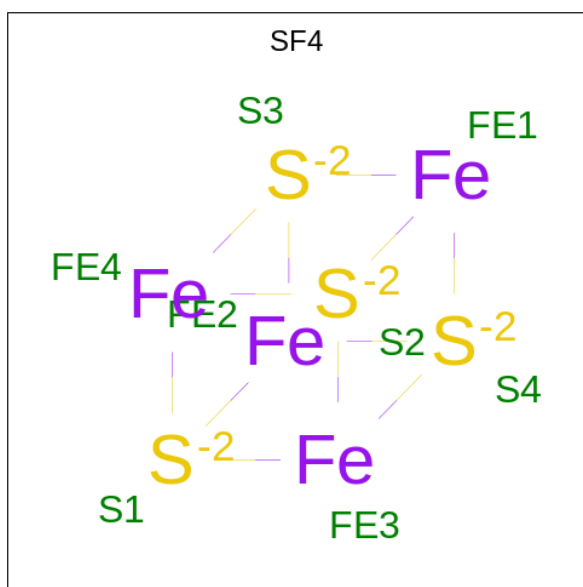
Mol	Chain	Residues	Atoms					AltConf
81	QD	1	Total 43	C 34	Fe 1	N 4	O 4	0
81	Qd	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 82 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



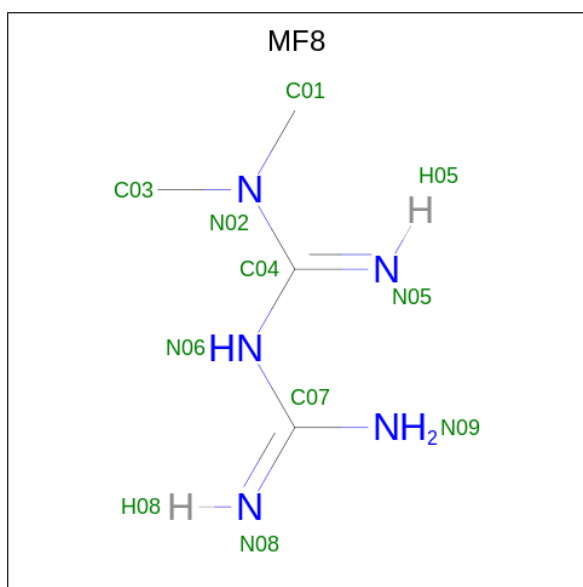
Mol	Chain	Residues	Atoms			AltConf
82	QE	1	Total	Fe	S	0
			4	2	2	
82	Qe	1	Total	Fe	S	0
			4	2	2	
82	S1	1	Total	Fe	S	0
			4	2	2	
82	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 83 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



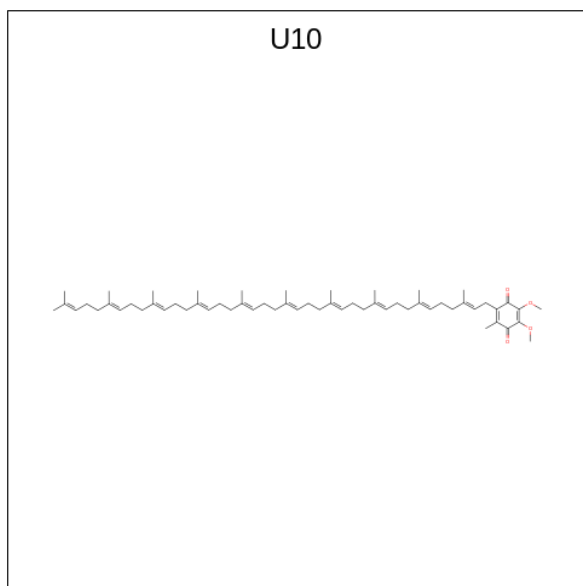
Mol	Chain	Residues	Atoms			AltConf
83	S1	1	Total	Fe	S	0
			8	4	4	
83	S1	1	Total	Fe	S	0
			8	4	4	
83	S7	1	Total	Fe	S	0
			8	4	4	
83	S8	1	Total	Fe	S	0
			8	4	4	
83	S8	1	Total	Fe	S	0
			8	4	4	
83	V1	1	Total	Fe	S	0
			8	4	4	

- Molecule 84 is Metformin (CCD ID: MF8) (formula: $C_4H_{11}N_5$) (labeled as "Ligand of Interest" by depositor).



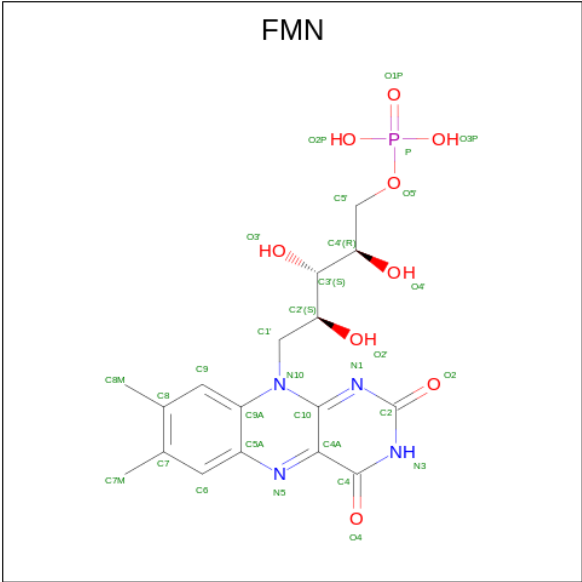
Mol	Chain	Residues	Atoms			AltConf
84	S2	1	Total	C	N	0
			9	4	5	

- Molecule 85 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
85	S7	1	Total	C	O	0
			63	59	4	

- Molecule 86 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).

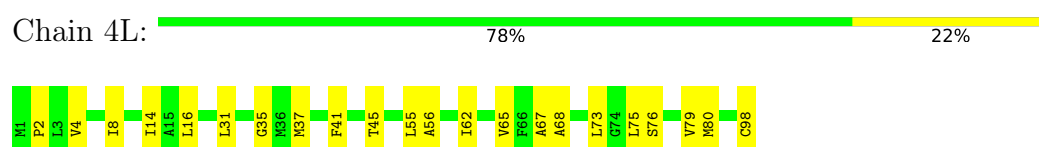


Mol	Chain	Residues	Atoms					AltConf
86	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

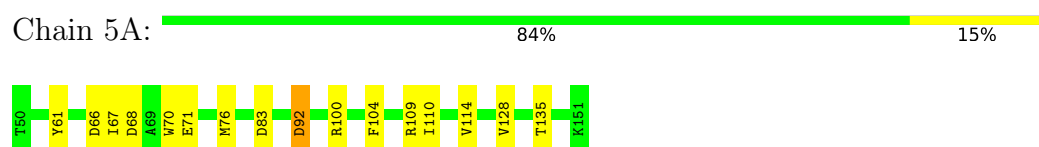
3 Residue-property plots [i](#)

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

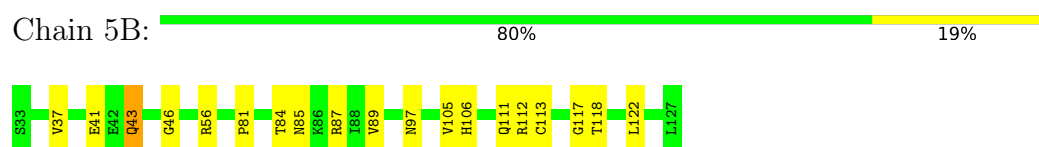
- Molecule 1: NADH-ubiquinone oxidoreductase chain 4L



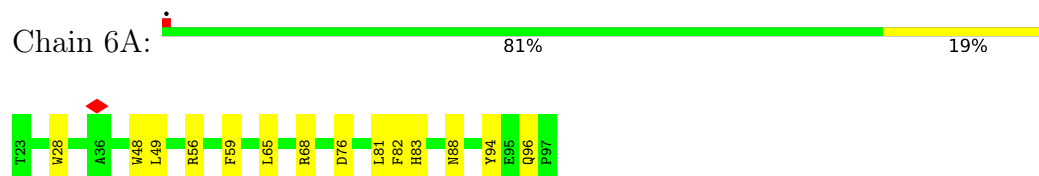
- Molecule 2: Cytochrome c oxidase subunit 5A, mitochondrial



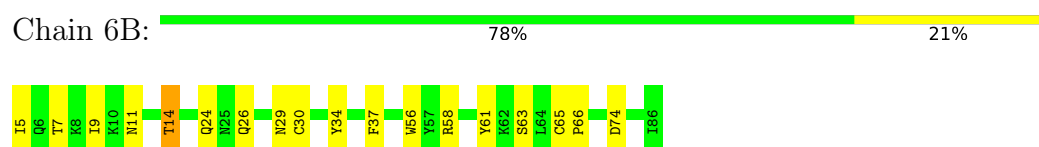
- Molecule 3: Cytochrome c oxidase subunit 5B, mitochondrial



- Molecule 4: Cytochrome c oxidase subunit



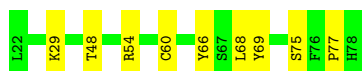
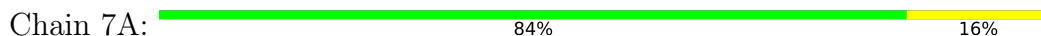
- Molecule 5: Cytochrome c oxidase subunit



- Molecule 6: Cytochrome c oxidase subunit 6C



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



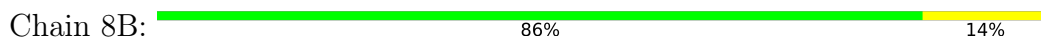
- Molecule 8: Cytochrome c oxidase subunit 7B, mitochondrial



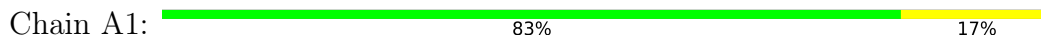
- Molecule 9: Cytochrome c oxidase subunit 7C, mitochondrial



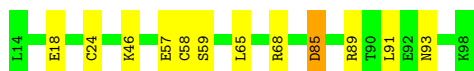
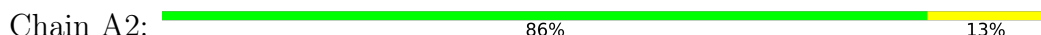
- Molecule 10: Cytochrome c oxidase subunit 8



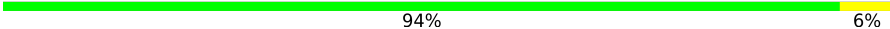
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain A3:  94% 6%



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

Chain A5:  88% 12%



- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain A6:  83% 17%



- Molecule 16: Complex I-B14.5a

Chain A7:  74% 12% 13%



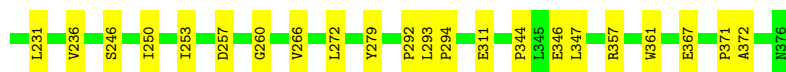
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8:  85% 15%



- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain A9:  84% 16%



- Molecule 19: Acyl carrier protein

Chain AB:  70% 18% 11%



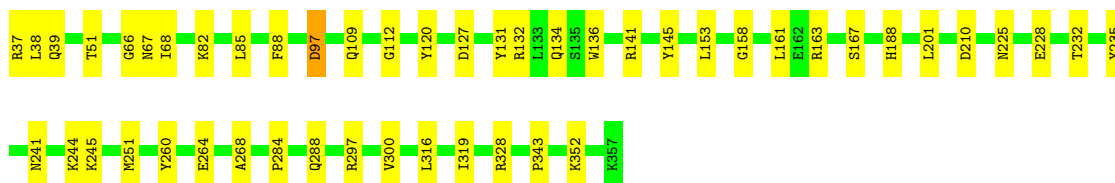
- Molecule 19: Acyl carrier protein

Chain AC: 86% 13%



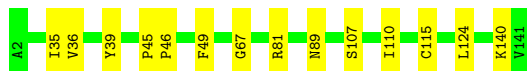
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain AK: 85% 15%



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain AL: 90% 10%



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AM: 89% 10%



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain AN: 83% 17%



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

Chain B1: 80% 20%



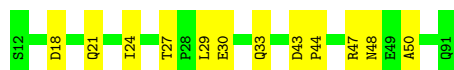
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain B2:  82% 18%



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain B3:  85% 15%



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain B4:  92% 8%



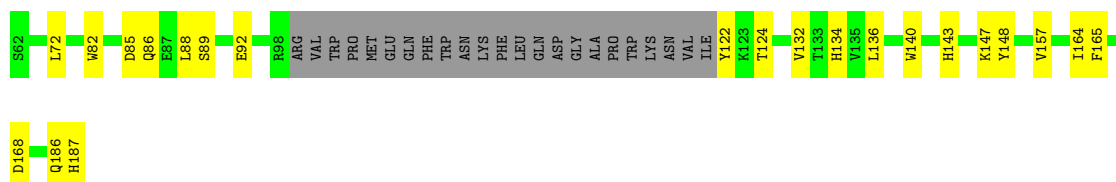
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain B5:  90% 10%



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain B6:  64% 17% 18%



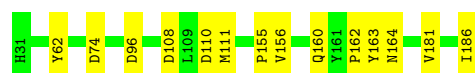
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain B7:  81% 19%



- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain B8:  91% 9%



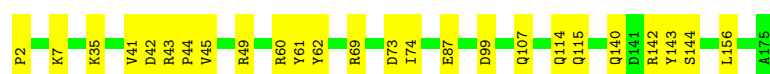
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain B9:  87% 13%



- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain BK:  86% 14%



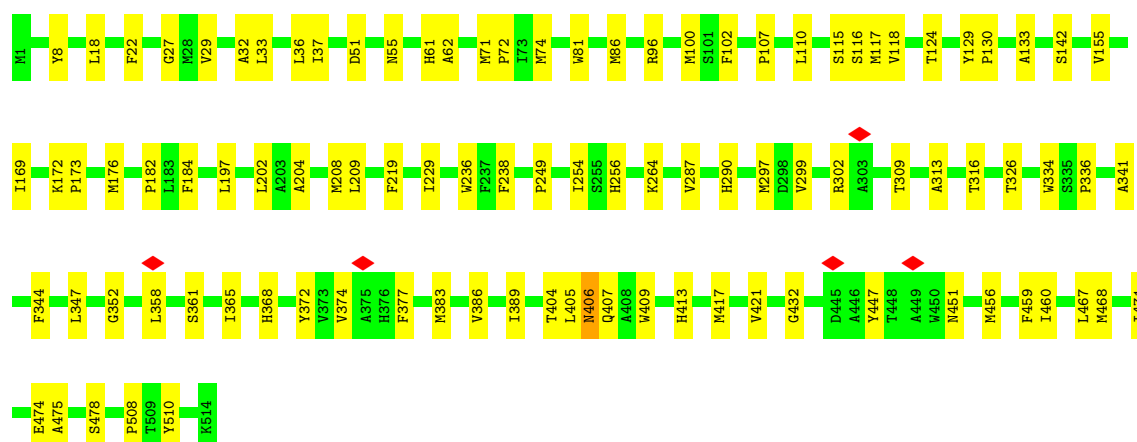
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain BL:  89% 11%



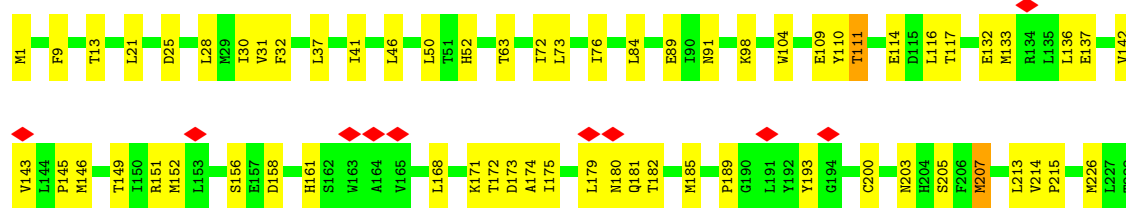
- Molecule 35: Cytochrome c oxidase subunit 1

Chain C1:  81% 19%

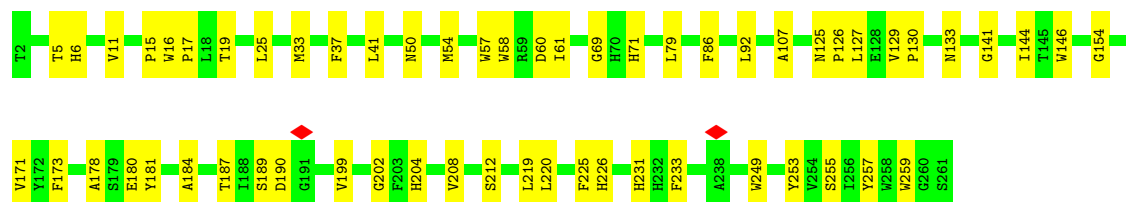
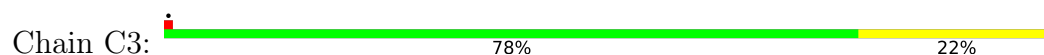


- Molecule 36: Cytochrome c oxidase subunit 2

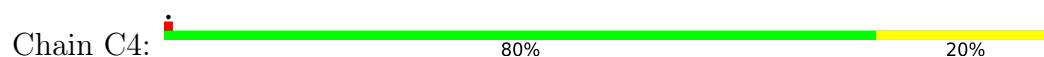
Chain C2:  72% 27%



• Molecule 37: Cytochrome c oxidase subunit 3



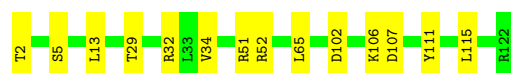
• Molecule 38: Cytochrome c oxidase subunit 4



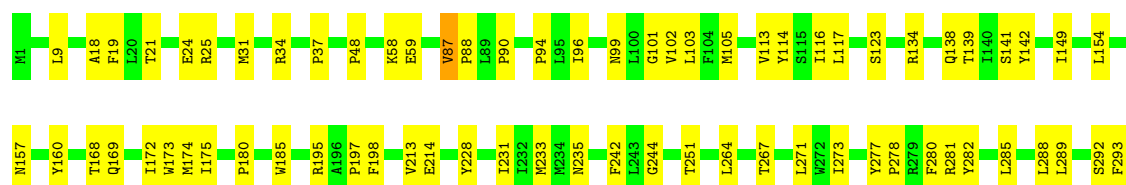
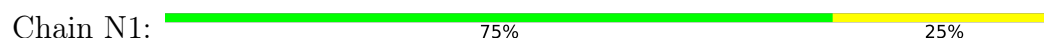
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



• Molecule 40: NADH dehydrogenase [ubiquinone] 1 subunit C2



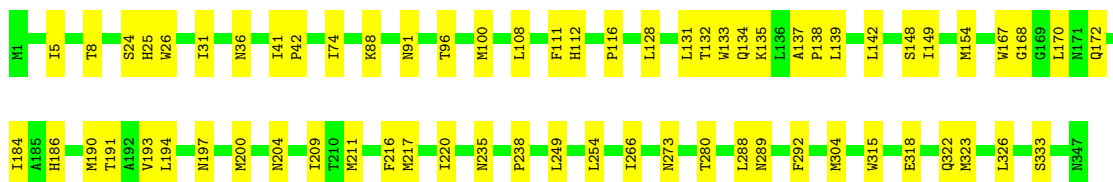
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1





• Molecule 42: NADH-ubiquinone oxidoreductase chain 2

Chain N2: 81% 19%



• Molecule 43: NADH-ubiquinone oxidoreductase chain 3

Chain N3: 83% 17%



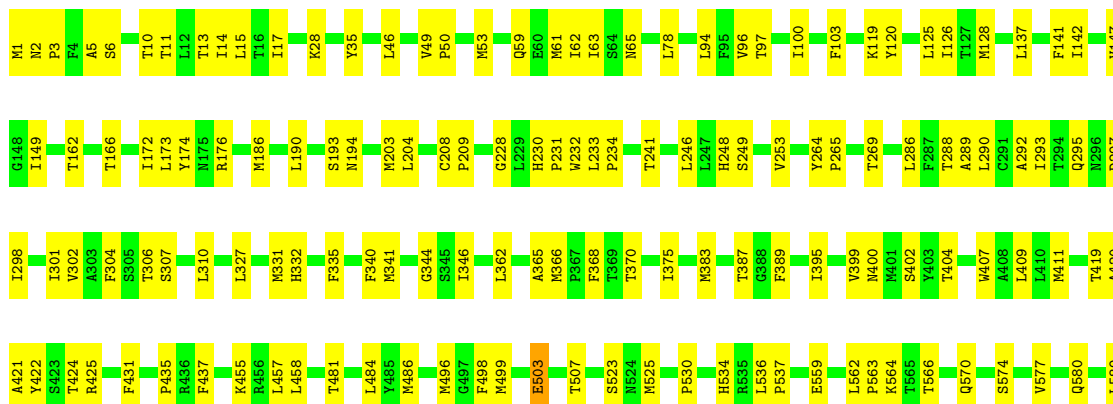
• Molecule 44: NADH-ubiquinone oxidoreductase chain 4

Chain N4: 82% 17%



• Molecule 45: NADH-ubiquinone oxidoreductase chain 5

Chain N5: 76% 24%





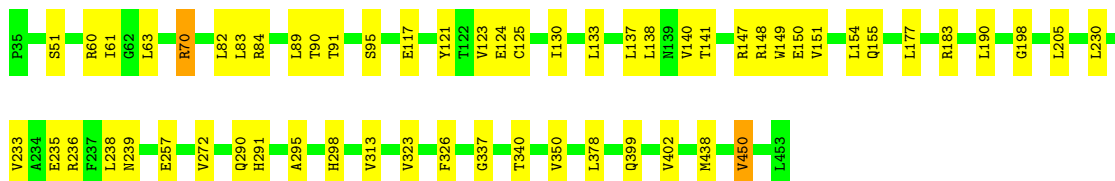
- Molecule 46: NADH-ubiquinone oxidoreductase chain 6

Chain N6: 80% 20%



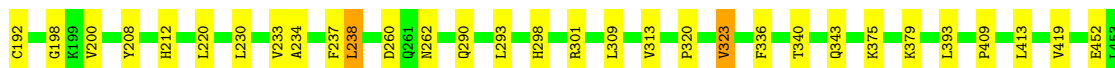
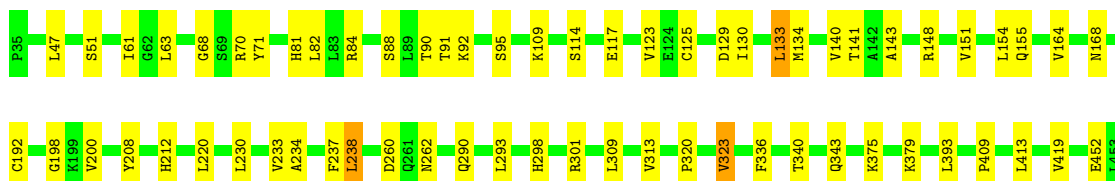
- Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain QA: 86% 13%



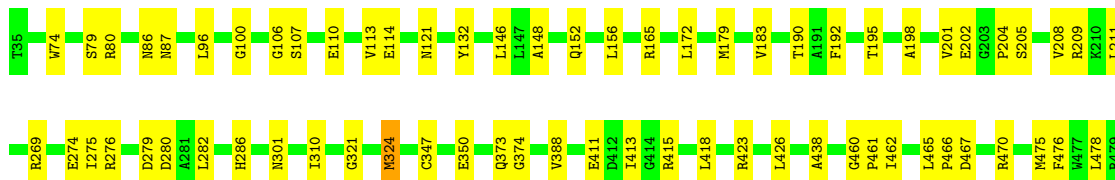
- Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain Qa: 85% 15%



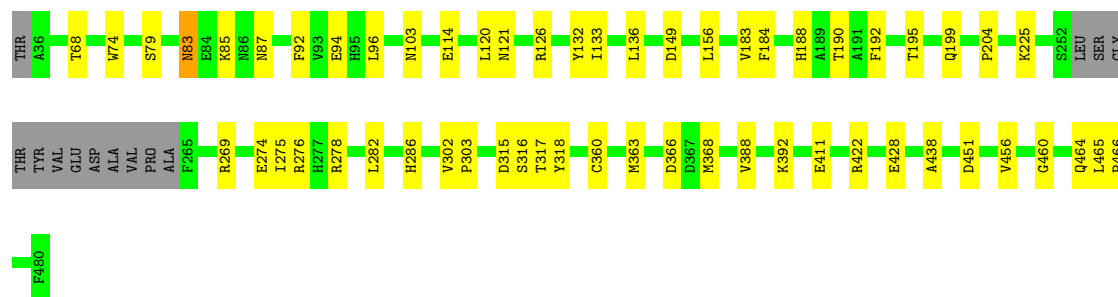
- Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain QB: 85% 15%



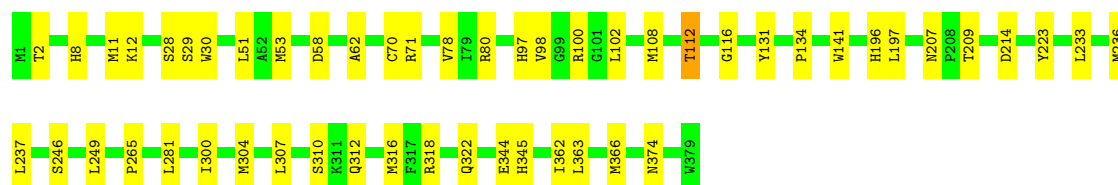
- Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain Qb: 84% 13%



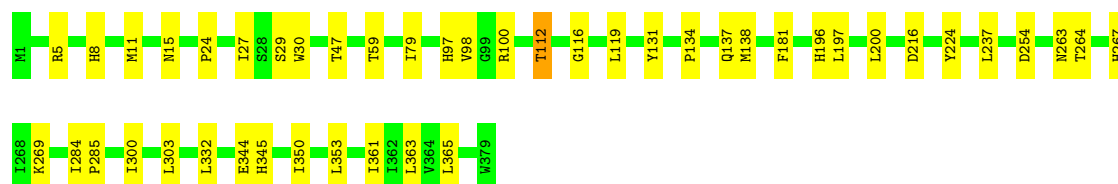
- Molecule 49: Cytochrome b

Chain QC: 86% 13%



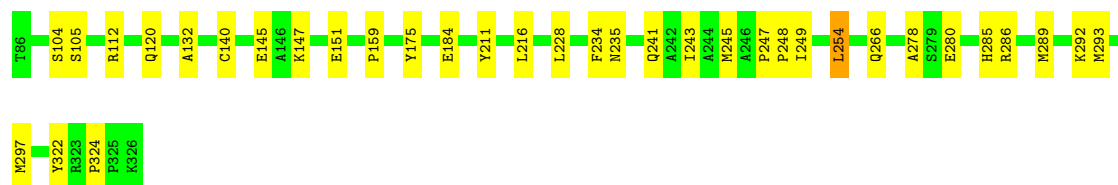
- Molecule 49: Cytochrome b

Chain Qc: 88% 12%



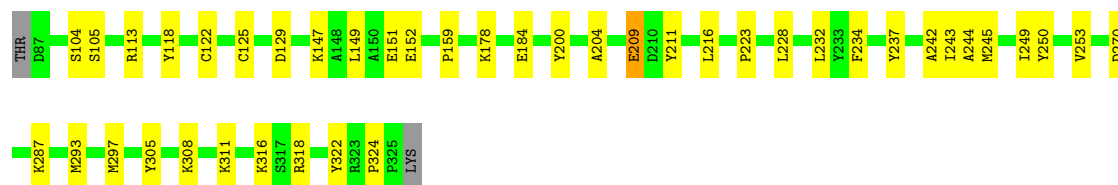
- Molecule 50: Cytochrome c1, heme protein, mitochondrial

Chain QD: 85% 14%



- Molecule 50: Cytochrome c1, heme protein, mitochondrial

Chain Qd: 82% 17%





- Molecule 53: Cytochrome b-c1 complex subunit 7

Chain QG: 88% 12%



- Molecule 53: Cytochrome b-c1 complex subunit 7

Chain Qg: 87% 12%



- Molecule 54: Cytochrome b-c1 complex subunit 8

Chain QH: 80% 19%



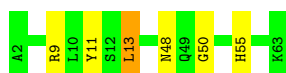
- Molecule 54: Cytochrome b-c1 complex subunit 8

Chain Qh: 87% 13%



- Molecule 55: Complex III subunit 9

Chain QI: 90% 8%



- Molecule 55: Complex III subunit 9

Chain Qi: 89% 8%



- Molecule 56: Cytochrome b-c1 complex subunit 10

Chain QJ: 81% 13% 6%



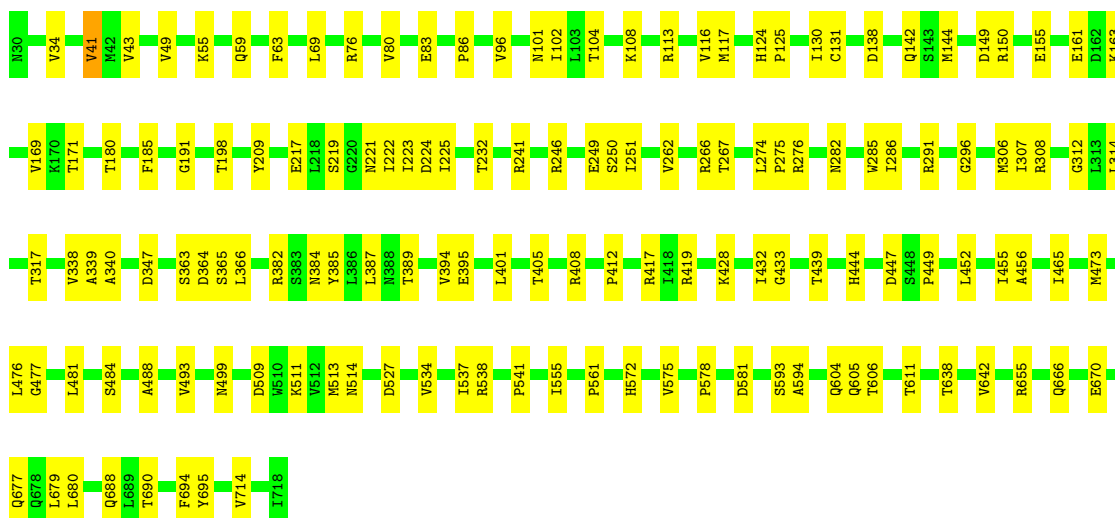
- Molecule 56: Cytochrome b-c1 complex subunit 10

Chain Qj: 83% 13% ..



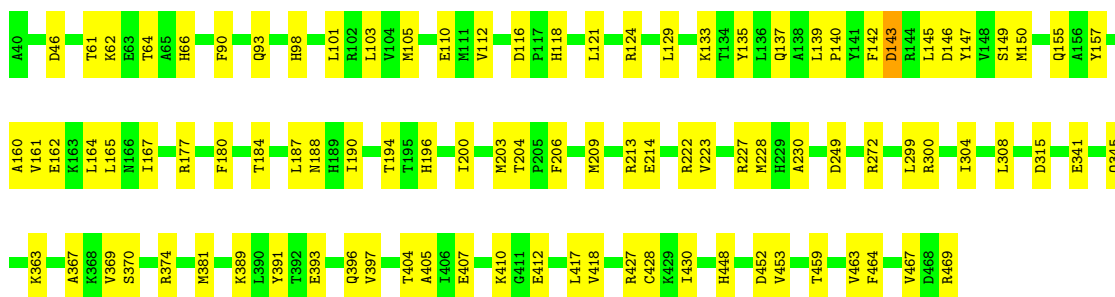
- Molecule 57: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain S1: 79% 21%



- Molecule 58: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain S2: 78% 22%



- Molecule 59: Complex I-30kD

Chain S3: 86% 14%

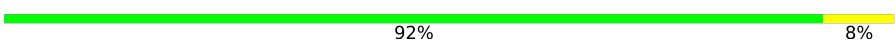


- Molecule 60: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain S4:  85% 15%



- Molecule 61: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain S5:  92% 8%



- Molecule 62: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain S6:  91% 9%



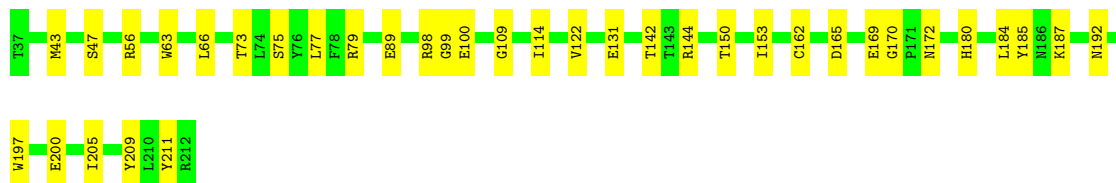
- Molecule 63: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain S7:  79% 19%



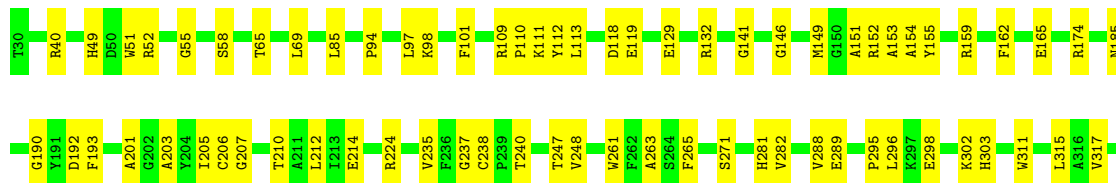
- Molecule 64: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

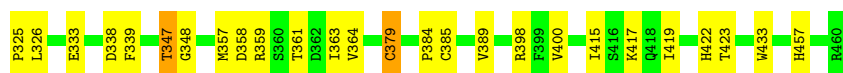
Chain S8:  80% 20%



- Molecule 65: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain V1:  78% 22%





- Molecule 66: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain V2: 86% 13%



- Molecule 67: NADH:ubiquinone oxidoreductase subunit V3

Chain V3: 74% 26%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	320129	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.9	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	46.884	Depositor
Minimum map value	-34.576	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.006	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	576.0, 576.0, 576.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, 2MR, FMN, 3PE, HEA, U10, PLX, ZN, NDP, PEE, MF8, ADP, CDL, HEM, ZMP, FES, SF4, PC1, CU, MG

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	4L	0.15	0/759	0.29	0/1029
2	5A	0.09	0/843	0.23	0/1145
3	5B	0.12	0/739	0.30	0/1002
4	6A	0.10	0/648	0.23	0/888
5	6B	0.11	0/704	0.26	0/951
6	6C	0.10	0/587	0.25	0/781
7	7A	0.11	0/457	0.23	0/620
8	7B	0.10	0/405	0.26	0/555
9	7C	0.11	0/400	0.22	0/536
10	8B	0.11	0/349	0.23	0/477
11	A1	0.14	0/577	0.32	0/777
12	A2	0.10	0/697	0.25	0/938
13	A3	0.10	0/664	0.23	0/912
14	A5	0.13	0/929	0.23	0/1258
15	A6	0.14	0/991	0.29	0/1335
16	A7	0.12	0/798	0.26	0/1079
17	A8	0.11	0/1436	0.25	0/1938
18	A9	0.14	0/2820	0.27	0/3823
19	AB	0.10	0/633	0.23	0/851
19	AC	0.13	0/714	0.23	0/965
20	AK	0.12	0/2661	0.27	0/3602
21	AL	0.12	0/1042	0.21	0/1411
22	AM	0.10	0/1245	0.23	0/1694
23	AN	0.14	0/1204	0.27	0/1624
24	B1	0.13	0/491	0.28	0/663
25	B2	0.12	0/610	0.23	0/836
26	B3	0.12	0/660	0.25	0/892
27	B4	0.14	0/1092	0.26	0/1481
28	B5	0.15	0/1184	0.28	0/1603
29	B6	0.15	0/910	0.33	0/1237
30	B7	0.12	0/1092	0.25	0/1459

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	B8	0.13	0/1371	0.26	0/1875
32	B9	0.14	0/1590	0.27	0/2155
33	BK	0.13	0/1489	0.25	0/2008
34	BL	0.13	0/851	0.27	0/1155
35	C1	0.14	0/4164	0.28	0/5689
36	C2	0.12	0/1880	0.28	0/2564
37	C3	0.13	0/2186	0.26	0/2991
38	C4	0.12	0/1187	0.26	0/1606
39	CA	0.10	0/430	0.19	0/581
40	CB	0.13	0/1031	0.26	0/1394
41	N1	0.18	0/2581	0.35	0/3529
42	N2	0.17	0/2773	0.33	0/3768
43	N3	0.16	0/938	0.28	0/1281
44	N4	0.17	0/3723	0.31	0/5078
45	N5	0.16	0/4914	0.34	0/6683
46	N6	0.14	0/1364	0.31	0/1850
47	QA	0.15	0/3200	0.29	0/4333
47	Qa	0.15	0/3200	0.29	0/4333
48	QB	0.15	0/3531	0.30	0/4793
48	Qb	0.14	0/3436	0.27	0/4659
49	QC	0.17	0/3123	0.31	0/4269
49	Qc	0.17	0/3123	0.32	0/4269
50	QD	0.15	0/1979	0.26	0/2684
50	Qd	0.15	0/1962	0.27	0/2663
51	QE	0.12	0/1550	0.25	0/2098
51	QK	0.11	0/528	0.27	0/716
51	Qe	0.12	0/1550	0.27	0/2098
52	QF	0.11	0/558	0.22	0/747
52	Qf	0.13	0/534	0.25	0/714
53	QG	0.14	0/913	0.25	0/1223
53	Qg	0.14	0/913	0.27	0/1223
54	QH	0.14	0/684	0.30	0/926
54	Qh	0.14	0/688	0.28	0/931
55	QI	0.11	0/520	0.20	0/701
55	Qi	0.16	0/506	0.27	0/683
56	QJ	0.10	0/420	0.22	0/576
56	Qj	0.14	0/437	0.31	0/598
57	S1	0.15	0/5378	0.32	2/7287 (0.0%)
58	S2	0.18	0/3538	0.31	0/4796
59	S3	0.15	0/1789	0.29	0/2436
60	S4	0.14	0/1030	0.27	0/1391
61	S5	0.11	0/889	0.23	0/1190
62	S6	0.13	0/755	0.29	0/1018

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
63	S7	0.17	0/1279	0.30	0/1730
64	S8	0.16	0/1443	0.29	0/1952
65	V1	0.15	0/3391	0.31	0/4583
66	V2	0.14	0/1711	0.30	0/2328
67	V3	0.11	0/365	0.27	0/493
All	All	0.14	0/115736	0.29	2/157010 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	S1	364	ASP	CA-C-N	-5.03	114.77	122.21
57	S1	364	ASP	C-N-CA	-5.03	114.77	122.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4L	748	0	799	23	0
2	5A	825	0	823	12	0
3	5B	724	0	705	15	0
4	6A	620	0	589	16	0
5	6B	684	0	649	12	0
6	6C	574	0	590	7	0
7	7A	447	0	443	13	0
8	7B	392	0	372	4	0
9	7C	387	0	385	13	0
10	8B	338	0	342	6	0
11	A1	562	0	557	9	0
12	A2	686	0	699	8	0
13	A3	643	0	642	5	0
14	A5	910	0	950	8	0
15	A6	967	0	972	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A7	780	0	808	9	0
17	A8	1398	0	1372	20	0
18	A9	2743	0	2762	33	0
19	AB	624	0	625	10	0
19	AC	702	0	694	9	0
20	AK	2601	0	2566	28	0
21	AL	1021	0	1025	13	0
22	AM	1204	0	1162	15	0
23	AN	1173	0	1166	20	0
24	B1	479	0	486	8	0
25	B2	584	0	529	10	0
26	B3	641	0	620	8	0
27	B4	1062	0	1072	7	0
28	B5	1151	0	1164	13	0
29	B6	882	0	899	20	0
30	B7	1068	0	1043	22	0
31	B8	1315	0	1208	11	0
32	B9	1534	0	1470	21	0
33	BK	1456	0	1426	23	0
34	BL	828	0	788	8	0
35	C1	4024	0	4005	82	0
36	C2	1833	0	1843	45	0
37	C3	2103	0	2034	50	0
38	C4	1153	0	1130	20	0
39	CA	417	0	422	4	0
40	CB	1000	0	994	13	0
41	N1	2508	0	2607	60	0
42	N2	2710	0	2874	46	0
43	N3	914	0	951	18	0
44	N4	3631	0	3839	55	0
45	N5	4785	0	4933	98	0
46	N6	1329	0	1326	31	0
47	QA	3147	0	3129	40	0
47	Qa	3147	0	3129	40	0
48	QB	3459	0	3350	45	0
48	Qb	3367	0	3262	34	0
49	QC	3025	0	3090	38	0
49	Qc	3025	0	3090	35	0
50	QD	1921	0	1867	26	0
50	Qd	1904	0	1849	32	0
51	QE	1517	0	1500	33	0
51	QK	520	0	554	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	Qe	1517	0	1500	21	0
52	QF	552	0	536	7	0
52	Qf	528	0	510	6	0
53	QG	893	0	888	8	0
53	Qg	893	0	888	10	0
54	QH	662	0	660	12	0
54	Qh	666	0	663	9	0
55	QI	507	0	509	5	0
55	Qi	493	0	491	5	0
56	QJ	405	0	405	6	0
56	Qj	421	0	418	5	0
57	S1	5290	0	5321	92	0
58	S2	3459	0	3396	68	0
59	S3	1738	0	1693	18	0
60	S4	1007	0	1008	17	0
61	S5	867	0	871	9	0
62	S6	741	0	701	7	0
63	S7	1248	0	1254	31	0
64	S8	1412	0	1363	30	0
65	V1	3316	0	3272	56	0
66	V2	1671	0	1673	20	0
67	V3	355	0	329	10	0
68	4L	92	0	137	8	0
68	7A	91	0	132	6	0
68	A7	51	0	46	1	0
68	A8	83	0	113	7	0
68	AK	68	0	80	3	0
68	AL	94	0	138	7	0
68	B4	80	0	107	4	0
68	B5	100	0	156	6	0
68	C3	170	0	240	7	0
68	CB	100	0	156	4	0
68	N1	78	0	103	4	0
68	N4	62	0	68	2	0
68	N5	189	0	284	15	0
68	QB	64	0	72	3	0
68	QC	55	0	54	2	0
68	QD	64	0	72	1	0
68	QH	125	0	138	7	0
68	Qb	64	0	72	2	0
69	5B	1	0	0	0	0
69	S6	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	6A	45	0	64	11	0
70	C1	183	0	274	14	0
70	C3	190	0	291	13	0
70	N1	48	0	73	3	0
70	N3	54	0	88	1	0
70	QB	51	0	79	2	0
70	Qb	48	0	73	2	0
70	Qc	54	0	88	4	0
70	Qh	54	0	88	1	0
71	6C	43	0	67	1	0
71	AL	47	0	75	2	0
71	AM	51	0	83	6	0
71	B1	52	0	88	1	0
71	CB	52	0	88	3	0
71	N4	49	0	79	4	0
71	N6	52	0	88	1	0
71	QI	52	0	88	2	0
71	Qi	46	0	73	5	0
71	S7	52	0	88	6	0
72	7A	43	0	60	6	0
72	B8	32	0	38	0	0
72	C1	85	0	124	1	0
72	CA	51	0	82	1	0
72	CB	46	0	69	1	0
72	N5	46	0	69	1	0
72	QE	44	0	65	1	0
72	QJ	34	0	42	1	0
72	Qc	48	0	73	2	0
72	Qj	29	0	32	0	0
72	S7	51	0	82	2	0
73	7C	51	0	82	5	0
73	A9	39	0	52	4	0
73	N1	31	0	36	0	0
73	N3	51	0	82	4	0
73	N4	49	0	75	5	0
73	N5	137	0	205	4	0
73	QB	34	0	42	1	0
73	QC	40	0	54	1	0
73	QE	47	0	71	2	0
73	Qc	42	0	61	1	0
73	Qe	75	0	104	8	0
73	S2	48	0	73	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	S8	51	0	82	7	0
74	A9	48	0	26	1	0
75	AB	36	0	47	2	0
75	AC	36	0	47	4	0
76	AK	27	0	12	3	0
77	C1	120	0	108	18	0
78	C1	1	0	0	0	0
78	C2	2	0	0	0	0
79	C1	1	0	0	0	0
79	S1	1	0	0	0	0
80	QC	86	0	60	8	0
80	Qc	86	0	60	7	0
81	QD	43	0	30	2	0
81	Qd	43	0	32	4	0
82	QE	4	0	0	2	0
82	Qe	4	0	0	2	0
82	S1	4	0	0	0	0
82	V2	4	0	0	0	0
83	S1	16	0	0	1	0
83	S7	8	0	0	1	0
83	S8	16	0	0	1	0
83	V1	8	0	0	0	0
84	S2	9	0	0	0	0
85	S7	63	0	90	6	0
86	V1	31	0	19	1	0
All	All	117589	0	118918	1583	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 7.

All (1583) 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)
33:BK:140:GLN:O	33:BK:144:SER:HB2	1.73	0.88
1:4L:37:MET:HG2	1:4L:67:ALA:HB2	1.62	0.81
49:QC:98:VAL:HG22	80:QC:402:HEM:HBC2	1.64	0.80
49:QC:237:LEU:HB2	50:QD:297:MET:HE2	1.64	0.80
68:4L:201:CDL:H521	46:N6:88:THR:HG23	1.65	0.78
29:B6:88:LEU:HD22	29:B6:92:GLU:HG2	1.64	0.78
49:Qc:98:VAL:HG22	80:Qc:403:HEM:HBC2	1.66	0.77
21:AL:140:LYS:H	42:N2:273:ASN:HD22	1.32	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:S2:272:ARG:HH11	73:S8:303:PEE:H2	1.52	0.74
57:S1:149:ASP:HB2	58:S2:367:ALA:HB3	1.68	0.74
26:B3:27:THR:HG22	26:B3:29:LEU:H	1.53	0.74
35:C1:447:TYR:O	35:C1:451:ASN:ND2	2.21	0.73
20:AK:120:TYR:HH	76:AK:401:ADP:HO2'	1.30	0.73
42:N2:88:LYS:HG3	42:N2:148:SER:HB3	1.68	0.73
1:4L:68:ALA:HB3	43:N3:67:LEU:HD11	1.69	0.73
66:V2:68:LYS:NZ	67:V3:407:SER:OG	2.22	0.72
30:B7:29:TYR:O	30:B7:104:ARG:NH2	2.23	0.71
36:C2:104:TRP:HA	36:C2:207:MET:HG2	1.73	0.71
45:N5:5:ALA:HB2	45:N5:61:MET:HE1	1.72	0.71
37:C3:129:VAL:HG11	37:C3:180:GLU:HG3	1.71	0.70
47:Qa:81:HIS:HD2	47:Qa:192:CYS:H	1.37	0.70
57:S1:124:HIS:HD2	58:S2:381:MET:HE2	1.57	0.70
47:Qa:155:GLN:HE22	47:Qa:200:VAL:HB	1.57	0.69
68:7A:102:CDL:H421	73:7C:101:PEE:H31	1.74	0.69
49:Qc:138:MET:HG2	49:Qc:254:ASP:HB2	1.75	0.69
5:6B:9:ILE:HG12	5:6B:56:TRP:HB2	1.75	0.69
12:A2:24:CYS:N	12:A2:58:CYS:SG	2.66	0.69
36:C2:132:GLU:HB3	36:C2:137:GLU:HG3	1.72	0.69
68:N5:703:CDL:H591	68:N5:703:CDL:H642	1.75	0.69
57:S1:493:VAL:HG23	57:S1:513:MET:HE1	1.75	0.69
1:4L:14:ILE:HG12	68:4L:201:CDL:H781	1.75	0.68
8:7B:53:TRP:HE1	38:C4:111:ILE:HG22	1.58	0.68
18:A9:188:GLU:HG3	18:A9:200:ILE:HD13	1.76	0.68
18:A9:212:ARG:NH1	18:A9:311:GLU:OE2	2.27	0.68
19:AC:114:ASP:OD1	32:B9:87:ARG:NH2	2.26	0.68
49:QC:246:SER:HB2	49:QC:249:LEU:HB2	1.75	0.68
20:AK:141:ARG:NH2	76:AK:401:ADP:N7	2.41	0.68
48:QB:100:GLY:HA2	48:QB:106:GLY:H	1.59	0.68
50:QD:266:GLN:HE22	52:Qf:91:LYS:H	1.42	0.68
57:S1:419:ARG:NH1	57:S1:439:THR:O	2.26	0.67
35:C1:107:PRO:HB3	37:C3:25:LEU:HB2	1.75	0.67
18:A9:173:ASP:HB3	18:A9:176:SER:HB2	1.75	0.67
43:N3:37:TYR:OH	58:S2:93:GLN:NE2	2.27	0.67
44:N4:391:ILE:HG23	44:N4:394:ILE:HD12	1.76	0.67
15:A6:42:SER:HB3	60:S4:52:LEU:HB3	1.75	0.67
45:N5:100:ILE:HG21	45:N5:246:LEU:HB2	1.77	0.67
63:S7:188:LYS:HB2	63:S7:191:ARG:HB2	1.74	0.67
47:Qa:155:GLN:NE2	47:Qa:200:VAL:O	2.27	0.67
51:Qe:190:VAL:HG21	51:Qe:250:ARG:HH22	1.59	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:A8:301:CDL:H112	40:CB:32:ARG:HG2	1.76	0.67
33:BK:2:PRO:O	33:BK:7:LYS:NZ	2.28	0.67
3:5B:113:CYS:HB3	3:5B:118:THR:HG22	1.76	0.66
65:V1:40:ARG:NH1	65:V1:289:GLU:O	2.27	0.66
44:N4:371:PRO:HD2	68:N5:703:CDL:H391	1.77	0.66
41:N1:102:VAL:HG11	41:N1:154:LEU:HD11	1.76	0.66
41:N1:141:SER:HB2	41:N1:289:LEU:HD12	1.78	0.66
42:N2:108:LEU:HD11	42:N2:191:THR:HG21	1.76	0.66
50:Qd:125:CYS:SG	81:Qd:401:HEC:HAC	2.35	0.66
13:A3:151:VAL:O	17:A8:207:LYS:NZ	2.27	0.66
15:A6:89:VAL:HG22	75:AB:201:ZMP:H2	1.76	0.66
57:S1:266:ARG:HD2	57:S1:267:THR:HG23	1.77	0.66
50:QD:280:GLU:OE2	50:QD:286:ARG:NH1	2.28	0.66
75:AC:201:ZMP:H14	32:B9:102:ALA:HB1	1.77	0.66
45:N5:126:ILE:HG21	68:N5:703:CDL:H621	1.77	0.66
51:QK:24:GLY:HA3	47:Qa:109:LYS:HE3	1.76	0.66
58:S2:300:ARG:NH2	58:S2:407:GLU:OE2	2.29	0.66
65:V1:235:VAL:HG12	65:V1:240:THR:HG21	1.78	0.66
12:A2:59:SER:HB2	57:S1:655:ARG:HD3	1.78	0.66
20:AK:66:GLY:O	20:AK:163:ARG:NH2	2.29	0.65
15:A6:66:TYR:O	15:A6:86:ARG:NH1	2.29	0.65
49:QC:316:MET:HE3	73:QC:403:PEE:H11	1.79	0.65
57:S1:433:GLY:HA2	57:S1:447:ASP:HA	1.78	0.65
21:AL:140:LYS:O	42:N2:273:ASN:ND2	2.30	0.65
36:C2:89:GLU:O	36:C2:91:ASN:ND2	2.30	0.65
70:6A:101:PC1:H321	37:C3:202:GLY:HA3	1.77	0.65
27:B4:15:PRO:HG2	27:B4:18:LEU:HB2	1.78	0.65
52:QF:56:ARG:NH1	52:QF:65:GLU:OE2	2.29	0.65
72:C1:609:3PE:H372	72:C1:609:3PE:H282	1.77	0.64
58:S2:374:ARG:NH2	64:S8:165:ASP:OD1	2.29	0.64
9:7C:42:THR:HG21	10:8B:45:VAL:HG12	1.79	0.64
18:A9:346:GLU:HG2	18:A9:371:PRO:HB3	1.80	0.64
2:5A:114:VAL:HG11	2:5A:128:VAL:HG11	1.79	0.64
65:V1:112:TYR:HB2	65:V1:240:THR:HG22	1.79	0.64
41:N1:58:LYS:HE2	63:S7:125:PRO:HG2	1.80	0.64
47:Qa:82:LEU:HD11	47:Qa:154:LEU:HB3	1.80	0.63
35:C1:51:ASP:O	35:C1:55:ASN:ND2	2.31	0.63
57:S1:250:SER:HB2	57:S1:606:THR:HG23	1.80	0.63
65:V1:111:LYS:HB2	65:V1:151:ALA:HA	1.78	0.63
4:6A:81:LEU:HB3	70:6A:101:PC1:H12	1.80	0.63
15:A6:88:LYS:NZ	15:A6:132:PHE:O	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:QC:214:ASP:OD1	54:Qh:3:ARG:NH2	2.31	0.63
70:6A:101:PC1:H112	37:C3:187:THR:HA	1.81	0.63
6:6C:69:GLY:HA3	8:7B:79:GLU:HG3	1.78	0.63
35:C1:129:TYR:OH	35:C1:236:TRP:NE1	2.31	0.63
52:Qf:60:ARG:NH1	54:Qh:78:TYR:O	2.31	0.63
57:S1:308:ARG:NH1	57:S1:312:GLY:O	2.31	0.63
33:BK:107:GLN:HE22	45:N5:194:ASN:HD22	1.46	0.63
41:N1:173:TRP:HB3	41:N1:175:ILE:HG22	1.80	0.63
22:AM:106:ARG:HB2	22:AM:109:ILE:HG13	1.81	0.63
44:N4:369:LEU:HD21	45:N5:149:ILE:HD13	1.81	0.63
59:S3:89:HIS:ND1	59:S3:91:ASP:OD1	2.26	0.62
15:A6:78:LEU:HD22	15:A6:130:MET:HE3	1.81	0.62
38:C4:41:ARG:NH1	38:C4:43:ASP:OD1	2.32	0.62
47:QA:121:TYR:HB3	47:QA:137:LEU:HD11	1.81	0.62
47:Qa:81:HIS:CD2	47:Qa:192:CYS:H	2.17	0.62
59:S3:187:ILE:HG23	59:S3:188:LEU:HG	1.80	0.62
65:V1:94:PRO:HB2	65:V1:97:LEU:HB2	1.82	0.62
18:A9:61:ALA:HB3	18:A9:82:VAL:HG13	1.82	0.62
29:B6:85:ASP:OD2	32:B9:167:TRP:NE1	2.27	0.62
70:C1:605:PC1:H241	70:C3:301:PC1:H241	1.82	0.62
58:S2:61:THR:H	58:S2:64:THR:HG1	1.47	0.62
36:C2:116:LEU:HD11	36:C2:226:MET:HB3	1.81	0.62
59:S3:83:GLU:OE1	59:S3:142:ARG:NH2	2.30	0.62
37:C3:178:ALA:HB2	70:C3:306:PC1:H2B2	1.81	0.62
45:N5:295:GLN:O	45:N5:425:ARG:NH1	2.33	0.62
57:S1:246:ARG:HH22	60:S4:123:ASN:HD21	1.48	0.62
60:S4:109:ASN:ND2	60:S4:111:LEU:O	2.33	0.62
35:C1:27:GLY:HA3	77:C1:601:HEA:H273	1.82	0.61
58:S2:90:PHE:HB3	58:S2:103:LEU:HB3	1.82	0.61
30:B7:92:HIS:ND1	45:N5:481:THR:OG1	2.29	0.61
44:N4:87:GLU:O	44:N4:92:LYS:NZ	2.28	0.61
47:Qa:84:ARG:NH1	47:Qa:114:SER:OG	2.32	0.61
18:A9:87:GLU:HG3	18:A9:89:TYR:H	1.65	0.61
36:C2:173:ASP:O	36:C2:180:ASN:ND2	2.32	0.61
58:S2:155:GLN:NE2	58:S2:315:ASP:OD2	2.28	0.61
65:V1:110:PRO:HB3	65:V1:152:ARG:HD3	1.81	0.61
24:B1:57:TRP:NE1	28:B5:134:GLU:OE1	2.25	0.61
47:Qa:70:ARG:HD2	47:Qa:117:GLU:HG2	1.83	0.61
58:S2:188:ASN:OD1	58:S2:410:LYS:NZ	2.29	0.61
41:N1:87:VAL:HG11	43:N3:6:THR:HG21	1.80	0.61
48:QB:411:GLU:OE2	48:QB:415:ARG:NH2	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:S8:63:TRP:HE1	73:S8:303:PEE:H13	1.64	0.61
65:V1:109:ARG:NH1	65:V1:237:GLY:O	2.33	0.61
3:5B:89:VAL:HG22	35:C1:510:TYR:HB3	1.83	0.61
9:7C:62:LYS:NZ	35:C1:117:MET:O	2.33	0.61
43:N3:68:GLU:HG3	43:N3:98:LEU:HD13	1.82	0.61
49:Qc:137:GLN:NE2	49:Qc:263:ASN:O	2.33	0.61
57:S1:161:GLU:OE2	66:V2:42:ARG:NH1	2.33	0.61
49:Qc:284:ILE:HD11	70:Qc:405:PC1:H241	1.83	0.61
58:S2:222:ARG:NH1	58:S2:249:ASP:OD2	2.23	0.61
66:V2:38:LEU:O	66:V2:124:ARG:NH2	2.34	0.61
66:V2:108:PRO:HB2	66:V2:111:ARG:HG2	1.82	0.61
1:4L:31:LEU:HD21	46:N6:67:VAL:HG11	1.81	0.61
34:BL:95:PHE:O	34:BL:99:LEU:HB2	2.01	0.61
35:C1:51:ASP:OD1	35:C1:55:ASN:ND2	2.34	0.61
48:QB:374:GLY:HA3	70:QB:503:PC1:H151	1.83	0.61
49:QC:233:LEU:HG	50:QD:297:MET:HE1	1.83	0.61
41:N1:99:ASN:N	70:N1:402:PC1:O12	2.26	0.60
41:N1:103:LEU:HD13	46:N6:55:MET:HE3	1.83	0.60
50:Qd:147:LYS:NZ	50:Qd:151:GLU:OE2	2.34	0.60
22:AM:34:ARG:NH2	64:S8:89:GLU:OE2	2.34	0.60
43:N3:70:ALA:HB2	46:N6:59:ILE:HD11	1.82	0.60
49:QC:71:ARG:NH2	50:QD:278:ALA:O	2.34	0.60
35:C1:155:VAL:HG11	70:C1:610:PC1:H3B1	1.83	0.60
35:C1:169:ILE:O	35:C1:172:LYS:NZ	2.34	0.60
51:QE:177:ARG:HH12	51:QE:233:GLY:HA2	1.65	0.60
49:Qc:100:ARG:NH2	80:Qc:403:HEM:O1A	2.34	0.60
51:Qe:204:ARG:NH2	51:Qe:258:LEU:O	2.27	0.60
65:V1:52:ARG:HH21	67:V3:390:GLN:HG2	1.66	0.60
65:V1:263:ALA:HA	65:V1:271:SER:HB3	1.84	0.60
48:Qb:121:ASN:ND2	48:Qb:132:TYR:OH	2.35	0.60
70:C1:608:PC1:H391	70:C1:608:PC1:H2A2	1.84	0.60
9:7C:59:GLN:NE2	35:C1:116:SER:O	2.34	0.60
37:C3:220:LEU:HG	68:C3:304:CDL:H751	1.84	0.60
5:6B:66:PRO:HD3	36:C2:179:LEU:HD11	1.84	0.60
41:N1:34:ARG:HG2	63:S7:82:PRO:HA	1.83	0.60
51:QE:207:LYS:HE3	51:QE:210:TRP:HD1	1.66	0.60
3:5B:43:GLN:NE2	37:C3:225:PHE:O	2.27	0.60
66:V2:187:GLN:HE21	66:V2:190:ASP:HA	1.66	0.60
1:4L:65:VAL:HA	43:N3:67:LEU:HD22	1.84	0.59
44:N4:403:THR:HA	44:N4:406:TYR:CE2	2.37	0.59
47:QA:399:GLN:HA	47:QA:402:VAL:HG22	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6B:7:THR:O	5:6B:11:ASN:ND2	2.35	0.59
12:A2:89:ARG:O	12:A2:93:ASN:ND2	2.35	0.59
29:B6:132:VAL:O	29:B6:136:LEU:HB3	2.02	0.59
72:7A:101:3PE:H292	45:N5:484:LEU:HD23	1.83	0.59
51:Qe:187:GLU:OE1	51:Qe:248:ARG:NH2	2.35	0.59
73:7C:101:PEE:H38	35:C1:22:PHE:HD1	1.67	0.59
19:AB:116:VAL:HG12	19:AB:120:MET:HE2	1.84	0.59
70:N3:202:PC1:H151	72:S7:204:3PE:H31	1.84	0.59
50:QD:216:LEU:HB3	50:QD:249:ILE:HD11	1.84	0.59
51:QE:234:TYR:HB2	51:QE:243:TYR:HB2	1.84	0.59
48:Qb:276:ARG:NH2	48:Qb:466:PRO:O	2.35	0.59
20:AK:109:GLN:OE1	20:AK:328:ARG:NH1	2.34	0.59
42:N2:42:PRO:HG2	46:N6:167:VAL:HG22	1.84	0.59
42:N2:289:ASN:HA	42:N2:292:PHE:CE2	2.38	0.59
44:N4:231:LEU:HD23	44:N4:235:LEU:HD12	1.85	0.59
57:S1:69:LEU:O	60:S4:158:LYS:NZ	2.32	0.59
66:V2:85:LEU:HD13	67:V3:400:LEU:HD22	1.83	0.59
35:C1:347:LEU:HD13	35:C1:383:MET:HB3	1.83	0.59
44:N4:447:LEU:HD11	71:N4:502:PLX:H381	1.85	0.59
47:QA:84:ARG:NH2	47:QA:190:LEU:O	2.33	0.59
44:N4:445:LEU:HD22	68:N5:703:CDL:H401	1.84	0.59
33:BK:60:ARG:NH1	33:BK:62:TYR:OH	2.35	0.59
68:C3:304:CDL:H231	68:C3:304:CDL:H352	1.84	0.59
35:C1:254:ILE:HD12	35:C1:341:ALA:HA	1.85	0.58
58:S2:162:GLU:OE2	58:S2:177:ARG:NH2	2.34	0.58
64:S8:205:ILE:O	64:S8:209:TYR:HB3	2.02	0.58
48:QB:165:ARG:NH1	48:QB:208:VAL:O	2.36	0.58
49:Qc:119:LEU:HD13	80:Qc:403:HEM:HBB2	1.85	0.58
57:S1:405:THR:HB	57:S1:477:GLY:HA3	1.84	0.58
65:V1:296:LEU:HD21	65:V1:317:VAL:HG11	1.85	0.58
34:BL:150:PRO:HG3	40:CB:115:LEU:HD22	1.85	0.58
35:C1:406:ASN:ND2	70:C1:608:PC1:O14	2.36	0.58
57:S1:488:ALA:HB2	57:S1:677:GLN:HG3	1.85	0.58
57:S1:666:GLN:NE2	57:S1:670:GLU:OE2	2.36	0.58
25:B2:57:ARG:NH1	25:B2:61:PHE:O	2.36	0.58
50:QD:105:SER:OG	55:Qi:44:TYR:OH	2.21	0.58
54:QH:37:ASN:ND2	68:QH:102:CDL:OB4	2.35	0.58
65:V1:118:ASP:HB3	65:V1:207:GLY:HA2	1.85	0.58
10:8B:36:PRO:HB3	70:C1:608:PC1:H261	1.84	0.58
53:QG:36:ASP:OD1	53:QG:90:TYR:OH	2.16	0.58
58:S2:308:LEU:HB2	58:S2:407:GLU:HB2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:S7:85:ASP:HB3	63:S7:88:ARG:HB3	1.86	0.58
65:V1:338:ASP:OD1	65:V1:339:PHE:N	2.37	0.58
21:AL:140:LYS:H	42:N2:273:ASN:ND2	2.01	0.58
37:C3:204:HIS:CE1	37:C3:249:TRP:HB2	2.39	0.58
49:QC:207:ASN:OD1	49:QC:209:THR:OG1	2.21	0.58
57:S1:198:THR:HG21	57:S1:209:TYR:HB2	1.85	0.58
42:N2:170:LEU:HD11	42:N2:288:LEU:HD22	1.86	0.57
48:QB:195:THR:HG21	48:QB:269:ARG:H	1.68	0.57
44:N4:392:THR:O	44:N4:396:MET:HG2	2.04	0.57
48:QB:478:LEU:HB3	68:QB:501:CDL:H522	1.86	0.57
49:QC:236:MET:HE3	71:Qi:301:PLX:H202	1.86	0.57
57:S1:534:VAL:HG22	57:S1:537:ILE:HB	1.85	0.57
18:A9:279:TYR:HB2	18:A9:372:ALA:HB2	1.86	0.57
45:N5:249:SER:HA	45:N5:306:THR:HG21	1.85	0.57
47:QA:151:VAL:O	47:QA:155:GLN:HG2	2.05	0.57
48:QB:301:ASN:ND2	48:QB:347:CYS:SG	2.78	0.57
57:S1:282:ASN:ND2	57:S1:285:TRP:O	2.37	0.57
45:N5:362:LEU:HA	45:N5:365:ALA:HB3	1.85	0.57
68:N5:703:CDL:H541	68:N5:703:CDL:HA4	1.86	0.57
48:QB:113:VAL:HG12	48:QB:146:LEU:HD13	1.85	0.57
50:QD:104:SER:HA	55:Qi:48:ASN:HD21	1.68	0.57
71:QI:301:PLX:H341	56:QJ:31:GLY:HA3	1.85	0.57
65:V1:113:LEU:O	65:V1:154:ALA:HA	2.05	0.57
14:A5:48:THR:HA	14:A5:51:ILE:HG12	1.86	0.57
40:CB:52:ARG:NH1	42:N2:318:GLU:OE1	2.37	0.57
44:N4:383:THR:HG21	45:N5:190:LEU:HD22	1.86	0.57
70:6A:101:PC1:H142	37:C3:181:TYR:O	2.05	0.57
47:Qa:151:VAL:O	47:Qa:155:GLN:HG2	2.05	0.57
48:Qb:360:CYS:SG	48:Qb:368:MET:HG3	2.45	0.57
60:S4:75:ARG:NH1	60:S4:119:ASP:OD1	2.35	0.57
11:A1:46:ASN:ND2	46:N6:132:ASP:OD2	2.38	0.57
15:A6:81:SER:OG	18:A9:367:GLU:OE2	2.22	0.57
48:QB:121:ASN:ND2	48:QB:132:TYR:OH	2.38	0.57
50:Qd:118:TYR:HA	50:Qd:122:CYS:SG	2.45	0.57
65:V1:112:TYR:O	65:V1:240:THR:HA	2.05	0.57
7:7A:66:TYR:HE1	72:7A:101:3PE:H2A2	1.68	0.57
41:N1:197:PRO:HB2	41:N1:280:PHE:HD1	1.70	0.57
73:N4:501:PEE:H46	73:S2:501:PEE:H37	1.87	0.57
53:Qg:14:LEU:HD12	53:Qg:17:ILE:HD11	1.86	0.57
66:V2:182:ASN:HB3	66:V2:194:GLU:HB3	1.86	0.57
44:N4:445:LEU:HB3	68:N5:703:CDL:H452	1.85	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:N5:419:THR:HA	45:N5:422:TYR:CE2	2.40	0.56
49:Qc:285:PRO:HG2	70:Qc:405:PC1:H3E2	1.87	0.56
63:S7:86:MET:HB2	63:S7:91:VAL:HB	1.87	0.56
3:5B:105:VAL:HA	3:5B:111:GLN:HG3	1.87	0.56
37:C3:58:TRP:HD1	37:C3:61:ILE:HD12	1.70	0.56
38:C4:90:PHE:HA	38:C4:93:MET:HG2	1.87	0.56
73:N5:701:PEE:H36	68:N5:703:CDL:H231	1.87	0.56
51:Qe:196:ARG:NH1	51:Qe:254:ALA:O	2.39	0.56
58:S2:140:PRO:HB2	63:S7:142:TYR:CE2	2.40	0.56
58:S2:464:PHE:HA	58:S2:467:VAL:HB	1.86	0.56
60:S4:112:MET:HG3	64:S8:184:LEU:HD23	1.87	0.56
63:S7:66:THR:HG22	85:S7:201:U10:H3M2	1.87	0.56
9:7C:31:VAL:HG13	9:7C:37:LEU:HD22	1.87	0.56
17:A8:146:ASP:OD1	17:A8:149:ARG:NH2	2.38	0.56
22:AM:88:ARG:HD3	64:S8:200:GLU:HG3	1.86	0.56
70:N1:402:PC1:H112	70:N1:402:PC1:H32	1.87	0.56
51:QE:160:PRO:HD2	51:QE:163:LYS:HG2	1.87	0.56
47:Qa:91:THR:HG21	47:Qa:140:VAL:HA	1.86	0.56
30:B7:29:TYR:OH	30:B7:111:ARG:NH2	2.36	0.56
42:N2:112:HIS:O	42:N2:116:PRO:HD2	2.05	0.56
42:N2:131:LEU:O	42:N2:135:LYS:HG2	2.06	0.56
44:N4:211:GLY:H	44:N4:213:HIS:HD2	1.52	0.56
57:S1:49:VAL:HG13	57:S1:102:ILE:HD13	1.87	0.56
58:S2:140:PRO:HA	58:S2:143:ASP:HB2	1.88	0.56
59:S3:128:ILE:HB	59:S3:145:THR:HG23	1.87	0.56
51:QK:1:MET:O	51:QK:7:ARG:NH1	2.38	0.56
51:Qe:244:ASP:OD2	51:Qe:250:ARG:NH2	2.39	0.56
29:B6:165:PHE:O	29:B6:168:ASP:HB2	2.05	0.56
68:N1:401:CDL:H791	46:N6:16:GLY:HA2	1.88	0.56
47:QA:148:ARG:NH2	53:QG:50:ARG:O	2.38	0.56
47:Qa:320:PRO:HG2	47:Qa:343:GLN:HE21	1.71	0.56
48:Qb:366:ASP:H	48:Qb:464:GLN:HE21	1.53	0.56
52:Qf:38:GLU:OE2	52:Qf:78:ARG:NH1	2.39	0.56
23:AN:51:MET:HE2	41:N1:311:THR:HB	1.87	0.56
33:BK:114:GLN:HG3	45:N5:203:MET:HG2	1.87	0.56
55:QI:48:ASN:HD21	50:Qd:104:SER:HA	1.71	0.56
57:S1:389:THR:OG1	57:S1:511:LYS:O	2.23	0.56
42:N2:142:LEU:HB3	42:N2:194:LEU:HD21	1.87	0.56
57:S1:433:GLY:O	57:S1:444:HIS:NE2	2.34	0.56
35:C1:358:LEU:HB3	77:C1:602:HEA:HMA	1.87	0.56
4:6A:82:PHE:O	70:6A:101:PC1:H143	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:A8:301:CDL:H572	68:A8:301:CDL:H532	1.88	0.55
68:A8:301:CDL:H782	72:CB:202:3PE:H281	1.87	0.55
36:C2:151:ARG:HG3	36:C2:181:GLN:HG3	1.89	0.55
48:QB:80:ARG:NH2	48:QB:350:GLU:OE1	2.39	0.55
47:Qa:164:VAL:HG21	48:Qb:317:THR:HG21	1.88	0.55
57:S1:163:LYS:O	57:S1:171:THR:OG1	2.25	0.55
23:AN:144:THR:HB	41:N1:96:ILE:HG23	1.89	0.55
36:C2:189:PRO:HA	36:C2:213:LEU:HB2	1.87	0.55
47:Qa:260:ASP:OD2	47:Qa:262:ASN:ND2	2.39	0.55
35:C1:197:LEU:HA	37:C3:92:LEU:HD13	1.88	0.55
35:C1:383:MET:HE3	35:C1:421:VAL:HG23	1.89	0.55
49:Qc:353:LEU:HD12	72:Qc:404:3PE:H351	1.88	0.55
51:Qe:239:HIS:HB2	82:Qe:303:FES:S2	2.46	0.55
64:S8:47:SER:O	64:S8:56:ARG:NH2	2.40	0.55
64:S8:100:GLU:OE1	64:S8:172:ASN:ND2	2.37	0.55
57:S1:191:GLY:HA3	57:S1:439:THR:HB	1.89	0.55
6:6C:60:LYS:NZ	6:6C:64:GLU:OE2	2.30	0.55
45:N5:6:SER:O	45:N5:10:THR:OG1	2.19	0.55
45:N5:331:MET:HB3	45:N5:387:THR:HG22	1.89	0.55
54:Qh:49:VAL:HG12	70:Qh:101:PC1:H131	1.88	0.55
57:S1:688:GLN:HE21	57:S1:694:PHE:HA	1.71	0.55
12:A2:65:LEU:HD11	12:A2:91:LEU:HD13	1.89	0.55
35:C1:264:LYS:NZ	35:C1:326:THR:O	2.36	0.55
50:Qd:211:TYR:OH	81:Qd:401:HEC:O1A	2.15	0.55
63:S7:62:LEU:O	63:S7:91:VAL:HA	2.06	0.55
37:C3:16:TRP:NE1	37:C3:60:ASP:OD2	2.35	0.55
42:N2:36:ASN:OD1	42:N2:134:GLN:NE2	2.29	0.55
49:QC:197:LEU:HD11	80:QC:402:HEM:HMA3	1.89	0.55
48:Qb:274:GLU:HG3	48:Qb:456:VAL:HB	1.88	0.55
58:S2:101:LEU:HB2	58:S2:464:PHE:CZ	2.42	0.55
63:S7:55:ASN:ND2	63:S7:187:GLU:O	2.35	0.55
20:AK:82:LYS:HZ2	20:AK:268:ALA:HB3	1.72	0.55
50:QD:228:LEU:HD11	50:QD:234:PHE:HB2	1.89	0.55
58:S2:146:ASP:OD2	58:S2:149:SER:OG	2.24	0.54
65:V1:295:PRO:HG2	65:V1:298:GLU:HB2	1.90	0.54
41:N1:123:SER:HB3	41:N1:214:GLU:HG3	1.89	0.54
49:QC:362:ILE:HG23	49:QC:366:MET:HE2	1.87	0.54
57:S1:484:SER:HB2	57:S1:680:LEU:HD11	1.88	0.54
18:A9:212:ARG:O	18:A9:216:TYR:N	2.32	0.54
22:AM:78:ASP:OD1	22:AM:78:ASP:N	2.37	0.54
41:N1:134:ARG:NH2	58:S2:110:GLU:OE2	2.36	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5B:46:GLY:HA3	37:C3:69:GLY:HA3	1.88	0.54
5:6B:24:GLN:OE1	35:C1:302:ARG:NH1	2.41	0.54
35:C1:508:PRO:HG3	37:C3:6:HIS:HB3	1.88	0.54
47:QA:233:VAL:HG22	47:QA:236:ARG:HH12	1.72	0.54
48:Qb:422:ARG:NH2	48:Qb:428:GLU:OE1	2.39	0.54
49:Qc:332:LEU:HD11	73:Qc:401:PEE:H44	1.90	0.54
57:S1:340:ALA:HB3	57:S1:366:LEU:HD23	1.90	0.54
58:S2:137:GLN:O	63:S7:142:TYR:OH	2.26	0.54
14:A5:44:TYR:O	14:A5:48:THR:HG22	2.08	0.54
48:Qb:388:VAL:HG21	48:Qb:438:ALA:HA	1.88	0.54
50:Qd:122:CYS:SG	81:Qd:401:HEC:HAB	2.47	0.54
19:AB:82:ARG:HH21	19:AB:125:GLU:HG3	1.72	0.54
41:N1:31:MET:HG2	64:S8:77:LEU:HB2	1.90	0.54
51:QE:187:GLU:OE1	51:QE:248:ARG:NH2	2.40	0.54
20:AK:145:TYR:OH	20:AK:201:LEU:O	2.18	0.54
22:AM:55:PHE:CZ	22:AM:58:ARG:HG3	2.43	0.54
54:QH:37:ASN:OD1	54:QH:40:ARG:NH2	2.36	0.54
57:S1:593:SER:HA	57:S1:606:THR:O	2.07	0.54
36:C2:104:TRP:CG	36:C2:203:ASN:HB2	2.42	0.54
68:Qb:501:CDL:HA32	70:Qb:502:PC1:H151	1.89	0.54
50:Qd:293:MET:HA	73:Qc:302:PEE:H49	1.90	0.54
64:S8:63:TRP:HB3	64:S8:66:LEU:HD12	1.89	0.54
18:A9:206:ILE:HG13	74:A9:401:NDP:H42N	1.90	0.54
20:AK:210:ASP:OD1	20:AK:244:LYS:NZ	2.32	0.54
59:S3:132:LEU:HB2	59:S3:141:ILE:HG22	1.90	0.54
8:7B:71:ARG:HG3	8:7B:72:VAL:HG23	1.89	0.53
35:C1:374:VAL:HA	35:C1:377:PHE:CE2	2.42	0.53
63:S7:69:LEU:HB2	63:S7:107:GLY:HA3	1.89	0.53
35:C1:299:VAL:HG23	36:C2:84:LEU:HG	1.90	0.53
41:N1:288:LEU:HD11	73:S8:303:PEE:H8	1.88	0.53
58:S2:430:ILE:HB	58:S2:469:ARG:HD2	1.90	0.53
45:N5:400:ASN:HB3	45:N5:486:MET:HE3	1.90	0.53
38:C4:115:ALA:HA	38:C4:118:LEU:HD12	1.90	0.53
48:QB:476:PHE:O	73:QB:502:PEE:N	2.41	0.53
58:S2:214:GLU:OE2	58:S2:227:ARG:NH2	2.41	0.53
28:B5:163:ARG:NH1	40:CB:102:ASP:OD2	2.29	0.53
32:B9:143:GLU:O	32:B9:164:ARG:NH2	2.42	0.53
17:A8:219:TYR:OH	28:B5:189:ASN:ND2	2.35	0.53
34:BL:129:ARG:NH1	34:BL:136:LEU:O	2.33	0.53
35:C1:130:PRO:HG3	35:C1:209:LEU:HD13	1.91	0.53
47:QA:60:ARG:NH1	47:QA:124:GLU:OE1	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:QA:70:ARG:HD2	47:QA:117:GLU:HG2	1.91	0.53
50:QD:120:GLN:HB2	50:QD:254:LEU:HD11	1.89	0.53
49:QC:8:HIS:HB3	49:QC:11:MET:HB2	1.90	0.53
70:Qb:502:PC1:H2A2	73:Qe:301:PEE:H76	1.90	0.53
37:C3:126:PRO:HB3	37:C3:257:TYR:HB3	1.91	0.53
45:N5:421:ALA:O	45:N5:424:THR:OG1	2.26	0.53
48:QB:165:ARG:HD3	48:QB:209:ARG:HA	1.91	0.53
19:AC:105:MET:HE3	19:AC:139:MET:HE1	1.89	0.53
34:BL:89:VAL:HG21	44:N4:25:ILE:HG23	1.90	0.53
35:C1:173:PRO:HD2	35:C1:176:MET:HE2	1.90	0.53
37:C3:226:HIS:HE1	70:C3:303:PC1:H3A1	1.72	0.53
38:C4:155:GLY:H	38:C4:158:ALA:HB3	1.74	0.53
68:CB:203:CDL:H422	68:CB:203:CDL:H812	1.90	0.53
48:QB:79:SER:OG	48:QB:201:VAL:HA	2.09	0.53
80:QC:401:HEM:HMC1	80:QC:401:HEM:HBC2	1.91	0.53
47:Qa:68:GLY:O	47:Qa:208:TYR:OH	2.27	0.53
4:6A:68:ARG:NH1	37:C3:189:SER:OG	2.42	0.53
29:B6:85:ASP:O	32:B9:163:LYS:NZ	2.42	0.53
36:C2:161:HIS:HB2	36:C2:174:ALA:HB3	1.91	0.53
45:N5:103:PHE:HB2	45:N5:341:MET:HE3	1.91	0.53
47:Qa:155:GLN:HB3	47:Qa:198:GLY:HA2	1.90	0.53
48:Qb:103:ASN:ND2	48:Qb:149:ASP:OD2	2.40	0.53
7:7A:77:PRO:HG3	9:7C:62:LYS:HG3	1.90	0.52
1:4L:37:MET:HG2	1:4L:67:ALA:CB	2.37	0.52
1:4L:75:LEU:O	1:4L:79:VAL:HG13	2.10	0.52
41:N1:139:THR:HA	41:N1:142:TYR:CE2	2.44	0.52
43:N3:66:ASP:O	43:N3:69:ILE:HG13	2.09	0.52
16:A7:14:TRP:O	23:AN:28:ARG:NH1	2.42	0.52
50:QD:211:TYR:OH	81:QD:401:HEC:O2A	2.19	0.52
57:S1:104:THR:O	57:S1:113:ARG:NH2	2.41	0.52
65:V1:281:HIS:ND1	65:V1:358:ASP:OD1	2.42	0.52
3:5B:106:HIS:NE2	38:C4:34:ALA:O	2.31	0.52
35:C1:86:MET:HB3	35:C1:182:PRO:HG2	1.90	0.52
36:C2:30:ILE:HD13	36:C2:76:ILE:HG12	1.92	0.52
41:N1:174:MET:HB2	41:N1:242:PHE:HA	1.91	0.52
51:QE:209:GLU:HG3	51:QE:210:TRP:CD1	2.44	0.52
29:B6:89:SER:HB2	29:B6:92:GLU:HB2	1.90	0.52
29:B6:143:HIS:CD2	33:BK:45:VAL:HG21	2.44	0.52
47:QA:61:ILE:HG12	47:QA:130:ILE:HD11	1.92	0.52
4:6A:83:HIS:HA	70:6A:101:PC1:H132	1.90	0.52
30:B7:96:VAL:HA	30:B7:99:MET:HE3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:S1:452:LEU:HD21	57:S1:493:VAL:HG13	1.92	0.52
68:4L:201:CDL:H181	45:N5:589:LEU:HD11	1.91	0.52
3:5B:112:ARG:HA	3:5B:118:THR:O	2.09	0.52
28:B5:83:ALA:HA	68:B5:201:CDL:H162	1.90	0.52
36:C2:109:GLU:HG2	36:C2:117:THR:HG23	1.92	0.52
43:N3:79:SER:HA	43:N3:87:MET:HE2	1.91	0.52
44:N4:318:ALA:HB2	44:N4:373:ILE:HG13	1.92	0.52
46:N6:86:ASN:HD22	46:N6:89:VAL:HG23	1.74	0.52
57:S1:347:ASP:OD1	57:S1:347:ASP:N	2.43	0.52
65:V1:311:TRP:NE1	65:V1:333:GLU:OE1	2.38	0.52
10:8B:43:LEU:HD12	70:C1:608:PC1:H2B1	1.91	0.52
77:C1:602:HEA:HHC	77:C1:602:HEA:H122	1.91	0.52
45:N5:248:HIS:O	45:N5:253:VAL:HG22	2.10	0.52
47:QA:323:VAL:HG23	47:QA:340:THR:HG22	1.91	0.52
48:QB:107:SER:HA	48:QB:110:GLU:HG2	1.90	0.52
72:QJ:101:3PE:H322	73:Qe:301:PEE:H49	1.92	0.52
17:A8:107:HIS:HB3	17:A8:197:PRO:HD2	1.92	0.52
29:B6:140:TRP:HD1	33:BK:41:VAL:HG13	1.75	0.52
41:N1:231:ILE:O	41:N1:235:ASN:ND2	2.42	0.52
73:N4:501:PEE:H53	73:N4:501:PEE:H24	1.92	0.52
50:QD:322:TYR:CE2	50:QD:324:PRO:HG3	2.45	0.52
57:S1:456:ALA:O	57:S1:499:ASN:ND2	2.43	0.52
65:V1:364:VAL:HG12	65:V1:400:VAL:HG12	1.92	0.52
18:A9:163:LYS:NZ	18:A9:253:ILE:O	2.37	0.52
35:C1:406:ASN:HB3	35:C1:409:TRP:HB2	1.91	0.52
71:N6:201:PLX:H151	71:N6:201:PLX:H332	1.91	0.52
65:V1:326:LEU:HD22	65:V1:363:ILE:HD11	1.92	0.52
6:6C:45:ARG:NH1	36:C2:25:ASP:OD2	2.42	0.51
44:N4:82:SER:HB2	44:N4:432:ARG:CZ	2.40	0.51
41:N1:24:GLU:HA	41:N1:271:LEU:HD13	1.93	0.51
42:N2:280:THR:HG21	73:N4:501:PEE:H19	1.93	0.51
49:Qc:24:PRO:O	49:Qc:224:TYR:OH	2.16	0.51
65:V1:113:LEU:HD13	65:V1:149:MET:HE1	1.93	0.51
49:QC:300:ILE:HD11	49:QC:363:LEU:HD21	1.93	0.51
35:C1:358:LEU:C	77:C1:602:HEA:HMA	2.36	0.51
47:QA:82:LEU:HD11	47:QA:154:LEU:HB3	1.92	0.51
49:QC:97:HIS:HD2	80:QC:402:HEM:C1C	2.28	0.51
54:QH:29:HIS:HB2	54:QH:33:LYS:HE2	1.92	0.51
17:A8:196:ARG:NH2	23:AN:63:GLU:OE2	2.43	0.51
20:AK:241:ASN:HB3	20:AK:245:LYS:HE2	1.91	0.51
35:C1:309:THR:HG22	77:C1:602:HEA:HMB1	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:QC:29:SER:OG	68:QC:404:CDL:OB9	2.25	0.51
41:N1:25:ARG:HD3	41:N1:37:PRO:HG2	1.93	0.51
42:N2:211:MET:HG2	42:N2:333:SER:HB2	1.93	0.51
49:QC:112:THR:HG22	49:QC:196:HIS:CE1	2.45	0.51
49:Qc:8:HIS:HB3	49:Qc:11:MET:HB2	1.91	0.51
58:S2:190:ILE:HG23	58:S2:209:MET:HB3	1.93	0.51
1:4L:55:LEU:H	61:S5:25:GLN:HE22	1.59	0.51
11:A1:40:HIS:N	11:A1:44:GLN:OE1	2.44	0.51
68:AL:201:CDL:H532	45:N5:577:VAL:HG22	1.93	0.51
41:N1:160:TYR:OH	43:N3:73:LEU:O	2.28	0.51
45:N5:530:PRO:O	45:N5:534:HIS:HB2	2.10	0.51
48:QB:192:PHE:HB3	48:QB:195:THR:OG1	2.10	0.51
53:Qg:46:GLU:OE2	53:Qg:49:ARG:NH1	2.38	0.51
65:V1:205:ILE:HG12	65:V1:379:CYS:HB3	1.92	0.51
1:4L:98:CYS:HB3	45:N5:580:GLN:HB2	1.93	0.51
18:A9:204:SER:HB2	18:A9:266:VAL:HG12	1.92	0.51
30:B7:103:GLU:O	30:B7:107:ARG:HG2	2.11	0.51
44:N4:375:LEU:HD11	45:N5:141:PHE:HE2	1.75	0.51
46:N6:82:VAL:HG12	46:N6:85:SER:HB2	1.92	0.51
26:B3:33:GLN:NE2	26:B3:43:ASP:OD1	2.44	0.51
28:B5:139:ILE:HG23	44:N4:54:LEU:HD23	1.92	0.51
40:CB:13:LEU:HD21	61:S5:4:PHE:HB3	1.93	0.51
42:N2:167:TRP:HB3	45:N5:574:SER:HA	1.92	0.51
45:N5:97:THR:HG21	45:N5:125:LEU:HD22	1.93	0.51
54:QH:25:ARG:NH1	51:Qe:92:ARG:O	2.44	0.51
70:6A:101:PC1:H153	37:C3:184:ALA:HB3	1.93	0.51
45:N5:228:GLY:H	45:N5:230:HIS:HD2	1.58	0.51
45:N5:399:VAL:HG12	45:N5:409:LEU:HD13	1.92	0.51
49:Qc:237:LEU:HD13	50:Qd:297:MET:HG2	1.93	0.51
45:N5:368:PHE:HZ	45:N5:455:LYS:HG3	1.76	0.50
47:QA:155:GLN:HE21	47:QA:198:GLY:H	1.59	0.50
18:A9:64:PHE:O	18:A9:67:ARG:HG2	2.11	0.50
25:B2:65:THR:HB	25:B2:68:GLN:HG2	1.92	0.50
68:B5:201:CDL:H191	68:B5:201:CDL:H762	1.93	0.50
35:C1:254:ILE:HG13	35:C1:344:PHE:CD2	2.46	0.50
41:N1:213:VAL:HG13	41:N1:214:GLU:HG2	1.93	0.50
42:N2:139:LEU:HD13	42:N2:190:MET:HE1	1.93	0.50
46:N6:113:VAL:HG13	46:N6:118:LYS:HG2	1.93	0.50
57:S1:395:GLU:OE2	57:S1:417:ARG:NH1	2.44	0.50
62:S6:61:GLU:OE2	64:S8:192:ASN:ND2	2.34	0.50
65:V1:129:GLU:OE2	65:V1:132:ARG:NH2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:V1:162:PHE:HB3	65:V1:165:GLU:HB2	1.93	0.50
3:5B:37:VAL:HB	37:C3:154:GLY:HA2	1.94	0.50
21:AL:35:ILE:HD12	68:AL:201:CDL:H811	1.92	0.50
29:B6:186:GLN:O	29:B6:187:HIS:ND1	2.44	0.50
45:N5:253:VAL:HG23	45:N5:310:LEU:HD21	1.93	0.50
48:QB:192:PHE:O	48:QB:198:ALA:HB2	2.11	0.50
51:QE:196:ARG:NH2	51:QE:252:GLY:O	2.24	0.50
5:6B:30:CYS:HB2	5:6B:65:CYS:SG	2.52	0.50
29:B6:147:LYS:NZ	33:BK:42:ASP:OD1	2.39	0.50
73:N4:501:PEE:H32	68:N4:503:CDL:H381	1.92	0.50
47:Qa:148:ARG:NH2	53:Qg:50:ARG:O	2.44	0.50
57:S1:251:ILE:HG21	57:S1:604:GLN:HB3	1.92	0.50
58:S2:393:GLU:OE2	58:S2:396:GLN:NE2	2.45	0.50
65:V1:203:ALA:HB3	65:V1:206:CYS:HB2	1.92	0.50
50:QD:132:ALA:HA	50:QD:175:TYR:HA	1.92	0.50
50:QD:147:LYS:NZ	50:QD:151:GLU:OE2	2.44	0.50
57:S1:34:VAL:HG23	57:S1:41:VAL:HG13	1.92	0.50
57:S1:389:THR:HG21	57:S1:473:MET:HE2	1.93	0.50
65:V1:385:CYS:O	65:V1:389:VAL:HB	2.12	0.50
35:C1:347:LEU:HD13	35:C1:383:MET:HE2	1.94	0.50
43:N3:42:ASP:OD1	63:S7:119:LYS:NZ	2.44	0.50
49:QC:78:VAL:HG11	51:QE:135:GLN:HE22	1.77	0.50
49:QC:304:MET:HE1	49:QC:366:MET:HE1	1.94	0.50
50:Qd:129:ASP:OD1	50:Qd:178:LYS:NZ	2.42	0.50
51:Qe:204:ARG:NE	51:Qe:246:SER:O	2.43	0.50
41:N1:138:GLN:HG3	41:N1:285:LEU:HD21	1.94	0.50
45:N5:562:LEU:HB3	45:N5:563:PRO:HD3	1.92	0.50
54:QH:67:PHE:HE1	49:Qc:344:GLU:HG3	1.75	0.50
47:Qa:298:HIS:HB2	48:Qb:114:GLU:HG2	1.94	0.50
57:S1:149:ASP:OD2	57:S1:150:ARG:NH2	2.44	0.50
35:C1:37:ILE:CG2	77:C1:601:HEA:HMA	2.42	0.50
49:QC:8:HIS:O	49:QC:12:LYS:N	2.38	0.50
68:A7:201:CDL:HA61	68:A7:201:CDL:H521	1.93	0.50
20:AK:225:ASN:HB3	20:AK:228:GLU:HG2	1.94	0.50
21:AL:124:LEU:HD11	73:N4:501:PEE:H70	1.93	0.50
42:N2:24:SER:OG	61:S5:15:ASP:OD1	2.25	0.50
43:N3:56:PHE:O	46:N6:70:TYR:OH	2.30	0.50
49:QC:344:GLU:HG3	54:Qh:67:PHE:HE1	1.77	0.50
50:QD:159:PRO:HB2	50:Qd:184:GLU:HG3	1.94	0.50
47:Qa:61:ILE:HG12	47:Qa:130:ILE:HD11	1.93	0.50
63:S7:108:THR:HA	63:S7:136:CYS:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6A:56:ARG:HH21	4:6A:94:TYR:HB3	1.76	0.49
46:N6:17:PHE:HA	46:N6:20:PHE:CE2	2.46	0.49
47:QA:90:THR:HG23	47:QA:95:SER:HA	1.94	0.49
48:QB:274:GLU:HG2	54:Qh:18:SER:HB2	1.92	0.49
51:QE:220:LEU:HD12	51:QE:239:HIS:CE1	2.47	0.49
51:Qe:267:SER:HB3	51:Qe:270:LEU:HB3	1.93	0.49
57:S1:387:LEU:HD12	57:S1:514:ASN:HB3	1.93	0.49
65:V1:357:MET:HB3	65:V1:361:THR:HG21	1.93	0.49
13:A3:127:ALA:HB2	41:N1:312:ALA:HA	1.94	0.49
17:A8:95:VAL:HG12	17:A8:97:VAL:HG22	1.94	0.49
47:QA:298:HIS:HB2	48:QB:114:GLU:HG2	1.93	0.49
47:Qa:47:LEU:HD21	47:Qa:234:ALA:HB1	1.92	0.49
2:5A:76:MET:HE2	2:5A:110:ILE:HG12	1.94	0.49
7:7A:54:ARG:HH12	68:7A:102:CDL:HB61	1.78	0.49
11:A1:12:MET:HE3	41:N1:264:LEU:HD22	1.95	0.49
18:A9:293:LEU:HD12	18:A9:294:PRO:HD2	1.92	0.49
44:N4:41:LEU:O	44:N4:44:GLN:NE2	2.45	0.49
68:QH:102:CDL:HB32	68:QH:102:CDL:HA22	1.93	0.49
11:A1:58:ASN:O	11:A1:59:ARG:NH1	2.41	0.49
17:A8:201:GLU:HA	17:A8:204:LYS:HD3	1.95	0.49
68:AL:201:CDL:H401	68:AL:201:CDL:H771	1.94	0.49
37:C3:178:ALA:HB1	68:C3:305:CDL:H122	1.94	0.49
44:N4:266:MET:HB3	44:N4:395:LEU:HD13	1.94	0.49
50:Qd:322:TYR:CZ	50:Qd:324:PRO:HG3	2.46	0.49
57:S1:449:PRO:HB2	57:S1:679:LEU:HD13	1.94	0.49
65:V1:288:VAL:HG21	65:V1:303:HIS:CD2	2.47	0.49
4:6A:56:ARG:NH2	4:6A:96:GLN:O	2.45	0.49
5:6B:63:SER:HA	36:C2:111:THR:HG23	1.94	0.49
17:A8:160:THR:HA	17:A8:163:TRP:CD1	2.47	0.49
21:AL:81:ARG:HH11	21:AL:89:ASN:HD21	1.61	0.49
36:C2:149:THR:OG1	36:C2:185:MET:SD	2.67	0.49
57:S1:246:ARG:HH12	60:S4:123:ASN:HD22	1.60	0.49
58:S2:121:LEU:HD23	63:S7:113:MET:SD	2.53	0.49
65:V1:119:GLU:O	65:V1:159:ARG:NH1	2.45	0.49
23:AN:93:GLU:HG3	61:S5:98:HIS:CD2	2.47	0.49
37:C3:33:MET:O	37:C3:37:PHE:N	2.44	0.49
71:N4:502:PLX:H192	68:N5:703:CDL:H611	1.94	0.49
50:Qd:149:LEU:O	50:Qd:152:GLU:HG2	2.13	0.49
51:Qe:145:ASP:OD1	51:Qe:145:ASP:N	2.42	0.49
51:Qe:228:ALA:HB3	51:Qe:235:TYR:HB3	1.95	0.49
58:S2:227:ARG:NH1	63:S7:75:GLU:OE1	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A9:50:SER:OG	59:S3:225:GLU:OE2	2.30	0.49
32:B9:87:ARG:NH1	32:B9:91:ASP:OD2	2.46	0.49
36:C2:72:ILE:O	36:C2:76:ILE:HG13	2.13	0.49
36:C2:156:SER:HB2	36:C2:174:ALA:HB1	1.95	0.49
42:N2:304:MET:HE3	44:N4:135:ARG:HH22	1.76	0.49
44:N4:296:LEU:HD21	44:N4:378:GLU:HG3	1.95	0.49
47:QA:89:LEU:HD22	47:QA:150:GLU:HB3	1.94	0.49
57:S1:83:GLU:HB2	57:S1:101:ASN:HB3	1.94	0.49
41:N1:281:ARG:NH1	58:S2:452:ASP:OD1	2.46	0.49
44:N4:369:LEU:HD23	68:N5:703:CDL:H362	1.95	0.49
48:QB:373:GLN:NE2	48:QB:475:MET:SD	2.86	0.49
48:Qb:83:ASN:HD22	48:Qb:85:LYS:H	1.61	0.49
49:Qc:47:THR:HG23	49:Qc:79:ILE:HG23	1.93	0.49
57:S1:538:ARG:HG2	57:S1:555:ILE:HD11	1.95	0.49
58:S2:90:PHE:HB2	58:S2:105:MET:HE2	1.93	0.49
58:S2:190:ILE:HG21	58:S2:213:ARG:HG3	1.95	0.49
11:A1:52:ARG:NH1	11:A1:58:ASN:OD1	2.44	0.49
20:AK:97:ASP:N	20:AK:97:ASP:OD1	2.45	0.49
24:B1:47:ARG:NH2	24:B1:53:GLU:OE2	2.46	0.49
36:C2:137:GLU:OE2	38:C4:144:ARG:NH1	2.44	0.49
57:S1:339:ALA:HA	57:S1:365:SER:HB2	1.93	0.49
58:S2:194:THR:HG21	58:S2:209:MET:HB2	1.94	0.49
67:V3:420:SER:HB3	67:V3:423:HIS:ND1	2.27	0.49
1:4L:73:LEU:HD21	42:N2:41:ILE:HG13	1.95	0.49
17:A8:84:LEU:O	23:AN:88:ARG:NH1	2.46	0.49
17:A8:86:THR:OG1	17:A8:88:GLU:OE1	2.27	0.49
45:N5:119:LYS:NZ	68:N5:703:CDL:OA3	2.39	0.49
53:QG:71:MET:HE2	50:Qd:316:LYS:HD3	1.95	0.49
48:Qb:126:ARG:NH1	48:Qb:199:GLN:O	2.46	0.49
57:S1:307:ILE:HG23	57:S1:317:THR:HG21	1.94	0.49
21:AL:67:GLY:HA2	68:AL:201:CDL:H221	1.93	0.48
70:C1:610:PC1:H111	37:C3:11:VAL:HG21	1.95	0.48
45:N5:15:LEU:HD11	45:N5:94:LEU:HD21	1.94	0.48
51:Qe:201:ASP:OD1	51:Qe:201:ASP:N	2.41	0.48
59:S3:61:PHE:HZ	59:S3:106:ALA:HB2	1.78	0.48
15:A6:66:TYR:CE2	15:A6:86:ARG:HD3	2.48	0.48
30:B7:17:PRO:HB3	30:B7:105:GLU:HG2	1.95	0.48
37:C3:219:LEU:HD23	68:C3:304:CDL:H761	1.95	0.48
41:N1:59:GLU:HG3	43:N3:27:LEU:HD13	1.94	0.48
42:N2:96:THR:HG22	42:N2:100:MET:HE2	1.95	0.48
42:N2:197:ASN:HD22	42:N2:200:MET:HG2	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:QB:465:LEU:HD12	48:QB:466:PRO:HD2	1.93	0.48
15:A6:90:ARG:HE	15:A6:94:MET:HE2	1.78	0.48
17:A8:178:ARG:NH1	17:A8:181:GLN:OE1	2.43	0.48
18:A9:220:MET:HG2	73:A9:402:PEE:H17	1.96	0.48
18:A9:257:ASP:OD1	18:A9:257:ASP:N	2.46	0.48
20:AK:297:ARG:HA	20:AK:300:VAL:HG22	1.95	0.48
23:AN:98:MET:HE3	23:AN:101:VAL:HG21	1.94	0.48
68:B4:201:CDL:OA7	54:Qh:39:LEU:HD13	2.14	0.48
33:BK:142:ARG:NH1	33:BK:143:TYR:OH	2.46	0.48
36:C2:28:LEU:HA	36:C2:31:VAL:HG22	1.95	0.48
43:N3:33:LYS:O	63:S7:98:ARG:NH1	2.37	0.48
45:N5:65:ASN:HD21	45:N5:78:LEU:HD23	1.78	0.48
52:QF:34:ARG:O	52:QF:38:GLU:HG2	2.12	0.48
63:S7:75:GLU:HB2	63:S7:133:MET:HE1	1.95	0.48
71:AL:202:PLX:H1A2	71:AL:202:PLX:H21	1.58	0.48
22:AM:144:TYR:OH	57:S1:581:ASP:OD1	2.24	0.48
35:C1:358:LEU:CB	77:C1:602:HEA:HMA	2.44	0.48
35:C1:413:HIS:CE1	35:C1:468:MET:HB2	2.48	0.48
44:N4:233:ALA:HA	44:N4:320:GLY:HA2	1.95	0.48
48:QB:190:THR:HG22	48:QB:275:ILE:HG23	1.95	0.48
68:4L:201:CDL:H262	68:4L:201:CDL:H371	1.95	0.48
9:7C:56:VAL:HG21	35:C1:36:LEU:HD13	1.94	0.48
27:B4:26:SER:OG	27:B4:28:GLU:OE1	2.28	0.48
33:BK:74:ILE:HG23	33:BK:156:LEU:HD22	1.96	0.48
37:C3:54:MET:HB3	37:C3:58:TRP:CZ3	2.48	0.48
38:C4:44:TYR:OH	38:C4:48:ASP:OD1	2.30	0.48
41:N1:113:VAL:HG13	41:N1:139:THR:HG21	1.95	0.48
44:N4:12:LEU:HB2	44:N4:13:PRO:HD3	1.95	0.48
45:N5:368:PHE:CZ	45:N5:455:LYS:HG3	2.49	0.48
48:QB:205:SER:HA	48:QB:208:VAL:HG12	1.96	0.48
56:QJ:14:ALA:O	56:QJ:18:ILE:HG12	2.13	0.48
47:Qa:375:LYS:NZ	47:Qa:419:VAL:O	2.32	0.48
51:Qe:262:THR:HB	51:Qe:274:GLY:O	2.13	0.48
57:S1:43:VAL:HG12	57:S1:55:LYS:HD2	1.94	0.48
57:S1:338:VAL:HB	57:S1:363:SER:CB	2.43	0.48
59:S3:145:THR:OG1	59:S3:146:TYR:N	2.46	0.48
16:A7:109:ASP:OD2	23:AN:21:TYR:OH	2.30	0.48
42:N2:26:TRP:HB3	42:N2:74:ILE:HD13	1.96	0.48
45:N5:241:THR:HG21	45:N5:344:GLY:HA3	1.94	0.48
47:Qa:237:PHE:CE2	47:Qa:238:LEU:HD12	2.48	0.48
48:Qb:302:VAL:HB	48:Qb:303:PRO:HD3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:S2:129:LEU:O	58:S2:133:LYS:HG2	2.13	0.48
62:S6:108:THR:HG22	62:S6:119:ARG:HD3	1.94	0.48
64:S8:75:SER:O	64:S8:79:ARG:HG3	2.14	0.48
23:AN:95:ALA:HA	23:AN:106:VAL:HG11	1.96	0.48
28:B5:53:ARG:NH2	29:B6:89:SER:O	2.45	0.48
45:N5:536:LEU:HB3	45:N5:537:PRO:HD3	1.96	0.48
68:QH:102:CDL:OA3	50:Qd:305:TYR:OH	2.28	0.48
55:QI:50:GLY:H	55:QI:55:HIS:CD2	2.32	0.48
17:A8:115:LYS:HB3	17:A8:116:PRO:HD3	1.96	0.48
33:BK:73:ASP:OD1	33:BK:73:ASP:N	2.44	0.48
36:C2:152:MET:HB2	36:C2:182:THR:HB	1.95	0.48
42:N2:42:PRO:HG3	46:N6:167:VAL:HG13	1.95	0.48
47:QA:438:MET:HB2	47:QA:450:VAL:HG13	1.94	0.48
53:QG:43:ASP:OD2	53:QG:102:ARG:NH1	2.47	0.48
47:Qa:409:PRO:O	47:Qa:413:LEU:HG	2.13	0.48
65:V1:174:ARG:HA	67:V3:406:LEU:HD21	1.94	0.48
3:5B:84:THR:OG1	3:5B:85:ASN:N	2.47	0.48
68:B5:201:CDL:HB21	73:N5:701:PEE:H49	1.95	0.48
49:Qc:5:ARG:HH11	49:Qc:15:ASN:ND2	2.12	0.48
60:S4:70:GLU:O	60:S4:74:THR:OG1	2.28	0.48
63:S7:56:TRP:CE2	71:S7:203:PLX:H101	2.49	0.48
65:V1:185:ASN:OD1	65:V1:190:GLY:N	2.42	0.48
2:5A:61:TYR:OH	2:5A:71:GLU:O	2.31	0.48
40:CB:107:ASP:OD1	40:CB:107:ASP:N	2.47	0.48
44:N4:106:LEU:HD13	44:N4:234:VAL:HG11	1.96	0.48
48:QB:74:TRP:CZ2	48:QB:411:GLU:HA	2.48	0.48
66:V2:111:ARG:NH1	66:V2:114:GLU:OE2	2.47	0.48
1:4L:4:VAL:O	1:4L:8:ILE:HG12	2.14	0.47
4:6A:88:ASN:ND2	70:6A:101:PC1:H151	2.29	0.47
6:6C:63:GLU:O	6:6C:67:LYS:NZ	2.44	0.47
14:A5:38:ILE:O	14:A5:45:ARG:NH1	2.47	0.47
19:AC:119:ILE:HG21	19:AC:135:ALA:HB1	1.95	0.47
55:Qi:38:GLN:NE2	56:Qj:47:TYR:OH	2.47	0.47
56:Qj:42:LEU:HA	56:Qj:45:VAL:HG22	1.96	0.47
60:S4:112:MET:O	64:S8:144:ARG:NH1	2.36	0.47
85:S7:201:U10:H401	85:S7:201:U10:H422	1.66	0.47
44:N4:196:TRP:CD1	44:N4:250:LEU:HB3	2.48	0.47
23:AN:49:SER:HB2	41:N1:172:ILE:HD13	1.95	0.47
68:C3:304:CDL:H802	68:C3:305:CDL:H273	1.96	0.47
47:Qa:71:TYR:HB3	47:Qa:212:HIS:CE1	2.50	0.47
47:Qa:313:VAL:HG21	47:Qa:323:VAL:HG11	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:S1:274:LEU:HD21	60:S4:87:MET:HE2	1.96	0.47
58:S2:299:LEU:HD22	58:S2:304:ILE:HD12	1.97	0.47
68:7A:102:CDL:H232	68:7A:102:CDL:H822	1.96	0.47
9:7C:60:LEU:HD23	10:8B:64:TYR:HB2	1.96	0.47
28:B5:94:GLY:O	33:BK:61:TYR:OH	2.29	0.47
29:B6:148:TYR:CE1	33:BK:49:ARG:HG2	2.49	0.47
70:C1:610:PC1:H341	70:C1:610:PC1:H2A2	1.95	0.47
36:C2:98:LYS:HZ3	36:C2:111:THR:HG21	1.80	0.47
36:C2:145:PRO:HA	36:C2:214:VAL:O	2.14	0.47
44:N4:210:TYR:CG	44:N4:268:GLY:HA3	2.49	0.47
65:V1:210:THR:HB	65:V1:224:ARG:H	1.80	0.47
65:V1:325:PRO:HG3	65:V1:433:TRP:HB3	1.95	0.47
9:7C:52:PRO:HG2	35:C1:32:ALA:HB3	1.97	0.47
18:A9:129:LEU:HD23	18:A9:167:ILE:HG13	1.97	0.47
36:C2:110:TYR:HB2	36:C2:116:LEU:HB3	1.96	0.47
44:N4:79:ALA:O	44:N4:82:SER:HB3	2.15	0.47
50:QD:292:LYS:HD2	73:QE:301:PEE:H3	1.96	0.47
51:Qe:126:ALA:HA	73:Qe:301:PEE:H74	1.96	0.47
65:V1:347:THR:HG22	65:V1:348:GLY:H	1.80	0.47
20:AK:316:LEU:HB2	20:AK:319:ILE:HG12	1.96	0.47
36:C2:161:HIS:CE1	36:C2:200:CYS:SG	3.06	0.47
37:C3:173:PHE:CE1	37:C3:208:VAL:HG21	2.49	0.47
42:N2:25:HIS:HB2	61:S5:15:ASP:HB2	1.97	0.47
68:QB:501:CDL:H512	70:QB:503:PC1:H361	1.96	0.47
48:Qb:68:THR:HG22	48:Qb:136:LEU:HD23	1.96	0.47
57:S1:217:GLU:HG3	57:S1:412:PRO:HB3	1.95	0.47
5:6B:14:THR:HG23	36:C2:151:ARG:HH12	1.80	0.47
12:A2:18:GLU:HG2	12:A2:68:ARG:HB3	1.96	0.47
13:A3:160:GLY:HA3	17:A8:204:LYS:HE3	1.97	0.47
17:A8:124:ARG:NE	23:AN:80:ASP:OD2	2.44	0.47
75:AC:201:ZMP:H11A	32:B9:58:VAL:HG23	1.97	0.47
35:C1:74:MET:HE3	35:C1:389:ILE:HG13	1.97	0.47
41:N1:113:VAL:O	41:N1:116:ILE:HG12	2.14	0.47
43:N3:35:SER:O	63:S7:98:ARG:NH2	2.47	0.47
44:N4:82:SER:HB2	44:N4:432:ARG:NH1	2.30	0.47
44:N4:211:GLY:H	44:N4:213:HIS:CD2	2.31	0.47
45:N5:292:ALA:HB2	45:N5:304:PHE:HB3	1.97	0.47
45:N5:366:MET:O	45:N5:370:THR:OG1	2.25	0.47
49:QC:29:SER:HB2	68:QD:402:CDL:H142	1.97	0.47
51:QE:143:SER:OG	51:QE:145:ASP:OD1	2.31	0.47
48:Qb:87:ASN:HD22	48:Qb:204:PRO:HD3	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Qb:96:LEU:HD13	48:Qb:156:LEU:HD22	1.96	0.47
66:V2:149:LEU:HD11	66:V2:160:VAL:HG23	1.95	0.47
18:A9:165:ILE:HD13	18:A9:199:THR:HB	1.97	0.47
34:BL:77:ASP:OD1	34:BL:78:LYS:N	2.48	0.47
40:CB:106:LYS:NZ	40:CB:107:ASP:OD1	2.37	0.47
44:N4:201:MET:HE1	44:N4:212:LEU:HD11	1.96	0.47
44:N4:361:VAL:HG22	68:N5:703:CDL:H311	1.96	0.47
51:QE:177:ARG:HB3	51:QE:211:VAL:HG13	1.96	0.47
52:QF:60:ARG:HD3	52:QF:63:THR:HG21	1.96	0.47
47:Qa:301:ARG:NH2	48:Qb:94:GLU:OE2	2.46	0.47
50:Qd:311:LYS:HD3	50:Qd:311:LYS:HA	1.75	0.47
53:Qg:44:VAL:O	53:Qg:48:ILE:HG12	2.15	0.47
57:S1:575:VAL:C	57:S1:578:PRO:HD2	2.39	0.47
1:4L:76:SER:O	1:4L:79:VAL:HG22	2.14	0.47
18:A9:231:LEU:HD13	18:A9:292:PRO:HG3	1.95	0.47
25:B2:108:ASP:OD1	30:B7:107:ARG:NH1	2.47	0.47
35:C1:352:GLY:HA3	77:C1:602:HEA:C14	2.45	0.47
44:N4:76:MET:SD	44:N4:230:VAL:HB	2.55	0.47
45:N5:49:VAL:HB	45:N5:50:PRO:HD3	1.97	0.47
45:N5:566:THR:O	45:N5:570:GLN:HG2	2.15	0.47
47:QA:138:LEU:HD12	47:QA:233:VAL:HG12	1.97	0.47
35:C1:405:LEU:HD23	35:C1:475:ALA:HB2	1.97	0.47
36:C2:13:THR:HB	36:C2:168:LEU:HD23	1.97	0.47
44:N4:267:TRP:O	44:N4:271:MET:HG2	2.15	0.47
47:QA:313:VAL:HG11	47:QA:350:VAL:HG13	1.97	0.47
48:QB:110:GLU:HA	48:QB:113:VAL:HG22	1.97	0.47
47:Qa:125:CYS:HB3	47:Qa:133:LEU:HD22	1.97	0.47
57:S1:222:ILE:HA	57:S1:225:ILE:HG12	1.97	0.47
58:S2:167:ILE:HD13	58:S2:369:VAL:HG11	1.97	0.47
59:S3:89:HIS:CG	59:S3:90:PRO:HD2	2.50	0.47
59:S3:118:ASP:OD2	59:S3:125:ARG:NH2	2.45	0.47
67:V3:386:TYR:CZ	67:V3:388:ASN:HB3	2.50	0.47
16:A7:62:GLU:OE2	59:S3:44:ARG:NH1	2.44	0.46
35:C1:336:PRO:HD3	35:C1:407:GLN:HG3	1.98	0.46
41:N1:90:PRO:HB3	41:N1:94:PRO:HD3	1.96	0.46
42:N2:149:ILE:HD13	42:N2:154:MET:HE3	1.96	0.46
44:N4:168:GLN:HB2	44:N4:174:LEU:HG	1.96	0.46
49:Qc:303:LEU:HD11	70:Qc:405:PC1:H122	1.97	0.46
52:Qf:40:ILE:HG13	52:Qf:43:CYS:H	1.80	0.46
65:V1:235:VAL:H	65:V1:240:THR:HG21	1.80	0.46
71:CB:201:PLX:H171	61:S5:9:ARG:HH22	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:N2:112:HIS:HB2	42:N2:184:ILE:HD13	1.97	0.46
44:N4:408:LEU:HD12	45:N5:172:ILE:HG21	1.97	0.46
47:QA:154:LEU:HD23	47:QA:154:LEU:HA	1.78	0.46
50:QD:184:GLU:HG3	50:Qd:159:PRO:HB2	1.97	0.46
47:Qa:290:GLN:HB2	47:Qa:336:PHE:HE1	1.80	0.46
62:S6:36:GLU:OE2	62:S6:60:LYS:NZ	2.41	0.46
65:V1:384:PRO:HG2	65:V1:422:HIS:O	2.15	0.46
1:4L:35:GLY:HA3	46:N6:20:PHE:CZ	2.51	0.46
1:4L:65:VAL:HG11	46:N6:157:THR:HG23	1.97	0.46
9:7C:41:MET:HG2	73:7C:101:PEE:H62	1.97	0.46
31:B8:108:ASP:HB3	31:B8:111:MET:HG2	1.98	0.46
36:C2:133:MET:HB2	36:C2:136:LEU:HB2	1.98	0.46
45:N5:327:LEU:O	45:N5:331:MET:HG2	2.15	0.46
50:QD:243:ILE:HG12	50:QD:245:MET:H	1.81	0.46
51:QE:154:ILE:HD13	51:QE:176:VAL:HG21	1.98	0.46
68:QH:102:CDL:HA32	50:Qd:308:LYS:HE3	1.95	0.46
51:QK:34:LEU:HD23	51:QK:34:LEU:H	1.79	0.46
47:Qa:68:GLY:H	47:Qa:71:TYR:HD2	1.63	0.46
57:S1:219:SER:O	57:S1:222:ILE:HG12	2.15	0.46
58:S2:145:LEU:HD13	58:S2:430:ILE:HG21	1.97	0.46
58:S2:418:VAL:HB	58:S2:427:ARG:HB3	1.96	0.46
64:S8:142:THR:O	64:S8:187:LYS:NZ	2.49	0.46
38:C4:142:THR:HG23	38:C4:156:PHE:HZ	1.80	0.46
42:N2:132:THR:HG23	42:N2:209:ILE:HG12	1.98	0.46
45:N5:288:THR:HG21	45:N5:307:SER:HB3	1.97	0.46
15:A6:48:SER:O	15:A6:50:ASP:N	2.49	0.46
19:AB:140:CYS:HB2	19:AB:143:GLU:HG3	1.98	0.46
30:B7:22:MET:HE1	30:B7:102:PHE:CD2	2.51	0.46
35:C1:8:TYR:CZ	37:C3:15:PRO:HB3	2.51	0.46
35:C1:368:HIS:O	36:C2:171:LYS:NZ	2.42	0.46
68:CB:203:CDL:H342	68:CB:203:CDL:H191	1.98	0.46
65:V1:65:THR:O	65:V1:69:LEU:HG	2.16	0.46
66:V2:144:ASN:HB3	66:V2:147:SER:OG	2.16	0.46
4:6A:59:PHE:HB2	4:6A:94:TYR:CE2	2.50	0.46
5:6B:5:ILE:HG13	5:6B:7:THR:H	1.80	0.46
31:B8:62:TYR:OH	31:B8:74:ASP:O	2.21	0.46
36:C2:146:MET:HE2	36:C2:215:PRO:HG3	1.96	0.46
45:N5:402:SER:HB2	45:N5:404:THR:HG23	1.97	0.46
45:N5:435:PRO:HB3	45:N5:437:PHE:CZ	2.51	0.46
48:QB:467:ASP:HB3	48:QB:470:ARG:HG2	1.97	0.46
51:QE:123:VAL:HG13	55:Qi:29:ALA:HA	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:S2:467:VAL:O	58:S2:469:ARG:NH1	2.49	0.46
65:V1:55:GLY:O	65:V1:58:SER:OG	2.20	0.46
3:5B:41:GLU:HG2	3:5B:56:ARG:NH2	2.29	0.46
15:A6:88:LYS:NZ	15:A6:133:PHE:HA	2.31	0.46
16:A7:112:TYR:HE2	64:S8:43:MET:HE2	1.80	0.46
18:A9:219:SER:HB3	73:A9:402:PEE:H1	1.98	0.46
71:AM:201:PLX:H341	71:AM:201:PLX:H372	1.70	0.46
34:BL:72:ASP:OD1	34:BL:72:ASP:N	2.38	0.46
41:N1:273:ILE:HG23	41:N1:277:TYR:HD2	1.81	0.46
45:N5:346:ILE:HD11	45:N5:431:PHE:CZ	2.51	0.46
47:QA:235:GLU:O	47:QA:239:ASN:ND2	2.48	0.46
50:QD:112:ARG:NH2	50:QD:145:GLU:OE1	2.49	0.46
50:Qd:104:SER:O	50:Qd:287:LYS:NZ	2.49	0.46
65:V1:49:HIS:NE2	67:V3:383:ASN:OD1	2.49	0.46
68:A8:301:CDL:HB61	40:CB:29:THR:HB	1.98	0.46
18:A9:176:SER:O	18:A9:182:ARG:NE	2.47	0.46
18:A9:223:PHE:HB3	73:A9:402:PEE:H28	1.98	0.46
68:AK:402:CDL:H342	68:AK:402:CDL:H142	1.96	0.46
35:C1:202:LEU:HD22	35:C1:238:PHE:CE2	2.51	0.46
47:QA:272:VAL:HA	47:QA:337:GLY:HA3	1.97	0.46
49:QC:141:TRP:CD1	49:QC:265:PRO:HD3	2.50	0.46
64:S8:131:GLU:HB2	64:S8:144:ARG:HB3	1.97	0.46
15:A6:92:MET:HB2	75:AB:201:ZMP:H4A	1.97	0.46
68:B4:201:CDL:HA31	54:Qh:43:ARG:HH22	1.81	0.46
32:B9:52:LEU:O	32:B9:57:LYS:NZ	2.47	0.46
37:C3:126:PRO:HA	37:C3:130:PRO:HG2	1.97	0.46
71:CB:201:PLX:H131	71:CB:201:PLX:H101	1.73	0.46
41:N1:301:CYS:O	41:N1:305:ILE:HG13	2.16	0.46
68:N1:401:CDL:H721	68:N1:401:CDL:H341	1.98	0.46
44:N4:216:LEU:HB3	44:N4:217:PRO:HD3	1.97	0.46
68:QH:102:CDL:H331	68:QH:102:CDL:H721	1.98	0.46
71:QI:301:PLX:H1A3	71:QI:301:PLX:H22	1.64	0.46
57:S1:476:LEU:HD21	57:S1:481:LEU:HD21	1.97	0.46
57:S1:509:ASP:OD1	57:S1:509:ASP:N	2.47	0.46
58:S2:180:PHE:CZ	58:S2:223:VAL:HG11	2.51	0.46
21:AL:110:ILE:HG12	73:N5:702:PEE:H14	1.97	0.46
35:C1:219:PHE:HZ	37:C3:199:VAL:HG21	1.81	0.46
35:C1:334:TRP:HH2	36:C2:46:LEU:HD13	1.81	0.46
36:C2:9:PHE:HB2	36:C2:21:LEU:HD21	1.97	0.46
48:QB:321:GLY:HA2	48:QB:324:MET:HE2	1.98	0.46
49:QC:312:GLN:HG3	53:Qg:37:THR:HG22	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:S7:84:TYR:CE1	63:S7:171:GLU:HG3	2.50	0.46
8:7B:34:HIS:CE1	38:C4:99:GLU:HG3	2.51	0.45
16:A7:39:PRO:HG3	64:S8:211:TYR:CZ	2.52	0.45
17:A8:160:THR:HA	17:A8:163:TRP:NE1	2.31	0.45
30:B7:12:ASP:OD1	30:B7:14:SER:OG	2.29	0.45
35:C1:124:THR:HG21	35:C1:133:ALA:HB2	1.97	0.45
35:C1:297:MET:O	35:C1:302:ARG:NH1	2.47	0.45
77:C1:602:HEA:H271	77:C1:602:HEA:H211	1.63	0.45
37:C3:107:ALA:HB3	70:C3:301:PC1:H121	1.97	0.45
44:N4:398:MET:O	44:N4:402:ILE:HG13	2.15	0.45
45:N5:496:MET:HE1	68:N5:704:CDL:H431	1.99	0.45
48:QB:276:ARG:NH2	48:QB:466:PRO:O	2.49	0.45
48:Qb:282:LEU:HD12	48:Qb:460:GLY:HA2	1.97	0.45
52:Qf:28:ASP:HB3	52:Qf:29:PRO:HD3	1.98	0.45
58:S2:410:LYS:HE2	58:S2:463:VAL:HG23	1.97	0.45
6:6C:15:LEU:HD13	36:C2:50:LEU:HB2	1.99	0.45
6:6C:73:SER:HB3	36:C2:143:VAL:HG21	1.98	0.45
42:N2:137:ALA:HB3	42:N2:138:PRO:HD3	1.98	0.45
42:N2:168:GLY:O	42:N2:172:GLN:HG2	2.15	0.45
48:QB:388:VAL:HG21	48:QB:438:ALA:HA	1.98	0.45
47:Qa:323:VAL:HG12	47:Qa:340:THR:HG22	1.96	0.45
50:Qd:228:LEU:HD11	50:Qd:234:PHE:HB2	1.98	0.45
59:S3:119:VAL:HG12	59:S3:121:THR:HG22	1.98	0.45
68:4L:201:CDL:HA61	21:AL:49:PHE:HA	1.98	0.45
68:A8:301:CDL:H192	40:CB:34:VAL:HG12	1.97	0.45
35:C1:372:TYR:N	35:C1:432:GLY:HA3	2.30	0.45
41:N1:309:ILE:HD11	43:N3:87:MET:HE1	1.98	0.45
45:N5:298:ILE:O	45:N5:302:VAL:HG23	2.16	0.45
50:QD:112:ARG:HB2	50:QD:140:CYS:HB2	1.98	0.45
51:QE:151:LYS:HB3	51:QE:272:ILE:HD11	1.99	0.45
57:S1:275:PRO:HG3	57:S1:286:ILE:HG12	1.98	0.45
58:S2:140:PRO:HB2	63:S7:142:TYR:HE2	1.80	0.45
58:S2:194:THR:HB	58:S2:206:PHE:HA	1.98	0.45
2:5A:67:ILE:HG22	2:5A:100:ARG:HH12	1.82	0.45
15:A6:127:THR:HG23	59:S3:219:VAL:O	2.16	0.45
71:AM:201:PLX:H82	71:S7:203:PLX:H72	1.99	0.45
30:B7:107:ARG:HA	30:B7:110:GLN:HG2	1.97	0.45
33:BK:115:GLN:HG2	45:N5:62:ILE:HG12	1.98	0.45
47:QA:123:VAL:HB	47:QA:133:LEU:HD23	1.98	0.45
47:QA:155:GLN:HB3	47:QA:198:GLY:HA2	1.97	0.45
50:QD:285:HIS:O	50:QD:289:MET:HG3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:Qb:501:CDL:H122	68:Qb:501:CDL:HB4	1.98	0.45
62:S6:70:LEU:HD13	64:S8:109:GLY:HA3	1.99	0.45
63:S7:59:ARG:HG3	63:S7:181:GLN:HB3	1.98	0.45
68:7A:102:CDL:H822	68:7A:102:CDL:H201	1.99	0.45
24:B1:50:ARG:HB2	24:B1:53:GLU:HG2	1.98	0.45
30:B7:37:ARG:NH1	31:B8:160:GLN:OE1	2.39	0.45
54:QH:11:MET:HE2	48:Qb:278:ARG:HD3	1.97	0.45
51:QK:64:LEU:HA	51:QK:77:ARG:O	2.16	0.45
47:Qa:379:LYS:HG2	47:Qa:413:LEU:HD22	1.99	0.45
57:S1:224:ASP:OD2	57:S1:291:ARG:NH2	2.47	0.45
1:4L:55:LEU:HD13	61:S5:17:TRP:HE3	1.82	0.45
20:AK:51:THR:HG21	20:AK:153:LEU:HD22	1.98	0.45
20:AK:85:LEU:HD22	20:AK:158:GLY:HA3	1.99	0.45
41:N1:114:TYR:OH	46:N6:61:LEU:O	2.23	0.45
41:N1:117:LEU:HD11	46:N6:65:LEU:HD12	1.97	0.45
42:N2:193:VAL:HG21	42:N2:266:ILE:HG12	1.99	0.45
51:QE:193:SER:OG	51:QE:194:GLN:OE1	2.34	0.45
49:Qc:200:LEU:CD2	80:Qc:403:HEM:HAA1	2.46	0.45
49:Qc:361:ILE:HG12	49:Qc:365:LEU:HD12	1.97	0.45
63:S7:107:GLY:HA2	83:S7:202:SF4:S4	2.57	0.45
65:V1:141:GLY:HA3	65:V1:248:VAL:O	2.15	0.45
75:AC:201:ZMP:H5A	32:B9:109:ALA:HB1	1.99	0.45
20:AK:343:PRO:HB2	39:CA:34:PRO:HB3	1.98	0.45
40:CB:2:THR:HB	40:CB:5:SER:HB3	1.98	0.45
42:N2:220:ILE:HG22	42:N2:323:MET:HE1	1.99	0.45
73:N3:201:PEE:H22	73:N3:201:PEE:H27	1.72	0.45
47:QA:51:SER:OG	47:QA:230:LEU:HD12	2.17	0.45
48:QB:86:ASN:HA	48:QB:211:LEU:HD21	1.97	0.45
51:QE:211:VAL:HG21	51:QE:246:SER:HA	1.97	0.45
71:Qi:301:PLX:H1A3	71:Qi:301:PLX:H22	1.63	0.45
57:S1:169:VAL:HG22	57:S1:223:ILE:HD11	1.97	0.45
57:S1:262:VAL:HG23	57:S1:276:ARG:HB2	1.99	0.45
57:S1:296:GLY:O	57:S1:572:HIS:NE2	2.41	0.45
57:S1:385:TYR:OH	57:S1:527:ASP:OD1	2.31	0.45
3:5B:81:PRO:O	3:5B:87:ARG:NH1	2.48	0.45
68:7A:102:CDL:H111	68:7A:102:CDL:H722	1.98	0.45
22:AM:60:ARG:HH22	22:AM:95:ASP:HA	1.82	0.45
26:B3:18:ASP:O	26:B3:21:GLN:HG2	2.17	0.45
37:C3:171:VAL:HG22	68:C3:305:CDL:H232	1.98	0.45
49:QC:70:CYS:SG	49:QC:80:ARG:HD2	2.57	0.45
51:QE:228:ALA:HB3	51:QE:235:TYR:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:S4:131:LYS:NZ	60:S4:132:GLU:OE2	2.48	0.45
1:4L:79:VAL:HG12	46:N6:74:MET:HE3	1.98	0.45
4:6A:59:PHE:HB2	4:6A:94:TYR:HE2	1.81	0.45
35:C1:361:SER:O	35:C1:365:ILE:HG12	2.16	0.45
35:C1:383:MET:HG2	35:C1:421:VAL:HB	1.99	0.45
45:N5:265:PRO:O	45:N5:269:THR:HG23	2.15	0.45
52:QF:65:GLU:HG3	54:QH:73:LYS:NZ	2.32	0.45
58:S2:203:MET:O	58:S2:206:PHE:HB3	2.16	0.45
58:S2:272:ARG:NH1	73:S8:303:PEE:H2	2.27	0.45
63:S7:188:LYS:HB3	63:S7:191:ARG:HE	1.82	0.45
37:C3:181:TYR:HE2	70:C3:306:PC1:H271	1.82	0.45
37:C3:204:HIS:NE2	37:C3:249:TRP:HB2	2.32	0.45
48:Qb:315:ASP:OD1	48:Qb:316:SER:N	2.50	0.45
49:Qc:300:ILE:HD11	49:Qc:363:LEU:HD21	1.99	0.45
58:S2:160:ALA:HA	58:S2:404:THR:HG21	1.99	0.45
73:S2:501:PEE:H34	73:S2:501:PEE:H27	1.73	0.45
65:V1:261:TRP:NE1	65:V1:265:PHE:HE2	2.13	0.45
4:6A:65:LEU:HD22	37:C3:190:ASP:HB3	1.99	0.44
7:7A:66:TYR:HB2	72:7A:101:3PE:H232	1.99	0.44
19:AB:93:ILE:HD12	19:AB:108:LEU:HD13	1.99	0.44
19:AC:120:MET:HE1	32:B9:66:LEU:HB3	1.99	0.44
20:AK:112:GLY:HA2	20:AK:136:TRP:CD2	2.52	0.44
29:B6:143:HIS:HE1	45:N5:1:MET:HB2	1.82	0.44
35:C1:409:TRP:HB3	35:C1:471:ILE:HG12	1.98	0.44
71:N4:502:PLX:H191	68:N5:703:CDL:H242	1.98	0.44
53:QG:19:LYS:NZ	53:QG:85:GLU:OE2	2.40	0.44
47:Qa:90:THR:HG23	47:Qa:95:SER:HA	1.98	0.44
48:Qb:192:PHE:O	48:Qb:195:THR:OG1	2.31	0.44
58:S2:187:LEU:HD23	58:S2:213:ARG:HG2	1.99	0.44
1:4L:62:ILE:HG21	42:N2:31:ILE:HD11	1.99	0.44
22:AM:75:TRP:HE1	71:AM:201:PLX:H11	1.82	0.44
24:B1:29:ARG:NH2	71:B1:101:PLX:O2	2.51	0.44
68:B4:201:CDL:HA62	68:B4:201:CDL:H521	1.98	0.44
33:BK:107:GLN:NE2	45:N5:194:ASN:HD22	2.14	0.44
34:BL:90:VAL:HG22	44:N4:28:THR:HG21	1.98	0.44
42:N2:111:PHE:HA	45:N5:591:PHE:CE1	2.52	0.44
73:N5:705:PEE:H76	73:N5:705:PEE:H71	1.70	0.44
46:N6:39:VAL:O	46:N6:43:ILE:HG13	2.18	0.44
47:QA:91:THR:HG21	47:QA:140:VAL:HA	1.99	0.44
49:QC:307:LEU:HD11	49:QC:363:LEU:HD23	1.98	0.44
48:Qb:388:VAL:O	48:Qb:392:LYS:HG3	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Qe:133:VAL:HG12	73:Qe:301:PEE:H57	1.99	0.44
20:AK:134:GLN:HE22	76:AK:401:ADP:HN62	1.65	0.44
30:B7:44:GLN:NE2	30:B7:48:ASP:OD1	2.50	0.44
30:B7:103:GLU:OE2	30:B7:106:ARG:NH2	2.43	0.44
51:Qe:201:ASP:C	51:Qe:203:GLU:H	2.25	0.44
19:AB:140:CYS:O	19:AB:144:ILE:HG12	2.16	0.44
70:C1:610:PC1:H321	70:C1:610:PC1:H291	2.00	0.44
36:C2:111:THR:O	36:C2:111:THR:OG1	2.29	0.44
44:N4:204:MET:O	44:N4:208:PRO:HA	2.18	0.44
45:N5:3:PRO:HB2	45:N5:53:MET:HE1	1.99	0.44
64:S8:100:GLU:OE2	64:S8:185:TYR:OH	2.33	0.44
66:V2:245:VAL:HG13	66:V2:249:LEU:HD13	1.99	0.44
3:5B:41:GLU:HG2	3:5B:56:ARG:HH22	1.83	0.44
18:A9:246:SER:O	18:A9:250:ILE:HG12	2.17	0.44
36:C2:158:ASP:OD1	36:C2:158:ASP:N	2.50	0.44
46:N6:129:ASP:HB2	61:S5:32:ARG:NH1	2.32	0.44
54:QH:19:LEU:HG	54:QH:20:SER:H	1.81	0.44
57:S1:131:CYS:O	57:S1:241:ARG:NH1	2.33	0.44
73:S2:501:PEE:H71	73:S2:501:PEE:H76	1.79	0.44
65:V1:192:ASP:HB3	67:V3:411:MET:SD	2.58	0.44
24:B1:32:ASP:OD1	28:B5:135:LYS:NZ	2.38	0.44
70:C3:301:PC1:H142	70:C3:301:PC1:H111	1.83	0.44
41:N1:169:GLN:HB3	41:N1:244:GLY:HA3	1.98	0.44
44:N4:221:VAL:HA	44:N4:283:LYS:HD3	1.98	0.44
46:N6:82:VAL:HG22	46:N6:83:TRP:H	1.83	0.44
47:Qa:134:MET:SD	47:Qa:233:VAL:HG21	2.57	0.44
50:Qd:216:LEU:HB3	50:Qd:249:ILE:HD11	1.98	0.44
57:S1:124:HIS:CG	57:S1:125:PRO:HD2	2.53	0.44
57:S1:155:GLU:OE2	65:V1:398:ARG:NH2	2.41	0.44
1:4L:55:LEU:HD23	1:4L:55:LEU:HA	1.87	0.44
12:A2:85:ASP:OD1	12:A2:85:ASP:N	2.51	0.44
17:A8:157:GLU:HB2	17:A8:158:PRO:HD3	2.00	0.44
25:B2:79:MET:SD	45:N5:375:ILE:HG12	2.58	0.44
72:CA:101:3PE:H261	72:CA:101:3PE:H2A2	1.99	0.44
40:CB:51:ARG:CZ	42:N2:322:GLN:HG2	2.48	0.44
45:N5:407:TRP:O	45:N5:411:MET:HG2	2.17	0.44
46:N6:24:PRO:HG3	46:N6:83:TRP:CE2	2.52	0.44
51:QE:241:SER:OG	82:QE:303:FES:S1	2.69	0.44
49:Qc:24:PRO:HB2	49:Qc:27:ILE:HG23	1.99	0.44
57:S1:43:VAL:HG21	57:S1:96:VAL:HG21	1.99	0.44
57:S1:338:VAL:O	57:S1:365:SER:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:S1:401:LEU:HD11	57:S1:432:ILE:HG13	1.99	0.44
5:6B:58:ARG:HA	5:6B:61:TYR:CD1	2.53	0.44
9:7C:18:HIS:CD2	9:7C:18:HIS:H	2.35	0.44
18:A9:64:PHE:HZ	18:A9:208:GLY:HA3	1.83	0.44
42:N2:235:ASN:O	42:N2:315:TRP:NE1	2.51	0.44
51:QE:156:LEU:HB3	51:QE:210:TRP:CZ2	2.53	0.44
55:QI:48:ASN:ND2	50:Qd:105:SER:H	2.16	0.44
50:Qd:209:GLU:H	50:Qd:209:GLU:HG2	1.48	0.44
57:S1:76:ARG:O	57:S1:116:VAL:HG21	2.18	0.44
57:S1:180:THR:N	83:S1:802:SF4:S4	2.85	0.44
71:S7:203:PLX:H393	71:S7:203:PLX:H362	1.84	0.44
64:S8:153:ILE:HG12	83:S8:302:SF4:S1	2.58	0.44
66:V2:93:LEU:HD12	66:V2:122:TYR:HB3	2.00	0.44
1:4L:2:PRO:HG3	46:N6:127:ILE:HD13	1.98	0.44
68:B4:201:CDL:H1	68:B4:201:CDL:H512	2.00	0.44
35:C1:352:GLY:HA3	77:C1:602:HEA:H162	1.99	0.44
41:N1:87:VAL:HG22	41:N1:88:PRO:HD3	2.00	0.44
41:N1:293:PHE:HE1	73:S8:303:PEE:H7	1.83	0.44
47:QA:147:ARG:HD3	47:QA:149:TRP:CZ2	2.52	0.44
48:QB:310:ILE:HD11	48:QB:388:VAL:HA	1.99	0.44
54:QH:20:SER:O	54:QH:24:GLN:HG2	2.18	0.44
48:Qb:120:LEU:HD13	48:Qb:133:ILE:HG12	2.00	0.44
48:Qb:195:THR:HG21	48:Qb:269:ARG:H	1.83	0.44
48:Qb:225:LYS:HE2	48:Qb:225:LYS:HB3	1.79	0.44
49:Qc:216:ASP:CG	50:Qd:318:ARG:HH22	2.26	0.44
53:Qg:79:GLU:H	53:Qg:79:GLU:HG3	1.48	0.44
56:Qj:41:ILE:H	56:Qj:41:ILE:HD12	1.83	0.44
2:5A:104:PHE:N	38:C4:66:GLU:OE2	2.48	0.43
7:7A:60:CYS:SG	37:C3:19:THR:HG23	2.58	0.43
72:7A:101:3PE:H342	72:7A:101:3PE:H291	2.00	0.43
11:A1:31:ASN:OD1	11:A1:60:TYR:OH	2.23	0.43
14:A5:59:VAL:HG23	14:A5:68:LEU:HD21	1.99	0.43
14:A5:75:GLY:O	16:A7:103:ARG:NH2	2.50	0.43
68:AK:402:CDL:H382	42:N2:133:TRP:HZ3	1.83	0.43
24:B1:30:ARG:O	24:B1:33:GLU:HG2	2.18	0.43
29:B6:82:TRP:O	29:B6:86:GLN:HG2	2.18	0.43
29:B6:122:TYR:HD2	29:B6:124:THR:H	1.66	0.43
35:C1:287:VAL:O	35:C1:290:HIS:HD2	2.00	0.43
41:N1:233:MET:HE3	41:N1:233:MET:HB3	1.88	0.43
48:QB:148:ALA:O	48:QB:152:GLN:HB2	2.18	0.43
56:QJ:9:ARG:HD3	53:Qg:109:ALA:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:S1:594:ALA:O	57:S1:605:GLN:HA	2.17	0.43
2:5A:70:TRP:CH2	3:5B:117:GLY:HA2	2.53	0.43
73:N3:201:PEE:H30	73:N3:201:PEE:H36	1.70	0.43
45:N5:174:TYR:CD2	45:N5:232:TRP:HB3	2.53	0.43
45:N5:559:GLU:O	45:N5:564:LYS:HB2	2.18	0.43
50:Qd:244:ALA:HB3	81:Qd:401:HEC:HBD2	2.00	0.43
58:S2:374:ARG:NH1	64:S8:162:CYS:O	2.38	0.43
5:6B:37:PHE:CE1	5:6B:58:ARG:HB2	2.54	0.43
20:AK:37:ARG:C	20:AK:39:GLN:H	2.25	0.43
20:AK:127:ASP:O	20:AK:132:ARG:NH1	2.50	0.43
35:C1:96:ARG:NE	70:C1:610:PC1:O14	2.44	0.43
41:N1:157:ASN:OD1	41:N1:168:THR:OG1	2.28	0.43
42:N2:249:LEU:HD22	42:N2:254:LEU:HD12	2.00	0.43
45:N5:120:TYR:OH	68:N5:703:CDL:OA4	2.33	0.43
46:N6:77:GLU:N	46:N6:77:GLU:OE1	2.51	0.43
68:QB:501:CDL:H572	71:Qi:301:PLX:H291	2.00	0.43
52:QF:71:LEU:HD22	50:Qd:223:PRO:HG3	2.01	0.43
53:Qg:36:ASP:OD1	53:Qg:90:TYR:OH	2.20	0.43
57:S1:611:THR:HG21	60:S4:105:GLU:HA	2.00	0.43
65:V1:146:GLY:HA3	65:V1:193:PHE:CE1	2.52	0.43
2:5A:92:ASP:OD1	2:5A:135:THR:OG1	2.36	0.43
13:A3:110:ILE:HD11	73:S8:303:PEE:H36	2.01	0.43
16:A7:28:TYR:CZ	22:AM:55:PHE:HB3	2.54	0.43
18:A9:198:ALA:O	18:A9:260:GLY:HA2	2.18	0.43
38:C4:70:TRP:HA	38:C4:73:LEU:HG	2.00	0.43
49:QC:97:HIS:CD2	80:QC:402:HEM:NC	2.86	0.43
49:QC:131:TYR:O	49:QC:134:PRO:HD2	2.18	0.43
58:S2:150:MET:SD	58:S2:228:MET:HB2	2.58	0.43
7:7A:54:ARG:HD2	45:N5:499:MET:HE2	2.00	0.43
16:A7:42:PRO:HG3	23:AN:6:VAL:HG11	1.99	0.43
68:A8:301:CDL:H202	68:A8:301:CDL:H781	2.01	0.43
19:AC:128:PHE:HZ	19:AC:148:ILE:HG12	1.82	0.43
75:AC:201:ZMP:H11A	32:B9:58:VAL:CG2	2.49	0.43
26:B3:47:ARG:HA	26:B3:50:ALA:HB3	1.99	0.43
30:B7:15:LYS:HG2	30:B7:113:LYS:HG3	2.01	0.43
35:C1:71:MET:HB2	35:C1:72:PRO:HD3	2.01	0.43
41:N1:21:THR:HG21	85:S7:201:U10:H311	2.01	0.43
41:N1:295:PRO:HB3	73:N3:201:PEE:H26	2.00	0.43
68:N1:401:CDL:H511	46:N6:83:TRP:HZ3	1.84	0.43
44:N4:405:LEU:HD21	45:N5:173:LEU:HD12	1.99	0.43
45:N5:162:THR:O	45:N5:166:THR:HG23	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N6:24:PRO:O	46:N6:81:GLU:HB2	2.19	0.43
50:QD:105:SER:H	55:Qi:48:ASN:ND2	2.16	0.43
51:QE:239:HIS:HB2	82:QE:303:FES:S1	2.59	0.43
51:QK:20:ARG:HH11	51:QK:23:ALA:HA	1.84	0.43
49:Qc:350:ILE:HG12	72:Qc:404:3PE:H352	1.99	0.43
51:Qe:241:SER:OG	82:Qe:303:FES:S2	2.56	0.43
58:S2:149:SER:HA	58:S2:184:THR:HG22	2.00	0.43
63:S7:53:LEU:HD13	71:S7:203:PLX:H322	2.00	0.43
7:7A:29:LYS:HZ2	70:C3:303:PC1:H3F2	1.84	0.43
72:7A:101:3PE:H3C2	37:C3:41:LEU:HB2	2.01	0.43
9:7C:36:ARG:HH22	73:7C:101:PEE:H3	1.84	0.43
14:A5:9:THR:HG23	14:A5:16:VAL:HG22	2.01	0.43
23:AN:24:ASN:ND2	23:AN:24:ASN:O	2.51	0.43
32:B9:123:ILE:HD13	32:B9:129:GLY:HA3	2.01	0.43
77:C1:601:HEA:H212	77:C1:601:HEA:H271	1.52	0.43
44:N4:70:THR:HA	44:N4:103:GLN:HE21	1.83	0.43
44:N4:357:THR:O	44:N4:361:VAL:HG23	2.19	0.43
57:S1:338:VAL:HB	57:S1:363:SER:HB2	2.00	0.43
57:S1:638:THR:O	57:S1:642:VAL:HG23	2.19	0.43
37:C3:212:SER:HB2	68:C3:305:CDL:H242	2.00	0.43
44:N4:243:MET:HB3	44:N4:301:ILE:HG21	2.00	0.43
45:N5:233:LEU:HB3	45:N5:234:PRO:HD3	2.00	0.43
45:N5:289:ALA:O	45:N5:293:ILE:HG23	2.19	0.43
48:QB:467:ASP:OD2	49:QC:223:TYR:OH	2.28	0.43
49:QC:318:ARG:O	49:QC:322:GLN:HG3	2.19	0.43
70:Qc:405:PC1:H2E1	70:Qc:405:PC1:H3D2	2.00	0.43
58:S2:150:MET:HE3	58:S2:150:MET:HB2	1.93	0.43
65:V1:315:LEU:HB2	65:V1:359:ARG:HA	2.00	0.43
1:4L:16:LEU:HD23	68:4L:201:CDL:H862	2.01	0.43
20:AK:38:LEU:O	20:AK:39:GLN:HG2	2.18	0.43
20:AK:88:PHE:HB2	20:AK:161:LEU:HD23	2.00	0.43
71:AL:202:PLX:H131	68:N4:503:CDL:H121	2.01	0.43
27:B4:48:LEU:HB3	32:B9:208:LEU:HD13	2.01	0.43
41:N1:180:PRO:HB3	73:S8:303:PEE:H21	2.01	0.43
42:N2:135:LYS:O	42:N2:139:LEU:HD12	2.19	0.43
47:QA:123:VAL:HG13	47:QA:137:LEU:HD13	1.99	0.43
47:Qa:51:SER:HB3	47:Qa:230:LEU:HD12	2.00	0.43
49:Qc:30:TRP:HB3	49:Qc:100:ARG:HG3	2.00	0.43
57:S1:144:MET:HG3	58:S2:389:LYS:HG3	2.00	0.43
58:S2:147:TYR:CB	63:S7:71:CYS:HB3	2.49	0.43
63:S7:196:ARG:NE	72:S7:204:3PE:O14	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:V1:384:PRO:HB2	65:V1:423:THR:HG22	2.00	0.43
6:6C:37:TYR:CZ	36:C2:28:LEU:HD23	2.53	0.43
12:A2:57:GLU:O	57:S1:655:ARG:NH2	2.51	0.43
23:AN:68:ARG:O	23:AN:72:MET:HG3	2.18	0.43
30:B7:22:MET:HE1	30:B7:102:PHE:HD2	1.84	0.43
33:BK:107:GLN:HE22	45:N5:194:ASN:ND2	2.14	0.43
35:C1:37:ILE:HG22	77:C1:601:HEA:HMA	2.01	0.43
37:C3:133:ASN:HB3	37:C3:173:PHE:HE2	1.82	0.43
41:N1:142:TYR:CD1	41:N1:142:TYR:C	2.97	0.43
45:N5:96:VAL:O	45:N5:100:ILE:HG12	2.19	0.43
45:N5:172:ILE:O	45:N5:176:ARG:HG2	2.18	0.43
47:QA:89:LEU:HD11	47:QA:154:LEU:HD12	2.00	0.43
47:QA:177:LEU:HD21	47:QA:272:VAL:HG11	2.01	0.43
47:QA:291:HIS:CD2	47:QA:378:LEU:HD13	2.54	0.43
49:QC:102:LEU:HD22	49:QC:304:MET:HE2	2.00	0.43
47:Qa:63:LEU:HD23	47:Qa:141:THR:HG21	2.00	0.43
57:S1:428:LYS:HE2	57:S1:465:ILE:HD13	2.00	0.43
57:S1:695:TYR:HE2	57:S1:714:VAL:HG11	1.84	0.43
65:V1:85:LEU:HD21	65:V1:247:THR:HG23	2.00	0.43
68:4L:201:CDL:H191	68:4L:201:CDL:H152	2.00	0.43
18:A9:201:ILE:HG22	18:A9:203:PRO:HD3	2.01	0.43
19:AC:112:SER:HB2	32:B9:59:LEU:HD21	2.00	0.43
22:AM:61:TRP:HB3	64:S8:89:GLU:HG2	2.01	0.43
35:C1:229:ILE:HD11	36:C2:175:ILE:HG12	2.01	0.43
35:C1:313:ALA:HB3	36:C2:73:LEU:HD11	1.99	0.43
70:C1:610:PC1:H371	37:C3:50:ASN:HD21	1.83	0.43
68:N1:401:CDL:H752	68:N1:401:CDL:H782	1.83	0.43
45:N5:2:ASN:ND2	45:N5:59:GLN:OE1	2.52	0.43
45:N5:341:MET:SD	45:N5:457:LEU:HD12	2.59	0.43
51:QE:125:VAL:HG21	71:Qi:301:PLX:H101	2.00	0.43
51:QE:178:HIS:CE1	51:QE:209:GLU:HB2	2.54	0.43
55:QI:11:TYR:OH	48:Qb:451:ASP:OD2	2.29	0.43
73:Qe:301:PEE:H48	73:Qe:301:PEE:H13	2.00	0.43
57:S1:246:ARG:HH12	60:S4:123:ASN:ND2	2.17	0.43
62:S6:39:THR:HG22	62:S6:62:VAL:HG22	2.01	0.43
65:V1:415:ILE:O	65:V1:419:ILE:HG13	2.19	0.43
7:7A:54:ARG:HE	45:N5:503:GLU:HG2	1.84	0.42
7:7A:75:SER:HA	35:C1:118:VAL:HA	2.00	0.42
13:A3:135:PRO:HB2	23:AN:69:ILE:HD11	2.01	0.42
18:A9:236:VAL:HG22	18:A9:272:LEU:HD23	2.01	0.42
44:N4:412:ILE:HA	44:N4:416:ARG:HD2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:N5:375:ILE:HD12	45:N5:458:LEU:HD11	2.01	0.42
48:Qb:74:TRP:CZ2	48:Qb:411:GLU:HA	2.54	0.42
57:S1:394:VAL:HA	57:S1:473:MET:HE1	2.01	0.42
60:S4:133:ASP:N	60:S4:133:ASP:OD1	2.52	0.42
4:6A:88:ASN:OD1	70:6A:101:PC1:H141	2.19	0.42
71:AM:201:PLX:H182	41:N1:19:PHE:HZ	1.84	0.42
28:B5:71:MET:HE3	44:N4:442:LEU:HD11	2.01	0.42
38:C4:39:VAL:HG22	38:C4:41:ARG:HG3	2.01	0.42
41:N1:197:PRO:HB3	41:N1:278:PRO:O	2.18	0.42
42:N2:91:ASN:HD21	46:N6:117:PHE:HE1	1.67	0.42
45:N5:503:GLU:O	45:N5:507:THR:HG23	2.20	0.42
58:S2:405:ALA:HB1	58:S2:412:GLU:HG3	2.01	0.42
65:V1:112:TYR:CD1	65:V1:153:ALA:HB3	2.54	0.42
66:V2:59:ASN:HD21	66:V2:89:GLN:HB2	1.84	0.42
19:AC:112:SER:HB3	32:B9:59:LEU:HD11	2.02	0.42
20:AK:328:ARG:HH21	34:BL:58:ASP:CG	2.27	0.42
25:B2:59:ARG:HH12	26:B3:48:ASN:HA	1.83	0.42
25:B2:65:THR:HG22	25:B2:67:SER:H	1.84	0.42
30:B7:95:TYR:CZ	31:B8:156:VAL:HG11	2.55	0.42
39:CA:55:TRP:O	39:CA:59:ILE:HG12	2.19	0.42
47:QA:125:CYS:HB3	47:QA:133:LEU:HD22	2.01	0.42
47:QA:183:ARG:NH1	47:Qa:452:GLU:OE1	2.52	0.42
48:QB:426:LEU:HD12	48:QB:426:LEU:HA	1.87	0.42
51:QE:178:HIS:HB2	51:QE:210:TRP:CZ3	2.54	0.42
57:S1:476:LEU:HD22	57:S1:493:VAL:HG21	2.01	0.42
58:S2:112:VAL:HG21	58:S2:453:VAL:HG21	2.02	0.42
19:AC:90:TYR:CE1	26:B3:44:PRO:HB2	2.54	0.42
21:AL:36:VAL:HG22	68:AL:201:CDL:H742	2.01	0.42
25:B2:64:LEU:HD13	25:B2:69:LEU:HD21	2.01	0.42
28:B5:75:ILE:HD12	68:B5:201:CDL:H871	2.00	0.42
29:B6:157:VAL:HG22	45:N5:63:ILE:HG23	2.01	0.42
32:B9:119:PRO:HB3	45:N5:525:MET:HE2	2.01	0.42
37:C3:141:GLY:O	37:C3:144:ILE:HG22	2.19	0.42
41:N1:101:GLY:O	41:N1:105:MET:HG3	2.19	0.42
51:QE:178:HIS:HE1	51:QE:209:GLU:HB2	1.83	0.42
53:QG:36:ASP:OD2	53:QG:62:ARG:NH1	2.50	0.42
49:Qc:97:HIS:HD2	80:Qc:403:HEM:C1C	2.37	0.42
49:Qc:112:THR:HG22	49:Qc:196:HIS:CE1	2.54	0.42
58:S2:62:LYS:O	58:S2:66:HIS:ND1	2.48	0.42
59:S3:120:PRO:HB3	60:S4:137:PHE:CE1	2.55	0.42
64:S8:100:GLU:O	64:S8:170:GLY:N	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:V1:98:LYS:O	65:V1:101:PHE:HB2	2.19	0.42
66:V2:59:ASN:ND2	66:V2:89:GLN:HB2	2.34	0.42
17:A8:246:PHE:HE1	68:A8:301:CDL:H341	1.83	0.42
20:AK:284:PRO:O	20:AK:288:GLN:HG2	2.20	0.42
28:B5:90:ASN:ND2	68:B5:201:CDL:OA7	2.42	0.42
29:B6:134:HIS:NE2	45:N5:35:TYR:OH	2.36	0.42
38:C4:149:LYS:HB3	38:C4:152:PRO:HB3	2.01	0.42
41:N1:293:PHE:O	41:N1:297:THR:OG1	2.34	0.42
47:QA:290:GLN:HG2	47:QA:295:ALA:HB2	2.01	0.42
48:QB:179:MET:HE1	48:QB:282:LEU:HD13	2.01	0.42
52:QF:56:ARG:O	52:QF:60:ARG:HG3	2.19	0.42
54:QH:49:VAL:O	54:QH:52:PRO:HD2	2.19	0.42
51:QK:71:ASN:OD1	51:QK:71:ASN:N	2.52	0.42
48:Qb:79:SER:HB3	48:Qb:126:ARG:HA	2.02	0.42
5:6B:34:TYR:OH	5:6B:74:ASP:OD1	2.24	0.42
33:BK:35:LYS:HE3	33:BK:35:LYS:HB3	1.90	0.42
35:C1:33:LEU:O	35:C1:37:ILE:HG13	2.19	0.42
45:N5:290:LEU:O	45:N5:523:SER:OG	2.37	0.42
49:Qc:267:HIS:CD2	49:Qc:269:LYS:HG2	2.54	0.42
58:S2:230:ALA:O	64:S8:98:ARG:NH2	2.52	0.42
64:S8:99:GLY:O	64:S8:169:GLU:HG2	2.19	0.42
65:V1:51:TRP:CD1	67:V3:388:ASN:HD22	2.38	0.42
73:7C:101:PEE:H34	73:7C:101:PEE:H40	1.76	0.42
14:A5:104:VAL:HG23	59:S3:71:LYS:HG2	2.00	0.42
17:A8:202:LEU:HD13	23:AN:70:ALA:HB2	2.01	0.42
23:AN:141:ILE:HA	70:N1:402:PC1:H153	2.01	0.42
25:B2:90:ASP:OD1	25:B2:90:ASP:N	2.52	0.42
36:C2:37:LEU:O	36:C2:41:ILE:HG12	2.20	0.42
42:N2:190:MET:HG2	42:N2:204:ASN:HB3	2.02	0.42
42:N2:217:MET:HE2	42:N2:326:LEU:HB2	2.02	0.42
45:N5:137:LEU:HD13	45:N5:186:MET:HG2	2.02	0.42
48:QB:172:LEU:HD21	48:QB:202:GLU:HB3	2.02	0.42
51:QE:241:SER:HA	51:QE:252:GLY:HA3	2.02	0.42
52:QF:79:ASP:OD2	50:Qd:237:TYR:OH	2.29	0.42
47:Qa:237:PHE:HE2	47:Qa:238:LEU:HD12	1.84	0.42
47:Qa:293:LEU:HB3	47:Qa:309:LEU:HG	2.00	0.42
49:Qc:267:HIS:HD2	49:Qc:269:LYS:HG2	1.84	0.42
54:Qh:20:SER:O	54:Qh:24:GLN:HG2	2.19	0.42
58:S2:341:GLU:O	58:S2:345:GLN:HG2	2.19	0.42
63:S7:63:TRP:HH2	85:S7:201:U10:H303	1.85	0.42
1:4L:56:ALA:HA	61:S5:18:MET:HE3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5A:83:ASP:HB2	36:C2:52:HIS:ND1	2.34	0.42
15:A6:48:SER:OG	15:A6:106:ASP:OD1	2.35	0.42
19:AB:78:ALA:HA	19:AB:81:ASP:OD2	2.20	0.42
29:B6:132:VAL:O	29:B6:136:LEU:CB	2.67	0.42
77:C1:601:HEA:CMA	77:C1:601:HEA:HBA2	2.50	0.42
70:C1:610:PC1:H2C1	70:C3:302:PC1:H3D2	2.01	0.42
43:N3:73:LEU:HD23	43:N3:73:LEU:HA	1.88	0.42
44:N4:370:PRO:HB2	45:N5:142:ILE:HA	2.01	0.42
46:N6:3:MET:HB3	46:N6:5:ILE:HG12	2.02	0.42
46:N6:24:PRO:HG2	46:N6:28:TYR:HB2	2.01	0.42
47:QA:138:LEU:HD22	47:QA:238:LEU:HD21	2.01	0.42
49:QC:116:GLY:HA3	80:QC:402:HEM:C3C	2.55	0.42
50:QD:248:PRO:HB2	81:QD:401:HEC:HBB2	2.00	0.42
51:QE:130:LYS:HA	72:QE:302:3PE:H2A1	2.01	0.42
48:Qb:184:PHE:O	48:Qb:188:HIS:HD2	2.02	0.42
48:Qb:465:LEU:HD12	48:Qb:466:PRO:HD2	2.02	0.42
57:S1:138:ASP:HB3	57:S1:142:GLN:HE21	1.83	0.42
57:S1:541:PRO:HB3	57:S1:561:PRO:HD3	2.02	0.42
58:S2:164:LEU:HD23	58:S2:164:LEU:HA	1.91	0.42
65:V1:214:GLU:OE2	65:V1:224:ARG:NE	2.26	0.42
2:5A:68:ASP:OD1	2:5A:68:ASP:N	2.52	0.42
9:7C:52:PRO:HG3	35:C1:29:VAL:HG13	2.02	0.42
21:AL:107:SER:HB3	21:AL:110:ILE:HB	2.02	0.42
27:B4:25:ILE:HG21	27:B4:30:ARG:CZ	2.50	0.42
30:B7:99:MET:HG3	31:B8:156:VAL:HG12	2.01	0.42
37:C3:125:ASN:HD21	37:C3:127:LEU:HB2	1.84	0.42
68:CB:203:CDL:HA31	42:N2:238:PRO:HG2	2.02	0.42
44:N4:225:ILE:HD13	44:N4:331:ASN:HB2	2.01	0.42
44:N4:318:ALA:HB1	44:N4:374:ASN:CG	2.45	0.42
45:N5:10:THR:O	45:N5:14:ILE:HG23	2.20	0.42
45:N5:264:TYR:CG	45:N5:265:PRO:HD3	2.55	0.42
45:N5:383:MET:O	45:N5:389:PHE:HB2	2.19	0.42
48:QB:413:ILE:HG12	48:QB:423:ARG:HD2	2.01	0.42
50:QD:247:PRO:HA	50:QD:248:PRO:HD3	1.86	0.42
54:Qh:49:VAL:O	54:Qh:52:PRO:HD2	2.19	0.42
58:S2:142:PHE:HZ	58:S2:428:CYS:HG	1.68	0.42
59:S3:147:THR:HB	59:S3:153:ILE:HD11	2.01	0.42
71:6C:101:PLX:H21	71:6C:101:PLX:H1C3	1.86	0.42
11:A1:19:PRO:HB3	41:N1:9:LEU:HD12	2.00	0.42
23:AN:88:ARG:O	23:AN:92:GLU:HG2	2.19	0.42
30:B7:4:HIS:NE2	31:B8:155:PRO:HD3	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:B9:218:GLU:HG2	32:B9:219:ARG:HG2	2.02	0.42
35:C1:184:PHE:H	35:C1:256:HIS:CE1	2.37	0.42
68:QH:102:CDL:OA7	49:Qc:29:SER:OG	2.37	0.42
48:Qb:315:ASP:HB3	48:Qb:318:TYR:CE1	2.54	0.42
50:Qd:113:ARG:NH1	50:Qd:270:ASP:OD1	2.53	0.42
50:Qd:250:TYR:H	50:Qd:253:VAL:CG2	2.33	0.42
57:S1:49:VAL:HG11	57:S1:80:VAL:HG21	2.02	0.42
58:S2:391:TYR:HD1	64:S8:122:VAL:HG21	1.84	0.42
66:V2:88:ARG:HH11	67:V3:396:THR:HG23	1.85	0.42
18:A9:37:HIS:CD2	18:A9:39:ALA:H	2.37	0.41
68:AK:402:CDL:H162	68:AK:402:CDL:H361	2.01	0.41
22:AM:85:GLU:HG2	22:AM:86:TRP:H	1.85	0.41
24:B1:42:SER:O	24:B1:46:LYS:HB2	2.20	0.41
25:B2:59:ARG:NH2	26:B3:48:ASN:OD1	2.44	0.41
26:B3:24:ILE:O	26:B3:30:GLU:HB3	2.20	0.41
30:B7:92:HIS:O	30:B7:96:VAL:HG13	2.20	0.41
31:B8:164:ASN:HA	31:B8:181:VAL:HB	2.01	0.41
32:B9:147:ASP:HB3	32:B9:164:ARG:HH12	1.84	0.41
35:C1:316:THR:HG21	77:C1:602:HEA:C14	2.51	0.41
42:N2:186:HIS:O	42:N2:190:MET:HG3	2.20	0.41
45:N5:11:THR:HG22	45:N5:46:LEU:HB3	2.01	0.41
47:QA:63:LEU:HD23	47:QA:141:THR:HG21	2.02	0.41
48:QB:279:ASP:H	48:QB:460:GLY:HA3	1.85	0.41
62:S6:104:LYS:HE2	62:S6:104:LYS:HB2	1.82	0.41
63:S7:94:ARG:HD3	85:S7:201:U10:H253	2.01	0.41
2:5A:70:TRP:HH2	3:5B:117:GLY:HA2	1.85	0.41
10:8B:27:ALA:HB2	35:C1:404:THR:HG21	2.02	0.41
11:A1:13:ALA:HB2	41:N1:264:LEU:HD11	2.01	0.41
17:A8:200:GLY:N	23:AN:66:GLU:OE2	2.45	0.41
19:AB:134:ASP:HA	19:AB:137:LYS:HE2	2.00	0.41
22:AM:127:TYR:OH	62:S6:61:GLU:O	2.27	0.41
71:AM:201:PLX:H271	71:S7:203:PLX:H111	2.02	0.41
32:B9:144:TRP:HA	32:B9:147:ASP:OD2	2.20	0.41
36:C2:104:TRP:CD2	36:C2:203:ASN:HB2	2.56	0.41
72:N5:706:3PE:H3D1	72:N5:706:3PE:H391	2.02	0.41
48:QB:74:TRP:HB3	48:QB:418:LEU:HD11	2.02	0.41
49:QC:30:TRP:HB3	49:QC:100:ARG:HG3	2.02	0.41
51:QE:169:TRP:HZ2	51:QE:274:GLY:HA2	1.84	0.41
57:S1:130:ILE:HG23	64:S8:114:ILE:HD12	2.02	0.41
57:S1:382:ARG:C	57:S1:384:ASN:H	2.28	0.41
57:S1:432:ILE:HD11	57:S1:455:ILE:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:V1:155:TYR:OH	66:V2:69:ASN:O	2.26	0.41
66:V2:137:THR:HG22	66:V2:138:THR:H	1.85	0.41
18:A9:357:ARG:HD3	18:A9:361:TRP:O	2.20	0.41
31:B8:162:PRO:HB2	31:B8:163:TYR:CD2	2.54	0.41
35:C1:352:GLY:HA2	77:C1:602:HEA:H121	2.02	0.41
36:C2:30:ILE:HG21	36:C2:76:ILE:HD11	2.02	0.41
39:CA:47:THR:HG23	40:CB:65:LEU:HD22	2.01	0.41
45:N5:420:ALA:HB1	45:N5:498:PHE:CD1	2.55	0.41
50:QD:235:ASN:O	50:QD:241:GLN:HA	2.21	0.41
49:Qc:131:TYR:O	49:Qc:134:PRO:HD2	2.19	0.41
85:S7:201:U10:H271	85:S7:201:U10:H251	1.70	0.41
20:AK:260:TYR:HB3	20:AK:264:GLU:HB2	2.02	0.41
22:AM:84:PRO:HB3	64:S8:197:TRP:CE3	2.55	0.41
29:B6:72:LEU:HD23	29:B6:72:LEU:HA	1.92	0.41
31:B8:96:ASP:OD1	31:B8:96:ASP:N	2.50	0.41
35:C1:386:VAL:HG11	77:C1:601:HEA:H261	2.03	0.41
37:C3:253:TYR:HA	37:C3:257:TYR:HD1	1.85	0.41
37:C3:255:SER:O	37:C3:259:TRP:HB3	2.21	0.41
41:N1:18:ALA:HB1	41:N1:48:PRO:HB3	2.01	0.41
44:N4:122:PHE:HE2	44:N4:206:LYS:HG3	1.85	0.41
71:N4:502:PLX:H22	71:N4:502:PLX:H1A3	1.79	0.41
45:N5:28:LYS:HD3	45:N5:28:LYS:HA	1.91	0.41
45:N5:193:SER:OG	45:N5:204:LEU:HD12	2.20	0.41
48:QB:183:VAL:HG21	48:QB:286:HIS:HB3	2.02	0.41
53:QG:46:GLU:OE2	53:QG:50:ARG:NH2	2.50	0.41
47:Qa:123:VAL:HB	47:Qa:133:LEU:HD23	2.01	0.41
51:Qe:199:GLN:HE22	51:Qe:204:ARG:HH11	1.67	0.41
57:S1:408:ARG:HD2	57:S1:439:THR:HG23	2.02	0.41
58:S2:135:TYR:HE1	58:S2:417:LEU:HD21	1.86	0.41
58:S2:363:LYS:HD3	58:S2:370:SER:HB2	2.01	0.41
65:V1:119:GLU:HA	86:V1:502:FMN:HM71	2.02	0.41
73:A9:402:PEE:H26	73:A9:402:PEE:H32	1.80	0.41
22:AM:144:TYR:HD1	22:AM:144:TYR:H	1.68	0.41
30:B7:34:ARG:HH21	31:B8:186:ILE:HB	1.86	0.41
35:C1:460:ILE:HG12	38:C4:114:THR:HG21	2.02	0.41
44:N4:176:PHE:HA	44:N4:179:ILE:HG12	2.02	0.41
47:QA:155:GLN:NE2	47:QA:198:GLY:H	2.17	0.41
47:QA:257:GLU:HG3	47:QA:438:MET:HB3	2.02	0.41
51:QE:155:LYS:HZ2	51:QE:158:ASP:CG	2.29	0.41
47:Qa:92:LYS:HB2	47:Qa:143:ALA:HB1	2.02	0.41
48:Qb:183:VAL:HG21	48:Qb:286:HIS:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Qe:153:GLU:HG2	51:Qe:272:ILE:HG12	2.02	0.41
58:S2:116:ASP:OD2	58:S2:118:HIS:NE2	2.54	0.41
59:S3:157:VAL:HG21	59:S3:182:PRO:HD3	2.01	0.41
4:6A:81:LEU:HD22	70:6A:101:PC1:H221	2.02	0.41
5:6B:26:GLN:NE2	5:6B:29:ASN:HD22	2.18	0.41
18:A9:76:MET:HE2	18:A9:76:MET:HB3	1.90	0.41
19:AC:140:CYS:HB3	19:AC:143:GLU:HG3	2.03	0.41
20:AK:131:TYR:OH	20:AK:188:HIS:ND1	2.34	0.41
21:AL:39:TYR:CZ	68:AL:201:CDL:H592	2.56	0.41
36:C2:1:MET:HB3	36:C2:193:TYR:CD1	2.56	0.41
71:CB:201:PLX:H302	71:CB:201:PLX:H271	1.88	0.41
41:N1:307:LEU:HB3	41:N1:308:PRO:HD3	2.03	0.41
42:N2:5:ILE:O	42:N2:8:THR:HG22	2.20	0.41
45:N5:174:TYR:HD2	45:N5:232:TRP:HB3	1.86	0.41
48:QB:96:LEU:HD13	48:QB:156:LEU:HD22	2.01	0.41
48:QB:280:ASP:HA	48:QB:461:PRO:HB3	2.02	0.41
50:QD:293:MET:HA	73:QE:301:PEE:H49	2.02	0.41
51:QE:223:VAL:HG23	49:Qc:264:THR:HG23	2.02	0.41
48:Qb:190:THR:HB	48:Qb:275:ILE:HG13	2.02	0.41
51:Qe:220:LEU:HD12	51:Qe:239:HIS:CE1	2.55	0.41
2:5A:66:ASP:OD1	2:5A:66:ASP:N	2.52	0.41
3:5B:105:VAL:HG12	3:5B:122:LEU:HB2	2.02	0.41
7:7A:68:LEU:HD21	35:C1:110:LEU:HD11	2.01	0.41
68:AL:201:CDL:H322	68:AL:201:CDL:H352	1.90	0.41
27:B4:4:PRO:HD2	32:B9:115:TYR:CE1	2.56	0.41
27:B4:77:TYR:OH	45:N5:564:LYS:HG2	2.21	0.41
33:BK:74:ILE:O	40:CB:111:TYR:HB2	2.21	0.41
70:C1:610:PC1:H381	70:C1:610:PC1:H352	1.97	0.41
38:C4:149:LYS:O	38:C4:152:PRO:HD3	2.20	0.41
41:N1:198:PHE:CD1	41:N1:285:LEU:HD13	2.55	0.41
44:N4:119:TYR:HA	44:N4:122:PHE:HD1	1.84	0.41
51:QE:196:ARG:NH1	51:QE:254:ALA:O	2.54	0.41
51:QE:207:LYS:HG2	51:QE:209:GLU:HG2	2.01	0.41
56:QJ:23:MET:O	56:QJ:27:VAL:HG23	2.20	0.41
49:Qc:197:LEU:HD11	80:Qc:403:HEM:HMA2	2.03	0.41
50:Qd:232:LEU:HD13	50:Qd:242:ALA:HB1	2.02	0.41
57:S1:534:VAL:HG23	57:S1:537:ILE:HD12	2.03	0.41
2:5A:109:ARG:NH2	38:C4:82:TYR:OH	2.45	0.41
28:B5:113:PHE:O	28:B5:119:ARG:NH1	2.48	0.41
28:B5:133:TYR:OH	33:BK:87:GLU:OE1	2.34	0.41
35:C1:62:ALA:HB2	77:C1:601:HEA:HBD1	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C1:417:MET:O	35:C1:421:VAL:HG22	2.21	0.41
37:C3:79:LEU:HB3	37:C3:233:PHE:CE2	2.56	0.41
37:C3:173:PHE:HD1	37:C3:208:VAL:HG11	1.86	0.41
45:N5:15:LEU:HD23	45:N5:15:LEU:HA	1.93	0.41
49:QC:53:MET:HE2	49:Qc:181:PHE:CE1	2.56	0.41
49:QC:58:ASP:O	49:QC:62:ALA:N	2.51	0.41
51:QK:21:GLY:O	47:Qa:88:SER:OG	2.35	0.41
51:Qe:88:PHE:O	51:Qe:92:ARG:HG3	2.21	0.41
52:Qf:42:LYS:HE2	52:Qf:42:LYS:HB3	1.92	0.41
58:S2:46:ASP:OD1	58:S2:46:ASP:N	2.53	0.41
58:S2:448:HIS:HB3	58:S2:452:ASP:HB2	2.03	0.41
63:S7:85:ASP:O	63:S7:88:ARG:HB3	2.20	0.41
1:4L:80:MET:SD	46:N6:172:THR:HA	2.60	0.41
4:6A:76:ASP:OD1	4:6A:76:ASP:N	2.54	0.41
4:6A:88:ASN:CG	70:6A:101:PC1:H131	2.45	0.41
7:7A:29:LYS:NZ	70:C3:303:PC1:H3F2	2.36	0.41
7:7A:69:TYR:CE2	72:7A:101:3PE:H281	2.56	0.41
20:AK:352:LYS:HE2	20:AK:352:LYS:HB2	1.92	0.41
21:AL:45:PRO:HA	21:AL:46:PRO:HD3	1.92	0.41
29:B6:164:ILE:HB	30:B7:48:ASP:HB3	2.02	0.41
31:B8:110:ASP:HB3	44:N4:278:ARG:NH1	2.36	0.41
32:B9:146:LEU:HD21	32:B9:160:TYR:HE2	1.85	0.41
35:C1:18:LEU:HB3	35:C1:102:PHE:CZ	2.55	0.41
35:C1:33:LEU:HB3	35:C1:61:HIS:HB2	2.02	0.41
35:C1:459:PHE:HB3	38:C4:114:THR:HG23	2.03	0.41
36:C2:32:PHE:HD1	36:C2:32:PHE:HA	1.74	0.41
37:C3:231:HIS:HB3	70:C3:302:PC1:H133	2.01	0.41
41:N1:267:THR:O	41:N1:271:LEU:HG	2.21	0.41
42:N2:128:LEU:HD12	42:N2:216:PHE:HB3	2.03	0.41
45:N5:13:THR:O	45:N5:17:ILE:HG13	2.21	0.41
45:N5:230:HIS:N	45:N5:231:PRO:HD3	2.36	0.41
47:QA:82:LEU:HD23	47:QA:205:LEU:HD11	2.02	0.41
48:QB:179:MET:O	48:QB:183:VAL:HG23	2.21	0.41
49:QC:51:LEU:HD13	80:QC:401:HEM:HBD1	2.03	0.41
49:Qc:5:ARG:HH11	49:Qc:15:ASN:HD21	1.68	0.41
73:Qe:301:PEE:H81	73:Qe:301:PEE:H75	1.87	0.41
56:Qj:2:LEU:HD22	56:Qj:4:ARG:HG2	2.02	0.41
57:S1:86:PRO:O	57:S1:108:LYS:NZ	2.53	0.41
58:S2:165:LEU:HD21	58:S2:397:VAL:HG22	2.02	0.41
73:S2:501:PEE:H13	73:S2:501:PEE:H1	1.77	0.41
64:S8:98:ARG:HB3	64:S8:169:GLU:CD	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:V1:110:PRO:HD2	65:V1:238:CYS:SG	2.60	0.41
65:V1:201:ALA:HB3	66:V2:119:TYR:CD1	2.55	0.41
66:V2:152:ILE:HG21	66:V2:171:LEU:HD13	2.02	0.41
11:A1:65:GLY:HA2	17:A8:97:VAL:HG12	2.02	0.41
19:AB:137:LYS:HE3	19:AB:137:LYS:HB2	1.93	0.41
20:AK:67:ASN:ND2	20:AK:68:ILE:H	2.19	0.41
35:C1:37:ILE:HG21	77:C1:601:HEA:HMA	2.03	0.41
41:N1:288:LEU:O	41:N1:292:SER:HB2	2.20	0.41
45:N5:264:TYR:CD2	45:N5:265:PRO:HD3	2.56	0.41
49:Qc:237:LEU:HB2	50:Qd:297:MET:HG2	2.02	0.41
66:V2:237:PRO:HA	66:V2:238:PRO:HD3	1.95	0.41
15:A6:63:ARG:HH12	19:AB:132:ASP:HA	1.86	0.40
23:AN:36:PHE:O	23:AN:40:ILE:HG12	2.21	0.40
33:BK:99:ASP:OD2	33:BK:142:ARG:NH1	2.54	0.40
35:C1:468:MET:HE2	35:C1:468:MET:HB3	1.97	0.40
70:C3:302:PC1:H272	70:C3:302:PC1:H241	1.84	0.40
68:CB:203:CDL:H851	68:CB:203:CDL:H242	2.03	0.40
45:N5:128:MET:HE2	45:N5:147:VAL:HG11	2.02	0.40
45:N5:297:ASP:O	45:N5:301:ILE:HG13	2.21	0.40
48:QB:324:MET:HE2	48:QB:324:MET:HB2	1.90	0.40
54:QH:6:GLY:HA3	48:Qb:363:MET:SD	2.61	0.40
57:S1:185:PHE:CZ	57:S1:221:ASN:HB2	2.56	0.40
57:S1:306:MET:HE2	57:S1:314:LEU:HB3	2.03	0.40
64:S8:150:THR:HG21	64:S8:180:HIS:CD2	2.56	0.40
68:4L:201:CDL:H172	68:4L:201:CDL:H211	2.03	0.40
4:6A:48:TRP:HE3	4:6A:49:LEU:HD12	1.86	0.40
9:7C:49:PHE:HE2	10:8B:54:ALA:HB2	1.85	0.40
68:B5:201:CDL:H362	33:BK:45:VAL:HG12	2.03	0.40
35:C1:74:MET:SD	35:C1:249:PRO:HG2	2.61	0.40
35:C1:474:GLU:OE2	35:C1:478:SER:OG	2.37	0.40
70:C1:610:PC1:H131	37:C3:71:HIS:NE2	2.35	0.40
39:CA:31:ILE:HG23	39:CA:32:ARG:HG3	2.03	0.40
41:N1:228:TYR:HA	41:N1:231:ILE:HD12	2.03	0.40
43:N3:90:MET:SD	46:N6:151:THR:HG23	2.61	0.40
45:N5:208:CYS:HA	45:N5:209:PRO:HD3	1.78	0.40
45:N5:395:ILE:O	45:N5:399:VAL:HG23	2.21	0.40
48:QB:100:GLY:HA2	48:QB:106:GLY:N	2.30	0.40
49:QC:97:HIS:CD2	80:QC:402:HEM:C1C	3.09	0.40
68:QH:102:CDL:H721	68:QH:102:CDL:H311	2.02	0.40
55:QI:9:ARG:O	55:QI:13:LEU:HB2	2.21	0.40
57:S1:249:GLU:OE1	60:S4:78:ARG:NH2	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:S7:53:LEU:HB2	71:S7:203:PLX:H301	2.03	0.40
68:7A:102:CDL:H811	68:7A:102:CDL:H782	1.77	0.40
19:AB:115:GLN:O	19:AB:119:ILE:HG12	2.21	0.40
20:AK:232:THR:HG23	20:AK:235:TYR:H	1.86	0.40
71:AM:201:PLX:H182	41:N1:19:PHE:CZ	2.57	0.40
27:B4:59:VAL:HG22	44:N4:423:ILE:HG12	2.02	0.40
35:C1:100:MET:N	37:C3:17:PRO:HB3	2.36	0.40
35:C1:115:SER:OG	35:C1:142:SER:O	2.38	0.40
35:C1:204:ALA:O	35:C1:208:MET:HG3	2.21	0.40
37:C3:57:TRP:O	37:C3:61:ILE:HG13	2.22	0.40
38:C4:148:MET:HG3	38:C4:150:VAL:HG23	2.03	0.40
41:N1:195:ARG:HD3	41:N1:231:ILE:HD11	2.02	0.40
54:QH:72:ARG:HD3	54:QH:72:ARG:HA	1.93	0.40
56:Qj:23:MET:O	56:Qj:27:VAL:HG23	2.22	0.40
57:S1:59:GLN:NE2	60:S4:89:SER:O	2.53	0.40
58:S2:98:HIS:HB2	58:S2:464:PHE:HE2	1.86	0.40
59:S3:213:ASP:HB3	59:S3:216:VAL:HG22	2.03	0.40
4:6A:28:TRP:HB3	37:C3:146:TRP:HB2	2.03	0.40
7:7A:48:THR:HG21	70:C3:303:PC1:H2A2	2.03	0.40
16:A7:12:ARG:HB3	16:A7:20:LEU:HD12	2.02	0.40
35:C1:409:TRP:CZ3	35:C1:467:LEU:HD11	2.56	0.40
73:N3:201:PEE:H49	73:N3:201:PEE:H8	1.71	0.40
45:N5:332:HIS:HA	45:N5:335:PHE:CZ	2.57	0.40
47:QA:326:PHE:HA	51:QK:61:GLY:HA2	2.03	0.40
49:QC:28:SER:HB2	68:QC:404:CDL:HB22	2.03	0.40
49:QC:310:SER:HA	49:QC:374:ASN:HD21	1.85	0.40
51:QE:125:VAL:HG11	71:Qi:301:PLX:H122	2.02	0.40
51:QE:176:VAL:HG22	51:QE:212:ILE:HG12	2.03	0.40
49:Qc:116:GLY:HA3	80:Qc:403:HEM:C3C	2.56	0.40
50:Qd:200:TYR:O	50:Qd:204:ALA:CB	2.69	0.40
73:Qe:301:PEE:H62	73:Qe:301:PEE:H68	1.80	0.40
57:S1:63:PHE:HZ	57:S1:117:MET:HE1	1.87	0.40
58:S2:139:LEU:HB3	58:S2:140:PRO:HD3	2.03	0.40
1:4L:41:PHE:O	1:4L:45:THR:HG22	2.21	0.40
12:A2:46:LYS:HE3	12:A2:46:LYS:HB2	1.85	0.40
14:A5:49:GLU:O	14:A5:53:ASN:ND2	2.55	0.40
18:A9:217:PHE:HA	18:A9:220:MET:HE2	2.04	0.40
18:A9:344:PRO:HG2	18:A9:347:LEU:HD13	2.04	0.40
22:AM:85:GLU:H	22:AM:85:GLU:CD	2.30	0.40
24:B1:43:LEU:O	33:BK:69:ARG:HD2	2.22	0.40
25:B2:101:PRO:HD2	30:B7:99:MET:HE1	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BK:43:ARG:HB2	33:BK:44:PRO:HD3	2.03	0.40
35:C1:456:MET:HA	38:C4:118:LEU:HD21	2.03	0.40
37:C3:86:PHE:HZ	70:C3:302:PC1:H3C1	1.87	0.40
41:N1:149:ILE:HG21	41:N1:185:TRP:HB2	2.03	0.40
43:N3:97:LEU:HD23	43:N3:97:LEU:HA	1.91	0.40
45:N5:293:ILE:HD11	68:N5:704:CDL:H721	2.04	0.40
47:QA:83:LEU:HD23	47:QA:83:LEU:HA	1.90	0.40
48:QB:87:ASN:HD22	48:QB:204:PRO:HD3	1.86	0.40
53:QG:44:VAL:O	53:QG:48:ILE:HG12	2.22	0.40
56:QJ:4:ARG:HA	53:Qg:110:LYS:HD3	2.02	0.40
56:QJ:18:ILE:HD13	56:QJ:18:ILE:HA	1.89	0.40
51:QK:34:LEU:HA	51:QK:35:PRO:HD3	1.97	0.40
50:Qd:243:ILE:HG12	50:Qd:245:MET:H	1.85	0.40
53:Qg:46:GLU:HA	53:Qg:49:ARG:HG2	2.03	0.40
58:S2:157:TYR:O	58:S2:161:VAL:HG23	2.22	0.40
58:S2:196:HIS:O	58:S2:200:ILE:HG12	2.21	0.40
65:V1:302:LYS:HE3	65:V1:303:HIS:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	4L	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
2	5A	100/102 (98%)	100 (100%)	0	0	100	100
3	5B	93/95 (98%)	91 (98%)	2 (2%)	0	100	100
4	6A	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
5	6B	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
6	6C	68/70 (97%)	68 (100%)	0	0	100	100
7	7A	55/57 (96%)	55 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	7B	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
9	7C	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
10	8B	41/43 (95%)	41 (100%)	0	0	100	100
11	A1	68/70 (97%)	68 (100%)	0	0	100	100
12	A2	83/85 (98%)	79 (95%)	4 (5%)	0	100	100
13	A3	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
14	A5	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
15	A6	112/114 (98%)	108 (96%)	3 (3%)	1 (1%)	14	28
16	A7	93/112 (83%)	91 (98%)	2 (2%)	0	100	100
17	A8	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
18	A9	339/341 (99%)	331 (98%)	8 (2%)	0	100	100
19	AB	75/87 (86%)	74 (99%)	1 (1%)	0	100	100
19	AC	85/87 (98%)	85 (100%)	0	0	100	100
20	AK	319/321 (99%)	310 (97%)	9 (3%)	0	100	100
21	AL	138/140 (99%)	138 (100%)	0	0	100	100
22	AM	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
23	AN	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
24	B1	54/56 (96%)	54 (100%)	0	0	100	100
25	B2	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
26	B3	78/80 (98%)	77 (99%)	1 (1%)	0	100	100
27	B4	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
28	B5	136/138 (99%)	135 (99%)	1 (1%)	0	100	100
29	B6	99/126 (79%)	94 (95%)	5 (5%)	0	100	100
30	B7	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
31	B8	154/156 (99%)	151 (98%)	3 (2%)	0	100	100
32	B9	176/178 (99%)	174 (99%)	2 (1%)	0	100	100
33	BK	172/174 (99%)	171 (99%)	1 (1%)	0	100	100
34	BL	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
35	C1	512/514 (100%)	498 (97%)	14 (3%)	0	100	100
36	C2	226/228 (99%)	219 (97%)	7 (3%)	0	100	100
37	C3	258/260 (99%)	252 (98%)	6 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	C4	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
39	CA	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
40	CB	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
41	N1	316/318 (99%)	309 (98%)	7 (2%)	0	100	100
42	N2	345/347 (99%)	337 (98%)	8 (2%)	0	100	100
43	N3	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
44	N4	457/459 (100%)	448 (98%)	9 (2%)	0	100	100
45	N5	601/603 (100%)	576 (96%)	25 (4%)	0	100	100
46	N6	172/174 (99%)	163 (95%)	9 (5%)	0	100	100
47	QA	417/419 (100%)	407 (98%)	10 (2%)	0	100	100
47	Qa	417/419 (100%)	408 (98%)	9 (2%)	0	100	100
48	QB	444/446 (100%)	431 (97%)	13 (3%)	0	100	100
48	Qb	429/446 (96%)	424 (99%)	5 (1%)	0	100	100
49	QC	377/379 (100%)	374 (99%)	3 (1%)	0	100	100
49	Qc	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
50	QD	239/241 (99%)	231 (97%)	8 (3%)	0	100	100
50	Qd	237/241 (98%)	233 (98%)	4 (2%)	0	100	100
51	QE	194/274 (71%)	189 (97%)	5 (3%)	0	100	100
51	QK	69/274 (25%)	69 (100%)	0	0	100	100
51	Qe	194/274 (71%)	189 (97%)	5 (3%)	0	100	100
52	QF	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
52	Qf	62/67 (92%)	62 (100%)	0	0	100	100
53	QG	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
53	Qg	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
54	QH	76/79 (96%)	74 (97%)	2 (3%)	0	100	100
54	Qh	77/79 (98%)	77 (100%)	0	0	100	100
55	QI	60/62 (97%)	60 (100%)	0	0	100	100
55	Qi	58/62 (94%)	58 (100%)	0	0	100	100
56	QJ	47/52 (90%)	46 (98%)	1 (2%)	0	100	100
56	Qj	49/52 (94%)	46 (94%)	3 (6%)	0	100	100
57	S1	687/689 (100%)	663 (96%)	24 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	S2	427/430 (99%)	413 (97%)	14 (3%)	0	100	100
59	S3	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
60	S4	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
61	S5	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
62	S6	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
63	S7	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
64	S8	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
65	V1	429/431 (100%)	411 (96%)	18 (4%)	0	100	100
66	V2	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
67	V3	40/42 (95%)	37 (92%)	3 (8%)	0	100	100
All	All	13972/14569 (96%)	13630 (98%)	341 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	A6	49	ARG

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	4L	85/85 (100%)	85 (100%)	0	100	100
2	5A	89/89 (100%)	88 (99%)	1 (1%)	65	81
3	5B	80/80 (100%)	78 (98%)	2 (2%)	42	66
4	6A	66/66 (100%)	66 (100%)	0	100	100
5	6B	73/73 (100%)	72 (99%)	1 (1%)	59	78
6	6C	57/57 (100%)	57 (100%)	0	100	100
7	7A	48/48 (100%)	48 (100%)	0	100	100
8	7B	39/39 (100%)	38 (97%)	1 (3%)	40	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	7C	40/40 (100%)	39 (98%)	1 (2%)	42	66
10	8B	37/37 (100%)	37 (100%)	0	100	100
11	A1	58/58 (100%)	58 (100%)	0	100	100
12	A2	76/76 (100%)	75 (99%)	1 (1%)	61	79
13	A3	69/69 (100%)	69 (100%)	0	100	100
14	A5	99/99 (100%)	98 (99%)	1 (1%)	68	83
15	A6	107/107 (100%)	107 (100%)	0	100	100
16	A7	87/97 (90%)	83 (95%)	4 (5%)	24	48
17	A8	153/153 (100%)	153 (100%)	0	100	100
18	A9	295/295 (100%)	292 (99%)	3 (1%)	68	83
19	AB	71/80 (89%)	71 (100%)	0	100	100
19	AC	80/80 (100%)	79 (99%)	1 (1%)	61	79
20	AK	284/284 (100%)	281 (99%)	3 (1%)	65	81
21	AL	101/101 (100%)	100 (99%)	1 (1%)	68	83
22	AM	130/130 (100%)	128 (98%)	2 (2%)	57	77
23	AN	123/123 (100%)	123 (100%)	0	100	100
24	B1	53/53 (100%)	53 (100%)	0	100	100
25	B2	62/62 (100%)	62 (100%)	0	100	100
26	B3	62/62 (100%)	62 (100%)	0	100	100
27	B4	113/113 (100%)	113 (100%)	0	100	100
28	B5	121/121 (100%)	121 (100%)	0	100	100
29	B6	98/119 (82%)	98 (100%)	0	100	100
30	B7	112/112 (100%)	112 (100%)	0	100	100
31	B8	141/141 (100%)	141 (100%)	0	100	100
32	B9	159/159 (100%)	159 (100%)	0	100	100
33	BK	155/155 (100%)	155 (100%)	0	100	100
34	BL	91/91 (100%)	91 (100%)	0	100	100
35	C1	425/425 (100%)	423 (100%)	2 (0%)	81	90
36	C2	212/212 (100%)	205 (97%)	7 (3%)	33	58
37	C3	224/224 (100%)	223 (100%)	1 (0%)	84	92
38	C4	123/123 (100%)	122 (99%)	1 (1%)	73	86

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	CA	45/45 (100%)	45 (100%)	0	100	100
40	CB	108/108 (100%)	108 (100%)	0	100	100
41	N1	275/275 (100%)	272 (99%)	3 (1%)	65	81
42	N2	311/311 (100%)	311 (100%)	0	100	100
43	N3	100/100 (100%)	99 (99%)	1 (1%)	68	83
44	N4	410/410 (100%)	408 (100%)	2 (0%)	81	90
45	N5	537/537 (100%)	534 (99%)	3 (1%)	78	89
46	N6	140/140 (100%)	139 (99%)	1 (1%)	76	87
47	QA	330/330 (100%)	328 (99%)	2 (1%)	78	89
47	Qa	330/330 (100%)	323 (98%)	7 (2%)	47	70
48	QB	372/372 (100%)	370 (100%)	2 (0%)	81	90
48	Qb	362/372 (97%)	360 (99%)	2 (1%)	78	89
49	QC	332/332 (100%)	327 (98%)	5 (2%)	57	77
49	Qc	332/332 (100%)	329 (99%)	3 (1%)	70	84
50	QD	206/206 (100%)	205 (100%)	1 (0%)	81	90
50	Qd	204/206 (99%)	203 (100%)	1 (0%)	81	90
51	QE	166/225 (74%)	165 (99%)	1 (1%)	78	89
51	QK	55/225 (24%)	54 (98%)	1 (2%)	51	73
51	Qe	166/225 (74%)	166 (100%)	0	100	100
52	QF	64/64 (100%)	63 (98%)	1 (2%)	55	76
52	Qf	61/64 (95%)	61 (100%)	0	100	100
53	QG	93/93 (100%)	93 (100%)	0	100	100
53	Qg	93/93 (100%)	92 (99%)	1 (1%)	65	81
54	QH	70/70 (100%)	70 (100%)	0	100	100
54	Qh	70/70 (100%)	70 (100%)	0	100	100
55	QI	50/50 (100%)	49 (98%)	1 (2%)	48	71
55	Qi	49/50 (98%)	48 (98%)	1 (2%)	48	71
56	QJ	40/42 (95%)	40 (100%)	0	100	100
56	Qj	41/42 (98%)	40 (98%)	1 (2%)	43	67
57	S1	579/579 (100%)	576 (100%)	3 (0%)	81	90
58	S2	370/370 (100%)	367 (99%)	3 (1%)	73	86

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	S3	190/190 (100%)	188 (99%)	2 (1%)	65	81
60	S4	112/112 (100%)	110 (98%)	2 (2%)	51	73
61	S5	93/93 (100%)	93 (100%)	0	100	100
62	S6	79/79 (100%)	79 (100%)	0	100	100
63	S7	132/132 (100%)	130 (98%)	2 (2%)	57	77
64	S8	151/151 (100%)	150 (99%)	1 (1%)	76	87
65	V1	344/344 (100%)	338 (98%)	6 (2%)	53	75
66	V2	183/183 (100%)	181 (99%)	2 (1%)	65	81
67	V3	41/41 (100%)	41 (100%)	0	100	100
All	All	12184/12531 (97%)	12090 (99%)	94 (1%)	70	86

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	5A	92	ASP
3	5B	43	GLN
3	5B	97	ASN
5	6B	14	THR
8	7B	63	GLU
9	7C	60	LEU
12	A2	85	ASP
14	A5	113	LYS
16	A7	5	THR
16	A7	7	VAL
16	A7	31	ILE
16	A7	43	VAL
18	A9	36	LEU
18	A9	129	LEU
18	A9	184	LYS
19	AC	112	SER
20	AK	97	ASP
20	AK	167	SER
20	AK	251	MET
21	AL	115	CYS
22	AM	78	ASP
22	AM	144	TYR
35	C1	81	TRP
35	C1	406	ASN
36	C2	63	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	C2	111	THR
36	C2	114	GLU
36	C2	142	VAL
36	C2	172	THR
36	C2	205	SER
36	C2	207	MET
37	C3	5	THR
38	C4	109	PHE
41	N1	87	VAL
41	N1	251	THR
41	N1	282	TYR
43	N3	38	GLU
44	N4	122	PHE
44	N4	375	LEU
45	N5	286	LEU
45	N5	340	PHE
45	N5	503	GLU
46	N6	135	PHE
47	QA	70	ARG
47	QA	450	VAL
48	QB	324	MET
48	QB	462	ILE
49	QC	2	THR
49	QC	108	MET
49	QC	112	THR
49	QC	281	LEU
49	QC	345	HIS
50	QD	254	LEU
51	QE	211	VAL
52	QF	43	CYS
55	QI	13	LEU
51	QK	14	VAL
47	Qa	129	ASP
47	Qa	133	LEU
47	Qa	168	ASN
47	Qa	220	LEU
47	Qa	238	LEU
47	Qa	323	VAL
47	Qa	393	LEU
48	Qb	83	ASN
48	Qb	92	PHE
49	Qc	59	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	Qc	112	THR
49	Qc	345	HIS
50	Qd	209	GLU
53	Qg	79	GLU
55	Qi	18	THR
56	Qj	2	LEU
57	S1	41	VAL
57	S1	232	THR
57	S1	690	THR
58	S2	143	ASP
58	S2	204	THR
58	S2	459	THR
59	S3	85	GLU
59	S3	145	THR
60	S4	86	ASN
60	S4	133	ASP
63	S7	71	CYS
63	S7	142	TYR
64	S8	73	THR
65	V1	212	LEU
65	V1	282	VAL
65	V1	347	THR
65	V1	379	CYS
65	V1	417	LYS
65	V1	457	HIS
66	V2	137	THR
66	V2	249	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (257) such sidechains are listed below:

Mol	Chain	Res	Type
1	4L	7	ASN
2	5A	77	ASN
3	5B	119	HIS
4	6A	50	HIS
4	6A	63	HIS
5	6B	26	GLN
5	6B	33	ASN
5	6B	38	HIS
6	6C	72	GLN
7	7A	50	ASN
8	7B	59	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	7C	59	GLN
11	A1	61	HIS
12	A2	25	GLN
12	A2	73	GLN
14	A5	53	ASN
14	A5	71	GLN
14	A5	86	ASN
15	A6	84	GLN
15	A6	152	HIS
16	A7	9	GLN
16	A7	21	GLN
16	A7	25	GLN
17	A8	141	ASN
17	A8	142	GLN
18	A9	37	HIS
18	A9	72	HIS
18	A9	122	HIS
18	A9	154	GLN
18	A9	295	HIS
18	A9	323	HIS
20	AK	39	GLN
20	AK	67	ASN
20	AK	134	GLN
20	AK	151	HIS
20	AK	221	GLN
20	AK	325	GLN
21	AL	79	GLN
21	AL	89	ASN
22	AM	112	ASN
23	AN	61	GLN
23	AN	90	ASN
24	B1	3	ASN
24	B1	6	GLN
25	B2	63	GLN
26	B3	91	GLN
27	B4	50	GLN
27	B4	79	ASN
27	B4	123	GLN
29	B6	143	HIS
30	B7	76	ASN
30	B7	85	HIS
30	B7	110	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	B8	56	ASN
31	B8	115	ASN
32	B9	104	GLN
32	B9	117	GLN
33	BK	28	ASN
33	BK	55	GLN
33	BK	107	GLN
33	BK	161	GLN
34	BL	86	ASN
34	BL	140	ASN
35	C1	12	HIS
35	C1	80	ASN
35	C1	138	HIS
35	C1	256	HIS
35	C1	328	HIS
35	C1	368	HIS
35	C1	413	HIS
35	C1	422	ASN
35	C1	503	HIS
36	C2	59	GLN
36	C2	91	ASN
37	C3	50	ASN
37	C3	103	HIS
37	C3	125	ASN
37	C3	148	HIS
37	C3	161	GLN
37	C3	222	GLN
37	C3	226	HIS
38	C4	98	ASN
39	CA	73	ASN
41	N1	138	GLN
41	N1	171	HIS
42	N2	2	ASN
42	N2	49	ASN
42	N2	112	HIS
42	N2	144	GLN
42	N2	186	HIS
42	N2	273	ASN
42	N2	316	GLN
42	N2	322	GLN
43	N3	10	ASN
43	N3	26	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	N4	103	GLN
44	N4	175	ASN
44	N4	213	HIS
44	N4	251	ASN
44	N4	338	HIS
44	N4	366	ASN
45	N5	2	ASN
45	N5	59	GLN
45	N5	109	HIS
45	N5	135	ASN
45	N5	136	ASN
45	N5	139	GLN
45	N5	199	GLN
45	N5	230	HIS
45	N5	248	HIS
45	N5	348	HIS
45	N5	447	ASN
45	N5	470	ASN
45	N5	518	GLN
45	N5	524	ASN
45	N5	580	GLN
46	N6	86	ASN
47	QA	168	ASN
47	QA	176	ASN
47	QA	206	HIS
47	QA	227	HIS
47	QA	284	ASN
47	QA	291	HIS
47	QA	319	GLN
47	QA	415	GLN
47	QA	426	ASN
47	QA	443	ASN
48	QB	49	GLN
48	QB	66	GLN
48	QB	87	ASN
48	QB	152	GLN
48	QB	173	GLN
48	QB	188	HIS
48	QB	239	HIS
48	QB	249	HIS
48	QB	301	ASN
48	QB	357	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	QC	32	ASN
49	QC	54	HIS
49	QC	85	ASN
49	QC	137	GLN
49	QC	255	ASN
49	QC	260	ASN
49	QC	267	HIS
49	QC	308	HIS
49	QC	322	GLN
49	QC	341	GLN
50	QD	99	HIS
50	QD	206	HIS
50	QD	251	ASN
50	QD	266	GLN
51	QE	135	GLN
51	QE	164	ASN
51	QE	186	GLN
51	QE	199	GLN
51	QE	257	ASN
52	QF	80	HIS
52	QF	88	ASN
53	QG	54	ASN
54	QH	7	HIS
55	QI	38	GLN
55	QI	48	ASN
55	QI	55	HIS
56	QJ	16	ASN
51	QK	31	GLN
51	QK	58	GLN
47	Qa	81	HIS
47	Qa	155	GLN
47	Qa	167	GLN
47	Qa	172	GLN
47	Qa	178	HIS
47	Qa	211	ASN
47	Qa	212	HIS
47	Qa	239	ASN
47	Qa	284	ASN
47	Qa	290	GLN
47	Qa	319	GLN
47	Qa	343	GLN
47	Qa	376	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	Qa	408	GLN
48	Qb	40	GLN
48	Qb	43	GLN
48	Qb	83	ASN
48	Qb	160	GLN
48	Qb	170	GLN
48	Qb	188	HIS
48	Qb	207	ASN
48	Qb	239	HIS
48	Qb	286	HIS
48	Qb	313	HIS
48	Qb	357	HIS
48	Qb	464	GLN
49	Qc	15	ASN
49	Qc	54	HIS
49	Qc	207	ASN
49	Qc	260	ASN
49	Qc	267	HIS
49	Qc	352	GLN
50	Qd	116	GLN
50	Qd	190	ASN
51	Qe	135	GLN
51	Qe	186	GLN
51	Qe	199	GLN
51	Qe	239	HIS
52	Qf	36	GLN
52	Qf	55	GLN
53	Qg	23	ASN
54	Qh	13	HIS
55	Qi	38	GLN
55	Qi	48	ASN
56	Qj	16	ASN
57	S1	39	GLN
57	S1	142	GLN
57	S1	260	ASN
57	S1	282	ASN
57	S1	331	GLN
57	S1	336	ASN
57	S1	425	ASN
57	S1	453	GLN
57	S1	498	GLN
57	S1	604	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	S1	652	ASN
57	S1	688	GLN
58	S2	89	ASN
58	S2	93	GLN
58	S2	166	ASN
58	S2	189	HIS
58	S2	239	HIS
59	S3	77	GLN
59	S3	82	ASN
59	S3	123	GLN
59	S3	196	HIS
59	S3	228	GLN
60	S4	86	ASN
60	S4	123	ASN
60	S4	163	ASN
61	S5	25	GLN
61	S5	45	HIS
62	S6	74	GLN
62	S6	117	GLN
65	V1	220	GLN
65	V1	270	ASN
65	V1	284	HIS
65	V1	303	HIS
65	V1	344	GLN
65	V1	376	HIS
65	V1	393	ASN
65	V1	422	HIS
65	V1	456	GLN
66	V2	74	HIS
66	V2	90	ASN
66	V2	131	HIS
66	V2	133	GLN
66	V2	153	GLN
66	V2	246	GLN
67	V3	388	ASN
67	V3	419	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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$
58	2MR	S2	124	58	10,12,13	2.45	3 (30%)	5,13,15	1.01	0

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
58	2MR	S2	124	58	-	3/10/13/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	S2	124	2MR	CZ-NE	5.20	1.45	1.34
58	S2	124	2MR	CZ-NH2	5.07	1.44	1.33
58	S2	124	2MR	CQ1-NH1	-2.03	1.42	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	S2	124	2MR	NE-CD-CG-CB
58	S2	124	2MR	CA-CB-CG-CD
58	S2	124	2MR	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 106 ligands modelled in this entry, 7 are monoatomic - leaving 99 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
83	SF4	S8	301	64	0,12,12	-	-	-		
83	SF4	V1	501	65	0,12,12	-	-	-		
72	3PE	C1	609	-	45,45,50	0.32	0	48,50,55	0.28	0
72	3PE	QJ	101	-	33,33,50	0.37	0	36,38,55	0.34	0
72	3PE	B8	201	-	31,31,50	0.37	0	34,36,55	0.34	0
68	CDL	B5	201	-	99,99,99	0.31	0	105,111,111	0.37	0
70	PC1	C3	303	-	53,53,53	0.31	0	59,61,61	0.43	0
82	FES	QE	303	51	0,4,4	-	-	-		
70	PC1	QB	503	-	50,50,53	0.30	0	56,58,61	0.36	0
72	3PE	Qc	404	-	47,47,50	0.31	0	50,52,55	0.29	0
72	3PE	QE	302	-	43,43,50	0.32	0	46,48,55	0.31	0
73	PEE	Qe	302	-	23,23,50	1.42	3 (13%)	26,28,55	1.34	3 (11%)
68	CDL	QD	402	-	63,63,99	0.37	0	69,75,111	0.39	0
72	3PE	Qj	101	-	28,28,50	0.39	0	31,33,55	0.36	0
71	PLX	QI	301	-	51,51,51	1.11	4 (7%)	55,59,59	0.87	1 (1%)
72	3PE	S7	204	-	50,50,50	0.32	0	53,55,55	0.37	0
68	CDL	QB	501	-	63,63,99	0.38	0	69,75,111	0.38	0
68	CDL	N4	503	-	61,61,99	0.37	0	67,73,111	0.35	0
68	CDL	N1	401	-	77,77,99	0.34	0	83,89,111	0.30	0
68	CDL	N5	704	-	99,99,99	0.30	0	105,111,111	0.27	0
71	PLX	N6	201	-	51,51,51	1.11	4 (7%)	55,59,59	0.86	1 (1%)
74	NDP	A9	401	-	49,52,52	0.35	0	66,80,80	0.34	0
68	CDL	QC	404	-	54,54,99	0.40	0	60,66,111	0.36	0
68	CDL	C3	305	-	82,82,99	0.32	0	88,94,111	0.27	0
73	PEE	S8	303	-	50,50,50	1.32	5 (10%)	53,55,55	1.20	3 (5%)
70	PC1	Qb	502	-	47,47,53	0.31	0	53,55,61	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
73	PEE	Qc	401	-	41,41,50	1.28	4 (9%)	44,46,55	1.17	3 (6%)
80	HEM	Qc	402	49	50,50,50	1.29	6 (12%)	66,82,82	1.66	14 (21%)
68	CDL	QH	102	-	63,63,99	0.37	0	69,75,111	0.35	0
76	ADP	AK	401	-	27,29,29	1.35	4 (14%)	42,45,45	1.95	10 (23%)
80	HEM	QC	402	49	50,50,50	1.30	6 (12%)	66,82,82	1.69	15 (22%)
70	PC1	Qc	405	-	53,53,53	0.29	0	59,61,61	0.33	0
77	HEA	C1	602	35	66,67,67	2.31	23 (34%)	78,103,103	2.56	29 (37%)
68	CDL	Qb	501	-	63,63,99	0.37	0	69,75,111	0.35	0
71	PLX	CB	201	-	51,51,51	1.10	3 (5%)	55,59,59	0.88	1 (1%)
71	PLX	Qi	301	-	45,45,51	1.18	6 (13%)	49,53,59	0.82	1 (2%)
70	PC1	C1	606	-	45,45,53	0.31	0	51,53,61	0.31	0
81	HEC	Qd	401	50	50,50,50	1.38	5 (10%)	68,82,82	1.22	5 (7%)
72	3PE	CA	101	-	50,50,50	0.31	0	53,55,55	0.28	0
75	ZMP	AC	201	19	29,35,36	0.65	1 (3%)	34,42,45	0.78	1 (2%)
70	PC1	6A	101	-	44,44,53	0.32	0	50,52,61	0.31	0
73	PEE	QB	502	-	33,33,50	1.41	4 (12%)	36,38,55	1.14	2 (5%)
68	CDL	7A	102	-	90,90,99	0.31	0	96,102,111	0.28	0
73	PEE	QC	403	-	39,39,50	1.31	4 (10%)	42,44,55	1.19	3 (7%)
73	PEE	N5	701	-	45,45,50	1.39	5 (11%)	48,50,55	1.18	3 (6%)
70	PC1	C1	605	-	32,32,53	0.36	0	38,40,61	0.35	0
70	PC1	C3	306	-	42,42,53	0.32	0	48,50,61	0.29	0
73	PEE	N1	403	-	30,30,50	1.28	3 (10%)	33,35,55	1.15	2 (6%)
70	PC1	N3	202	-	53,53,53	0.30	0	59,61,61	0.29	0
71	PLX	B1	101	-	51,51,51	1.11	4 (7%)	55,59,59	0.89	1 (1%)
83	SF4	S1	801	57	0,12,12	-	-	-	-	-
75	ZMP	AB	201	19	29,35,36	0.69	1 (3%)	34,42,45	0.77	1 (2%)
72	3PE	7A	101	-	42,42,50	0.33	0	45,47,55	0.28	0
73	PEE	7C	101	-	50,50,50	1.33	5 (10%)	53,55,55	1.16	4 (7%)
73	PEE	N3	201	-	50,50,50	1.32	5 (10%)	53,55,55	1.15	3 (5%)
71	PLX	AL	202	-	46,46,51	1.16	5 (10%)	50,54,59	0.87	1 (2%)
73	PEE	N5	705	-	50,50,50	1.31	5 (10%)	53,55,55	1.16	3 (5%)
68	CDL	A7	201	-	50,50,99	0.40	0	56,62,111	0.33	0
73	PEE	N5	702	-	39,39,50	1.49	5 (12%)	41,44,55	1.22	2 (4%)
82	FES	Qe	303	51	0,4,4	-	-	-	-	-
68	CDL	A8	301	-	82,82,99	0.33	0	88,94,111	0.33	0
68	CDL	N5	703	-	88,88,99	0.31	0	94,100,111	0.31	0
70	PC1	C3	301	-	43,43,53	0.31	0	49,51,61	0.30	0
72	3PE	N5	706	-	45,45,50	0.33	0	48,50,55	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	CDL	CB	203	-	99,99,99	0.30	0	105,111,111	0.27	0
68	CDL	AK	402	-	67,67,99	0.36	0	73,79,111	0.38	0
86	FMN	V1	502	-	33,33,33	0.23	0	48,50,50	0.41	0
71	PLX	AM	201	-	50,50,51	1.12	4 (8%)	54,58,59	0.85	1 (1%)
71	PLX	N4	502	-	48,48,51	1.13	4 (8%)	52,56,59	0.91	2 (3%)
85	U10	S7	201	-	63,63,63	2.17	21 (33%)	76,79,79	1.68	21 (27%)
71	PLX	6C	101	-	42,42,51	1.17	4 (9%)	46,50,59	0.85	1 (2%)
80	HEM	Qc	403	49	50,50,50	1.31	6 (12%)	66,82,82	1.66	16 (24%)
70	PC1	C1	608	-	53,53,53	0.29	0	59,61,61	0.32	0
68	CDL	B4	201	-	79,79,99	0.33	0	85,91,111	0.32	0
70	PC1	C1	610	-	49,49,53	0.30	0	55,57,61	0.35	0
73	PEE	N4	501	-	48,48,50	1.34	5 (10%)	51,53,55	1.23	2 (3%)
73	PEE	QE	301	-	46,46,50	1.36	5 (10%)	49,51,55	1.24	5 (10%)
73	PEE	A9	402	-	38,38,50	1.48	5 (13%)	41,43,55	1.23	3 (7%)
73	PEE	Qe	301	-	50,50,50	1.32	5 (10%)	53,55,55	1.19	3 (5%)
68	CDL	AL	201	-	93,93,99	0.31	0	99,105,111	0.31	0
68	CDL	C3	304	-	86,86,99	0.32	0	92,98,111	0.28	0
70	PC1	Qh	101	-	53,53,53	0.30	0	59,61,61	0.26	0
80	HEM	QC	401	49	50,50,50	1.28	6 (12%)	66,82,82	1.68	14 (21%)
77	HEA	C1	601	35	66,67,67	2.21	23 (34%)	78,103,103	2.65	31 (39%)
68	CDL	QH	101	-	60,60,99	0.38	0	66,72,111	0.32	0
68	CDL	4L	201	-	91,91,99	0.32	0	97,103,111	0.36	0
73	PEE	S2	501	-	47,47,50	1.35	5 (10%)	50,52,55	1.20	4 (8%)
82	FES	V2	301	66	0,4,4	-	-	-	-	-
84	MF8	S2	502	-	7,8,8	1.06	0	7,10,10	1.40	1 (14%)
70	PC1	C3	302	-	48,48,53	0.31	0	54,56,61	0.37	0
83	SF4	S8	302	64	0,12,12	-	-	-	-	-
72	3PE	C1	607	-	38,38,50	0.35	0	41,43,55	0.37	0
72	3PE	CB	202	-	45,45,50	0.32	0	48,50,55	0.29	0
83	SF4	S1	802	57	0,12,12	-	-	-	-	-
81	HEC	QD	401	50	50,50,50	1.32	5 (10%)	68,82,82	1.24	6 (8%)
83	SF4	S7	202	63	0,12,12	-	-	-	-	-
71	PLX	S7	203	-	51,51,51	1.11	3 (5%)	55,59,59	0.88	2 (3%)
82	FES	S1	803	57	0,4,4	-	-	-	-	-
70	PC1	N1	402	-	47,47,53	0.31	0	53,55,61	0.30	0

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
83	SF4	S8	301	64	-	-	0/6/5/5
83	SF4	V1	501	65	-	-	0/6/5/5
72	3PE	C1	609	-	-	15/49/49/54	-
72	3PE	QJ	101	-	-	10/37/37/54	-
72	3PE	B8	201	-	-	8/35/35/54	-
68	CDL	B5	201	-	-	17/110/110/110	-
70	PC1	C3	303	-	-	14/57/57/57	-
82	FES	QE	303	51	-	-	0/1/1/1
70	PC1	QB	503	-	-	8/54/54/57	-
72	3PE	Qc	404	-	-	10/51/51/54	-
72	3PE	QE	302	-	-	7/47/47/54	-
73	PEE	Qe	302	-	-	9/27/27/54	-
68	CDL	QD	402	-	-	17/74/74/110	-
72	3PE	Qj	101	-	-	7/32/32/54	-
71	PLX	QI	301	-	-	15/55/55/55	-
72	3PE	S7	204	-	-	12/54/54/54	-
68	CDL	QB	501	-	-	15/74/74/110	-
68	CDL	N4	503	-	-	22/72/72/110	-
68	CDL	N1	401	-	-	14/88/88/110	-
68	CDL	N5	704	-	-	19/110/110/110	-
71	PLX	N6	201	-	-	22/55/55/55	-
74	NDP	A9	401	-	-	6/34/77/77	0/5/5/5
68	CDL	QC	404	-	-	19/65/65/110	-
68	CDL	C3	305	-	-	11/93/93/110	-
73	PEE	S8	303	-	-	24/54/54/54	-
70	PC1	Qb	502	-	-	12/51/51/57	-
73	PEE	Qc	401	-	-	27/45/45/54	-
80	HEM	Qc	402	49	-	7/14/54/54	-
68	CDL	QH	102	-	-	21/74/74/110	-
76	ADP	AK	401	-	-	4/16/32/32	0/3/3/3
80	HEM	QC	402	49	-	6/14/54/54	-
70	PC1	Qc	405	-	-	11/57/57/57	-
77	HEA	C1	602	35	-	14/36/76/76	-
68	CDL	Qb	501	-	-	18/74/74/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	PLX	CB	201	-	-	26/55/55/55	-
71	PLX	Qi	301	-	-	24/49/49/55	-
70	PC1	C1	606	-	-	7/49/49/57	-
81	HEC	Qd	401	50	1/1/3/7	7/14/54/54	-
72	3PE	CA	101	-	-	10/54/54/54	-
75	ZMP	AC	201	19	-	19/40/42/43	-
70	PC1	6A	101	-	-	10/48/48/57	-
73	PEE	QB	502	-	-	22/37/37/54	-
68	CDL	7A	102	-	-	18/101/101/110	-
73	PEE	QC	403	-	-	14/43/43/54	-
73	PEE	N5	701	-	-	26/49/49/54	-
70	PC1	C1	605	-	-	8/36/36/57	-
70	PC1	C3	306	-	-	8/46/46/57	-
73	PEE	N1	403	-	-	22/34/34/54	-
70	PC1	N3	202	-	-	15/57/57/57	-
71	PLX	B1	101	-	-	18/55/55/55	-
83	SF4	S1	801	57	-	-	0/6/5/5
75	ZMP	AB	201	19	-	8/40/42/43	-
72	3PE	7A	101	-	-	13/46/46/54	-
73	PEE	7C	101	-	-	16/54/54/54	-
73	PEE	N3	201	-	-	26/54/54/54	-
71	PLX	AL	202	-	-	19/50/50/55	-
73	PEE	N5	705	-	-	27/54/54/54	-
68	CDL	A7	201	-	-	12/61/61/110	-
73	PEE	N5	702	-	-	20/43/43/54	-
82	FES	Qe	303	51	-	-	0/1/1/1
68	CDL	A8	301	-	-	20/93/93/110	-
68	CDL	N5	703	-	-	23/99/99/110	-
70	PC1	C3	301	-	-	12/47/47/57	-
72	3PE	N5	706	-	-	12/49/49/54	-
68	CDL	CB	203	-	-	25/110/110/110	-
68	CDL	AK	402	-	-	18/78/78/110	-
86	FMN	V1	502	-	-	0/18/18/18	0/3/3/3
71	PLX	AM	201	-	-	20/54/54/55	-
71	PLX	N4	502	-	-	17/52/52/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	U10	S7	201	-	-	22/63/87/87	0/1/1/1
71	PLX	6C	101	-	-	16/46/46/55	-
80	HEM	Qc	403	49	-	11/14/54/54	-
70	PC1	C1	608	-	-	14/57/57/57	-
68	CDL	B4	201	-	-	21/90/90/110	-
70	PC1	C1	610	-	-	7/53/53/57	-
73	PEE	N4	501	-	-	24/52/52/54	-
73	PEE	QE	301	-	-	24/50/50/54	-
73	PEE	A9	402	-	-	20/42/42/54	-
73	PEE	Qe	301	-	-	28/54/54/54	-
68	CDL	AL	201	-	-	25/104/104/110	-
68	CDL	C3	304	-	-	13/97/97/110	-
70	PC1	Qh	101	-	-	5/57/57/57	-
80	HEM	QC	401	49	-	7/14/54/54	-
77	HEA	C1	601	35	-	12/36/76/76	-
68	CDL	QH	101	-	-	11/71/71/110	-
68	CDL	4L	201	-	-	22/102/102/110	-
73	PEE	S2	501	-	-	30/51/51/54	-
82	FES	V2	301	66	-	-	0/1/1/1
84	MF8	S2	502	-	-	5/8/8/8	-
70	PC1	C3	302	-	-	16/52/52/57	-
83	SF4	S8	302	64	-	-	0/6/5/5
72	3PE	C1	607	-	-	13/42/42/54	-
72	3PE	CB	202	-	-	12/49/49/54	-
83	SF4	S1	802	57	-	-	0/6/5/5
81	HEC	QD	401	50	1/1/3/7	4/14/54/54	-
83	SF4	S7	202	63	-	-	0/6/5/5
71	PLX	S7	203	-	-	22/55/55/55	-
82	FES	S1	803	57	-	-	0/1/1/1
70	PC1	N1	402	-	-	14/51/51/57	-

All (221) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	S7	201	U10	C6-C1	10.34	1.54	1.35
77	C1	602	HEA	FE-NB	5.67	2.12	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	C1	601	HEA	FE-NB	5.56	2.12	1.94
77	C1	602	HEA	C3B-C2B	5.37	1.46	1.34
77	C1	601	HEA	C3B-C2B	5.05	1.46	1.34
77	C1	601	HEA	C3A-C2A	4.95	1.47	1.36
77	C1	602	HEA	C3A-C2A	4.70	1.46	1.36
77	C1	601	HEA	C4B-NB	-4.69	1.32	1.40
76	AK	401	ADP	C5-C4	4.44	1.47	1.39
77	C1	602	HEA	C1C-NC	-4.35	1.31	1.39
77	C1	602	HEA	FE-NC	4.33	2.09	1.95
85	S7	201	U10	C4-C3	4.28	1.53	1.36
77	C1	601	HEA	FE-NC	4.23	2.09	1.95
77	C1	601	HEA	C3D-C2D	4.12	1.45	1.36
77	C1	602	HEA	C4C-NC	-4.06	1.31	1.39
73	N5	701	PEE	C18-C19	4.05	1.55	1.31
77	C1	602	HEA	CHC-C4B	4.05	1.46	1.38
73	A9	402	PEE	C18-C19	4.05	1.55	1.31
73	Qe	301	PEE	C18-C19	4.05	1.55	1.31
73	QE	301	PEE	C18-C19	4.05	1.55	1.31
73	N5	702	PEE	C18-C19	4.05	1.55	1.31
73	7C	101	PEE	C18-C19	4.04	1.55	1.31
73	N3	201	PEE	C18-C19	4.04	1.55	1.31
73	N5	705	PEE	C18-C19	4.04	1.55	1.31
73	S8	303	PEE	C18-C19	4.03	1.55	1.31
73	S2	501	PEE	C18-C19	4.03	1.55	1.31
73	QC	403	PEE	C18-C19	4.02	1.55	1.31
73	N4	501	PEE	C18-C19	4.02	1.55	1.31
77	C1	602	HEA	FE-ND	4.01	2.07	1.94
73	Qc	401	PEE	C18-C19	4.01	1.55	1.31
73	S8	303	PEE	C39-C38	3.96	1.54	1.31
73	N5	702	PEE	C39-C38	3.96	1.54	1.31
73	N4	501	PEE	C39-C38	3.96	1.54	1.31
73	Qe	301	PEE	C39-C38	3.96	1.54	1.31
73	S2	501	PEE	C39-C38	3.94	1.54	1.31
73	QE	301	PEE	C39-C38	3.94	1.54	1.31
73	7C	101	PEE	C39-C38	3.93	1.54	1.31
73	QB	502	PEE	C39-C38	3.93	1.54	1.31
73	N3	201	PEE	C39-C38	3.93	1.54	1.31
73	N5	705	PEE	C39-C38	3.92	1.54	1.31
73	N5	701	PEE	C39-C38	3.92	1.54	1.31
77	C1	601	HEA	FE-ND	3.90	2.06	1.94
73	A9	402	PEE	C39-C38	3.88	1.54	1.28
77	C1	602	HEA	CHD-C1D	3.84	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	C1	602	HEA	C4B-NB	-3.81	1.33	1.40
80	Qc	403	HEM	C4D-ND	-3.78	1.33	1.40
77	C1	602	HEA	C1D-ND	-3.66	1.34	1.40
80	QC	402	HEM	C4D-ND	-3.65	1.34	1.40
77	C1	602	HEA	C1A-NA	3.63	1.46	1.39
77	C1	601	HEA	CHA-C1A	3.63	1.45	1.38
77	C1	602	HEA	CHA-C1A	3.62	1.45	1.38
77	C1	601	HEA	CHC-C4B	3.61	1.45	1.38
77	C1	602	HEA	C3D-C2D	3.59	1.44	1.36
77	C1	601	HEA	C1D-ND	-3.58	1.34	1.40
80	Qc	402	HEM	C4D-ND	-3.54	1.34	1.40
80	QC	401	HEM	C4D-ND	-3.54	1.34	1.40
81	Qd	401	HEC	CBC-CAC	-3.51	1.35	1.51
77	C1	601	HEA	CHB-C1B	3.40	1.47	1.39
77	C1	601	HEA	CHA-C4D	3.37	1.46	1.39
81	QD	401	HEC	CBC-CAC	-3.31	1.36	1.51
77	C1	602	HEA	CHC-C1C	3.29	1.46	1.39
77	C1	602	HEA	C4A-NA	3.29	1.46	1.39
73	N3	201	PEE	O3-C30	3.28	1.42	1.33
73	N1	403	PEE	O3-C30	3.28	1.42	1.33
73	Qe	301	PEE	O3-C30	3.26	1.42	1.33
80	Qc	403	HEM	C1B-NB	-3.26	1.34	1.40
77	C1	601	HEA	CHC-C1C	3.26	1.46	1.39
73	QB	502	PEE	O3-C30	3.25	1.42	1.33
73	N5	701	PEE	O3-C30	3.25	1.42	1.33
73	Qc	401	PEE	O3-C30	3.25	1.42	1.33
73	7C	101	PEE	O3-C30	3.22	1.42	1.33
73	QC	403	PEE	O3-C30	3.22	1.42	1.33
73	N5	702	PEE	O3-C30	3.20	1.42	1.33
73	Qe	302	PEE	O3-C30	3.19	1.42	1.33
73	S2	501	PEE	O3-C30	3.19	1.42	1.33
73	A9	402	PEE	O3-C30	3.19	1.42	1.33
73	S8	303	PEE	O3-C30	3.17	1.42	1.33
77	C1	602	HEA	C1B-NB	-3.16	1.32	1.38
73	N4	501	PEE	O3-C30	3.15	1.42	1.33
73	QE	301	PEE	O3-C30	3.14	1.42	1.33
80	QC	402	HEM	C1B-NB	-3.12	1.34	1.40
73	N5	705	PEE	O3-C30	3.11	1.42	1.33
80	Qc	402	HEM	C1B-NB	-3.04	1.35	1.40
71	S7	203	PLX	O6-C4	-3.02	1.40	1.44
71	CB	201	PLX	O6-C4	-2.99	1.40	1.44
71	Qi	301	PLX	O6-C4	-2.98	1.40	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	N4	502	PLX	O6-C4	-2.98	1.40	1.44
85	S7	201	U10	C41-C39	2.98	1.57	1.51
80	QC	401	HEM	C1B-NB	-2.96	1.35	1.40
77	C1	602	HEA	CHA-C4D	2.95	1.46	1.39
77	C1	601	HEA	CHD-C4C	2.95	1.46	1.39
71	B1	101	PLX	O6-C4	-2.94	1.40	1.44
85	S7	201	U10	C7-C8	2.91	1.54	1.50
71	6C	101	PLX	O6-C4	-2.90	1.40	1.44
77	C1	601	HEA	C1C-NC	-2.90	1.34	1.39
71	AL	202	PLX	O6-C4	-2.89	1.40	1.44
73	QB	502	PEE	O2-C10	2.88	1.42	1.34
71	AM	201	PLX	O6-C4	-2.87	1.40	1.44
80	QC	402	HEM	C1C-C2C	-2.87	1.39	1.45
71	N6	201	PLX	O6-C4	-2.85	1.40	1.44
81	QD	401	HEC	CAC-C3C	2.85	1.58	1.51
80	Qc	403	HEM	C1C-C2C	-2.81	1.39	1.45
71	QI	301	PLX	O6-C4	-2.80	1.40	1.44
77	C1	601	HEA	C1B-NB	-2.79	1.33	1.38
77	C1	601	HEA	C1A-NA	2.75	1.45	1.39
77	C1	602	HEA	CHB-C4A	2.75	1.43	1.38
85	S7	201	U10	C7-C6	2.73	1.55	1.51
73	7C	101	PEE	O2-C10	2.71	1.42	1.34
85	S7	201	U10	C26-C24	2.69	1.56	1.51
73	S8	303	PEE	O2-C10	2.69	1.41	1.34
73	Qe	301	PEE	O2-C10	2.68	1.41	1.34
73	N5	702	PEE	O2-C10	2.66	1.41	1.34
76	AK	401	ADP	C5-C6	2.64	1.48	1.41
73	Qe	302	PEE	O2-C10	2.64	1.41	1.34
85	S7	201	U10	C31-C29	2.64	1.56	1.51
85	S7	201	U10	C21-C19	2.64	1.56	1.51
80	Qc	403	HEM	C1D-ND	-2.63	1.33	1.38
73	S2	501	PEE	O2-C10	2.63	1.41	1.34
75	AB	201	ZMP	C9-C10	-2.63	1.48	1.50
73	N5	701	PEE	O2-C10	2.61	1.41	1.34
73	QE	301	PEE	O2-C10	2.60	1.41	1.34
73	N3	201	PEE	O2-C10	2.60	1.41	1.34
80	Qc	402	HEM	C1C-C2C	-2.60	1.40	1.45
80	QC	402	HEM	C1D-ND	-2.58	1.33	1.38
73	N5	705	PEE	O2-C10	2.58	1.41	1.34
73	N4	501	PEE	O2-C2	-2.58	1.40	1.46
73	N1	403	PEE	O2-C10	2.57	1.41	1.34
73	QC	403	PEE	O2-C2	-2.57	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	QE	301	PEE	O2-C2	-2.56	1.40	1.46
73	N5	705	PEE	O2-C2	-2.55	1.40	1.46
73	Qc	401	PEE	O2-C2	-2.55	1.40	1.46
73	A9	402	PEE	O2-C10	2.55	1.41	1.34
81	Qd	401	HEC	CBB-CAB	-2.54	1.40	1.51
77	C1	601	HEA	CHB-C4A	2.54	1.43	1.38
80	QC	401	HEM	C1D-ND	-2.54	1.33	1.38
73	N1	403	PEE	O2-C2	-2.54	1.40	1.46
81	Qd	401	HEC	CAC-C3C	2.53	1.57	1.51
73	Qe	302	PEE	O2-C2	-2.53	1.40	1.46
77	C1	602	HEA	CHD-C4C	2.52	1.45	1.39
73	S8	303	PEE	O2-C2	-2.52	1.40	1.46
73	Qc	401	PEE	O2-C10	2.51	1.41	1.34
80	QC	401	HEM	C1C-C2C	-2.50	1.40	1.45
80	Qc	402	HEM	C1D-ND	-2.50	1.33	1.38
73	N4	501	PEE	O2-C10	2.49	1.41	1.34
73	S2	501	PEE	O2-C2	-2.49	1.40	1.46
77	C1	601	HEA	CHD-C1D	2.49	1.43	1.38
73	QC	403	PEE	O2-C10	2.48	1.41	1.34
73	A9	402	PEE	O2-C2	-2.48	1.40	1.46
80	QC	402	HEM	FE-NB	2.47	2.02	1.94
73	N5	702	PEE	O2-C2	-2.47	1.40	1.46
77	C1	602	HEA	C4D-ND	-2.47	1.33	1.38
73	Qe	301	PEE	O2-C2	-2.47	1.40	1.46
80	QC	401	HEM	FE-NB	2.45	2.02	1.94
80	Qc	402	HEM	FE-NB	2.45	2.02	1.94
75	AC	201	ZMP	C9-C10	-2.43	1.48	1.50
73	N5	701	PEE	O2-C2	-2.43	1.40	1.46
73	N3	201	PEE	O2-C2	-2.43	1.40	1.46
85	S7	201	U10	O5-C5	-2.42	1.18	1.23
85	S7	201	U10	C36-C34	2.42	1.56	1.51
77	C1	601	HEA	O2D-CGD	-2.42	1.22	1.30
80	Qc	403	HEM	FE-NB	2.42	2.02	1.94
77	C1	601	HEA	C4B-C3B	2.41	1.48	1.44
73	7C	101	PEE	O2-C2	-2.40	1.40	1.46
81	Qd	401	HEC	CMD-C2D	2.40	1.55	1.50
81	QD	401	HEC	CBB-CAB	-2.40	1.40	1.51
85	S7	201	U10	C46-C44	2.38	1.56	1.51
77	C1	602	HEA	O2D-CGD	-2.38	1.22	1.30
76	AK	401	ADP	C8-N7	2.36	1.36	1.31
85	S7	201	U10	C51-C49	2.34	1.56	1.51
85	S7	201	U10	O2-C2	-2.33	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	C1	601	HEA	O2A-CGA	-2.33	1.22	1.30
85	S7	201	U10	C11-C9	2.31	1.56	1.51
85	S7	201	U10	C6-C5	2.30	1.53	1.46
71	Qi	301	PLX	C1B-N1	-2.27	1.43	1.50
81	QD	401	HEC	CAB-C3B	2.23	1.56	1.51
71	QI	301	PLX	C1B-N1	-2.22	1.43	1.50
77	C1	602	HEA	O2A-CGA	-2.22	1.23	1.30
80	Qc	402	HEM	FE-ND	2.21	2.01	1.94
71	B1	101	PLX	C1B-N1	-2.20	1.43	1.50
76	AK	401	ADP	C5-N7	-2.19	1.34	1.39
80	QC	401	HEM	FE-ND	2.18	2.01	1.94
71	AL	202	PLX	C1B-N1	-2.17	1.43	1.50
71	Qi	301	PLX	C1A-N1	-2.17	1.43	1.50
85	S7	201	U10	C16-C14	2.16	1.55	1.51
71	N6	201	PLX	C1B-N1	-2.16	1.43	1.50
71	N4	502	PLX	C1B-N1	-2.15	1.43	1.50
81	Qd	401	HEC	CMA-C3A	2.14	1.55	1.50
71	S7	203	PLX	C1B-N1	-2.13	1.43	1.50
71	CB	201	PLX	C1B-N1	-2.13	1.43	1.50
85	S7	201	U10	C27-C28	2.12	1.57	1.50
81	QD	401	HEC	FE-ND	2.12	2.01	1.94
71	QI	301	PLX	C1A-N1	-2.12	1.43	1.50
85	S7	201	U10	O3-C3M	-2.11	1.40	1.45
71	6C	101	PLX	C1B-N1	-2.11	1.43	1.50
71	AM	201	PLX	C1B-N1	-2.10	1.43	1.50
77	C1	601	HEA	C4C-NC	-2.09	1.35	1.39
85	S7	201	U10	C22-C23	2.08	1.57	1.50
71	6C	101	PLX	P1-O4	2.08	1.67	1.59
73	QB	502	PEE	O2-C2	-2.08	1.41	1.46
71	CB	201	PLX	C1A-N1	-2.07	1.44	1.50
85	S7	201	U10	C42-C43	2.06	1.57	1.50
71	AM	201	PLX	P1-O4	2.06	1.67	1.59
71	AL	202	PLX	C1A-N1	-2.06	1.44	1.50
71	S7	203	PLX	C1A-N1	-2.05	1.44	1.50
71	N4	502	PLX	C1A-N1	-2.04	1.44	1.50
71	N6	201	PLX	C1A-N1	-2.04	1.44	1.50
85	S7	201	U10	O4-C4M	-2.04	1.40	1.45
71	AL	202	PLX	P1-O4	2.04	1.67	1.59
71	Qi	301	PLX	C7-C6	2.03	1.55	1.50
71	N6	201	PLX	P1-O4	2.03	1.67	1.59
71	N4	502	PLX	P1-O4	2.03	1.67	1.59
71	AL	202	PLX	C7-C6	2.02	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	B1	101	PLX	C1A-N1	-2.02	1.44	1.50
80	QC	402	HEM	C3C-C4C	-2.02	1.42	1.46
71	Qi	301	PLX	P1-O4	2.02	1.67	1.59
71	AM	201	PLX	C7-C6	2.01	1.55	1.50
80	Qc	403	HEM	FE-ND	2.01	2.01	1.94
71	QI	301	PLX	P1-O3	-2.01	1.45	1.55
71	6C	101	PLX	C1A-N1	-2.01	1.44	1.50
71	B1	101	PLX	P1-O4	2.01	1.67	1.59
71	Qi	301	PLX	P1-O3	-2.00	1.45	1.55

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	C1	601	HEA	CAD-CBD-CGD	-7.00	98.54	113.60
77	C1	602	HEA	CAD-CBD-CGD	-6.96	98.63	113.60
77	C1	602	HEA	CAA-CBA-CGA	-6.75	99.07	113.60
77	C1	601	HEA	C3D-C4D-ND	6.31	116.46	110.36
76	AK	401	ADP	C5-C4-N3	-6.17	118.69	126.75
77	C1	602	HEA	C3C-C4C-NC	6.11	114.01	110.25
77	C1	601	HEA	CAA-CBA-CGA	-5.95	100.80	113.60
77	C1	601	HEA	C3C-C2C-C1C	-5.95	99.98	107.16
77	C1	602	HEA	C2D-C1D-ND	5.64	116.52	109.84
77	C1	602	HEA	C1D-C2D-C3D	-5.62	101.05	106.96
77	C1	601	HEA	C3C-C4C-NC	5.58	113.68	110.25
77	C1	601	HEA	C13-C12-C11	-5.35	106.32	114.35
77	C1	602	HEA	C3C-C2C-C1C	-5.32	100.74	107.16
77	C1	602	HEA	C3D-C4D-ND	5.18	115.37	110.36
77	C1	602	HEA	C13-C12-C11	-5.16	106.60	114.35
77	C1	601	HEA	C2D-C1D-ND	5.05	115.82	109.84
76	AK	401	ADP	N3-C4-N9	4.87	135.10	127.08
77	C1	601	HEA	CHB-C1B-C2B	-4.86	117.39	124.98
80	QC	401	HEM	CHC-C4B-NB	4.82	129.66	124.42
80	Qc	402	HEM	CHC-C4B-NB	4.68	129.50	124.42
77	C1	601	HEA	C2C-C1C-NC	4.68	117.21	110.08
73	Qe	301	PEE	O2-C10-C11	4.47	121.13	111.50
73	S8	303	PEE	O2-C10-C11	4.46	121.12	111.50
80	QC	402	HEM	CHC-C4B-NB	4.44	129.25	124.42
77	C1	601	HEA	C2B-C1B-NB	4.43	115.19	109.88
77	C1	601	HEA	C1D-C2D-C3D	-4.38	102.35	106.96
80	Qc	403	HEM	CHC-C4B-NB	4.36	129.16	124.42
80	Qc	402	HEM	CHD-C4C-NC	4.33	129.12	124.44
77	C1	602	HEA	CHB-C1B-C2B	-4.29	118.28	124.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	QC	401	HEM	CHD-C4C-NC	4.24	129.03	124.44
73	N4	501	PEE	O2-C10-C11	4.24	120.64	111.50
80	QC	402	HEM	C4D-ND-C1D	4.21	109.42	105.07
77	C1	601	HEA	CHA-C4D-C3D	-4.21	118.66	124.84
73	Qe	302	PEE	O2-C10-C11	4.15	120.45	111.50
73	QE	301	PEE	O2-C10-C11	4.09	120.31	111.50
73	N5	702	PEE	O2-C10-C11	4.08	120.29	111.50
73	S2	501	PEE	O2-C10-C11	4.08	120.29	111.50
80	Qc	403	HEM	CHD-C4C-NC	4.08	128.85	124.44
80	QC	401	HEM	CHB-C1B-NB	4.03	129.34	124.37
73	QC	403	PEE	O2-C10-C11	4.00	120.12	111.50
80	QC	402	HEM	CHD-C4C-NC	4.00	128.76	124.44
77	C1	602	HEA	C2B-C1B-NB	3.99	114.66	109.88
73	7C	101	PEE	O2-C10-C11	3.95	120.02	111.50
73	N3	201	PEE	O2-C10-C11	3.95	120.01	111.50
77	C1	602	HEA	C4B-C3B-C2B	-3.95	100.67	107.41
73	N5	701	PEE	O2-C10-C11	3.94	119.98	111.50
73	A9	402	PEE	O2-C10-C11	3.93	119.98	111.50
77	C1	602	HEA	C3B-C4B-NB	3.93	114.50	109.84
80	Qc	402	HEM	CHB-C1B-NB	3.92	129.21	124.37
73	N1	403	PEE	O2-C10-C11	3.91	119.92	111.50
76	AK	401	ADP	C2-N3-C4	3.86	120.88	111.75
85	S7	201	U10	C7-C8-C9	-3.82	120.43	126.79
80	Qc	403	HEM	CHB-C1B-NB	3.82	129.08	124.37
73	N5	705	PEE	O2-C10-C11	3.77	119.62	111.50
73	Qc	401	PEE	O2-C10-C11	3.73	119.55	111.50
80	Qc	403	HEM	C4D-ND-C1D	3.71	108.90	105.07
80	QC	402	HEM	CHB-C1B-NB	3.63	128.85	124.37
80	QC	401	HEM	C4D-ND-C1D	3.60	108.79	105.07
80	Qc	402	HEM	C4D-ND-C1D	3.49	108.68	105.07
77	C1	601	HEA	C3B-C4B-NB	3.39	113.86	109.84
80	QC	401	HEM	C1B-NB-C4B	3.35	108.53	105.07
84	S2	502	MF8	C07-N06-C04	3.33	131.84	124.55
73	Qe	302	PEE	O3-C30-C31	3.32	120.10	111.38
76	AK	401	ADP	PA-O3A-PB	-3.32	121.42	132.83
73	QB	502	PEE	O2-C10-C11	3.30	118.61	111.50
80	Qc	403	HEM	C1B-NB-C4B	3.26	108.44	105.07
76	AK	401	ADP	C4-C5-N7	-3.24	106.67	110.62
85	S7	201	U10	C22-C23-C24	-3.23	119.87	127.66
85	S7	201	U10	C17-C18-C19	-3.21	119.94	127.66
77	C1	602	HEA	C2C-C1C-NC	3.18	114.92	110.08
80	QC	402	HEM	C1B-NB-C4B	3.16	108.34	105.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	C1	601	HEA	C4B-C3B-C2B	-3.16	102.01	107.41
76	AK	401	ADP	N3-C2-N1	-3.16	123.66	128.60
77	C1	602	HEA	CHA-C4D-C3D	-3.09	120.29	124.84
77	C1	602	HEA	C27-C19-C20	3.05	120.40	115.27
80	Qc	402	HEM	C1B-NB-C4B	3.04	108.22	105.07
85	S7	201	U10	C12-C13-C14	-3.03	120.36	127.66
85	S7	201	U10	C30-C29-C31	3.01	120.33	115.27
77	C1	601	HEA	CMB-C2B-C1B	-2.97	120.51	125.04
85	S7	201	U10	C47-C48-C49	-2.94	120.57	127.66
77	C1	601	HEA	CMB-C2B-C3B	2.93	135.93	130.34
85	S7	201	U10	C45-C44-C46	2.92	120.18	115.27
80	QC	401	HEM	CHA-C4D-ND	2.91	127.96	124.37
85	S7	201	U10	C20-C19-C21	2.88	120.11	115.27
73	Qc	401	PEE	O3-C30-C31	2.88	120.94	111.91
85	S7	201	U10	C42-C43-C44	-2.88	120.74	127.66
80	Qc	402	HEM	CHA-C4D-ND	2.85	127.89	124.37
77	C1	602	HEA	C13-C14-C15	-2.84	120.81	127.66
73	QE	301	PEE	O3-C30-C31	2.84	120.82	111.91
80	QC	401	HEM	CHD-C1D-ND	2.83	127.50	124.42
80	QC	402	HEM	CHD-C1D-ND	2.82	127.49	124.42
85	S7	201	U10	C37-C38-C39	-2.82	120.88	127.66
81	QD	401	HEC	O1D-CGD-CBD	-2.79	114.12	123.08
85	S7	201	U10	C32-C33-C34	-2.79	120.95	127.66
81	Qd	401	HEC	O1D-CGD-CBD	-2.79	114.13	123.08
77	C1	601	HEA	C1D-ND-C4D	-2.78	102.20	105.07
85	S7	201	U10	C50-C49-C51	2.78	119.95	115.27
76	AK	401	ADP	C5-N7-C8	2.78	107.46	103.51
77	C1	601	HEA	C27-C19-C20	2.78	119.94	115.27
80	QC	402	HEM	CHA-C4D-ND	2.76	127.78	124.37
85	S7	201	U10	C10-C9-C11	2.75	119.90	115.27
77	C1	601	HEA	C17-C18-C19	-2.75	121.03	127.66
80	QC	402	HEM	C4C-NC-C1C	2.75	108.04	105.35
77	C1	601	HEA	C13-C14-C15	-2.75	121.04	127.66
81	Qd	401	HEC	CHA-C4D-ND	2.75	127.41	124.42
77	C1	601	HEA	CHB-C1B-NB	2.74	127.39	124.42
80	QC	402	HEM	C4A-NA-C1A	2.74	108.03	105.35
73	N5	705	PEE	O3-C30-C31	2.73	120.49	111.91
77	C1	602	HEA	C17-C18-C19	-2.73	121.08	127.66
77	C1	602	HEA	CMD-C2D-C1D	2.73	129.19	125.04
77	C1	602	HEA	CHC-C4B-NB	-2.72	121.02	124.37
85	S7	201	U10	C40-C39-C41	2.72	119.84	115.27
73	QB	502	PEE	O3-C30-C31	2.71	120.42	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	C1	601	HEA	C1B-C2B-C3B	-2.71	103.56	106.80
73	N4	501	PEE	O3-C30-C31	2.70	120.38	111.91
77	C1	601	HEA	CMD-C2D-C1D	2.70	129.15	125.04
80	QC	401	HEM	CHA-C1A-NA	2.69	128.79	123.85
80	Qc	403	HEM	CHA-C4D-ND	2.69	127.69	124.37
80	Qc	403	HEM	CHD-C1D-ND	2.68	127.33	124.42
73	S2	501	PEE	O3-C30-C31	2.68	120.30	111.91
85	S7	201	U10	C35-C34-C36	2.67	119.77	115.27
80	Qc	403	HEM	C4C-NC-C1C	2.67	107.97	105.35
76	AK	401	ADP	C4-N9-C8	2.67	108.62	105.73
73	QC	403	PEE	O3-C30-C31	2.66	120.26	111.91
73	N1	403	PEE	O3-C30-C31	2.66	120.25	111.91
80	Qc	402	HEM	CHA-C1A-NA	2.65	128.72	123.85
80	Qc	402	HEM	C4C-NC-C1C	2.62	107.92	105.35
77	C1	601	HEA	C4D-C3D-C2D	-2.62	103.08	106.90
85	S7	201	U10	C27-C28-C29	-2.61	121.37	127.66
85	S7	201	U10	C25-C24-C26	2.61	119.66	115.27
73	7C	101	PEE	O3-C30-C31	2.59	120.04	111.91
73	S8	303	PEE	O3-C30-C31	2.58	120.02	111.91
73	Qe	301	PEE	O3-C30-C31	2.57	119.96	111.91
73	N3	201	PEE	O3-C30-C31	2.56	119.95	111.91
77	C1	602	HEA	CMB-C2B-C1B	-2.56	121.14	125.04
85	S7	201	U10	C15-C14-C16	2.55	119.56	115.27
73	A9	402	PEE	O3-C30-C31	2.55	119.90	111.91
73	N5	702	PEE	O3-C30-C31	2.54	119.89	111.91
77	C1	601	HEA	C26-C15-C16	2.54	119.54	115.27
73	A9	402	PEE	C37-C38-C39	-2.54	109.59	126.84
73	N5	701	PEE	O3-C30-C31	2.50	119.75	111.91
80	Qc	403	HEM	C4A-NA-C1A	2.47	107.77	105.35
81	Qd	401	HEC	O1A-CGA-CBA	-2.47	115.13	123.08
80	Qc	402	HEM	CHD-C1D-ND	2.46	127.09	124.42
81	Qd	401	HEC	C1D-ND-C4D	2.46	107.61	105.07
81	QD	401	HEC	O1A-CGA-CBA	-2.46	115.18	123.08
80	Qc	403	HEM	CAD-CBD-CGD	-2.45	108.33	113.60
77	C1	601	HEA	OMA-CMA-C3A	-2.45	120.15	125.69
75	AC	201	ZMP	O1-C10-C9	-2.44	121.11	123.99
80	QC	402	HEM	C2A-C1A-NA	-2.43	107.43	110.15
77	C1	602	HEA	CHB-C1B-NB	2.42	127.05	124.42
77	C1	602	HEA	C1D-ND-C4D	-2.42	102.57	105.07
80	QC	402	HEM	CHA-C1A-NA	2.39	128.25	123.85
85	S7	201	U10	C1M-C1-C6	-2.37	120.53	124.40
85	S7	201	U10	C56-C54-C55	2.37	119.83	114.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	C1	601	HEA	C27-C19-C18	-2.36	117.63	123.68
80	QC	402	HEM	C1C-CHC-C4B	-2.36	120.97	126.06
77	C1	601	HEA	C4C-NC-C1C	-2.34	103.06	105.35
80	QC	401	HEM	CAD-CBD-CGD	-2.33	108.59	113.60
80	Qc	402	HEM	CHB-C1B-C2B	-2.32	120.28	126.73
80	QC	402	HEM	C4A-CHB-C1B	-2.29	120.92	126.34
71	B1	101	PLX	O3-P1-O2	-2.28	100.98	112.24
80	Qc	402	HEM	C1C-CHC-C4B	-2.27	121.15	126.06
71	6C	101	PLX	O3-P1-O2	-2.27	101.01	112.24
71	CB	201	PLX	O3-P1-O2	-2.27	101.02	112.24
80	Qc	402	HEM	CAD-CBD-CGD	-2.27	108.72	113.60
80	QC	401	HEM	CHB-C1B-C2B	-2.27	120.43	126.73
80	Qc	403	HEM	C1C-CHC-C4B	-2.26	121.18	126.06
71	N6	201	PLX	O3-P1-O2	-2.25	101.11	112.24
71	AL	202	PLX	O3-P1-O2	-2.25	101.11	112.24
71	AM	201	PLX	O3-P1-O2	-2.24	101.17	112.24
81	Qd	401	HEC	O2A-CGA-O1A	2.24	128.88	123.30
77	C1	602	HEA	O1D-CGD-CBD	-2.24	115.90	123.08
80	Qc	403	HEM	CHB-C1B-C2B	-2.23	120.52	126.73
71	QI	301	PLX	O3-P1-O2	-2.23	101.23	112.24
71	N4	502	PLX	O3-P1-O2	-2.22	101.25	112.24
81	QD	401	HEC	O2A-CGA-O1A	2.20	128.79	123.30
71	Qi	301	PLX	O3-P1-O2	-2.20	101.35	112.24
71	S7	203	PLX	O3-P1-O2	-2.20	101.36	112.24
80	QC	402	HEM	CHB-C1B-C2B	-2.19	120.65	126.73
77	C1	602	HEA	CHC-C1C-C2C	-2.18	121.07	127.24
77	C1	601	HEA	CHC-C4B-NB	-2.18	121.69	124.37
80	QC	401	HEM	C4C-NC-C1C	2.18	107.48	105.35
77	C1	602	HEA	CHD-C1D-C2D	-2.17	120.70	126.73
77	C1	601	HEA	CMC-C2C-C3C	2.17	131.84	126.59
77	C1	602	HEA	CMC-C2C-C3C	2.16	131.81	126.59
76	AK	401	ADP	C6-C5-N7	2.16	136.04	132.02
77	C1	602	HEA	O1A-CGA-CBA	-2.16	116.15	123.08
80	Qc	403	HEM	C4A-CHB-C1B	-2.16	121.22	126.34
73	Qe	302	PEE	C2-O2-C10	-2.14	112.53	117.79
80	Qc	403	HEM	CHA-C1A-NA	2.14	127.78	123.85
80	QC	402	HEM	C4C-CHD-C1D	-2.13	121.46	126.06
73	QE	301	PEE	C2-O2-C10	-2.13	112.55	117.79
80	QC	401	HEM	C1C-CHC-C4B	-2.13	121.47	126.06
76	AK	401	ADP	N9-C8-N7	-2.10	111.04	113.91
85	S7	201	U10	C52-C53-C54	-2.10	120.58	127.75
81	QD	401	HEC	C1D-ND-C4D	2.10	107.24	105.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	Qc	402	HEM	C4A-NA-C1A	2.09	107.40	105.35
77	C1	602	HEA	C26-C15-C16	2.09	118.78	115.27
80	QC	401	HEM	C4A-NA-C1A	2.08	107.38	105.35
80	Qc	403	HEM	C2A-C1A-NA	-2.08	107.82	110.15
71	N4	502	PLX	C26-C25-C24	-2.07	108.59	113.38
77	C1	601	HEA	O1D-CGD-CBD	-2.07	116.45	123.08
73	Qc	401	PEE	C17-C18-C19	-2.06	108.90	124.73
77	C1	602	HEA	C27-C19-C18	-2.06	118.39	123.68
73	QC	403	PEE	C17-C18-C19	-2.06	108.95	124.73
80	QC	401	HEM	C4A-CHB-C1B	-2.05	121.47	126.34
73	S2	501	PEE	C20-C19-C18	-2.05	109.01	124.73
73	S8	303	PEE	C17-C18-C19	-2.04	109.05	124.73
73	Qe	301	PEE	C17-C18-C19	-2.04	109.05	124.73
81	QD	401	HEC	CMC-C2C-C3C	2.04	130.02	125.61
81	QD	401	HEC	CAA-C2A-C1A	-2.04	121.05	124.89
73	QE	301	PEE	C40-C39-C38	-2.04	109.09	124.73
73	S2	501	PEE	C37-C38-C39	-2.03	109.15	124.73
73	N5	705	PEE	C37-C38-C39	-2.03	109.16	124.73
75	AB	201	ZMP	C15-C14-C13	-2.03	108.98	112.36
80	Qc	402	HEM	C4A-CHB-C1B	-2.03	121.53	126.34
73	N5	701	PEE	C37-C38-C39	-2.02	109.21	124.73
73	7C	101	PEE	C40-C39-C38	-2.02	109.24	124.73
73	7C	101	PEE	C20-C19-C18	-2.02	109.25	124.73
73	N3	201	PEE	C37-C38-C39	-2.01	109.28	124.73
73	QE	301	PEE	C20-C19-C18	-2.01	109.34	124.73
80	Qc	403	HEM	C4C-CHD-C1D	-2.01	121.73	126.06
71	S7	203	PLX	C8-C7-C6	-2.00	108.75	113.38

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
81	QD	401	HEC	NA
81	Qd	401	HEC	NA

All (1361) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
68	4L	201	CDL	CA2-OA2-PA1-OA3
68	4L	201	CDL	CB2-OB2-PB2-OB3
68	4L	201	CDL	CB2-OB2-PB2-OB4
68	4L	201	CDL	CB2-OB2-PB2-OB5
68	7A	102	CDL	CA2-OA2-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
68	7A	102	CDL	CA2-OA2-PA1-OA4
68	7A	102	CDL	CA2-OA2-PA1-OA5
68	7A	102	CDL	CB3-OB5-PB2-OB3
68	A7	201	CDL	CB2-OB2-PB2-OB3
68	A7	201	CDL	CB3-OB5-PB2-OB2
68	A7	201	CDL	CB3-OB5-PB2-OB3
68	A7	201	CDL	CB3-OB5-PB2-OB4
68	A8	301	CDL	CA2-OA2-PA1-OA3
68	A8	301	CDL	CA2-OA2-PA1-OA4
68	A8	301	CDL	CA2-OA2-PA1-OA5
68	A8	301	CDL	CB3-OB5-PB2-OB4
68	AK	402	CDL	CA2-OA2-PA1-OA3
68	AK	402	CDL	CA2-OA2-PA1-OA4
68	AK	402	CDL	CA3-OA5-PA1-OA3
68	AK	402	CDL	CA3-OA5-PA1-OA4
68	AK	402	CDL	CB2-OB2-PB2-OB3
68	AK	402	CDL	CB2-OB2-PB2-OB4
68	AK	402	CDL	CB2-OB2-PB2-OB5
68	AL	201	CDL	CA2-OA2-PA1-OA3
68	AL	201	CDL	CB3-OB5-PB2-OB3
68	AL	201	CDL	CB3-OB5-PB2-OB4
68	B4	201	CDL	CA3-OA5-PA1-OA3
68	B4	201	CDL	CB2-OB2-PB2-OB3
68	B5	201	CDL	CA2-OA2-PA1-OA3
68	B5	201	CDL	CB3-OB5-PB2-OB2
68	C3	304	CDL	CA2-OA2-PA1-OA3
68	C3	304	CDL	CA2-OA2-PA1-OA4
68	C3	304	CDL	CA2-OA2-PA1-OA5
68	C3	304	CDL	CA3-OA5-PA1-OA4
68	C3	305	CDL	CA2-OA2-PA1-OA4
68	C3	305	CDL	CA3-OA5-PA1-OA3
68	CB	203	CDL	CA2-OA2-PA1-OA3
68	CB	203	CDL	CB2-OB2-PB2-OB3
68	N1	401	CDL	CB2-OB2-PB2-OB4
68	N4	503	CDL	CA2-OA2-PA1-OA3
68	N5	703	CDL	CA2-OA2-PA1-OA3
68	N5	703	CDL	CA3-OA5-PA1-OA2
68	N5	703	CDL	CA3-OA5-PA1-OA3
68	N5	703	CDL	CA3-OA5-PA1-OA4
68	N5	703	CDL	CB2-OB2-PB2-OB3
68	N5	703	CDL	CB2-OB2-PB2-OB4
68	N5	703	CDL	CB3-OB5-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
68	QB	501	CDL	CA2-OA2-PA1-OA3
68	QB	501	CDL	CA3-OA5-PA1-OA4
68	QC	404	CDL	CA2-OA2-PA1-OA4
68	QC	404	CDL	CA3-OA5-PA1-OA2
68	QC	404	CDL	CA3-OA5-PA1-OA3
68	QC	404	CDL	CA3-OA5-PA1-OA4
68	QC	404	CDL	OA6-CA4-CA6-OA8
68	QC	404	CDL	CB2-OB2-PB2-OB3
68	QC	404	CDL	CB3-OB5-PB2-OB3
68	QC	404	CDL	CB3-OB5-PB2-OB4
68	QD	402	CDL	CA2-OA2-PA1-OA3
68	QD	402	CDL	CA2-OA2-PA1-OA4
68	QD	402	CDL	CA2-OA2-PA1-OA5
68	QD	402	CDL	CA3-OA5-PA1-OA3
68	QD	402	CDL	CB3-OB5-PB2-OB2
68	QD	402	CDL	CB3-OB5-PB2-OB3
68	QD	402	CDL	CB3-OB5-PB2-OB4
68	QH	101	CDL	CA2-OA2-PA1-OA3
68	QH	102	CDL	CA2-OA2-PA1-OA3
68	QH	102	CDL	CA3-OA5-PA1-OA2
68	QH	102	CDL	CA3-OA5-PA1-OA3
68	QH	102	CDL	CA3-OA5-PA1-OA4
68	QH	102	CDL	CB2-OB2-PB2-OB4
68	Qb	501	CDL	CA2-OA2-PA1-OA3
68	Qb	501	CDL	CB2-OB2-PB2-OB5
68	Qb	501	CDL	CB3-OB5-PB2-OB2
68	Qb	501	CDL	CB3-OB5-PB2-OB3
68	Qb	501	CDL	CB3-OB5-PB2-OB4
68	Qb	501	CDL	OB5-CB3-CB4-OB6
70	6A	101	PC1	C11-O13-P-O14
70	C1	606	PC1	C11-O13-P-O12
70	C1	606	PC1	C11-O13-P-O14
70	C1	606	PC1	C11-O13-P-O11
70	C1	610	PC1	C11-O13-P-O12
70	C1	610	PC1	C11-O13-P-O14
70	C1	610	PC1	C11-O13-P-O11
70	C3	301	PC1	C11-O13-P-O14
70	C3	302	PC1	C11-O13-P-O14
70	C3	302	PC1	C1-O11-P-O12
70	C3	302	PC1	C1-O11-P-O14
70	C3	302	PC1	C1-O11-P-O13
70	C3	303	PC1	C1-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
70	C3	303	PC1	C1-O11-P-O14
70	C3	303	PC1	C1-O11-P-O13
70	N1	402	PC1	C11-O13-P-O12
70	N1	402	PC1	C11-O13-P-O14
70	N1	402	PC1	C11-O13-P-O11
70	N1	402	PC1	C1-O11-P-O12
70	N1	402	PC1	C1-O11-P-O14
70	Qc	405	PC1	C1-O11-P-O14
71	6C	101	PLX	O7-C6-O6-C4
71	AL	202	PLX	O7-C6-C7-C8
71	AL	202	PLX	O7-C6-O6-C4
71	AL	202	PLX	C3-O4-P1-O2
71	AL	202	PLX	C25-C24-O8-C5
71	AL	202	PLX	O9-C24-C25-C26
71	AM	201	PLX	O7-C6-O6-C4
71	AM	201	PLX	C2-O1-P1-O4
71	AM	201	PLX	C2-O1-P1-O2
71	AM	201	PLX	N1-C1-C2-O1
71	B1	101	PLX	O7-C6-O6-C4
71	B1	101	PLX	C3-O4-P1-O2
71	B1	101	PLX	C3-O4-P1-O3
71	B1	101	PLX	C2-O1-P1-O2
71	B1	101	PLX	C2-O1-P1-O3
71	CB	201	PLX	O7-C6-O6-C4
71	CB	201	PLX	C2-O1-P1-O2
71	CB	201	PLX	O9-C24-O8-C5
71	CB	201	PLX	O9-C24-C25-C26
71	N4	502	PLX	O7-C6-O6-C4
71	N4	502	PLX	C5-C4-O6-C6
71	N4	502	PLX	C3-O4-P1-O2
71	N4	502	PLX	C3-O4-P1-O3
71	N6	201	PLX	O7-C6-O6-C4
71	N6	201	PLX	N1-C1-C2-O1
71	N6	201	PLX	O8-C24-C25-C26
71	N6	201	PLX	O9-C24-C25-C26
71	QI	301	PLX	C2-O1-P1-O2
71	QI	301	PLX	O9-C24-O8-C5
71	QI	301	PLX	O9-C24-C25-C26
71	Qi	301	PLX	O7-C6-C7-C8
71	Qi	301	PLX	O7-C6-O6-C4
71	Qi	301	PLX	C2-O1-P1-O2
71	Qi	301	PLX	O9-C24-O8-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	Qi	301	PLX	O9-C24-C25-C26
71	S7	203	PLX	O7-C6-C7-C8
71	S7	203	PLX	C2-O1-P1-O3
71	S7	203	PLX	O9-C24-C25-C26
72	B8	201	3PE	C1-O11-P-O13
72	B8	201	3PE	O13-C11-C12-N
72	C1	609	3PE	C1-O11-P-O12
72	C1	609	3PE	C1-O11-P-O13
72	C1	609	3PE	C1-O11-P-O14
72	C1	609	3PE	C11-O13-P-O12
72	C1	609	3PE	C11-O13-P-O14
72	C1	609	3PE	O13-C11-C12-N
72	CB	202	3PE	C1-O11-P-O12
72	CB	202	3PE	C11-O13-P-O12
72	CB	202	3PE	C11-O13-P-O14
72	N5	706	3PE	C1-O11-P-O12
72	N5	706	3PE	C1-O11-P-O13
72	N5	706	3PE	C1-O11-P-O14
72	N5	706	3PE	O13-C11-C12-N
72	QE	302	3PE	O13-C11-C12-N
72	QJ	101	3PE	C11-O13-P-O12
72	QJ	101	3PE	C11-O13-P-O14
72	QJ	101	3PE	O13-C11-C12-N
72	Qc	404	3PE	C11-O13-P-O11
72	Qc	404	3PE	C11-O13-P-O12
72	Qc	404	3PE	C11-O13-P-O14
72	Qc	404	3PE	O13-C11-C12-N
72	Qj	101	3PE	C11-O13-P-O12
72	Qj	101	3PE	C11-O13-P-O14
72	Qj	101	3PE	O13-C11-C12-N
72	S7	204	3PE	C1-O11-P-O12
72	S7	204	3PE	C1-O11-P-O14
72	S7	204	3PE	O13-C11-C12-N
73	A9	402	PEE	C11-C10-O2-C2
73	A9	402	PEE	C1-O3P-P-O1P
73	A9	402	PEE	C4-O4P-P-O3P
73	A9	402	PEE	C4-O4P-P-O2P
73	N1	403	PEE	C1-O3P-P-O2P
73	N1	403	PEE	C1-O3P-P-O1P
73	N1	403	PEE	C4-O4P-P-O3P
73	N1	403	PEE	C4-O4P-P-O2P
73	N1	403	PEE	C4-O4P-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
73	N3	201	PEE	C17-C18-C19-C20
73	N3	201	PEE	C1-O3P-P-O2P
73	N3	201	PEE	C4-O4P-P-O3P
73	N3	201	PEE	C31-C30-O3-C3
73	N4	501	PEE	C1-O3P-P-O2P
73	N4	501	PEE	C1-O3P-P-O1P
73	N4	501	PEE	O4P-C4-C5-N
73	N4	501	PEE	C37-C38-C39-C40
73	N5	702	PEE	C11-C10-O2-C2
73	N5	702	PEE	C1-O3P-P-O2P
73	N5	702	PEE	C1-O3P-P-O1P
73	N5	702	PEE	C1-O3P-P-O4P
73	N5	702	PEE	C37-C38-C39-C40
73	N5	705	PEE	C1-O3P-P-O2P
73	N5	705	PEE	C4-O4P-P-O2P
73	N5	705	PEE	C4-O4P-P-O1P
73	QB	502	PEE	C4-O4P-P-O2P
73	QB	502	PEE	C4-O4P-P-O1P
73	QB	502	PEE	O5-C30-O3-C3
73	QB	502	PEE	C31-C30-O3-C3
73	QC	403	PEE	O2-C2-C3-O3
73	QE	301	PEE	C1-O3P-P-O2P
73	QE	301	PEE	C1-O3P-P-O1P
73	QE	301	PEE	C4-O4P-P-O1P
73	Qc	401	PEE	O4P-C4-C5-N
73	Qe	301	PEE	C11-C10-O2-C2
73	Qe	301	PEE	O4-C10-O2-C2
73	Qe	301	PEE	C1-O3P-P-O2P
73	Qe	301	PEE	C4-O4P-P-O1P
73	S2	501	PEE	C11-C10-O2-C2
73	S2	501	PEE	O4-C10-O2-C2
73	S2	501	PEE	C1-O3P-P-O1P
73	S2	501	PEE	C4-O4P-P-O3P
73	S2	501	PEE	C4-O4P-P-O2P
73	S2	501	PEE	C4-O4P-P-O1P
73	S2	501	PEE	O4P-C4-C5-N
73	S8	303	PEE	O4-C10-O2-C2
73	S8	303	PEE	O3P-C1-C2-O2
73	S8	303	PEE	C1-O3P-P-O1P
73	S8	303	PEE	C1-O3P-P-O4P
75	AC	201	ZMP	C17-C18-C21-O5
75	AC	201	ZMP	N2-C16-C17-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	AC	201	ZMP	C12-C11-S1-C10
75	AC	201	ZMP	O1-C10-S1-C11
75	AC	201	ZMP	C9-C10-S1-C11
75	AC	201	ZMP	S1-C10-C9-C8
75	AC	201	ZMP	C7-C8-C9-C10
76	AK	401	ADP	C5'-O5'-PA-O2A
76	AK	401	ADP	C5'-O5'-PA-O3A
77	C1	601	HEA	C1A-C2A-CAA-CBA
77	C1	601	HEA	C2A-C3A-CMA-OMA
77	C1	601	HEA	C4A-C3A-CMA-OMA
77	C1	601	HEA	C17-C18-C19-C27
77	C1	601	HEA	C27-C19-C20-C21
77	C1	602	HEA	C2A-C3A-CMA-OMA
77	C1	602	HEA	C4A-C3A-CMA-OMA
77	C1	602	HEA	C18-C19-C20-C21
77	C1	602	HEA	C27-C19-C20-C21
80	QC	401	HEM	C2B-C3B-CAB-CBB
80	QC	402	HEM	C2B-C3B-CAB-CBB
80	Qc	403	HEM	C2B-C3B-CAB-CBB
80	Qc	403	HEM	C4B-C3B-CAB-CBB
85	S7	201	U10	C9-C11-C12-C13
85	S7	201	U10	C18-C19-C21-C22
85	S7	201	U10	C20-C19-C21-C22
85	S7	201	U10	C23-C24-C26-C27
85	S7	201	U10	C25-C24-C26-C27
85	S7	201	U10	C34-C36-C37-C38
85	S7	201	U10	C38-C39-C41-C42
85	S7	201	U10	C40-C39-C41-C42
73	N3	201	PEE	O5-C30-O3-C3
73	Qe	301	PEE	O5-C30-O3-C3
73	Qe	301	PEE	C31-C30-O3-C3
73	N1	403	PEE	O5-C30-O3-C3
73	N4	501	PEE	O5-C30-O3-C3
73	N5	702	PEE	O5-C30-O3-C3
73	Qc	401	PEE	O5-C30-O3-C3
73	A9	402	PEE	O4-C10-O2-C2
73	N5	702	PEE	O4-C10-O2-C2
73	N5	705	PEE	O4-C10-O2-C2
73	N4	501	PEE	C31-C30-O3-C3
73	Qc	401	PEE	C31-C30-O3-C3
73	N5	705	PEE	C11-C10-O2-C2
73	S8	303	PEE	C11-C10-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
77	C1	601	HEA	C3A-C2A-CAA-CBA
85	S7	201	U10	C35-C34-C36-C37
73	N1	403	PEE	C31-C30-O3-C3
73	N5	702	PEE	C31-C30-O3-C3
73	N5	701	PEE	C17-C18-C19-C20
73	N5	701	PEE	C37-C38-C39-C40
73	N5	705	PEE	C37-C38-C39-C40
73	S8	303	PEE	C37-C38-C39-C40
77	C1	602	HEA	C17-C18-C19-C27
77	C1	601	HEA	C17-C18-C19-C20
77	C1	602	HEA	C17-C18-C19-C20
73	A9	402	PEE	O5-C30-O3-C3
68	A7	201	CDL	O1-C1-CA2-OA2
73	A9	402	PEE	C31-C30-O3-C3
73	7C	101	PEE	C21-C22-C23-C24
80	Qc	403	HEM	C1A-C2A-CAA-CBA
68	AL	201	CDL	C1-CA2-OA2-PA1
77	C1	601	HEA	C15-C16-C17-C18
77	C1	602	HEA	C19-C20-C21-C22
85	S7	201	U10	C19-C21-C22-C23
85	S7	201	U10	C29-C31-C32-C33
85	S7	201	U10	C49-C51-C52-C53
68	A8	301	CDL	CA2-C1-CB2-OB2
70	C1	605	PC1	C11-C12-N-C14
70	C3	303	PC1	C11-C12-N-C14
68	A8	301	CDL	O1-C1-CB2-OB2
68	B4	201	CDL	O1-C1-CA2-OA2
73	N1	403	PEE	C10-C11-C12-C13
73	7C	101	PEE	O2-C2-C3-O3
77	C1	601	HEA	C18-C19-C20-C21
85	S7	201	U10	C33-C34-C36-C37
73	N3	201	PEE	C10-C11-C12-C13
73	QC	403	PEE	C10-C11-C12-C13
73	Qc	401	PEE	C30-C31-C32-C33
73	N5	702	PEE	C30-C31-C32-C33
73	Qe	302	PEE	C10-C11-C12-C13
70	C1	608	PC1	C2-C1-O11-P
72	7A	101	3PE	C2-C1-O11-P
70	C1	605	PC1	C11-C12-N-C13
70	C3	303	PC1	C11-C12-N-C13
73	N1	403	PEE	C30-C31-C32-C33
80	Qc	403	HEM	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
72	7A	101	3PE	C31-C32-C33-C34
77	C1	601	HEA	C19-C20-C21-C22
85	S7	201	U10	C14-C16-C17-C18
73	QE	301	PEE	C10-C11-C12-C13
68	N1	401	CDL	O1-C1-CB2-OB2
73	N1	403	PEE	C33-C34-C35-C36
73	Qc	401	PEE	C17-C18-C19-C20
68	4L	201	CDL	CA2-OA2-PA1-OA5
68	4L	201	CDL	CA3-OA5-PA1-OA2
68	7A	102	CDL	CB2-OB2-PB2-OB5
68	A8	301	CDL	CB2-OB2-PB2-OB5
68	A8	301	CDL	CB3-OB5-PB2-OB2
68	AK	402	CDL	CA2-OA2-PA1-OA5
68	AK	402	CDL	CA3-OA5-PA1-OA2
68	AL	201	CDL	CA2-OA2-PA1-OA5
68	AL	201	CDL	CB3-OB5-PB2-OB2
68	B4	201	CDL	CA2-OA2-PA1-OA5
68	B5	201	CDL	CA3-OA5-PA1-OA2
68	C3	304	CDL	CA3-OA5-PA1-OA2
68	C3	305	CDL	CA2-OA2-PA1-OA5
68	CB	203	CDL	CA2-OA2-PA1-OA5
68	CB	203	CDL	CB2-OB2-PB2-OB5
68	CB	203	CDL	CB3-OB5-PB2-OB2
68	N1	401	CDL	CB2-OB2-PB2-OB5
68	N1	401	CDL	CB3-OB5-PB2-OB2
68	N4	503	CDL	CA2-OA2-PA1-OA5
68	N4	503	CDL	CA3-OA5-PA1-OA2
68	N4	503	CDL	CB2-OB2-PB2-OB5
68	N5	703	CDL	CA2-OA2-PA1-OA5
68	N5	703	CDL	CB2-OB2-PB2-OB5
68	N5	703	CDL	CB3-OB5-PB2-OB2
68	QB	501	CDL	CA2-OA2-PA1-OA5
68	QB	501	CDL	CA3-OA5-PA1-OA2
68	QC	404	CDL	CB3-OB5-PB2-OB2
68	QH	102	CDL	CB2-OB2-PB2-OB5
68	QH	102	CDL	CB3-OB5-PB2-OB2
68	Qb	501	CDL	CA2-OA2-PA1-OA5
70	6A	101	PC1	C11-O13-P-O11
70	C1	605	PC1	C11-O13-P-O11
70	C1	606	PC1	C1-O11-P-O13
70	C1	608	PC1	C1-O11-P-O13
70	C3	301	PC1	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
70	C3	302	PC1	C11-O13-P-O11
70	N1	402	PC1	C1-O11-P-O13
70	N3	202	PC1	C11-O13-P-O11
70	N3	202	PC1	C1-O11-P-O13
70	Qc	405	PC1	C1-O11-P-O13
71	B1	101	PLX	C3-O4-P1-O1
71	B1	101	PLX	C2-O1-P1-O4
71	CB	201	PLX	C2-O1-P1-O4
71	N4	502	PLX	C3-O4-P1-O1
71	N6	201	PLX	C3-O4-P1-O1
71	QI	301	PLX	C2-O1-P1-O4
71	S7	203	PLX	C2-O1-P1-O4
72	7A	101	3PE	C1-O11-P-O13
72	7A	101	3PE	C11-O13-P-O11
72	B8	201	3PE	C11-O13-P-O11
72	C1	609	3PE	C11-O13-P-O11
72	CA	101	3PE	C11-O13-P-O11
72	CB	202	3PE	C11-O13-P-O11
72	QE	302	3PE	C1-O11-P-O13
72	QJ	101	3PE	C11-O13-P-O11
72	Qc	404	3PE	C1-O11-P-O13
72	Qj	101	3PE	C11-O13-P-O11
72	S7	204	3PE	C1-O11-P-O13
73	N1	403	PEE	C1-O3P-P-O4P
73	N3	201	PEE	C1-O3P-P-O4P
73	N4	501	PEE	C1-O3P-P-O4P
73	N5	701	PEE	C4-O4P-P-O3P
73	QB	502	PEE	C4-O4P-P-O3P
73	QC	403	PEE	C4-O4P-P-O3P
73	QE	301	PEE	C1-O3P-P-O4P
73	Qc	401	PEE	C1-O3P-P-O4P
73	Qe	301	PEE	C1-O3P-P-O4P
73	Qe	301	PEE	C4-O4P-P-O3P
68	A7	201	CDL	CB2-C1-CA2-OA2
68	B4	201	CDL	CB2-C1-CA2-OA2
68	N1	401	CDL	CA2-C1-CB2-OB2
85	S7	201	U10	C45-C44-C46-C47
73	S8	303	PEE	C31-C30-O3-C3
73	N5	705	PEE	C33-C34-C35-C36
71	AL	202	PLX	O6-C6-C7-C8
71	AM	201	PLX	O6-C6-C7-C8
71	S7	203	PLX	O6-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	S7	203	PLX	O8-C24-C25-C26
71	N4	502	PLX	C9-C10-C11-C12
73	N3	201	PEE	C32-C33-C34-C35
73	N5	702	PEE	C14-C15-C16-C17
71	AL	202	PLX	C29-C30-C31-C32
71	AM	201	PLX	C12-C13-C14-C15
71	CB	201	PLX	C29-C30-C31-C32
71	Qi	301	PLX	C26-C27-C28-C29
71	S7	203	PLX	C7-C8-C9-C10
73	N5	701	PEE	C21-C22-C23-C24
73	Qc	401	PEE	C31-C32-C33-C34
75	AC	201	ZMP	C19-C18-C21-O5
75	AC	201	ZMP	C20-C18-C21-O5
71	B1	101	PLX	C29-C30-C31-C32
71	N6	201	PLX	C34-C35-C36-C37
71	S7	203	PLX	C13-C14-C15-C16
73	N5	701	PEE	C31-C32-C33-C34
73	N5	702	PEE	C12-C13-C14-C15
73	N5	702	PEE	C11-C12-C13-C14
73	N5	702	PEE	C10-C11-C12-C13
71	Qi	301	PLX	C18-C19-C20-C21
72	C1	609	3PE	C25-C26-C27-C28
73	N3	201	PEE	C33-C34-C35-C36
73	N4	501	PEE	C23-C24-C25-C26
73	N5	701	PEE	C12-C13-C14-C15
70	Qb	502	PC1	C36-C37-C38-C39
71	B1	101	PLX	C25-C26-C27-C28
73	7C	101	PEE	C12-C13-C14-C15
73	N5	701	PEE	C14-C15-C16-C17
73	QC	403	PEE	C21-C22-C23-C24
71	QI	301	PLX	C29-C30-C31-C32
68	N4	503	CDL	CA7-C31-C32-C33
70	N3	202	PC1	C23-C24-C25-C26
71	Qi	301	PLX	C25-C26-C27-C28
72	C1	607	3PE	C2C-C2D-C2E-C2F
73	Qc	401	PEE	C33-C34-C35-C36
73	S8	303	PEE	C33-C34-C35-C36
68	N1	401	CDL	C76-C77-C78-C79
71	AL	202	PLX	C12-C13-C14-C15
73	A9	402	PEE	C12-C13-C14-C15
68	4L	201	CDL	C39-C40-C41-C42
68	CB	203	CDL	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	CB	201	PLX	C31-C32-C33-C34
73	N1	403	PEE	C12-C13-C14-C15
73	N5	701	PEE	C32-C33-C34-C35
73	QE	301	PEE	C32-C33-C34-C35
73	S2	501	PEE	C11-C12-C13-C14
75	AC	201	ZMP	C1-C22-C23-C24
73	N3	201	PEE	C22-C23-C24-C25
73	N5	705	PEE	C14-C15-C16-C17
73	Qe	301	PEE	C33-C34-C35-C36
73	N4	501	PEE	C11-C10-O2-C2
73	QE	301	PEE	C11-C10-O2-C2
73	N1	403	PEE	C13-C14-C15-C16
73	S2	501	PEE	C20-C21-C22-C23
73	N4	501	PEE	C35-C36-C37-C38
73	N4	501	PEE	C39-C40-C41-C42
73	QB	502	PEE	C35-C36-C37-C38
70	C3	301	PC1	C29-C2A-C2B-C2C
70	C3	306	PC1	C29-C2A-C2B-C2C
71	N4	502	PLX	C16-C17-C18-C19
72	CA	101	3PE	C2A-C2B-C2C-C2D
73	Qe	301	PEE	C14-C15-C16-C17
75	AB	201	ZMP	C2-C1-C22-C23
70	C3	303	PC1	C11-C12-N-C15
85	S7	201	U10	C39-C41-C42-C43
73	7C	101	PEE	C11-C12-C13-C14
72	7A	101	3PE	O13-C11-C12-N
73	QE	301	PEE	O4P-C4-C5-N
68	CB	203	CDL	C38-C39-C40-C41
71	QI	301	PLX	C7-C8-C9-C10
73	S8	303	PEE	C11-C12-C13-C14
68	CB	203	CDL	C22-C23-C24-C25
68	A8	301	CDL	C38-C39-C40-C41
68	N4	503	CDL	C13-C14-C15-C16
73	Qc	401	PEE	C22-C23-C24-C25
71	CB	201	PLX	C7-C8-C9-C10
73	N3	201	PEE	C21-C22-C23-C24
68	AL	201	CDL	C52-C53-C54-C55
68	N5	704	CDL	C22-C23-C24-C25
73	Qe	302	PEE	C11-C12-C13-C14
68	AL	201	CDL	C33-C34-C35-C36
73	S8	303	PEE	O5-C30-O3-C3
71	AM	201	PLX	O9-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	B1	101	PLX	O9-C24-C25-C26
68	N5	704	CDL	C72-C73-C74-C75
68	QB	501	CDL	C51-C52-C53-C54
68	QH	102	CDL	C51-C52-C53-C54
73	N3	201	PEE	C35-C36-C37-C38
73	N5	701	PEE	C15-C16-C17-C18
72	C1	607	3PE	C2E-C2F-C2G-C2H
70	Qh	101	PC1	C35-C36-C37-C38
73	QE	301	PEE	C12-C13-C14-C15
68	QH	101	CDL	C31-C32-C33-C34
72	N5	706	3PE	C35-C36-C37-C38
73	N1	403	PEE	C11-C12-C13-C14
73	Qc	401	PEE	C12-C13-C14-C15
73	Qe	301	PEE	C22-C23-C24-C25
70	C1	605	PC1	C11-C12-N-C15
70	C3	302	PC1	C11-C12-N-C15
68	CB	203	CDL	C78-C79-C80-C81
80	QC	401	HEM	C3D-CAD-CBD-CGD
73	QE	301	PEE	C11-C12-C13-C14
73	N5	702	PEE	C18-C19-C20-C21
73	A9	402	PEE	C35-C36-C37-C38
73	S2	501	PEE	C19-C20-C21-C22
73	N4	501	PEE	O4-C10-O2-C2
73	N5	701	PEE	O4-C10-O2-C2
73	QE	301	PEE	O4-C10-O2-C2
72	S7	204	3PE	C21-C22-C23-C24
73	S2	501	PEE	C31-C30-O3-C3
75	AC	201	ZMP	C22-C23-C24-C25
72	QJ	101	3PE	C24-C25-C26-C27
73	S2	501	PEE	C14-C15-C16-C17
68	N5	703	CDL	C60-C61-C62-C63
73	Qc	401	PEE	C32-C33-C34-C35
72	C1	607	3PE	C27-C28-C29-C2A
80	Qc	402	HEM	C2B-C3B-CAB-CBB
71	AL	202	PLX	C33-C34-C35-C36
71	Qi	301	PLX	C13-C14-C15-C16
73	7C	101	PEE	C31-C32-C33-C34
73	S8	303	PEE	C22-C23-C24-C25
68	CB	203	CDL	C61-C62-C63-C64
73	N5	701	PEE	C11-C12-C13-C14
68	4L	201	CDL	CA5-C11-C12-C13
73	N5	701	PEE	C11-C10-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
73	Qe	302	PEE	C11-C10-O2-C2
71	CB	201	PLX	O4-C3-C4-O6
71	Qi	301	PLX	O4-C3-C4-O6
73	Qe	302	PEE	O3P-C1-C2-O2
68	N1	401	CDL	C31-C32-C33-C34
73	N4	501	PEE	C22-C23-C24-C25
73	S8	303	PEE	C13-C14-C15-C16
75	AB	201	ZMP	C22-C23-C24-C25
80	QC	401	HEM	C4B-C3B-CAB-CBB
80	QC	402	HEM	C4B-C3B-CAB-CBB
71	N4	502	PLX	C29-C30-C31-C32
75	AB	201	ZMP	C6-C7-C8-C9
73	Qe	302	PEE	O4-C10-O2-C2
68	A8	301	CDL	OB6-CB4-CB6-OB8
70	C1	608	PC1	O21-C2-C3-O31
71	6C	101	PLX	O6-C4-C5-O8
72	QJ	101	3PE	O21-C2-C3-O31
68	N5	703	CDL	C59-C60-C61-C62
71	N4	502	PLX	C11-C12-C13-C14
73	Qe	301	PEE	C12-C13-C14-C15
75	AC	201	ZMP	C6-C7-C8-C9
70	Qh	101	PC1	C11-C12-N-C14
75	AC	201	ZMP	C3-C4-C5-C6
73	7C	101	PEE	C35-C36-C37-C38
73	N5	701	PEE	C35-C36-C37-C38
73	N5	705	PEE	C35-C36-C37-C38
73	S2	501	PEE	C15-C16-C17-C18
73	S8	303	PEE	C35-C36-C37-C38
85	S7	201	U10	C43-C44-C46-C47
73	N4	501	PEE	C11-C12-C13-C14
73	QE	301	PEE	C33-C34-C35-C36
73	N4	501	PEE	C17-C18-C19-C20
73	A9	402	PEE	C33-C34-C35-C36
73	S2	501	PEE	C40-C41-C42-C43
73	N5	702	PEE	C33-C34-C35-C36
75	AC	201	ZMP	C1-C2-C3-C4
73	QE	301	PEE	C16-C17-C18-C19
68	7A	102	CDL	CA3-OA5-PA1-OA2
68	AL	201	CDL	CB2-OB2-PB2-OB5
68	B5	201	CDL	CA2-OA2-PA1-OA5
68	QC	404	CDL	CB2-OB2-PB2-OB5
68	QH	101	CDL	CA2-OA2-PA1-OA5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
70	C3	301	PC1	C1-O11-P-O13
71	AL	202	PLX	C3-O4-P1-O1
71	Qi	301	PLX	C2-O1-P1-O4
73	N5	705	PEE	C1-O3P-P-O4P
73	N5	705	PEE	C4-O4P-P-O3P
73	S2	501	PEE	C1-O3P-P-O4P
72	QJ	101	3PE	C26-C27-C28-C29
70	C3	301	PC1	C2-C1-O11-P
68	7A	102	CDL	OB5-CB3-CB4-CB6
68	QD	402	CDL	OA5-CA3-CA4-CA6
70	C3	301	PC1	O11-C1-C2-C3
73	Qc	401	PEE	O3P-C1-C2-C3
73	S2	501	PEE	C42-C43-C44-C45
75	AC	201	ZMP	C14-C15-N2-C16
73	Qe	301	PEE	C10-C11-C12-C13
73	N5	705	PEE	C21-C22-C23-C24
73	QB	502	PEE	C32-C33-C34-C35
75	AC	201	ZMP	C2-C3-C4-C5
73	Qe	301	PEE	C35-C36-C37-C38
68	B5	201	CDL	CB2-C1-CA2-OA2
80	Qc	403	HEM	C3A-C2A-CAA-CBA
72	CB	202	3PE	C21-C22-C23-C24
73	S2	501	PEE	O5-C30-O3-C3
70	Qc	405	PC1	C3A-C3B-C3C-C3D
68	A8	301	CDL	CB3-CB4-CB6-OB8
68	N4	503	CDL	CA3-CA4-CA6-OA8
68	QC	404	CDL	CA3-CA4-CA6-OA8
68	QH	102	CDL	CA3-CA4-CA6-OA8
70	C1	608	PC1	C39-C3A-C3B-C3C
70	C3	306	PC1	C1-C2-C3-O31
73	N1	403	PEE	C1-C2-C3-O3
73	N5	701	PEE	C1-C2-C3-O3
73	QB	502	PEE	C1-C2-C3-O3
73	Qc	401	PEE	C1-C2-C3-O3
71	S7	203	PLX	C32-C33-C34-C35
70	QB	503	PC1	C29-C2A-C2B-C2C
73	N5	702	PEE	C32-C33-C34-C35
73	S2	501	PEE	C21-C22-C23-C24
71	N6	201	PLX	O6-C6-C7-C8
75	AB	201	ZMP	O3-C16-C17-O4
75	AC	201	ZMP	O3-C16-C17-O4
73	QC	403	PEE	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
73	S8	303	PEE	C21-C22-C23-C24
73	QC	403	PEE	C16-C17-C18-C19
68	B5	201	CDL	C21-C22-C23-C24
73	N5	701	PEE	C33-C34-C35-C36
73	7C	101	PEE	C39-C40-C41-C42
73	N5	705	PEE	C19-C20-C21-C22
75	AC	201	ZMP	C22-C1-C2-C3
73	QE	301	PEE	C40-C41-C42-C43
73	N5	701	PEE	C30-C31-C32-C33
68	CB	203	CDL	C63-C64-C65-C66
70	Qc	405	PC1	C28-C29-C2A-C2B
72	CA	101	3PE	C35-C36-C37-C38
68	B4	201	CDL	C80-C81-C82-C83
73	Qe	301	PEE	C38-C39-C40-C41
73	S2	501	PEE	C38-C39-C40-C41
71	CB	201	PLX	C11-C12-C13-C14
68	C3	304	CDL	OB5-CB3-CB4-OB6
73	N1	403	PEE	O3P-C1-C2-O2
70	C3	302	PC1	C11-C12-N-C13
71	QI	301	PLX	C34-C35-C36-C37
73	QC	403	PEE	C14-C15-C16-C17
73	Qe	301	PEE	C41-C42-C43-C44
73	A9	402	PEE	C31-C32-C33-C34
71	N4	502	PLX	C34-C35-C36-C37
73	S8	303	PEE	O2-C2-C3-O3
71	QI	301	PLX	C16-C17-C18-C19
73	N3	201	PEE	C42-C43-C44-C45
68	N1	401	CDL	C75-C76-C77-C78
71	Qi	301	PLX	C29-C30-C31-C32
70	N3	202	PC1	C32-C33-C34-C35
73	S8	303	PEE	C34-C35-C36-C37
71	S7	203	PLX	C14-C15-C16-C17
74	A9	401	NDP	PN-O3-PA-O1A
73	A9	402	PEE	C11-C12-C13-C14
70	Qc	405	PC1	C2D-C2E-C2F-C2G
68	A8	301	CDL	C11-C12-C13-C14
68	N5	704	CDL	C17-C18-C19-C20
73	A9	402	PEE	C17-C18-C19-C20
73	S2	501	PEE	C18-C19-C20-C21
73	S2	501	PEE	C16-C17-C18-C19
68	AL	201	CDL	OB5-CB3-CB4-CB6
68	C3	304	CDL	OB5-CB3-CB4-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
68	QB	501	CDL	OB5-CB3-CB4-CB6
70	C1	608	PC1	O11-C1-C2-C3
71	6C	101	PLX	O4-C3-C4-C5
71	CB	201	PLX	O4-C3-C4-C5
71	Qi	301	PLX	O4-C3-C4-C5
72	7A	101	3PE	O11-C1-C2-C3
73	A9	402	PEE	O3P-C1-C2-C3
73	QB	502	PEE	O3P-C1-C2-C3
73	QC	403	PEE	O3P-C1-C2-C3
73	Qe	301	PEE	O3P-C1-C2-C3
73	Qe	302	PEE	O3P-C1-C2-C3
68	QB	501	CDL	CA7-C31-C32-C33
72	CA	101	3PE	O13-C11-C12-N
71	N6	201	PLX	C7-C8-C9-C10
72	Qc	404	3PE	C3A-C3B-C3C-C3D
73	N4	501	PEE	C24-C25-C26-C27
73	QE	301	PEE	C14-C15-C16-C17
68	7A	102	CDL	C78-C79-C80-C81
73	7C	101	PEE	C41-C42-C43-C44
73	N3	201	PEE	C40-C41-C42-C43
71	AL	202	PLX	C32-C33-C34-C35
71	CB	201	PLX	C20-C21-C22-C23
71	N6	201	PLX	C35-C36-C37-C38
72	CB	202	3PE	C39-C3A-C3B-C3C
68	QD	402	CDL	CA4-CA3-OA5-PA1
68	QH	102	CDL	CA4-CA3-OA5-PA1
70	C3	303	PC1	C2-C1-O11-P
70	N1	402	PC1	C2-C1-O11-P
73	N5	705	PEE	C24-C25-C26-C27
68	CB	203	CDL	C81-C82-C83-C84
71	6C	101	PLX	C13-C14-C15-C16
71	AM	201	PLX	C25-C26-C27-C28
71	Qi	301	PLX	C19-C20-C21-C22
72	QJ	101	3PE	C33-C34-C35-C36
80	Qc	402	HEM	C3D-CAD-CBD-CGD
68	4L	201	CDL	C15-C16-C17-C18
68	Qb	501	CDL	C54-C55-C56-C57
68	QD	402	CDL	CA3-CA4-CA6-OA8
70	C1	608	PC1	C1-C2-C3-O31
71	N4	502	PLX	C3-C4-C5-O8
71	N6	201	PLX	C3-C4-C5-O8
72	QJ	101	3PE	C1-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
73	7C	101	PEE	C1-C2-C3-O3
73	N5	705	PEE	C1-C2-C3-O3
73	Qe	302	PEE	C1-C2-C3-O3
73	N5	701	PEE	C22-C23-C24-C25
73	N3	201	PEE	C11-C12-C13-C14
75	AB	201	ZMP	N2-C16-C17-C18
68	N1	401	CDL	C13-C14-C15-C16
73	Qc	401	PEE	C35-C36-C37-C38
68	B4	201	CDL	CA3-OA5-PA1-OA2
68	C3	305	CDL	CA3-OA5-PA1-OA2
71	B1	101	PLX	C5-C4-O6-C6
71	CB	201	PLX	C3-C4-O6-C6
71	N6	201	PLX	C5-C4-O6-C6
72	CA	101	3PE	C1-O11-P-O13
73	N5	702	PEE	C4-O4P-P-O3P
70	Qh	101	PC1	C38-C39-C3A-C3B
71	CB	201	PLX	O7-C6-C7-C8
68	CB	203	CDL	C33-C34-C35-C36
75	AB	201	ZMP	C3-C4-C5-C6
68	7A	102	CDL	OB5-CB3-CB4-OB6
68	A8	301	CDL	OB5-CB3-CB4-OB6
68	B4	201	CDL	OB5-CB3-CB4-OB6
68	B5	201	CDL	OB5-CB3-CB4-OB6
71	AM	201	PLX	O4-C3-C4-O6
71	QI	301	PLX	O4-C3-C4-O6
72	7A	101	3PE	O11-C1-C2-O21
73	N5	701	PEE	O3P-C1-C2-O2
73	QB	502	PEE	O3P-C1-C2-O2
73	Qe	301	PEE	O3P-C1-C2-O2
73	Qc	401	PEE	C23-C24-C25-C26
73	S2	501	PEE	C35-C36-C37-C38
73	QE	301	PEE	C34-C35-C36-C37
68	QH	102	CDL	C73-C74-C75-C76
68	QD	402	CDL	OA6-CA4-CA6-OA8
70	C3	306	PC1	O21-C2-C3-O31
71	N6	201	PLX	O6-C4-C5-O8
71	Qi	301	PLX	O6-C4-C5-O8
72	S7	204	3PE	O21-C2-C3-O31
73	N5	701	PEE	O2-C2-C3-O3
73	Qe	302	PEE	O2-C2-C3-O3
68	7A	102	CDL	C37-C38-C39-C40
72	Qc	404	3PE	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
73	N3	201	PEE	C20-C21-C22-C23
71	S7	203	PLX	C35-C36-C37-C38
73	Qe	301	PEE	C31-C32-C33-C34
71	AM	201	PLX	C31-C32-C33-C34
71	CB	201	PLX	C9-C10-C11-C12
68	A8	301	CDL	C17-C18-C19-C20
68	AK	402	CDL	C53-C54-C55-C56
68	B5	201	CDL	C17-C18-C19-C20
73	N4	501	PEE	C32-C33-C34-C35
68	A7	201	CDL	C1-CA2-OA2-PA1
68	AK	402	CDL	C1-CA2-OA2-PA1
68	N4	503	CDL	CB4-CB3-OB5-PB2
68	N5	703	CDL	C1-CB2-OB2-PB2
68	QH	101	CDL	CB4-CB3-OB5-PB2
71	6C	101	PLX	C4-C3-O4-P1
76	AK	401	ADP	C4'-C5'-O5'-PA
68	B4	201	CDL	C74-C75-C76-C77
68	C3	304	CDL	C74-C75-C76-C77
71	N6	201	PLX	C26-C27-C28-C29
70	Qh	101	PC1	C11-C12-N-C15
73	N1	403	PEE	C14-C15-C16-C17
73	N5	705	PEE	C22-C23-C24-C25
68	N5	704	CDL	C51-C52-C53-C54
73	QC	403	PEE	C30-C31-C32-C33
75	AC	201	ZMP	O1-C10-C9-C8
71	CB	201	PLX	O8-C24-C25-C26
71	QI	301	PLX	O8-C24-C25-C26
71	Qi	301	PLX	O6-C6-C7-C8
68	B5	201	CDL	OB5-CB3-CB4-CB6
68	N4	503	CDL	OB5-CB3-CB4-CB6
68	Qb	501	CDL	OB5-CB3-CB4-CB6
71	N6	201	PLX	O4-C3-C4-C5
73	S8	303	PEE	O3P-C1-C2-C3
77	C1	602	HEA	C26-C15-C16-C17
68	4L	201	CDL	C23-C24-C25-C26
73	S2	501	PEE	C44-C45-C46-C47
73	N5	702	PEE	C31-C32-C33-C34
72	C1	607	3PE	O21-C21-C22-C23
73	QB	502	PEE	C1-C2-O2-C10
80	QC	402	HEM	C2C-C3C-CAC-CBC
80	Qc	403	HEM	C2C-C3C-CAC-CBC
68	4L	201	CDL	C76-C77-C78-C79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
68	CB	203	CDL	CB3-CB4-CB6-OB8
68	N4	503	CDL	C1-CA2-OA2-PA1
68	N4	503	CDL	CA4-CA3-OA5-PA1
71	6C	101	PLX	C3-C4-C5-O8
71	AM	201	PLX	C3-C4-C5-O8
71	N4	502	PLX	C4-C3-O4-P1
71	Qi	301	PLX	C3-C4-C5-O8
72	S7	204	3PE	C1-C2-C3-O31
73	QC	403	PEE	C1-C2-C3-O3
68	AK	402	CDL	OA5-CA3-CA4-OA6
68	AL	201	CDL	OB5-CB3-CB4-OB6
68	N4	503	CDL	OB5-CB3-CB4-OB6
68	QB	501	CDL	OA5-CA3-CA4-OA6
70	C1	608	PC1	O11-C1-C2-O21
70	C3	301	PC1	O11-C1-C2-O21
70	QB	503	PC1	O11-C1-C2-O21
71	6C	101	PLX	O4-C3-C4-O6
73	A9	402	PEE	O3P-C1-C2-O2
73	QC	403	PEE	O3P-C1-C2-O2
73	Qc	401	PEE	O3P-C1-C2-O2
80	Qc	402	HEM	C4B-C3B-CAB-CBB
84	S2	502	MF8	N06-C04-N02-C01
71	S7	203	PLX	C6-C7-C8-C9
68	Qb	501	CDL	CB5-C51-C52-C53
68	N5	704	CDL	C59-C60-C61-C62
73	Qe	301	PEE	C11-C12-C13-C14
68	B4	201	CDL	C78-C79-C80-C81
72	C1	609	3PE	C2A-C2B-C2C-C2D
68	N4	503	CDL	OA6-CA4-CA6-OA8
68	QH	102	CDL	OA6-CA4-CA6-OA8
68	Qb	501	CDL	OB6-CB4-CB6-OB8
71	AL	202	PLX	O6-C4-C5-O8
71	AM	201	PLX	O6-C4-C5-O8
73	N5	705	PEE	O2-C2-C3-O3
73	QB	502	PEE	O2-C2-C3-O3
73	Qc	401	PEE	O2-C2-C3-O3
71	B1	101	PLX	C31-C32-C33-C34
68	CB	203	CDL	C77-C78-C79-C80
70	N1	402	PC1	C11-C12-N-C15
70	C3	303	PC1	C37-C38-C39-C3A
70	Qb	502	PC1	C23-C24-C25-C26
73	QB	502	PEE	O4-C10-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	CB	201	PLX	C28-C29-C30-C31
73	Qc	401	PEE	C11-C12-C13-C14
73	S8	303	PEE	C42-C43-C44-C45
73	A9	402	PEE	C10-C11-C12-C13
71	6C	101	PLX	C14-C15-C16-C17
71	N4	502	PLX	C31-C32-C33-C34
72	CA	101	3PE	C27-C28-C29-C2A
72	N5	706	3PE	C3A-C3B-C3C-C3D
68	N5	703	CDL	CA7-C31-C32-C33
71	CB	201	PLX	C15-C16-C17-C18
71	QI	301	PLX	C11-C10-C9-C8
68	B4	201	CDL	CB2-OB2-PB2-OB5
68	C3	305	CDL	CB3-OB5-PB2-OB2
68	QH	101	CDL	CA3-OA5-PA1-OA2
68	QH	102	CDL	CA2-OA2-PA1-OA5
70	C1	608	PC1	C11-O13-P-O11
70	C3	303	PC1	C11-O13-P-O11
71	N6	201	PLX	C2-O1-P1-O4
72	CB	202	3PE	C1-O11-P-O13
68	B5	201	CDL	O1-C1-CA2-OA2
68	B5	201	CDL	CB4-CB3-OB5-PB2
72	QE	302	3PE	C2-C1-O11-P
72	Qj	101	3PE	C2-C1-O11-P
73	7C	101	PEE	C2-C1-O3P-P
73	S2	501	PEE	C2-C1-O3P-P
68	4L	201	CDL	CA2-OA2-PA1-OA4
68	4L	201	CDL	CA3-OA5-PA1-OA3
68	4L	201	CDL	CA3-OA5-PA1-OA4
68	7A	102	CDL	CA3-OA5-PA1-OA3
68	7A	102	CDL	CA3-OA5-PA1-OA4
68	7A	102	CDL	CB2-OB2-PB2-OB3
68	7A	102	CDL	CB2-OB2-PB2-OB4
68	A8	301	CDL	CB2-OB2-PB2-OB3
68	AL	201	CDL	CA2-OA2-PA1-OA4
68	B4	201	CDL	CA2-OA2-PA1-OA3
68	B4	201	CDL	CB2-OB2-PB2-OB4
68	B5	201	CDL	CA2-OA2-PA1-OA4
68	B5	201	CDL	CA3-OA5-PA1-OA3
68	B5	201	CDL	CA3-OA5-PA1-OA4
68	B5	201	CDL	CB3-OB5-PB2-OB3
68	C3	304	CDL	CA3-OA5-PA1-OA3
68	CB	203	CDL	CA2-OA2-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
68	CB	203	CDL	CB3-OB5-PB2-OB3
68	N1	401	CDL	CB3-OB5-PB2-OB3
68	N4	503	CDL	CA2-OA2-PA1-OA4
68	N4	503	CDL	CA3-OA5-PA1-OA3
68	N4	503	CDL	CA3-OA5-PA1-OA4
68	N4	503	CDL	CB2-OB2-PB2-OB3
68	N5	703	CDL	CA2-OA2-PA1-OA4
68	N5	703	CDL	CB3-OB5-PB2-OB4
68	QB	501	CDL	CA2-OA2-PA1-OA4
68	QC	404	CDL	CB2-OB2-PB2-OB4
68	QH	101	CDL	CA2-OA2-PA1-OA4
68	QH	102	CDL	CA2-OA2-PA1-OA4
68	QH	102	CDL	CB3-OB5-PB2-OB3
68	QH	102	CDL	CB3-OB5-PB2-OB4
68	Qb	501	CDL	CA2-OA2-PA1-OA4
68	Qb	501	CDL	CB2-OB2-PB2-OB4
70	6A	101	PC1	C11-O13-P-O12
70	C1	605	PC1	C11-O13-P-O12
70	C1	605	PC1	C11-O13-P-O14
70	C1	606	PC1	C1-O11-P-O14
70	C1	608	PC1	C1-O11-P-O14
70	C3	301	PC1	C11-O13-P-O12
70	C3	301	PC1	C1-O11-P-O12
70	C3	302	PC1	C11-O13-P-O12
70	N1	402	PC1	C11-C12-N-C14
70	N3	202	PC1	C11-O13-P-O14
70	N3	202	PC1	C1-O11-P-O12
70	N3	202	PC1	C1-O11-P-O14
70	Qc	405	PC1	C1-O11-P-O12
71	AL	202	PLX	C3-O4-P1-O3
71	AM	201	PLX	C3-O4-P1-O2
71	CB	201	PLX	C2-C1-N1-C1C
71	CB	201	PLX	C2-C1-N1-C1A
71	N6	201	PLX	C3-O4-P1-O2
71	N6	201	PLX	C3-O4-P1-O3
71	QI	301	PLX	C2-O1-P1-O3
71	Qi	301	PLX	C2-O1-P1-O3
71	S7	203	PLX	C2-O1-P1-O2
72	7A	101	3PE	C1-O11-P-O12
72	7A	101	3PE	C1-O11-P-O14
72	7A	101	3PE	C11-O13-P-O14
72	B8	201	3PE	C1-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
72	B8	201	3PE	C11-O13-P-O12
72	B8	201	3PE	C11-O13-P-O14
72	CA	101	3PE	C11-O13-P-O14
72	CB	202	3PE	C1-O11-P-O14
72	QE	302	3PE	C1-O11-P-O14
72	Qc	404	3PE	C1-O11-P-O12
72	Qc	404	3PE	C1-O11-P-O14
73	A9	402	PEE	C4-O4P-P-O1P
73	N3	201	PEE	C1-O3P-P-O1P
73	N5	701	PEE	C4-O4P-P-O2P
73	N5	701	PEE	C4-O4P-P-O1P
73	N5	705	PEE	C1-O3P-P-O1P
73	QC	403	PEE	C4-O4P-P-O2P
73	QC	403	PEE	C4-O4P-P-O1P
73	Qc	401	PEE	C1-O3P-P-O2P
73	Qe	301	PEE	C1-O3P-P-O1P
73	Qe	301	PEE	C4-O4P-P-O2P
73	Qe	302	PEE	C1-O3P-P-O1P
73	S2	501	PEE	C1-O3P-P-O2P
73	S8	303	PEE	C4-O4P-P-O2P
68	N5	704	CDL	CB5-C51-C52-C53
68	4L	201	CDL	OB5-CB3-CB4-CB6
68	A8	301	CDL	OB5-CB3-CB4-CB6
70	QB	503	PC1	O11-C1-C2-C3
70	Qb	502	PC1	O11-C1-C2-C3
73	N1	403	PEE	O3P-C1-C2-C3
73	N5	701	PEE	O3P-C1-C2-C3
73	N5	705	PEE	C12-C13-C14-C15
73	Qe	301	PEE	C13-C14-C15-C16
70	C1	608	PC1	O21-C21-C22-C23
73	Qe	301	PEE	C37-C38-C39-C40
71	6C	101	PLX	C25-C24-O8-C5
71	B1	101	PLX	C1-C2-O1-P1
71	N4	502	PLX	C25-C24-O8-C5
71	N6	201	PLX	C25-C24-O8-C5
71	S7	203	PLX	C25-C24-O8-C5
72	7A	101	3PE	C12-C11-O13-P
72	CA	101	3PE	C12-C11-O13-P
72	CB	202	3PE	C12-C11-O13-P
81	QD	401	HEC	C1A-C2A-CAA-CBA
72	QE	302	3PE	O31-C31-C32-C33
68	B4	201	CDL	CA7-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
70	QB	503	PC1	C21-C22-C23-C24
68	QB	501	CDL	OB5-CB3-CB4-OB6
68	QD	402	CDL	OA5-CA3-CA4-OA6
70	C3	303	PC1	O11-C1-C2-O21
70	Qb	502	PC1	O11-C1-C2-O21
71	AL	202	PLX	C7-C8-C9-C10
71	B1	101	PLX	C14-C15-C16-C17
73	QB	502	PEE	C31-C32-C33-C34
70	C3	302	PC1	C11-C12-N-C14
68	Qb	501	CDL	CB3-CB4-CB6-OB8
70	6A	101	PC1	O13-C11-C12-N
70	C1	605	PC1	O13-C11-C12-N
70	C1	606	PC1	O13-C11-C12-N
70	C1	608	PC1	O13-C11-C12-N
70	C3	302	PC1	O13-C11-C12-N
70	C3	303	PC1	O13-C11-C12-N
70	C3	306	PC1	O13-C11-C12-N
70	N3	202	PC1	O13-C11-C12-N
70	Qc	405	PC1	O13-C11-C12-N
71	6C	101	PLX	N1-C1-C2-O1
71	B1	101	PLX	N1-C1-C2-O1
71	CB	201	PLX	C3-C4-C5-O8
73	N4	501	PEE	C1-C2-C3-O3
73	QE	301	PEE	C1-C2-C3-O3
73	Qe	301	PEE	C32-C33-C34-C35
71	CB	201	PLX	O6-C4-C5-O8
71	N4	502	PLX	O6-C4-C5-O8
73	N4	501	PEE	O2-C2-C3-O3
73	QE	301	PEE	O2-C2-C3-O3
68	C3	304	CDL	C54-C55-C56-C57
73	N4	501	PEE	C12-C13-C14-C15
73	Qc	401	PEE	C16-C17-C18-C19
68	B4	201	CDL	C34-C35-C36-C37
68	B5	201	CDL	C1-CA2-OA2-PA1
68	CB	203	CDL	CB4-CB3-OB5-PB2
68	N5	704	CDL	CA4-CA3-OA5-PA1
70	C3	302	PC1	C37-C38-C39-C3A
68	CB	203	CDL	C12-C13-C14-C15
71	AL	202	PLX	O8-C24-C25-C26
71	Qi	301	PLX	O8-C24-C25-C26
85	S7	201	U10	C24-C26-C27-C28
73	N4	501	PEE	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
84	S2	502	MF8	N06-C04-N02-C03
70	Qh	101	PC1	C11-C12-N-C13
71	S7	203	PLX	C12-C13-C14-C15
68	QC	404	CDL	O1-C1-CA2-OA2
73	QB	502	PEE	C11-C10-O2-C2
71	AM	201	PLX	C27-C28-C29-C30
73	S2	501	PEE	C33-C34-C35-C36
74	A9	401	NDP	C2D-C1D-N1N-C6N
72	C1	607	3PE	C24-C25-C26-C27
73	QE	301	PEE	C21-C22-C23-C24
70	C1	610	PC1	C22-C23-C24-C25
70	C3	303	PC1	C1-C2-O21-C21
73	S8	303	PEE	C3-C2-O2-C10
68	N5	704	CDL	OB5-CB3-CB4-CB6
71	AM	201	PLX	O4-C3-C4-C5
77	C1	602	HEA	C11-C12-C13-C14
73	N3	201	PEE	C30-C31-C32-C33
70	C1	608	PC1	C38-C39-C3A-C3B
68	AL	201	CDL	CB4-CB3-OB5-PB2
68	B4	201	CDL	C73-C74-C75-C76
68	4L	201	CDL	OB5-CB3-CB4-OB6
68	N5	704	CDL	OB5-CB3-CB4-OB6
71	N6	201	PLX	O4-C3-C4-O6
72	Qj	101	3PE	O31-C31-C32-C33
71	CB	201	PLX	C2-C1-N1-C1B
74	A9	401	NDP	O4D-C1D-N1N-C6N
70	C1	606	PC1	C31-C32-C33-C34
71	AL	202	PLX	C11-C10-C9-C8
71	B1	101	PLX	C11-C12-C13-C14
81	QD	401	HEC	C3A-C2A-CAA-CBA
70	6A	101	PC1	C21-C22-C23-C24
73	N1	403	PEE	O2-C2-C3-O3
68	7A	102	CDL	CB3-OB5-PB2-OB2
68	A7	201	CDL	CA2-OA2-PA1-OA5
68	A7	201	CDL	CB2-OB2-PB2-OB5
68	AL	201	CDL	CA3-OA5-PA1-OA2
68	C3	304	CDL	CB2-OB2-PB2-OB5
68	CB	203	CDL	CA3-OA5-PA1-OA2
68	N1	401	CDL	CA2-OA2-PA1-OA5
68	N5	704	CDL	CA3-OA5-PA1-OA2
70	6A	101	PC1	C1-O11-P-O13
70	C3	306	PC1	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
70	C3	306	PC1	C1-O11-P-O13
70	QB	503	PC1	C1-O11-P-O13
71	6C	101	PLX	C2-O1-P1-O4
71	N4	502	PLX	C2-O1-P1-O4
71	S7	203	PLX	C3-O4-P1-O1
72	C1	607	3PE	C11-O13-P-O11
73	7C	101	PEE	C1-O3P-P-O4P
73	QC	403	PEE	C1-O3P-P-O4P
70	N3	202	PC1	C22-C23-C24-C25
73	S8	303	PEE	C1-C2-C3-O3
68	N1	401	CDL	C73-C74-C75-C76
71	6C	101	PLX	C6-C7-C8-C9
68	N4	503	CDL	C72-C71-CB7-OB8
68	7A	102	CDL	CB4-CB3-OB5-PB2
70	C3	302	PC1	C2-C1-O11-P
73	N3	201	PEE	C2-C1-O3P-P
80	Qc	403	HEM	CAA-CBA-CGA-O1A
84	S2	502	MF8	N08-C07-N06-C04
73	N3	201	PEE	C41-C42-C43-C44
73	N5	705	PEE	C18-C19-C20-C21
68	AL	201	CDL	C36-C37-C38-C39
73	S8	303	PEE	C14-C15-C16-C17
76	AK	401	ADP	O4'-C4'-C5'-O5'
85	S7	201	U10	C44-C46-C47-C48
72	C1	607	3PE	O13-C11-C12-N
68	B4	201	CDL	C12-C13-C14-C15
68	N5	703	CDL	C36-C37-C38-C39
80	QC	402	HEM	C4C-C3C-CAC-CBC
73	N5	701	PEE	C13-C14-C15-C16
80	QC	401	HEM	CAA-CBA-CGA-O2A
71	QI	301	PLX	C12-C13-C14-C15
75	AB	201	ZMP	C2-C3-C4-C5
73	S8	303	PEE	C15-C16-C17-C18
75	AB	201	ZMP	O3-C16-C17-C18
70	N3	202	PC1	C26-C27-C28-C29
71	S7	203	PLX	C11-C10-C9-C8
71	Qi	301	PLX	C24-C25-C26-C27
80	Qc	403	HEM	CAD-CBD-CGD-O1D
68	AL	201	CDL	OB6-CB4-CB6-OB8
70	Qc	405	PC1	O21-C2-C3-O31
70	C3	306	PC1	C2-C1-O11-P
72	C1	607	3PE	C2-C1-O11-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
85	S7	201	U10	C5-C4-O4-C4M
68	7A	102	CDL	C81-C82-C83-C84
71	AM	201	PLX	C9-C10-C11-C12
73	QE	301	PEE	C15-C16-C17-C18
68	QC	404	CDL	C31-C32-C33-C34
81	Qd	401	HEC	C3D-CAD-CBD-CGD
70	N3	202	PC1	C28-C29-C2A-C2B
70	Qb	502	PC1	C35-C36-C37-C38
71	N4	502	PLX	C33-C34-C35-C36
71	QI	301	PLX	C13-C14-C15-C16
70	Qc	405	PC1	C1-C2-C3-O31
71	AL	202	PLX	C3-C4-C5-O8
72	QE	302	3PE	C23-C24-C25-C26
72	C1	609	3PE	C33-C34-C35-C36
72	N5	706	3PE	C22-C23-C24-C25
73	7C	101	PEE	C23-C24-C25-C26
80	QC	402	HEM	CAA-CBA-CGA-O1A
80	Qc	402	HEM	CAD-CBD-CGD-O1D
73	QE	301	PEE	C31-C32-C33-C34
68	4L	201	CDL	CA6-CA4-OA6-CA5
68	AL	201	CDL	CA6-CA4-OA6-CA5
68	Qb	501	CDL	CA3-CA4-OA6-CA5
70	C3	302	PC1	C3-C2-O21-C21
72	S7	204	3PE	C3-C2-O21-C21
70	N1	402	PC1	C11-C12-N-C13
68	QD	402	CDL	CA3-OA5-PA1-OA2
71	AM	201	PLX	C5-C4-O6-C6
84	S2	502	MF8	N05-C04-N02-C01
71	N6	201	PLX	C25-C26-C27-C28
68	C3	304	CDL	C72-C71-CB7-OB8
70	C1	605	PC1	C32-C33-C34-C35
68	QD	402	CDL	OB5-CB3-CB4-OB6
77	C1	601	HEA	CAD-CBD-CGD-O1D
71	S7	203	PLX	C25-C26-C27-C28
71	QI	301	PLX	O4-C3-C4-C5
70	N3	202	PC1	C38-C39-C3A-C3B
80	Qc	403	HEM	CAA-CBA-CGA-O2A
71	N6	201	PLX	C10-C11-C12-C13
73	QB	502	PEE	C33-C34-C35-C36
70	C3	302	PC1	C32-C33-C34-C35
68	CB	203	CDL	OB6-CB4-CB6-OB8
70	C3	302	PC1	O21-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
80	QC	402	HEM	CAA-CBA-CGA-O2A
68	C3	305	CDL	C57-C58-C59-C60
73	QE	301	PEE	C22-C23-C24-C25
80	QC	401	HEM	CAA-CBA-CGA-O1A
80	Qc	402	HEM	CAA-CBA-CGA-O2A
81	Qd	401	HEC	CAA-CBA-CGA-O2A
80	Qc	403	HEM	CAD-CBD-CGD-O2D
77	C1	602	HEA	CAD-CBD-CGD-O2D
71	Qi	301	PLX	C15-C16-C17-C18
70	C3	301	PC1	C2A-C2B-C2C-C2D
73	N5	705	PEE	O5-C30-O3-C3
68	CB	203	CDL	C72-C71-CB7-OB8
70	Qb	502	PC1	O21-C21-C22-C23
73	A9	402	PEE	C18-C19-C20-C21
68	N1	401	CDL	C12-C13-C14-C15
72	N5	706	3PE	C1-C2-C3-O31
72	C1	609	3PE	C3B-C3C-C3D-C3E
73	N5	705	PEE	C17-C18-C19-C20
73	QB	502	PEE	C37-C38-C39-C40
73	Qe	301	PEE	C30-C31-C32-C33
80	Qc	402	HEM	CAA-CBA-CGA-O1A
71	CB	201	PLX	C11-C10-C9-C8
73	N4	501	PEE	C33-C34-C35-C36
73	N5	702	PEE	O3P-C1-C2-O2
74	A9	401	NDP	C2D-C1D-N1N-C2N
68	AL	201	CDL	C52-C51-CB5-OB6
71	AM	201	PLX	O8-C24-C25-C26
81	Qd	401	HEC	CAA-CBA-CGA-O1A
72	CA	101	3PE	C29-C2A-C2B-C2C
68	B4	201	CDL	OB5-CB3-CB4-CB6
68	C3	305	CDL	OB5-CB3-CB4-CB6
72	S7	204	3PE	O11-C1-C2-C3
68	QD	402	CDL	C52-C51-CB5-OB6
73	N5	705	PEE	O4P-C4-C5-N
68	QH	101	CDL	C72-C73-C74-C75
70	N3	202	PC1	C29-C2A-C2B-C2C
71	6C	101	PLX	C18-C19-C20-C21
68	4L	201	CDL	C79-C80-C81-C82
70	Qb	502	PC1	C22-C23-C24-C25
71	S7	203	PLX	O6-C4-C5-O8
71	B1	101	PLX	C30-C31-C32-C33
71	S7	203	PLX	C27-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
72	7A	101	3PE	C32-C33-C34-C35
73	N1	403	PEE	O2-C10-C11-C12
85	S7	201	U10	C50-C49-C51-C52
68	AK	402	CDL	C72-C73-C74-C75
72	Qj	101	3PE	C33-C34-C35-C36
73	A9	402	PEE	C1-O3P-P-O4P
73	S8	303	PEE	C4-O4P-P-O3P
73	N5	705	PEE	C31-C30-O3-C3
68	C3	305	CDL	C12-C11-CA5-OA6
70	C3	301	PC1	O31-C31-C32-C33
72	B8	201	3PE	O21-C21-C22-C23
72	C1	609	3PE	O21-C21-C22-C23
73	QE	301	PEE	C37-C38-C39-C40
80	QC	401	HEM	CAD-CBD-CGD-O1D
81	Qd	401	HEC	C3A-C2A-CAA-CBA
73	N4	501	PEE	O2-C10-C11-C12
73	QB	502	PEE	O2-C10-C11-C12
73	S2	501	PEE	O2-C10-C11-C12
73	7C	101	PEE	C38-C39-C40-C41
73	N5	701	PEE	C16-C17-C18-C19
73	N5	702	PEE	C36-C37-C38-C39
73	Qc	401	PEE	C13-C14-C15-C16
81	QD	401	HEC	CAD-CBD-CGD-O2D
68	AK	402	CDL	CA6-CA4-OA6-CA5
68	B5	201	CDL	CB3-CB4-OB6-CB5
68	N4	503	CDL	CB6-CB4-OB6-CB5
68	QB	501	CDL	CA6-CA4-OA6-CA5
68	QD	402	CDL	CB6-CB4-OB6-CB5
68	QH	102	CDL	CA3-CA4-OA6-CA5
70	QB	503	PC1	C3-C2-O21-C21
70	Qb	502	PC1	C3-C2-O21-C21
72	C1	607	3PE	C3-C2-O21-C21
72	Qc	404	3PE	C39-C3A-C3B-C3C
74	A9	401	NDP	O4D-C1D-N1N-C2N
73	N3	201	PEE	O2-C10-C11-C12
81	Qd	401	HEC	CAD-CBD-CGD-O1D
71	Qi	301	PLX	C16-C17-C18-C19
68	A7	201	CDL	C72-C71-CB7-OB8
73	N5	705	PEE	O3-C30-C31-C32
68	N5	704	CDL	C1-CA2-OA2-PA1
71	AL	202	PLX	C7-C6-O6-C4
77	C1	601	HEA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
68	QC	404	CDL	OB5-CB3-CB4-OB6
68	QH	102	CDL	OB5-CB3-CB4-OB6
68	N5	703	CDL	C12-C11-CA5-OA6
68	QB	501	CDL	C32-C31-CA7-OA8
72	CB	202	3PE	O31-C31-C32-C33
73	N5	701	PEE	O2-C10-C11-C12
73	Qc	401	PEE	O2-C10-C11-C12
77	C1	602	HEA	CAD-CBD-CGD-O1D
80	Qc	402	HEM	CAD-CBD-CGD-O2D
68	N5	704	CDL	C42-C43-C44-C45
80	Qc	403	HEM	C4C-C3C-CAC-CBC
74	A9	401	NDP	O4B-C4B-C5B-O5B
68	C3	304	CDL	CA5-C11-C12-C13
73	Qe	301	PEE	C18-C19-C20-C21
68	7A	102	CDL	C57-C58-C59-C60
73	Qc	401	PEE	C2-C3-O3-C30
68	AL	201	CDL	C32-C31-CA7-OA8
68	A8	301	CDL	OA5-CA3-CA4-CA6
68	AK	402	CDL	OA5-CA3-CA4-CA6
77	C1	602	HEA	C2D-C3D-CAD-CBD
81	QD	401	HEC	CAD-CBD-CGD-O1D
68	A8	301	CDL	C33-C34-C35-C36
73	7C	101	PEE	C14-C15-C16-C17
73	N3	201	PEE	C23-C24-C25-C26
68	N5	704	CDL	OA6-CA4-CA6-OA8
68	N5	704	CDL	OB6-CB4-CB6-OB8
70	Qb	502	PC1	O21-C2-C3-O31
72	CB	202	3PE	O21-C2-C3-O31
72	N5	706	3PE	O21-C2-C3-O31
71	Qi	301	PLX	C6-C7-C8-C9
68	N5	703	CDL	C61-C62-C63-C64
68	AL	201	CDL	C12-C11-CA5-OA6
68	QC	404	CDL	C52-C51-CB5-OB6
68	QH	101	CDL	C32-C31-CA7-OA8
68	QH	102	CDL	C32-C31-CA7-OA8
70	C1	610	PC1	O21-C21-C22-C23
70	N1	402	PC1	O21-C21-C22-C23
70	Qc	405	PC1	O21-C21-C22-C23
72	S7	204	3PE	C3B-C3C-C3D-C3E
81	Qd	401	HEC	CAD-CBD-CGD-O2D
68	QH	101	CDL	CA4-CA3-OA5-PA1
73	Qe	301	PEE	C2-C1-O3P-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
73	Qc	401	PEE	O4-C10-O2-C2
68	N5	704	CDL	C72-C71-CB7-OB8
70	Qb	502	PC1	O31-C31-C32-C33
80	QC	401	HEM	CAD-CBD-CGD-O2D
68	CB	203	CDL	CB5-C51-C52-C53
85	S7	201	U10	C3-C4-O4-C4M
70	C3	303	PC1	C2B-C2C-C2D-C2E
71	S7	203	PLX	C15-C16-C17-C18
71	B1	101	PLX	C15-C16-C17-C18
70	C3	301	PC1	O32-C31-C32-C33
73	N3	201	PEE	O4-C10-C11-C12
68	N5	703	CDL	C12-C11-CA5-OA7
73	N1	403	PEE	O4-C10-C11-C12
68	A7	201	CDL	C72-C71-CB7-OB9
68	AL	201	CDL	C12-C11-CA5-OA7
68	AL	201	CDL	C32-C31-CA7-OA9
68	C3	305	CDL	C12-C11-CA5-OA7
72	C1	609	3PE	O22-C21-C22-C23
72	CB	202	3PE	O32-C31-C32-C33
73	N5	705	PEE	O5-C30-C31-C32
68	4L	201	CDL	C52-C51-CB5-OB6
68	B4	201	CDL	C12-C11-CA5-OA6
70	N1	402	PC1	C2F-C2G-C2H-C2I
72	QJ	101	3PE	C23-C24-C25-C26
73	QE	301	PEE	C4-O4P-P-O3P
71	AL	202	PLX	C14-C15-C16-C17
71	AM	201	PLX	C30-C31-C32-C33
71	Qi	301	PLX	C27-C28-C29-C30
68	N5	704	CDL	C72-C71-CB7-OB9
72	B8	201	3PE	O22-C21-C22-C23
68	N5	703	CDL	C72-C71-CB7-OB8
72	N5	706	3PE	O21-C21-C22-C23
68	QH	102	CDL	C32-C31-CA7-OA9
70	Qb	502	PC1	O32-C31-C32-C33
68	A7	201	CDL	CA2-OA2-PA1-OA3
68	CB	203	CDL	CB2-OB2-PB2-OB4
68	N4	503	CDL	CB3-OB5-PB2-OB3
68	N5	704	CDL	CB3-OB5-PB2-OB3
68	QC	404	CDL	CA2-OA2-PA1-OA3
68	Qb	501	CDL	CA3-OA5-PA1-OA3
70	C1	608	PC1	C11-O13-P-O12
70	C1	608	PC1	C1-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
70	C3	306	PC1	C1-O11-P-O14
71	6C	101	PLX	C2-O1-P1-O2
71	N6	201	PLX	C2-O1-P1-O2
72	C1	607	3PE	C11-O13-P-O14
72	S7	204	3PE	C11-O13-P-O14
73	QB	502	PEE	C1-O3P-P-O1P
73	Qc	401	PEE	C4-O4P-P-O2P
72	C1	607	3PE	O22-C21-C22-C23
73	QB	502	PEE	O4-C10-C11-C12
73	S2	501	PEE	O4-C10-C11-C12
70	6A	101	PC1	C34-C35-C36-C37
77	C1	602	HEA	CAA-CBA-CGA-O2A
68	QC	404	CDL	C52-C51-CB5-OB7
73	N4	501	PEE	O4-C10-C11-C12
73	N5	701	PEE	O4-C10-C11-C12
73	Qc	401	PEE	O4-C10-C11-C12
84	S2	502	MF8	N09-C07-N06-C04
72	CA	101	3PE	C23-C24-C25-C26
68	Qb	501	CDL	C72-C71-CB7-OB8
68	N4	503	CDL	C34-C35-C36-C37
68	B4	201	CDL	C12-C11-CA5-OA7
73	Qc	401	PEE	C11-C10-O2-C2
68	AL	201	CDL	CA3-CA4-OA6-CA5
68	N4	503	CDL	CB3-CB4-OB6-CB5
68	QB	501	CDL	CA3-CA4-OA6-CA5
68	QH	102	CDL	CA6-CA4-OA6-CA5
68	Qb	501	CDL	CA6-CA4-OA6-CA5
70	6A	101	PC1	C12-C11-O13-P
70	C3	302	PC1	C1-C2-O21-C21
70	N1	402	PC1	C12-C11-O13-P
70	QB	503	PC1	C1-C2-O21-C21
70	Qb	502	PC1	C1-C2-O21-C21
71	AM	201	PLX	C1-C2-O1-P1
72	C1	607	3PE	C1-C2-O21-C21
72	N5	706	3PE	C12-C11-O13-P
72	QE	302	3PE	C12-C11-O13-P
72	S7	204	3PE	C1-C2-O21-C21
73	N1	403	PEE	C5-C4-O4P-P
73	N3	201	PEE	C5-C4-O4P-P
68	QB	501	CDL	C32-C31-CA7-OA9
73	7C	101	PEE	C13-C14-C15-C16
68	AK	402	CDL	C12-C11-CA5-OA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
72	7A	101	3PE	O21-C21-C22-C23
73	A9	402	PEE	O2-C10-C11-C12
68	B4	201	CDL	C33-C34-C35-C36
68	N5	704	CDL	C11-C12-C13-C14
71	CB	201	PLX	C17-C18-C19-C20
70	6A	101	PC1	C25-C26-C27-C28
73	QB	502	PEE	C11-C12-C13-C14
68	QD	402	CDL	C71-C72-C73-C74
73	QB	502	PEE	C36-C37-C38-C39
72	C1	609	3PE	O31-C31-C32-C33
73	N3	201	PEE	O3-C30-C31-C32
70	C1	610	PC1	C3E-C3F-C3G-C3H
71	6C	101	PLX	C7-C8-C9-C10
73	S2	501	PEE	C43-C44-C45-C46
70	Qc	405	PC1	C21-C22-C23-C24
73	7C	101	PEE	C33-C34-C35-C36
68	C3	305	CDL	C32-C31-CA7-OA8
68	QH	101	CDL	C12-C11-CA5-OA6
68	C3	305	CDL	C32-C31-CA7-OA9
70	N1	402	PC1	O22-C21-C22-C23
70	QB	503	PC1	C3A-C3B-C3C-C3D
71	6C	101	PLX	C11-C12-C13-C14
68	QC	404	CDL	CA4-CA3-OA5-PA1
68	N1	401	CDL	CB5-C51-C52-C53
71	S7	203	PLX	O4-C3-C4-O6
68	4L	201	CDL	C12-C11-CA5-OA7
68	N5	703	CDL	C72-C71-CB7-OB9
70	C1	610	PC1	O22-C21-C22-C23
72	C1	609	3PE	O32-C31-C32-C33
68	CB	203	CDL	C39-C40-C41-C42
70	N3	202	PC1	C3B-C3C-C3D-C3E
68	4L	201	CDL	C12-C11-CA5-OA6
73	N5	705	PEE	C31-C32-C33-C34
70	C3	303	PC1	C21-C22-C23-C24
72	N5	706	3PE	O22-C21-C22-C23
77	C1	602	HEA	CAA-CBA-CGA-O1A
81	Qd	401	HEC	C1A-C2A-CAA-CBA
68	4L	201	CDL	C32-C31-CA7-OA8
68	N5	704	CDL	C52-C51-CB5-OB6
68	A8	301	CDL	C54-C55-C56-C57
68	QB	501	CDL	C73-C74-C75-C76
68	QH	101	CDL	C12-C11-CA5-OA7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
73	N3	201	PEE	O5-C30-C31-C32
68	A8	301	CDL	C22-C23-C24-C25
70	N3	202	PC1	C36-C37-C38-C39
71	CB	201	PLX	C24-C25-C26-C27
68	AK	402	CDL	C72-C71-CB7-OB8
68	N5	703	CDL	C52-C51-CB5-OB6
70	6A	101	PC1	O31-C31-C32-C33
68	AL	201	CDL	C32-C33-C34-C35
68	AL	201	CDL	C34-C35-C36-C37
72	C1	607	3PE	C2A-C2B-C2C-C2D
73	S2	501	PEE	C31-C32-C33-C34
68	AK	402	CDL	C32-C31-CA7-OA8

There are no ring outliers.

86 monomers are involved in 277 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	C1	609	3PE	1	0
72	QJ	101	3PE	1	0
68	B5	201	CDL	6	0
70	C3	303	PC1	4	0
82	QE	303	FES	2	0
70	QB	503	PC1	2	0
72	Qc	404	3PE	2	0
72	QE	302	3PE	1	0
73	Qe	302	PEE	1	0
68	QD	402	CDL	1	0
71	QI	301	PLX	2	0
72	S7	204	3PE	2	0
68	QB	501	CDL	3	0
68	N4	503	CDL	2	0
68	N1	401	CDL	4	0
68	N5	704	CDL	2	0
71	N6	201	PLX	1	0
74	A9	401	NDP	1	0
68	QC	404	CDL	2	0
68	C3	305	CDL	4	0
73	S8	303	PEE	7	0
70	Qb	502	PC1	2	0
73	Qc	401	PEE	1	0
68	QH	102	CDL	7	0
76	AK	401	ADP	3	0

Continued on next page...

Continued from previous page...

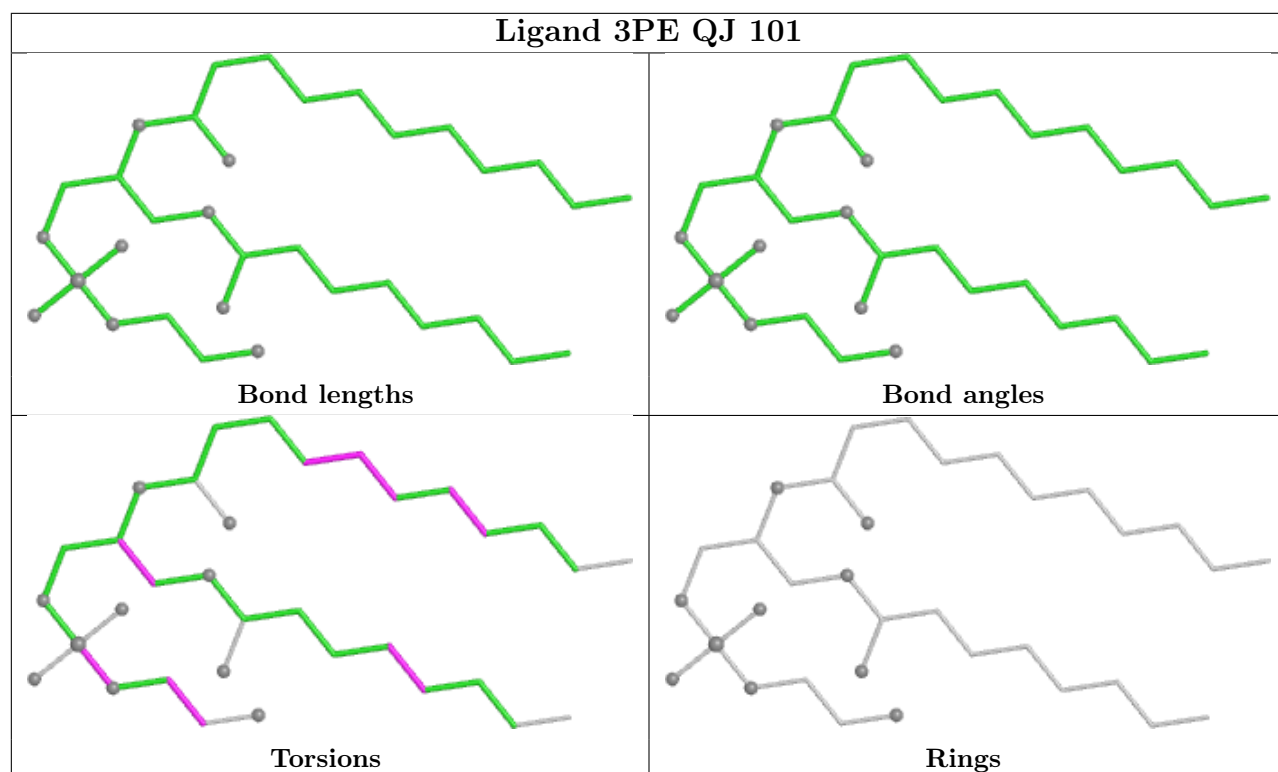
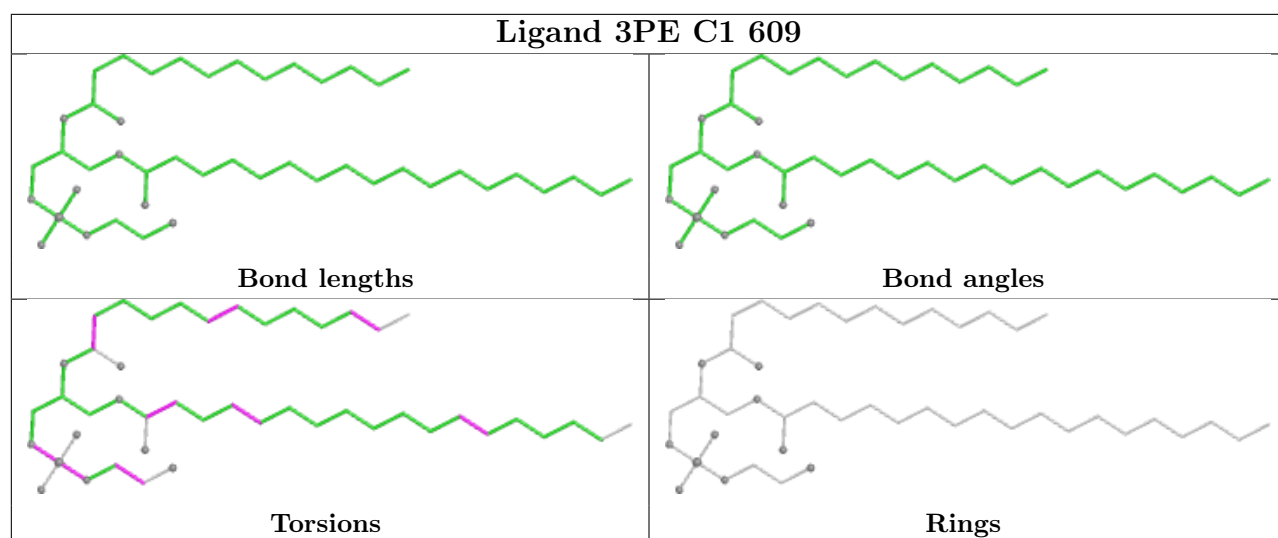
Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	QC	402	HEM	6	0
70	Qc	405	PC1	4	0
77	C1	602	HEA	10	0
68	Qb	501	CDL	2	0
71	CB	201	PLX	3	0
71	Qi	301	PLX	5	0
81	Qd	401	HEC	4	0
72	CA	101	3PE	1	0
75	AC	201	ZMP	4	0
70	6A	101	PC1	11	0
73	QB	502	PEE	1	0
68	7A	102	CDL	6	0
73	QC	403	PEE	1	0
73	N5	701	PEE	2	0
70	C1	605	PC1	1	0
70	C3	306	PC1	2	0
70	N3	202	PC1	1	0
71	B1	101	PLX	1	0
75	AB	201	ZMP	2	0
72	7A	101	3PE	6	0
73	7C	101	PEE	5	0
73	N3	201	PEE	4	0
71	AL	202	PLX	2	0
73	N5	705	PEE	1	0
68	A7	201	CDL	1	0
73	N5	702	PEE	1	0
82	Qe	303	FES	2	0
68	A8	301	CDL	7	0
68	N5	703	CDL	13	0
70	C3	301	PC1	3	0
72	N5	706	3PE	1	0
68	CB	203	CDL	4	0
68	AK	402	CDL	3	0
86	V1	502	FMN	1	0
71	AM	201	PLX	6	0
71	N4	502	PLX	4	0
85	S7	201	U10	6	0
71	6C	101	PLX	1	0
80	Qc	403	HEM	7	0
70	C1	608	PC1	4	0
68	B4	201	CDL	4	0
70	C1	610	PC1	9	0

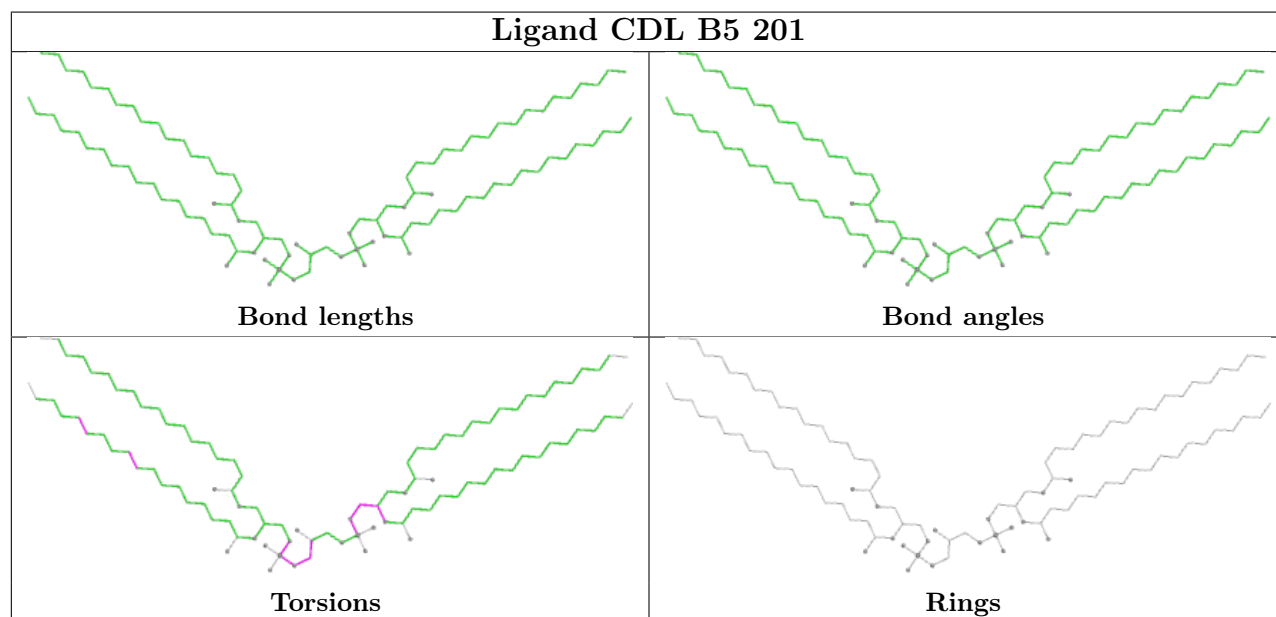
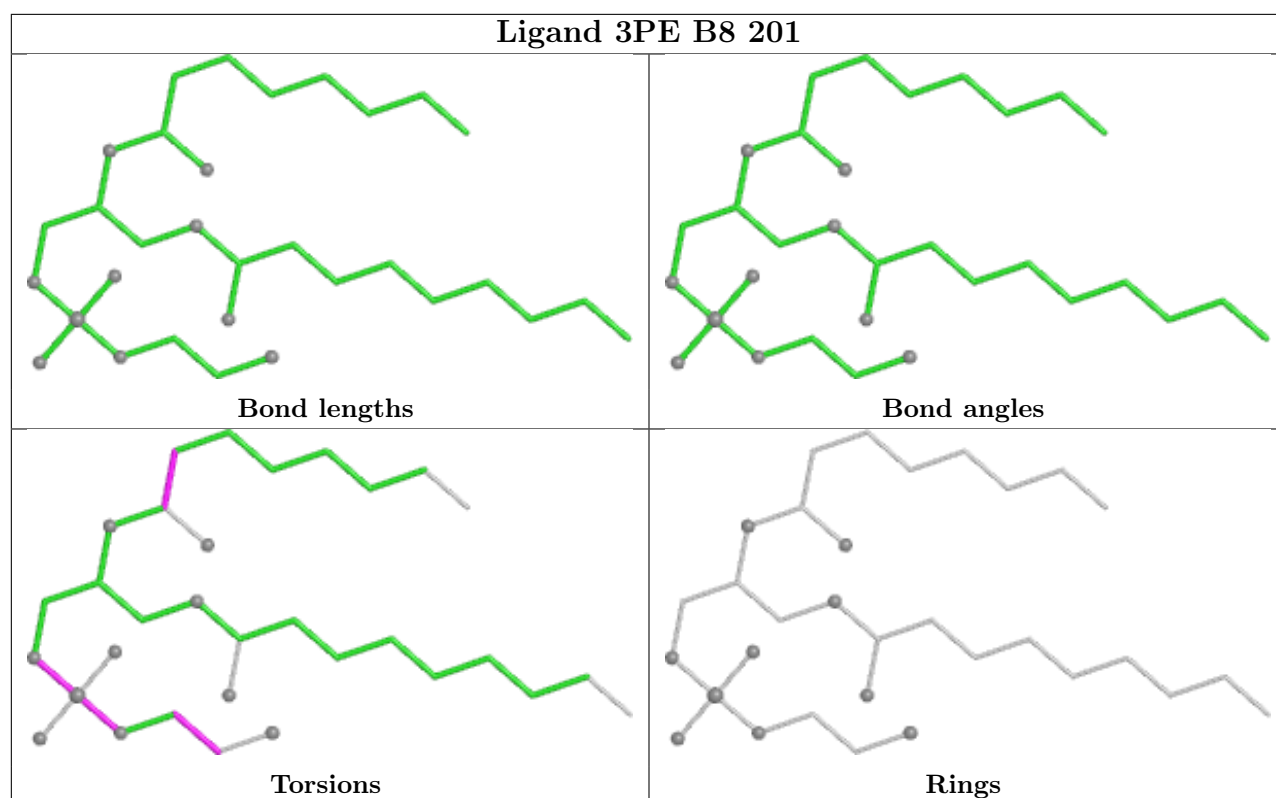
Continued on next page...

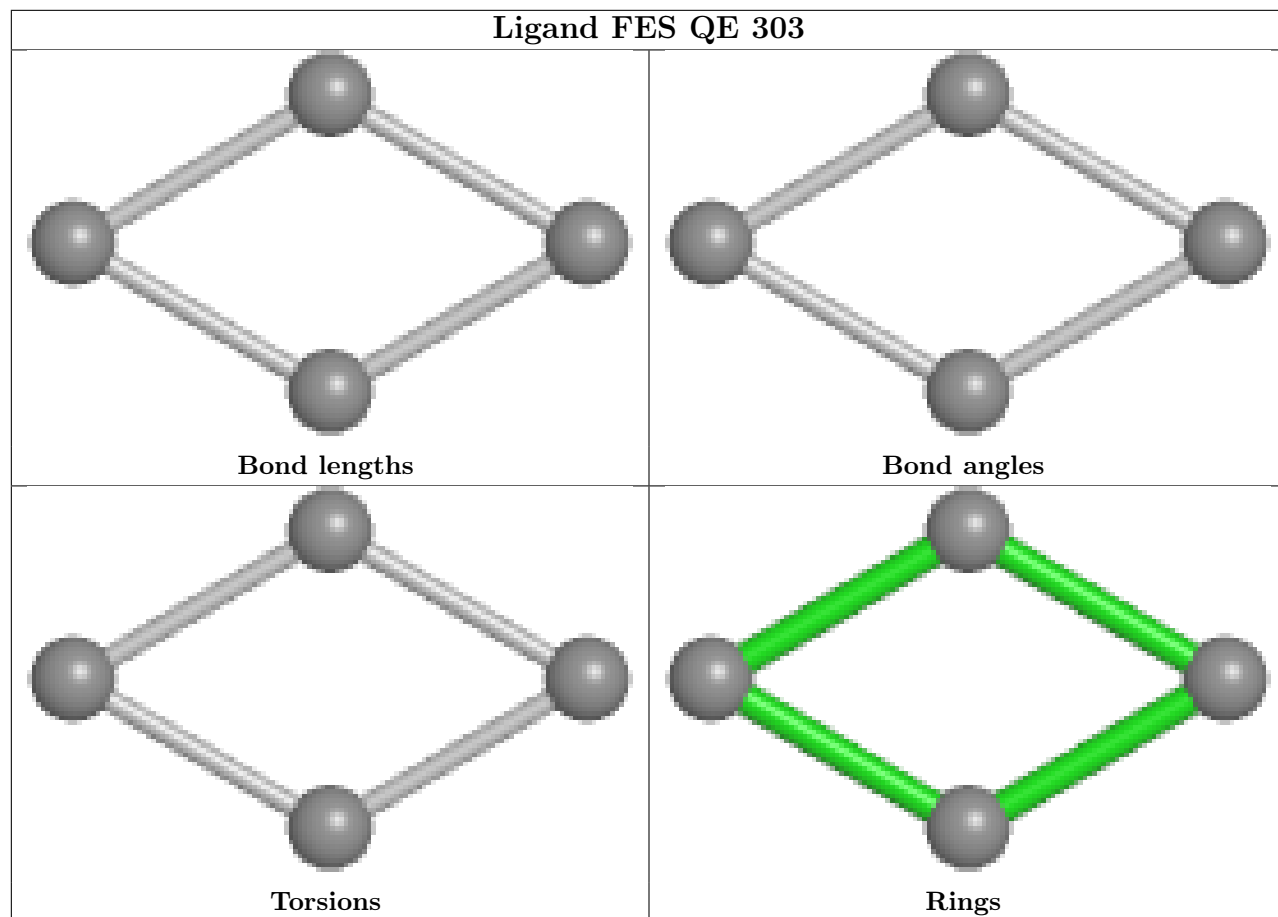
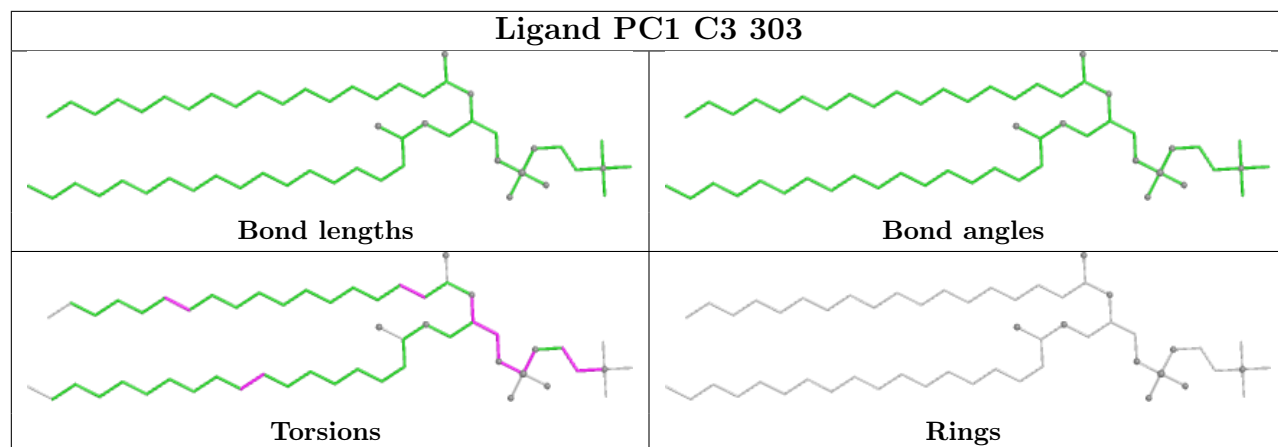
Continued from previous page...

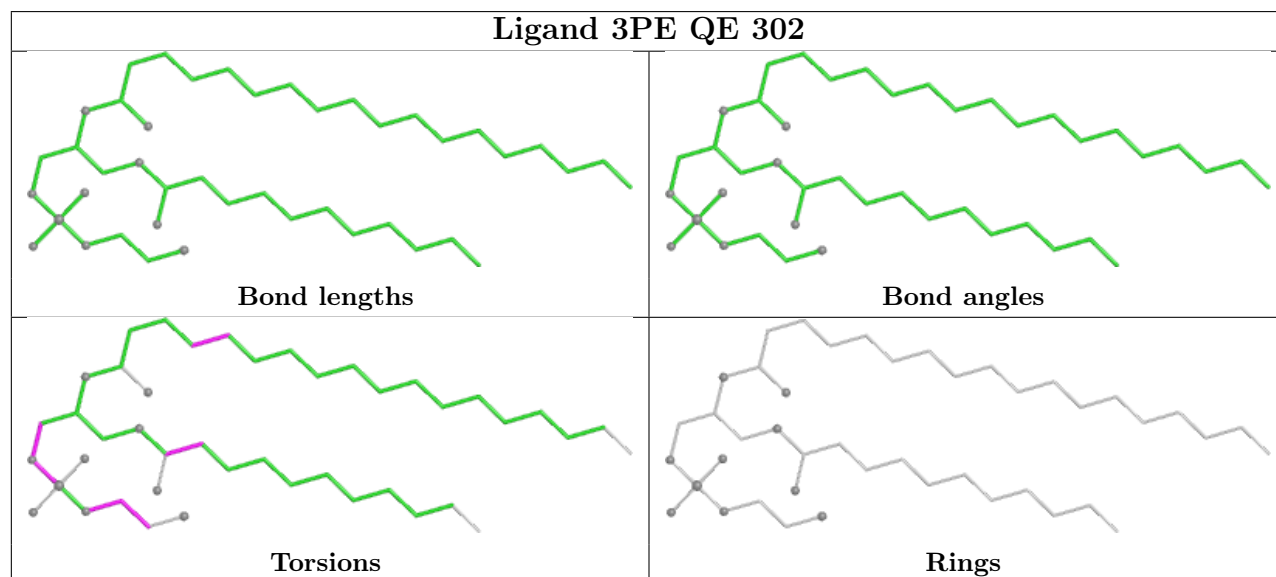
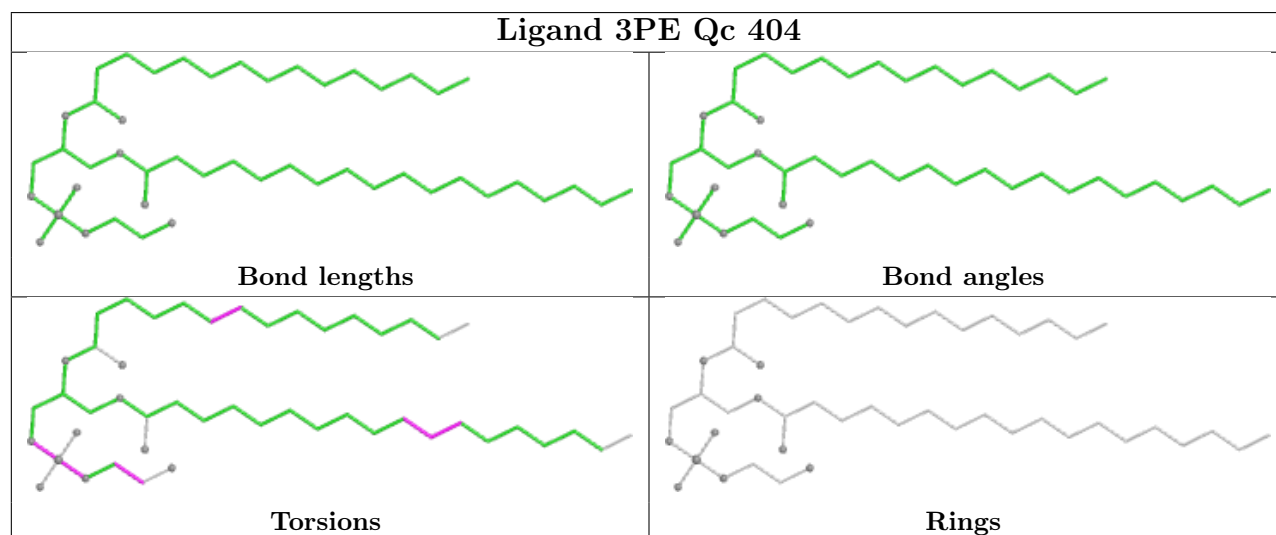
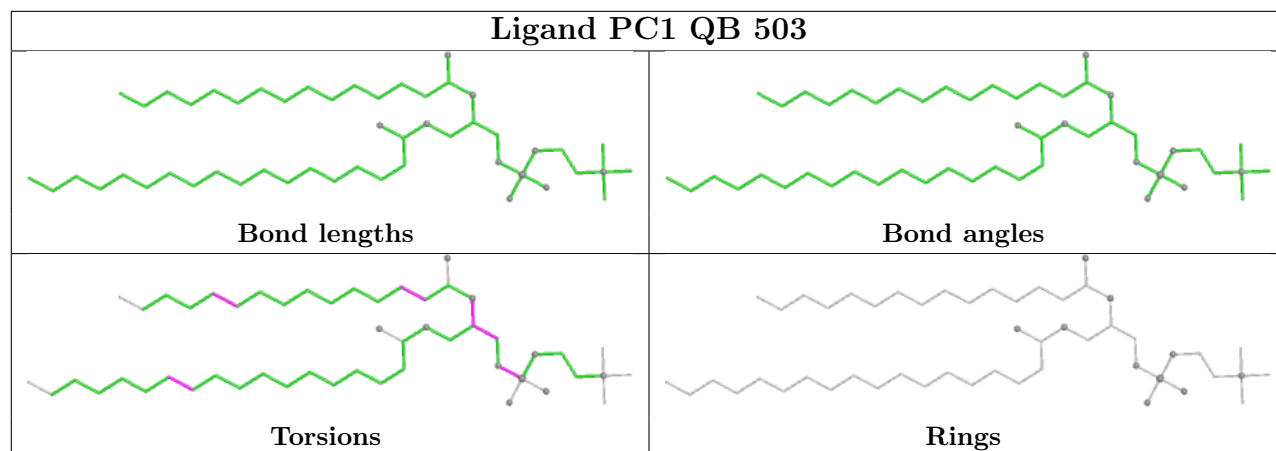
Mol	Chain	Res	Type	Clashes	Symm-Clashes
73	N4	501	PEE	5	0
73	QE	301	PEE	2	0
73	A9	402	PEE	4	0
73	Qe	301	PEE	7	0
68	AL	201	CDL	7	0
68	C3	304	CDL	4	0
70	Qh	101	PC1	1	0
80	QC	401	HEM	2	0
77	C1	601	HEA	8	0
68	4L	201	CDL	8	0
73	S2	501	PEE	4	0
70	C3	302	PC1	4	0
83	S8	302	SF4	1	0
72	CB	202	3PE	1	0
83	S1	802	SF4	1	0
81	QD	401	HEC	2	0
83	S7	202	SF4	1	0
71	S7	203	PLX	6	0
70	N1	402	PC1	3	0

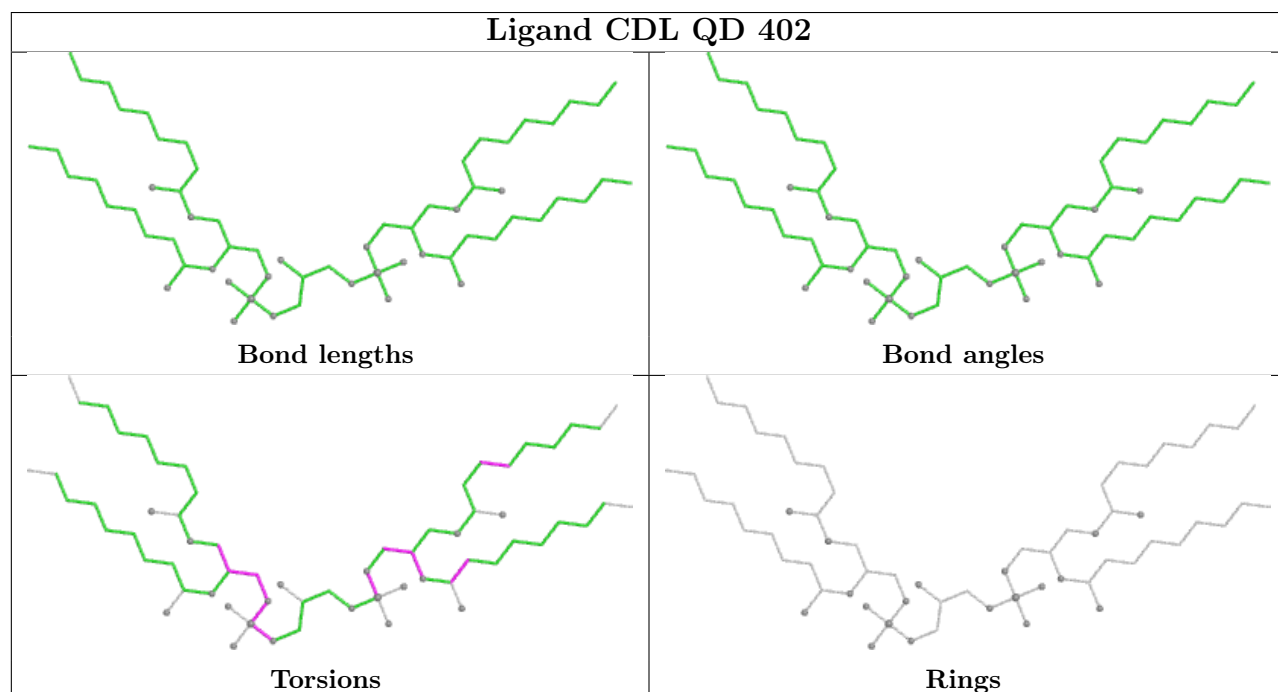
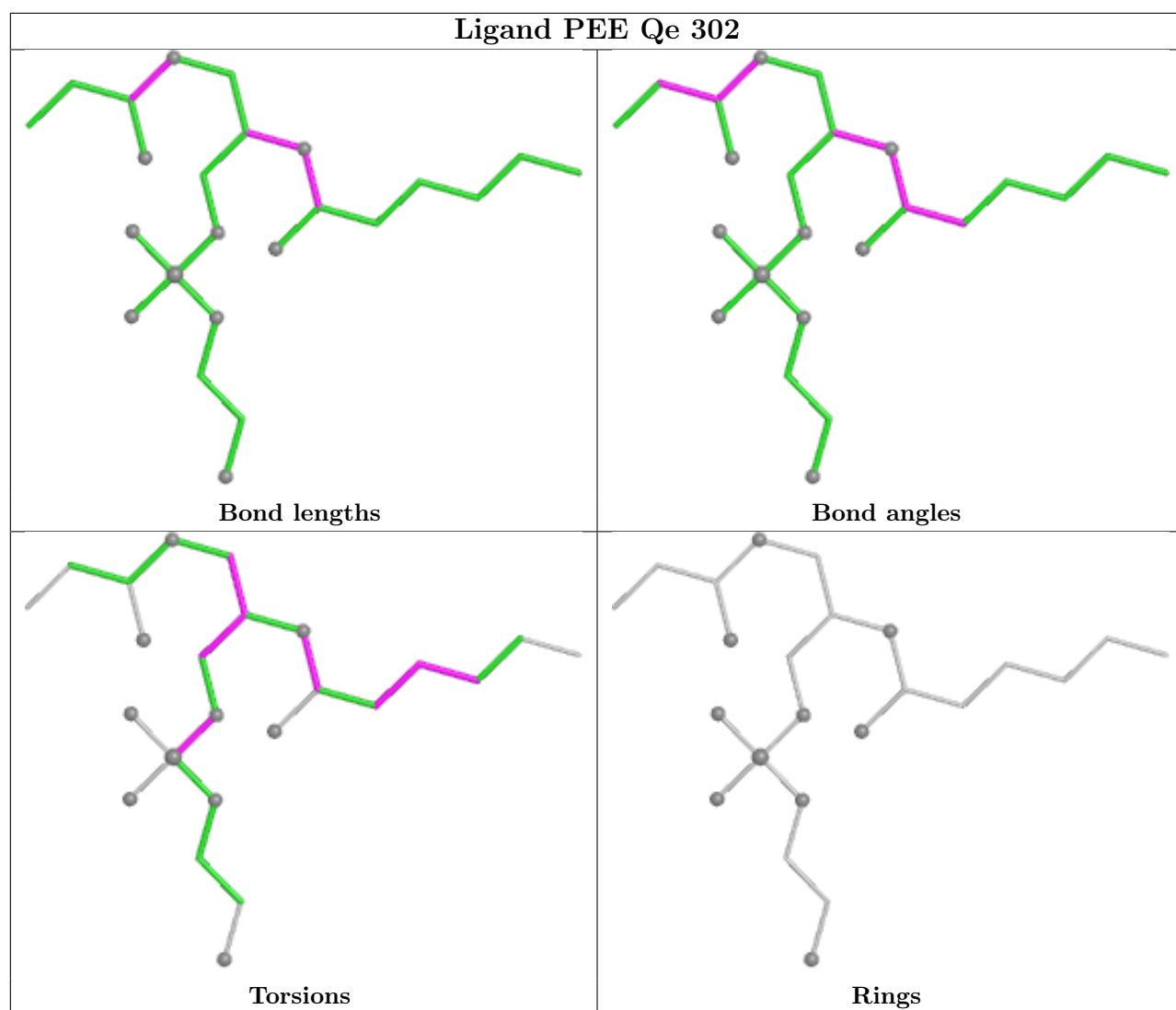
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

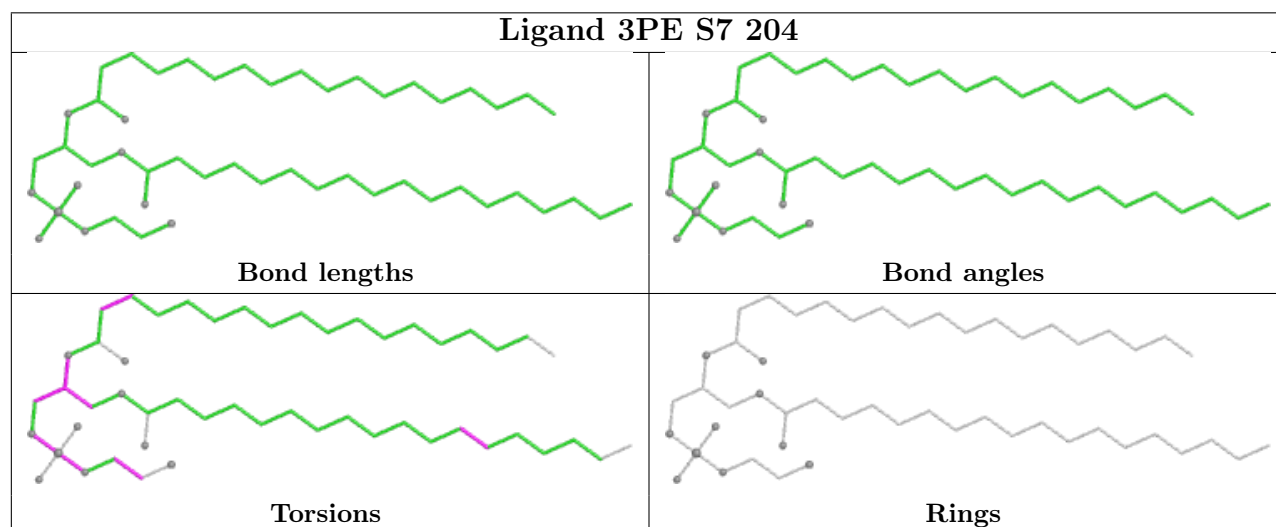
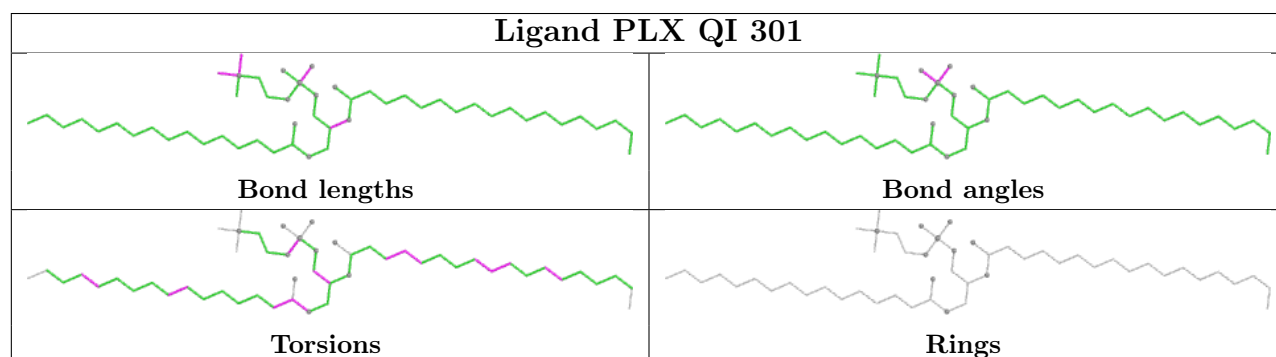
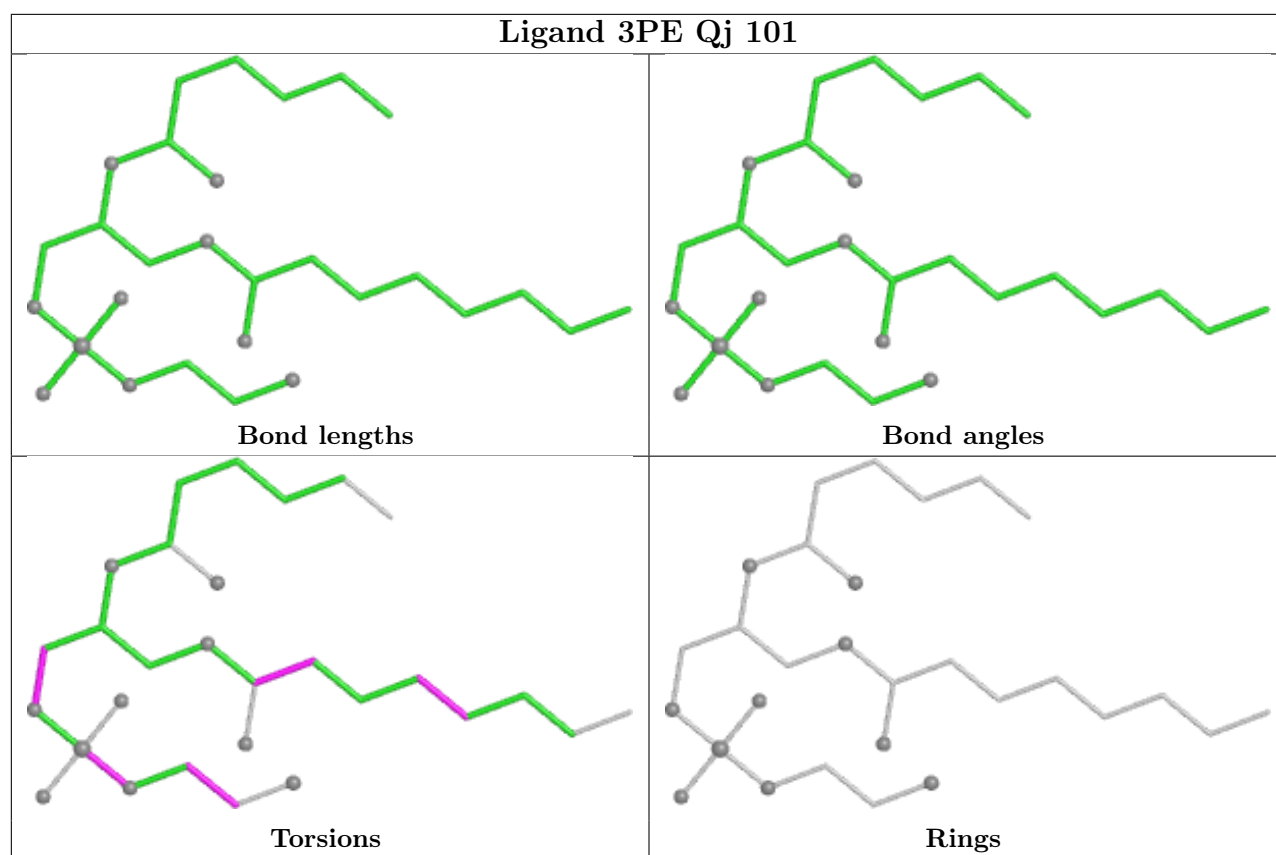


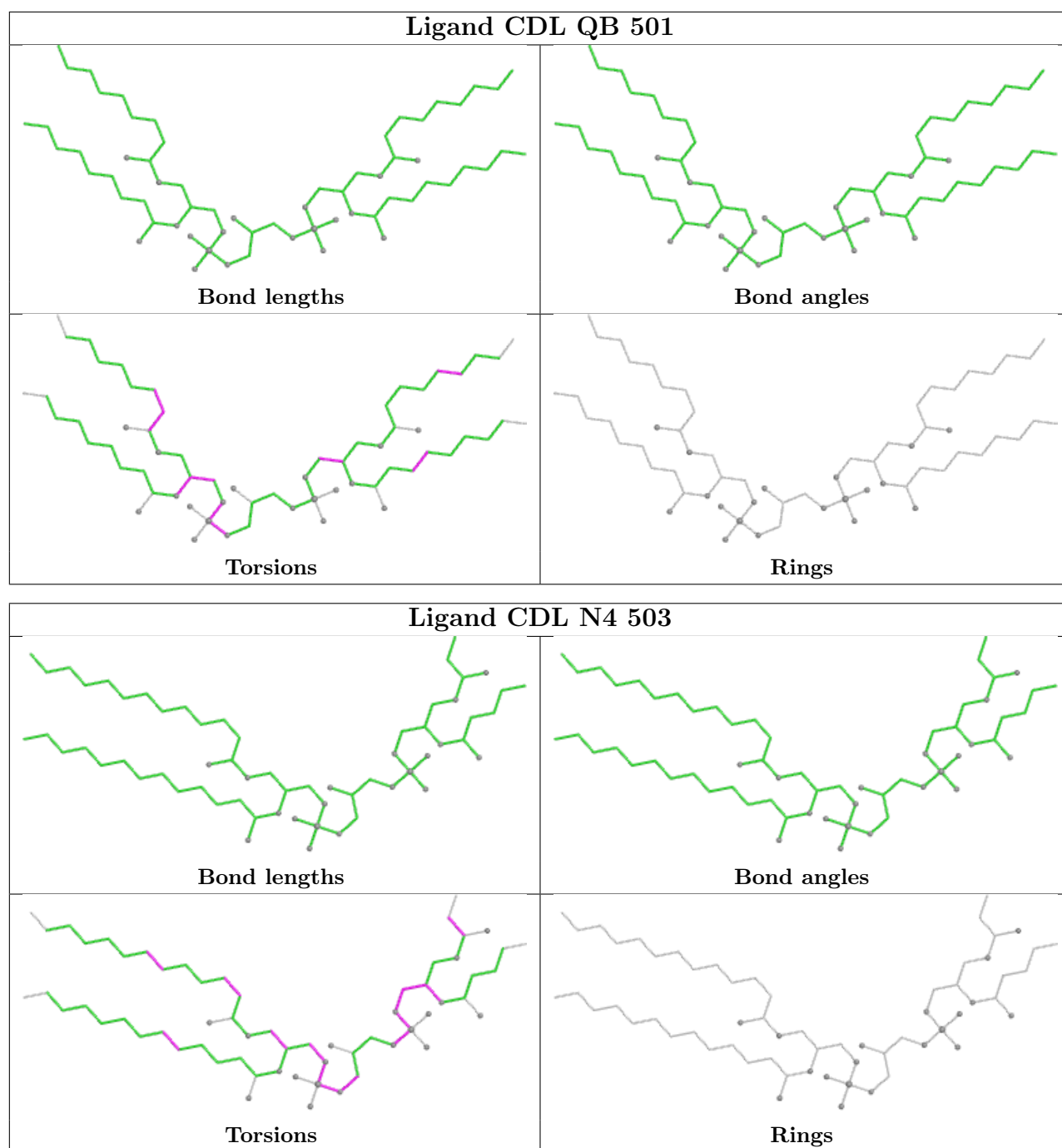


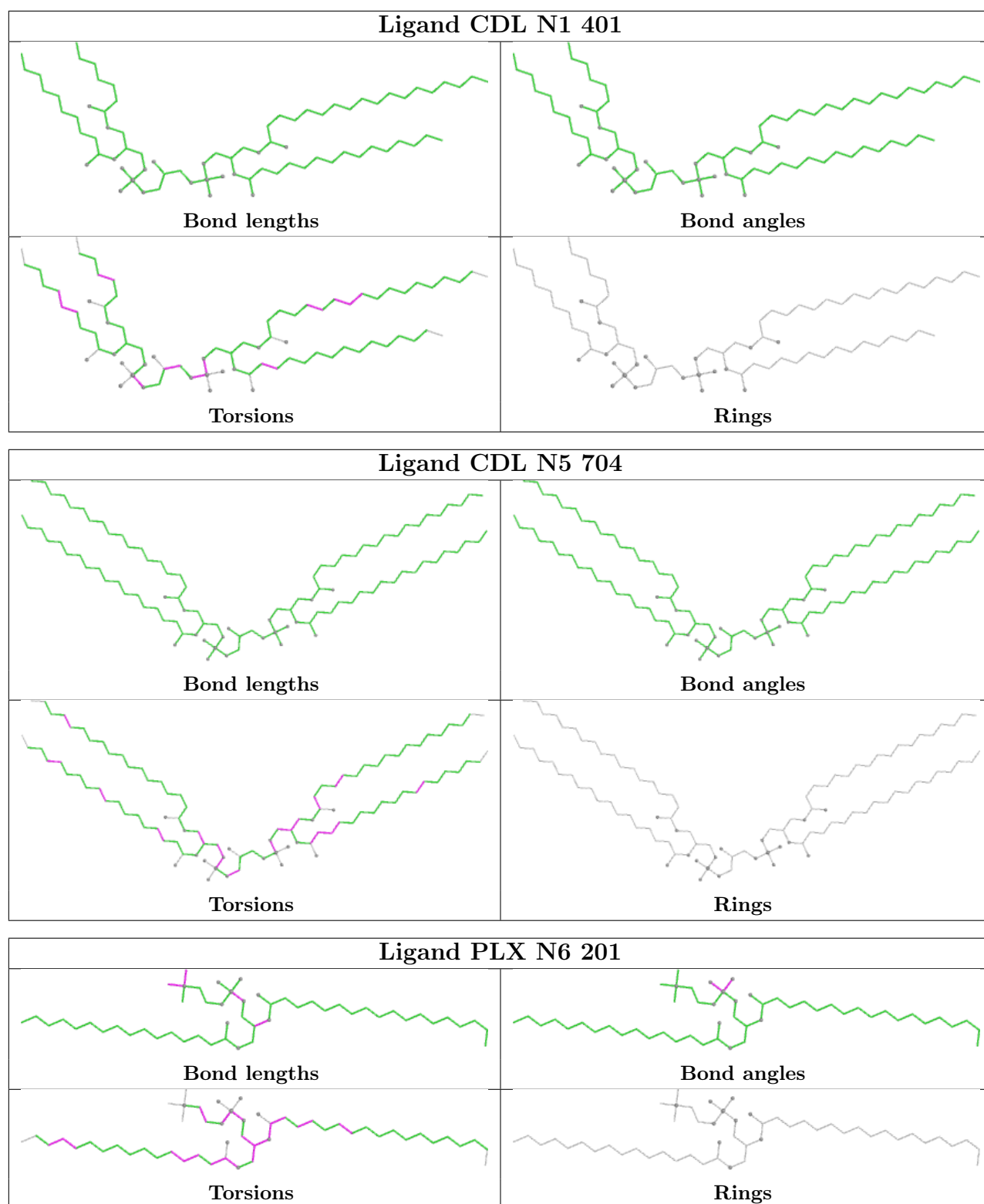




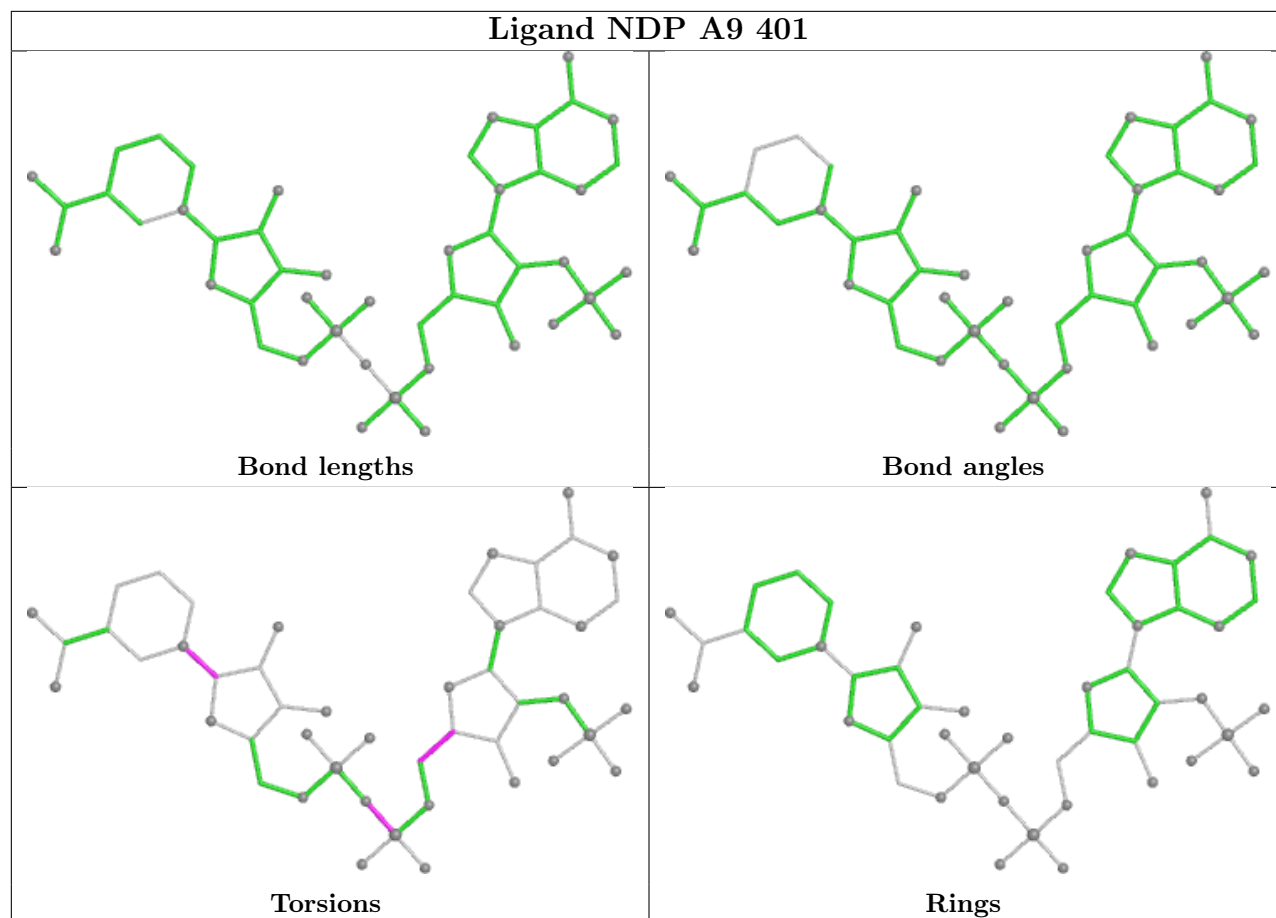




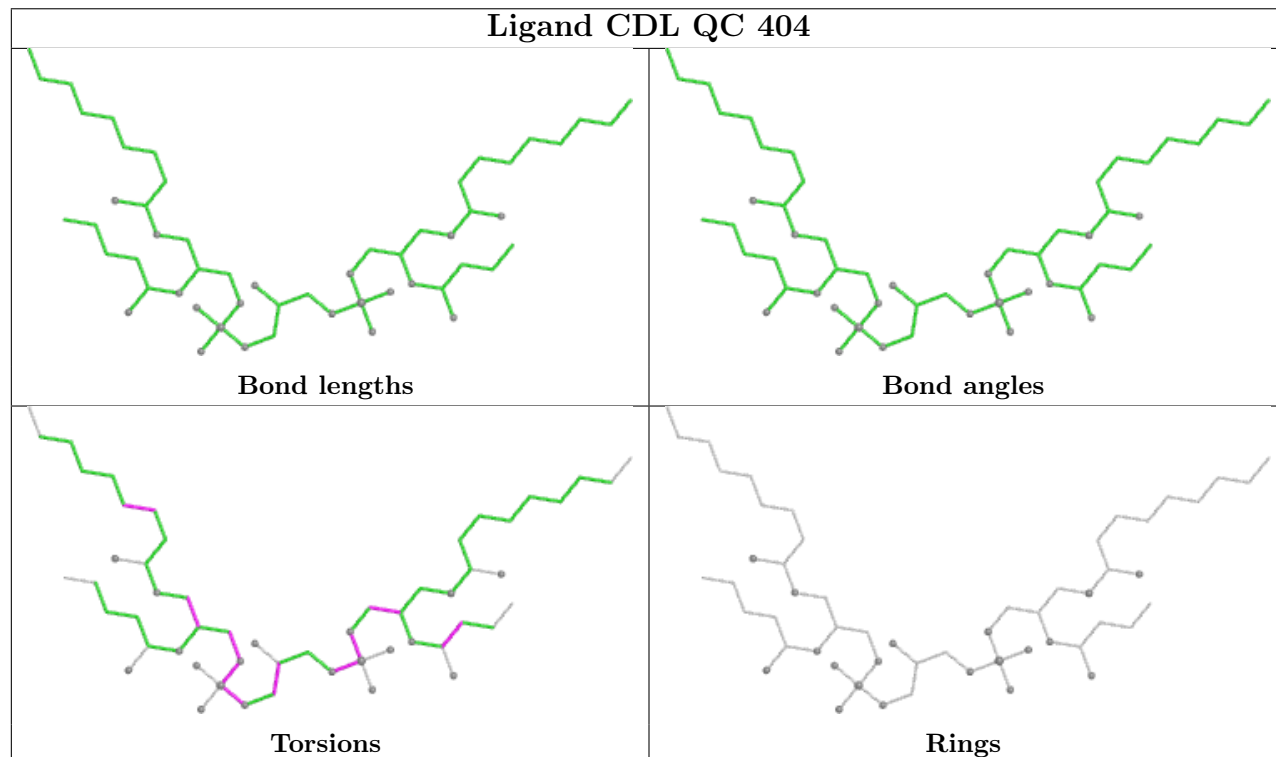


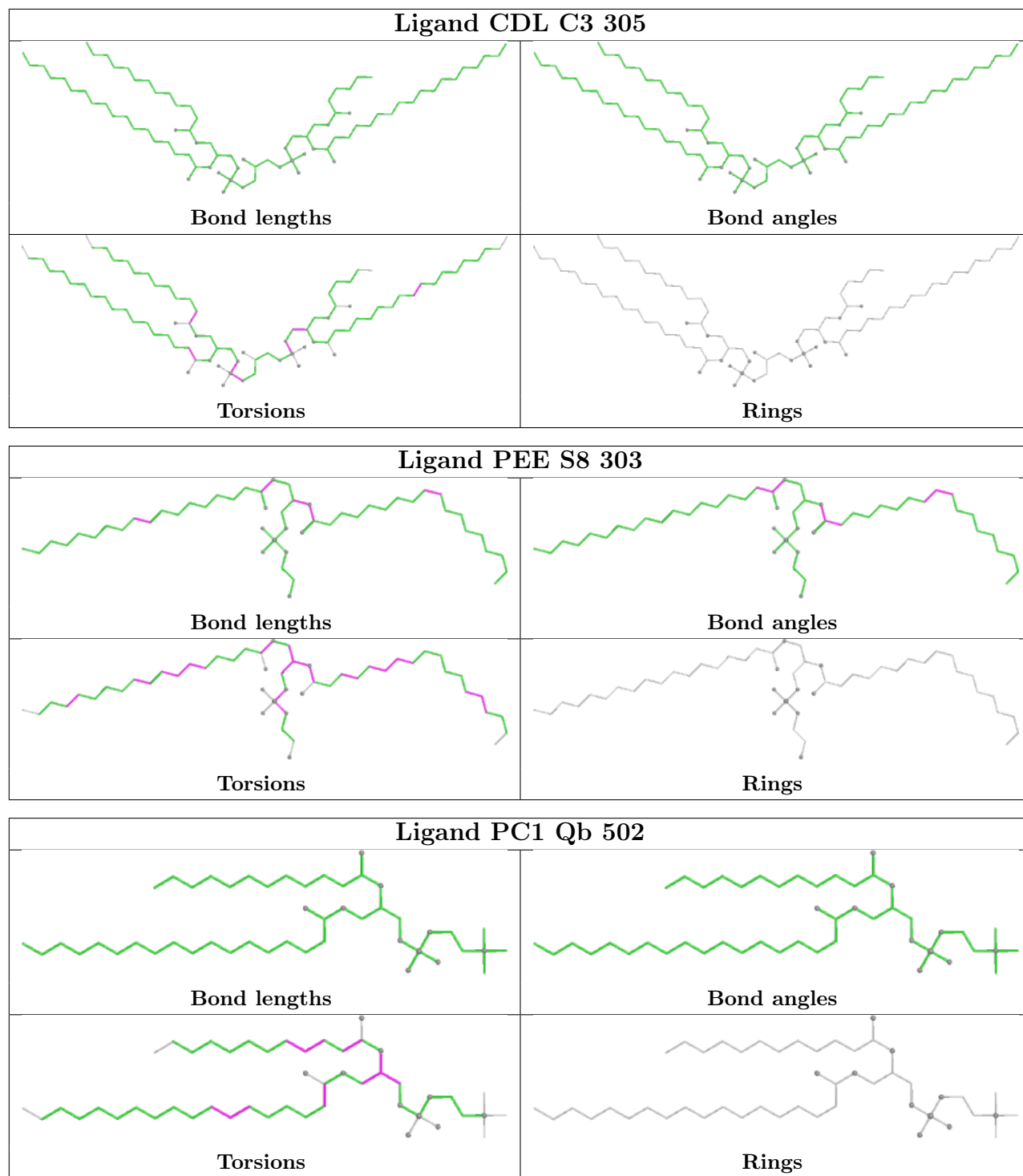


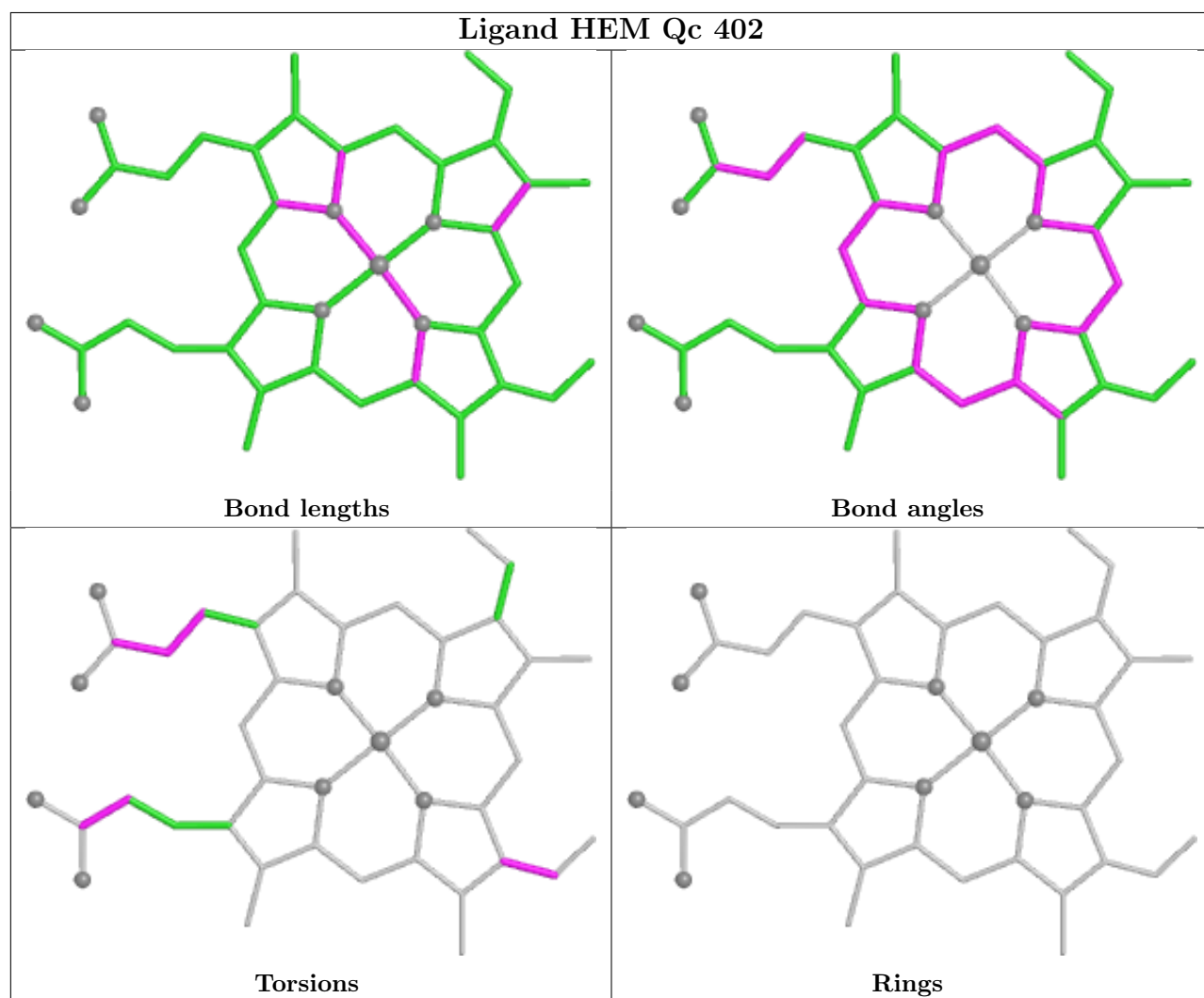
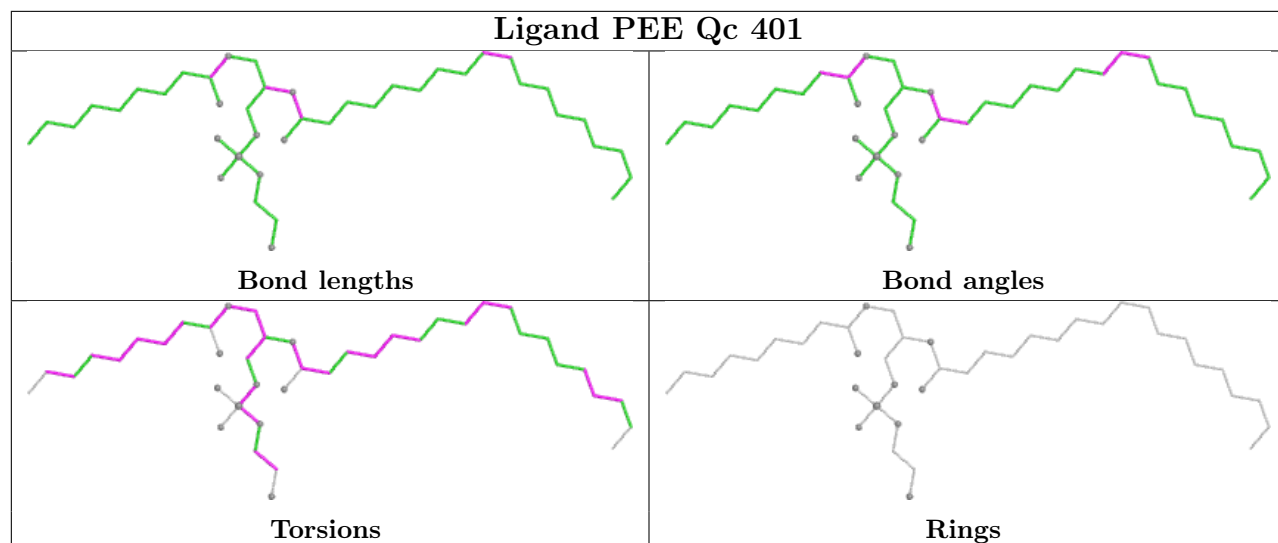
Ligand NDP A9 401

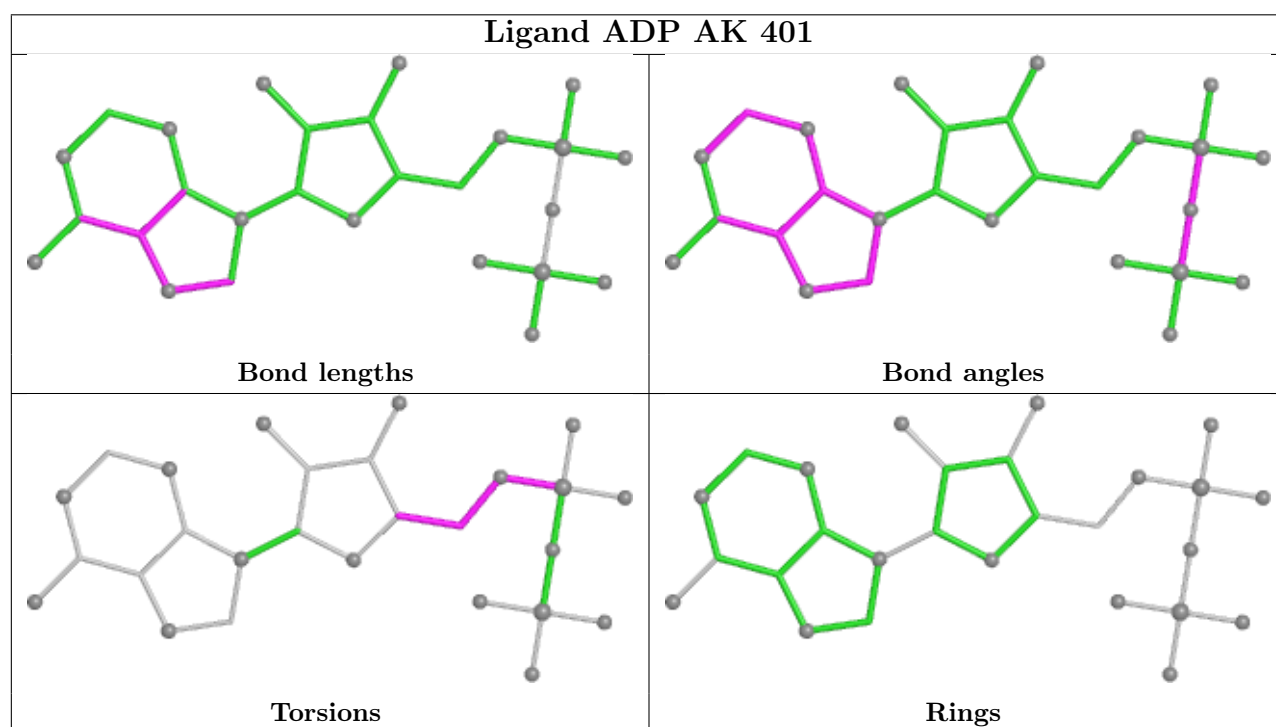
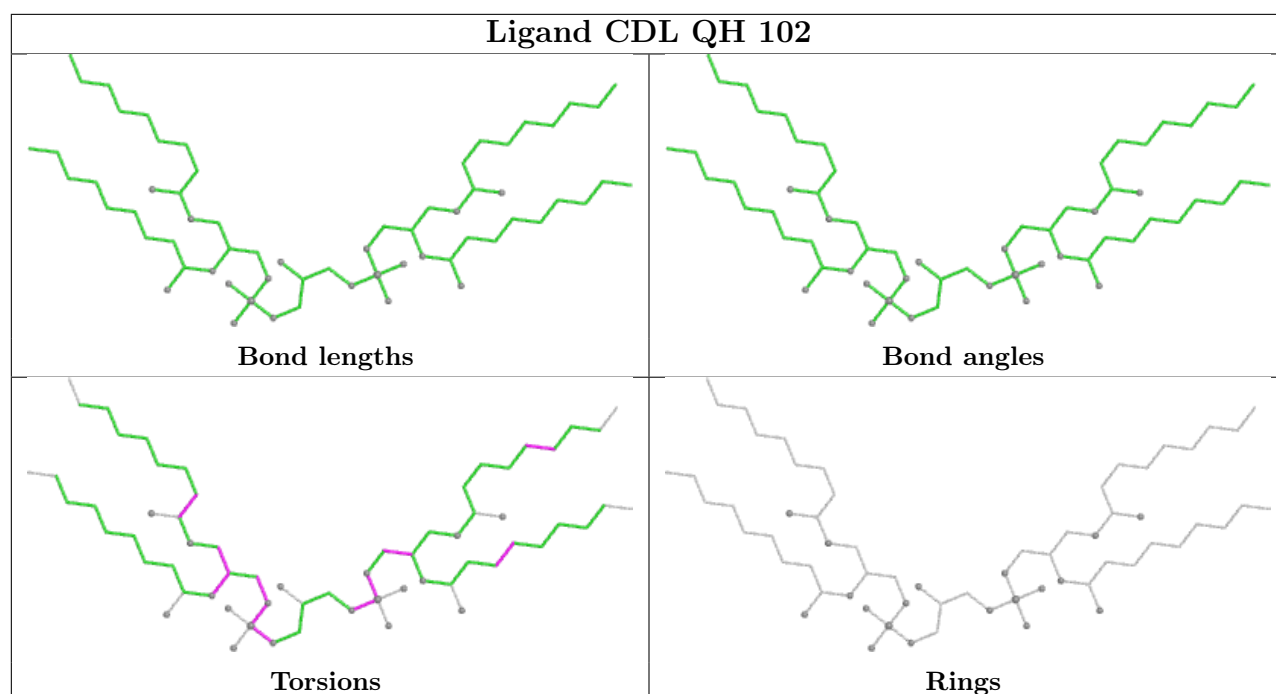


Ligand CDL QC 404

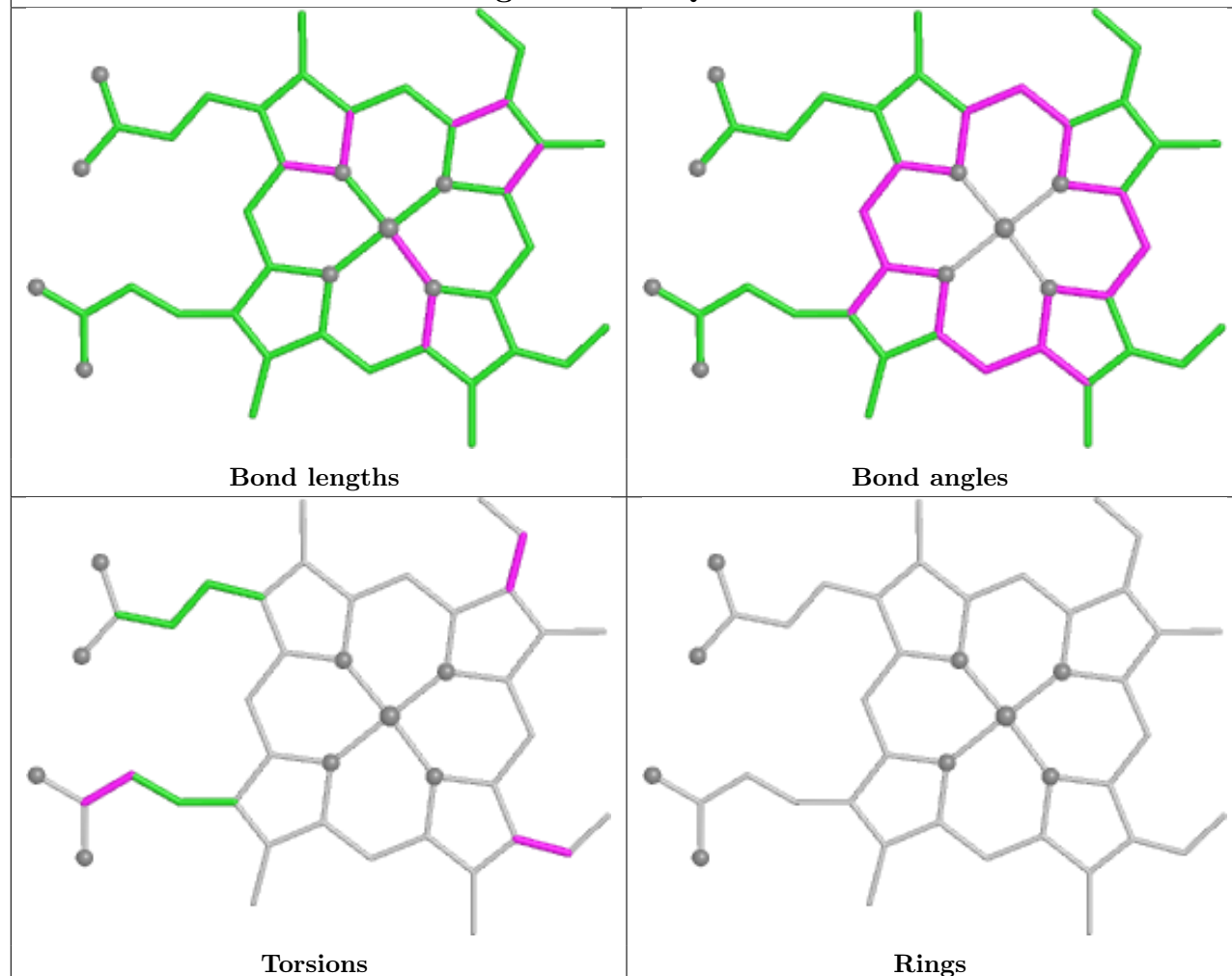




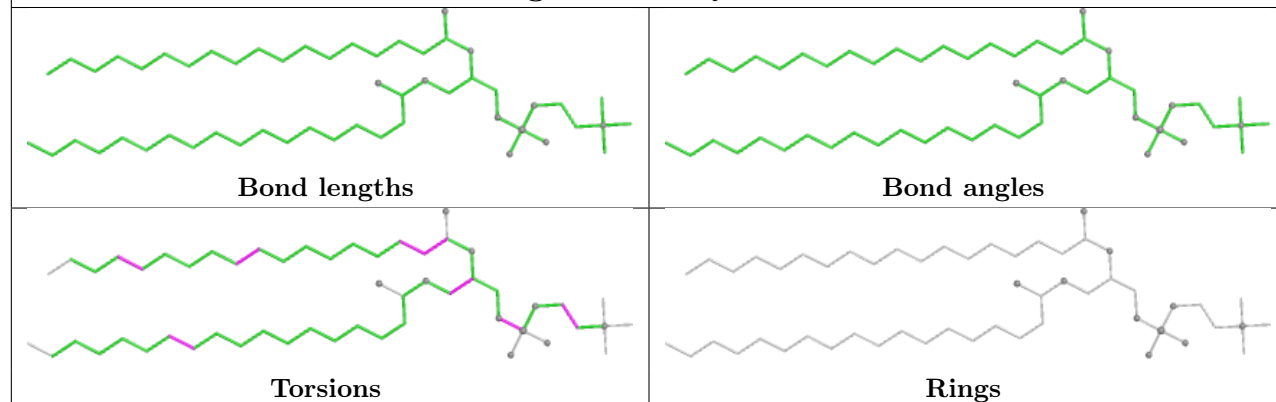


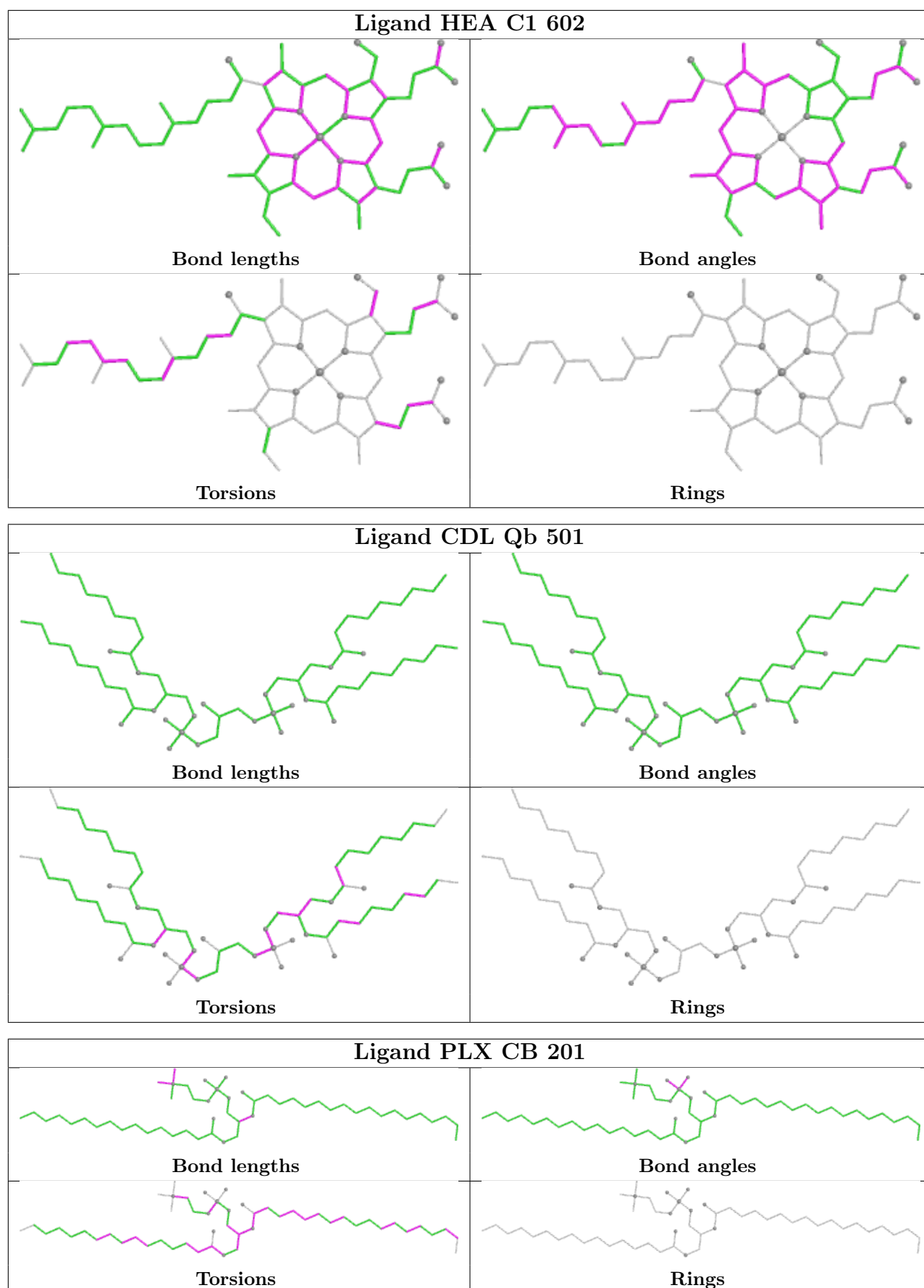


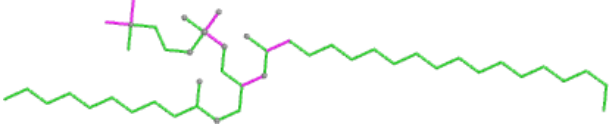
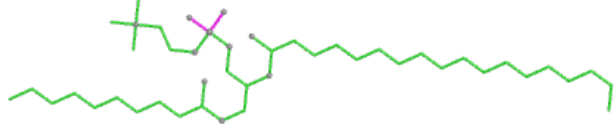
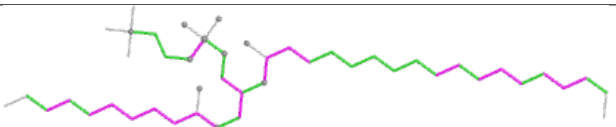
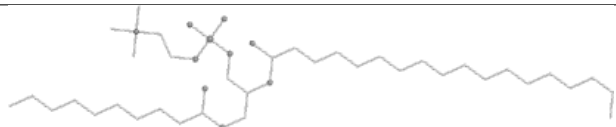
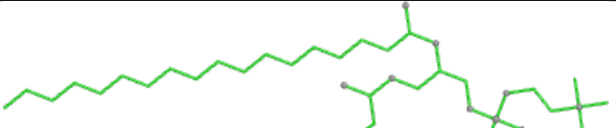
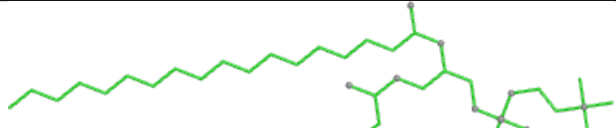
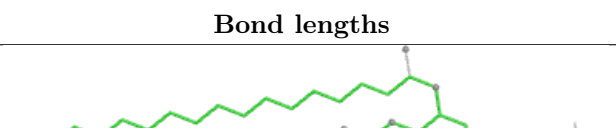
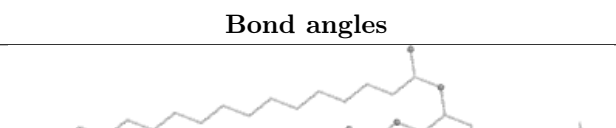
Ligand HEM QC 402



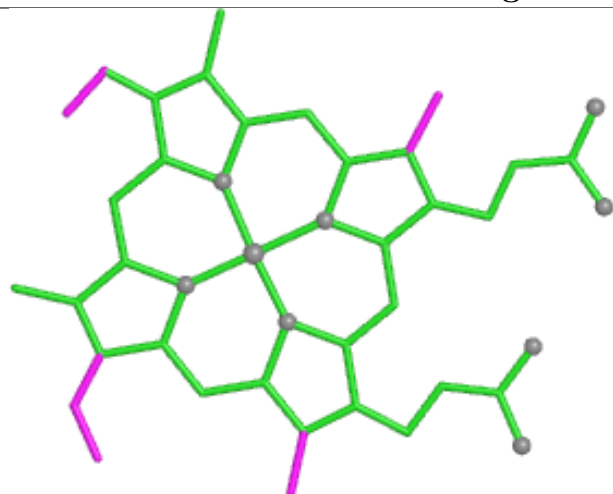
Ligand PC1 Qc 405



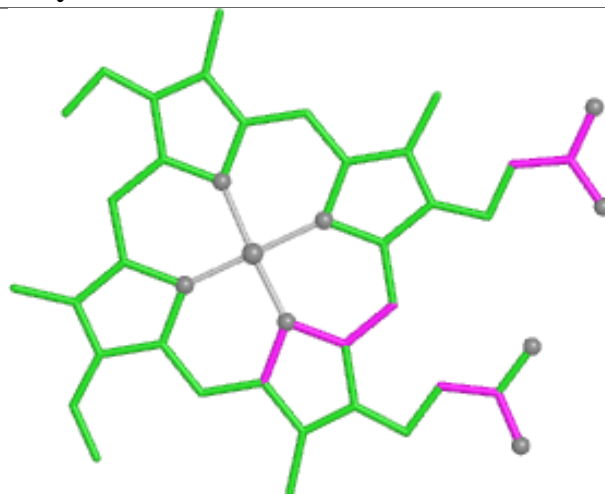


Ligand PLX Qi 301	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 C1 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

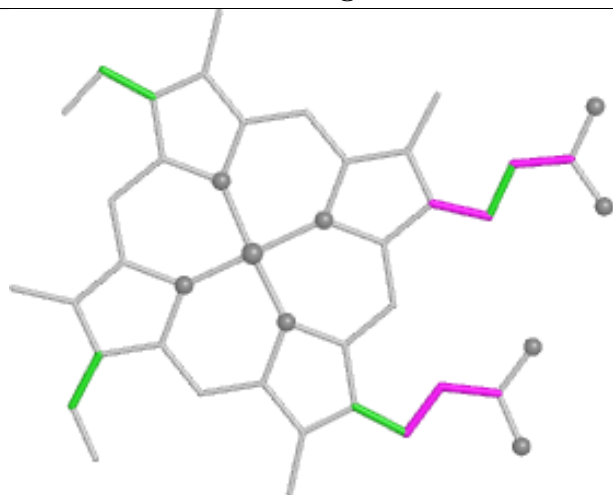
Ligand HEC Qd 401



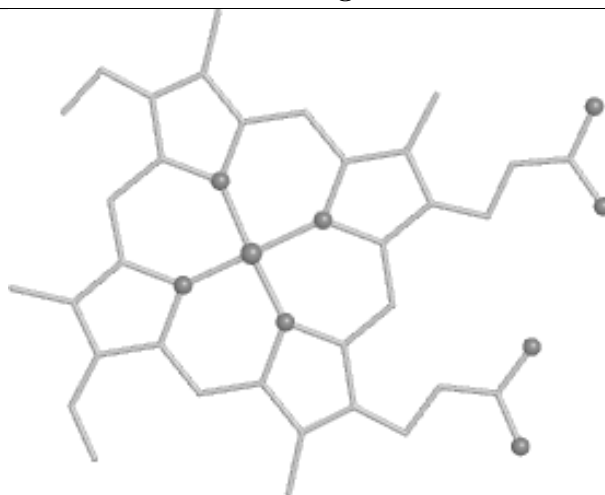
Bond lengths



Bond angles

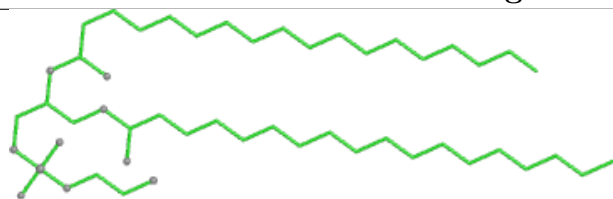


Torsions

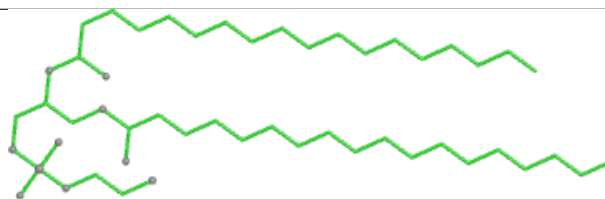


Rings

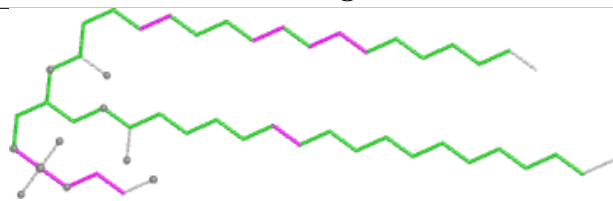
Ligand 3PE CA 101



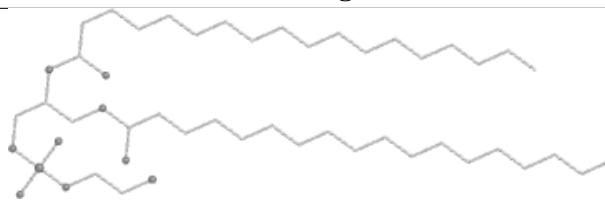
Bond lengths



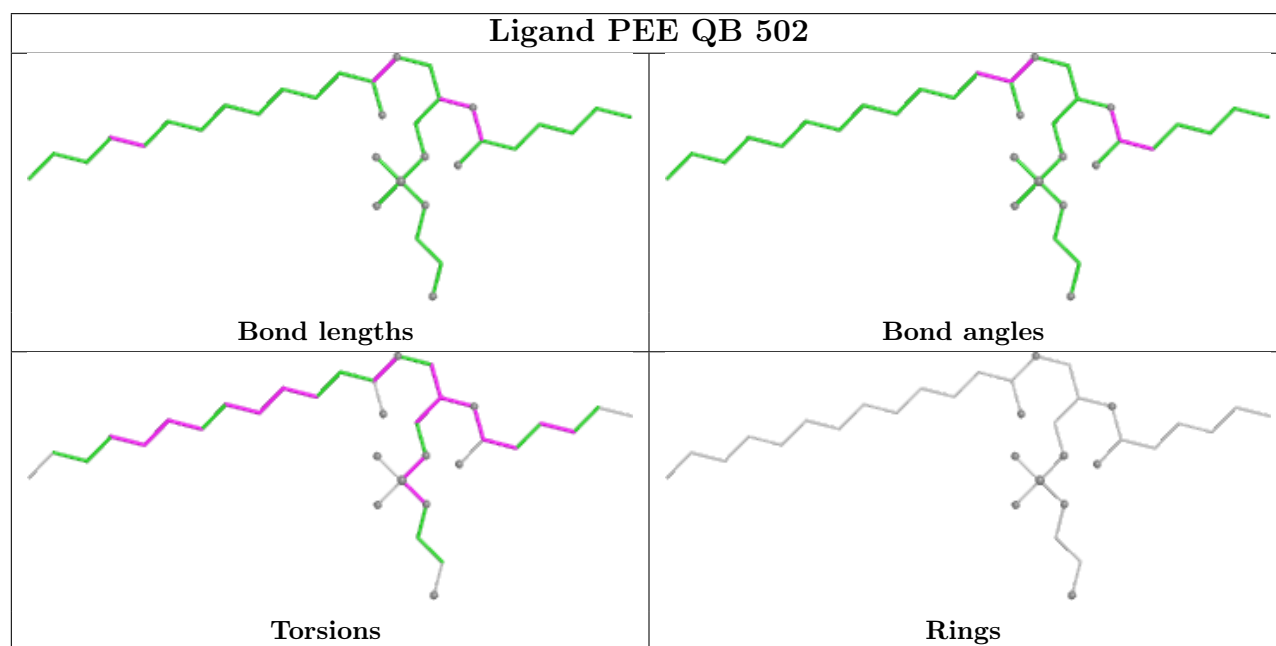
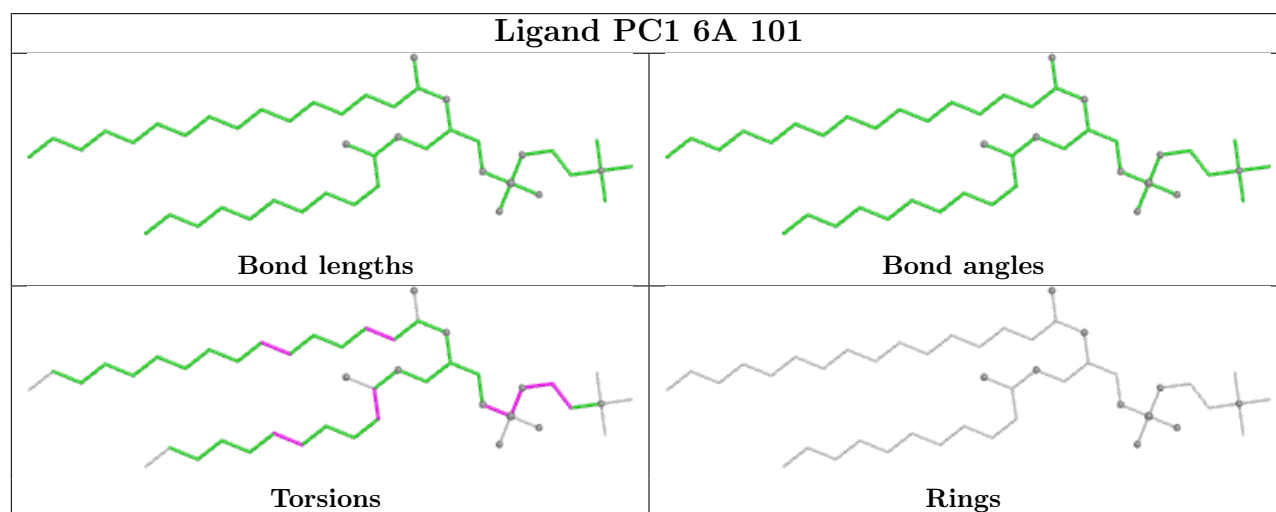
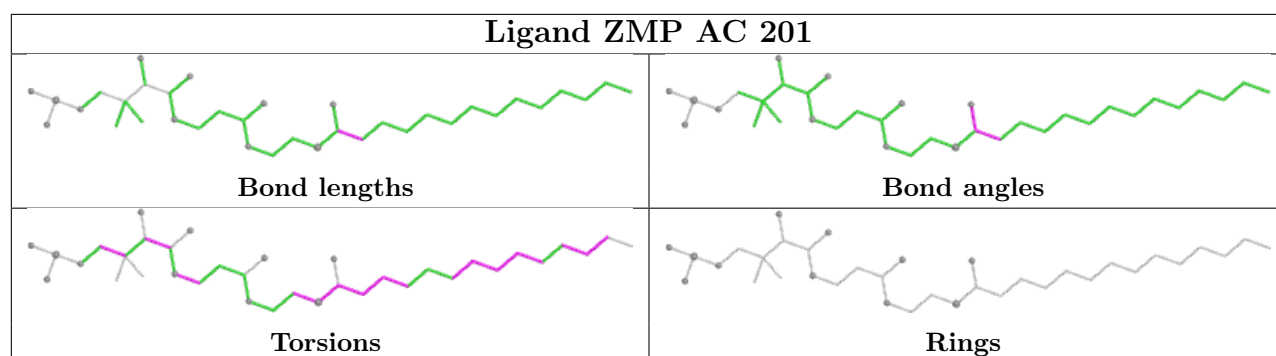
Bond angles

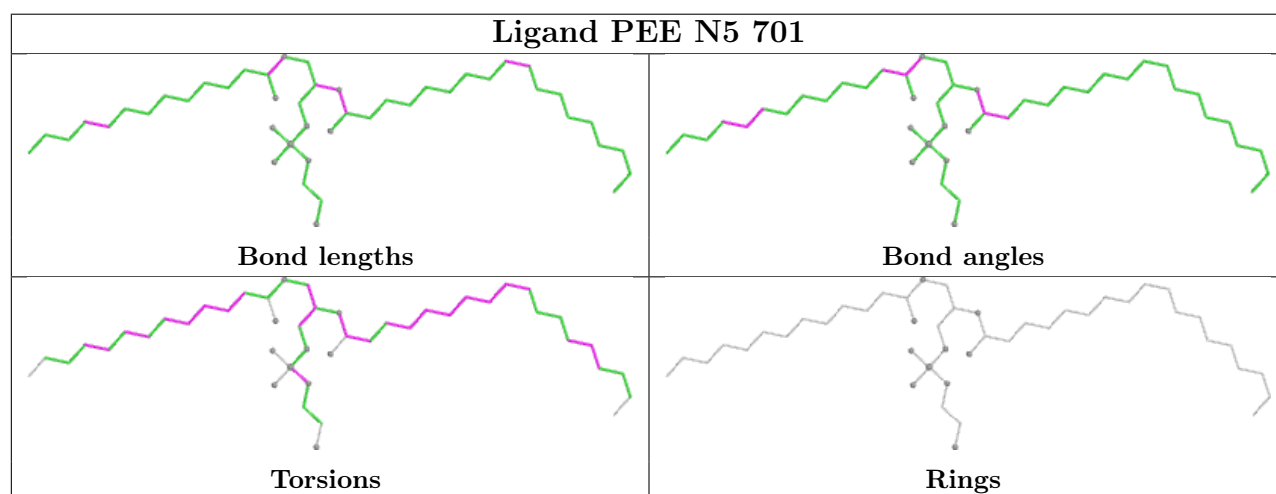
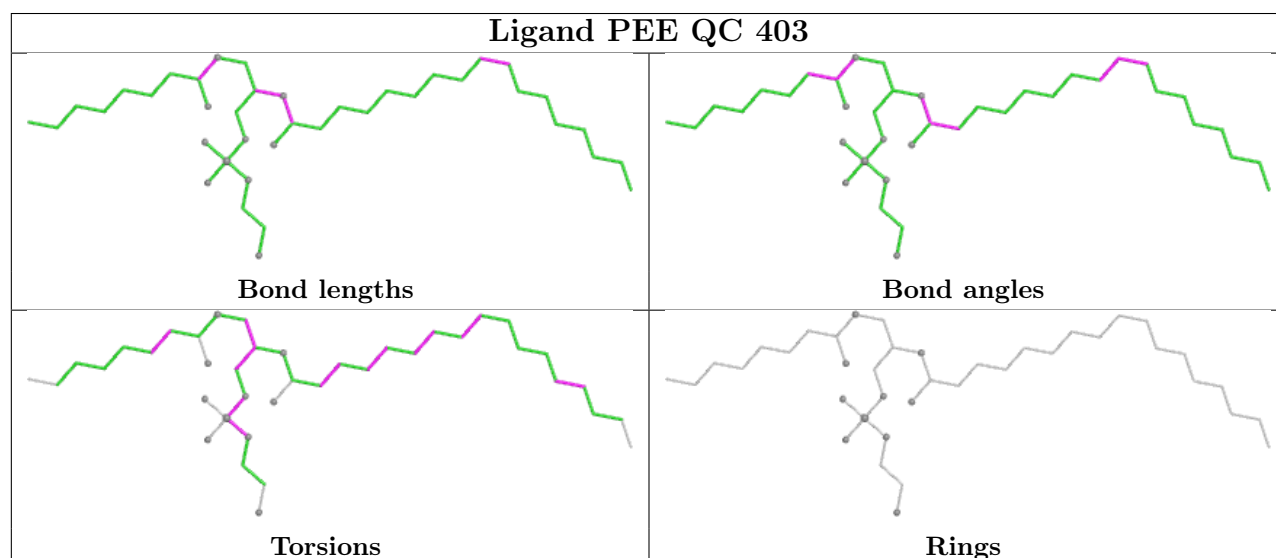
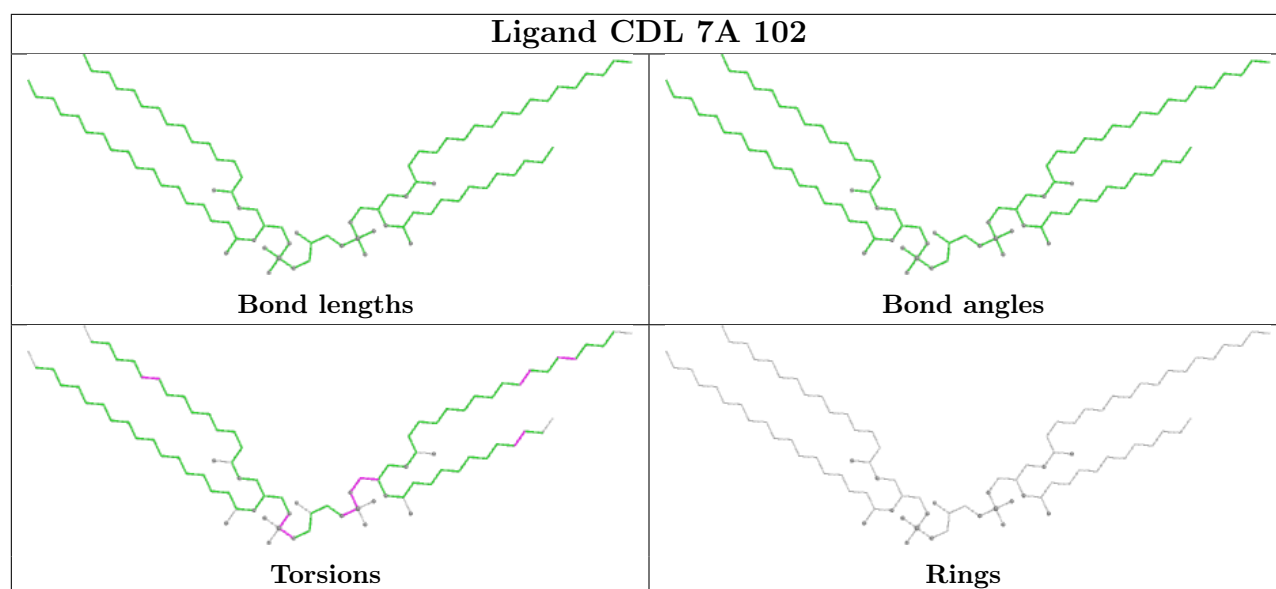


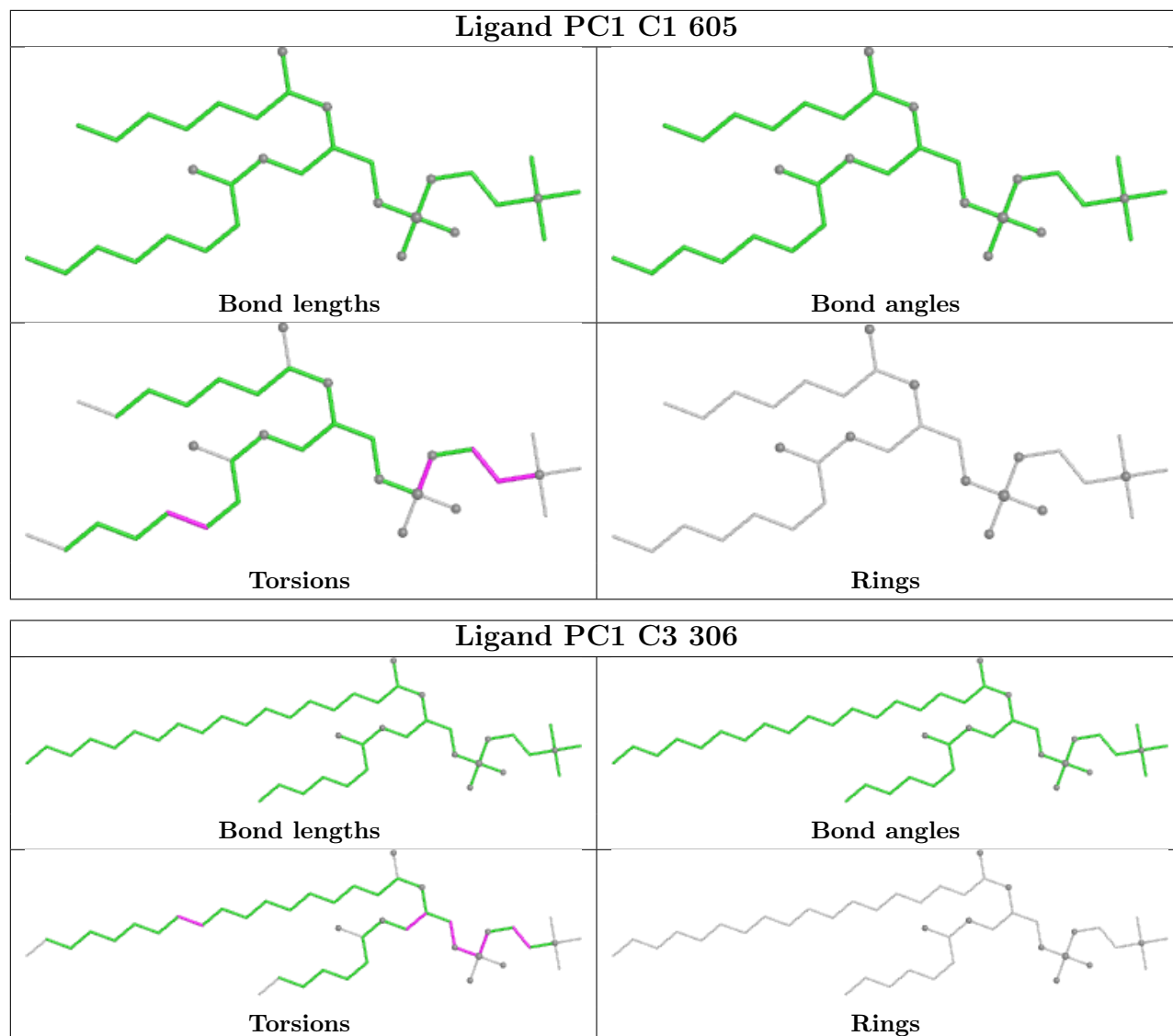
Torsions

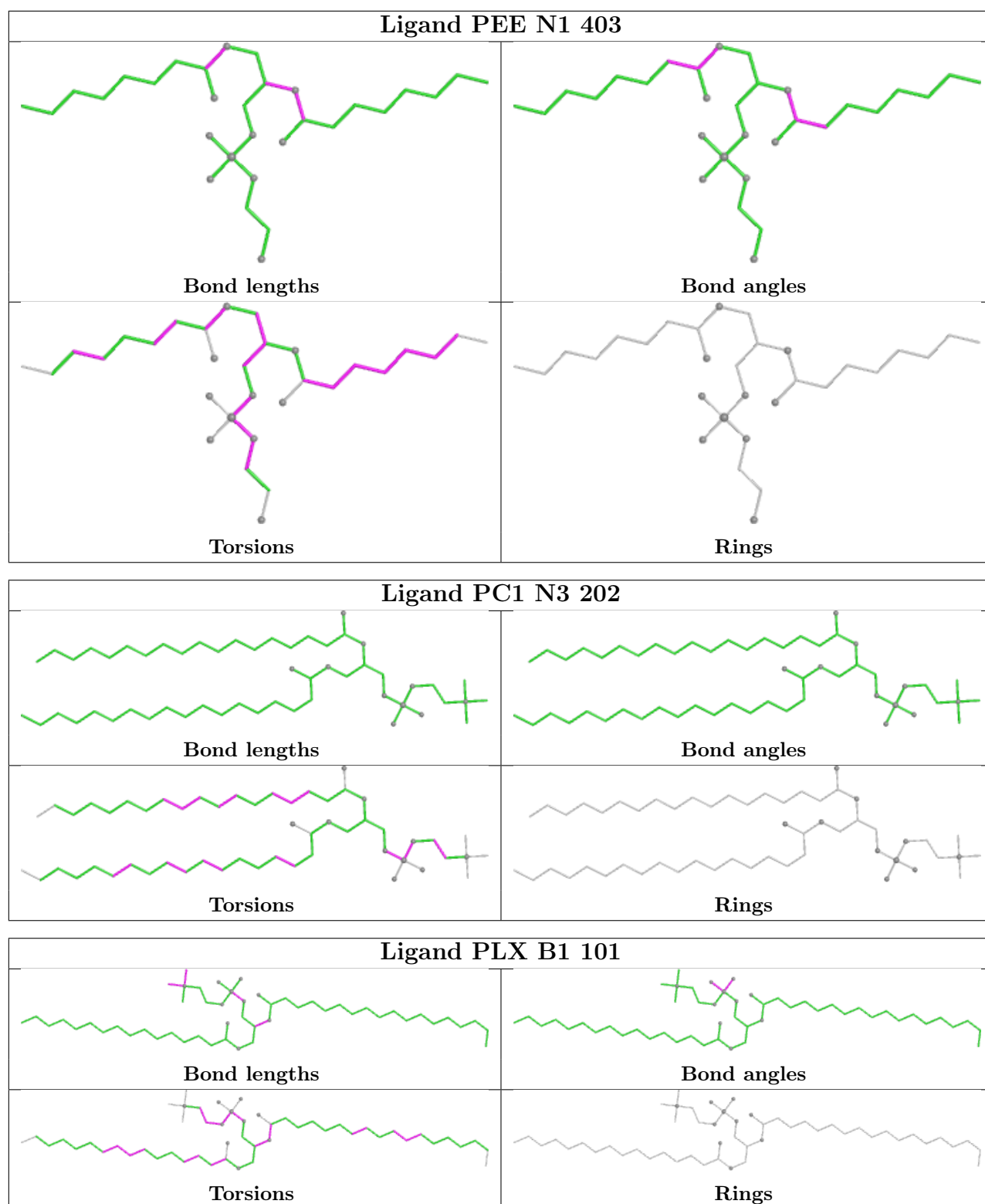


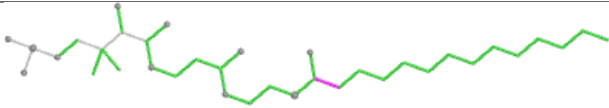
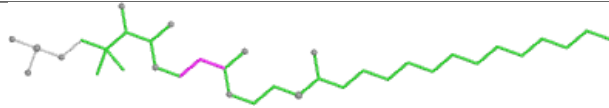
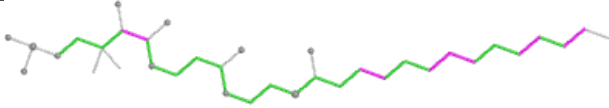
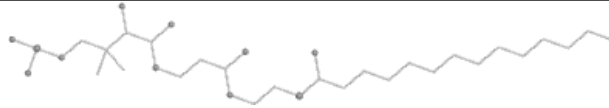
Rings

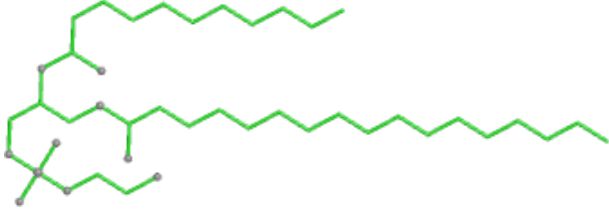
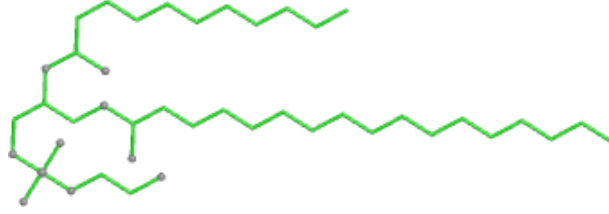
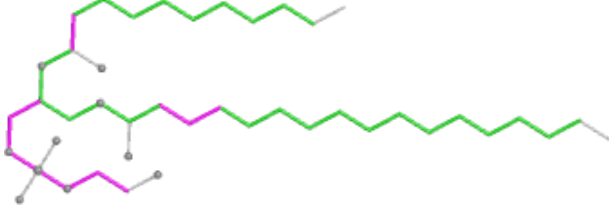
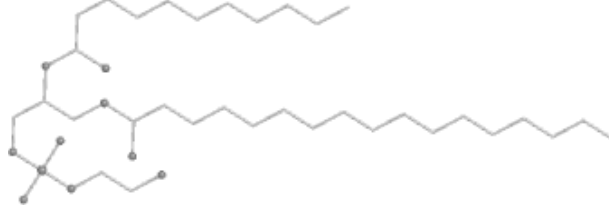


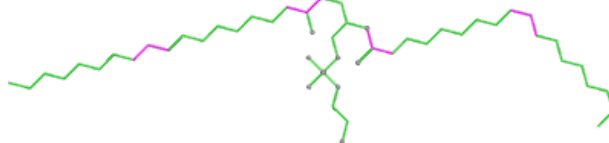
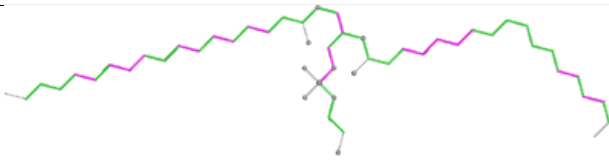
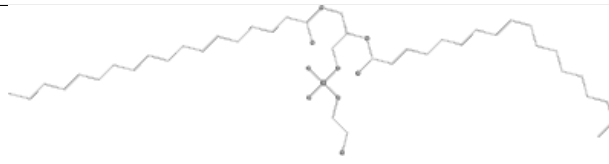


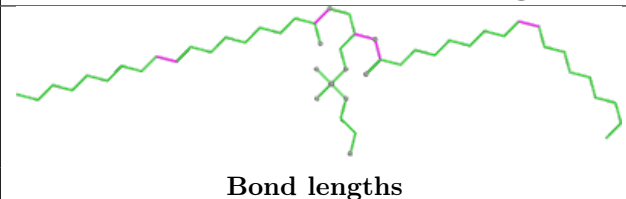
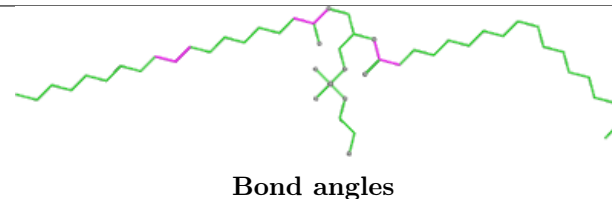
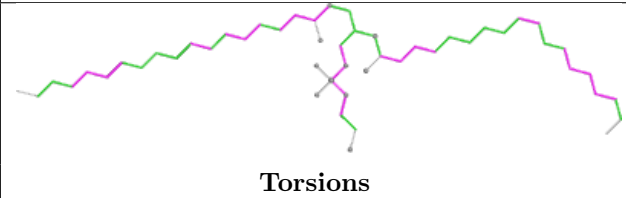
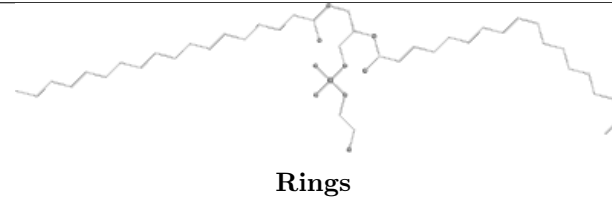


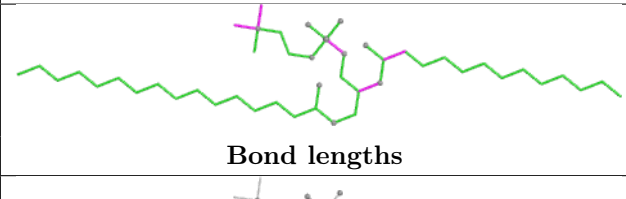
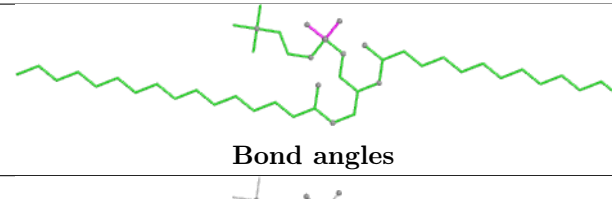
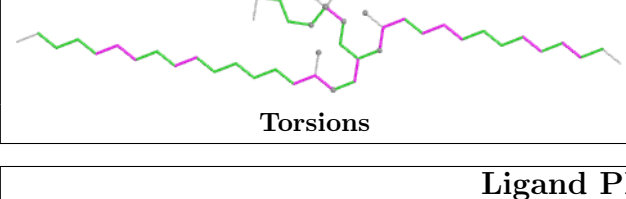


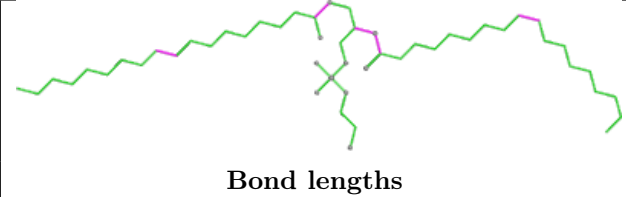
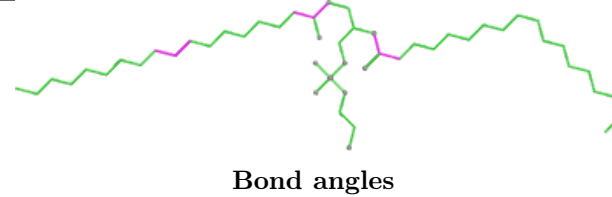
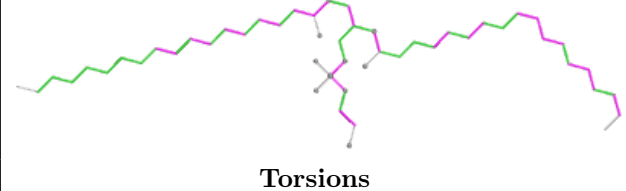
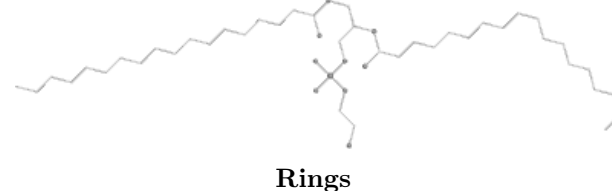
Ligand ZMP AB 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

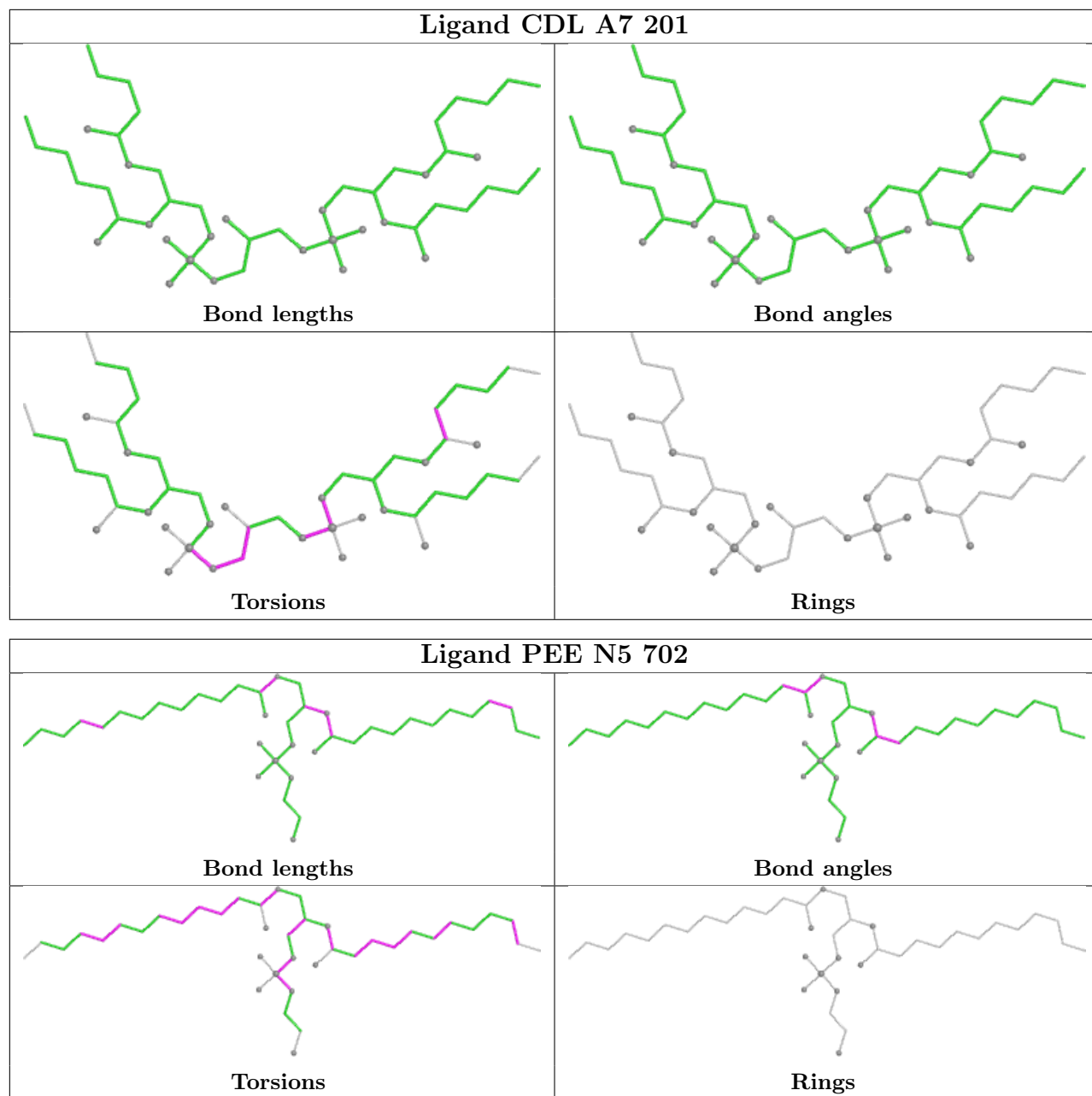
Ligand 3PE 7A 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

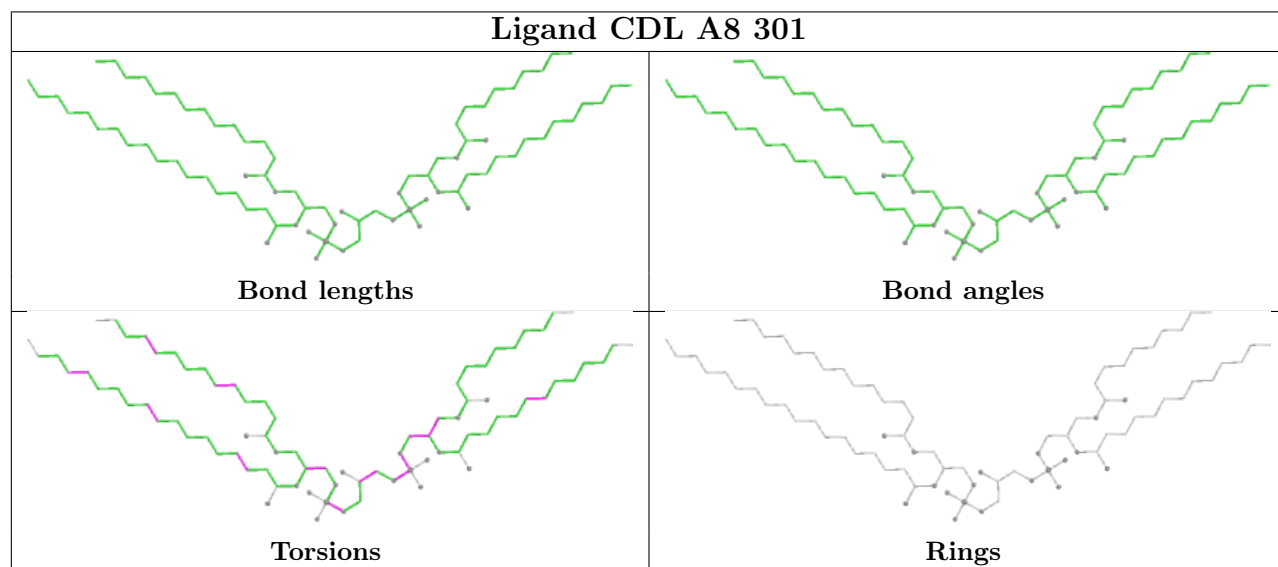
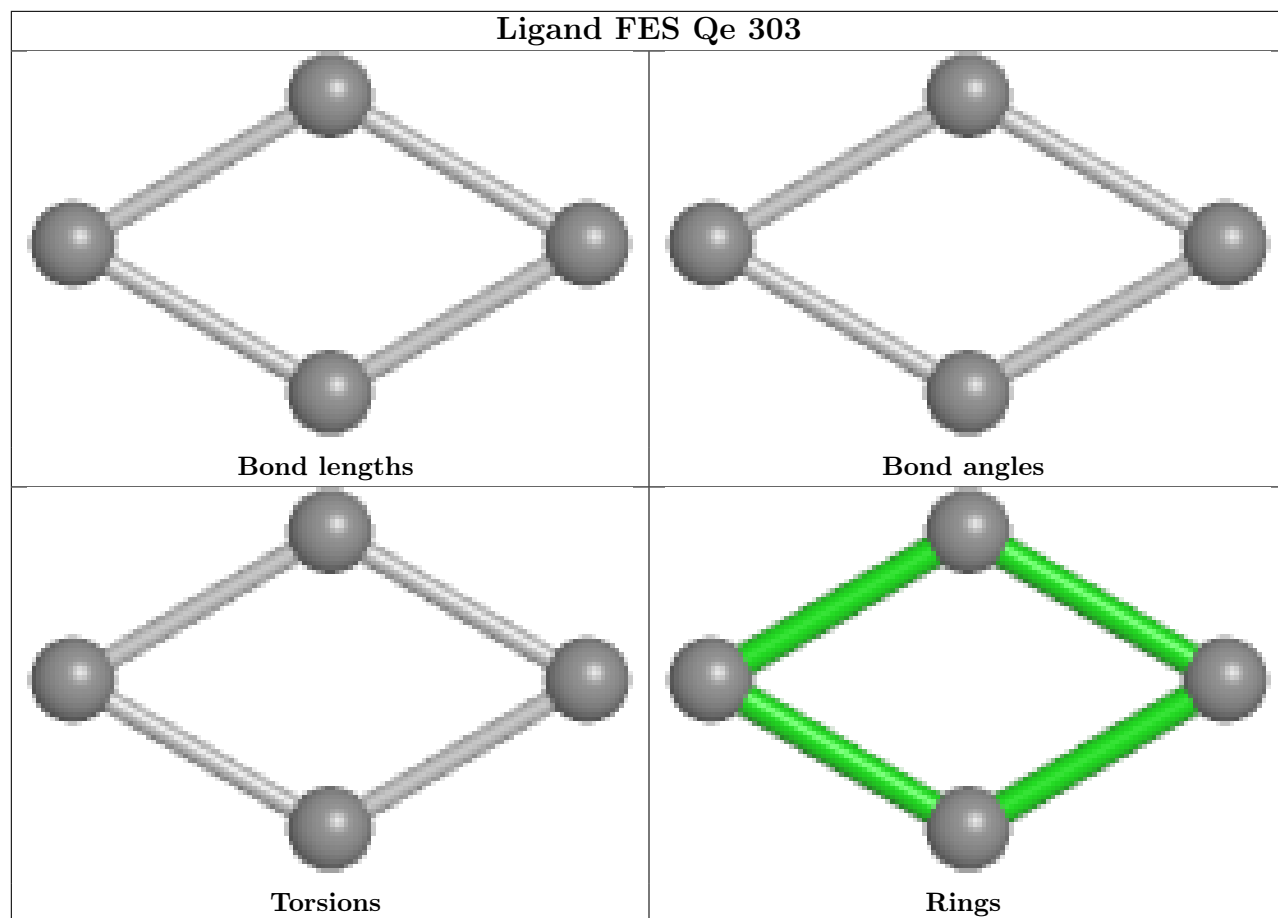
Ligand PEE 7C 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

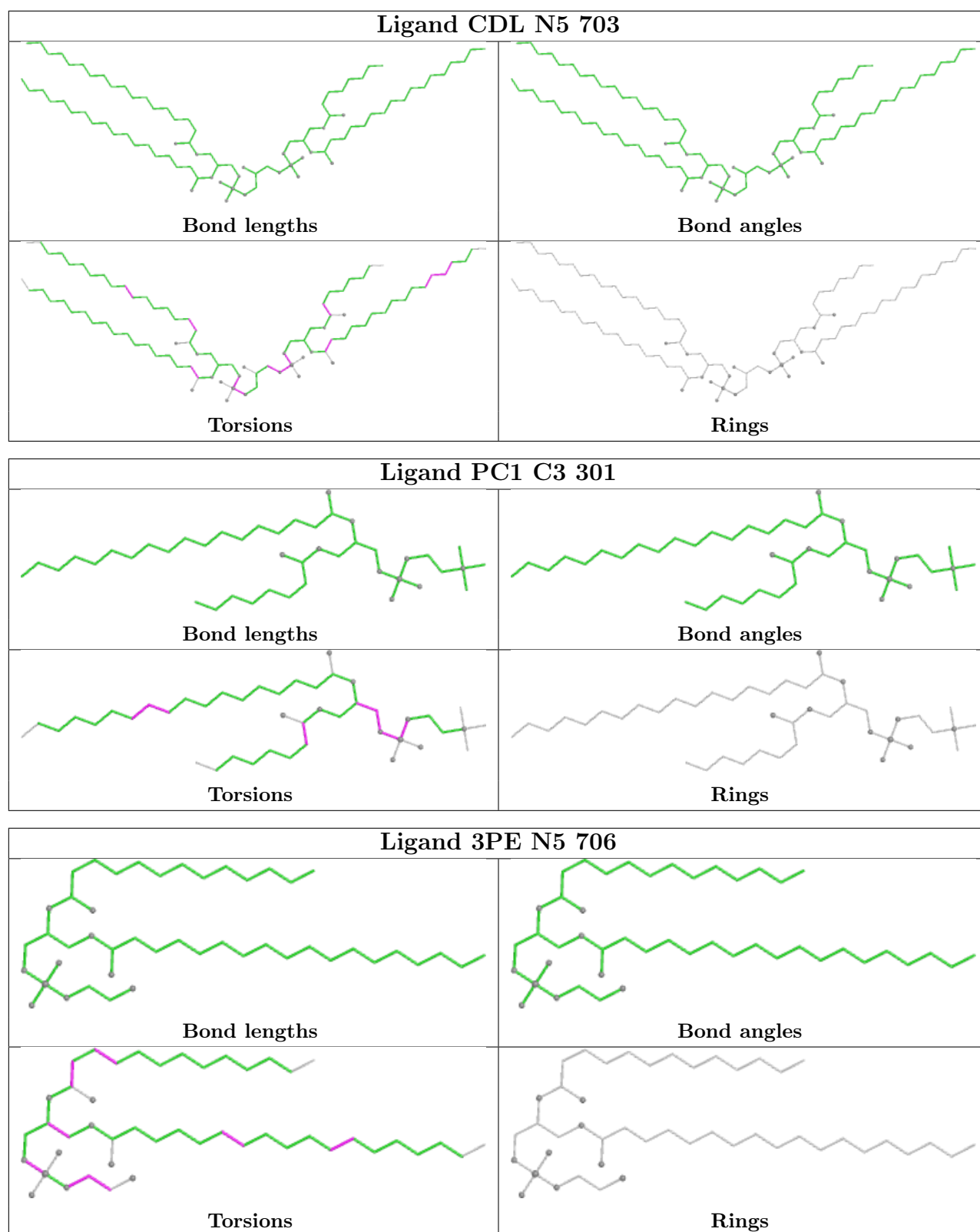
Ligand PEE N3 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

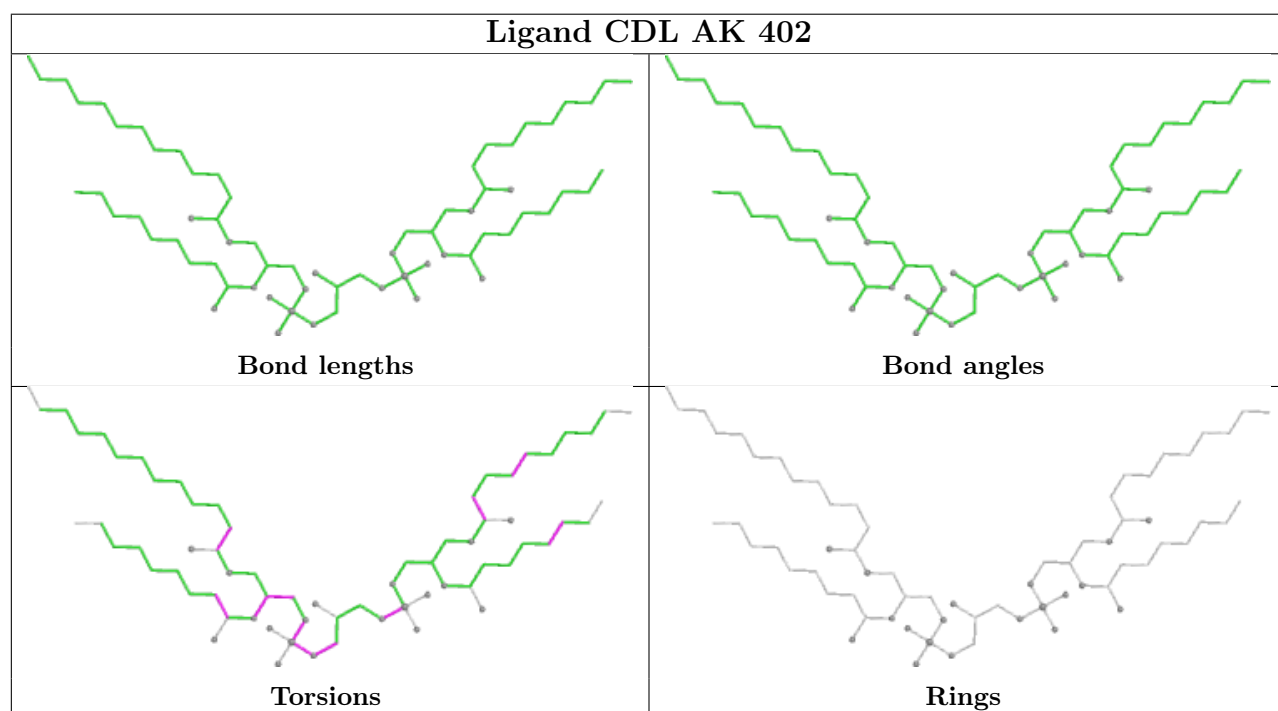
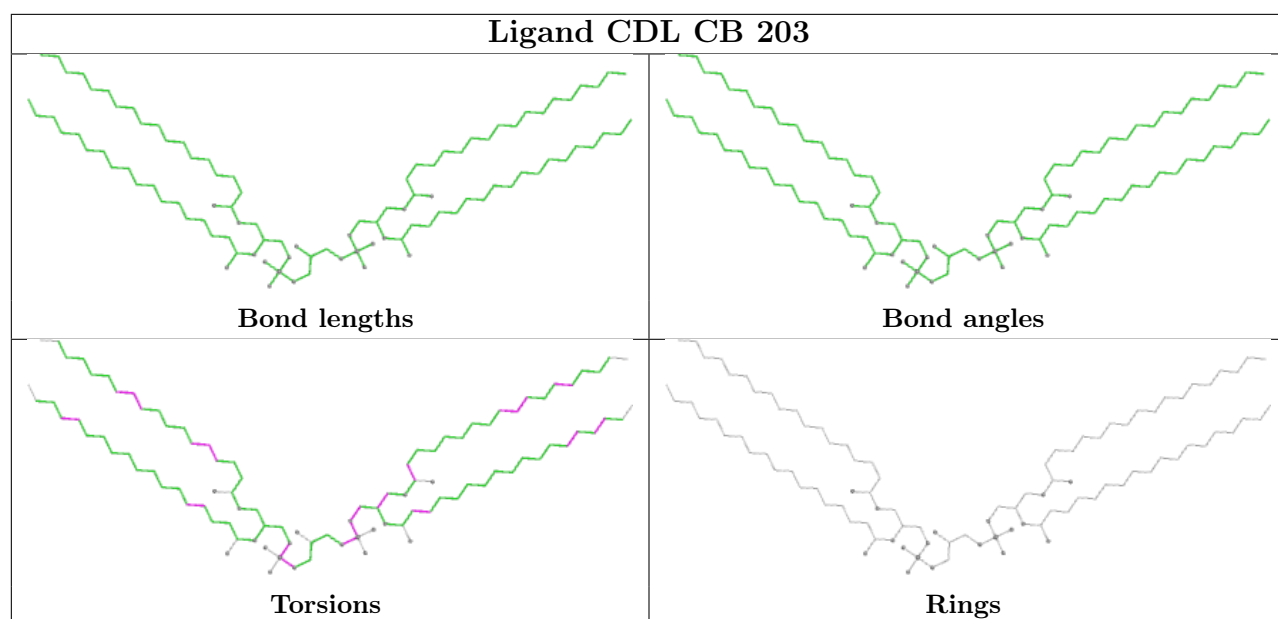
Ligand PLX AL 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

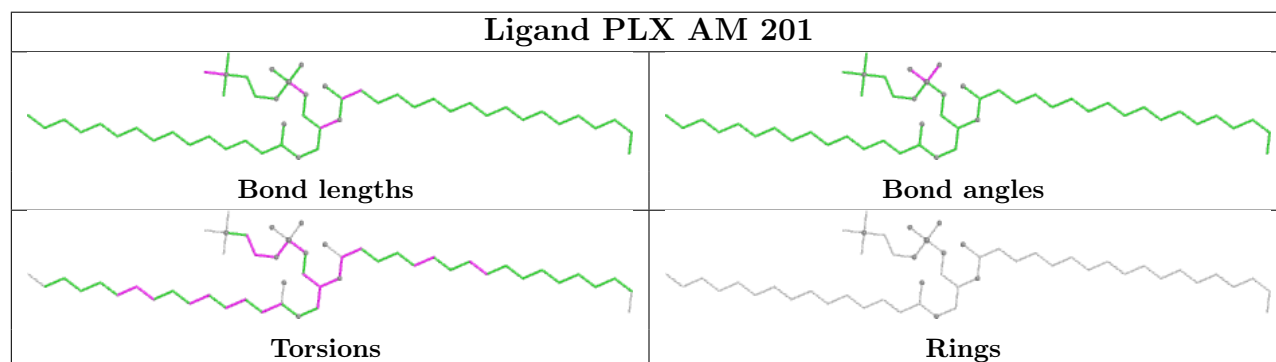
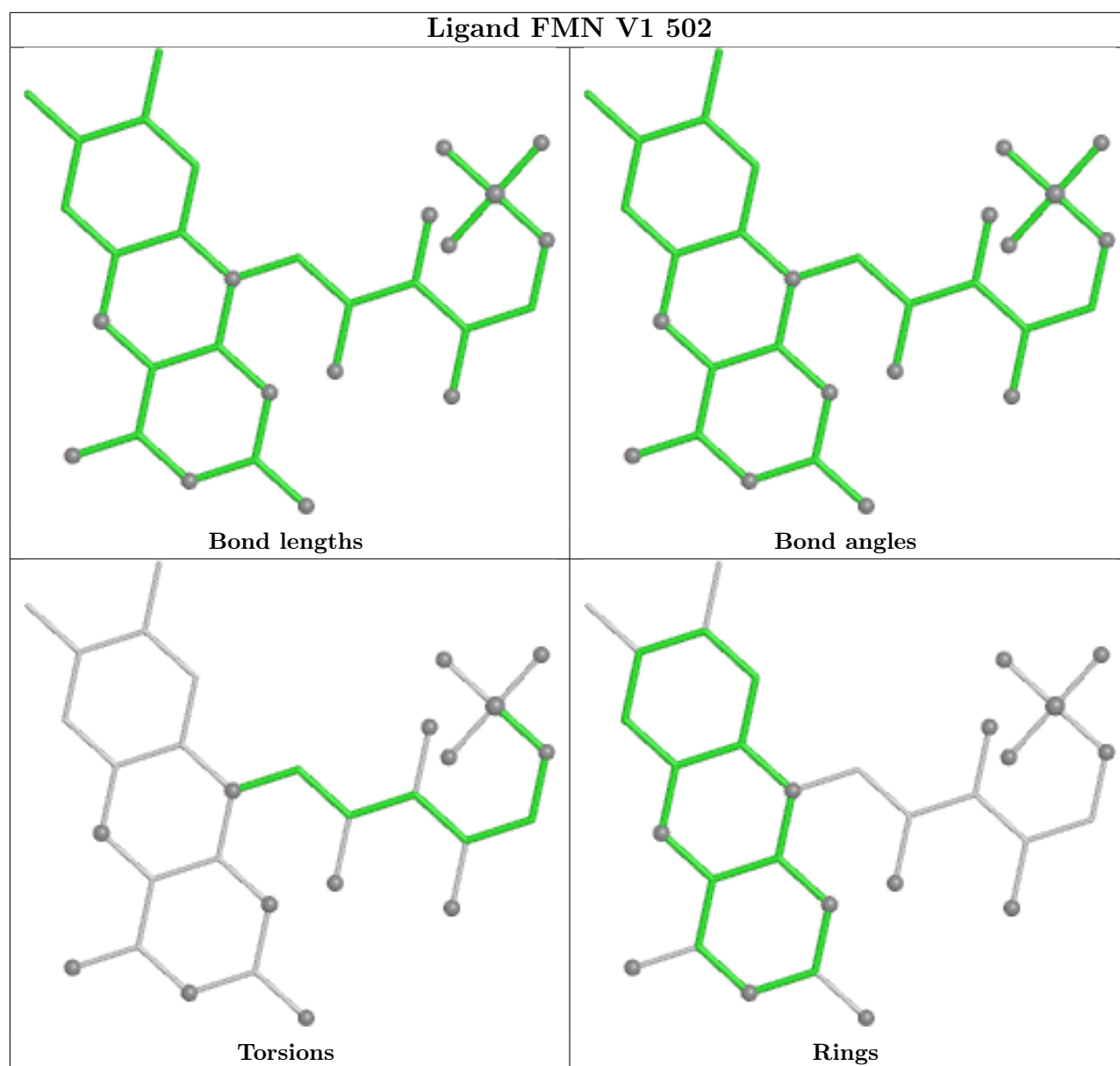
Ligand PEE N5 705	
 Bond lengths	 Bond angles
 Torsions	 Rings

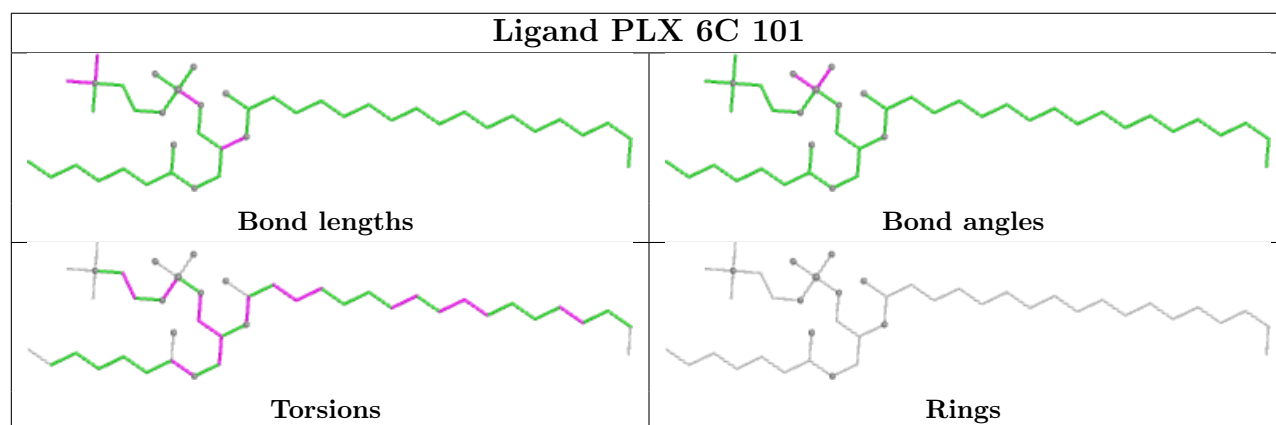
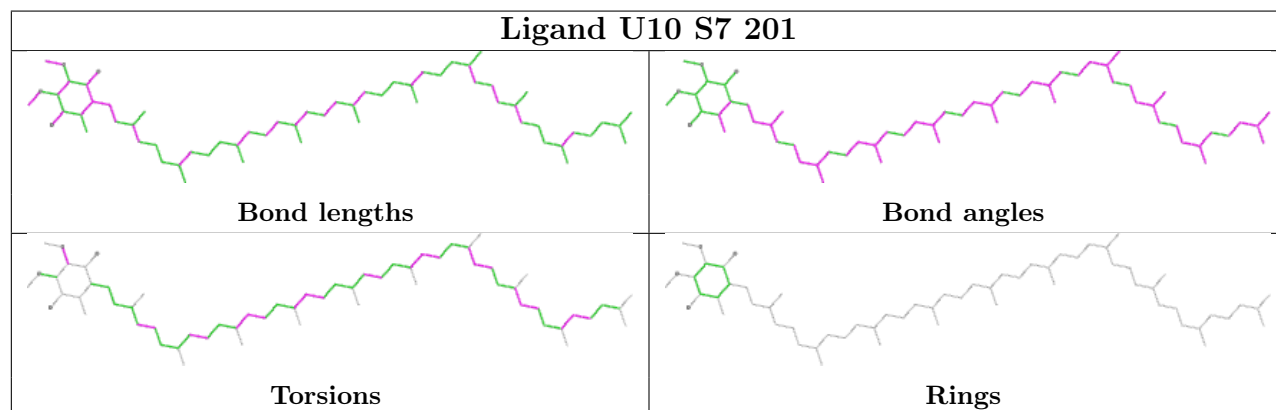
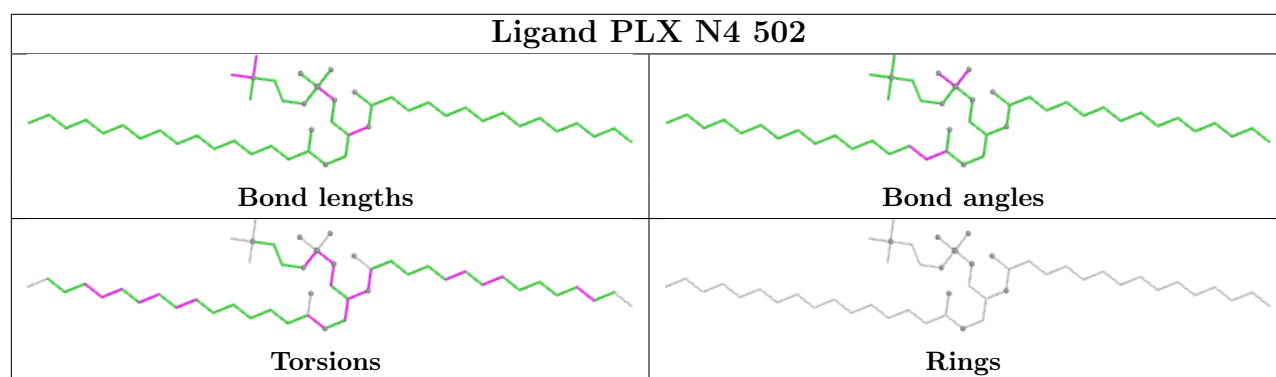




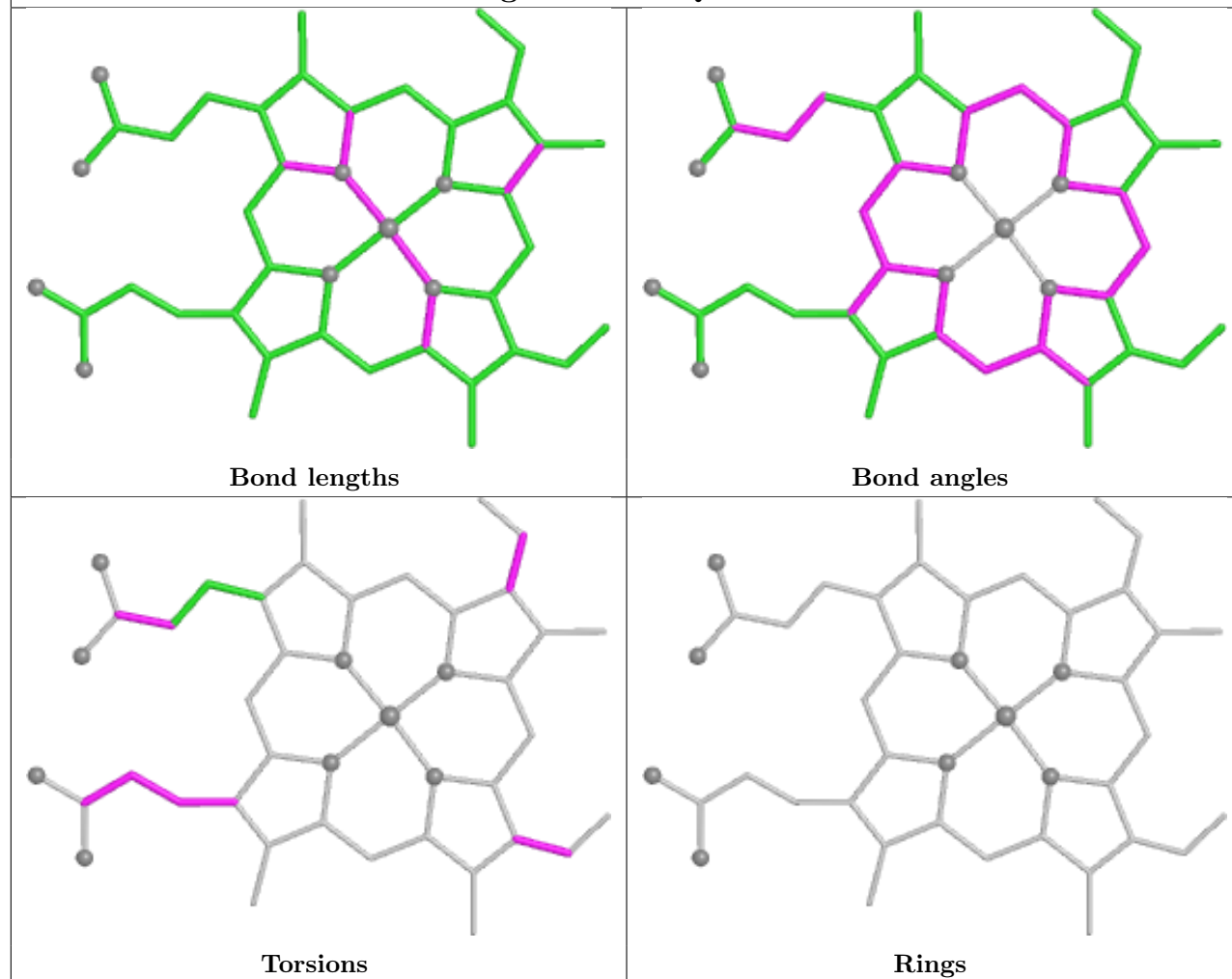




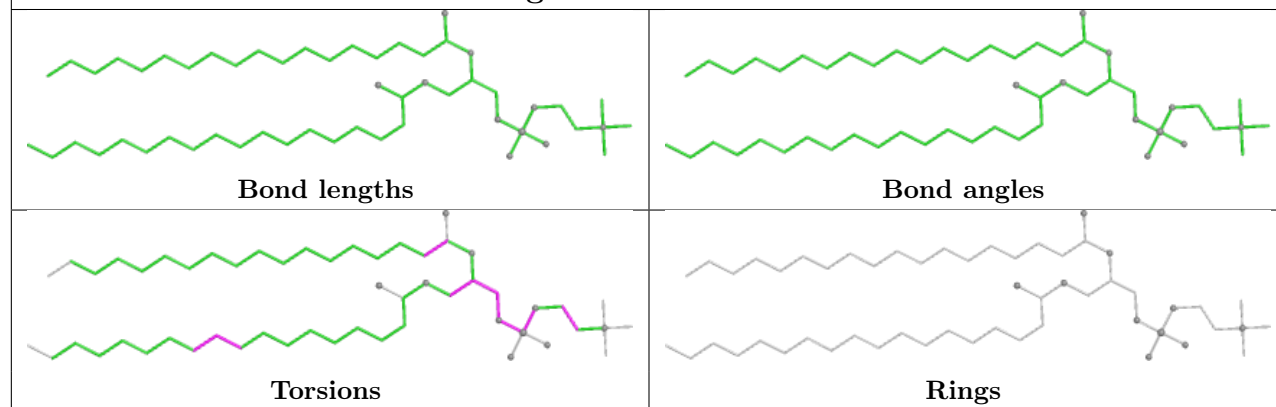


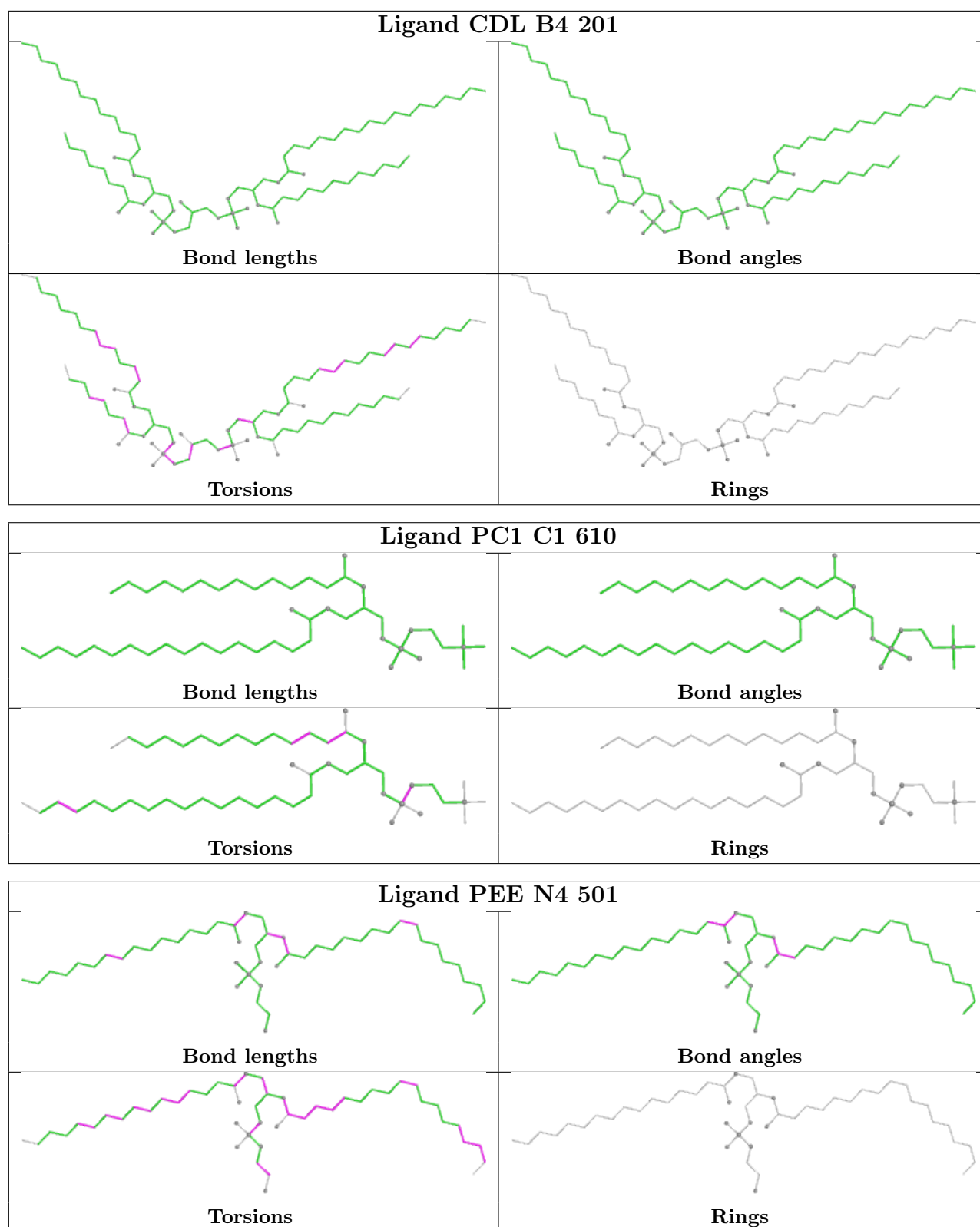


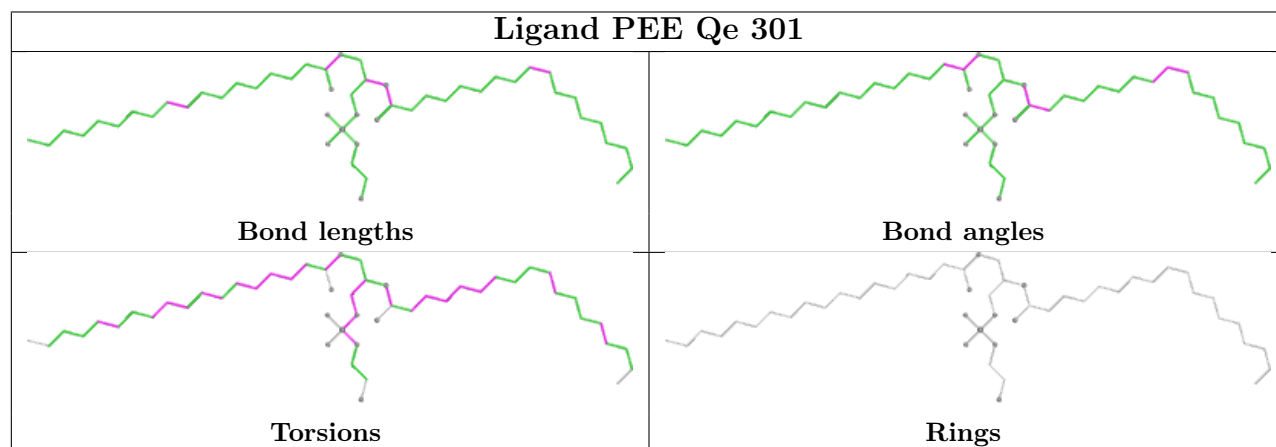
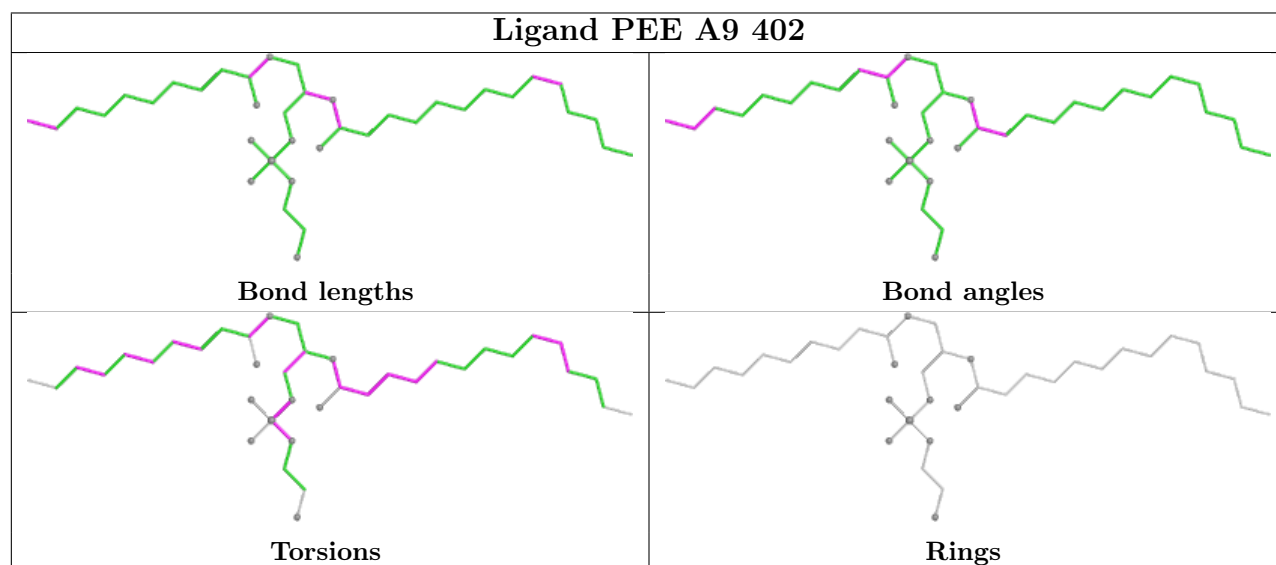
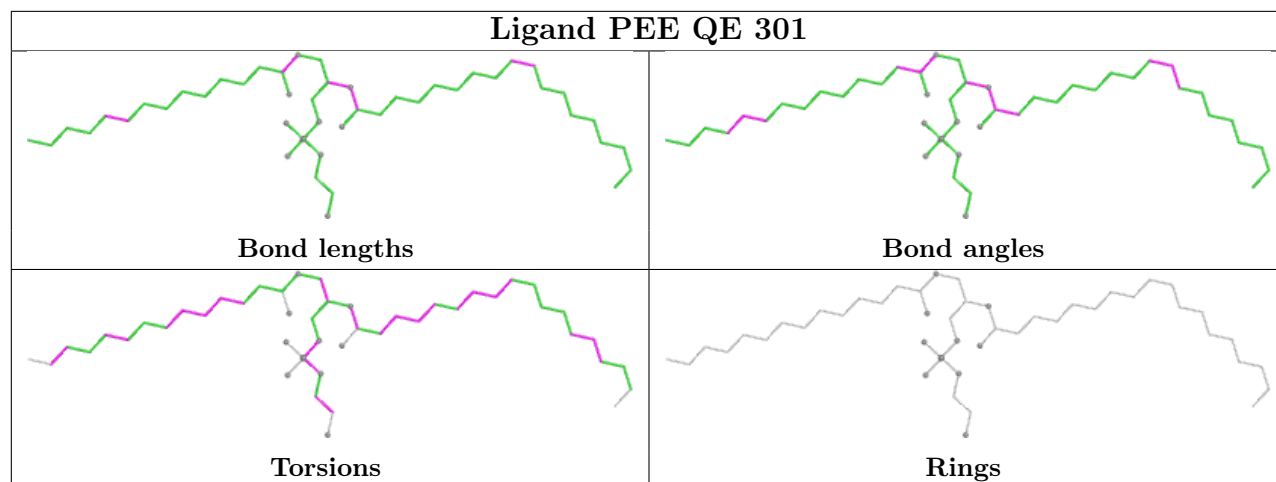
Ligand HEM Qc 403

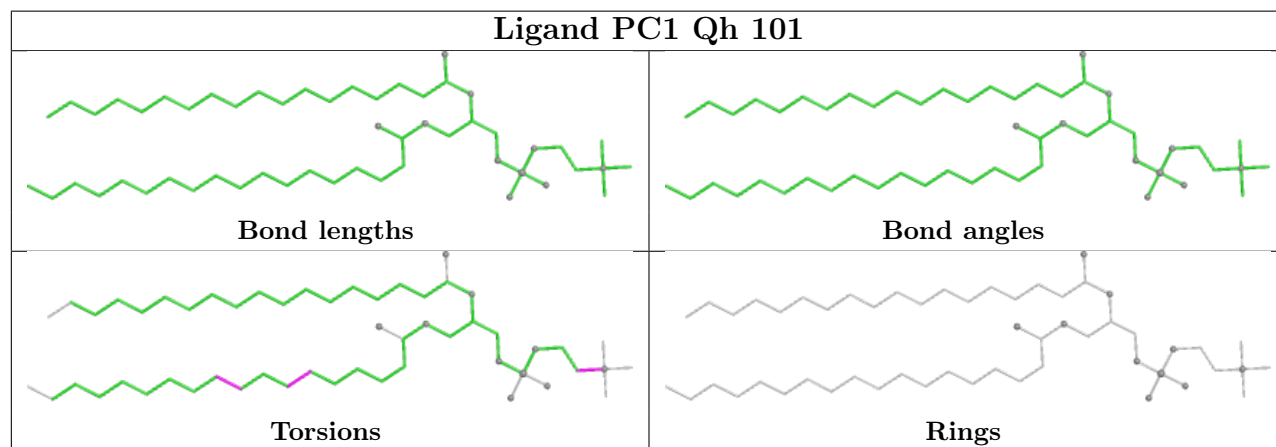
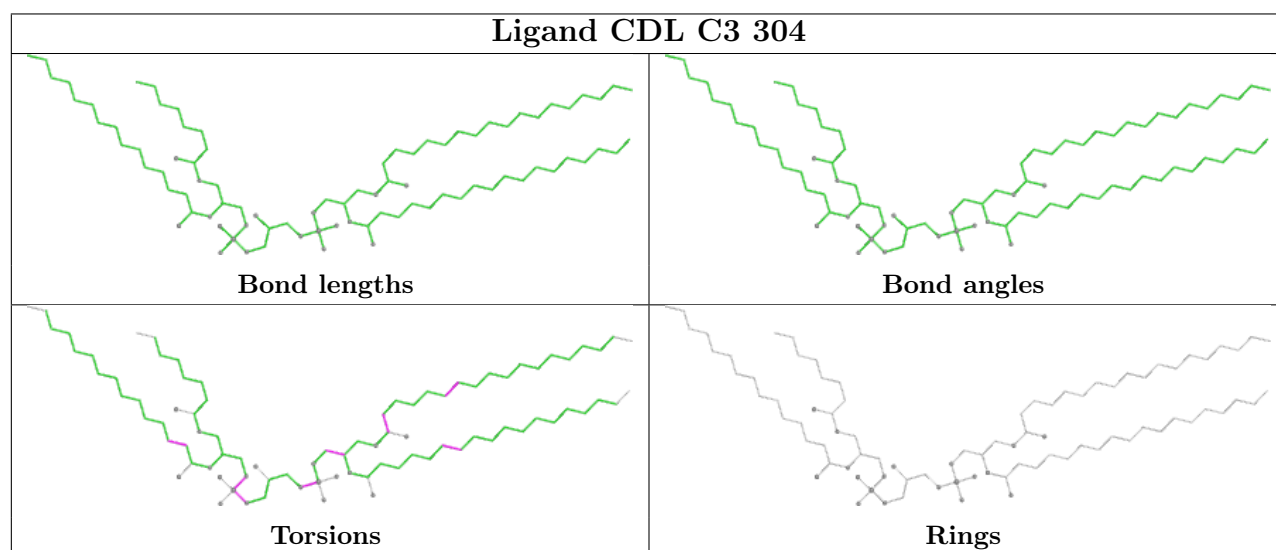
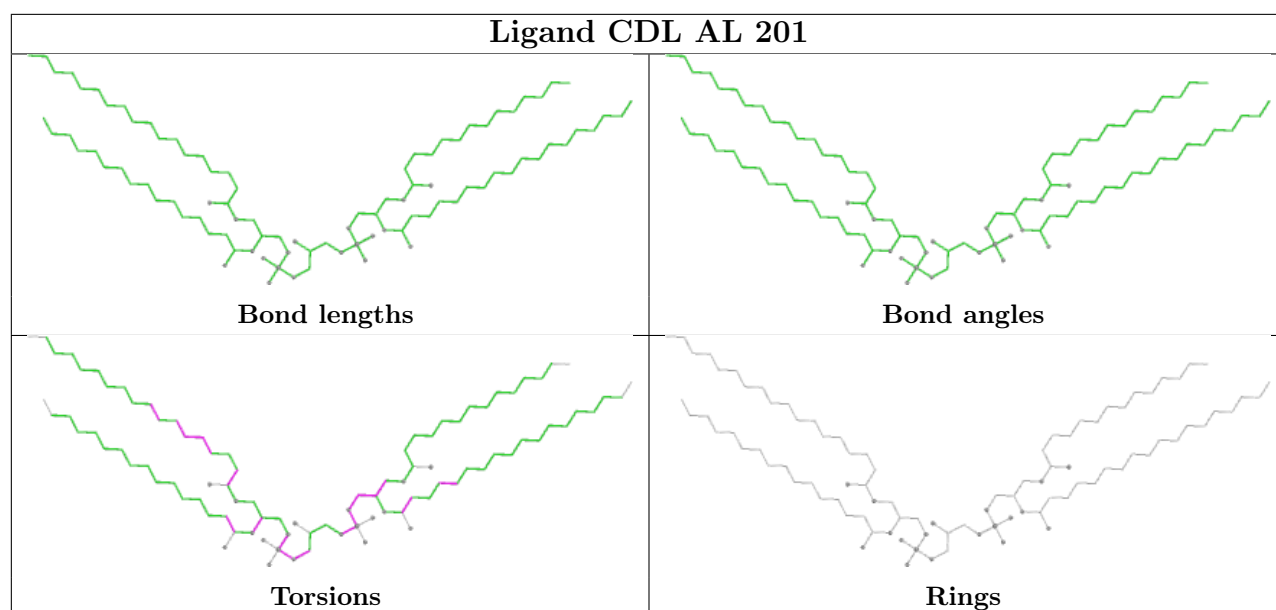


Ligand PC1 C1 608

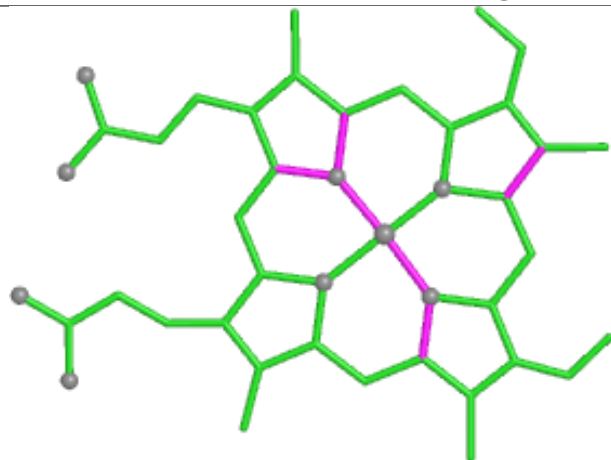




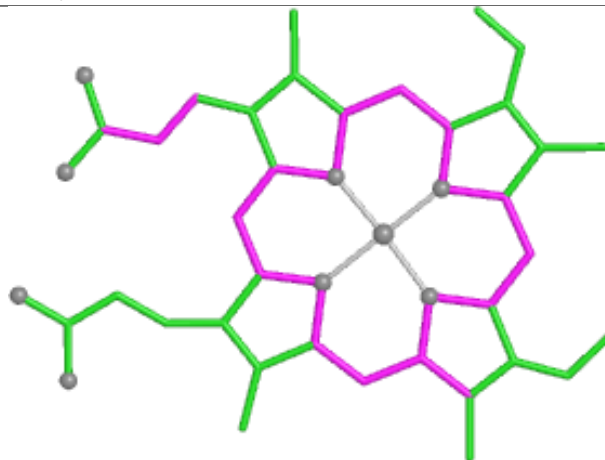




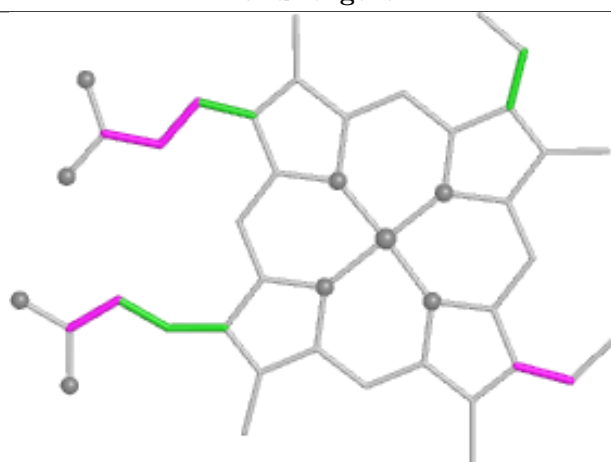
Ligand HEM QC 401



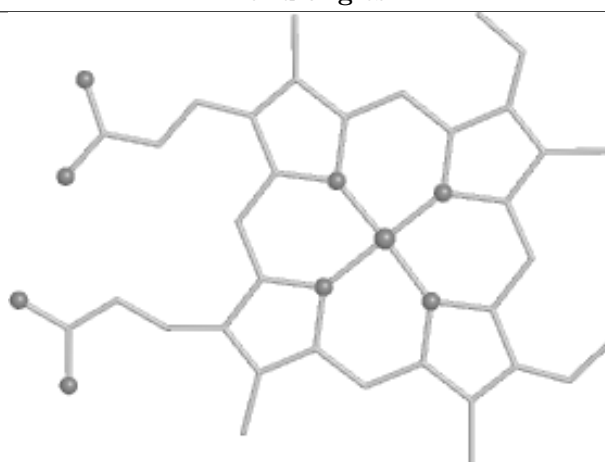
Bond lengths



Bond angles

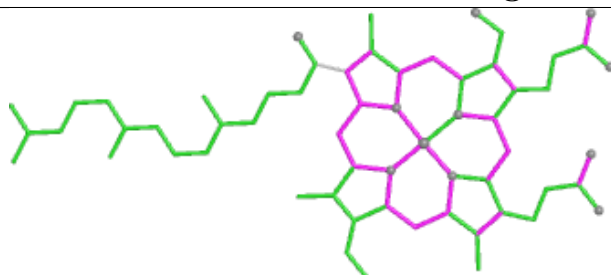


Torsions

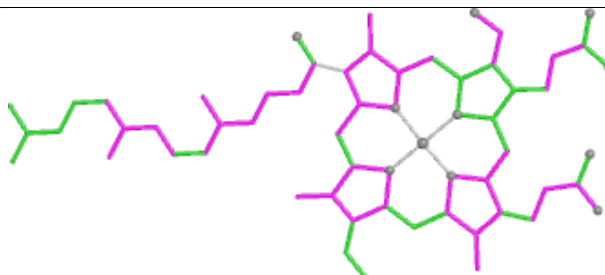


Rings

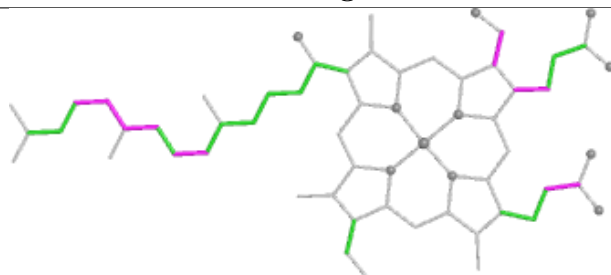
Ligand HEA C1 601



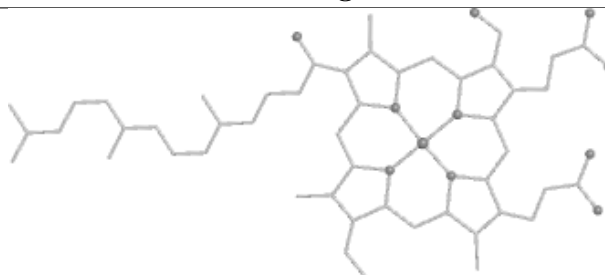
Bond lengths



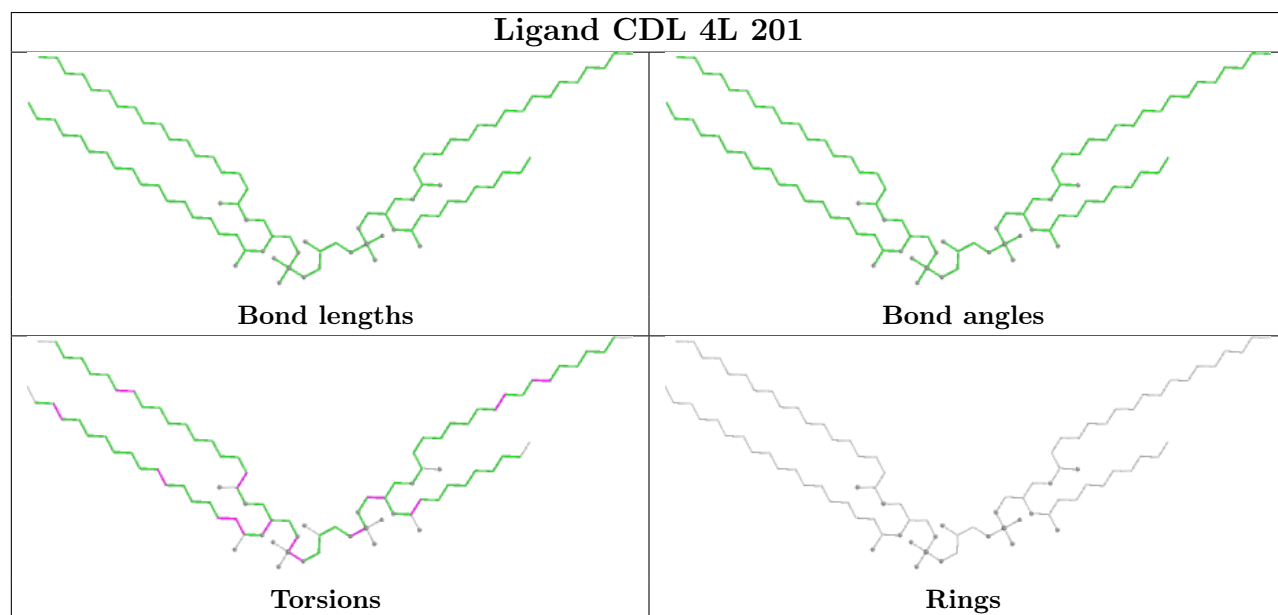
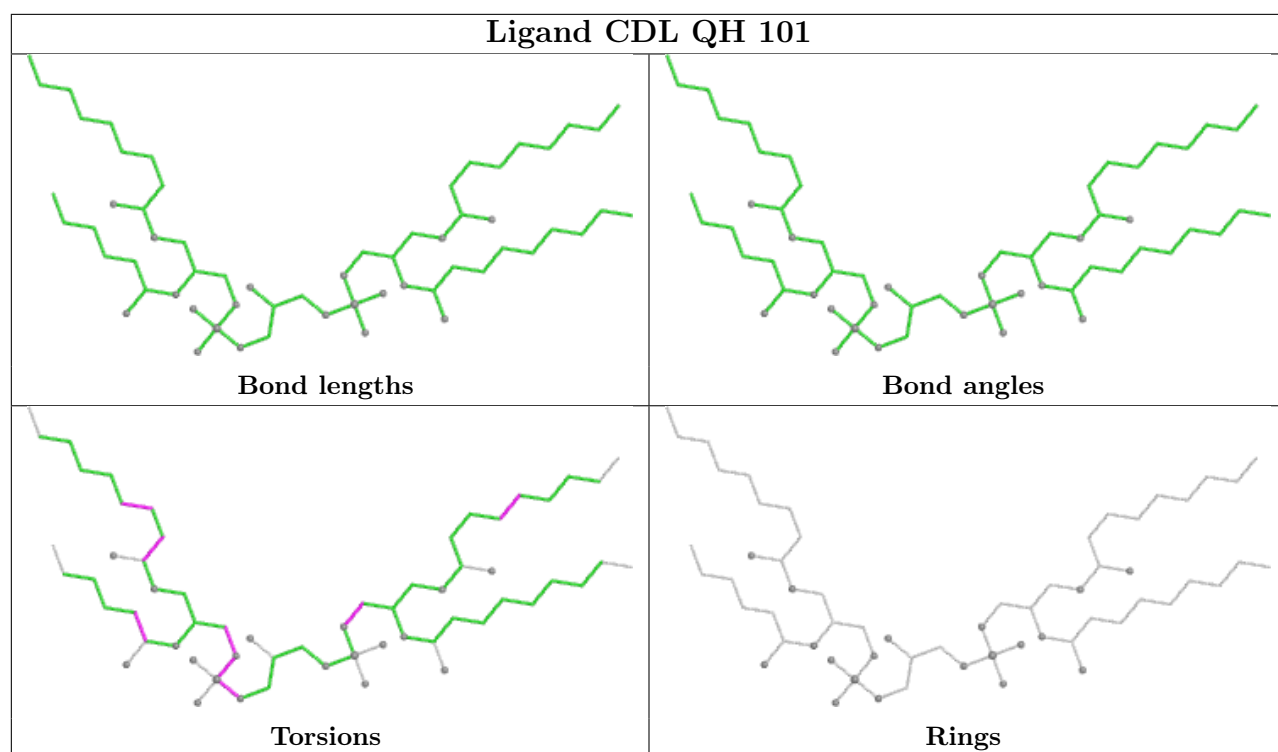
Bond angles

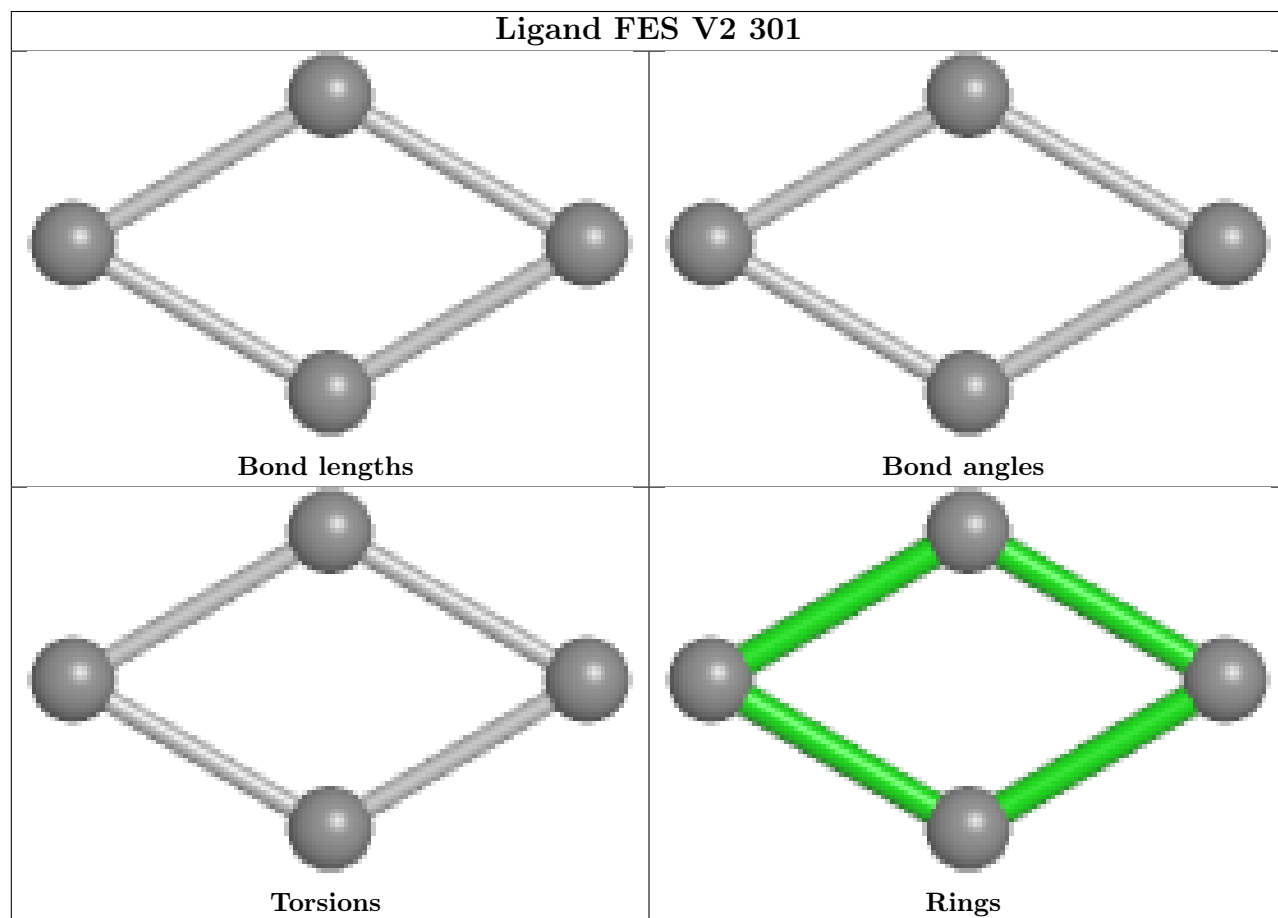
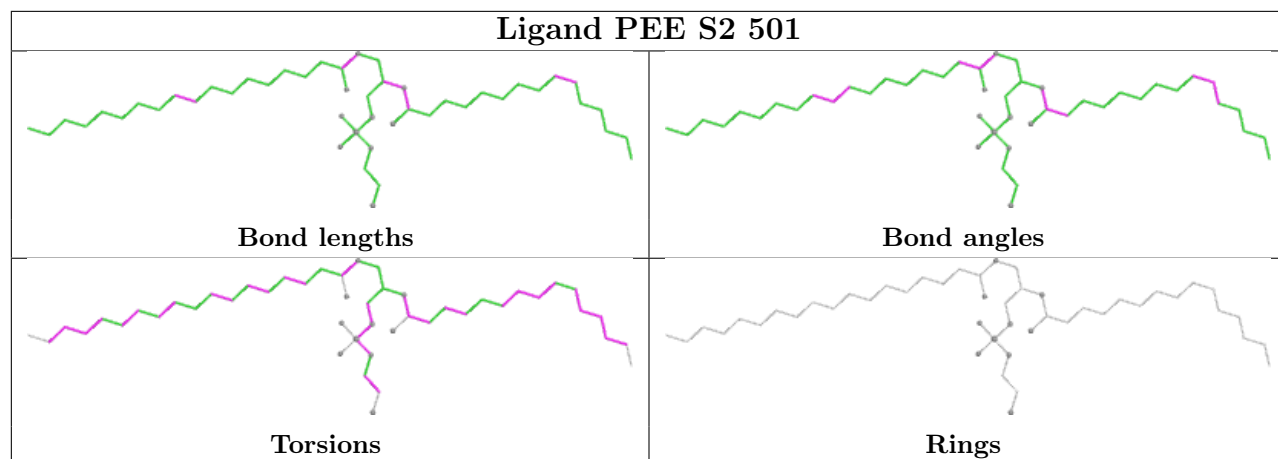


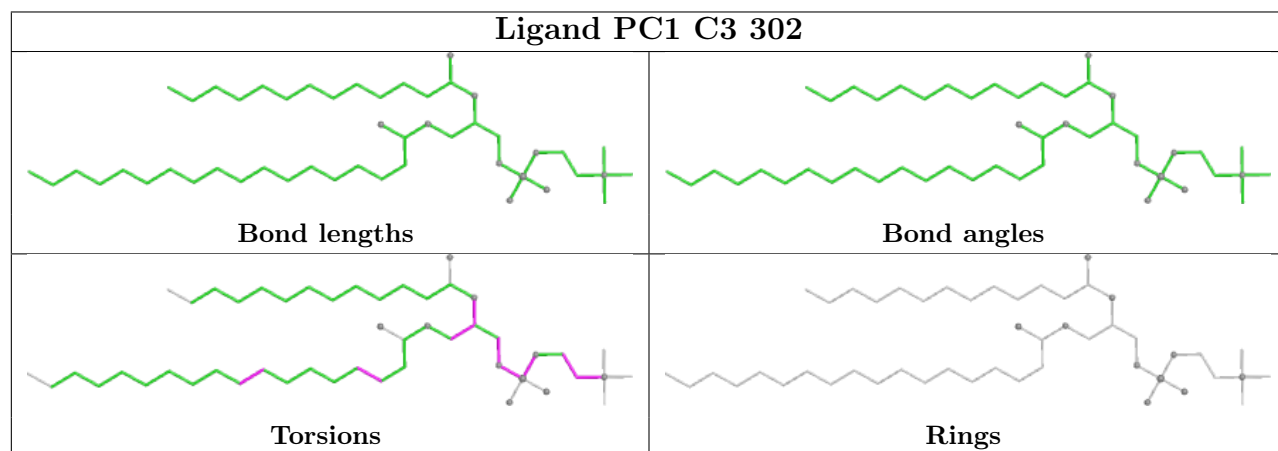
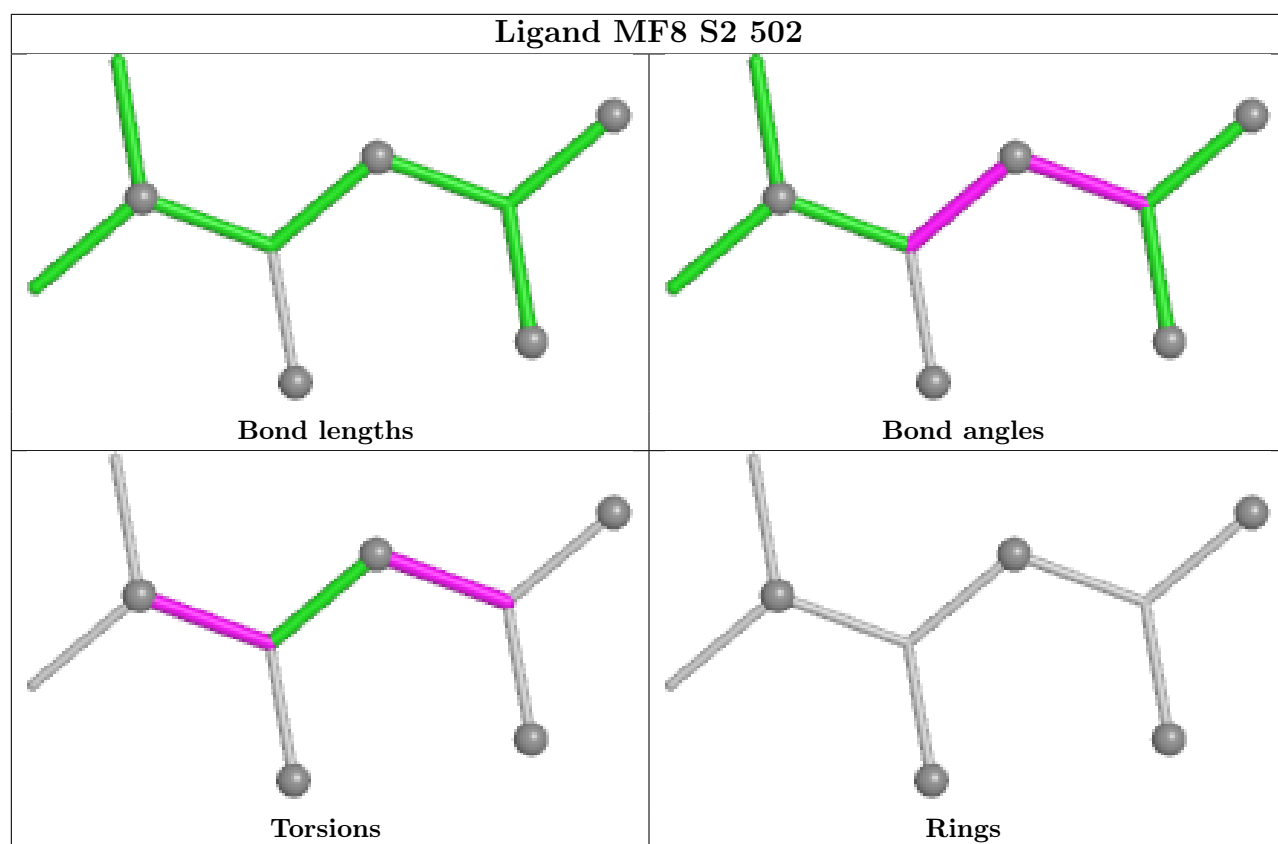
Torsions

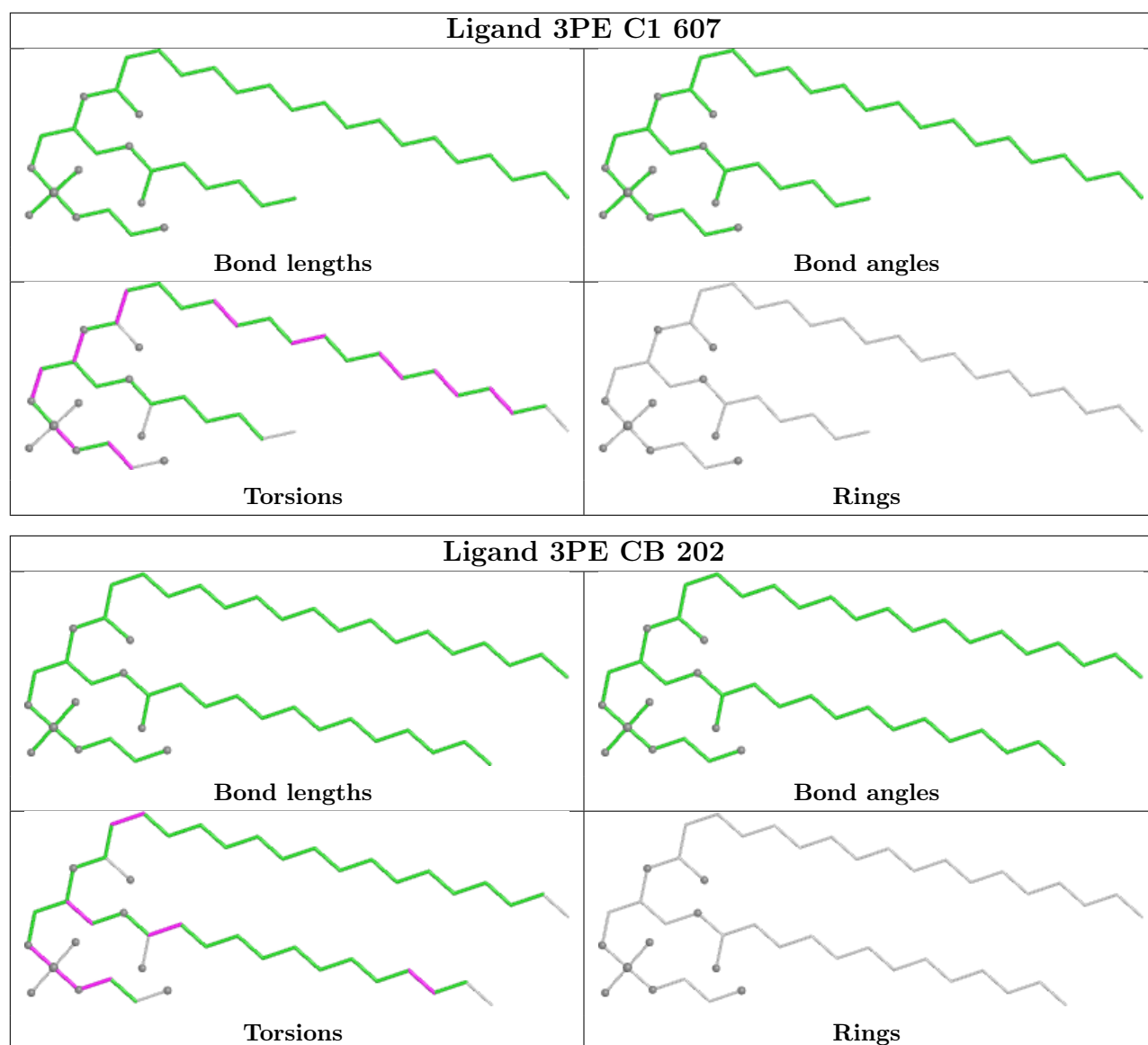


Rings

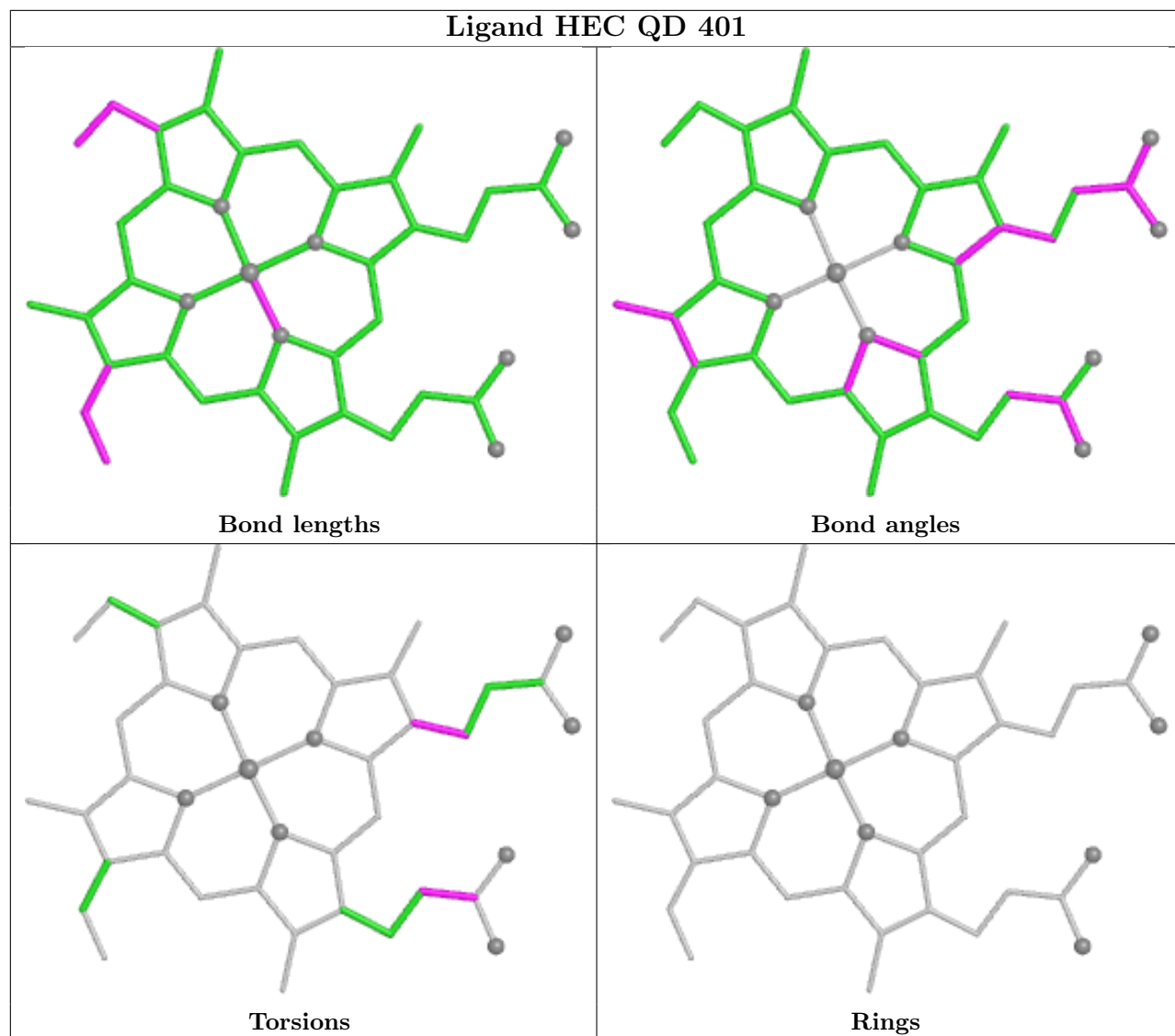




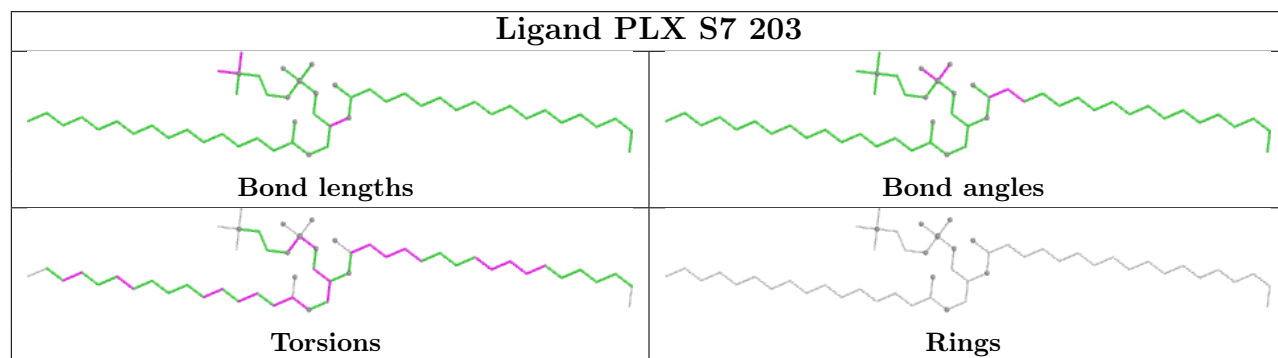


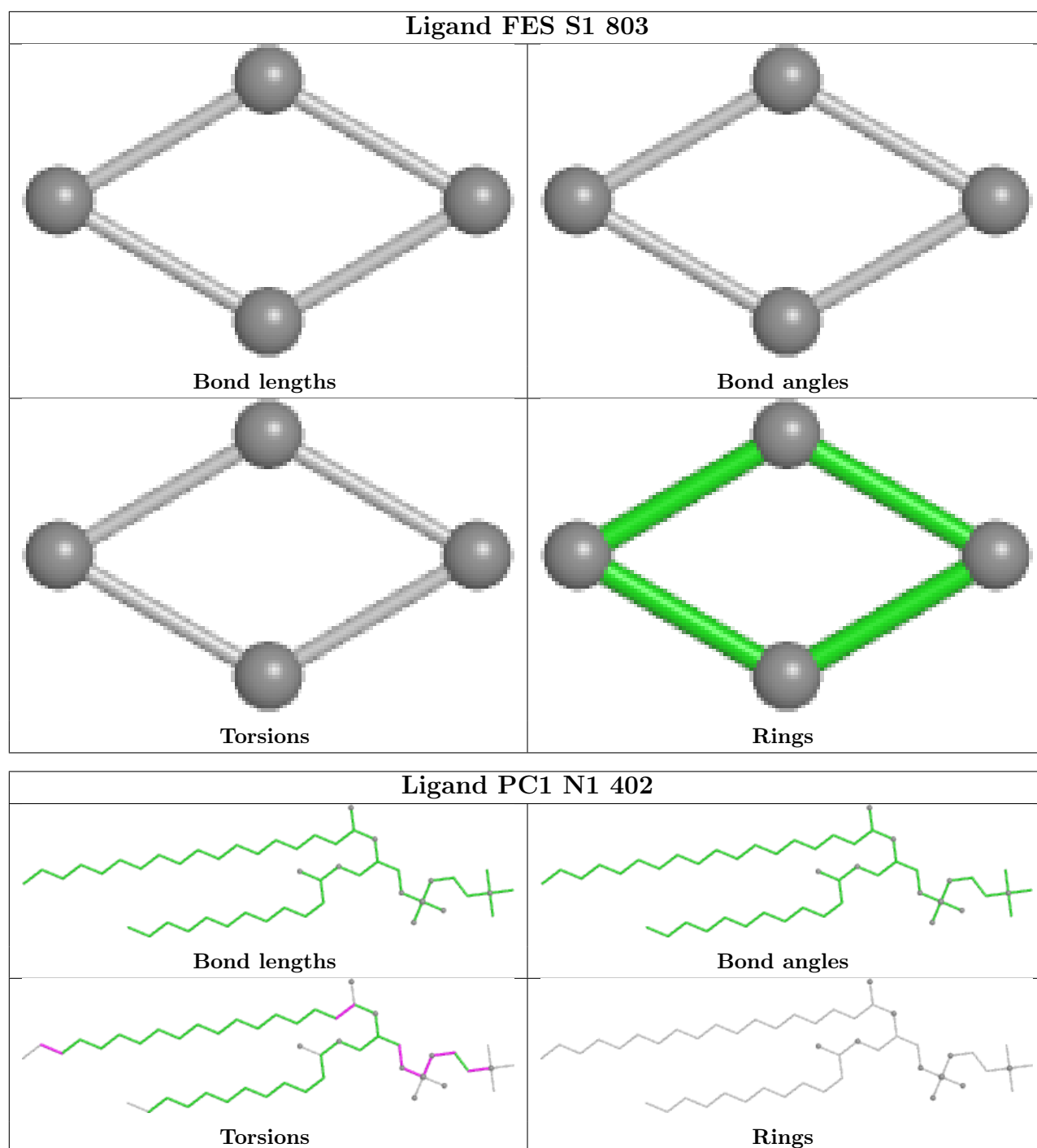


Ligand HEC QD 401



Ligand PLX S7 203





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

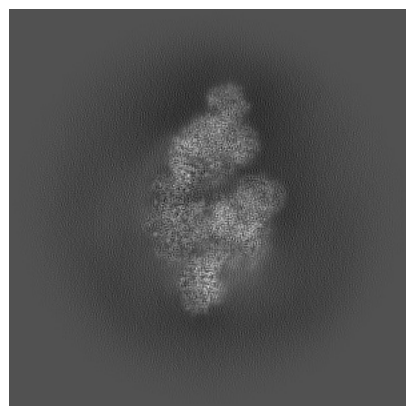
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60424. These allow visual inspection of the internal detail of the map and identification of artifacts.

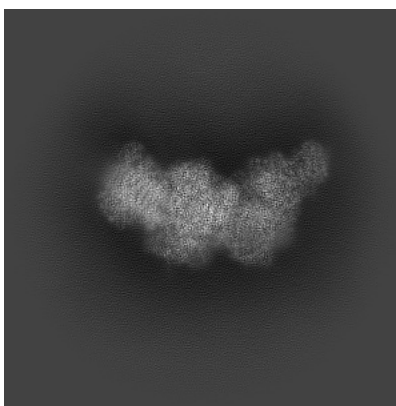
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

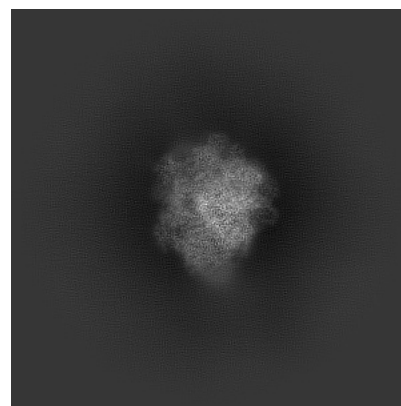
6.1.1 Primary map



X

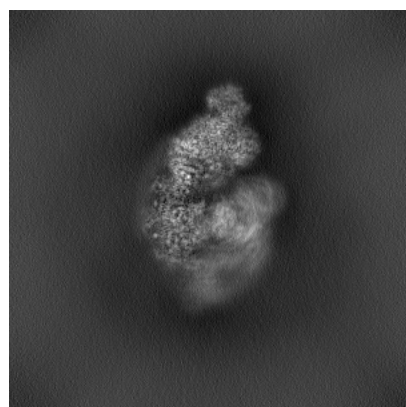


Y

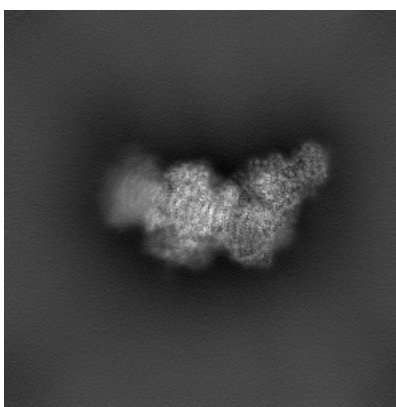


Z

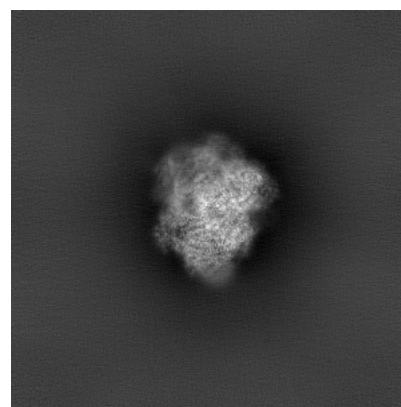
6.1.2 Raw map



X



Y

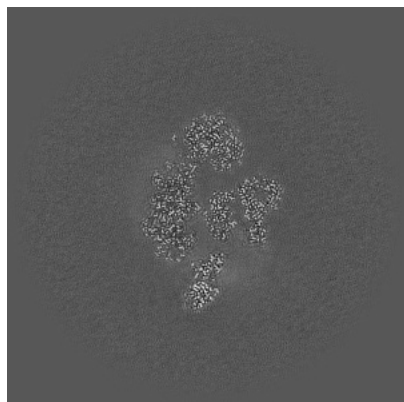


Z

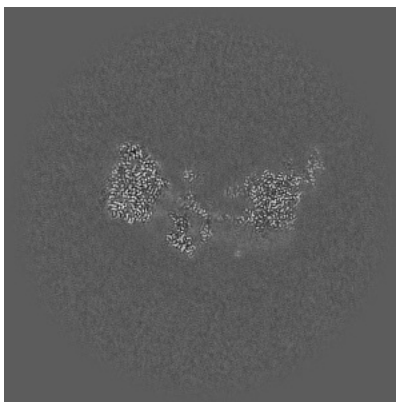
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

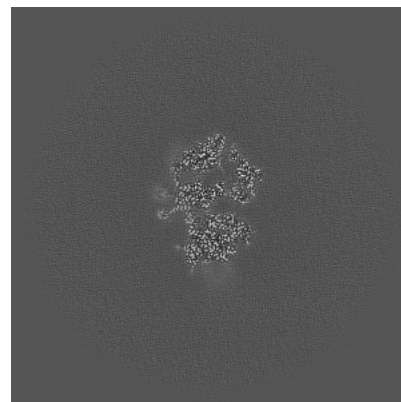
6.2.1 Primary map



X Index: 240

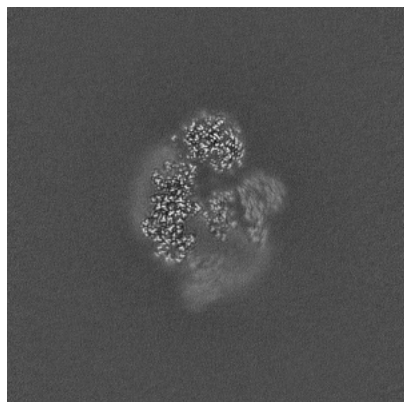


Y Index: 240

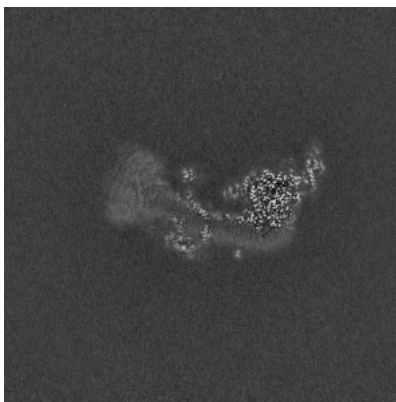


Z Index: 240

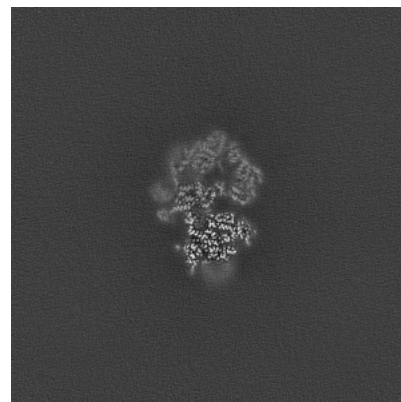
6.2.2 Raw map



X Index: 240



Y Index: 240

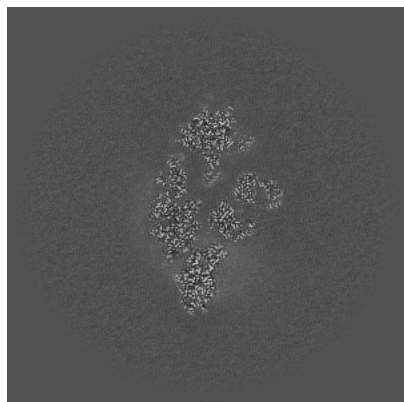


Z Index: 240

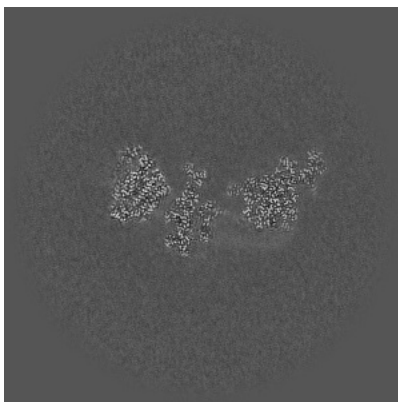
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

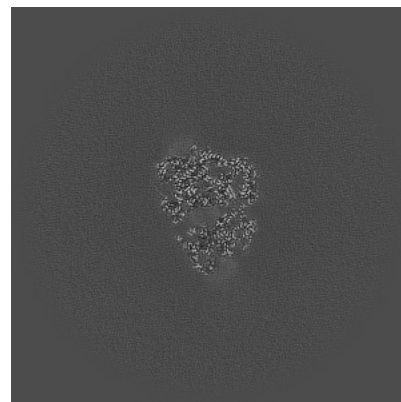
6.3.1 Primary map



X Index: 255

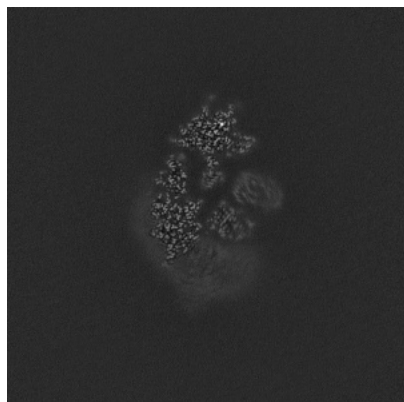


Y Index: 245

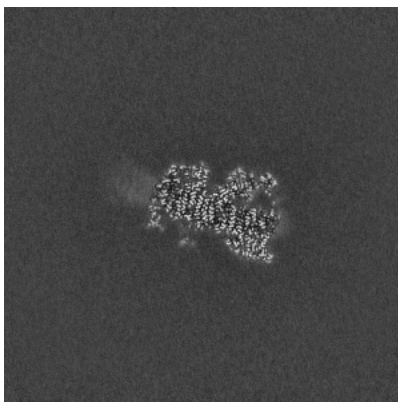


Z Index: 219

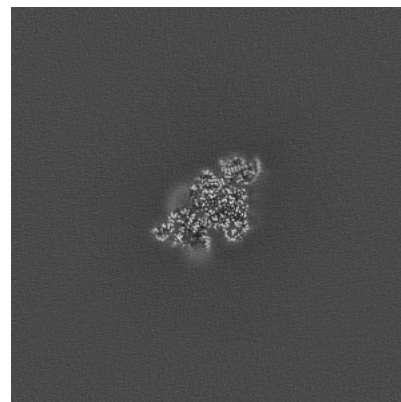
6.3.2 Raw map



X Index: 256



Y Index: 205

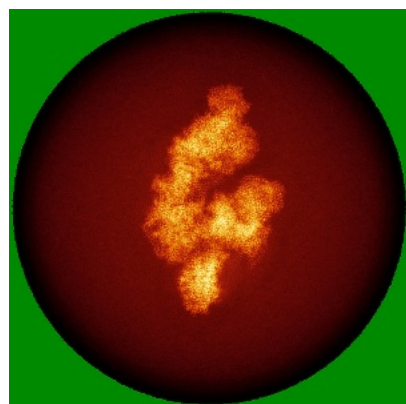


Z Index: 314

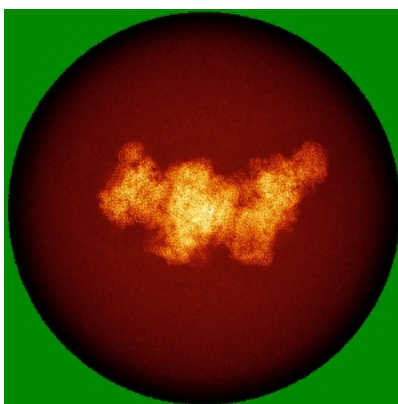
The images above show the largest variance slices of the map in three orthogonal directions.

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

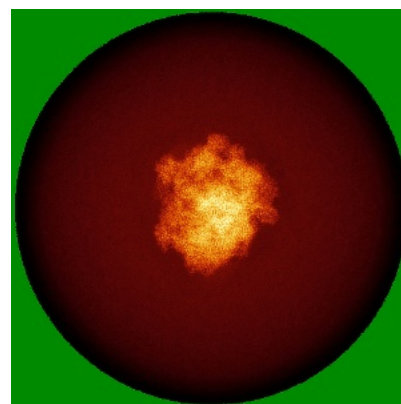
6.4.1 Primary map



X

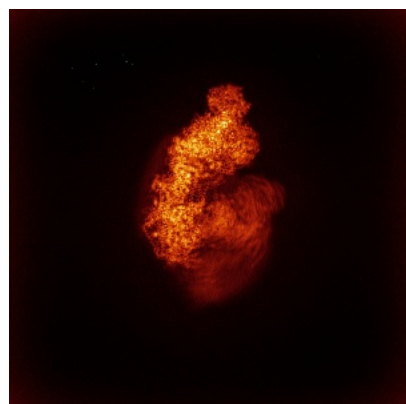


Y

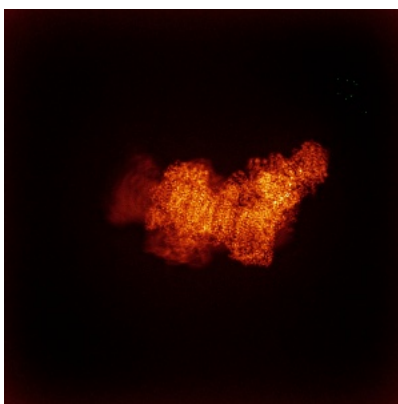


Z

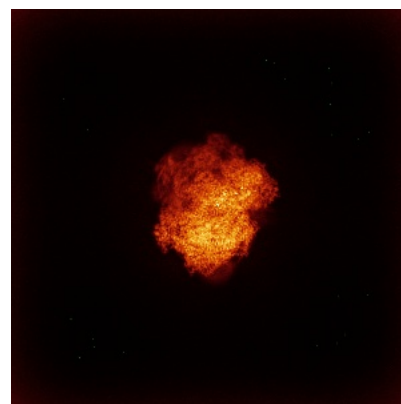
6.4.2 Raw map



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



X



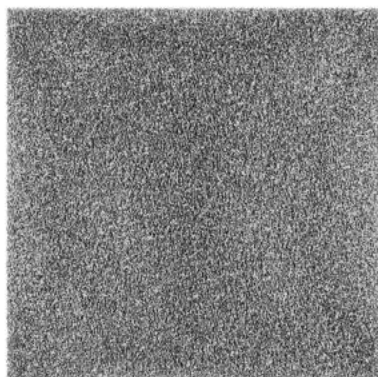
Y



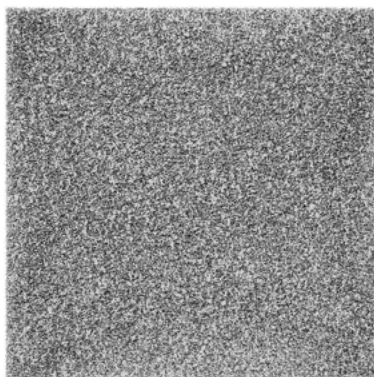
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

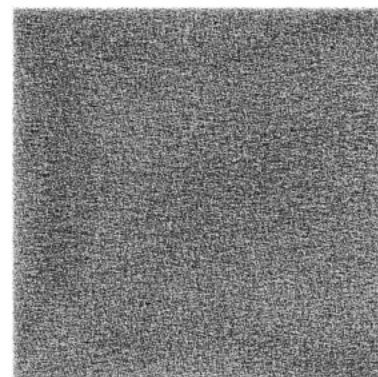
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

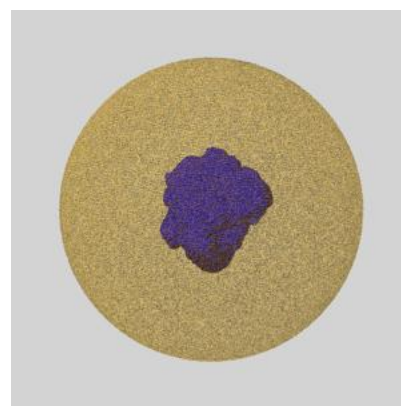
6.6.1 emd_60424_msk_1.map [i](#)



X



Y

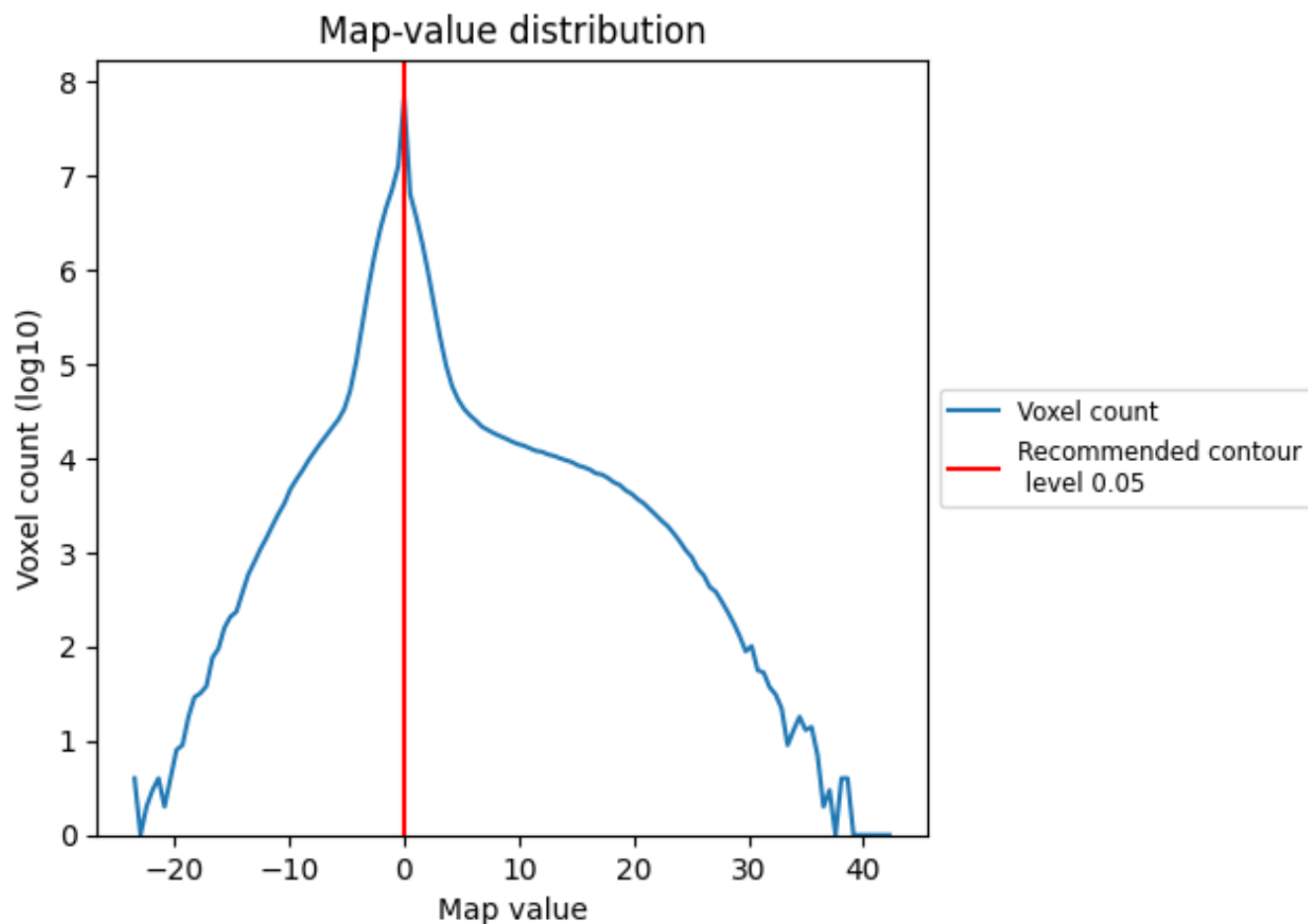


Z

7 Map analysis [i](#)

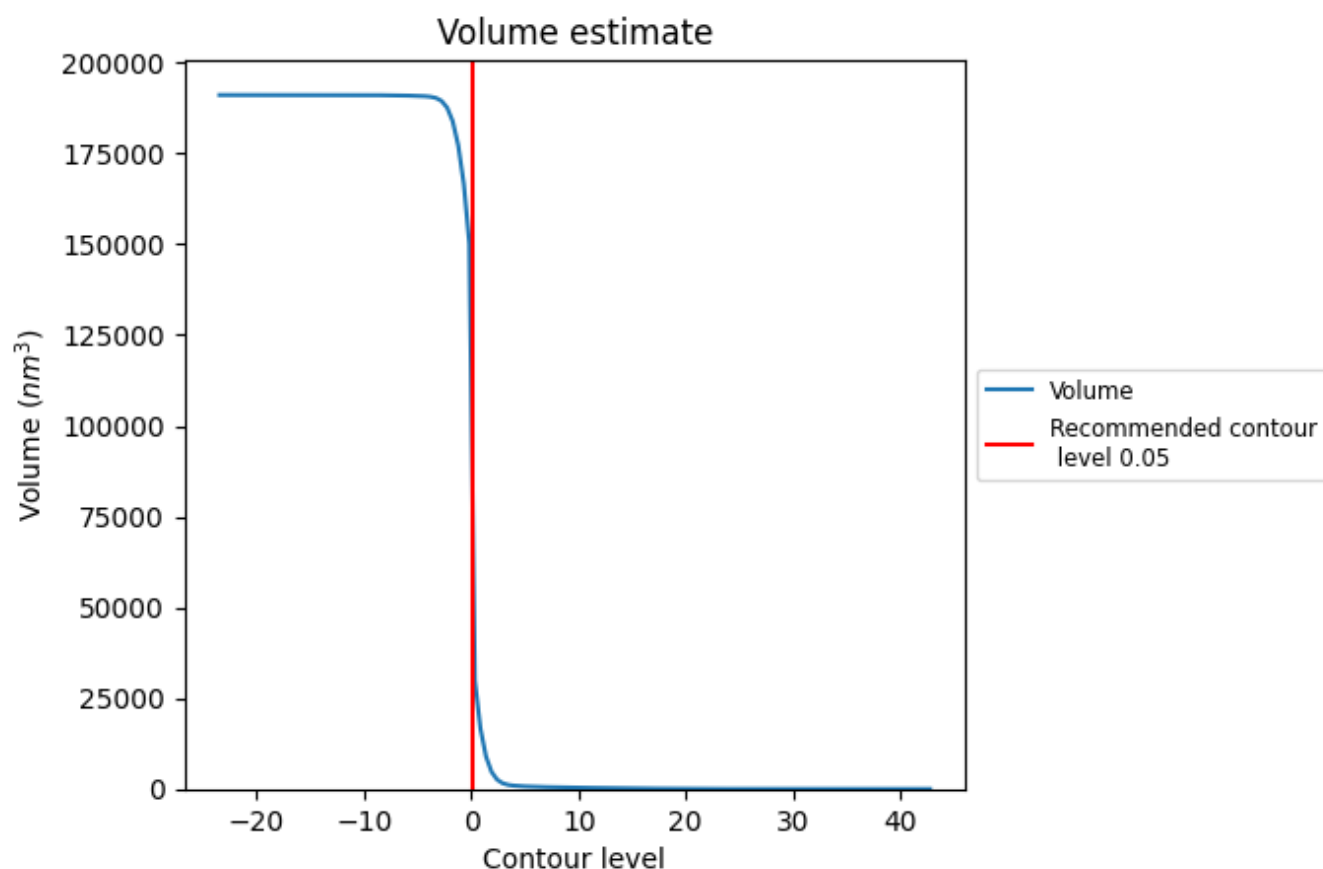
This section contains the results of statistical analysis of the map.

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.

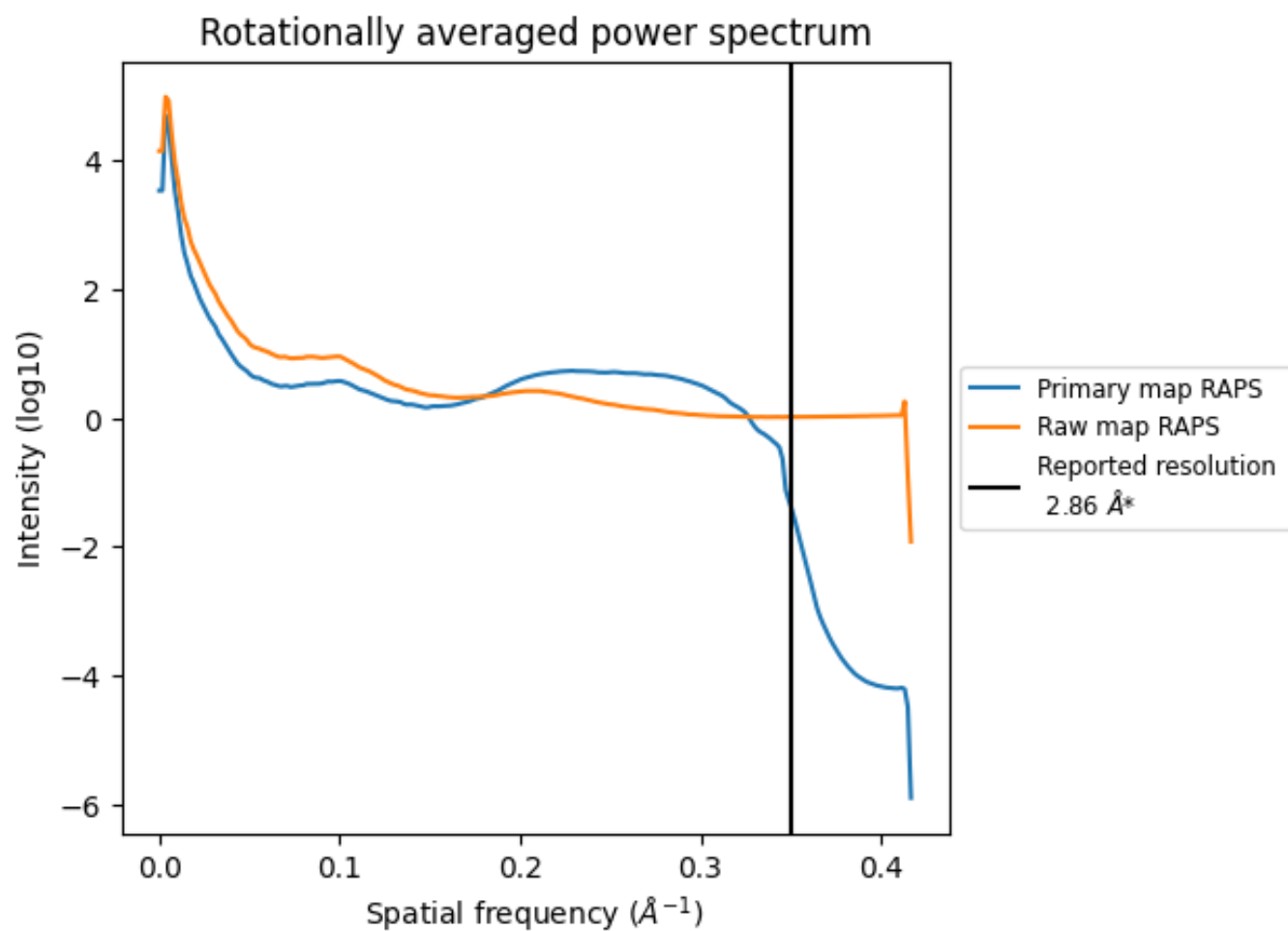
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 97381 nm³; this corresponds to an approximate mass of 87967 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 ⓘ

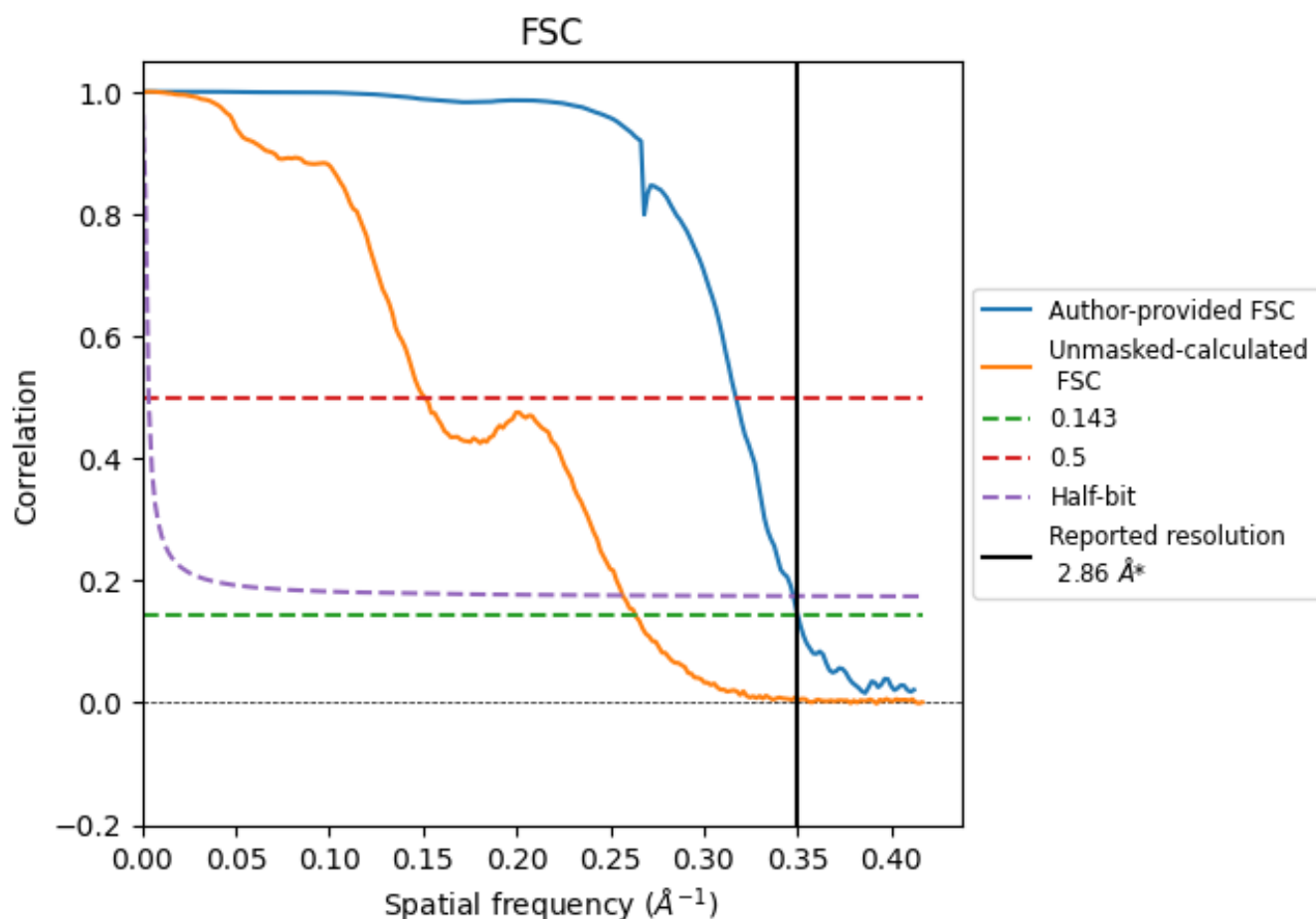


*Reported resolution corresponds to spatial frequency of 0.350 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.350 Å⁻¹

8.2 Resolution estimates [i](#)

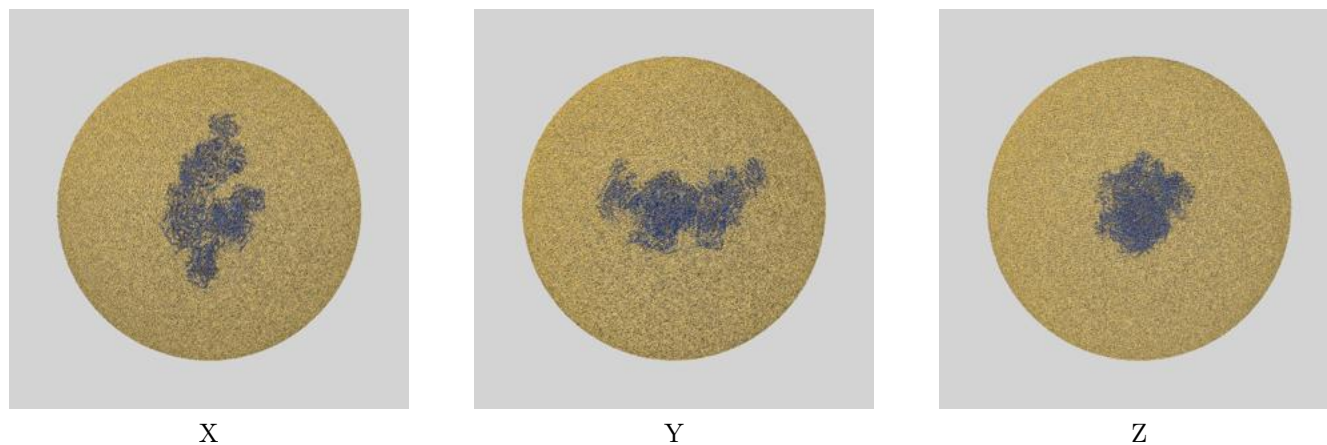
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.86	3.15	2.88
Unmasked-calculated*	3.80	6.63	3.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 2.86 by more than 10 %

9 Map-model fit [i](#)

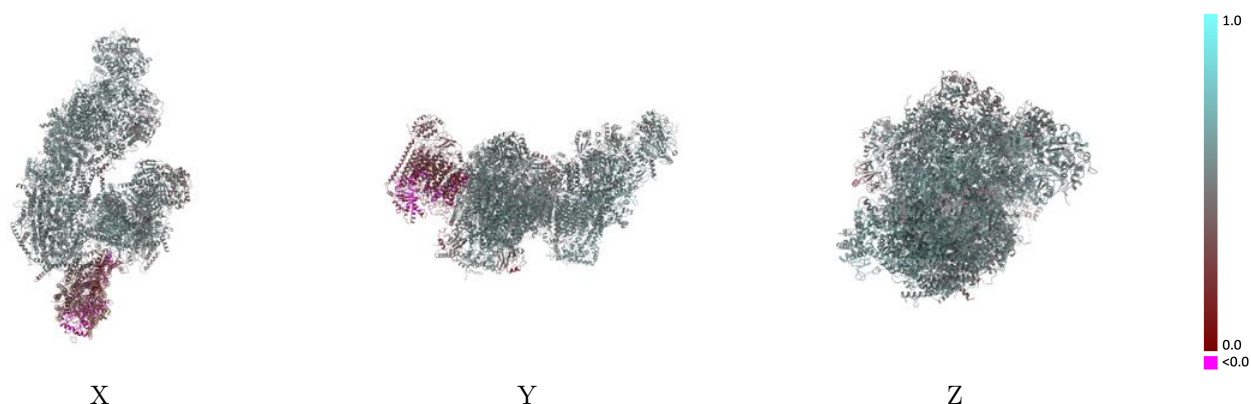
This section contains information regarding the fit between EMDB map EMD-60424 and PDB model 8ZSQ. Per-residue inclusion information can be found in [section 3](#) on [page 32](#).

9.1 Map-model overlay [i](#)



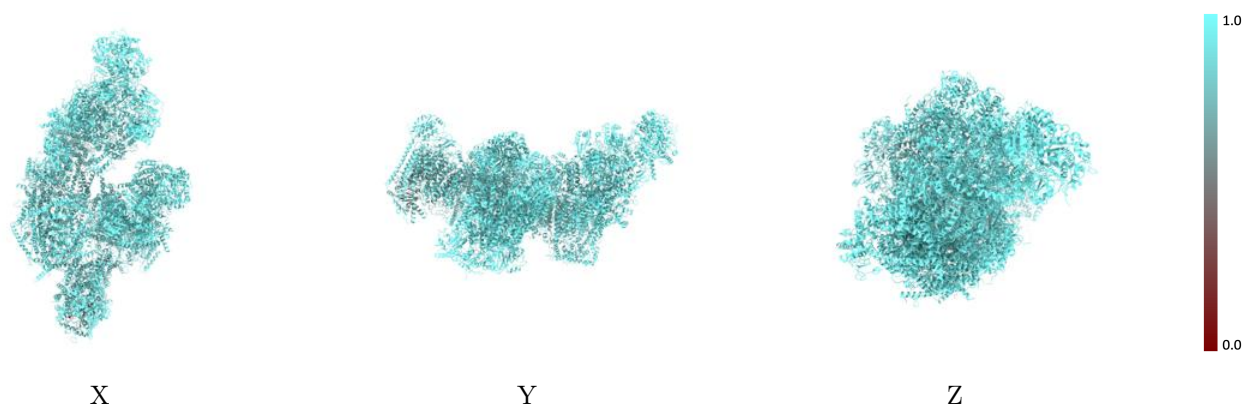
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



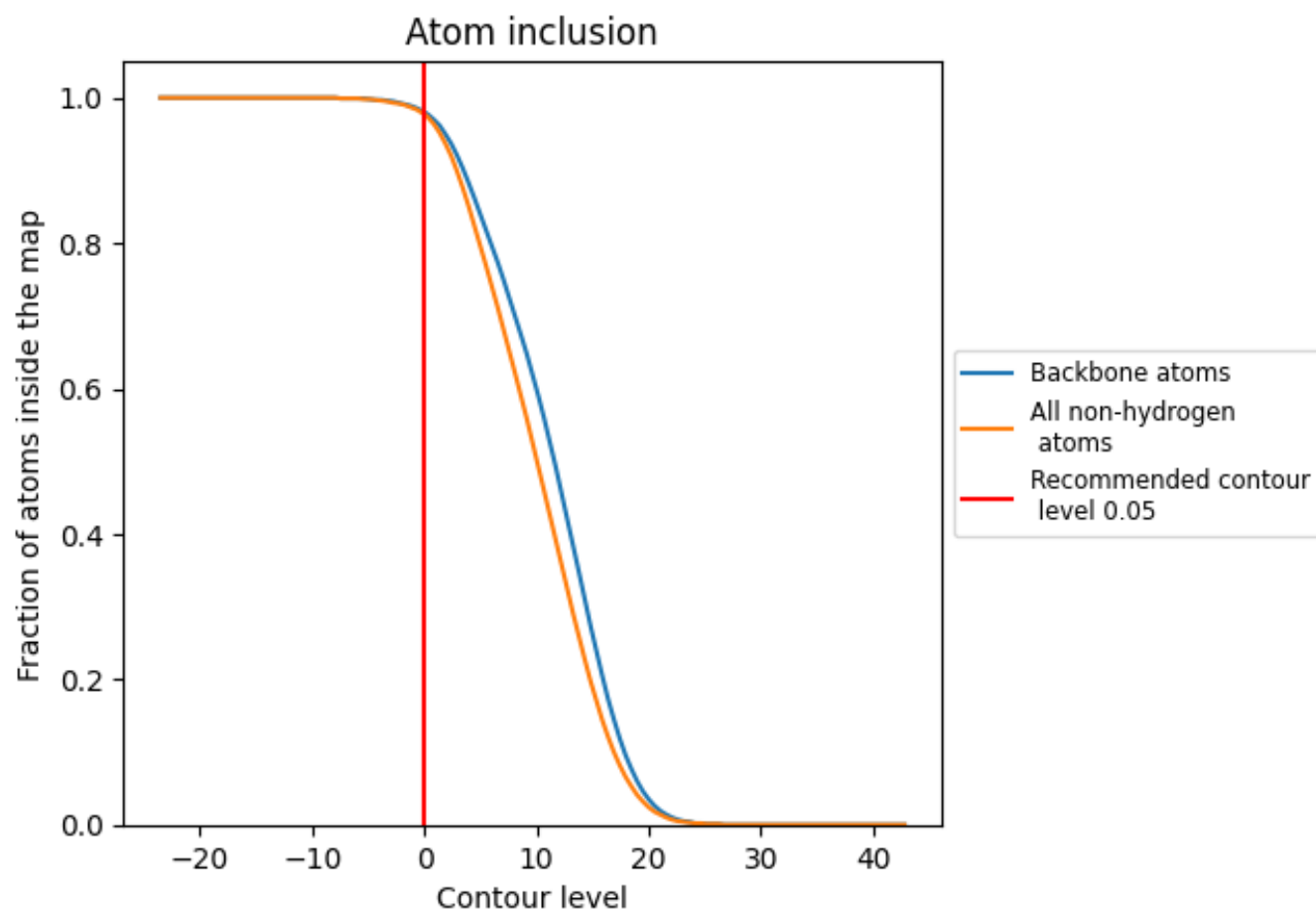
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9770	 0.5010
4L	 0.9980	 0.5900
5A	 0.9340	 0.3250
5B	 0.9410	 0.2880
6A	 0.8750	 0.1680
6B	 0.8540	 0.1040
6C	 0.8800	 0.2080
7A	 0.9620	 0.3680
7B	 0.9370	 0.2730
7C	 0.9260	 0.3160
8B	 0.9460	 0.3220
A1	 0.9980	 0.5820
A2	 0.9900	 0.4670
A3	 1.0000	 0.5660
A5	 0.9910	 0.5260
A6	 0.9930	 0.5300
A7	 0.9990	 0.5370
A8	 0.9990	 0.5720
A9	 0.9970	 0.5550
AB	 0.9910	 0.4550
AC	 0.9840	 0.5280
AK	 0.9940	 0.5360
AL	 0.9990	 0.5640
AM	 0.9980	 0.5510
AN	 0.9970	 0.5710
B1	 0.9920	 0.5020
B2	 0.9950	 0.5290
B3	 0.9940	 0.4910
B4	 0.9960	 0.5560
B5	 0.9910	 0.5400
B6	 0.9930	 0.4920
B7	 0.9950	 0.5250
B8	 0.9950	 0.5680
B9	 0.9940	 0.5480
BK	 0.9820	 0.5200



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BL	 0.9880	 0.5140
C1	 0.8590	 0.2160
C2	 0.7950	 0.1000
C3	 0.8800	 0.2140
C4	 0.9010	 0.2690
CA	 0.9960	 0.5340
CB	 0.9950	 0.5620
N1	 0.9940	 0.5840
N2	 0.9950	 0.5890
N3	 0.9990	 0.5810
N4	 0.9900	 0.5550
N5	 0.9920	 0.5520
N6	 0.9900	 0.5500
QA	 0.9880	 0.5170
QB	 0.9920	 0.5650
QC	 0.9960	 0.5870
QD	 0.9970	 0.5640
QE	 0.9890	 0.4590
QF	 0.9930	 0.4580
QG	 0.9840	 0.5110
QH	 0.9800	 0.5020
QI	 0.9840	 0.5180
QJ	 0.9880	 0.5250
QK	 0.9960	 0.5060
Qa	 0.9790	 0.5100
Qb	 0.9840	 0.5160
Qc	 0.9870	 0.5500
Qd	 0.9890	 0.5270
Qe	 0.9800	 0.4240
Qf	 0.9900	 0.5140
Qg	 0.9880	 0.5720
Qh	 0.9960	 0.5710
Qi	 0.9980	 0.5700
Qj	 0.9910	 0.5600
S1	 0.9880	 0.5210
S2	 0.9940	 0.5710
S3	 0.9950	 0.5640
S4	 0.9920	 0.5480
S5	 0.9970	 0.5620
S6	 0.9990	 0.5600
S7	 0.9940	 0.5760
S8	 0.9990	 0.5880

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
V1	 0.9920	 0.5350
V2	 0.9950	 0.5350
V3	 0.9970	 0.5290