



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 11:07 PM JST

PDB ID : 8ZSN / pdb_00008zsn
EMDB ID : EMD-60421
Title : Respirasome closed state 1 in the absence of biguanide (SC-ApoC)
Authors : Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.
Deposited on : 2024-06-05
Resolution : 2.88 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:

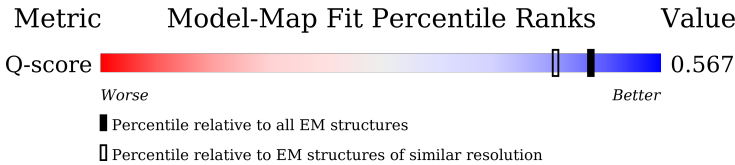
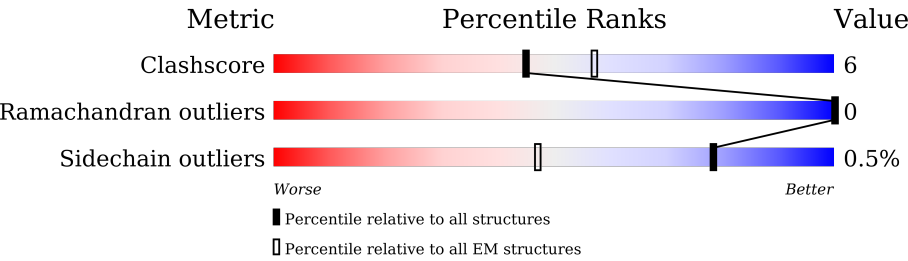
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 2.88 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.



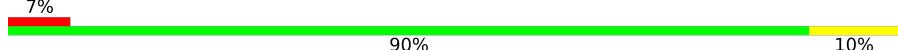
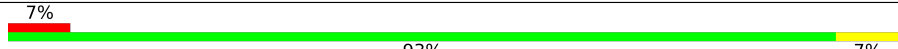
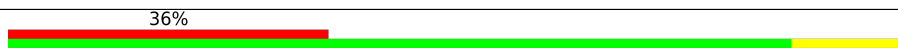
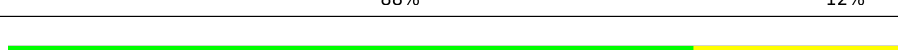
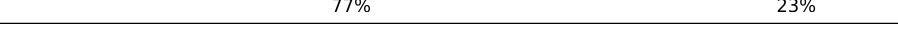
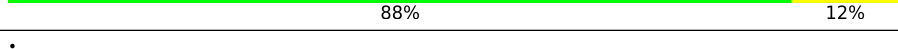
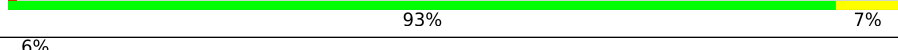
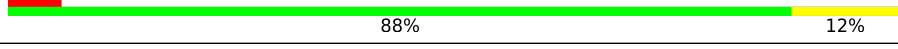
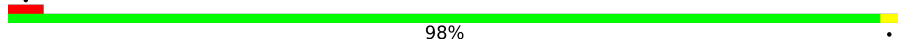
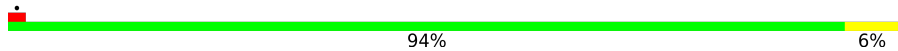
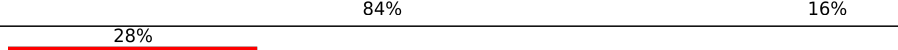
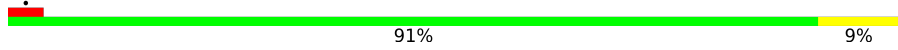
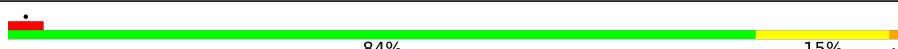
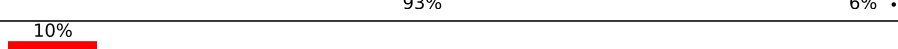
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12111 (2.38 - 3.38)

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	
2	5A	102	
3	5B	95	
4	6A	75	

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

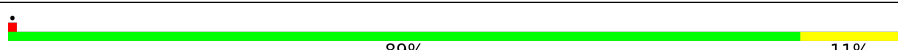
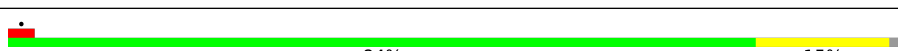
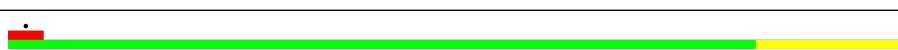
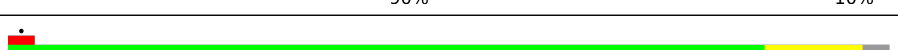
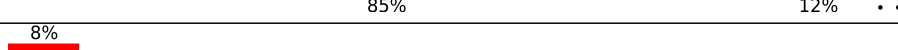
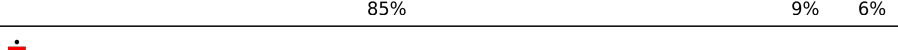
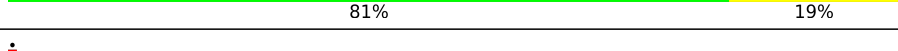
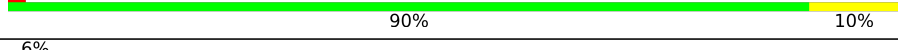
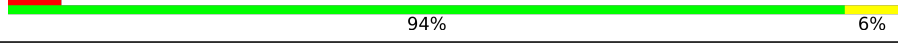
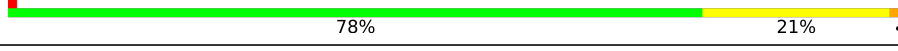
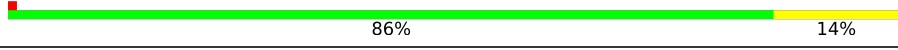
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Mol	Chain	Length	Quality of chain
29	B6	126	
30	B7	125	
31	B8	156	
32	B9	178	
33	BK	174	
34	BL	99	
35	C1	514	
36	C2	228	
37	C3	260	
38	C4	138	
39	CA	49	
40	CB	121	
41	N1	318	
42	N2	347	
43	N3	115	
44	N4	459	
45	N5	603	
46	N6	174	
47	QA	419	
47	Qa	419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

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Mol	Chain	Length	Quality of chain
50	Qd	241	
51	QE	196	
51	Qe	196	
52	QF	67	
52	Qf	67	
53	QG	101	
53	Qg	101	
54	QH	79	
54	Qh	79	
55	QI	62	
55	Qi	62	
56	QJ	52	
56	Qj	52	
57	QK	78	
58	S1	689	
59	S2	430	
60	S3	208	
61	S4	124	
62	S5	105	
63	S6	96	
64	S7	156	
65	S8	176	
66	V1	431	
67	V2	217	
68	V3	42	

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
82	HEC	QD	401	X	-	-	-
82	HEC	Qd	401	X	-	-	-

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 117287 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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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	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 Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	QK	73	Total	C	N	O	S	0	0
			520	328	98	92	2		

- Molecule 58 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

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

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

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

- Molecule 60 is a protein called Complex I-30kD.

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

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

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

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

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

- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

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

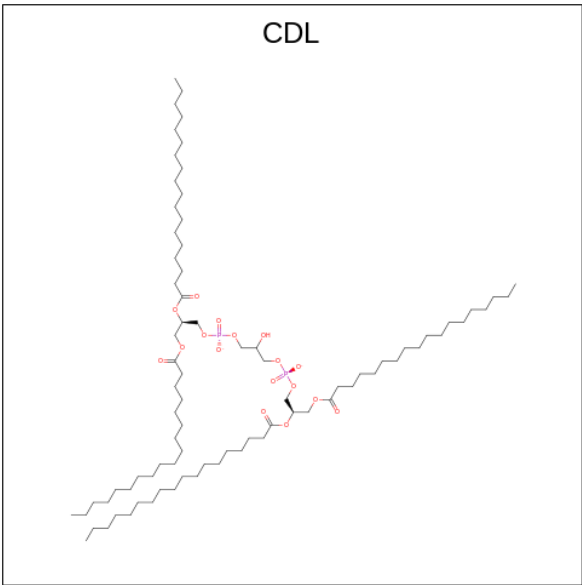
- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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

- Molecule 68 is a protein called NADH:ubiquinone oxidoreductase subunit V3.

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

- Molecule 69 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
69	4L	1	Total	C	O	P	0
			92	73	17	2	
69	6A	1	Total	C	O	P	0
			83	64	17	2	
69	A7	1	Total	C	O	P	0
			51	32	17	2	
69	AK	1	Total	C	O	P	0
			68	49	17	2	
69	AL	1	Total	C	O	P	0
			94	75	17	2	
69	AL	1	Total	C	O	P	0
			80	61	17	2	
69	B5	1	Total	C	O	P	0
			100	81	17	2	
69	CB	1	Total	C	O	P	0
			83	64	17	2	
69	N1	1	Total	C	O	P	0
			78	59	17	2	
69	N4	1	Total	C	O	P	0
			100	81	17	2	
69	N4	1	Total	C	O	P	0
			62	43	17	2	
69	N5	1	Total	C	O	P	0
			89	70	17	2	
69	N5	1	Total	C	O	P	0
			100	81	17	2	
69	QB	1	Total	C	O	P	0
			64	45	17	2	

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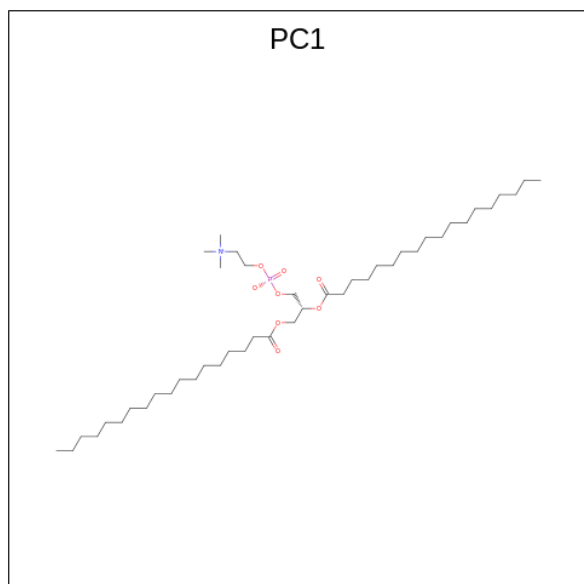
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Mol	Chain	Residues	Atoms				AltConf
69	QD	1	Total	C	O	P	0
			58	39	17	2	
69	QH	1	Total	C	O	P	0
			64	45	17	2	
69	Qb	1	Total	C	O	P	0
			64	45	17	2	
69	Qc	1	Total	C	O	P	0
			61	42	17	2	
69	Qh	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 70 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
70	5B	1	Total	Zn	0
			1	1	
70	S6	1	Total	Zn	0
			1	1	

- Molecule 71 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



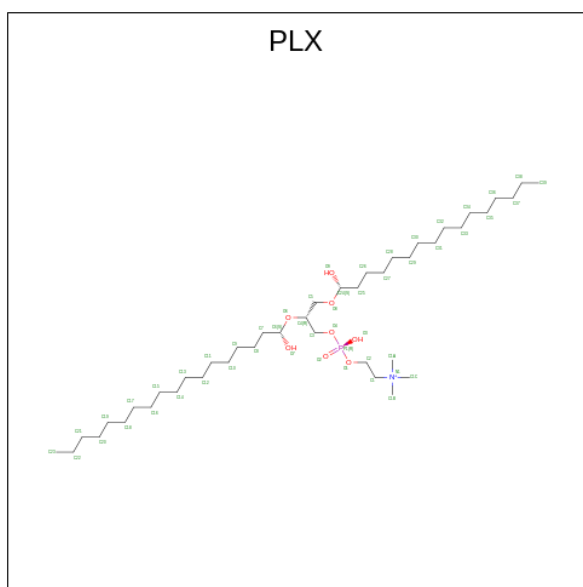
Mol	Chain	Residues	Atoms					AltConf
71	6A	1	Total	C	N	O	P	0
			45	35	1	8	1	

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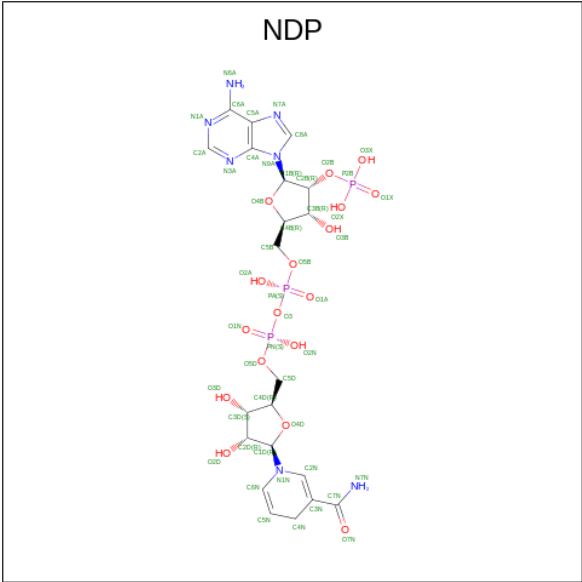
Mol	Chain	Residues	Atoms					AltConf
71	6A	1	Total	C	N	O	P	0
			38	28	1	8	1	
71	C1	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	C1	1	Total	C	N	O	P	0
			33	23	1	8	1	
71	C1	1	Total	C	N	O	P	0
			46	36	1	8	1	
71	C3	1	Total	C	N	O	P	0
			44	34	1	8	1	
71	C3	1	Total	C	N	O	P	0
			49	39	1	8	1	
71	C3	1	Total	C	N	O	P	0
			50	40	1	8	1	
71	N1	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	N1	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	N3	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	QB	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	Qb	1	Total	C	N	O	P	0
			48	38	1	8	1	
71	Qc	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	Qh	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 72 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).



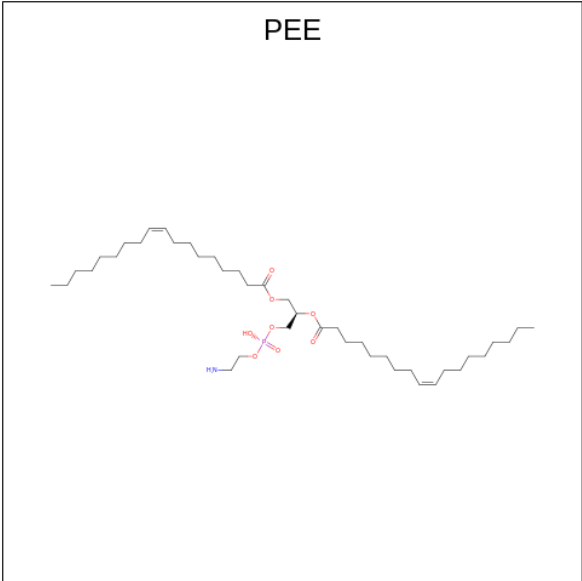
Mol	Chain	Residues	Atoms					AltConf
72	6C	1	Total	C	N	O	P	0
			43	33	1	8	1	
72	AL	1	Total	C	N	O	P	0
			47	37	1	8	1	
72	AM	1	Total	C	N	O	P	0
			52	42	1	8	1	
72	B5	1	Total	C	N	O	P	0
			52	42	1	8	1	
72	CB	1	Total	C	N	O	P	0
			52	42	1	8	1	
72	N3	1	Total	C	N	O	P	0
			52	42	1	8	1	
72	N4	1	Total	C	N	O	P	0
			52	42	1	8	1	
72	QB	1	Total	C	N	O	P	0
			46	36	1	8	1	
72	QI	1	Total	C	N	O	P	0
			52	42	1	8	1	
72	S7	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 73 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
73	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 74 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
74	A9	1	Total	C	N	O	P	0
			39	29	1	8	1	
74	AL	1	Total	C	N	O	P	0
			49	39	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
74	C3	1	Total	C	N	O	P	0
			51	41	1	8	1	
74	N1	1	Total	C	N	O	P	0
			31	21	1	8	1	
74	N3	1	Total	C	N	O	P	0
			51	41	1	8	1	
74	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
74	N5	1	Total	C	N	O	P	0
			40	30	1	8	1	
74	N5	1	Total	C	N	O	P	0
			51	41	1	8	1	
74	QB	1	Total	C	N	O	P	0
			34	24	1	8	1	
74	QC	1	Total	C	N	O	P	0
			40	30	1	8	1	
74	QE	1	Total	C	N	O	P	0
			47	37	1	8	1	
74	QJ	1	Total	C	N	O	P	0
			51	41	1	8	1	
74	Qc	1	Total	C	N	O	P	0
			42	32	1	8	1	
74	Qd	1	Total	C	N	O	P	0
			24	14	1	8	1	
74	S2	1	Total	C	N	O	P	0
			45	35	1	8	1	
74	S8	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 75 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



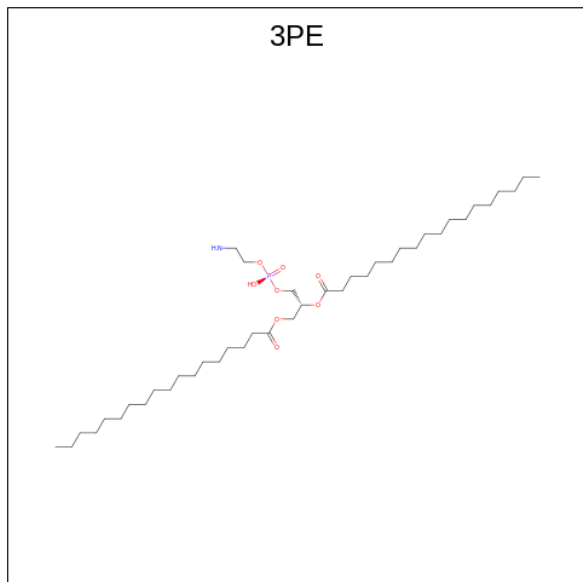
Mol	Chain	Residues	Atoms						AltConf
75	AB	1	Total 36	C 25	N 2	O 7	P 1	S 1	0
75	AC	1	Total 36	C 25	N 2	O 7	P 1	S 1	0

- Molecule 76 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



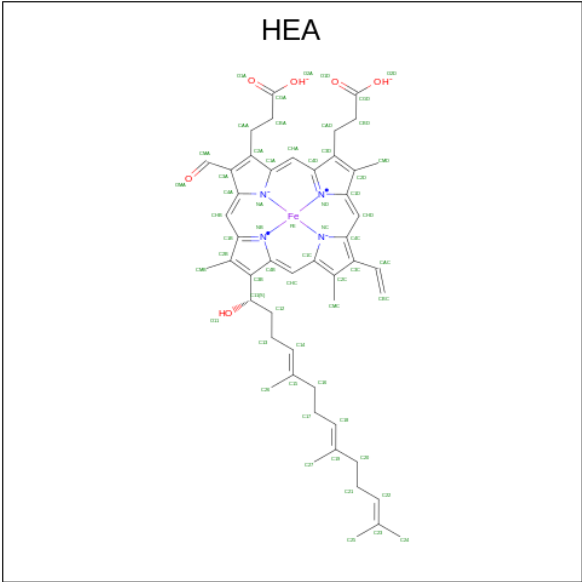
Mol	Chain	Residues	Atoms					AltConf
76	AK	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 77 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
77	B8	1	Total	C	N	O	P	0
			32	22	1	8	1	
77	C1	1	Total	C	N	O	P	0
			45	35	1	8	1	
77	C1	1	Total	C	N	O	P	0
			46	36	1	8	1	
77	CA	1	Total	C	N	O	P	0
			46	36	1	8	1	
77	CB	1	Total	C	N	O	P	0
			48	38	1	8	1	
77	N5	1	Total	C	N	O	P	0
			38	28	1	8	1	
77	QE	1	Total	C	N	O	P	0
			44	34	1	8	1	
77	QJ	1	Total	C	N	O	P	0
			34	24	1	8	1	
77	Qc	1	Total	C	N	O	P	0
			48	38	1	8	1	
77	Qj	1	Total	C	N	O	P	0
			29	19	1	8	1	
77	S7	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 78 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

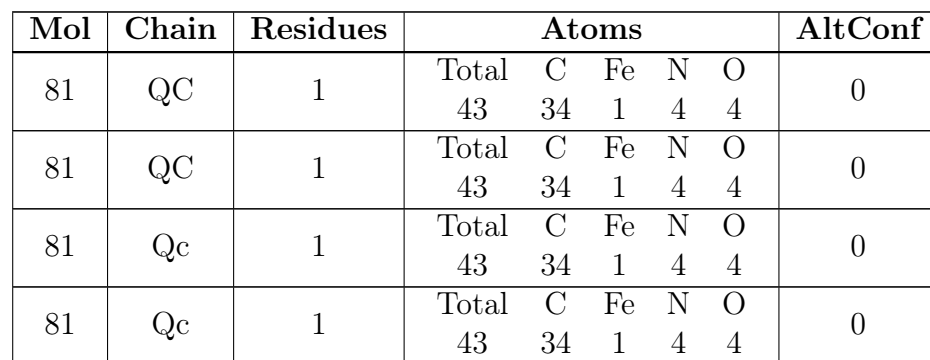
- Molecule 79 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

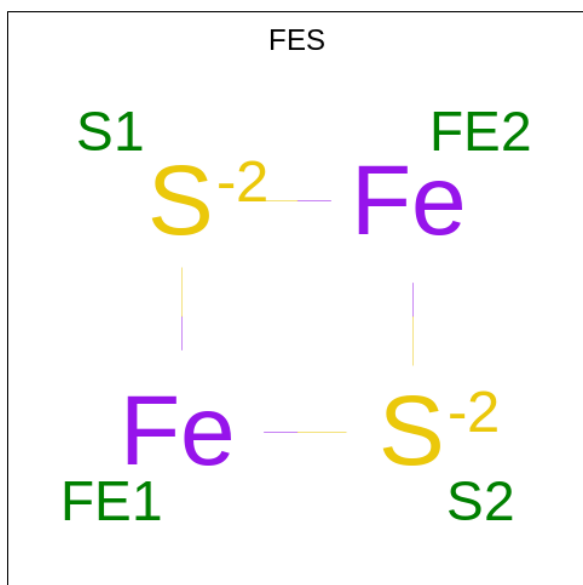
- Molecule 81 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



- [illegible]

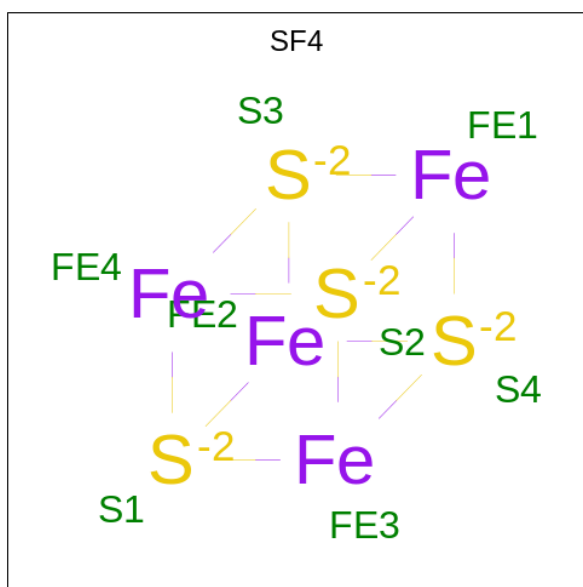
Mol	Chain	Residues	Atoms					AltConf
82	QD	1	Total 43	C 34	Fe 1	N 4	O 4	0
82	Qd	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 83 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



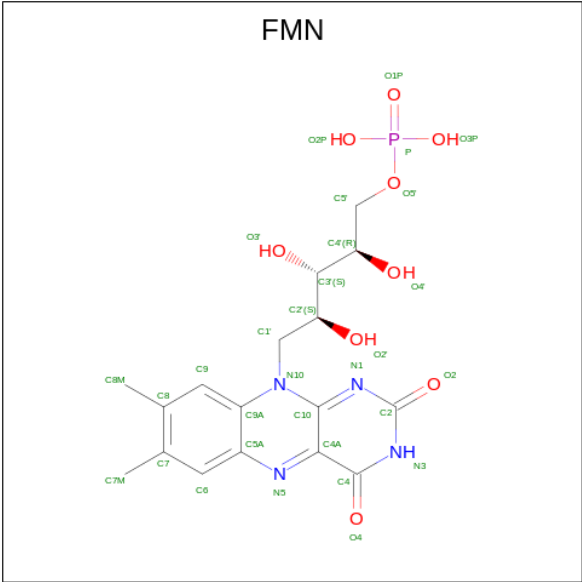
Mol	Chain	Residues	Atoms			AltConf
83	QE	1	Total	Fe	S	0
			4	2	2	
83	Qe	1	Total	Fe	S	0
			4	2	2	
83	S1	1	Total	Fe	S	0
			4	2	2	
83	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 84 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 85 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).

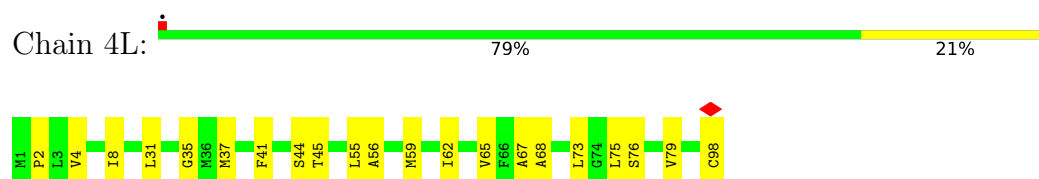


Mol	Chain	Residues	Atoms					AltConf
85	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

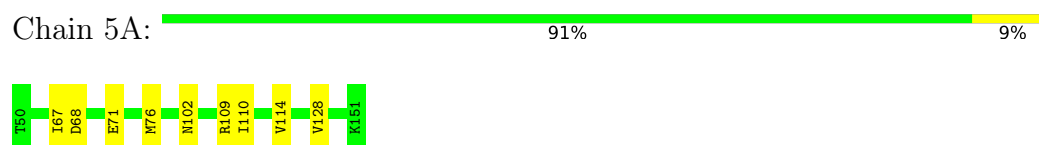
3 Residue-property plots [i](#)

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.

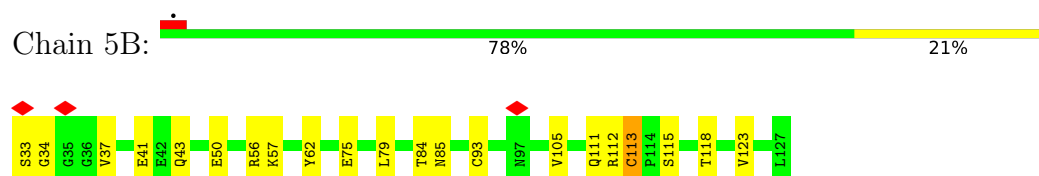
- Molecule 1: NADH-ubiquinone oxidoreductase chain 4L



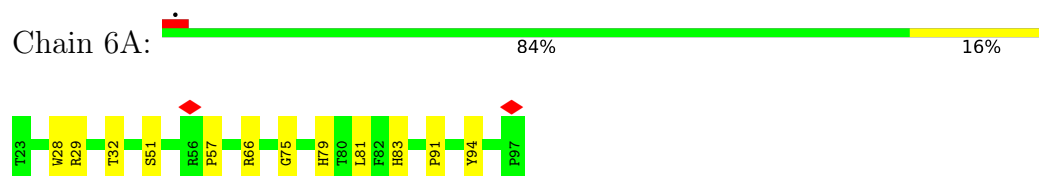
- Molecule 2: Cytochrome c oxidase subunit 5A, mitochondrial



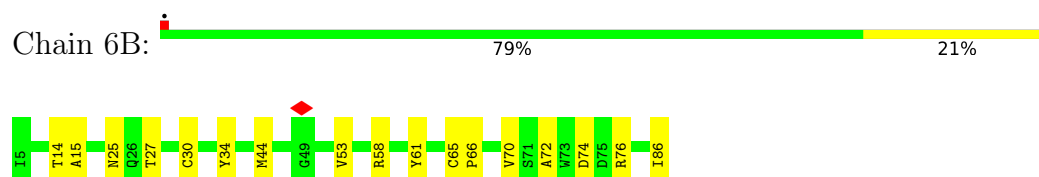
- Molecule 3: Cytochrome c oxidase subunit 5B, mitochondrial



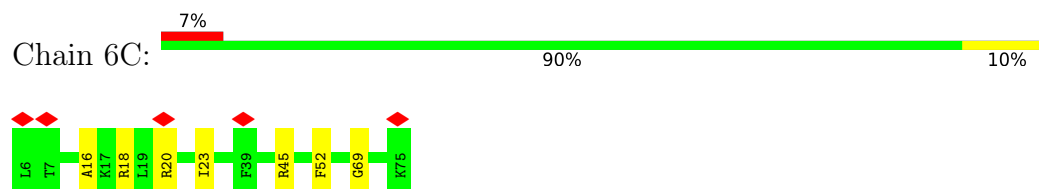
- Molecule 4: Cytochrome c oxidase subunit



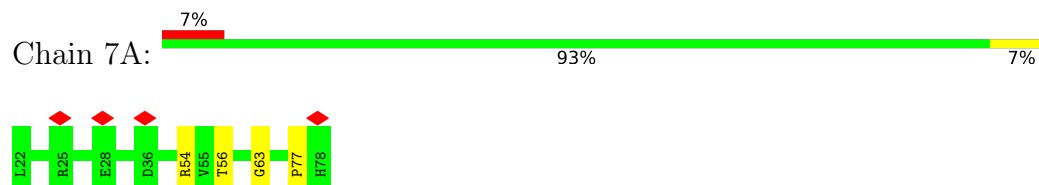
- Molecule 5: Cytochrome c oxidase subunit



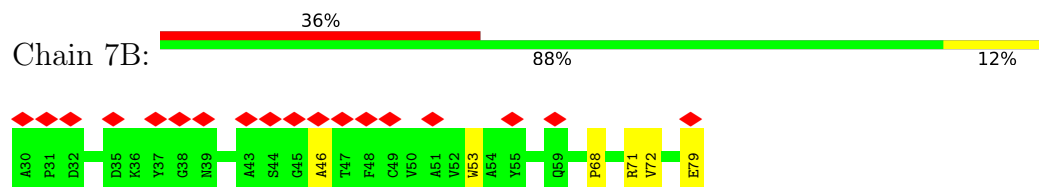
- Molecule 6: Cytochrome c oxidase subunit 6C



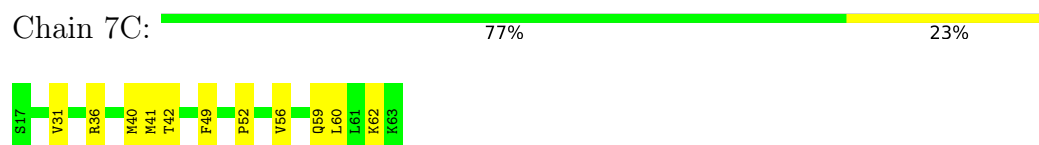
- Molecule 7: Cytochrome c oxidase subunit 7A1, mitochondrial



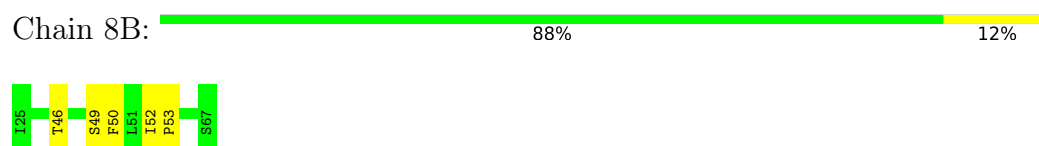
- Molecule 8: Cytochrome c oxidase subunit 7B, mitochondrial



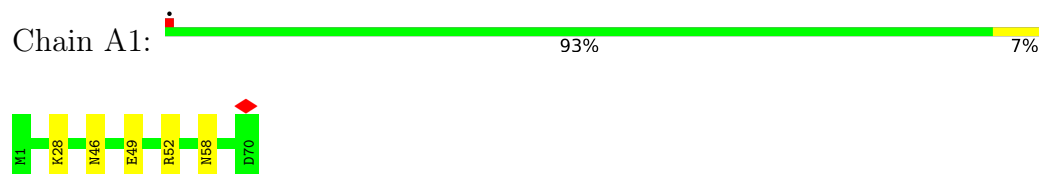
- Molecule 9: Cytochrome c oxidase subunit 7C, mitochondrial



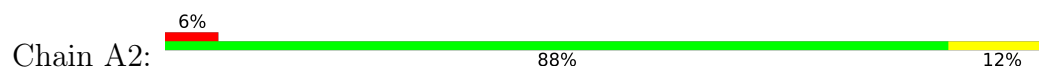
- Molecule 10: Cytochrome c oxidase subunit 8

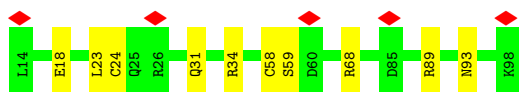


- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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





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



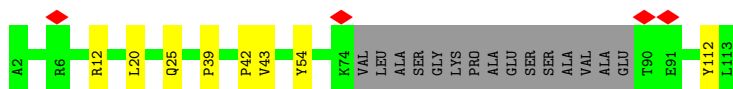
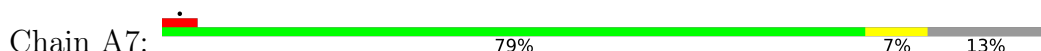
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



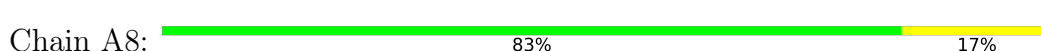
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



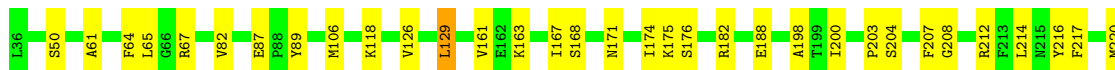
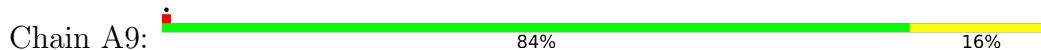
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

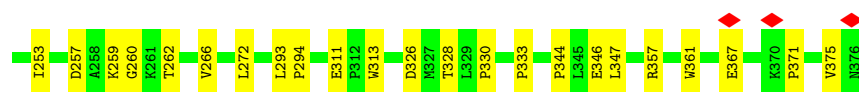


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

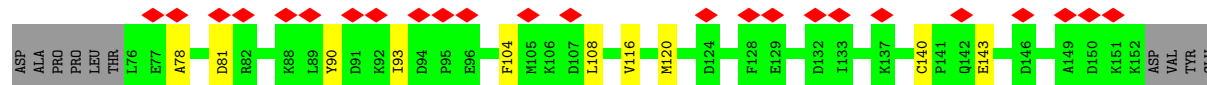
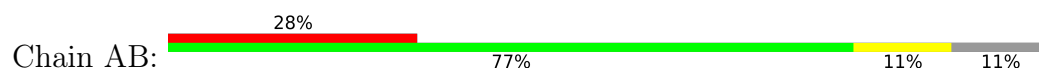


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

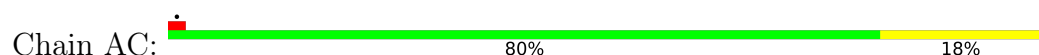




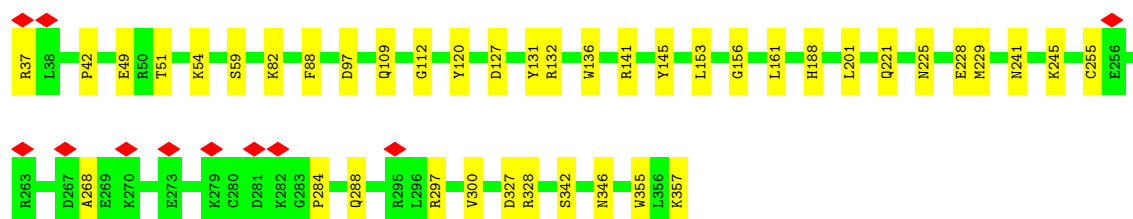
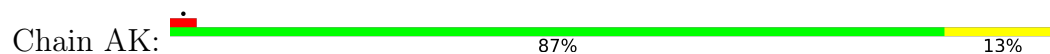
- Molecule 19: Acyl carrier protein



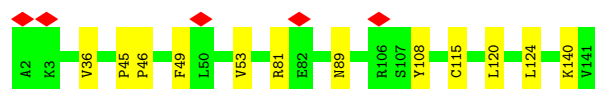
- Molecule 19: Acyl carrier protein



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



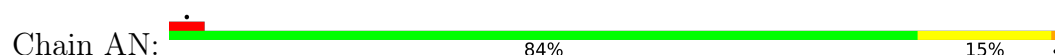
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



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

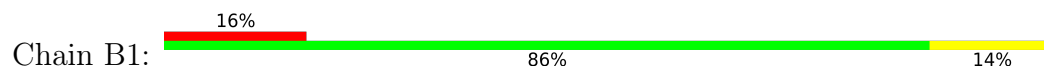


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

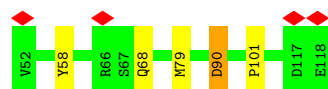




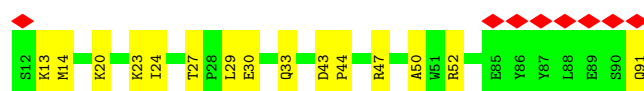
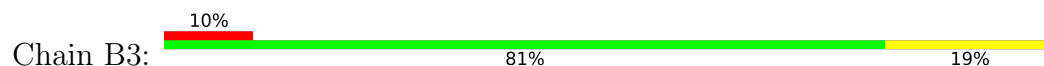
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



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



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



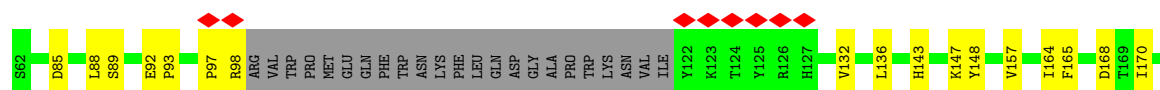
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

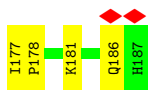


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

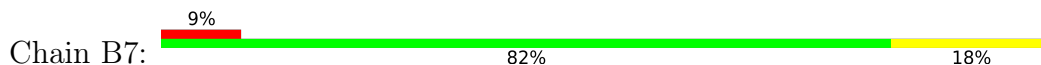


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6





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



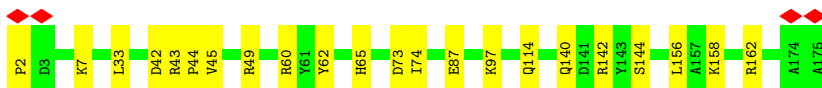
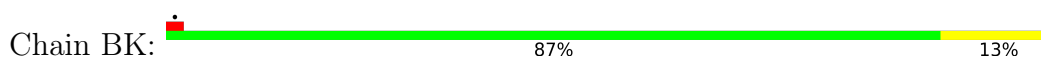
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



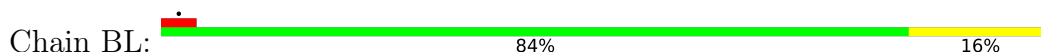
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



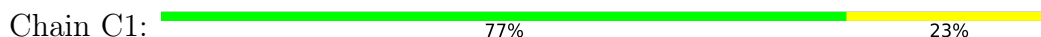
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



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

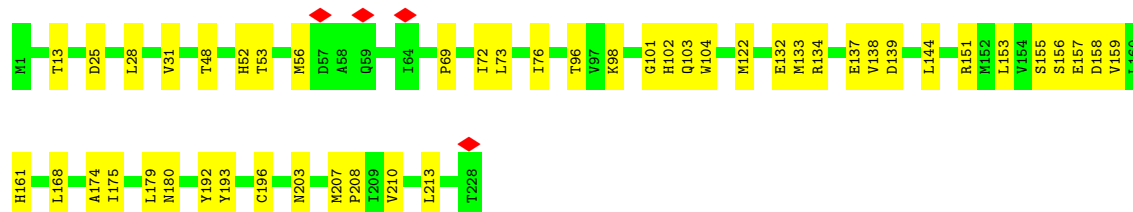
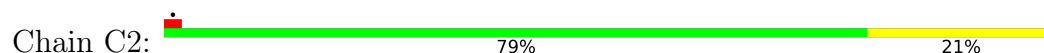


- Molecule 35: Cytochrome c oxidase subunit 1

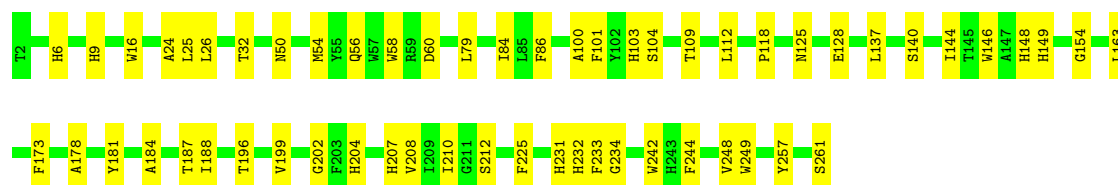
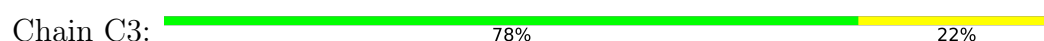




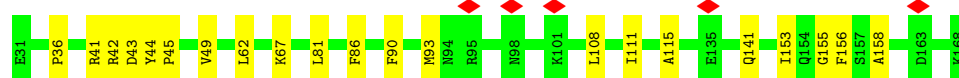
- Molecule 36: Cytochrome c oxidase subunit 2



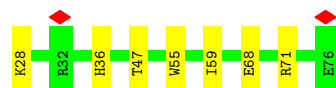
- Molecule 37: Cytochrome c oxidase subunit 3



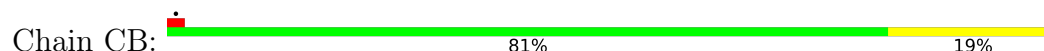
- Molecule 38: Cytochrome c oxidase subunit 4



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

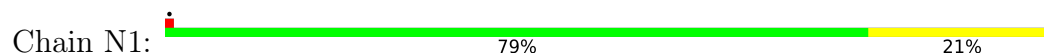


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 subunit C2

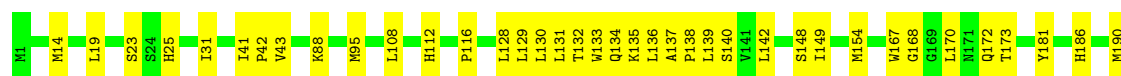
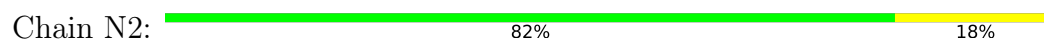




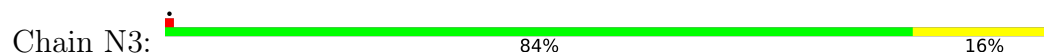
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



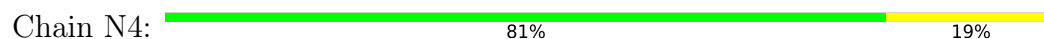
- Molecule 42: NADH-ubiquinone oxidoreductase chain 2



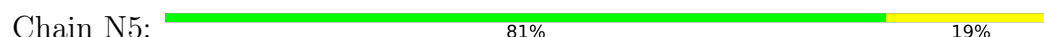
- Molecule 43: NADH-ubiquinone oxidoreductase chain 3

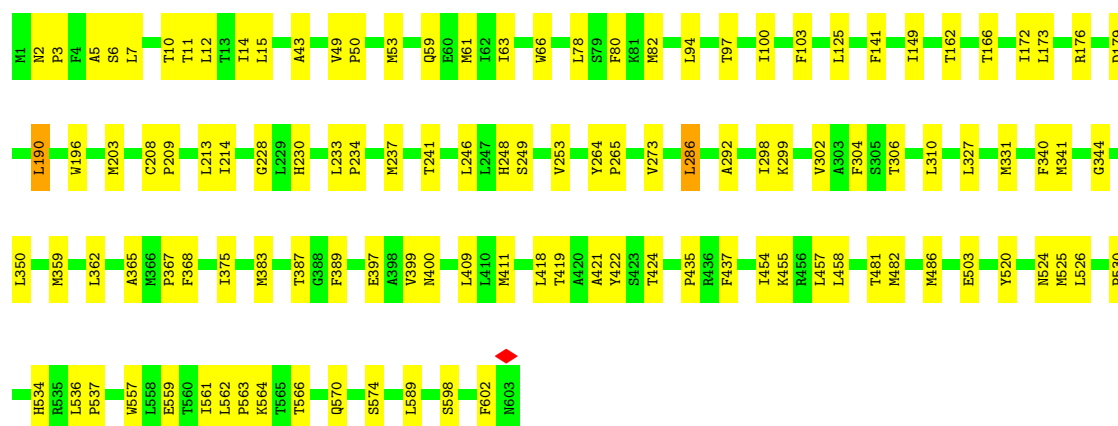


- Molecule 44: NADH-ubiquinone oxidoreductase chain 4

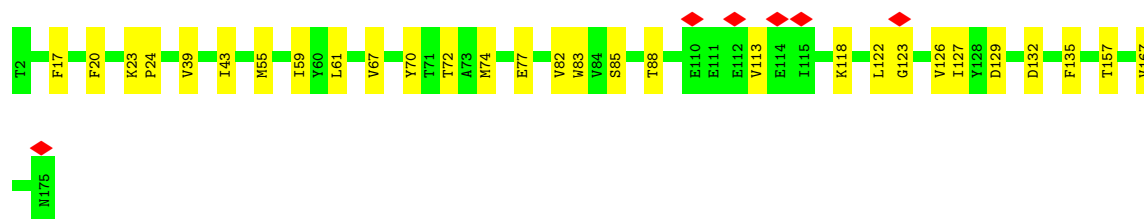
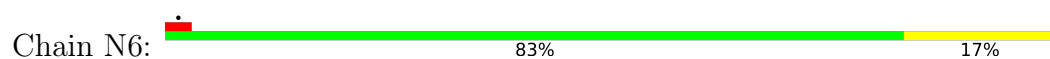


- Molecule 45: NADH-ubiquinone oxidoreductase chain 5

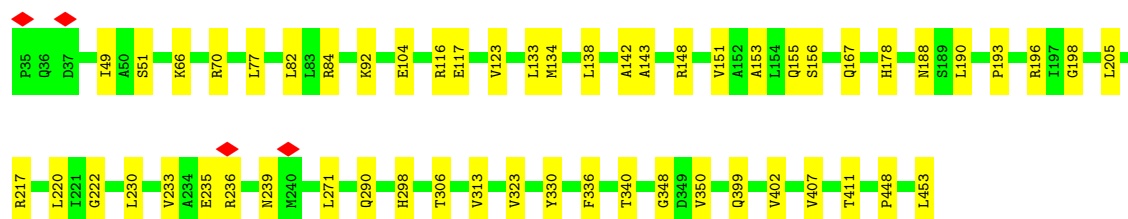
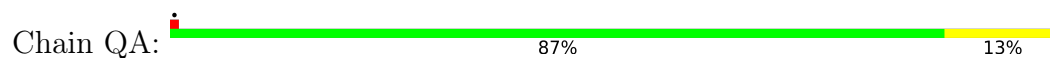




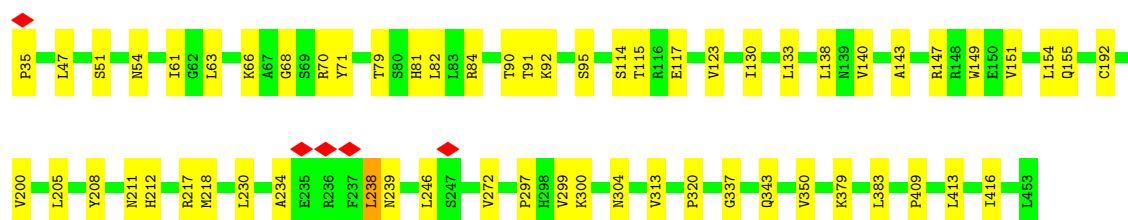
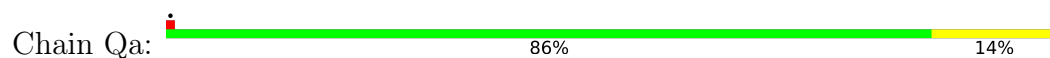
- Molecule 46: NADH-ubiquinone oxidoreductase chain 6



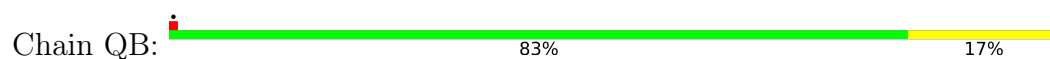
- Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial

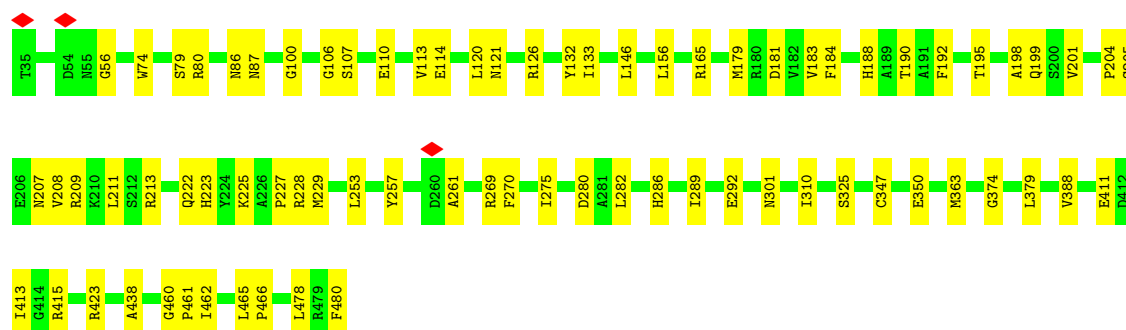


- Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial



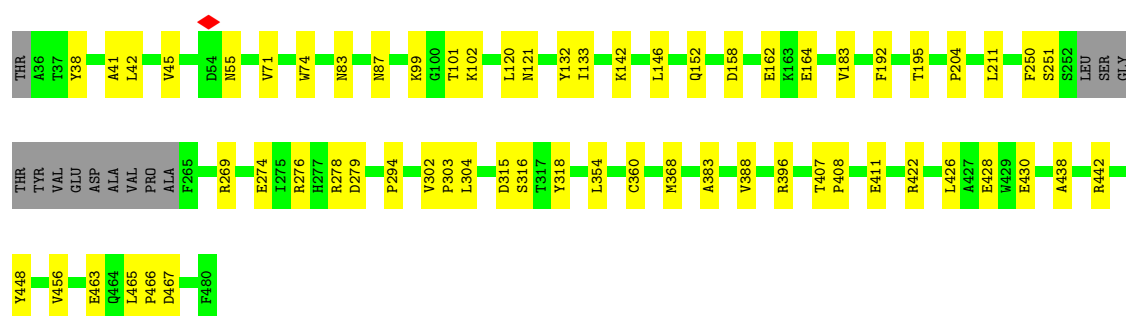
- Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial





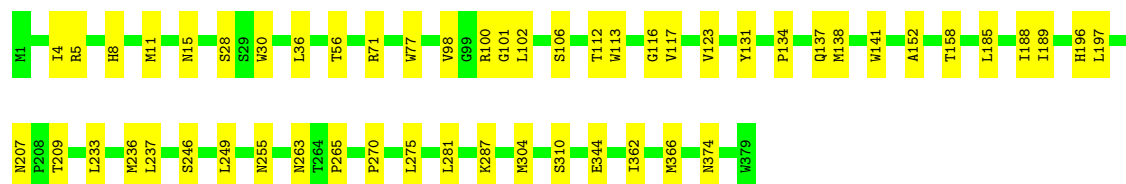
- Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain Qb: 83% 14%



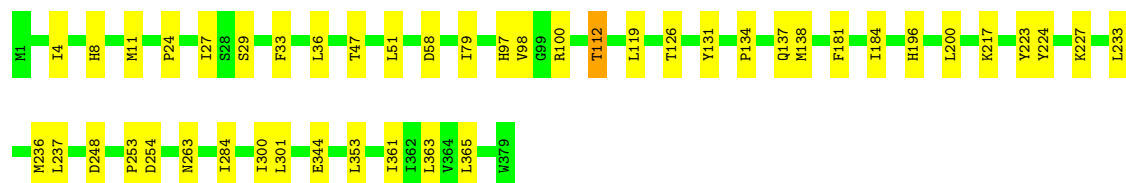
- Molecule 49: Cytochrome b

Chain Qc: 86% 14%



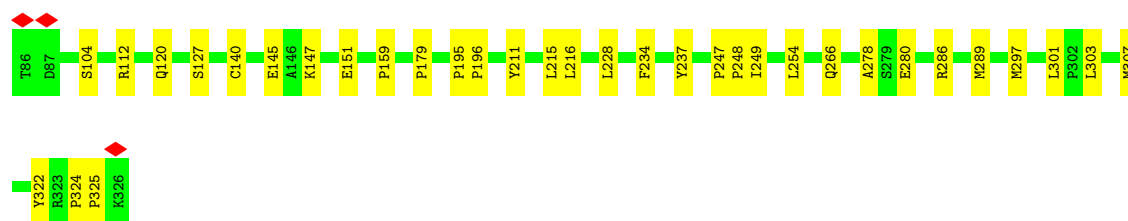
- Molecule 49: Cytochrome b

Chain Qc: 88% 12%

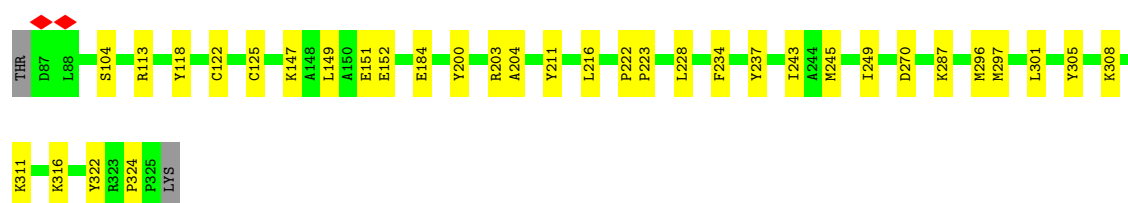


- Molecule 50: Cytochrome c1, heme protein, mitochondrial

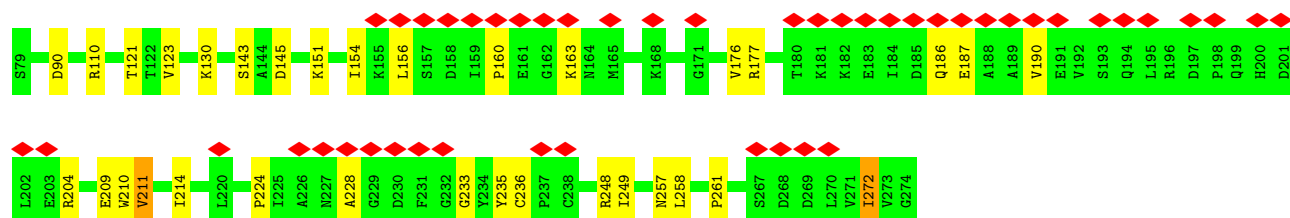
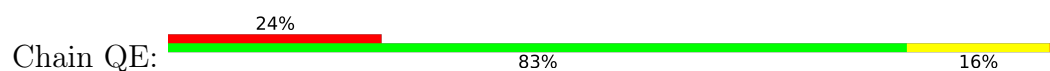
Chain QD: 86% 14%



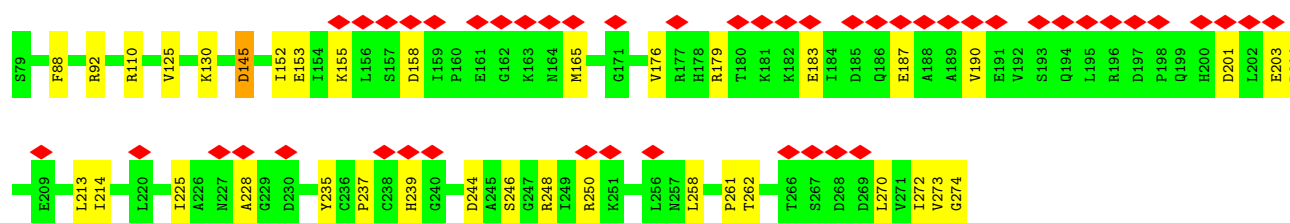
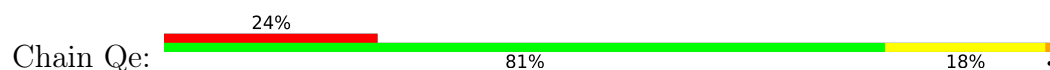
- Molecule 50: Cytochrome c1, heme protein, mitochondrial



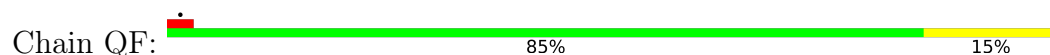
- Molecule 51: Cytochrome b-c1 complex subunit Rieske, mitochondrial



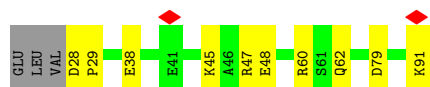
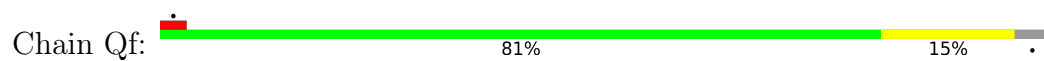
- Molecule 51: Cytochrome b-c1 complex subunit Rieske, mitochondrial



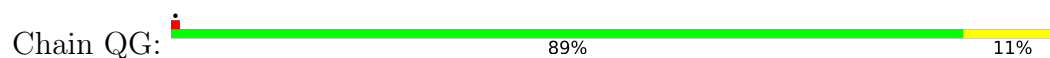
- Molecule 52: Cytochrome b-c1 complex subunit 6



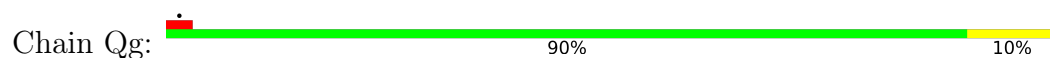
- Molecule 52: Cytochrome b-c1 complex subunit 6



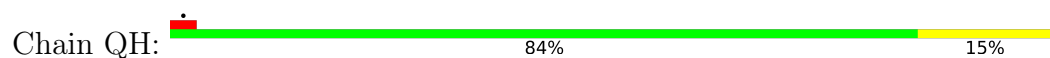
- Molecule 53: Cytochrome b-c1 complex subunit 7



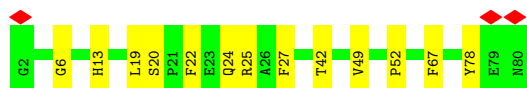
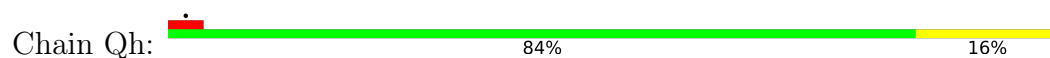
- Molecule 53: Cytochrome b-c1 complex subunit 7



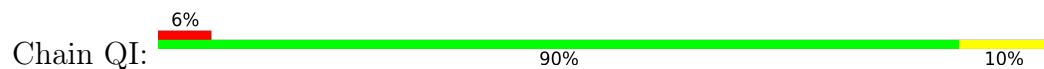
- Molecule 54: Cytochrome b-c1 complex subunit 8



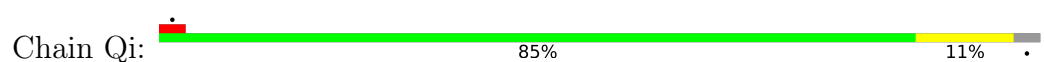
- Molecule 54: Cytochrome b-c1 complex subunit 8



- Molecule 55: Complex III subunit 9

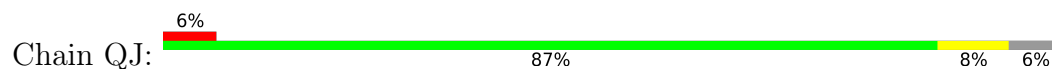


- Molecule 55: Complex III subunit 9

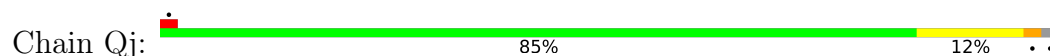




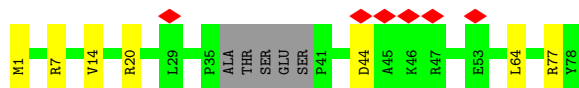
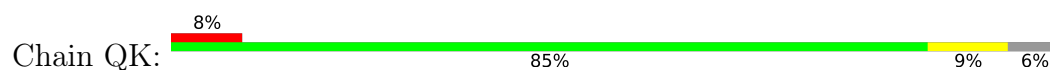
- Molecule 56: Cytochrome b-c1 complex subunit 10



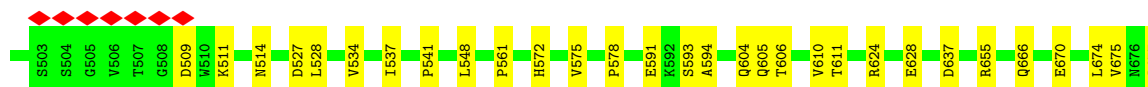
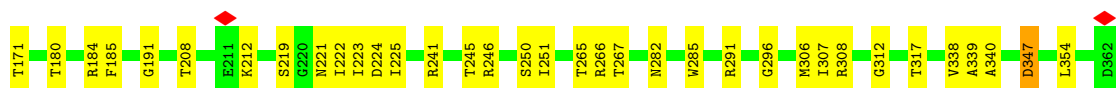
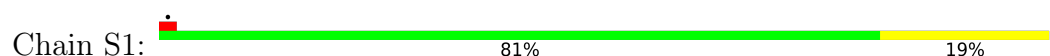
- Molecule 56: Cytochrome b-c1 complex subunit 10



- Molecule 57: Cytochrome b-c1 complex subunit Rieske, mitochondrial

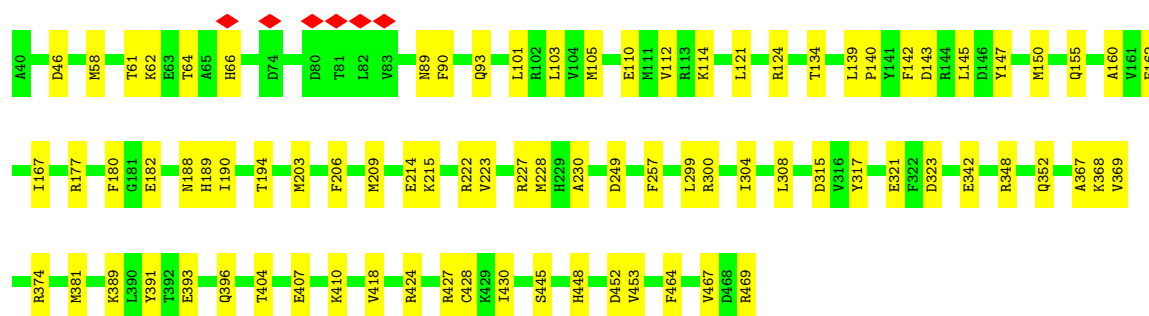


- Molecule 58: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



- Molecule 59: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain S2:  81% 19%



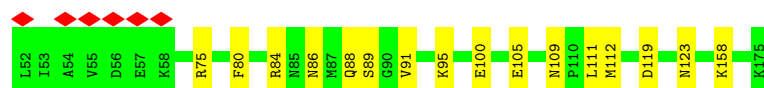
• Molecule 60: Complex I-30kD

Chain S3:  88% 12%



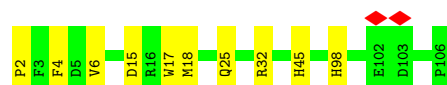
• Molecule 61: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain S4:  5% 87% 13%



• Molecule 62: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain S5:  90% 10%



• Molecule 63: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain S6:  6% 94% 6%



• Molecule 64: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain S7:  78% 21%

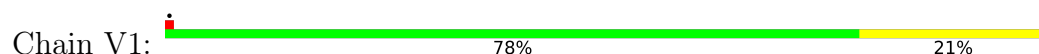




- Molecule 65: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



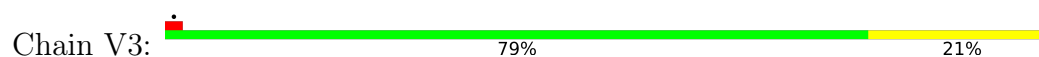
- Molecule 66: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



- Molecule 67: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 68: NADH:ubiquinone oxidoreductase subunit V3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	168528	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS 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	63.880	Depositor
Minimum map value	-46.757	Depositor
Average map value	0.003	Depositor
Map value standard deviation	1.241	Depositor
Recommended contour level	5	Depositor
Map size (Å)	576.0, 576.0, 576.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ADP, PEE, FES, HEA, SF4, PLX, ZMP, HEC, CDL, ZN, FMN, CU, NDP, 2MR, HEM, 3PE, MG, PC1

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	0.14	0/759	0.30	0/1029
2	5A	0.11	0/843	0.23	0/1145
3	5B	0.17	0/739	0.33	0/1002
4	6A	0.12	0/648	0.27	0/888
5	6B	0.13	0/704	0.23	0/951
6	6C	0.11	0/587	0.23	0/781
7	7A	0.11	0/457	0.27	0/620
8	7B	0.11	0/405	0.26	0/555
9	7C	0.16	0/400	0.24	0/536
10	8B	0.12	0/349	0.27	0/477
11	A1	0.13	0/577	0.33	0/777
12	A2	0.10	0/697	0.26	0/938
13	A3	0.10	0/664	0.23	0/912
14	A5	0.11	0/929	0.22	0/1258
15	A6	0.13	0/991	0.27	0/1335
16	A7	0.11	0/798	0.26	0/1079
17	A8	0.11	0/1436	0.24	0/1938
18	A9	0.13	0/2820	0.27	0/3823
19	AB	0.08	0/633	0.21	0/851
19	AC	0.12	0/714	0.23	0/965
20	AK	0.11	0/2661	0.26	0/3602
21	AL	0.11	0/1042	0.21	0/1411
22	AM	0.12	0/1245	0.25	0/1694
23	AN	0.13	0/1204	0.26	0/1624
24	B1	0.11	0/491	0.24	0/663
25	B2	0.12	0/610	0.27	0/836
26	B3	0.11	0/660	0.26	0/892
27	B4	0.13	0/1092	0.25	0/1481
28	B5	0.14	0/1184	0.25	0/1603
29	B6	0.15	0/910	0.31	0/1237
30	B7	0.12	0/1092	0.24	0/1459

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	B8	0.12	0/1371	0.24	0/1875
32	B9	0.13	0/1590	0.28	0/2155
33	BK	0.14	0/1489	0.25	0/2008
34	BL	0.14	0/851	0.27	0/1155
35	C1	0.18	0/4164	0.32	0/5689
36	C2	0.17	0/1880	0.29	0/2564
37	C3	0.16	0/2186	0.29	0/2991
38	C4	0.13	0/1187	0.25	0/1606
39	CA	0.11	0/430	0.20	0/581
40	CB	0.14	0/1031	0.25	0/1394
41	N1	0.17	0/2581	0.34	0/3529
42	N2	0.18	0/2773	0.33	0/3768
43	N3	0.15	0/938	0.28	0/1281
44	N4	0.17	0/3723	0.32	0/5078
45	N5	0.16	0/4914	0.34	0/6683
46	N6	0.14	0/1364	0.30	0/1850
47	QA	0.14	0/3200	0.28	0/4333
47	Qa	0.14	0/3200	0.28	0/4333
48	QB	0.14	0/3531	0.30	0/4793
48	Qb	0.14	0/3436	0.29	0/4659
49	QC	0.16	0/3123	0.31	0/4269
49	Qc	0.18	0/3123	0.32	0/4269
50	QD	0.13	0/1979	0.25	0/2684
50	Qd	0.14	0/1962	0.27	0/2663
51	QE	0.11	0/1550	0.26	0/2098
51	Qe	0.12	0/1550	0.27	0/2098
52	QF	0.11	0/558	0.22	0/747
52	Qf	0.11	0/534	0.22	0/714
53	QG	0.14	0/913	0.25	0/1223
53	Qg	0.12	0/913	0.25	0/1223
54	QH	0.15	0/684	0.31	0/926
54	Qh	0.14	0/688	0.29	0/931
55	QI	0.10	0/520	0.20	0/701
55	Qi	0.14	0/506	0.25	0/683
56	QJ	0.10	0/420	0.24	0/576
56	Qj	0.13	0/437	0.32	0/598
57	QK	0.11	0/528	0.26	0/716
58	S1	0.14	0/5378	0.30	0/7287
59	S2	0.16	0/3538	0.29	0/4796
60	S3	0.14	0/1789	0.27	0/2436
61	S4	0.13	0/1030	0.26	0/1391
62	S5	0.11	0/889	0.23	0/1190
63	S6	0.12	0/755	0.27	0/1018

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
64	S7	0.16	0/1279	0.31	0/1730
65	S8	0.16	0/1443	0.28	0/1952
66	V1	0.14	0/3391	0.29	0/4583
67	V2	0.13	0/1711	0.29	0/2328
68	V3	0.10	0/365	0.26	0/493
All	All	0.14	0/115736	0.28	0/157010

There are no bond length outliers.

There are no bond angle outliers.

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	21	0
2	5A	825	0	823	6	0
3	5B	724	0	705	14	0
4	6A	620	0	589	9	0
5	6B	684	0	649	10	0
6	6C	574	0	590	7	0
7	7A	447	0	443	4	0
8	7B	392	0	372	7	0
9	7C	387	0	385	12	0
10	8B	338	0	342	4	0
11	A1	562	0	557	4	0
12	A2	686	0	699	6	0
13	A3	643	0	642	2	0
14	A5	910	0	950	4	0
15	A6	967	0	972	10	0
16	A7	780	0	808	6	0
17	A8	1398	0	1372	24	0
18	A9	2743	0	2762	32	0
19	AB	624	0	625	6	0
19	AC	702	0	694	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	AK	2601	0	2566	24	0
21	AL	1021	0	1025	11	0
22	AM	1204	0	1162	12	0
23	AN	1173	0	1166	21	0
24	B1	479	0	486	6	0
25	B2	584	0	529	6	0
26	B3	641	0	620	11	0
27	B4	1062	0	1072	6	0
28	B5	1151	0	1164	11	0
29	B6	882	0	899	20	0
30	B7	1068	0	1043	18	0
31	B8	1315	0	1208	9	0
32	B9	1534	0	1470	19	0
33	BK	1456	0	1426	19	0
34	BL	828	0	788	13	0
35	C1	4024	0	4005	81	0
36	C2	1833	0	1843	40	0
37	C3	2103	0	2034	53	0
38	C4	1153	0	1130	18	0
39	CA	417	0	422	4	0
40	CB	1000	0	994	19	0
41	N1	2508	0	2607	53	0
42	N2	2710	0	2874	48	0
43	N3	914	0	951	16	0
44	N4	3631	0	3839	60	0
45	N5	4785	0	4933	87	0
46	N6	1329	0	1326	28	0
47	QA	3147	0	3129	35	0
47	Qa	3147	0	3129	37	0
48	QB	3459	0	3350	48	0
48	Qb	3367	0	3262	36	0
49	QC	3025	0	3090	35	0
49	Qc	3025	0	3090	40	0
50	QD	1921	0	1867	25	0
50	Qd	1904	0	1849	29	0
51	QE	1517	0	1500	21	0
51	Qe	1517	0	1500	27	0
52	QF	552	0	536	7	0
52	Qf	528	0	510	7	0
53	QG	893	0	888	7	0
53	Qg	893	0	888	6	0
54	QH	662	0	660	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	Qh	666	0	663	11	0
55	QI	507	0	509	5	0
55	Qi	493	0	491	6	0
56	QJ	405	0	405	5	0
56	Qj	421	0	418	6	0
57	QK	520	0	554	5	0
58	S1	5290	0	5321	86	0
59	S2	3459	0	3396	68	0
60	S3	1738	0	1693	15	0
61	S4	1007	0	1008	10	0
62	S5	867	0	871	11	0
63	S6	741	0	701	4	0
64	S7	1248	0	1254	26	0
65	S8	1412	0	1363	21	0
66	V1	3316	0	3272	61	0
67	V2	1671	0	1673	15	0
68	V3	355	0	329	8	0
69	4L	92	0	137	7	0
69	6A	83	0	116	5	0
69	A7	51	0	46	1	0
69	AK	68	0	80	4	0
69	AL	174	0	245	10	0
69	B5	100	0	156	3	0
69	CB	83	0	113	4	0
69	N1	78	0	103	6	0
69	N4	162	0	224	10	0
69	N5	189	0	284	9	0
69	QB	64	0	72	2	0
69	QD	58	0	60	1	0
69	QH	64	0	72	4	0
69	Qb	64	0	72	3	0
69	Qc	61	0	66	1	0
69	Qh	55	0	54	3	0
70	5B	1	0	0	0	0
70	S6	1	0	0	0	0
71	6A	83	0	114	8	0
71	C1	133	0	197	1	0
71	C3	143	0	217	22	0
71	N1	108	0	176	9	0
71	N3	54	0	88	1	0
71	QB	51	0	79	4	0
71	Qb	48	0	73	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
71	Qc	54	0	88	1	0
71	Qh	54	0	88	3	0
72	6C	43	0	67	1	0
72	AL	47	0	75	1	0
72	AM	52	0	88	5	0
72	B5	52	0	88	1	0
72	CB	52	0	88	7	0
72	N3	52	0	88	3	0
72	N4	52	0	88	3	0
72	QB	46	0	73	3	0
72	QI	52	0	88	5	0
72	S7	52	0	88	4	0
73	A9	48	0	26	0	0
74	A9	39	0	52	1	0
74	AL	49	0	75	4	0
74	C3	51	0	82	6	0
74	N1	31	0	36	1	0
74	N3	51	0	82	2	0
74	N5	137	0	205	5	0
74	QB	34	0	42	3	0
74	QC	40	0	54	0	0
74	QE	47	0	71	1	0
74	QJ	51	0	82	3	0
74	Qc	42	0	61	1	0
74	Qd	24	0	22	0	0
74	S2	45	0	67	1	0
74	S8	51	0	82	2	0
75	AB	36	0	47	0	0
75	AC	36	0	47	3	0
76	AK	27	0	12	2	0
77	B8	32	0	38	0	0
77	C1	91	0	136	4	0
77	CA	46	0	69	0	0
77	CB	48	0	73	5	0
77	N5	38	0	50	1	0
77	QE	44	0	65	0	0
77	QJ	34	0	42	1	0
77	Qc	48	0	73	3	0
77	Qj	29	0	32	1	0
77	S7	51	0	82	4	0
78	C1	120	0	108	13	0
79	C1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
79	C2	2	0	0	0	0
80	C1	1	0	0	0	0
80	S1	1	0	0	0	0
81	QC	86	0	60	6	0
81	Qc	86	0	60	10	0
82	QD	43	0	30	2	0
82	Qd	43	0	32	3	0
83	QE	4	0	0	0	0
83	Qe	4	0	0	1	0
83	S1	4	0	0	1	0
83	V2	4	0	0	0	0
84	S1	16	0	0	1	0
84	S7	8	0	0	0	0
84	S8	16	0	0	0	0
84	V1	8	0	0	1	0
85	V1	31	0	19	0	0
All	All	117287	0	118494	1475	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 6.

All (1475) 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	1.71	0.89
30:B7:92:HIS:HD1	45:N5:481:THR:HG1	1.24	0.85
77:CB:202:3PE:H381	42:N2:325:LEU:H	1.42	0.84
21:AL:108:TYR:HB2	69:AL:202:CDL:HB32	1.62	0.80
1:4L:37:MET:HG2	1:4L:67:ALA:HB2	1.63	0.79
29:B6:88:LEU:HD22	29:B6:92:GLU:HG2	1.62	0.79
58:S1:149:ASP:HB2	59:S2:367:ALA:HB3	1.66	0.78
20:AK:141:ARG:NH2	76:AK:401:ADP:N7	2.33	0.77
49:QC:237:LEU:HB2	50:QD:297:MET:HE2	1.66	0.77
44:N4:445:LEU:HB3	69:N5:703:CDL:H452	1.67	0.76
12:A2:59:SER:HB2	58:S1:655:ARG:HD3	1.68	0.76
26:B3:27:THR:HG22	26:B3:29:LEU:H	1.50	0.76
42:N2:88:LYS:HG3	42:N2:148:SER:HB3	1.66	0.75
74:C3:304:PEE:H2	74:C3:304:PEE:H11	1.69	0.74
33:BK:2:PRO:O	33:BK:7:LYS:NZ	2.21	0.74
37:C3:16:TRP:NE1	37:C3:60:ASP:OD2	2.19	0.74
47:QA:70:ARG:HD2	47:QA:117:GLU:HG2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:AC:201:ZMP:H14	32:B9:102:ALA:HB1	1.70	0.73
1:4L:68:ALA:HB3	43:N3:67:LEU:HD11	1.69	0.72
22:AM:34:ARG:NH2	65:S8:89:GLU:OE2	2.23	0.71
47:Qa:155:GLN:HE22	47:Qa:200:VAL:HB	1.55	0.71
64:S7:85:ASP:HB3	64:S7:88:ARG:HB3	1.72	0.71
54:QH:55:VAL:HG11	77:Qc:405:3PE:H3I2	1.73	0.71
7:7A:77:PRO:HG3	9:7C:62:LYS:HG3	1.73	0.70
21:AL:140:LYS:O	42:N2:273:ASN:ND2	2.23	0.70
47:Qa:138:LEU:HB3	47:Qa:238:LEU:HG	1.73	0.70
1:4L:2:PRO:HG3	46:N6:127:ILE:HD13	1.72	0.70
9:7C:62:LYS:NZ	35:C1:117:MET:O	2.24	0.70
21:AL:140:LYS:H	42:N2:273:ASN:HD22	1.38	0.69
51:Qe:204:ARG:NH2	51:Qe:258:LEU:O	2.23	0.69
59:S2:308:LEU:HB2	59:S2:407:GLU:HB2	1.75	0.69
35:C1:443:TYR:O	36:C2:134:ARG:NH2	2.25	0.69
48:QB:100:GLY:HA2	48:QB:106:GLY:H	1.56	0.69
49:Qc:98:VAL:HG22	81:Qc:404:HEM:HBC2	1.74	0.69
50:QD:266:GLN:HE22	52:Qf:91:LYS:H	1.41	0.68
49:QC:71:ARG:NH2	50:QD:278:ALA:O	2.26	0.68
50:QD:211:TYR:OH	82:QD:401:HEC:O2A	2.11	0.68
59:S2:155:GLN:NE2	59:S2:315:ASP:OD2	2.27	0.68
35:C1:155:VAL:HG11	71:C3:303:PC1:H3B1	1.74	0.68
42:N2:108:LEU:HD11	42:N2:191:THR:HG21	1.74	0.68
49:QC:138:MET:HB2	49:QC:255:ASN:HD22	1.59	0.68
51:Qe:190:VAL:HG21	51:Qe:250:ARG:HH22	1.58	0.68
9:7C:59:GLN:NE2	35:C1:116:SER:O	2.26	0.68
64:S7:188:LYS:HB2	64:S7:191:ARG:HB2	1.74	0.68
69:N5:703:CDL:H602	69:N5:703:CDL:H212	1.76	0.68
18:A9:212:ARG:NH1	18:A9:311:GLU:OE2	2.27	0.67
57:QK:1:MET:O	57:QK:7:ARG:NH1	2.27	0.67
41:N1:108:MET:HE1	71:N1:402:PC1:H282	1.76	0.67
12:A2:24:CYS:N	12:A2:58:CYS:SG	2.68	0.67
60:S3:83:GLU:OE1	60:S3:142:ARG:NH2	2.26	0.67
51:QE:187:GLU:OE1	51:QE:248:ARG:NH2	2.27	0.67
41:N1:87:VAL:HG11	43:N3:6:THR:HG21	1.76	0.67
54:Qh:25:ARG:HG2	71:Qh:101:PC1:H111	1.75	0.67
58:S1:433:GLY:HA2	58:S1:447:ASP:HA	1.77	0.67
44:N4:122:PHE:HZ	44:N4:206:LYS:HG3	1.60	0.67
15:A6:66:TYR:O	15:A6:86:ARG:NH1	2.28	0.67
19:AC:114:ASP:OD1	32:B9:87:ARG:NH2	2.28	0.66
41:N1:173:TRP:HB3	41:N1:175:ILE:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B6:132:VAL:O	29:B6:136:LEU:HB3	1.94	0.66
41:N1:141:SER:HB2	41:N1:289:LEU:HD12	1.78	0.66
50:Qd:125:CYS:SG	82:Qd:401:HEC:HAC	2.36	0.66
35:C1:406:ASN:HD22	35:C1:409:TRP:CD1	2.13	0.66
51:Qe:187:GLU:OE1	51:Qe:248:ARG:NH2	2.26	0.66
58:S1:282:ASN:ND2	58:S1:285:TRP:O	2.29	0.66
59:S2:374:ARG:NH2	65:S8:165:ASP:OD1	2.27	0.66
69:4L:201:CDL:H521	46:N6:88:THR:HG23	1.78	0.66
9:7C:42:THR:HG23	10:8B:49:SER:HB3	1.77	0.66
66:V1:112:TYR:HB2	66:V1:240:THR:HG22	1.76	0.66
36:C2:175:ILE:HD12	36:C2:180:ASN:HD21	1.61	0.66
36:C2:104:TRP:HA	36:C2:207:MET:HG2	1.76	0.66
44:N4:122:PHE:CZ	44:N4:206:LYS:HG3	2.31	0.66
58:S1:419:ARG:NH1	58:S1:439:THR:O	2.29	0.65
71:C3:302:PC1:H3B2	71:C3:303:PC1:H2A1	1.79	0.65
51:Qe:145:ASP:OD1	51:Qe:145:ASP:N	2.30	0.65
72:AL:204:PLX:H81	69:N4:503:CDL:HA31	1.76	0.65
45:N5:362:LEU:HA	45:N5:365:ALA:HB3	1.77	0.65
49:Qc:300:ILE:HD11	49:Qc:363:LEU:HD21	1.77	0.65
45:N5:418:LEU:HD21	69:N5:704:CDL:H762	1.78	0.65
69:4L:201:CDL:H341	21:AL:53:VAL:HG22	1.79	0.65
20:AK:120:TYR:OH	76:AK:401:ADP:O2'	2.15	0.65
36:C2:132:GLU:HB3	36:C2:137:GLU:HG3	1.79	0.65
71:N3:203:PC1:H141	77:S7:303:3PE:H31	1.78	0.65
61:S4:91:VAL:O	61:S4:95:LYS:NZ	2.29	0.65
59:S2:393:GLU:OE2	59:S2:396:GLN:NE2	2.29	0.64
30:B7:29:TYR:O	30:B7:104:ARG:NH2	2.30	0.64
36:C2:161:HIS:HB2	36:C2:174:ALA:HB3	1.78	0.64
49:QC:246:SER:HB2	49:QC:249:LEU:HB2	1.80	0.64
42:N2:142:LEU:HB3	42:N2:194:LEU:HD21	1.79	0.64
8:7B:53:TRP:HE1	38:C4:111:ILE:HG22	1.63	0.64
45:N5:530:PRO:O	45:N5:534:HIS:HB2	1.97	0.64
51:Qe:153:GLU:HG2	51:Qe:272:ILE:HG12	1.79	0.64
51:Qe:262:THR:HB	51:Qe:274:GLY:O	1.98	0.64
69:AL:202:CDL:H751	69:AL:202:CDL:H601	1.79	0.63
36:C2:52:HIS:HD2	36:C2:56:MET:HE2	1.63	0.63
43:N3:37:TYR:OH	59:S2:93:GLN:NE2	2.30	0.63
46:N6:113:VAL:HG13	46:N6:118:LYS:HG2	1.79	0.63
69:AL:202:CDL:H801	45:N5:557:TRP:HB3	1.80	0.63
49:Qc:126:THR:HG21	81:Qc:403:HEM:HBB2	1.79	0.63
50:Qd:147:LYS:NZ	50:Qd:151:GLU:OE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:V1:214:GLU:OE2	66:V1:224:ARG:NE	2.28	0.63
67:V2:108:PRO:HB2	67:V2:111:ARG:HG2	1.79	0.63
18:A9:188:GLU:HG3	18:A9:200:ILE:HD13	1.80	0.63
41:N1:53:LEU:HD11	72:S7:302:PLX:H192	1.80	0.63
41:N1:99:ASN:N	71:N1:402:PC1:O12	2.31	0.63
58:S1:433:GLY:O	58:S1:444:HIS:NE2	2.26	0.63
59:S2:162:GLU:OE2	59:S2:177:ARG:NH2	2.31	0.63
69:4L:201:CDL:H181	45:N5:589:LEU:HD11	1.81	0.63
20:AK:82:LYS:HZ2	20:AK:268:ALA:HB3	1.64	0.63
47:Qa:51:SER:HB3	47:Qa:230:LEU:HD12	1.80	0.63
59:S2:90:PHE:HB3	59:S2:103:LEU:HB3	1.80	0.63
13:A3:151:VAL:O	17:A8:207:LYS:NZ	2.28	0.63
35:C1:406:ASN:HD22	35:C1:409:TRP:HD1	1.47	0.63
47:Qa:84:ARG:NH1	47:Qa:114:SER:OG	2.29	0.63
35:C1:264:LYS:HE2	36:C2:53:THR:HA	1.81	0.63
35:C1:347:LEU:HD13	35:C1:383:MET:HE2	1.80	0.63
19:AB:116:VAL:HG12	19:AB:120:MET:HE2	1.80	0.63
58:S1:83:GLU:HB2	58:S1:101:ASN:HB3	1.80	0.63
69:Qc:401:CDL:H311	69:Qc:401:CDL:H512	1.80	0.62
66:V1:40:ARG:NH1	66:V1:289:GLU:O	2.32	0.62
29:B6:147:LYS:NZ	33:BK:42:ASP:OD1	2.31	0.62
44:N4:391:ILE:HG23	44:N4:394:ILE:HD12	1.80	0.62
11:A1:46:ASN:ND2	46:N6:132:ASP:OD2	2.32	0.62
25:B2:101:PRO:HD2	30:B7:99:MET:HE1	1.81	0.62
33:BK:60:ARG:NH1	33:BK:62:TYR:OH	2.32	0.62
55:QI:48:ASN:HD21	50:Qd:104:SER:HA	1.65	0.62
58:S1:104:THR:O	58:S1:113:ARG:NH2	2.31	0.62
49:QC:5:ARG:NH1	49:QC:15:ASN:OD1	2.32	0.62
48:Qb:422:ARG:NH2	48:Qb:428:GLU:OE1	2.31	0.62
3:5B:41:GLU:HG2	3:5B:56:ARG:HH22	1.64	0.62
18:A9:87:GLU:HG3	18:A9:89:TYR:H	1.64	0.62
35:C1:107:PRO:HB3	37:C3:25:LEU:HB2	1.80	0.62
71:N1:403:PC1:H372	71:N1:403:PC1:H3B2	1.81	0.62
69:QH:401:CDL:H312	69:QH:401:CDL:H721	1.81	0.62
45:N5:100:ILE:HG21	45:N5:246:LEU:HB2	1.81	0.62
53:Qg:36:ASP:OD1	53:Qg:90:TYR:OH	2.16	0.62
36:C2:133:MET:SD	38:C4:141:GLN:NE2	2.73	0.62
12:A2:89:ARG:O	12:A2:93:ASN:ND2	2.33	0.61
48:QB:204:PRO:HG2	48:QB:207:ASN:HB2	1.82	0.61
66:V1:110:PRO:HB3	66:V1:152:ARG:HD3	1.80	0.61
35:C1:358:LEU:HB3	78:C1:602:HEA:HMA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:N3:70:ALA:HB2	46:N6:59:ILE:HD11	1.81	0.61
59:S2:214:GLU:OE2	59:S2:227:ARG:NH2	2.34	0.61
25:B2:68:GLN:NE2	45:N5:367:PRO:HD2	2.16	0.61
69:N4:502:CDL:H832	69:N4:502:CDL:H231	1.81	0.61
12:A2:31:GLN:OE1	12:A2:34:ARG:NH2	2.32	0.61
35:C1:409:TRP:HB3	35:C1:471:ILE:HG12	1.82	0.61
41:N1:231:ILE:O	41:N1:235:ASN:ND2	2.33	0.61
2:5A:114:VAL:HG11	2:5A:128:VAL:HG11	1.83	0.61
18:A9:346:GLU:HG2	18:A9:371:PRO:HB3	1.81	0.61
72:CB:201:PLX:H362	42:N2:336:VAL:HB	1.82	0.61
47:QA:193:PRO:HG2	47:QA:196:ARG:HG3	1.82	0.61
66:V1:235:VAL:HG12	66:V1:240:THR:HG21	1.82	0.61
74:C3:304:PEE:H65	74:C3:304:PEE:H14	1.83	0.61
66:V1:52:ARG:HH21	68:V3:390:GLN:HG2	1.65	0.61
66:V1:338:ASP:OD1	66:V1:339:PHE:N	2.34	0.61
18:A9:313:TRP:HB3	74:A9:402:PEE:H15	1.83	0.61
38:C4:155:GLY:H	38:C4:158:ALA:HB3	1.64	0.61
48:Qb:87:ASN:HD22	48:Qb:204:PRO:HD3	1.66	0.61
71:6A:101:PC1:H32	37:C3:188:ILE:HD12	1.83	0.60
58:S1:456:ALA:O	58:S1:499:ASN:ND2	2.35	0.60
17:A8:196:ARG:NH2	23:AN:63:GLU:OE2	2.34	0.60
38:C4:41:ARG:NH1	38:C4:43:ASP:OD1	2.35	0.60
59:S2:469:ARG:NH2	60:S3:169:GLU:OE2	2.34	0.60
65:S8:131:GLU:HB2	65:S8:144:ARG:HB3	1.83	0.60
17:A8:107:HIS:HB3	17:A8:197:PRO:HD2	1.82	0.60
58:S1:59:GLN:NE2	61:S4:89:SER:O	2.33	0.60
50:QD:228:LEU:HD11	50:QD:234:PHE:HB2	1.83	0.60
47:Qa:90:THR:HG23	47:Qa:95:SER:HA	1.84	0.60
51:Qe:179:ARG:NH1	51:Qe:246:SER:OG	2.35	0.60
64:S7:55:ASN:ND2	64:S7:187:GLU:O	2.33	0.60
28:B5:163:ARG:NH1	40:CB:102:ASP:OD2	2.31	0.60
45:N5:97:THR:HG21	45:N5:125:LEU:HD22	1.84	0.60
59:S2:61:THR:H	59:S2:64:THR:HG1	1.49	0.60
5:6B:34:TYR:OH	5:6B:74:ASP:OD1	2.17	0.60
37:C3:24:ALA:HB2	71:C3:303:PC1:H3A1	1.82	0.60
54:QH:11:MET:HE2	48:Qb:278:ARG:HD3	1.82	0.60
58:S1:340:ALA:HB3	58:S1:366:LEU:HD23	1.84	0.60
77:C1:609:3PE:H322	77:C1:609:3PE:H361	1.84	0.60
41:N1:34:ARG:HG2	64:S7:82:PRO:HA	1.83	0.60
58:S1:338:VAL:O	58:S1:365:SER:HB2	2.02	0.60
66:V1:111:LYS:HB2	66:V1:151:ALA:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A8:239:LYS:HD3	28:B5:149:LEU:HD11	1.84	0.59
41:N1:24:GLU:OE2	41:N1:274:ARG:NH1	2.35	0.59
50:QD:147:LYS:NZ	50:QD:151:GLU:OE2	2.35	0.59
69:4L:201:CDL:H262	69:4L:201:CDL:H382	1.84	0.59
69:N1:401:CDL:H162	74:N1:404:PEE:H23	1.82	0.59
58:S1:224:ASP:OD2	58:S1:291:ARG:NH2	2.33	0.59
35:C1:101:SER:O	35:C1:156:SER:OG	2.20	0.59
47:Qa:155:GLN:NE2	47:Qa:200:VAL:O	2.35	0.59
67:V2:111:ARG:NH1	67:V2:114:GLU:OE2	2.32	0.59
52:QF:71:LEU:HD22	50:Qd:223:PRO:HG3	1.83	0.59
47:Qa:123:VAL:HB	47:Qa:133:LEU:HD23	1.84	0.59
30:B7:103:GLU:OE2	30:B7:106:ARG:NH2	2.36	0.59
47:Qa:151:VAL:O	47:Qa:155:GLN:HG2	2.02	0.59
60:S3:44:ARG:HE	60:S3:47:ILE:HD12	1.68	0.59
67:V2:187:GLN:HE21	67:V2:190:ASP:HA	1.68	0.59
50:Qd:216:LEU:HB3	50:Qd:249:ILE:HD11	1.83	0.59
2:5A:67:ILE:HG13	2:5A:71:GLU:HB2	1.83	0.59
20:AK:127:ASP:O	20:AK:132:ARG:NH1	2.34	0.59
71:C3:303:PC1:H341	71:C3:303:PC1:H292	1.85	0.59
58:S1:64:CYS:O	58:S1:184:ARG:NH2	2.27	0.59
66:V1:296:LEU:HD21	66:V1:317:VAL:HG11	1.85	0.59
44:N4:251:ASN:HD21	44:N4:304:GLN:HE22	1.48	0.59
67:V2:59:ASN:ND2	67:V2:89:GLN:OE1	2.35	0.59
5:6B:30:CYS:HB2	5:6B:65:CYS:SG	2.43	0.59
6:6C:45:ARG:NH2	72:6C:101:PLX:O2	2.31	0.59
48:Qb:467:ASP:OD2	49:Qc:223:TYR:OH	2.10	0.59
34:BL:95:PHE:O	34:BL:99:LEU:HB2	2.02	0.58
35:C1:313:ALA:HB3	36:C2:73:LEU:HD11	1.84	0.58
69:N4:502:CDL:H792	69:N4:502:CDL:H381	1.84	0.58
47:QA:92:LYS:HD2	47:QA:143:ALA:HB1	1.85	0.58
42:N2:42:PRO:HG2	46:N6:167:VAL:HG22	1.85	0.58
54:QH:3:ARG:HH22	49:Qc:217:LYS:HE2	1.67	0.58
47:Qa:81:HIS:HD2	47:Qa:192:CYS:H	1.51	0.58
34:BL:89:VAL:HG21	44:N4:25:ILE:HG23	1.85	0.58
47:QA:148:ARG:NH2	53:QG:50:ARG:O	2.34	0.58
42:N2:289:ASN:HA	42:N2:292:PHE:CE2	2.38	0.58
54:QH:67:PHE:HE1	49:Qc:344:GLU:HG3	1.67	0.58
58:S1:49:VAL:HG13	58:S1:102:ILE:HD13	1.85	0.58
41:N1:58:LYS:HE2	64:S7:125:PRO:HG2	1.84	0.58
41:N1:102:VAL:HG11	41:N1:154:LEU:HD11	1.85	0.58
47:QA:151:VAL:O	47:QA:155:GLN:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:QE:160:PRO:HD2	51:QE:163:LYS:HG2	1.84	0.58
41:N1:25:ARG:HD3	41:N1:37:PRO:HG2	1.85	0.58
48:QB:280:ASP:HA	48:QB:461:PRO:HB3	1.85	0.58
65:S8:205:ILE:O	65:S8:209:TYR:HB3	2.02	0.58
23:AN:51:MET:HE2	41:N1:311:THR:HB	1.84	0.58
47:QA:138:LEU:O	47:QA:142:ALA:HB3	2.04	0.58
50:QD:280:GLU:OE2	50:QD:286:ARG:NH1	2.36	0.58
58:S1:666:GLN:NE2	58:S1:670:GLU:OE2	2.36	0.58
29:B6:181:LYS:HG3	30:B7:40:VAL:HG13	1.84	0.58
69:Qb:501:CDL:H712	49:Qc:4:ILE:HD11	1.85	0.58
60:S3:187:ILE:HG23	60:S3:188:LEU:HG	1.84	0.58
1:4L:56:ALA:HA	62:S5:18:MET:HE3	1.85	0.58
3:5B:113:CYS:HB3	3:5B:118:THR:HG22	1.86	0.58
41:N1:103:LEU:HD13	46:N6:55:MET:HE3	1.86	0.58
58:S1:624:ARG:NH1	58:S1:628:GLU:OE1	2.32	0.58
1:4L:65:VAL:HA	43:N3:67:LEU:HD22	1.86	0.58
69:6A:102:CDL:H122	37:C3:178:ALA:HB1	1.86	0.58
51:Qe:155:LYS:HG3	51:Qe:158:ASP:H	1.68	0.58
35:C1:184:PHE:H	35:C1:256:HIS:CE1	2.22	0.57
53:QG:43:ASP:OD2	53:QG:102:ARG:NH1	2.37	0.57
66:V1:118:ASP:HB3	66:V1:207:GLY:HA2	1.85	0.57
37:C3:234:GLY:N	71:C3:302:PC1:O12	2.35	0.57
22:AM:88:ARG:HD3	65:S8:200:GLU:HG3	1.86	0.57
37:C3:148:HIS:HE1	37:C3:232:HIS:HE1	1.50	0.57
48:QB:411:GLU:OE2	48:QB:415:ARG:NH2	2.33	0.57
49:QC:207:ASN:OD1	49:QC:209:THR:OG1	2.20	0.57
47:Qa:379:LYS:HG2	47:Qa:413:LEU:HD22	1.86	0.57
18:A9:257:ASP:OD1	18:A9:257:ASP:N	2.38	0.57
44:N4:392:THR:O	44:N4:396:MET:HG2	2.04	0.57
51:Qe:201:ASP:OD1	51:Qe:201:ASP:N	2.38	0.57
30:B7:12:ASP:OD1	30:B7:14:SER:OG	2.23	0.57
37:C3:9:HIS:HD2	71:C3:303:PC1:H133	1.68	0.57
47:QA:233:VAL:HG22	47:QA:236:ARG:HH12	1.69	0.57
35:C1:352:GLY:HA3	78:C1:602:HEA:H162	1.85	0.57
22:AM:106:ARG:HB2	22:AM:109:ILE:HG13	1.87	0.57
45:N5:561:ILE:HG23	74:N5:702:PEE:H62	1.86	0.57
35:C1:447:TYR:O	35:C1:451:ASN:ND2	2.33	0.57
36:C2:137:GLU:OE2	36:C2:193:TYR:OH	2.21	0.57
10:8B:46:THR:O	10:8B:49:SER:OG	2.22	0.57
25:B2:90:ASP:N	25:B2:90:ASP:OD1	2.37	0.57
49:QC:28:SER:HB2	69:Qh:102:CDL:HB22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:QH:37:ASN:ND2	69:QH:401:CDL:OB4	2.37	0.57
49:Qc:100:ARG:NH2	81:Qc:404:HEM:O1A	2.37	0.57
29:B6:143:HIS:HD2	33:BK:45:VAL:HG21	1.69	0.56
42:N2:131:LEU:O	42:N2:135:LYS:HG2	2.05	0.56
43:N3:68:GLU:HG3	43:N3:98:LEU:HD13	1.87	0.56
59:S2:90:PHE:HB2	59:S2:105:MET:HE2	1.86	0.56
67:V2:130:TYR:HA	67:V2:189:ASN:HD21	1.70	0.56
48:QB:478:LEU:HD11	74:QB:502:PEE:H2	1.86	0.56
47:Qa:82:LEU:HD11	47:Qa:154:LEU:HB3	1.86	0.56
35:C1:91:ASP:OD1	35:C1:92:MET:N	2.33	0.56
49:QC:233:LEU:HG	50:QD:297:MET:HE1	1.86	0.56
52:QF:34:ARG:O	52:QF:38:GLU:HG2	2.05	0.56
61:S4:84:ARG:NH1	61:S4:88:GLN:O	2.37	0.56
66:V1:94:PRO:HB2	66:V1:97:LEU:HB2	1.87	0.56
48:Qb:388:VAL:HG21	48:Qb:438:ALA:HA	1.86	0.56
59:S2:418:VAL:HB	59:S2:427:ARG:HB3	1.87	0.56
15:A6:81:SER:OG	18:A9:367:GLU:OE2	2.23	0.56
51:Qe:204:ARG:NE	51:Qe:246:SER:O	2.35	0.56
64:S7:86:MET:HB2	64:S7:91:VAL:HB	1.87	0.56
29:B6:143:HIS:CD2	33:BK:45:VAL:HG21	2.40	0.56
38:C4:36:PRO:HB2	38:C4:49:VAL:HG13	1.88	0.56
48:QB:195:THR:HG21	48:QB:269:ARG:H	1.70	0.56
49:Qc:138:MET:HG2	49:Qc:254:ASP:HB2	1.87	0.56
58:S1:593:SER:HA	58:S1:606:THR:O	2.05	0.56
61:S4:109:ASN:ND2	61:S4:111:LEU:O	2.37	0.56
36:C2:104:TRP:CG	36:C2:203:ASN:HB2	2.40	0.56
52:Qf:62:GLN:O	52:Qf:62:GLN:NE2	2.39	0.56
21:AL:140:LYS:H	42:N2:273:ASN:ND2	2.03	0.56
71:C3:302:PC1:H3D2	71:C3:303:PC1:H2C1	1.88	0.56
67:V2:85:LEU:HD13	68:V3:400:LEU:HD22	1.88	0.56
28:B5:152:LYS:HD3	40:CB:96:VAL:HG21	1.88	0.56
33:BK:114:GLN:HG3	45:N5:203:MET:HG2	1.87	0.56
41:N1:133:LEU:HD11	46:N6:72:THR:HG21	1.88	0.56
66:V1:205:ILE:HG12	66:V1:379:CYS:HB3	1.88	0.56
77:C1:608:3PE:H371	38:C4:111:ILE:HG21	1.88	0.55
41:N1:180:PRO:HB3	74:S8:303:PEE:H21	1.88	0.55
18:A9:129:LEU:HD23	18:A9:167:ILE:HG13	1.88	0.55
26:B3:33:GLN:NE2	26:B3:43:ASP:OD1	2.39	0.55
52:QF:79:ASP:OD2	50:Qd:237:TYR:OH	2.24	0.55
42:N2:235:ASN:O	42:N2:315:TRP:NE1	2.40	0.55
50:Qd:243:ILE:HG12	50:Qd:245:MET:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:S1:266:ARG:HD2	58:S1:267:THR:HG23	1.89	0.55
18:A9:163:LYS:NZ	18:A9:253:ILE:O	2.30	0.55
48:Qb:55:ASN:HD22	48:Qb:251:SER:HA	1.71	0.55
4:6A:66:ARG:HB3	4:6A:91:PRO:HG3	1.89	0.55
5:6B:14:THR:OG1	36:C2:96:THR:OG1	2.25	0.55
35:C1:27:GLY:HA3	78:C1:601:HEA:H273	1.88	0.55
35:C1:31:THR:OG1	78:C1:601:HEA:H14	2.06	0.55
51:QE:154:ILE:HD13	51:QE:176:VAL:HG21	1.89	0.55
1:4L:65:VAL:HG11	46:N6:157:THR:HG23	1.88	0.55
4:6A:57:PRO:O	4:6A:94:TYR:OH	2.22	0.55
20:AK:145:TYR:OH	20:AK:201:LEU:O	2.20	0.55
33:BK:33:LEU:HD13	45:N5:49:VAL:HG13	1.89	0.55
37:C3:248:VAL:HG22	71:C3:301:PC1:H2H1	1.89	0.55
45:N5:214:ILE:HD13	77:N5:706:3PE:H252	1.89	0.55
50:QD:216:LEU:HB3	50:QD:249:ILE:HD11	1.87	0.55
58:S1:124:HIS:HD2	59:S2:381:MET:HE2	1.71	0.55
4:6A:75:GLY:H	71:6A:103:PC1:H141	1.72	0.55
37:C3:54:MET:HG2	71:C3:303:PC1:H362	1.88	0.55
49:QC:98:VAL:HG22	81:QC:402:HEM:HBC2	1.89	0.55
50:QD:104:SER:HA	55:Qi:48:ASN:HD21	1.72	0.55
66:V1:109:ARG:NH1	66:V1:237:GLY:O	2.39	0.55
7:7A:54:ARG:HG2	45:N5:503:GLU:OE1	2.07	0.55
14:A5:44:TYR:O	14:A5:48:THR:HG22	2.06	0.55
40:CB:32:ARG:HG2	69:CB:203:CDL:H112	1.88	0.55
58:S1:534:VAL:HG22	58:S1:537:ILE:HB	1.89	0.55
69:4L:201:CDL:H261	69:4L:201:CDL:H221	1.88	0.55
42:N2:211:MET:HG2	42:N2:333:SER:HB2	1.89	0.55
44:N4:211:GLY:H	44:N4:213:HIS:HD2	1.54	0.55
44:N4:403:THR:HA	44:N4:406:TYR:CE2	2.42	0.55
61:S4:75:ARG:NH1	61:S4:119:ASP:OD1	2.37	0.55
69:AL:201:CDL:H751	69:AL:201:CDL:H381	1.88	0.55
67:V2:182:ASN:HB3	67:V2:194:GLU:HB3	1.89	0.55
20:AK:131:TYR:OH	20:AK:188:HIS:ND1	2.32	0.54
17:A8:86:THR:OG1	17:A8:88:GLU:OE1	2.23	0.54
45:N5:3:PRO:HB2	45:N5:53:MET:HE1	1.90	0.54
25:B2:58:TYR:HB2	26:B3:14:MET:HE1	1.90	0.54
19:AB:93:ILE:HD12	19:AB:108:LEU:HD13	1.88	0.54
33:BK:73:ASP:OD1	33:BK:73:ASP:N	2.39	0.54
48:Qb:192:PHE:O	48:Qb:195:THR:OG1	2.23	0.54
58:S1:246:ARG:HH22	61:S4:123:ASN:HD21	1.56	0.54
37:C3:50:ASN:HD21	71:C3:303:PC1:H371	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:N2:14:MET:HA	42:N2:133:TRP:HE1	1.73	0.54
45:N5:149:ILE:HD11	69:N5:703:CDL:H171	1.88	0.54
45:N5:249:SER:HA	45:N5:306:THR:HG21	1.88	0.54
58:S1:408:ARG:HD2	58:S1:439:THR:HG23	1.89	0.54
64:S7:62:LEU:O	64:S7:91:VAL:HA	2.07	0.54
5:6B:15:ALA:O	36:C2:151:ARG:NH2	2.31	0.54
36:C2:138:VAL:HG12	36:C2:208:PRO:HG2	1.90	0.54
49:Qc:301:LEU:HD21	74:Qc:402:PEE:H47	1.89	0.54
53:Qg:97:GLU:OE1	53:Qg:100:ARG:NH1	2.40	0.54
66:V1:140:GLU:OE2	66:V1:256:ARG:NH1	2.40	0.54
40:CB:106:LYS:NZ	40:CB:107:ASP:OD1	2.33	0.54
41:N1:173:TRP:HE1	71:N1:403:PC1:H122	1.73	0.54
51:QE:151:LYS:HE2	51:QE:272:ILE:HD11	1.90	0.54
59:S2:464:PHE:HA	59:S2:467:VAL:HB	1.89	0.54
69:AL:201:CDL:H452	69:AL:201:CDL:H191	1.89	0.54
59:S2:160:ALA:HA	59:S2:404:THR:HG21	1.90	0.54
17:A8:95:VAL:HG12	17:A8:97:VAL:HG22	1.90	0.54
23:AN:144:THR:HG22	41:N1:96:ILE:HA	1.90	0.54
44:N4:408:LEU:HD12	45:N5:172:ILE:HG21	1.89	0.54
45:N5:253:VAL:HG23	45:N5:310:LEU:HD21	1.90	0.54
45:N5:536:LEU:HB3	45:N5:537:PRO:HD3	1.91	0.53
49:Qc:8:HIS:HB3	49:Qc:11:MET:HB2	1.89	0.53
58:S1:69:LEU:O	61:S4:158:LYS:NZ	2.29	0.53
59:S2:182:GLU:OE2	59:S2:317:TYR:OH	2.22	0.53
74:C3:304:PEE:H77	74:C3:304:PEE:H25	1.90	0.53
41:N1:160:TYR:OH	43:N3:73:LEU:O	2.26	0.53
49:Qc:24:PRO:HB2	49:Qc:27:ILE:HG23	1.91	0.53
49:Qc:237:LEU:HD13	50:Qd:297:MET:HG2	1.89	0.53
69:6A:102:CDL:HB62	56:Qj:44:TRP:HH2	1.73	0.53
32:B9:146:LEU:HD21	32:B9:160:TYR:HE2	1.74	0.53
35:C1:95:PRO:HD2	71:C3:303:PC1:H111	1.90	0.53
58:S1:449:PRO:HB2	58:S1:679:LEU:HD13	1.91	0.53
36:C2:102:HIS:CD2	36:C2:157:GLU:HG3	2.44	0.53
28:B5:147:ALA:HB2	44:N4:173:SER:HB2	1.91	0.53
38:C4:90:PHE:HA	38:C4:93:MET:HG2	1.91	0.53
45:N5:375:ILE:HD12	45:N5:458:LEU:HD11	1.90	0.53
58:S1:208:THR:HG21	58:S1:212:LYS:HB3	1.89	0.53
66:V1:55:GLY:O	66:V1:58:SER:OG	2.21	0.53
67:V2:93:LEU:HD12	67:V2:122:TYR:HB3	1.91	0.53
26:B3:20:LYS:O	26:B3:23:LYS:NZ	2.41	0.53
41:N1:139:THR:HA	41:N1:142:TYR:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:N4:133:ILE:HD11	44:N4:231:LEU:HD11	1.89	0.53
47:QA:399:GLN:HA	47:QA:402:VAL:HG22	1.90	0.53
47:Qa:35:PRO:HD2	47:Qa:54:ASN:HA	1.89	0.53
58:S1:347:ASP:OD1	58:S1:347:ASP:N	2.41	0.53
3:5B:105:VAL:HG22	3:5B:111:GLN:HB2	1.91	0.53
17:A8:246:PHE:HE1	69:CB:203:CDL:H341	1.74	0.53
35:C1:374:VAL:HA	35:C1:377:PHE:CE2	2.43	0.53
37:C3:112:LEU:HD13	37:C3:118:PRO:HG3	1.89	0.53
45:N5:241:THR:HG21	45:N5:344:GLY:HA3	1.91	0.53
48:QB:192:PHE:O	48:QB:198:ALA:HB2	2.09	0.53
69:Qb:501:CDL:HB22	71:Qb:502:PC1:H141	1.90	0.53
59:S2:227:ARG:NH1	64:S7:75:GLU:OE1	2.42	0.53
42:N2:170:LEU:HD11	42:N2:288:LEU:HD22	1.90	0.53
65:S8:63:TRP:HB3	65:S8:66:LEU:HD12	1.89	0.53
44:N4:318:ALA:HB2	44:N4:373:ILE:HG13	1.91	0.53
44:N4:375:LEU:HD11	45:N5:141:PHE:HE2	1.72	0.53
30:B7:34:ARG:HH21	31:B8:186:ILE:HB	1.74	0.52
41:N1:174:MET:HB2	41:N1:242:PHE:HA	1.91	0.52
47:QA:116:ARG:HH21	57:QK:64:LEU:HD21	1.73	0.52
48:Qb:396:ARG:NE	48:Qb:430:GLU:OE2	2.37	0.52
37:C3:101:PHE:HB2	37:C3:196:THR:HG21	1.91	0.52
39:CA:68:GLU:OE2	39:CA:71:ARG:NH2	2.42	0.52
43:N3:38:GLU:HG3	59:S2:89:ASN:HB2	1.91	0.52
66:V1:210:THR:HB	66:V1:224:ARG:H	1.73	0.52
5:6B:44:MET:HE3	5:6B:53:VAL:HG11	1.91	0.52
47:QA:123:VAL:HB	47:QA:133:LEU:HD23	1.91	0.52
49:QC:362:ILE:HA	49:QC:366:MET:HG3	1.90	0.52
20:AK:109:GLN:OE1	20:AK:328:ARG:NH1	2.36	0.52
23:AN:144:THR:HG22	41:N1:97:ASN:H	1.75	0.52
37:C3:204:HIS:NE2	37:C3:249:TRP:HB2	2.25	0.52
71:C3:303:PC1:H2B1	71:C3:303:PC1:H361	1.92	0.52
60:S3:93:VAL:HG22	60:S3:145:THR:HG21	1.92	0.52
1:4L:55:LEU:H	62:S5:25:GLN:HE22	1.56	0.52
48:QB:165:ARG:HD3	48:QB:209:ARG:HA	1.89	0.52
61:S4:112:MET:HG3	65:S8:184:LEU:HD23	1.91	0.52
18:A9:61:ALA:HB3	18:A9:82:VAL:HG13	1.92	0.52
30:B7:17:PRO:HB3	30:B7:105:GLU:HG2	1.91	0.52
36:C2:28:LEU:HA	36:C2:31:VAL:HG22	1.92	0.52
41:N1:273:ILE:HG23	41:N1:277:TYR:HD2	1.75	0.52
44:N4:405:LEU:HD21	45:N5:173:LEU:HD12	1.90	0.52
49:Qc:51:LEU:HD13	81:Qc:403:HEM:HBD1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:N4:502:CDL:H751	69:N4:502:CDL:H262	1.91	0.52
45:N5:400:ASN:HB3	45:N5:486:MET:HE3	1.90	0.52
47:QA:66:LYS:O	47:QA:217:ARG:NH2	2.42	0.52
64:S7:86:MET:HE3	64:S7:91:VAL:HG12	1.90	0.52
47:QA:167:GLN:NE2	57:QK:44:ASP:O	2.42	0.52
49:QC:100:ARG:NH1	81:QC:402:HEM:HBD1	2.25	0.52
59:S2:112:VAL:HG21	59:S2:453:VAL:HG21	1.91	0.52
58:S1:338:VAL:HB	58:S1:363:SER:HB2	1.92	0.52
58:S1:387:LEU:HD12	58:S1:514:ASN:HB3	1.92	0.52
1:4L:37:MET:HG2	1:4L:67:ALA:CB	2.38	0.51
20:AK:88:PHE:HB2	20:AK:161:LEU:HD23	1.92	0.51
45:N5:6:SER:O	45:N5:10:THR:OG1	2.18	0.51
17:A8:219:TYR:OH	28:B5:189:ASN:ND2	2.42	0.51
30:B7:29:TYR:OH	30:B7:111:ARG:NH2	2.44	0.51
47:QA:235:GLU:O	47:QA:239:ASN:ND2	2.43	0.51
50:QD:112:ARG:HB2	50:QD:140:CYS:HB2	1.92	0.51
50:QD:237:TYR:OH	52:Qf:79:ASP:OD2	2.28	0.51
59:S2:190:ILE:HG23	59:S2:209:MET:HB3	1.93	0.51
5:6B:65:CYS:O	36:C2:98:LYS:NZ	2.43	0.51
18:A9:50:SER:OG	60:S3:225:GLU:OE2	2.28	0.51
35:C1:18:LEU:HB3	35:C1:102:PHE:CZ	2.45	0.51
41:N1:123:SER:HB3	41:N1:214:GLU:HG3	1.93	0.51
49:QC:36:LEU:HD11	69:QD:402:CDL:H161	1.92	0.51
51:QE:177:ARG:HB3	51:QE:211:VAL:HG13	1.92	0.51
58:S1:405:THR:HB	58:S1:477:GLY:HA3	1.92	0.51
59:S2:180:PHE:CZ	59:S2:223:VAL:HG11	2.46	0.51
72:B5:201:PLX:H32	44:N4:3:LYS:HE2	1.91	0.51
42:N2:112:HIS:O	42:N2:116:PRO:HD2	2.11	0.51
48:QB:301:ASN:ND2	48:QB:347:CYS:SG	2.84	0.51
59:S2:101:LEU:HB2	59:S2:464:PHE:CZ	2.44	0.51
69:B5:202:CDL:H671	45:N5:12:LEU:HD13	1.92	0.51
51:QE:209:GLU:HG3	51:QE:210:TRP:CD1	2.46	0.51
53:QG:36:ASP:OD1	53:QG:90:TYR:OH	2.18	0.51
20:AK:342:SER:O	20:AK:346:ASN:ND2	2.44	0.51
45:N5:15:LEU:HD11	45:N5:94:LEU:HD21	1.93	0.51
69:N5:703:CDL:H161	69:N5:703:CDL:H592	1.92	0.51
49:QC:197:LEU:HD11	81:QC:402:HEM:HMA3	1.93	0.51
51:QE:177:ARG:HH12	51:QE:233:GLY:HA2	1.75	0.51
66:V1:357:MET:HB3	66:V1:361:THR:HG21	1.92	0.51
45:N5:419:THR:HA	45:N5:422:TYR:CE2	2.46	0.51
51:QE:151:LYS:HB3	51:QE:272:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B7:22:MET:HE1	30:B7:102:PHE:HD2	1.75	0.51
37:C3:140:SER:HB2	37:C3:242:TRP:HE1	1.75	0.51
41:N1:228:TYR:HA	41:N1:231:ILE:HD12	1.93	0.51
44:N4:76:MET:SD	44:N4:230:VAL:HB	2.51	0.51
45:N5:562:LEU:HB3	45:N5:563:PRO:HD3	1.93	0.51
48:Qb:152:GLN:HE22	48:Qb:250:PHE:HA	1.75	0.51
55:Qi:45:GLU:OE2	55:Qi:54:LYS:NZ	2.35	0.51
4:6A:51:SER:HB3	69:6A:102:CDL:H731	1.92	0.51
19:AC:156:GLU:OE1	28:B5:52:LYS:NZ	2.41	0.51
20:AK:241:ASN:HB3	20:AK:245:LYS:HE2	1.93	0.51
35:C1:229:ILE:HD11	36:C2:175:ILE:HD13	1.92	0.51
43:N3:66:ASP:O	43:N3:69:ILE:HG13	2.11	0.51
37:C3:137:LEU:HD12	37:C3:249:TRP:CD1	2.46	0.51
44:N4:211:GLY:H	44:N4:213:HIS:CD2	2.28	0.51
72:QI:301:PLX:H152	71:Qb:502:PC1:H3G1	1.92	0.51
58:S1:144:MET:HG3	59:S2:389:LYS:HG3	1.92	0.51
58:S1:611:THR:HG21	61:S4:105:GLU:HA	1.92	0.51
34:BL:77:ASP:OD1	34:BL:78:LYS:N	2.44	0.50
35:C1:260:TYR:OH	35:C1:486:GLU:OE1	2.26	0.50
16:A7:112:TYR:HE2	65:S8:43:MET:HE2	1.76	0.50
23:AN:93:GLU:HG3	62:S5:98:HIS:CD2	2.46	0.50
27:B4:14:LEU:HD12	27:B4:15:PRO:HD2	1.93	0.50
30:B7:107:ARG:HA	30:B7:110:GLN:HG2	1.92	0.50
47:Qa:115:THR:HG23	47:Qa:117:GLU:H	1.75	0.50
66:V1:119:GLU:O	66:V1:159:ARG:NH1	2.44	0.50
1:4L:62:ILE:HG21	42:N2:31:ILE:HD11	1.94	0.50
14:A5:48:THR:HA	14:A5:51:ILE:HG12	1.91	0.50
19:AB:104:PHE:HD1	19:AB:108:LEU:HD12	1.75	0.50
21:AL:124:LEU:HD11	74:AL:203:PEE:H70	1.92	0.50
36:C2:139:ASP:OD1	36:C2:139:ASP:N	2.42	0.50
44:N4:16:TRP:CE2	69:N4:502:CDL:H272	2.46	0.50
49:QC:344:GLU:HG3	54:Qh:67:PHE:HE1	1.77	0.50
48:Qb:121:ASN:ND2	48:Qb:132:TYR:OH	2.40	0.50
11:A1:49:GLU:OE1	11:A1:52:ARG:NH2	2.36	0.50
15:A6:88:LYS:NZ	15:A6:133:PHE:HA	2.26	0.50
43:N3:38:GLU:HB2	43:N3:43:PRO:HG3	1.93	0.50
44:N4:1:MET:HE2	44:N4:111:THR:HG21	1.92	0.50
51:Qe:183:GLU:O	51:Qe:187:GLU:HG2	2.12	0.50
58:S1:161:GLU:OE2	67:V2:42:ARG:NH1	2.44	0.50
60:S3:132:LEU:HB2	60:S3:141:ILE:HG22	1.93	0.50
1:4L:55:LEU:HD13	62:S5:17:TRP:HE3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4L:73:LEU:HD21	42:N2:41:ILE:HG13	1.94	0.50
11:A1:28:LYS:NZ	17:A8:168:TYR:OH	2.33	0.50
15:A6:78:LEU:HD22	15:A6:130:MET:HE3	1.93	0.50
37:C3:231:HIS:HB3	71:C3:302:PC1:H133	1.93	0.50
43:N3:35:SER:O	64:S7:98:ARG:NH2	2.44	0.50
47:QA:153:ALA:O	47:QA:156:SER:OG	2.20	0.50
60:S3:89:HIS:CG	60:S3:90:PRO:HD2	2.47	0.50
17:A8:137:GLY:O	17:A8:141:ASN:ND2	2.35	0.50
42:N2:42:PRO:HG3	46:N6:167:VAL:HG13	1.93	0.50
53:Qg:36:ASP:OD2	53:Qg:62:ARG:NH1	2.42	0.50
58:S1:43:VAL:HG12	58:S1:55:LYS:HD2	1.93	0.50
48:QB:413:ILE:HG12	48:QB:423:ARG:HD2	1.94	0.50
69:QB:501:CDL:H512	71:QB:503:PC1:H361	1.94	0.50
49:Qc:284:ILE:HD12	71:Qc:406:PC1:H352	1.93	0.50
51:Qe:244:ASP:OD2	51:Qe:250:ARG:NH2	2.41	0.50
35:C1:254:ILE:HG13	35:C1:344:PHE:CD2	2.46	0.50
44:N4:73:LEU:HA	44:N4:76:MET:HE2	1.93	0.50
66:V1:326:LEU:HD22	66:V1:363:ILE:HD11	1.92	0.50
41:N1:32:GLN:HE22	59:S2:203:MET:HE2	1.77	0.50
41:N1:113:VAL:HG13	41:N1:139:THR:HG21	1.94	0.50
46:N6:17:PHE:HA	46:N6:20:PHE:CE2	2.47	0.50
77:Qc:405:3PE:H2D2	77:Qc:405:3PE:H292	1.93	0.50
59:S2:150:MET:SD	59:S2:228:MET:HB2	2.52	0.50
77:S7:303:3PE:H352	77:S7:303:3PE:H291	1.94	0.50
66:V1:203:ALA:HB3	66:V1:206:CYS:HB2	1.92	0.50
1:4L:98:CYS:HG	42:N2:181:TYR:HH	1.56	0.49
47:Qa:61:ILE:HG12	47:Qa:130:ILE:HD11	1.93	0.49
47:Qa:81:HIS:CD2	47:Qa:192:CYS:H	2.30	0.49
49:Qc:353:LEU:HD12	77:Qc:405:3PE:H351	1.94	0.49
66:V1:112:TYR:O	66:V1:240:THR:HA	2.12	0.49
23:AN:98:MET:HE3	23:AN:101:VAL:HG21	1.94	0.49
72:CB:201:PLX:H1B3	62:S5:2:PRO:HD2	1.94	0.49
42:N2:128:LEU:HD12	42:N2:216:PHE:HB3	1.93	0.49
45:N5:534:HIS:CD2	74:N5:705:PEE:H13	2.47	0.49
48:QB:156:LEU:O	48:QB:213:ARG:NH1	2.42	0.49
51:QE:228:ALA:HB3	51:QE:235:TYR:HB3	1.94	0.49
67:V2:149:LEU:HD11	67:V2:160:VAL:HG23	1.94	0.49
31:B8:96:ASP:OD1	31:B8:96:ASP:N	2.46	0.49
49:QC:56:THR:HG21	49:Qc:58:ASP:HB2	1.95	0.49
58:S1:131:CYS:O	58:S1:241:ARG:NH1	2.39	0.49
58:S1:149:ASP:OD2	58:S1:150:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:S2:300:ARG:NH2	59:S2:407:GLU:OE2	2.45	0.49
9:7C:56:VAL:HG13	35:C1:53:ILE:HD11	1.94	0.49
18:A9:64:PHE:O	18:A9:67:ARG:HG2	2.13	0.49
28:B5:133:TYR:OH	33:BK:87:GLU:OE1	2.21	0.49
45:N5:327:LEU:O	45:N5:331:MET:HG2	2.13	0.49
49:Qc:227:LYS:HG2	50:Qd:308:LYS:HE2	1.95	0.49
58:S1:250:SER:HB2	58:S1:606:THR:HG23	1.93	0.49
65:S8:66:LEU:HD13	74:S8:303:PEE:H54	1.94	0.49
3:5B:50:GLU:OE1	3:5B:62:TYR:OH	2.30	0.49
12:A2:23:LEU:HD12	12:A2:34:ARG:HG2	1.95	0.49
17:A8:141:ASN:HD21	23:AN:81:ARG:HH21	1.61	0.49
77:C1:608:3PE:H2B1	77:C1:608:3PE:H272	1.94	0.49
48:Qb:74:TRP:CZ2	48:Qb:411:GLU:HA	2.47	0.49
66:V1:65:THR:O	66:V1:69:LEU:HG	2.11	0.49
29:B6:89:SER:HB2	29:B6:92:GLU:HB2	1.94	0.49
35:C1:38:ARG:HG3	35:C1:458:SER:HB2	1.95	0.49
47:Qa:68:GLY:O	47:Qa:208:TYR:OH	2.31	0.49
66:V1:64:LYS:HD2	67:V2:249:LEU:HD11	1.94	0.49
7:7A:63:GLY:C	37:C3:26:LEU:HD21	2.37	0.49
72:AM:201:PLX:H292	72:AM:201:PLX:H102	1.94	0.49
44:N4:233:ALA:HA	44:N4:320:GLY:HA2	1.95	0.49
47:QA:155:GLN:HE21	47:QA:198:GLY:H	1.59	0.49
69:Qb:501:CDL:HA32	71:Qb:502:PC1:H151	1.95	0.49
69:6A:102:CDL:H332	71:6A:103:PC1:H232	1.95	0.49
23:AN:49:SER:HB2	41:N1:172:ILE:HD13	1.95	0.49
35:C1:181:THR:O	35:C1:270:TYR:OH	2.19	0.49
45:N5:248:HIS:O	45:N5:253:VAL:HG22	2.12	0.49
47:Qa:66:LYS:HB2	47:Qa:217:ARG:HB3	1.95	0.49
58:S1:163:LYS:O	58:S1:171:THR:OG1	2.31	0.49
64:S7:69:LEU:HB2	64:S7:107:GLY:HA3	1.94	0.49
66:V1:162:PHE:HB3	66:V1:165:GLU:HB2	1.95	0.49
66:V1:281:HIS:ND1	66:V1:358:ASP:OD1	2.46	0.49
17:A8:202:LEU:HD13	23:AN:70:ALA:HB2	1.94	0.49
69:AL:201:CDL:H521	69:AL:201:CDL:H562	1.94	0.49
37:C3:58:TRP:CD2	71:C3:302:PC1:H252	2.48	0.49
42:N2:95:MET:HE2	42:N2:149:ILE:HA	1.94	0.49
42:N2:136:LEU:HD12	42:N2:205:LEU:HD21	1.95	0.49
44:N4:94:LEU:HD11	69:N4:502:CDL:H312	1.94	0.49
47:QA:116:ARG:NH1	47:QA:188:ASN:O	2.46	0.49
51:QE:143:SER:OG	51:QE:145:ASP:OD1	2.28	0.49
58:S1:674:LEU:HD12	58:S1:675:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AB:140:CYS:HB2	19:AB:143:GLU:HG3	1.95	0.49
22:AM:144:TYR:HD1	22:AM:144:TYR:H	1.59	0.49
69:B5:202:CDL:H821	69:N5:703:CDL:H473	1.94	0.49
29:B6:186:GLN:HG3	30:B7:89:TYR:HE2	1.77	0.49
32:B9:181:GLN:NE2	32:B9:198:PRO:O	2.44	0.49
36:C2:13:THR:HB	36:C2:168:LEU:HD23	1.95	0.49
72:CB:201:PLX:H211	42:N2:332:LEU:HD13	1.95	0.49
42:N2:238:PRO:HG2	69:N4:502:CDL:HA31	1.94	0.49
45:N5:190:LEU:HB2	45:N5:196:TRP:NE1	2.28	0.49
45:N5:399:VAL:HG12	45:N5:409:LEU:HD13	1.94	0.49
47:QA:104:GLU:OE1	48:QB:325:SER:OG	2.30	0.49
48:QB:100:GLY:HA2	48:QB:106:GLY:N	2.25	0.49
52:QF:60:ARG:HD3	52:QF:63:THR:HG21	1.95	0.49
52:Qf:28:ASP:HB3	52:Qf:29:PRO:HD3	1.94	0.49
58:S1:389:THR:HG21	58:S1:473:MET:HE2	1.94	0.49
58:S1:624:ARG:NH2	58:S1:637:ASP:OD1	2.41	0.49
66:V1:302:LYS:HE3	66:V1:303:HIS:CE1	2.47	0.49
14:A5:49:GLU:O	14:A5:53:ASN:ND2	2.42	0.48
48:QB:80:ARG:NH2	48:QB:350:GLU:OE1	2.44	0.48
10:8B:52:ILE:HB	10:8B:53:PRO:HD3	1.95	0.48
18:A9:344:PRO:HG2	18:A9:347:LEU:HD13	1.95	0.48
42:N2:173:THR:HG22	59:S2:58:MET:HG2	1.95	0.48
45:N5:566:THR:O	45:N5:570:GLN:HG2	2.14	0.48
48:QB:107:SER:HA	48:QB:110:GLU:HG2	1.96	0.48
48:QB:465:LEU:HD12	48:QB:466:PRO:HD2	1.94	0.48
66:V1:192:ASP:HB3	68:V3:411:MET:SD	2.53	0.48
66:V1:347:THR:HG22	66:V1:348:GLY:H	1.78	0.48
35:C1:251:PHE:HB3	35:C1:319:LYS:HE2	1.95	0.48
41:N1:176:PHE:HE2	71:N1:403:PC1:H3I2	1.78	0.48
43:N3:79:SER:HA	43:N3:87:MET:HE2	1.95	0.48
59:S2:142:PHE:HZ	59:S2:428:CYS:SG	2.36	0.48
66:V1:112:TYR:CD1	66:V1:153:ALA:HB3	2.48	0.48
66:V1:288:VAL:HG21	66:V1:303:HIS:CD2	2.48	0.48
68:V3:420:SER:HB3	68:V3:423:HIS:ND1	2.28	0.48
17:A8:115:LYS:HB3	17:A8:116:PRO:HD3	1.95	0.48
48:QB:460:GLY:HA2	48:QB:462:ILE:HG12	1.95	0.48
49:QC:112:THR:HG22	49:QC:196:HIS:CE1	2.48	0.48
48:Qb:383:ALA:HB3	48:Qb:442:ARG:HG3	1.96	0.48
51:Qe:214:ILE:HG13	51:Qe:261:PRO:HD3	1.94	0.48
51:Qe:228:ALA:HB3	51:Qe:235:TYR:HB3	1.95	0.48
59:S2:445:SER:HB2	59:S2:453:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:V1:263:ALA:HA	66:V1:271:SER:HB3	1.95	0.48
17:A8:124:ARG:NE	23:AN:80:ASP:OD2	2.44	0.48
37:C3:140:SER:O	37:C3:144:ILE:HG12	2.12	0.48
44:N4:216:LEU:HB3	44:N4:217:PRO:HD3	1.95	0.48
48:QB:126:ARG:NH1	48:QB:199:GLN:O	2.46	0.48
19:AB:90:TYR:HD2	19:AB:93:ILE:HG12	1.79	0.48
23:AN:95:ALA:HA	23:AN:106:VAL:HG11	1.95	0.48
37:C3:187:THR:OG1	37:C3:188:ILE:N	2.47	0.48
41:N1:24:GLU:HA	41:N1:271:LEU:HD13	1.96	0.48
49:QC:141:TRP:CD1	49:QC:265:PRO:HD3	2.49	0.48
53:QG:71:MET:HE2	50:Qd:316:LYS:HD3	1.96	0.48
48:Qb:360:CYS:SG	48:Qb:368:MET:HG3	2.53	0.48
12:A2:18:GLU:HG2	12:A2:68:ARG:HB3	1.95	0.48
30:B7:103:GLU:O	30:B7:107:ARG:HG2	2.13	0.48
32:B9:150:HIS:CD2	32:B9:151:PRO:HD2	2.49	0.48
36:C2:103:GLN:HG2	36:C2:158:ASP:CG	2.39	0.48
37:C3:125:ASN:HD22	37:C3:128:GLU:HG3	1.78	0.48
45:N5:292:ALA:HB2	45:N5:304:PHE:HB3	1.96	0.48
45:N5:383:MET:O	45:N5:389:PHE:HB2	2.14	0.48
21:AL:81:ARG:HH11	21:AL:89:ASN:HD21	1.62	0.48
49:QC:8:HIS:HB3	49:QC:11:MET:HB2	1.96	0.48
59:S2:140:PRO:HB2	64:S7:142:TYR:CE2	2.49	0.48
66:V1:113:LEU:O	66:V1:154:ALA:HA	2.13	0.48
35:C1:173:PRO:HD2	35:C1:176:MET:HE2	1.94	0.48
40:CB:32:ARG:O	40:CB:36:MET:HG2	2.14	0.48
45:N5:341:MET:HE2	45:N5:454:ILE:HG12	1.96	0.48
48:QB:222:GLN:NE2	48:QB:261:ALA:O	2.47	0.48
59:S2:143:ASP:OD1	59:S2:150:MET:HB3	2.13	0.48
59:S2:180:PHE:HZ	59:S2:223:VAL:HG11	1.79	0.48
66:V1:364:VAL:HG12	66:V1:400:VAL:HG12	1.96	0.48
32:B9:119:PRO:HB3	45:N5:525:MET:HE2	1.96	0.48
36:C2:151:ARG:HD3	36:C2:153:LEU:HD21	1.95	0.48
67:V2:137:THR:HG22	67:V2:138:THR:H	1.79	0.48
1:4L:31:LEU:HD21	46:N6:67:VAL:HG11	1.96	0.47
71:6A:101:PC1:H142	37:C3:181:TYR:O	2.13	0.47
22:AM:55:PHE:CZ	22:AM:58:ARG:HG3	2.49	0.47
48:QB:110:GLU:HA	48:QB:113:VAL:HG22	1.95	0.47
53:Qg:44:VAL:O	53:Qg:48:ILE:HG12	2.14	0.47
58:S1:509:ASP:OD1	58:S1:509:ASP:N	2.44	0.47
7:7A:56:THR:HG21	37:C3:56:GLN:HE22	1.80	0.47
18:A9:328:THR:HG22	18:A9:330:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C1:413:HIS:CE1	35:C1:468:MET:HB2	2.49	0.47
44:N4:12:LEU:HB2	44:N4:13:PRO:HD3	1.96	0.47
48:QB:79:SER:OG	48:QB:201:VAL:HA	2.14	0.47
56:QJ:14:ALA:O	56:QJ:18:ILE:HG12	2.14	0.47
58:S1:219:SER:O	58:S1:222:ILE:HG12	2.15	0.47
58:S1:308:ARG:NH1	58:S1:312:GLY:O	2.45	0.47
72:AM:201:PLX:H81	72:S7:302:PLX:H72	1.95	0.47
24:B1:30:ARG:NH1	24:B1:33:GLU:OE2	2.47	0.47
29:B6:165:PHE:O	29:B6:168:ASP:HB2	2.14	0.47
37:C3:257:TYR:O	37:C3:261:SER:OG	2.23	0.47
41:N1:202:GLU:HG3	41:N1:212:ASN:HD21	1.79	0.47
44:N4:82:SER:HB2	44:N4:432:ARG:CZ	2.45	0.47
45:N5:559:GLU:O	45:N5:564:LYS:HB2	2.14	0.47
49:QC:116:GLY:HA3	81:QC:402:HEM:C3C	2.50	0.47
48:Qb:152:GLN:NE2	48:Qb:250:PHE:HA	2.30	0.47
81:Qc:404:HEM:HHA	81:Qc:404:HEM:HBA1	1.96	0.47
64:S7:108:THR:HA	64:S7:136:CYS:HB3	1.96	0.47
18:A9:272:LEU:HG	18:A9:375:VAL:HG21	1.97	0.47
34:BL:90:VAL:HG22	44:N4:28:THR:HG21	1.95	0.47
36:C2:96:THR:OG1	36:C2:151:ARG:NH1	2.47	0.47
44:N4:82:SER:HB2	44:N4:432:ARG:NH1	2.29	0.47
44:N4:369:LEU:HD21	45:N5:149:ILE:HD13	1.97	0.47
45:N5:368:PHE:HZ	45:N5:455:LYS:HG3	1.80	0.47
49:Qc:248:ASP:OD2	50:Qd:203:ARG:NE	2.46	0.47
50:Qd:211:TYR:OH	82:Qd:401:HEC:O1A	2.14	0.47
59:S2:145:LEU:HD13	59:S2:430:ILE:HG21	1.96	0.47
63:S6:74:GLN:HG3	65:S8:108:SER:HB2	1.96	0.47
3:5B:105:VAL:HA	3:5B:111:GLN:HG3	1.95	0.47
15:A6:66:TYR:CE2	15:A6:86:ARG:HD3	2.49	0.47
17:A8:160:THR:HA	17:A8:163:TRP:CD1	2.49	0.47
47:Qa:70:ARG:HD2	47:Qa:117:GLU:HG2	1.97	0.47
48:Qb:99:LYS:NZ	48:Qb:164:GLU:OE2	2.47	0.47
48:Qb:302:VAL:HB	48:Qb:303:PRO:HD3	1.95	0.47
53:Qg:14:LEU:HD12	53:Qg:17:ILE:HD11	1.96	0.47
58:S1:251:ILE:HG21	58:S1:604:GLN:HB3	1.95	0.47
58:S1:428:LYS:HE2	58:S1:465:ILE:HD13	1.97	0.47
59:S2:323:ASP:OD1	65:S8:37:THR:OG1	2.31	0.47
34:BL:106:VAL:HG13	44:N4:453:MET:HE3	1.96	0.47
35:C1:124:THR:HG22	35:C1:132:LEU:HG	1.96	0.47
36:C2:158:ASP:OD1	36:C2:159:VAL:N	2.46	0.47
41:N1:213:VAL:HG13	41:N1:214:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:QD:248:PRO:HB2	82:QD:401:HEC:HBB2	1.95	0.47
49:Qc:200:LEU:HD22	81:Qc:404:HEM:HAA1	1.95	0.47
50:Qd:322:TYR:CZ	50:Qd:324:PRO:HG3	2.50	0.47
58:S1:86:PRO:O	58:S1:108:LYS:NZ	2.47	0.47
2:5A:68:ASP:OD1	2:5A:68:ASP:N	2.47	0.47
5:6B:25:ASN:ND2	5:6B:27:THR:OG1	2.46	0.47
74:AL:203:PEE:H27	74:AL:203:PEE:H64	1.97	0.47
31:B8:110:ASP:HB3	44:N4:278:ARG:HH11	1.80	0.47
32:B9:143:GLU:O	32:B9:164:ARG:NH2	2.48	0.47
35:C1:51:ASP:O	35:C1:55:ASN:ND2	2.46	0.47
35:C1:383:MET:HE3	35:C1:421:VAL:HG23	1.97	0.47
78:C1:601:HEA:HHa	78:C1:601:HEA:HBD2	1.96	0.47
40:CB:19:GLU:OE2	40:CB:83:TYR:OH	2.26	0.47
40:CB:51:ARG:CZ	42:N2:322:GLN:HG2	2.45	0.47
45:N5:2:ASN:ND2	45:N5:59:GLN:OE1	2.48	0.47
49:QC:237:LEU:HD22	50:QD:301:LEU:HD11	1.96	0.47
48:Qb:120:LEU:HD13	48:Qb:133:ILE:HG12	1.96	0.47
52:Qf:60:ARG:NH1	54:Qh:78:TYR:O	2.46	0.47
58:S1:476:LEU:HD21	58:S1:481:LEU:HD21	1.96	0.47
59:S2:147:TYR:CB	64:S7:71:CYS:HB3	2.44	0.47
66:V1:113:LEU:HD13	66:V1:149:MET:HE1	1.96	0.47
66:V1:326:LEU:HD23	66:V1:367:ILE:HD11	1.96	0.47
21:AL:36:VAL:HG22	69:AL:201:CDL:H742	1.97	0.47
26:B3:47:ARG:HA	26:B3:50:ALA:HB3	1.96	0.47
42:N2:210:THR:HG22	42:N2:333:SER:HB3	1.97	0.47
44:N4:443:PRO:HB3	72:N4:501:PLX:H351	1.97	0.47
48:QB:56:GLY:HA3	48:QB:227:PRO:HB3	1.97	0.47
51:Qe:165:MET:HB3	51:Qe:176:VAL:HG23	1.97	0.47
58:S1:127:ASP:O	58:S1:131:CYS:HB2	2.14	0.47
71:6A:101:PC1:H151	37:C3:184:ALA:O	2.15	0.47
35:C1:176:MET:HE3	35:C1:181:THR:HG22	1.97	0.47
78:C1:601:HEA:H212	78:C1:601:HEA:H271	1.51	0.47
38:C4:41:ARG:HB2	38:C4:44:TYR:HB3	1.97	0.47
49:QC:152:ALA:HB2	49:QC:287:LYS:HG2	1.96	0.47
50:Qd:228:LEU:HD11	50:Qd:234:PHE:HB2	1.96	0.47
59:S2:167:ILE:HD13	59:S2:369:VAL:HG11	1.97	0.47
59:S2:188:ASN:OD1	59:S2:410:LYS:NZ	2.48	0.47
74:S2:501:PEE:H30	74:S2:501:PEE:H23	1.49	0.47
2:5A:76:MET:HE2	2:5A:110:ILE:HG12	1.96	0.47
8:7B:53:TRP:NE1	38:C4:111:ILE:HG22	2.29	0.47
24:B1:57:TRP:NE1	28:B5:134:GLU:OE1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:N4:79:ALA:O	44:N4:82:SER:HB3	2.15	0.47
44:N4:106:LEU:HD13	44:N4:234:VAL:HG11	1.96	0.47
72:QI:301:PLX:H192	49:Qc:236:MET:HG3	1.97	0.47
59:S2:448:HIS:HB3	59:S2:452:ASP:HB2	1.97	0.47
1:4L:75:LEU:O	1:4L:79:VAL:HG13	2.15	0.46
2:5A:109:ARG:HD2	38:C4:86:PHE:CE1	2.50	0.46
35:C1:371:TYR:HE2	35:C1:436:MET:HE2	1.80	0.46
42:N2:243:LEU:HD22	42:N2:330:ILE:HG21	1.96	0.46
48:Qb:465:LEU:HD12	48:Qb:466:PRO:HD2	1.97	0.46
69:4L:201:CDL:HA61	21:AL:49:PHE:HA	1.97	0.46
3:5B:112:ARG:HA	3:5B:118:THR:O	2.16	0.46
9:7C:49:PHE:CG	10:8B:50:PHE:HD2	2.33	0.46
13:A3:135:PRO:HB2	23:AN:69:ILE:HD11	1.95	0.46
17:A8:141:ASN:HD21	23:AN:81:ARG:NH2	2.13	0.46
17:A8:248:THR:OG1	69:CB:203:CDL:HA31	2.16	0.46
71:N1:403:PC1:H2E2	71:N1:403:PC1:H2A2	1.97	0.46
42:N2:186:HIS:O	42:N2:190:MET:HG3	2.15	0.46
45:N5:78:LEU:HD13	74:N5:701:PEE:H40	1.97	0.46
47:QA:134:MET:HE2	47:QA:233:VAL:HG21	1.97	0.46
47:QA:306:THR:OG1	48:QB:114:GLU:OE1	2.27	0.46
3:5B:43:GLN:NE2	37:C3:225:PHE:O	2.38	0.46
35:C1:440:TYR:OH	36:C2:196:CYS:O	2.28	0.46
51:QE:110:ARG:NH1	54:Qh:22:PHE:O	2.39	0.46
48:Qb:42:LEU:HD22	48:Qb:426:LEU:HB3	1.96	0.46
50:Qd:118:TYR:HA	50:Qd:122:CYS:SG	2.55	0.46
50:Qd:122:CYS:SG	82:Qd:401:HEC:HAB	2.55	0.46
1:4L:76:SER:O	1:4L:79:VAL:HG22	2.15	0.46
18:A9:293:LEU:HD12	18:A9:294:PRO:HD2	1.98	0.46
69:AL:202:CDL:H162	69:AL:202:CDL:H332	1.97	0.46
29:B6:132:VAL:O	29:B6:136:LEU:CB	2.63	0.46
35:C1:62:ALA:HB2	78:C1:601:HEA:HBD1	1.98	0.46
57:QK:64:LEU:HA	57:QK:77:ARG:O	2.15	0.46
75:AC:201:ZMP:H5A	32:B9:109:ALA:HB1	1.96	0.46
45:N5:213:LEU:HD23	45:N5:213:LEU:HA	1.76	0.46
45:N5:526:LEU:HD12	45:N5:530:PRO:HG3	1.97	0.46
49:Qc:112:THR:HG22	49:Qc:196:HIS:CE1	2.50	0.46
60:S3:119:VAL:HG12	60:S3:121:THR:HG22	1.97	0.46
69:N1:401:CDL:H342	69:N1:401:CDL:H721	1.97	0.46
47:Qa:92:LYS:HD3	47:Qa:143:ALA:HB1	1.97	0.46
59:S2:391:TYR:HD1	65:S8:122:VAL:HG21	1.80	0.46
18:A9:198:ALA:O	18:A9:260:GLY:HA2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A9:217:PHE:HA	18:A9:220:MET:HE2	1.97	0.46
27:B4:25:ILE:HG21	27:B4:30:ARG:CZ	2.45	0.46
29:B6:181:LYS:NZ	30:B7:38:GLU:OE2	2.49	0.46
72:N4:501:PLX:H22	72:N4:501:PLX:H1C3	1.72	0.46
47:QA:298:HIS:HB2	48:QB:114:GLU:HG2	1.97	0.46
55:QI:30:LEU:HD13	56:QJ:34:TRP:HB2	1.98	0.46
48:Qb:315:ASP:OD1	48:Qb:316:SER:N	2.48	0.46
58:S1:180:THR:N	84:S1:802:SF4:S4	2.83	0.46
58:S1:488:ALA:HB2	58:S1:677:GLN:HG3	1.97	0.46
68:V3:386:TYR:CZ	68:V3:388:ASN:HB3	2.50	0.46
8:7B:71:ARG:HG3	8:7B:72:VAL:HG23	1.97	0.46
74:AL:203:PEE:H1	44:N4:191:SER:HB3	1.98	0.46
35:C1:98:ASN:HB2	35:C1:163:ASN:ND2	2.31	0.46
37:C3:100:ALA:O	37:C3:104:SER:OG	2.27	0.46
40:CB:13:LEU:HD21	62:S5:4:PHE:HB3	1.96	0.46
71:N1:402:PC1:H221	43:N3:3:ILE:HG12	1.96	0.46
43:N3:56:PHE:O	46:N6:70:TYR:OH	2.32	0.46
47:QA:313:VAL:HG11	47:QA:350:VAL:HG13	1.98	0.46
58:S1:385:TYR:OH	58:S1:527:ASP:OD1	2.24	0.46
58:S1:389:THR:OG1	58:S1:511:LYS:O	2.34	0.46
59:S2:194:THR:HG21	59:S2:209:MET:HB2	1.97	0.46
1:4L:4:VAL:O	1:4L:8:ILE:HG12	2.15	0.46
71:6A:101:PC1:H341	37:C3:202:GLY:HA3	1.97	0.46
18:A9:64:PHE:HZ	18:A9:208:GLY:HA3	1.80	0.46
19:AC:112:SER:HB3	32:B9:59:LEU:HD11	1.98	0.46
24:B1:42:SER:O	24:B1:46:LYS:HB2	2.16	0.46
36:C2:101:GLY:HA3	36:C2:161:HIS:HD2	1.80	0.46
44:N4:267:TRP:O	44:N4:271:MET:HG2	2.16	0.46
45:N5:298:ILE:O	45:N5:302:VAL:HG23	2.15	0.46
54:QH:29:HIS:O	54:QH:33:LYS:HG2	2.16	0.46
72:QI:301:PLX:H22	72:QI:301:PLX:H1C3	1.62	0.46
47:Qa:66:LYS:O	47:Qa:217:ARG:NH2	2.41	0.46
47:Qa:71:TYR:HB3	47:Qa:212:HIS:CE1	2.51	0.46
5:6B:66:PRO:HD3	36:C2:179:LEU:HD11	1.97	0.46
22:AM:127:TYR:OH	63:S6:61:GLU:O	2.22	0.46
42:N2:19:LEU:O	42:N2:23:SER:OG	2.31	0.46
46:N6:122:LEU:HG	46:N6:123:GLY:H	1.80	0.46
48:QB:388:VAL:HG21	48:QB:438:ALA:HA	1.98	0.46
49:QC:101:GLY:HA2	49:QC:106:SER:HB2	1.97	0.46
58:S1:338:VAL:HB	58:S1:363:SER:CB	2.46	0.46
59:S2:321:GLU:O	59:S2:352:GLN:NE2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A8:174:PHE:HB3	17:A8:178:ARG:HH12	1.82	0.45
27:B4:26:SER:OG	27:B4:28:GLU:OE1	2.33	0.45
28:B5:139:ILE:HG23	44:N4:54:LEU:HD23	1.98	0.45
35:C1:508:PRO:HG3	37:C3:6:HIS:HB3	1.98	0.45
51:Qe:239:HIS:HB2	83:Qe:301:FES:S2	2.56	0.45
54:Qh:27:PHE:CD1	71:Qh:101:PC1:H12	2.50	0.45
19:AC:120:MET:HE1	32:B9:66:LEU:HB3	1.98	0.45
69:AK:402:CDL:H362	69:AK:402:CDL:H141	1.98	0.45
29:B6:157:VAL:HG22	45:N5:63:ILE:HG23	1.99	0.45
33:BK:144:SER:HB3	33:BK:158:LYS:NZ	2.31	0.45
41:N1:59:GLU:HG3	43:N3:27:LEU:HD13	1.99	0.45
41:N1:142:TYR:CE1	41:N1:192:GLU:HG2	2.51	0.45
56:Qj:38:TRP:CG	77:Qj:101:3PE:H221	2.51	0.45
58:S1:130:ILE:HG23	65:S8:114:ILE:HD12	1.97	0.45
66:V1:88:ARG:HD2	66:V1:274:LYS:HE2	1.98	0.45
66:V1:118:ASP:HA	66:V1:159:ARG:HB3	1.97	0.45
66:V1:141:GLY:HA2	66:V1:252:PRO:HD3	1.98	0.45
16:A7:12:ARG:HB3	16:A7:20:LEU:HD12	1.97	0.45
32:B9:77:ASP:OD1	32:B9:77:ASP:N	2.48	0.45
35:C1:230:LEU:HB2	37:C3:103:HIS:CD2	2.50	0.45
35:C1:375:ALA:HB1	35:C1:429:HIS:CE1	2.52	0.45
37:C3:86:PHE:CZ	71:C3:302:PC1:H3A1	2.51	0.45
37:C3:204:HIS:CE1	37:C3:249:TRP:HB2	2.51	0.45
41:N1:134:ARG:NH2	59:S2:110:GLU:OE2	2.43	0.45
47:Qa:79:THR:HG23	47:Qa:205:LEU:HD23	1.99	0.45
48:Qb:276:ARG:NH2	48:Qb:466:PRO:O	2.46	0.45
67:V2:128:GLY:H	67:V2:170:THR:HG1	1.59	0.45
25:B2:79:MET:SD	45:N5:375:ILE:HG12	2.57	0.45
33:BK:74:ILE:HG23	33:BK:156:LEU:HD22	1.98	0.45
36:C2:192:TYR:CE2	36:C2:213:LEU:HD12	2.52	0.45
71:QB:503:PC1:H222	49:QC:4:ILE:HD11	1.98	0.45
69:QH:401:CDL:OA7	49:Qc:29:SER:OG	2.20	0.45
50:Qd:149:LEU:O	50:Qd:152:GLU:HG2	2.16	0.45
58:S1:107:GLU:OE2	58:S1:111:LYS:NZ	2.49	0.45
5:6B:58:ARG:HA	5:6B:61:TYR:CE2	2.52	0.45
16:A7:39:PRO:HG3	65:S8:211:TYR:CZ	2.51	0.45
72:N3:202:PLX:H72	72:N3:202:PLX:H4	1.65	0.45
45:N5:66:TRP:HZ3	74:N5:701:PEE:H36	1.82	0.45
47:Qa:91:THR:HG21	47:Qa:140:VAL:HA	1.97	0.45
15:A6:127:THR:HG23	60:S3:219:VAL:O	2.16	0.45
29:B6:164:ILE:HD12	29:B6:170:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:C3:9:HIS:CD2	71:C3:303:PC1:H133	2.50	0.45
58:S1:575:VAL:C	58:S1:578:PRO:HD2	2.41	0.45
66:V1:325:PRO:HG3	66:V1:433:TRP:HB3	1.98	0.45
2:5A:102:ASN:HD22	38:C4:67:LYS:HG2	1.80	0.45
3:5B:79:LEU:HD13	3:5B:123:VAL:HG21	1.98	0.45
35:C1:423:MET:HE3	77:C1:608:3PE:H321	1.99	0.45
40:CB:35:TYR:OH	42:N2:335:LEU:O	2.33	0.45
74:N3:201:PEE:H30	74:N3:201:PEE:H36	1.76	0.45
74:N3:201:PEE:H67	74:N3:201:PEE:H72	1.63	0.45
44:N4:383:THR:HG21	45:N5:190:LEU:HD22	1.98	0.45
72:QB:504:PLX:H82	50:QD:307:MET:HE1	1.99	0.45
47:Qa:234:ALA:O	47:Qa:239:ASN:HB2	2.17	0.45
47:Qa:320:PRO:HG2	47:Qa:343:GLN:HE21	1.82	0.45
58:S1:339:ALA:HA	58:S1:365:SER:HB2	1.99	0.45
58:S1:422:TRP:HA	58:S1:427:LEU:HB3	1.98	0.45
17:A8:117:ASN:HB3	23:AN:73:PRO:HG2	1.99	0.45
41:N1:114:TYR:OH	46:N6:61:LEU:O	2.25	0.45
44:N4:119:TYR:CZ	44:N4:161:LEU:HB2	2.51	0.45
47:QA:271:LEU:HD22	47:QA:453:LEU:HD13	1.98	0.45
50:QD:112:ARG:NH2	50:QD:145:GLU:OE1	2.49	0.45
58:S1:47:THR:O	58:S1:96:VAL:HG22	2.16	0.45
67:V2:59:ASN:HD21	67:V2:89:GLN:HB2	1.81	0.45
4:6A:28:TRP:CD1	37:C3:149:HIS:HD1	2.35	0.45
4:6A:79:HIS:HD2	4:6A:83:HIS:CD2	2.34	0.45
71:C3:301:PC1:H292	71:C3:301:PC1:H2D2	1.98	0.45
40:CB:2:THR:HB	40:CB:5:SER:HB3	1.98	0.45
42:N2:137:ALA:HB3	42:N2:138:PRO:HD3	1.99	0.45
48:QB:374:GLY:HA3	71:QB:503:PC1:H151	1.99	0.45
47:Qa:313:VAL:HG11	47:Qa:350:VAL:HG13	1.98	0.45
59:S2:190:ILE:HD11	59:S2:257:PHE:HZ	1.82	0.45
59:S2:194:THR:HB	59:S2:206:PHE:HA	1.99	0.45
59:S2:222:ARG:NH1	59:S2:249:ASP:OD2	2.24	0.45
66:V1:235:VAL:H	66:V1:240:THR:HG21	1.82	0.45
20:AK:357:LYS:HD3	39:CA:36:HIS:O	2.17	0.45
35:C1:48:LEU:HD13	35:C1:57:ILE:HD12	1.98	0.45
52:QF:65:GLU:HG3	54:QH:73:LYS:NZ	2.32	0.45
59:S2:190:ILE:HD11	59:S2:257:PHE:CZ	2.52	0.45
6:6C:20:ARG:O	6:6C:23:ILE:HG22	2.17	0.44
9:7C:52:PRO:HG3	35:C1:29:VAL:HG13	1.99	0.44
16:A7:54:TYR:CE2	59:S2:368:LYS:HD2	2.53	0.44
33:BK:74:ILE:O	40:CB:111:TYR:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C1:265:LYS:HD2	35:C1:490:THR:HG21	1.99	0.44
42:N2:25:HIS:HB2	62:S5:15:ASP:HB2	2.00	0.44
45:N5:230:HIS:H	45:N5:230:HIS:CD2	2.34	0.44
50:QD:120:GLN:HB2	50:QD:254:LEU:HD11	1.99	0.44
58:S1:124:HIS:CG	58:S1:125:PRO:HD2	2.52	0.44
58:S1:382:ARG:C	58:S1:384:ASN:H	2.25	0.44
59:S2:46:ASP:OD1	59:S2:46:ASP:N	2.49	0.44
59:S2:430:ILE:HB	59:S2:469:ARG:HD2	1.99	0.44
69:4L:201:CDL:OB9	46:N6:23:LYS:NZ	2.49	0.44
6:6C:16:ALA:O	6:6C:20:ARG:HG3	2.17	0.44
17:A8:235:LEU:HD23	17:A8:235:LEU:HA	1.86	0.44
48:QB:310:ILE:HD11	48:QB:388:VAL:HA	1.99	0.44
49:QC:236:MET:HG2	74:QE:301:PEE:H61	1.98	0.44
49:Qc:200:LEU:CD2	81:Qc:404:HEM:HAA1	2.47	0.44
8:7B:53:TRP:CE2	38:C4:115:ALA:HB2	2.51	0.44
35:C1:378:HIS:HE1	78:C1:601:HEA:NA	2.09	0.44
36:C2:144:LEU:HB2	36:C2:213:LEU:HD23	1.99	0.44
72:CB:201:PLX:H112	72:CB:201:PLX:H81	1.72	0.44
46:N6:129:ASP:HB2	62:S5:32:ARG:NH1	2.32	0.44
57:QK:20:ARG:HD2	48:Qb:318:TYR:CE1	2.52	0.44
48:Qb:294:PRO:HG3	48:Qb:448:TYR:CZ	2.53	0.44
52:Qf:45:LYS:O	52:Qf:48:GLU:HG2	2.17	0.44
72:S7:302:PLX:H381	77:S7:303:3PE:H3C2	1.99	0.44
66:V1:375:LYS:HD2	66:V1:393:ASN:ND2	2.32	0.44
6:6C:69:GLY:HA3	8:7B:79:GLU:HG3	1.98	0.44
9:7C:36:ARG:HG2	9:7C:40:MET:HE2	1.99	0.44
18:A9:126:VAL:HG23	18:A9:161:VAL:HG11	2.00	0.44
37:C3:173:PHE:CE2	37:C3:208:VAL:HG21	2.53	0.44
42:N2:43:VAL:HG11	42:N2:129:LEU:HD23	1.98	0.44
19:AC:90:TYR:HE1	26:B3:44:PRO:HB2	1.83	0.44
69:AL:201:CDL:H401	69:AL:201:CDL:H771	1.99	0.44
32:B9:218:GLU:HG2	32:B9:219:ARG:HG2	2.00	0.44
35:C1:3:VAL:HG13	35:C1:7:LEU:HD12	1.98	0.44
36:C2:161:HIS:CE1	36:C2:207:MET:HE1	2.53	0.44
37:C3:79:LEU:HD21	71:C3:303:PC1:H143	2.00	0.44
45:N5:49:VAL:HB	45:N5:50:PRO:HD3	1.99	0.44
47:QA:84:ARG:NH2	47:QA:190:LEU:O	2.50	0.44
47:Qa:230:LEU:HD23	47:Qa:230:LEU:HA	1.88	0.44
50:Qd:200:TYR:O	50:Qd:204:ALA:CB	2.66	0.44
58:S1:222:ILE:HA	58:S1:225:ILE:HG12	2.00	0.44
16:A7:25:GLN:O	59:S2:215:LYS:NZ	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:AC:201:ZMP:H1	32:B9:113:PHE:HA	1.98	0.44
35:C1:184:PHE:H	35:C1:256:HIS:HE1	1.65	0.44
42:N2:168:GLY:O	42:N2:172:GLN:HG2	2.17	0.44
44:N4:210:TYR:CG	44:N4:268:GLY:HA3	2.52	0.44
46:N6:82:VAL:HG22	46:N6:83:TRP:H	1.83	0.44
72:QB:504:PLX:H251	72:QB:504:PLX:H52	1.78	0.44
49:QC:102:LEU:HD22	49:QC:304:MET:HE2	1.99	0.44
51:QE:186:GLN:O	51:QE:190:VAL:HG23	2.17	0.44
55:Qi:54:LYS:HA	55:Qi:57:LYS:HE3	1.99	0.44
66:V1:174:ARG:HA	68:V3:406:LEU:HD21	2.00	0.44
66:V1:384:PRO:HG2	66:V1:422:HIS:O	2.18	0.44
30:B7:95:TYR:CZ	31:B8:156:VAL:HG11	2.53	0.44
35:C1:331:ASN:OD1	38:C4:42:ARG:NH1	2.49	0.44
72:N4:501:PLX:H181	72:N4:501:PLX:H211	1.77	0.44
49:Qc:119:LEU:HD22	81:Qc:404:HEM:HBB2	1.98	0.44
58:S1:241:ARG:HG2	65:S8:117:LYS:HD2	2.00	0.44
20:AK:42:PRO:HG2	69:AK:402:CDL:HB62	1.99	0.44
37:C3:210:ILE:HD13	71:C3:302:PC1:H3B1	2.00	0.44
46:N6:77:GLU:N	46:N6:77:GLU:OE1	2.51	0.44
46:N6:82:VAL:HG12	46:N6:85:SER:HB2	1.99	0.44
48:QB:74:TRP:CZ2	48:QB:411:GLU:HA	2.53	0.44
56:QJ:4:ARG:HA	53:Qg:110:LYS:HD3	1.98	0.44
47:Qa:299:VAL:HG22	48:Qb:120:LEU:HB3	1.99	0.44
58:S1:476:LEU:HD22	58:S1:493:VAL:HG21	1.99	0.44
58:S1:692:LYS:HD3	58:S1:715:THR:HG22	2.00	0.44
66:V1:140:GLU:CD	66:V1:256:ARG:HH12	2.25	0.44
66:V1:269:ARG:NH1	66:V1:340:ASP:OD2	2.50	0.44
69:AK:402:CDL:H402	42:N2:133:TRP:HZ3	1.82	0.44
41:N1:273:ILE:HG23	41:N1:277:TYR:CD2	2.51	0.44
72:QB:504:PLX:H22	72:QB:504:PLX:H1C3	1.79	0.44
50:Qd:104:SER:O	50:Qd:287:LYS:NZ	2.51	0.44
63:S6:111:CYS:O	63:S6:115:GLY:N	2.51	0.44
74:AL:203:PEE:H31	74:AL:203:PEE:H26	1.78	0.43
35:C1:372:TYR:N	35:C1:432:GLY:HA3	2.33	0.43
37:C3:244:PHE:HB2	74:C3:304:PEE:H70	2.00	0.43
42:N2:298:TYR:O	42:N2:303:THR:OG1	2.26	0.43
44:N4:197:LEU:HD21	69:N4:503:CDL:H111	1.99	0.43
45:N5:5:ALA:HB2	45:N5:61:MET:HE1	1.98	0.43
45:N5:237:MET:HB3	45:N5:299:LYS:HE3	2.00	0.43
47:Qa:147:ARG:HD3	47:Qa:149:TRP:CZ2	2.53	0.43
48:Qb:38:TYR:CZ	48:Qb:42:LEU:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:Qj:2:LEU:HB2	56:Qj:3:SER:H	1.63	0.43
66:V1:381:GLN:N	84:V1:501:SF4:S4	2.90	0.43
67:V2:186:VAL:HG22	67:V2:196:LEU:HD11	2.00	0.43
17:A8:160:THR:HA	17:A8:163:TRP:NE1	2.34	0.43
24:B1:30:ARG:O	24:B1:33:GLU:HG2	2.18	0.43
69:N1:401:CDL:HB31	46:N6:82:VAL:HG21	2.00	0.43
42:N2:197:ASN:HB2	42:N2:269:GLU:HG2	1.99	0.43
69:N5:704:CDL:H181	69:N5:704:CDL:H221	2.01	0.43
47:QA:155:GLN:NE2	47:QA:198:GLY:H	2.16	0.43
48:QB:480:PHE:O	55:Qi:18:THR:HG22	2.18	0.43
51:QE:123:VAL:HG13	55:Qi:29:ALA:HA	1.99	0.43
55:QI:36:PHE:CZ	50:Qd:296:MET:HG2	2.53	0.43
51:Qe:225:ILE:HG12	51:Qe:237:PRO:HD3	2.00	0.43
58:S1:169:VAL:HG22	58:S1:223:ILE:HD11	1.99	0.43
18:A9:262:THR:O	18:A9:333:PRO:HD2	2.18	0.43
25:B2:68:GLN:HE21	45:N5:367:PRO:HD2	1.83	0.43
29:B6:148:TYR:CE1	33:BK:49:ARG:HG2	2.53	0.43
35:C1:263:GLY:HA2	35:C1:487:LEU:HD11	2.00	0.43
40:CB:13:LEU:HD11	62:S5:6:VAL:HG12	2.00	0.43
66:V1:115:VAL:HG21	66:V1:142:CYS:SG	2.58	0.43
1:4L:55:LEU:HD23	1:4L:55:LEU:HA	1.89	0.43
20:AK:297:ARG:HA	20:AK:300:VAL:HG22	2.00	0.43
29:B6:97:PRO:O	29:B6:98:ARG:NE	2.42	0.43
72:CB:201:PLX:H321	72:CB:201:PLX:H352	1.71	0.43
41:N1:157:ASN:OD1	41:N1:168:THR:OG1	2.25	0.43
41:N1:281:ARG:NH1	59:S2:452:ASP:OD1	2.49	0.43
43:N3:38:GLU:HB3	43:N3:41:PHE:O	2.18	0.43
44:N4:357:THR:O	44:N4:361:VAL:HG23	2.19	0.43
44:N4:398:MET:O	44:N4:402:ILE:HG13	2.18	0.43
45:N5:162:THR:O	45:N5:166:THR:HG23	2.18	0.43
48:QB:121:ASN:ND2	48:QB:132:TYR:OH	2.39	0.43
81:QC:401:HEM:HMC1	81:QC:401:HEM:HBC2	2.00	0.43
72:QI:301:PLX:H81	71:Qb:502:PC1:H331	2.01	0.43
58:S1:185:PHE:CZ	58:S1:221:ASN:HB2	2.54	0.43
61:S4:80:PHE:HE1	61:S4:100:GLU:HG2	1.83	0.43
66:V1:244:ASN:OD1	66:V1:245:VAL:N	2.51	0.43
1:4L:44:SER:OG	1:4L:59:MET:SD	2.71	0.43
4:6A:81:LEU:HB3	71:6A:101:PC1:H12	2.00	0.43
18:A9:212:ARG:O	18:A9:216:TYR:N	2.35	0.43
29:B6:92:GLU:HG3	32:B9:157:TYR:HD1	1.82	0.43
36:C2:155:SER:OG	36:C2:156:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:C4:62:LEU:HG	38:C4:81:LEU:HD21	1.99	0.43
47:Qa:272:VAL:HA	47:Qa:337:GLY:HA3	2.01	0.43
3:5B:33:SER:OG	3:5B:34:GLY:N	2.50	0.43
15:A6:107:LEU:HD23	15:A6:107:LEU:HA	1.87	0.43
32:B9:120:GLN:HB2	45:N5:524:ASN:HD21	1.83	0.43
35:C1:75:ILE:HD11	35:C1:249:PRO:HG3	2.00	0.43
35:C1:319:LYS:HE3	35:C1:319:LYS:HB3	1.80	0.43
42:N2:167:TRP:HB3	45:N5:574:SER:HA	2.01	0.43
49:QC:137:GLN:NE2	49:QC:263:ASN:O	2.52	0.43
58:S1:191:GLY:HA3	58:S1:439:THR:HB	2.01	0.43
1:4L:35:GLY:HA3	46:N6:20:PHE:CZ	2.54	0.43
19:AC:119:ILE:HG21	19:AC:135:ALA:HB1	2.00	0.43
72:AM:201:PLX:H341	72:AM:201:PLX:H372	1.86	0.43
35:C1:130:PRO:HG3	35:C1:209:LEU:HD13	2.01	0.43
40:CB:66:TYR:CE1	77:CB:202:3PE:H262	2.53	0.43
44:N4:243:MET:HB3	44:N4:301:ILE:HG21	2.01	0.43
46:N6:24:PRO:HG3	46:N6:83:TRP:CE2	2.54	0.43
48:QB:80:ARG:HH22	48:QB:350:GLU:CD	2.26	0.43
47:Qa:211:ASN:HB3	47:Qa:246:LEU:HG	2.00	0.43
49:Qc:47:THR:HG23	49:Qc:79:ILE:HG23	2.01	0.43
58:S1:594:ALA:O	58:S1:605:GLN:HA	2.18	0.43
59:S2:147:TYR:HB2	64:S7:71:CYS:HB3	2.00	0.43
3:5B:37:VAL:HB	37:C3:154:GLY:HA2	2.01	0.43
26:B3:52:ARG:HD3	45:N5:435:PRO:O	2.19	0.43
37:C3:79:LEU:HB3	37:C3:233:PHE:CE2	2.54	0.43
37:C3:163:LEU:HD23	37:C3:163:LEU:HA	1.84	0.43
41:N1:113:VAL:O	41:N1:116:ILE:HG12	2.19	0.43
48:QB:179:MET:HE1	48:QB:282:LEU:HD13	2.00	0.43
48:QB:223:HIS:HA	48:QB:228:ARG:NH2	2.34	0.43
49:QC:131:TYR:O	49:QC:134:PRO:HD2	2.19	0.43
52:QF:56:ARG:O	52:QF:60:ARG:HG3	2.19	0.43
54:QH:3:ARG:NH2	49:Qc:217:LYS:HE2	2.33	0.43
51:Qe:153:GLU:HB3	51:Qe:270:LEU:HD11	2.01	0.43
58:S1:432:ILE:HG12	58:S1:445:LEU:HB2	2.00	0.43
58:S1:534:VAL:HG23	58:S1:537:ILE:HD12	2.00	0.43
60:S3:211:ARG:NH2	60:S3:222:GLU:OE2	2.48	0.43
18:A9:176:SER:O	18:A9:182:ARG:NE	2.52	0.43
28:B5:176:LYS:H	62:S5:45:HIS:CD2	2.36	0.43
33:BK:142:ARG:NE	34:BL:138:GLU:O	2.42	0.43
39:CA:47:THR:HG23	40:CB:65:LEU:HD22	2.00	0.43
41:N1:138:GLN:HG3	41:N1:285:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:QA:49:ILE:HD13	47:QA:220:LEU:HB3	2.01	0.43
55:QI:24:THR:HG23	74:QJ:101:PEE:H22	2.00	0.43
74:QJ:101:PEE:H8	74:QJ:101:PEE:H48	1.67	0.43
50:Qd:322:TYR:CE2	50:Qd:324:PRO:HG3	2.54	0.43
59:S2:121:LEU:HD23	64:S7:113:MET:SD	2.59	0.43
23:AN:10:MET:HE3	23:AN:11:PRO:HD2	2.01	0.43
32:B9:201:LYS:HE3	32:B9:201:LYS:HB2	1.86	0.43
35:C1:365:ILE:HD13	35:C1:365:ILE:HA	1.91	0.43
42:N2:140:SER:HB3	62:S5:2:PRO:HA	2.01	0.43
44:N4:347:GLY:O	44:N4:350:THR:HG22	2.18	0.43
45:N5:14:ILE:HD11	45:N5:43:ALA:HA	2.01	0.43
74:QB:502:PEE:H68	74:QB:502:PEE:H63	1.52	0.43
51:QE:130:LYS:HD2	56:Qj:34:TRP:CE2	2.53	0.43
53:QG:44:VAL:O	53:QG:48:ILE:HG12	2.19	0.43
8:7B:68:PRO:HD2	38:C4:156:PHE:HE1	1.84	0.42
19:AC:105:MET:HE3	19:AC:139:MET:HE1	2.01	0.42
21:AL:120:LEU:HD22	69:N4:503:CDL:H321	2.01	0.42
23:AN:68:ARG:HD3	46:N6:135:PHE:CD2	2.54	0.42
31:B8:96:ASP:OD2	44:N4:346:ARG:NH1	2.52	0.42
46:N6:39:VAL:O	46:N6:43:ILE:HG13	2.19	0.42
50:QD:322:TYR:CE2	50:QD:324:PRO:HG3	2.54	0.42
77:QJ:102:3PE:H262	77:QJ:102:3PE:H352	2.01	0.42
58:S1:307:ILE:HG23	58:S1:317:THR:HG21	2.01	0.42
58:S1:354:LEU:HD22	58:S1:548:LEU:HD22	2.01	0.42
66:V1:168:ASN:ND2	68:V3:388:ASN:HD21	2.17	0.42
3:5B:93:CYS:SG	3:5B:115:SER:HB2	2.59	0.42
17:A8:157:GLU:HB2	17:A8:158:PRO:HD3	2.01	0.42
18:A9:204:SER:HB2	18:A9:266:VAL:HG12	2.00	0.42
19:AB:78:ALA:HA	19:AB:81:ASP:OD2	2.20	0.42
19:AC:104:PHE:HD1	19:AC:108:LEU:HD12	1.84	0.42
20:AK:59:SER:OG	20:AK:156:GLY:O	2.24	0.42
35:C1:240:HIS:O	35:C1:243:VAL:HG22	2.20	0.42
69:N1:401:CDL:H771	69:N1:401:CDL:H801	1.85	0.42
45:N5:286:LEU:HD22	45:N5:411:MET:SD	2.60	0.42
49:QC:106:SER:HB3	81:QC:402:HEM:HBD2	2.01	0.42
56:QJ:34:TRP:CZ2	51:Qe:130:LYS:HD2	2.54	0.42
56:QJ:34:TRP:CE2	51:Qe:130:LYS:HD2	2.54	0.42
20:AK:51:THR:HG21	20:AK:153:LEU:HD22	2.00	0.42
29:B6:92:GLU:HB3	29:B6:93:PRO:HD3	2.01	0.42
35:C1:202:LEU:HD22	35:C1:238:PHE:CE2	2.54	0.42
42:N2:149:ILE:HD13	42:N2:154:MET:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:N5:7:LEU:O	45:N5:11:THR:HG23	2.19	0.42
48:QB:113:VAL:HG12	48:QB:146:LEU:HD23	2.01	0.42
51:QE:204:ARG:NH2	51:QE:258:LEU:O	2.46	0.42
56:Qj:2:LEU:HD22	56:Qj:4:ARG:HG2	2.01	0.42
58:S1:484:SER:HB2	58:S1:680:LEU:HD11	2.01	0.42
59:S2:134:THR:HG22	59:S2:424:ARG:HG2	2.01	0.42
65:S8:75:SER:O	65:S8:79:ARG:HG3	2.19	0.42
33:BK:43:ARG:HB2	33:BK:44:PRO:HD3	2.01	0.42
35:C1:71:MET:HB2	35:C1:72:PRO:HD3	2.00	0.42
78:C1:601:HEA:CMA	78:C1:601:HEA:HBA2	2.49	0.42
36:C2:28:LEU:HA	36:C2:28:LEU:HD12	1.85	0.42
72:N3:202:PLX:H281	72:N3:202:PLX:H311	1.67	0.42
45:N5:103:PHE:HB2	45:N5:341:MET:HE3	2.00	0.42
48:QB:86:ASN:HA	48:QB:211:LEU:HD21	2.00	0.42
49:Qc:137:GLN:NE2	49:Qc:263:ASN:O	2.53	0.42
50:Qd:113:ARG:NH1	50:Qd:270:ASP:OD1	2.53	0.42
59:S2:62:LYS:O	59:S2:66:HIS:ND1	2.41	0.42
3:5B:75:GLU:H	3:5B:75:GLU:CD	2.27	0.42
9:7C:60:LEU:HD23	9:7C:60:LEU:HA	1.84	0.42
18:A9:171:ASN:HD21	18:A9:326:ASP:HA	1.84	0.42
20:AK:328:ARG:HH21	34:BL:58:ASP:CG	2.27	0.42
27:B4:48:LEU:HB3	32:B9:208:LEU:HD13	2.02	0.42
45:N5:228:GLY:H	45:N5:230:HIS:CD2	2.37	0.42
47:Qa:297:PRO:HB3	47:Qa:304:ASN:HD21	1.84	0.42
48:Qb:274:GLU:HG3	48:Qb:456:VAL:HB	2.00	0.42
49:Qc:36:LEU:HD23	49:Qc:36:LEU:HA	1.86	0.42
20:AK:355:TRP:H	20:AK:355:TRP:CD1	2.38	0.42
22:AM:44:TYR:OH	22:AM:113:HIS:N	2.48	0.42
31:B8:161:TYR:HB3	31:B8:166:LEU:HG	2.00	0.42
35:C1:191:THR:HG23	35:C1:245:ILE:HG23	2.02	0.42
45:N5:228:GLY:H	45:N5:230:HIS:HD2	1.66	0.42
45:N5:368:PHE:CZ	45:N5:455:LYS:HG3	2.55	0.42
54:QH:67:PHE:CE1	49:Qc:344:GLU:HG3	2.52	0.42
48:Qb:195:THR:HG21	48:Qb:269:ARG:H	1.85	0.42
49:Qc:97:HIS:HD2	81:Qc:404:HEM:C1C	2.38	0.42
64:S7:161:ILE:HG13	64:S7:180:LEU:HB2	2.02	0.42
66:V1:86:ARG:O	66:V1:88:ARG:NH1	2.53	0.42
4:6A:29:ARG:HB2	37:C3:146:TRP:CE2	2.55	0.42
35:C1:105:LEU:HB2	35:C1:106:PRO:HD3	2.02	0.42
35:C1:280:ILE:HG13	35:C1:315:PRO:HB2	2.02	0.42
72:N3:202:PLX:H132	72:N3:202:PLX:H101	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:N4:232:ALA:O	44:N4:237:LYS:NZ	2.52	0.42
45:N5:264:TYR:CD2	45:N5:265:PRO:HD3	2.54	0.42
47:QA:51:SER:OG	47:QA:230:LEU:HD12	2.19	0.42
48:QB:192:PHE:HB3	48:QB:195:THR:OG1	2.18	0.42
50:QD:303:LEU:HB3	51:QE:121:THR:OG1	2.20	0.42
69:A7:201:CDL:HA61	69:A7:201:CDL:H521	2.02	0.42
19:AC:94:ASP:HB3	19:AC:97:LYS:HG2	2.01	0.42
21:AL:45:PRO:HA	21:AL:46:PRO:HD3	1.92	0.42
22:AM:12:GLN:O	22:AM:16:GLY:N	2.52	0.42
23:AN:43:LEU:HG	41:N1:179:TRP:HE1	1.84	0.42
31:B8:88:PRO:HB3	31:B8:98:ARG:NH2	2.35	0.42
37:C3:207:HIS:NE2	71:C3:302:PC1:H3H1	2.34	0.42
42:N2:139:LEU:HD13	42:N2:190:MET:HE1	2.02	0.42
42:N2:190:MET:HE2	42:N2:190:MET:HB3	1.73	0.42
45:N5:264:TYR:CG	45:N5:265:PRO:HD3	2.54	0.42
45:N5:331:MET:HB3	45:N5:387:THR:HG22	2.02	0.42
47:QA:82:LEU:HD23	47:QA:205:LEU:HD11	1.99	0.42
47:QA:222:GLY:HA3	47:QA:230:LEU:HD11	2.02	0.42
48:QB:270:PHE:CG	48:QB:292:GLU:HB2	2.55	0.42
53:QG:40:GLU:HA	53:QG:44:VAL:HB	2.01	0.42
54:QH:12:ARG:NH1	48:Qb:279:ASP:OD1	2.53	0.42
47:Qa:379:LYS:HG3	47:Qa:416:ILE:HG21	2.02	0.42
49:Qc:24:PRO:O	49:Qc:224:TYR:OH	2.19	0.42
50:Qd:311:LYS:HA	50:Qd:311:LYS:HD3	1.89	0.42
51:Qe:190:VAL:HG11	51:Qe:250:ARG:NH2	2.35	0.42
59:S2:299:LEU:HD22	59:S2:304:ILE:HD12	2.01	0.42
20:AK:284:PRO:O	20:AK:288:GLN:HG2	2.20	0.42
72:AM:201:PLX:H182	41:N1:19:PHE:HZ	1.85	0.42
26:B3:13:LYS:HA	26:B3:13:LYS:HD2	1.83	0.42
29:B6:177:ILE:HA	29:B6:178:PRO:HD3	1.88	0.42
30:B7:43:GLN:NE2	31:B8:169:GLU:OE2	2.43	0.42
30:B7:92:HIS:O	30:B7:96:VAL:HG13	2.20	0.42
31:B8:108:ASP:HB3	31:B8:111:MET:HG2	2.01	0.42
35:C1:145:LEU:HD21	37:C3:32:THR:HG21	2.01	0.42
40:CB:4:MET:O	40:CB:10:ARG:NH1	2.51	0.42
44:N4:131:ILE:O	44:N4:135:ARG:HB3	2.20	0.42
44:N4:231:LEU:HD23	44:N4:235:LEU:HD12	2.02	0.42
49:Qc:253:PRO:HB3	50:Qd:204:ALA:HA	2.00	0.42
58:S1:76:ARG:O	58:S1:116:VAL:HG21	2.20	0.42
60:S3:213:ASP:HB3	60:S3:216:VAL:HG22	2.01	0.42
66:V1:382:CYS:HB3	66:V1:384:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4L:79:VAL:HG12	46:N6:74:MET:HE3	2.02	0.42
37:C3:84:ILE:HG12	74:C3:304:PEE:H16	2.01	0.42
48:QB:183:VAL:HG21	48:QB:286:HIS:HB3	2.01	0.42
49:QC:123:VAL:HG22	49:QC:189:ILE:HD13	2.01	0.42
51:QE:214:ILE:HG13	51:QE:261:PRO:HD3	2.02	0.42
49:Qc:233:LEU:HD23	49:Qc:233:LEU:HA	1.82	0.42
58:S1:395:GLU:OE2	58:S1:417:ARG:NH1	2.53	0.42
64:S7:188:LYS:HB3	64:S7:191:ARG:NH2	2.35	0.42
66:V1:116:ASN:O	66:V1:245:VAL:HG23	2.20	0.42
18:A9:106:MET:HE2	18:A9:118:LYS:HE3	2.02	0.41
29:B6:85:ASP:OD2	32:B9:167:TRP:NE1	2.43	0.41
35:C1:124:THR:OG1	35:C1:128:VAL:HG12	2.19	0.41
36:C2:72:ILE:O	36:C2:76:ILE:HG13	2.20	0.41
37:C3:173:PHE:HD2	37:C3:208:VAL:HG11	1.85	0.41
45:N5:419:THR:HA	45:N5:422:TYR:CZ	2.54	0.41
49:QC:310:SER:HA	49:QC:374:ASN:HD21	1.85	0.41
72:QI:301:PLX:H111	51:Qe:125:VAL:HG21	2.02	0.41
49:Qc:237:LEU:HB2	50:Qd:297:MET:HG2	2.01	0.41
58:S1:62:ARG:HB2	83:S1:803:FES:S1	2.59	0.41
59:S2:228:MET:SD	64:S7:167:PRO:HG3	2.60	0.41
1:4L:41:PHE:O	1:4L:45:THR:HG22	2.19	0.41
14:A5:30:LYS:HE3	14:A5:88:LEU:HD21	2.02	0.41
15:A6:88:LYS:NZ	15:A6:132:PHE:O	2.36	0.41
20:AK:37:ARG:NH1	20:AK:49:GLU:OE1	2.52	0.41
20:AK:54:LYS:NZ	20:AK:297:ARG:HH12	2.18	0.41
24:B1:47:ARG:NH2	24:B1:53:GLU:OE2	2.46	0.41
34:BL:150:PRO:HG3	40:CB:115:LEU:HD22	2.02	0.41
41:N1:212:ASN:O	64:S7:99:GLN:NE2	2.53	0.41
71:N1:403:PC1:H322	71:N1:403:PC1:H3D2	2.02	0.41
44:N4:193:ILE:HD13	69:N4:503:CDL:OA4	2.20	0.41
44:N4:266:MET:HB3	44:N4:395:LEU:HD13	2.02	0.41
45:N5:435:PRO:HB3	45:N5:437:PHE:CE2	2.55	0.41
48:Qb:158:ASP:O	48:Qb:162:GLU:HG2	2.20	0.41
64:S7:173:LEU:O	64:S7:177:ILE:HG12	2.21	0.41
66:V1:295:PRO:HG2	66:V1:298:GLU:HB2	2.02	0.41
71:6A:101:PC1:H133	37:C3:187:THR:HA	2.03	0.41
8:7B:46:ALA:HA	38:C4:108:LEU:HD13	2.02	0.41
15:A6:88:LYS:HD2	15:A6:88:LYS:HA	1.65	0.41
16:A7:42:PRO:HG3	23:AN:6:VAL:HG11	2.01	0.41
17:A8:246:PHE:HD2	44:N4:116:ILE:HG23	1.85	0.41
18:A9:259:LYS:HE3	18:A9:259:LYS:HB3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AC:140:CYS:HB3	19:AC:143:GLU:HG3	2.02	0.41
41:N1:173:TRP:NE1	41:N1:244:GLY:O	2.53	0.41
44:N4:201:MET:HE1	44:N4:212:LEU:HD11	2.03	0.41
47:QA:348:GLY:HA2	47:QA:448:PRO:HD3	2.02	0.41
48:QB:181:ASP:OD1	48:QB:181:ASP:N	2.52	0.41
74:QB:502:PEE:H48	74:QB:502:PEE:H7	1.83	0.41
50:QD:195:PRO:HA	50:QD:196:PRO:HD3	1.96	0.41
49:Qc:33:PHE:HA	49:Qc:36:LEU:HB2	2.03	0.41
51:Qe:201:ASP:C	51:Qe:203:GLU:H	2.27	0.41
54:Qh:42:THR:OG1	69:Qh:102:CDL:H111	2.20	0.41
5:6B:72:ALA:O	5:6B:76:ARG:HD3	2.21	0.41
17:A8:201:GLU:HA	17:A8:204:LYS:HD3	2.00	0.41
69:AK:402:CDL:H381	42:N2:132:THR:HG21	2.03	0.41
26:B3:24:ILE:O	26:B3:30:GLU:HB3	2.20	0.41
71:C3:302:PC1:H342	71:C3:302:PC1:H371	1.92	0.41
41:N1:142:TYR:CD1	41:N1:142:TYR:C	2.98	0.41
48:QB:87:ASN:H	48:QB:207:ASN:ND2	2.17	0.41
58:S1:245:THR:HA	58:S1:265:THR:O	2.19	0.41
4:6A:28:TRP:O	4:6A:32:THR:OG1	2.23	0.41
28:B5:110:TRP:O	28:B5:119:ARG:HG2	2.20	0.41
36:C2:69:PRO:O	36:C2:73:LEU:HG	2.21	0.41
40:CB:62:ARG:HD3	77:CB:202:3PE:H342	2.03	0.41
44:N4:259:TYR:O	44:N4:263:MET:HG2	2.20	0.41
45:N5:15:LEU:HD23	45:N5:15:LEU:HA	1.89	0.41
46:N6:123:GLY:O	46:N6:126:VAL:HB	2.21	0.41
47:QA:77:LEU:O	47:QA:196:ARG:HD3	2.20	0.41
51:QE:90:ASP:OD1	51:QE:90:ASP:N	2.44	0.41
54:QH:22:PHE:O	51:Qe:110:ARG:HD2	2.20	0.41
54:QH:69:LYS:HE3	54:QH:69:LYS:HB2	1.85	0.41
48:Qb:304:LEU:HD13	48:Qb:354:LEU:HD22	2.01	0.41
49:Qc:181:PHE:HA	49:Qc:184:ILE:HG22	2.02	0.41
51:Qe:213:LEU:HD13	51:Qe:258:LEU:HD12	2.03	0.41
52:Qf:38:GLU:OE1	52:Qf:47:ARG:NH2	2.40	0.41
64:S7:121:TYR:O	64:S7:128:ARG:NH1	2.54	0.41
72:S7:302:PLX:H322	72:S7:302:PLX:H291	1.89	0.41
66:V1:110:PRO:HD2	66:V1:238:CYS:SG	2.61	0.41
66:V1:115:VAL:HG11	66:V1:138:LEU:HD11	2.02	0.41
18:A9:65:LEU:HG	18:A9:129:LEU:HD22	2.03	0.41
19:AC:155:TYR:CD2	19:AC:156:GLU:HG3	2.55	0.41
35:C1:236:TRP:O	35:C1:288:TRP:HB2	2.20	0.41
35:C1:381:LEU:HD21	78:C1:602:HEA:HBC2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:C3:54:MET:HB3	37:C3:58:TRP:CZ3	2.55	0.41
37:C3:196:THR:HA	37:C3:199:VAL:HG22	2.02	0.41
41:N1:31:MET:HG2	65:S8:77:LEU:HB2	2.03	0.41
41:N1:146:LEU:HG	41:N1:188:SER:HB3	2.03	0.41
45:N5:233:LEU:HB3	45:N5:234:PRO:HD3	2.01	0.41
48:QB:379:LEU:HD23	48:QB:379:LEU:HA	1.90	0.41
49:QC:270:PRO:HG2	49:QC:275:LEU:HD23	2.03	0.41
50:QD:325:PRO:HD3	54:Qh:13:HIS:CD2	2.55	0.41
66:V1:369:ARG:HA	66:V1:369:ARG:HD2	1.90	0.41
18:A9:168:SER:O	18:A9:203:PRO:HD2	2.21	0.41
22:AM:78:ASP:OD1	22:AM:78:ASP:N	2.53	0.41
35:C1:74:MET:HE3	35:C1:389:ILE:HG13	2.02	0.41
36:C2:122:MET:HE2	36:C2:122:MET:HB3	2.00	0.41
40:CB:65:LEU:HD23	77:CB:202:3PE:C21	2.51	0.41
44:N4:200:ILE:O	44:N4:204:MET:HG2	2.21	0.41
45:N5:80:PHE:HB3	45:N5:82:MET:HE2	2.02	0.41
45:N5:520:TYR:CE1	69:N5:704:CDL:HB22	2.56	0.41
47:QA:178:HIS:NE2	47:QA:330:TYR:OH	2.46	0.41
48:QB:363:MET:SD	54:Qh:6:GLY:HA3	2.61	0.41
49:QC:113:TRP:O	49:QC:117:VAL:HG23	2.20	0.41
51:QE:156:LEU:HB3	51:QE:210:TRP:CZ2	2.55	0.41
69:QH:401:CDL:OA3	50:Qd:305:TYR:OH	2.32	0.41
47:Qa:63:LEU:HD21	47:Qa:218:MET:HE3	2.01	0.41
51:Qe:88:PHE:O	51:Qe:92:ARG:HG3	2.21	0.41
55:Qi:34:ARG:HH21	56:Qj:50:GLY:HA3	1.86	0.41
64:S7:98:ARG:HA	64:S7:125:PRO:HD3	2.03	0.41
65:S8:49:ASP:OD1	65:S8:49:ASP:N	2.49	0.41
11:A1:52:ARG:NH1	11:A1:58:ASN:OD1	2.54	0.41
18:A9:207:PHE:HB2	18:A9:214:LEU:HG	2.03	0.41
20:AK:112:GLY:HA2	20:AK:136:TRP:CD2	2.56	0.41
20:AK:327:ASP:OD1	44:N4:91:ARG:NH2	2.44	0.41
22:AM:139:PRO:HG3	58:S1:306:MET:HE1	2.03	0.41
29:B6:147:LYS:HE3	29:B6:148:TYR:CZ	2.56	0.41
33:BK:97:LYS:HB3	33:BK:97:LYS:HE3	1.85	0.41
35:C1:197:LEU:HD12	71:C1:607:PC1:H381	2.02	0.41
35:C1:442:ASP:OD1	35:C1:443:TYR:N	2.54	0.41
74:C3:304:PEE:H49	74:C3:304:PEE:H7	1.89	0.41
42:N2:290:LEU:HD21	44:N4:150:LEU:HD21	2.03	0.41
69:N5:703:CDL:H561	69:N5:703:CDL:H532	1.85	0.41
48:QB:120:LEU:HD13	48:QB:133:ILE:HG12	2.01	0.41
50:QD:127:SER:HB3	50:QD:179:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:QE:224:PRO:HA	51:QE:236:CYS:HA	2.02	0.41
52:QF:40:ILE:HG22	52:QF:43:CYS:H	1.86	0.41
54:Qh:20:SER:O	54:Qh:24:GLN:HG2	2.21	0.41
54:Qh:49:VAL:O	54:Qh:52:PRO:HD2	2.21	0.41
58:S1:296:GLY:O	58:S1:572:HIS:NE2	2.45	0.41
59:S2:105:MET:HE3	59:S2:105:MET:HB2	1.85	0.41
59:S2:145:LEU:HD22	59:S2:469:ARG:HG2	2.03	0.41
66:V1:412:LEU:HD12	66:V1:415:ILE:HD11	2.03	0.41
27:B4:77:TYR:CZ	45:N5:564:LYS:HG2	2.56	0.41
34:BL:98:VAL:HG11	44:N4:71:TRP:CZ3	2.55	0.41
34:BL:117:TRP:CZ2	34:BL:121:GLU:HG3	2.56	0.41
35:C1:28:MET:HE3	35:C1:469:ILE:HD11	2.01	0.41
35:C1:360:ASN:O	35:C1:364:ASP:N	2.49	0.41
35:C1:436:MET:HE3	35:C1:443:TYR:HB3	2.03	0.41
78:C1:601:HEA:CMA	78:C1:601:HEA:CBA	2.99	0.41
71:C3:303:PC1:H153	71:C3:303:PC1:H112	1.88	0.41
77:CB:202:3PE:H351	77:CB:202:3PE:H392	2.03	0.41
69:N1:401:CDL:H511	46:N6:83:TRP:HZ3	1.85	0.41
74:N5:705:PEE:H76	74:N5:705:PEE:H71	1.83	0.41
47:QA:290:GLN:HB2	47:QA:336:PHE:HE1	1.86	0.41
48:QB:205:SER:HA	48:QB:208:VAL:HG12	2.03	0.41
69:QB:501:CDL:H342	71:QB:503:PC1:H2D1	2.02	0.41
49:QC:30:TRP:HE1	69:Qh:102:CDL:H1	1.86	0.41
50:QD:159:PRO:HB2	50:Qd:184:GLU:HG3	2.03	0.41
47:Qa:409:PRO:O	47:Qa:413:LEU:HG	2.20	0.41
58:S1:347:ASP:CB	58:S1:594:ALA:HB1	2.51	0.41
59:S2:203:MET:O	59:S2:206:PHE:HB3	2.21	0.41
60:S3:147:THR:HB	60:S3:153:ILE:HD11	2.03	0.41
64:S7:154:ASP:OD1	64:S7:154:ASP:N	2.54	0.41
66:V1:313:ASN:O	66:V1:359:ARG:HG2	2.21	0.41
66:V1:385:CYS:O	66:V1:389:VAL:HB	2.21	0.41
3:5B:84:THR:OG1	3:5B:85:ASN:N	2.54	0.41
19:AC:91:ASP:OD1	26:B3:47:ARG:NH2	2.49	0.41
69:AL:202:CDL:H792	69:AL:202:CDL:H762	1.94	0.41
36:C2:155:SER:HB2	36:C2:179:LEU:HD23	2.03	0.41
37:C3:148:HIS:HE1	37:C3:232:HIS:CE1	2.36	0.41
41:N1:267:THR:O	41:N1:271:LEU:HG	2.22	0.41
44:N4:328:CYS:HB3	44:N4:437:MET:HE1	2.02	0.41
45:N5:176:ARG:HD3	45:N5:179:ASP:HB2	2.03	0.41
45:N5:213:LEU:HB3	45:N5:273:VAL:HG11	2.03	0.41
45:N5:598:SER:HA	45:N5:602:PHE:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Qc:237:LEU:HD22	50:Qd:301:LEU:HD11	2.02	0.41
51:Qe:152:ILE:HG22	51:Qe:273:VAL:HB	2.03	0.41
64:S7:51:ASP:HB3	64:S7:190:LEU:HB2	2.03	0.41
23:AN:36:PHE:O	23:AN:40:ILE:HG12	2.21	0.40
27:B4:15:PRO:HG2	27:B4:18:LEU:HB2	2.03	0.40
32:B9:178:GLU:OE2	32:B9:209:TRP:NE1	2.54	0.40
35:C1:73:ILE:HD13	78:C1:601:HEA:H253	2.02	0.40
38:C4:45:PRO:HB3	38:C4:90:PHE:HZ	1.86	0.40
69:N1:401:CDL:H751	69:N1:401:CDL:H532	2.02	0.40
45:N5:350:LEU:HD12	45:N5:359:MET:HG2	2.02	0.40
48:QB:184:PHE:O	48:QB:188:HIS:HD2	2.04	0.40
48:QB:190:THR:HG22	48:QB:275:ILE:HG23	2.04	0.40
49:Qc:361:ILE:HG12	49:Qc:365:LEU:HD12	2.03	0.40
58:S1:43:VAL:HG21	58:S1:96:VAL:HG21	2.03	0.40
60:S3:231:ARG:NH2	65:S8:128:ILE:O	2.54	0.40
66:V1:63:TYR:HB3	66:V1:256:ARG:HD3	2.03	0.40
68:V3:383:ASN:O	68:V3:383:ASN:ND2	2.54	0.40
6:6C:52:PHE:CD2	38:C4:153:ILE:HG12	2.56	0.40
9:7C:41:MET:HE2	9:7C:41:MET:HB3	1.88	0.40
9:7C:52:PRO:HG2	35:C1:32:ALA:HB3	2.02	0.40
15:A6:145:LEU:HD12	15:A6:145:LEU:HA	1.96	0.40
19:AC:91:ASP:HB2	26:B3:44:PRO:HB3	2.03	0.40
22:AM:25:ARG:O	22:AM:29:ARG:HG2	2.21	0.40
30:B7:22:MET:HE1	30:B7:102:PHE:CD2	2.54	0.40
33:BK:65:HIS:CD2	34:BL:124:ARG:HH12	2.39	0.40
34:BL:72:ASP:OD1	34:BL:72:ASP:N	2.48	0.40
35:C1:417:MET:O	35:C1:421:VAL:HG22	2.21	0.40
35:C1:442:ASP:CG	36:C2:134:ARG:HH22	2.25	0.40
41:N1:173:TRP:NE1	71:N1:403:PC1:H122	2.34	0.40
41:N1:306:SER:O	41:N1:310:MET:HG2	2.21	0.40
42:N2:130:LEU:HD12	42:N2:134:GLN:HG3	2.03	0.40
45:N5:208:CYS:HA	45:N5:209:PRO:HD3	1.78	0.40
45:N5:341:MET:SD	45:N5:457:LEU:HD12	2.62	0.40
47:QA:138:LEU:O	47:QA:142:ALA:CB	2.68	0.40
51:QE:249:ILE:HG22	51:QE:257:ASN:ND2	2.35	0.40
48:Qb:101:THR:HG22	48:Qb:102:LYS:H	1.85	0.40
48:Qb:142:LYS:HA	48:Qb:142:LYS:HD3	1.91	0.40
50:Qd:222:PRO:HA	50:Qd:223:PRO:HD3	1.94	0.40
58:S1:528:LEU:HD23	58:S1:528:LEU:HA	1.93	0.40
59:S2:114:LYS:HE3	59:S2:114:LYS:HB2	1.89	0.40
59:S2:139:LEU:HB3	59:S2:140:PRO:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:S3:196:HIS:HA	60:S3:197:PRO:HD3	1.90	0.40
64:S7:130:VAL:HB	64:S7:159:VAL:HA	2.03	0.40
69:6A:102:CDL:H251	37:C3:212:SER:HB3	2.04	0.40
20:AK:221:GLN:HE22	20:AK:229:MET:HE3	1.86	0.40
20:AK:225:ASN:HB3	20:AK:228:GLU:HG2	2.04	0.40
23:AN:21:TYR:CE2	59:S2:348:ARG:HD2	2.56	0.40
23:AN:120:MET:HE2	23:AN:120:MET:HB3	1.88	0.40
33:BK:162:ARG:NH1	34:BL:140:ASN:OD1	2.54	0.40
35:C1:37:ILE:CG2	78:C1:601:HEA:HMA	2.52	0.40
35:C1:436:MET:HA	35:C1:437:PRO:HD3	1.94	0.40
37:C3:137:LEU:HD23	37:C3:137:LEU:HA	1.86	0.40
39:CA:55:TRP:O	39:CA:59:ILE:HG12	2.21	0.40
72:CB:201:PLX:H31	72:CB:201:PLX:H6	1.88	0.40
45:N5:397:GLU:HB3	45:N5:482:MET:HE1	2.02	0.40
45:N5:421:ALA:O	45:N5:424:THR:OG1	2.32	0.40
49:QC:185:LEU:HD23	49:QC:188:ILE:HD12	2.04	0.40
53:QG:34:ARG:O	53:QG:37:THR:HG22	2.22	0.40
55:QI:11:TYR:HA	55:QI:15:PHE:HB2	2.04	0.40
74:QJ:101:PEE:H71	74:QJ:101:PEE:H77	1.74	0.40
47:Qa:300:LYS:HE3	47:Qa:300:LYS:HB2	1.92	0.40
48:Qb:407:THR:HB	48:Qb:408:PRO:HD3	2.04	0.40
71:Qb:502:PC1:H3C1	71:Qb:502:PC1:H381	2.04	0.40
49:Qc:131:TYR:O	49:Qc:134:PRO:HD2	2.21	0.40
81:Qc:403:HEM:HMC1	81:Qc:403:HEM:HBC2	2.01	0.40
59:S2:189:HIS:NE2	59:S2:342:GLU:OE1	2.43	0.40
59:S2:230:ALA:O	65:S8:98:ARG:NH2	2.54	0.40
63:S6:84:ILE:HD12	63:S6:84:ILE:HA	1.95	0.40
66:V1:314:LEU:HD11	66:V1:317:VAL:HG23	2.03	0.40
3:5B:57:LYS:HB3	3:5B:57:LYS:HE2	1.87	0.40
6:6C:18:ARG:CZ	36:C2:48:THR:HB	2.52	0.40
18:A9:174:ILE:HG23	18:A9:175:LYS:HG3	2.02	0.40
18:A9:357:ARG:HD3	18:A9:361:TRP:O	2.21	0.40
22:AM:85:GLU:HG2	22:AM:86:TRP:H	1.87	0.40
69:B5:202:CDL:H762	69:B5:202:CDL:H211	2.03	0.40
36:C2:193:TYR:CD1	36:C2:210:VAL:HG22	2.56	0.40
69:CB:203:CDL:H581	44:N4:56:PHE:HE2	1.85	0.40
41:N1:2:PHE:CE2	41:N1:6:ILE:HD11	2.57	0.40
42:N2:135:LYS:O	42:N2:139:LEU:HD12	2.22	0.40
45:N5:304:PHE:CZ	45:N5:526:LEU:HD22	2.55	0.40
47:QA:323:VAL:HG23	47:QA:340:THR:HG22	2.03	0.40
47:QA:407:VAL:HG13	47:QA:411:THR:HB	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:QD:247:PRO:HA	50:QD:248:PRO:HD3	1.86	0.40
54:QH:8:LEU:HB2	48:Qb:463:GLU:OE2	2.21	0.40
47:Qa:47:LEU:HD21	47:Qa:234:ALA:HB1	2.03	0.40
54:Qh:27:PHE:HD1	71:Qh:101:PC1:H12	1.86	0.40
59:S2:145:LEU:HD11	59:S2:430:ILE:HD13	2.03	0.40
65:S8:150:THR:HG21	65:S8:180:HIS:CD2	2.56	0.40
6:6C:45:ARG:NH1	36:C2:25:ASP:OD2	2.53	0.40
9:7C:31:VAL:HG12	35:C1:479:LYS:HE3	2.03	0.40
72:AM:201:PLX:H21	72:AM:201:PLX:H1B2	1.87	0.40
24:B1:50:ARG:HB2	24:B1:53:GLU:HG2	2.02	0.40
35:C1:140:GLY:O	35:C1:213:ARG:NH2	2.55	0.40
35:C1:433:LEU:HA	35:C1:433:LEU:HD23	1.81	0.40
40:CB:30:ASP:OD1	40:CB:31:PRO:HD2	2.22	0.40
72:CB:201:PLX:H171	72:CB:201:PLX:H282	2.03	0.40
41:N1:127:TYR:OH	59:S2:89:ASN:O	2.37	0.40
48:QB:225:LYS:HD2	48:QB:257:TYR:CE1	2.56	0.40
48:QB:229:MET:SD	48:QB:253:LEU:HD21	2.62	0.40
49:QC:77:TRP:CH2	50:QD:289:MET:HE2	2.57	0.40
48:Qb:41:ALA:O	48:Qb:45:VAL:HG23	2.21	0.40
48:Qb:211:LEU:HD23	48:Qb:211:LEU:HA	1.98	0.40
58:S1:541:PRO:HB3	58:S1:561:PRO:HD3	2.03	0.40
58:S1:591:GLU:HG2	58:S1:610:VAL:HG23	2.03	0.40
77:S7:303:3PE:H3D1	77:S7:303:3PE:H3H2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4L	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
2	5A	100/102 (98%)	99 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	5B	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
4	6A	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
5	6B	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
6	6C	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
7	7A	55/57 (96%)	55 (100%)	0	0	100	100
8	7B	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
9	7C	45/47 (96%)	43 (96%)	2 (4%)	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%)	80 (96%)	3 (4%)	0	100	100
13	A3	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
14	A5	110/112 (98%)	109 (99%)	1 (1%)	0	100	100
15	A6	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
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%)	327 (96%)	12 (4%)	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%)	309 (97%)	10 (3%)	0	100	100
21	AL	138/140 (99%)	138 (100%)	0	0	100	100
22	AM	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
23	AN	140/142 (99%)	129 (92%)	11 (8%)	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%)	123 (98%)	3 (2%)	0	100	100
28	B5	136/138 (99%)	133 (98%)	3 (2%)	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%)	175 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	BK	172/174 (99%)	171 (99%)	1 (1%)	0	100	100
34	BL	97/99 (98%)	88 (91%)	9 (9%)	0	100	100
35	C1	512/514 (100%)	493 (96%)	19 (4%)	0	100	100
36	C2	226/228 (99%)	221 (98%)	5 (2%)	0	100	100
37	C3	258/260 (99%)	248 (96%)	10 (4%)	0	100	100
38	C4	136/138 (99%)	128 (94%)	8 (6%)	0	100	100
39	CA	47/49 (96%)	47 (100%)	0	0	100	100
40	CB	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
41	N1	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
42	N2	345/347 (99%)	335 (97%)	10 (3%)	0	100	100
43	N3	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
44	N4	457/459 (100%)	453 (99%)	4 (1%)	0	100	100
45	N5	601/603 (100%)	576 (96%)	25 (4%)	0	100	100
46	N6	172/174 (99%)	161 (94%)	11 (6%)	0	100	100
47	QA	417/419 (100%)	410 (98%)	7 (2%)	0	100	100
47	Qa	417/419 (100%)	411 (99%)	6 (1%)	0	100	100
48	QB	444/446 (100%)	432 (97%)	12 (3%)	0	100	100
48	Qb	429/446 (96%)	423 (99%)	6 (1%)	0	100	100
49	QC	377/379 (100%)	371 (98%)	6 (2%)	0	100	100
49	Qc	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
50	QD	239/241 (99%)	230 (96%)	9 (4%)	0	100	100
50	Qd	237/241 (98%)	232 (98%)	5 (2%)	0	100	100
51	QE	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
51	Qe	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
52	QF	65/67 (97%)	65 (100%)	0	0	100	100
52	Qf	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
53	QG	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
53	Qg	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
54	QH	76/79 (96%)	74 (97%)	2 (3%)	0	100	100
54	Qh	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
55	QI	60/62 (97%)	59 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	48 (98%)	1 (2%)	0	100	100
57	QK	69/78 (88%)	69 (100%)	0	0	100	100
58	S1	687/689 (100%)	662 (96%)	25 (4%)	0	100	100
59	S2	427/430 (99%)	413 (97%)	14 (3%)	0	100	100
60	S3	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
61	S4	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
62	S5	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
63	S6	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
64	S7	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
65	S8	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
66	V1	429/431 (100%)	412 (96%)	17 (4%)	0	100	100
67	V2	215/217 (99%)	208 (97%)	7 (3%)	0	100	100
68	V3	40/42 (95%)	37 (92%)	3 (8%)	0	100	100
All	All	13972/14217 (98%)	13598 (97%)	374 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	89 (100%)	0	100	100
3	5B	80/80 (100%)	79 (99%)	1 (1%)	61	84
4	6A	66/66 (100%)	66 (100%)	0	100	100
5	6B	73/73 (100%)	71 (97%)	2 (3%)	39	70
6	6C	57/57 (100%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	7A	48/48 (100%)	48 (100%)	0	100	100
8	7B	39/39 (100%)	39 (100%)	0	100	100
9	7C	40/40 (100%)	40 (100%)	0	100	100
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%)	76 (100%)	0	100	100
13	A3	69/69 (100%)	69 (100%)	0	100	100
14	A5	99/99 (100%)	99 (100%)	0	100	100
15	A6	107/107 (100%)	107 (100%)	0	100	100
16	A7	87/97 (90%)	86 (99%)	1 (1%)	65	86
17	A8	153/153 (100%)	153 (100%)	0	100	100
18	A9	295/295 (100%)	294 (100%)	1 (0%)	86	95
19	AB	71/80 (89%)	71 (100%)	0	100	100
19	AC	80/80 (100%)	79 (99%)	1 (1%)	61	84
20	AK	284/284 (100%)	282 (99%)	2 (1%)	76	90
21	AL	101/101 (100%)	100 (99%)	1 (1%)	68	87
22	AM	130/130 (100%)	128 (98%)	2 (2%)	57	82
23	AN	123/123 (100%)	122 (99%)	1 (1%)	73	89
24	B1	53/53 (100%)	53 (100%)	0	100	100
25	B2	62/62 (100%)	61 (98%)	1 (2%)	55	81
26	B3	62/62 (100%)	61 (98%)	1 (2%)	55	81
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%)	420 (99%)	5 (1%)	63	84
36	C2	212/212 (100%)	212 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	C3	224/224 (100%)	223 (100%)	1 (0%)	84	94
38	C4	123/123 (100%)	123 (100%)	0	100	100
39	CA	45/45 (100%)	44 (98%)	1 (2%)	45	75
40	CB	108/108 (100%)	107 (99%)	1 (1%)	70	88
41	N1	275/275 (100%)	272 (99%)	3 (1%)	65	86
42	N2	311/311 (100%)	311 (100%)	0	100	100
43	N3	100/100 (100%)	100 (100%)	0	100	100
44	N4	410/410 (100%)	407 (99%)	3 (1%)	76	90
45	N5	537/537 (100%)	534 (99%)	3 (1%)	78	92
46	N6	140/140 (100%)	140 (100%)	0	100	100
47	QA	330/330 (100%)	330 (100%)	0	100	100
47	Qa	330/330 (100%)	328 (99%)	2 (1%)	78	92
48	QB	372/372 (100%)	371 (100%)	1 (0%)	86	95
48	Qb	362/372 (97%)	358 (99%)	4 (1%)	65	86
49	QC	332/332 (100%)	330 (99%)	2 (1%)	78	92
49	Qc	332/332 (100%)	331 (100%)	1 (0%)	86	95
50	QD	206/206 (100%)	205 (100%)	1 (0%)	81	93
50	Qd	204/206 (99%)	204 (100%)	0	100	100
51	QE	166/166 (100%)	164 (99%)	2 (1%)	63	84
51	Qe	166/166 (100%)	165 (99%)	1 (1%)	78	92
52	QF	64/64 (100%)	64 (100%)	0	100	100
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%)	93 (100%)	0	100	100
54	QH	70/70 (100%)	70 (100%)	0	100	100
54	Qh	70/70 (100%)	69 (99%)	1 (1%)	59	83
55	QI	50/50 (100%)	50 (100%)	0	100	100
55	Qi	49/50 (98%)	49 (100%)	0	100	100
56	QJ	40/42 (95%)	40 (100%)	0	100	100
56	Qj	41/42 (98%)	40 (98%)	1 (2%)	43	73
57	QK	55/59 (93%)	54 (98%)	1 (2%)	51	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	S1	579/579 (100%)	577 (100%)	2 (0%)	86	95
59	S2	370/370 (100%)	370 (100%)	0	100	100
60	S3	190/190 (100%)	189 (100%)	1 (0%)	81	93
61	S4	112/112 (100%)	111 (99%)	1 (1%)	70	88
62	S5	93/93 (100%)	93 (100%)	0	100	100
63	S6	79/79 (100%)	78 (99%)	1 (1%)	61	84
64	S7	132/132 (100%)	127 (96%)	5 (4%)	29	61
65	S8	151/151 (100%)	151 (100%)	0	100	100
66	V1	344/344 (100%)	341 (99%)	3 (1%)	70	88
67	V2	183/183 (100%)	180 (98%)	3 (2%)	55	81
68	V3	41/41 (100%)	41 (100%)	0	100	100
All	All	12184/12247 (100%)	12120 (100%)	64 (0%)	78	93

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	5B	113	CYS
5	6B	70	VAL
5	6B	86	ILE
16	A7	43	VAL
18	A9	129	LEU
19	AC	112	SER
20	AK	97	ASP
20	AK	255	CYS
21	AL	115	CYS
22	AM	78	ASP
22	AM	144	TYR
23	AN	144	THR
25	B2	90	ASP
26	B3	91	GLN
35	C1	52	GLN
35	C1	81	TRP
35	C1	151	HIS
35	C1	465	VAL
35	C1	512	ASN
37	C3	109	THR
39	CA	28	LYS
40	CB	56	VAL

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Mol	Chain	Res	Type
41	N1	224	PHE
41	N1	251	THR
41	N1	282	TYR
44	N4	114	GLU
44	N4	375	LEU
44	N4	444	LEU
45	N5	190	LEU
45	N5	286	LEU
45	N5	340	PHE
48	QB	289	ILE
49	QC	158	THR
49	QC	281	LEU
50	QD	215	LEU
51	QE	211	VAL
51	QE	272	ILE
57	QK	14	VAL
47	Qa	238	LEU
47	Qa	383	LEU
48	Qb	71	VAL
48	Qb	83	ASN
48	Qb	146	LEU
48	Qb	183	VAL
49	Qc	112	THR
51	Qe	145	ASP
54	Qh	19	LEU
56	Qj	2	LEU
58	S1	100	TRP
58	S1	347	ASP
60	S3	145	THR
61	S4	86	ASN
63	S6	102	LEU
64	S7	71	CYS
64	S7	88	ARG
64	S7	101	ASP
64	S7	117	LEU
64	S7	142	TYR
66	V1	210	THR
66	V1	235	VAL
66	V1	347	THR
67	V2	137	THR
67	V2	245	VAL
67	V2	249	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (251) such sidechains are listed below:

Mol	Chain	Res	Type
1	4L	50	ASN
2	5A	77	ASN
2	5A	102	ASN
4	6A	50	HIS
4	6A	54	HIS
4	6A	64	HIS
4	6A	83	HIS
4	6A	84	ASN
5	6B	11	ASN
5	6B	24	GLN
5	6B	25	ASN
5	6B	26	GLN
6	6C	22	HIS
7	7A	34	GLN
7	7A	50	ASN
8	7B	34	HIS
8	7B	59	GLN
8	7B	65	ASN
9	7C	18	HIS
12	A2	73	GLN
12	A2	86	GLN
13	A3	156	GLN
14	A5	71	GLN
14	A5	86	ASN
15	A6	84	GLN
15	A6	134	HIS
15	A6	152	HIS
16	A7	9	GLN
16	A7	21	GLN
17	A8	141	ASN
17	A8	142	GLN
18	A9	38	HIS
18	A9	72	HIS
18	A9	122	HIS
18	A9	138	ASN
18	A9	154	GLN
18	A9	356	HIS
19	AC	142	GLN
20	AK	67	ASN
20	AK	217	GLN
20	AK	221	GLN

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Mol	Chain	Res	Type
21	AL	89	ASN
22	AM	17	HIS
23	AN	61	GLN
23	AN	90	ASN
24	B1	3	ASN
24	B1	6	GLN
24	B1	14	HIS
25	B2	63	GLN
25	B2	71	GLN
26	B3	33	GLN
26	B3	91	GLN
27	B4	50	GLN
27	B4	79	ASN
27	B4	123	GLN
30	B7	85	HIS
30	B7	110	GLN
31	B8	56	ASN
31	B8	115	ASN
31	B8	132	HIS
32	B9	104	GLN
32	B9	117	GLN
33	BK	107	GLN
34	BL	86	ASN
35	C1	12	HIS
35	C1	52	GLN
35	C1	80	ASN
35	C1	99	ASN
35	C1	163	ASN
35	C1	170	ASN
35	C1	256	HIS
35	C1	328	HIS
35	C1	360	ASN
35	C1	422	ASN
35	C1	496	HIS
35	C1	512	ASN
36	C2	52	HIS
36	C2	59	GLN
36	C2	91	ASN
36	C2	102	HIS
36	C2	161	HIS
36	C2	180	ASN
37	C3	38	ASN

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Mol	Chain	Res	Type
37	C3	50	ASN
37	C3	56	GLN
37	C3	103	HIS
37	C3	125	ASN
37	C3	133	ASN
37	C3	161	GLN
37	C3	204	HIS
37	C3	232	HIS
38	C4	154	GLN
41	N1	138	GLN
41	N1	171	HIS
41	N1	317	GLN
42	N2	49	ASN
42	N2	83	GLN
42	N2	144	GLN
42	N2	186	HIS
42	N2	273	ASN
42	N2	310	ASN
42	N2	322	GLN
43	N3	26	GLN
44	N4	30	HIS
44	N4	213	HIS
44	N4	251	ASN
44	N4	279	GLN
44	N4	366	ASN
45	N5	2	ASN
45	N5	59	GLN
45	N5	135	ASN
45	N5	139	GLN
45	N5	199	GLN
45	N5	230	HIS
45	N5	248	HIS
45	N5	296	ASN
45	N5	518	GLN
45	N5	524	ASN
45	N5	540	HIS
45	N5	580	GLN
46	N6	175	ASN
47	QA	167	GLN
47	QA	168	ASN
47	QA	176	ASN
47	QA	184	ASN

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Mol	Chain	Res	Type
47	QA	284	ASN
47	QA	291	HIS
47	QA	365	ASN
47	QA	415	GLN
47	QA	426	ASN
48	QB	49	GLN
48	QB	66	GLN
48	QB	119	HIS
48	QB	188	HIS
48	QB	239	HIS
48	QB	301	ASN
48	QB	397	ASN
48	QB	464	GLN
49	QC	54	HIS
49	QC	97	HIS
49	QC	255	ASN
49	QC	308	HIS
49	QC	322	GLN
50	QD	206	HIS
50	QD	266	GLN
50	QD	310	HIS
51	QE	186	GLN
51	QE	199	GLN
51	QE	227	ASN
51	QE	257	ASN
52	QF	88	ASN
55	QI	38	GLN
55	QI	48	ASN
55	QI	55	HIS
56	QJ	16	ASN
47	Qa	81	HIS
47	Qa	139	ASN
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	290	GLN
47	Qa	291	HIS
47	Qa	304	ASN

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Mol	Chain	Res	Type
47	Qa	311	GLN
47	Qa	319	GLN
47	Qa	343	GLN
47	Qa	376	ASN
47	Qa	408	GLN
48	Qb	43	GLN
48	Qb	83	ASN
48	Qb	87	ASN
48	Qb	160	GLN
48	Qb	170	GLN
48	Qb	188	HIS
48	Qb	207	ASN
48	Qb	223	HIS
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	114	ASN
49	Qc	207	ASN
49	Qc	341	GLN
50	Qd	190	ASN
50	Qd	206	HIS
50	Qd	241	GLN
50	Qd	251	ASN
50	Qd	283	HIS
50	Qd	310	HIS
51	Qe	135	GLN
51	Qe	186	GLN
51	Qe	199	GLN
51	Qe	239	HIS
52	Qf	36	GLN
52	Qf	55	GLN
52	Qf	62	GLN
52	Qf	80	HIS
52	Qf	84	HIS
53	Qg	23	ASN
54	Qh	7	HIS
54	Qh	13	HIS
54	Qh	65	GLN

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Mol	Chain	Res	Type
55	Qi	38	GLN
55	Qi	48	ASN
56	Qj	16	ASN
58	S1	39	GLN
58	S1	278	HIS
58	S1	282	ASN
58	S1	331	GLN
58	S1	336	ASN
58	S1	425	ASN
58	S1	453	GLN
58	S1	498	GLN
58	S1	604	GLN
58	S1	677	GLN
58	S1	688	GLN
59	S2	93	GLN
59	S2	166	ASN
59	S2	239	HIS
60	S3	77	GLN
60	S3	82	ASN
60	S3	123	GLN
60	S3	196	HIS
61	S4	123	ASN
61	S4	163	ASN
62	S5	25	GLN
62	S5	34	HIS
62	S5	45	HIS
63	S6	117	GLN
64	S7	144	HIS
66	V1	220	GLN
66	V1	270	ASN
66	V1	303	HIS
66	V1	344	GLN
66	V1	393	ASN
67	V2	87	GLN
67	V2	90	ASN
67	V2	131	HIS
67	V2	133	GLN
67	V2	153	GLN
67	V2	182	ASN
67	V2	187	GLN
68	V3	388	ASN
68	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	$\# Z > 2$
59	2MR	S2	124	59	10,12,13	2.45	2 (20%)	5,13,15	1.07	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
59	2MR	S2	124	59	-	3/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	S2	124	2MR	CZ-NE	5.21	1.45	1.34
59	S2	124	2MR	CZ-NH2	5.08	1.44	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	S2	124	2MR	NE-CD-CG-CB
59	S2	124	2MR	CA-CB-CG-CD
59	S2	124	2MR	CG-CD-NE-CZ

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 101 ligands modelled in this entry, 7 are monoatomic - leaving 94 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	$\# Z > 2$
74	PEE	Qc	402	-	41,41,50	1.27	4 (9%)	44,46,55	1.17	4 (9%)
74	PEE	C3	304	-	50,50,50	1.32	5 (10%)	53,55,55	1.22	4 (7%)
69	CDL	Qc	401	-	60,60,99	0.38	0	66,72,111	0.37	0
71	PC1	QB	503	-	50,50,53	0.31	0	56,58,61	0.34	0
71	PC1	Qc	406	-	53,53,53	0.29	0	59,61,61	0.34	0
69	CDL	A7	201	-	50,50,99	0.41	0	56,62,111	0.34	0
69	CDL	AK	402	-	67,67,99	0.36	0	73,79,111	0.36	0
72	PLX	N4	501	-	51,51,51	1.11	3 (5%)	55,59,59	0.88	1 (1%)
77	3PE	C1	609	-	45,45,50	0.32	0	48,50,55	0.29	0
84	SF4	V1	501	66	0,12,12	-	-	-	-	-
69	CDL	4L	201	-	91,91,99	0.32	0	97,103,111	0.35	0
77	3PE	QJ	102	-	33,33,50	0.37	0	36,38,55	0.34	0
71	PC1	C1	605	-	53,53,53	0.30	0	59,61,61	0.34	0
74	PEE	Qd	402	-	23,23,50	1.41	3 (13%)	26,28,55	1.38	3 (11%)
71	PC1	6A	101	-	44,44,53	0.33	0	50,52,61	0.32	0
71	PC1	C1	607	-	45,45,53	0.31	0	51,53,61	0.32	0
77	3PE	Qc	405	-	47,47,50	0.32	0	50,52,55	0.36	0
72	PLX	AL	204	-	46,46,51	1.16	5 (10%)	50,54,59	0.88	1 (2%)
81	HEM	Qc	404	49	50,50,50	1.32	5 (10%)	66,82,82	1.68	18 (27%)
71	PC1	C1	606	-	32,32,53	0.36	0	38,40,61	0.35	0
71	PC1	N3	203	-	53,53,53	0.30	0	59,61,61	0.37	0
69	CDL	6A	102	-	82,82,99	0.33	0	88,94,111	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	HEM	QC	401	49	50,50,50	1.32	6 (12%)	66,82,82	1.66	15 (22%)
78	HEA	C1	602	35	66,67,67	2.21	25 (37%)	78,103,103	2.68	32 (41%)
84	SF4	S7	301	64	0,12,12	-	-	-	-	-
69	CDL	N5	703	-	88,88,99	0.32	0	94,100,111	0.33	0
74	PEE	QE	301	-	46,46,50	1.37	5 (10%)	49,51,55	1.18	4 (8%)
77	3PE	N5	706	-	37,37,50	0.35	0	40,42,55	0.30	0
72	PLX	QB	504	-	45,45,51	1.17	4 (8%)	49,53,59	0.91	1 (2%)
84	SF4	S8	301	65	0,12,12	-	-	-	-	-
76	ADP	AK	401	-	27,29,29	1.35	4 (14%)	42,45,45	1.98	11 (26%)
69	CDL	QD	402	-	57,57,99	0.38	0	63,69,111	0.39	0
74	PEE	N5	702	-	39,39,50	1.49	5 (12%)	41,44,55	1.21	2 (4%)
69	CDL	N5	704	-	99,99,99	0.30	0	105,111,111	0.28	0
77	3PE	CA	101	-	45,45,50	0.32	0	48,50,55	0.31	0
74	PEE	N5	705	-	50,50,50	1.32	5 (10%)	53,55,55	1.18	5 (9%)
75	ZMP	AB	201	19	29,35,36	0.70	1 (3%)	34,42,45	0.78	0
74	PEE	N3	201	-	50,50,50	1.32	5 (10%)	53,55,55	1.17	4 (7%)
71	PC1	C3	303	-	49,49,53	0.30	0	55,57,61	0.31	0
69	CDL	Qh	102	-	54,54,99	0.39	0	60,66,111	0.47	1 (1%)
72	PLX	6C	101	-	42,42,51	1.17	4 (9%)	46,50,59	0.90	2 (4%)
69	CDL	AL	201	-	93,93,99	0.31	0	99,105,111	0.32	0
77	3PE	Qj	101	-	28,28,50	0.39	0	31,33,55	0.34	0
72	PLX	B5	201	-	51,51,51	1.10	3 (5%)	55,59,59	0.89	1 (1%)
77	3PE	C1	608	-	44,44,50	0.33	0	47,49,55	0.38	0
71	PC1	Qh	101	-	53,53,53	0.29	0	59,61,61	0.28	0
72	PLX	QI	301	-	51,51,51	1.11	5 (9%)	55,59,59	0.88	1 (1%)
85	FMN	V1	502	-	33,33,33	0.24	0	48,50,50	0.46	1 (2%)
82	HEC	QD	401	50	50,50,50	1.32	6 (12%)	68,82,82	1.19	5 (7%)
75	ZMP	AC	201	19	29,35,36	0.65	1 (3%)	34,42,45	0.73	0
69	CDL	N1	401	-	77,77,99	0.34	0	83,89,111	0.32	0
74	PEE	QB	502	-	33,33,50	1.43	4 (12%)	36,38,55	1.20	2 (5%)
77	3PE	CB	202	-	47,47,50	0.31	0	50,52,55	0.34	0
84	SF4	S1	802	58	0,12,12	-	-	-	-	-
69	CDL	QH	401	-	63,63,99	0.38	0	69,75,111	0.36	0
74	PEE	N1	404	-	30,30,50	1.28	3 (10%)	33,35,55	1.20	2 (6%)
74	PEE	QJ	101	-	50,50,50	1.32	5 (10%)	53,55,55	1.21	4 (7%)
83	FES	Qe	301	51	0,4,4	-	-	-	-	-
71	PC1	N1	402	-	53,53,53	0.30	0	59,61,61	0.31	0
71	PC1	C3	301	-	43,43,53	0.32	0	49,51,61	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	PEE	S2	501	-	44,44,50	1.40	5 (11%)	46,49,55	1.20	3 (6%)
69	CDL	QB	501	-	63,63,99	0.37	0	69,75,111	0.39	0
69	CDL	AL	202	-	79,79,99	0.33	0	85,91,111	0.33	0
74	PEE	A9	402	-	38,38,50	1.49	6 (15%)	41,43,55	1.20	3 (7%)
71	PC1	Qb	502	-	47,47,53	0.32	0	53,55,61	0.36	0
72	PLX	AM	201	-	51,51,51	1.10	4 (7%)	55,59,59	0.90	1 (1%)
74	PEE	AL	203	-	48,48,50	1.34	5 (10%)	51,53,55	1.20	2 (3%)
77	3PE	S7	303	-	50,50,50	0.32	0	53,55,55	0.34	0
81	HEM	Qc	403	49	50,50,50	1.31	6 (12%)	66,82,82	1.68	14 (21%)
73	NDP	A9	401	-	49,52,52	0.34	0	66,80,80	0.42	0
72	PLX	S7	302	-	51,51,51	1.11	3 (5%)	55,59,59	0.91	2 (3%)
84	SF4	S1	801	58	0,12,12	-	-	-	-	-
78	HEA	C1	601	35	66,67,67	2.21	25 (37%)	78,103,103	2.67	29 (37%)
71	PC1	N1	403	-	53,53,53	0.29	0	59,61,61	0.30	0
72	PLX	CB	201	-	51,51,51	1.11	4 (7%)	55,59,59	0.88	1 (1%)
83	FES	S1	803	58	0,4,4	-	-	-	-	-
71	PC1	6A	103	-	37,37,53	0.34	0	43,45,61	0.30	0
72	PLX	N3	202	-	51,51,51	1.10	4 (7%)	55,59,59	3.03	7 (12%)
81	HEM	QC	402	49	50,50,50	1.33	6 (12%)	66,82,82	1.67	16 (24%)
69	CDL	CB	203	-	82,82,99	0.32	0	88,94,111	0.32	0
82	HEC	Qd	401	50	50,50,50	1.32	6 (12%)	68,82,82	1.23	4 (5%)
84	SF4	S8	302	65	0,12,12	-	-	-	-	-
71	PC1	C3	302	-	48,48,53	0.31	0	54,56,61	0.36	0
74	PEE	S8	303	-	50,50,50	1.32	5 (10%)	53,55,55	1.15	3 (5%)
69	CDL	N4	502	-	99,99,99	0.30	0	105,111,111	0.27	0
77	3PE	B8	201	-	31,31,50	0.37	0	34,36,55	0.32	0
77	3PE	QE	302	-	43,43,50	0.32	0	46,48,55	0.32	0
74	PEE	N5	701	-	45,45,50	1.37	6 (13%)	48,50,55	1.23	3 (6%)
69	CDL	N4	503	-	61,61,99	0.37	0	67,73,111	0.33	0
69	CDL	Qb	501	-	63,63,99	0.37	0	69,75,111	0.36	0
83	FES	QE	303	51	0,4,4	-	-	-	-	-
83	FES	V2	301	67	0,4,4	-	-	-	-	-
69	CDL	B5	202	-	99,99,99	0.30	0	105,111,111	0.29	0
74	PEE	QC	403	-	39,39,50	1.31	4 (10%)	42,44,55	1.18	3 (7%)

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
74	PEE	Qc	402	-	-	27/45/45/54	-
74	PEE	C3	304	-	-	21/54/54/54	-
69	CDL	Qc	401	-	-	18/71/71/110	-
71	PC1	QB	503	-	-	18/54/54/57	-
71	PC1	Qc	406	-	-	11/57/57/57	-
69	CDL	A7	201	-	-	11/61/61/110	-
69	CDL	AK	402	-	-	25/78/78/110	-
72	PLX	N4	501	-	-	25/55/55/55	-
77	3PE	C1	609	-	-	9/49/49/54	-
84	SF4	V1	501	66	-	-	0/6/5/5
69	CDL	4L	201	-	-	19/102/102/110	-
77	3PE	QJ	102	-	-	5/37/37/54	-
71	PC1	C1	605	-	-	17/57/57/57	-
74	PEE	Qd	402	-	-	9/27/27/54	-
71	PC1	6A	101	-	-	14/48/48/57	-
71	PC1	C1	607	-	-	13/49/49/57	-
77	3PE	Qc	405	-	-	11/51/51/54	-
72	PLX	AL	204	-	-	18/50/50/55	-
81	HEM	Qc	404	49	-	8/14/54/54	-
71	PC1	C1	606	-	-	9/36/36/57	-
71	PC1	N3	203	-	-	14/57/57/57	-
69	CDL	6A	102	-	-	21/93/93/110	-
81	HEM	QC	401	49	-	7/14/54/54	-
78	HEA	C1	602	35	-	13/36/76/76	-
84	SF4	S7	301	64	-	-	0/6/5/5
69	CDL	N5	703	-	-	22/99/99/110	-
74	PEE	QE	301	-	-	23/50/50/54	-
77	3PE	N5	706	-	-	7/41/41/54	-
72	PLX	QB	504	-	-	18/49/49/55	-
84	SF4	S8	301	65	-	-	0/6/5/5
76	ADP	AK	401	-	-	1/16/32/32	0/3/3/3
69	CDL	QD	402	-	-	20/68/68/110	-
74	PEE	N5	702	-	-	27/43/43/54	-
69	CDL	N5	704	-	-	18/110/110/110	-
77	3PE	CA	101	-	-	6/49/49/54	-
74	PEE	N5	705	-	-	29/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	ZMP	AB	201	19	-	12/40/42/43	-
74	PEE	N3	201	-	-	29/54/54/54	-
71	PC1	C3	303	-	-	8/53/53/57	-
69	CDL	Qh	102	-	-	12/65/65/110	-
72	PLX	6C	101	-	-	20/46/46/55	-
69	CDL	AL	201	-	-	23/104/104/110	-
77	3PE	Qj	101	-	-	5/32/32/54	-
72	PLX	B5	201	-	-	19/55/55/55	-
77	3PE	C1	608	-	-	11/48/48/54	-
71	PC1	Qh	101	-	-	18/57/57/57	-
72	PLX	QI	301	-	-	18/55/55/55	-
85	FMN	V1	502	-	-	6/18/18/18	0/3/3/3
82	HEC	QD	401	50	1/1/3/7	2/14/54/54	-
75	ZMP	AC	201	19	-	17/40/42/43	-
69	CDL	N1	401	-	-	16/88/88/110	-
74	PEE	QB	502	-	-	24/37/37/54	-
77	3PE	CB	202	-	-	11/51/51/54	-
84	SF4	S1	802	58	-	-	0/6/5/5
69	CDL	QH	401	-	-	17/74/74/110	-
74	PEE	N1	404	-	-	15/34/34/54	-
74	PEE	QJ	101	-	-	28/54/54/54	-
83	FES	Qe	301	51	-	-	0/1/1/1
71	PC1	N1	402	-	-	16/57/57/57	-
71	PC1	C3	301	-	-	18/47/47/57	-
74	PEE	S2	501	-	-	20/48/48/54	-
69	CDL	QB	501	-	-	17/74/74/110	-
69	CDL	AL	202	-	-	25/90/90/110	-
74	PEE	A9	402	-	-	17/42/42/54	-
71	PC1	Qb	502	-	-	15/51/51/57	-
72	PLX	AM	201	-	-	19/55/55/55	-
74	PEE	AL	203	-	-	31/52/52/54	-
77	3PE	S7	303	-	-	15/54/54/54	-
81	HEM	Qc	403	49	-	7/14/54/54	-
73	NDP	A9	401	-	-	5/34/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	PLX	S7	302	-	-	24/55/55/55	-
84	SF4	S1	801	58	-	-	0/6/5/5
78	HEA	C1	601	35	-	12/36/76/76	-
71	PC1	N1	403	-	-	20/57/57/57	-
72	PLX	CB	201	-	-	25/55/55/55	-
83	FES	S1	803	58	-	-	0/1/1/1
71	PC1	6A	103	-	-	9/41/41/57	-
72	PLX	N3	202	-	-	32/55/55/55	-
81	HEM	QC	402	49	-	6/14/54/54	-
69	CDL	CB	203	-	-	28/93/93/110	-
82	HEC	Qd	401	50	1/1/3/7	4/14/54/54	-
84	SF4	S8	302	65	-	-	0/6/5/5
71	PC1	C3	302	-	-	13/52/52/57	-
74	PEE	S8	303	-	-	22/54/54/54	-
69	CDL	N4	502	-	-	15/110/110/110	-
77	3PE	B8	201	-	-	10/35/35/54	-
77	3PE	QE	302	-	-	16/47/47/54	-
74	PEE	N5	701	-	-	26/49/49/54	-
69	CDL	N4	503	-	-	28/72/72/110	-
69	CDL	Qb	501	-	-	16/74/74/110	-
83	FES	QE	303	51	-	-	0/1/1/1
83	FES	V2	301	67	-	-	0/1/1/1
69	CDL	B5	202	-	-	23/110/110/110	-
74	PEE	QC	403	-	-	23/43/43/54	-

All (205) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	C1	601	HEA	C3B-C2B	5.33	1.46	1.34
78	C1	602	HEA	C3B-C2B	5.12	1.46	1.34
78	C1	602	HEA	FE-ND	4.91	2.10	1.94
78	C1	601	HEA	FE-NB	4.67	2.09	1.94
78	C1	602	HEA	FE-NB	4.64	2.09	1.94
78	C1	601	HEA	FE-ND	4.64	2.09	1.94
78	C1	602	HEA	C3A-C2A	4.55	1.46	1.36
78	C1	601	HEA	C3A-C2A	4.49	1.46	1.36
76	AK	401	ADP	C5-C4	4.45	1.47	1.39
78	C1	602	HEA	FE-NC	4.22	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	C1	601	HEA	FE-NC	4.18	2.09	1.95
78	C1	602	HEA	C1D-ND	-4.12	1.33	1.40
78	C1	601	HEA	CHC-C4B	4.10	1.46	1.38
74	QE	301	PEE	C18-C19	4.06	1.55	1.31
74	A9	402	PEE	C18-C19	4.05	1.55	1.31
78	C1	601	HEA	C4B-NB	-4.04	1.33	1.40
74	N5	702	PEE	C18-C19	4.04	1.55	1.31
74	C3	304	PEE	C18-C19	4.04	1.55	1.31
74	N5	705	PEE	C18-C19	4.04	1.55	1.31
74	S2	501	PEE	C18-C19	4.04	1.55	1.31
74	N5	701	PEE	C18-C19	4.03	1.55	1.31
74	QC	403	PEE	C18-C19	4.03	1.55	1.31
74	N3	201	PEE	C18-C19	4.03	1.55	1.31
74	S8	303	PEE	C18-C19	4.03	1.55	1.31
74	Qc	402	PEE	C18-C19	4.03	1.55	1.31
74	AL	203	PEE	C18-C19	4.03	1.55	1.31
74	QJ	101	PEE	C18-C19	4.01	1.55	1.31
74	QB	502	PEE	C39-C38	3.96	1.54	1.31
74	S8	303	PEE	C39-C38	3.96	1.54	1.31
78	C1	601	HEA	C1D-ND	-3.95	1.33	1.40
74	QE	301	PEE	C39-C38	3.95	1.54	1.31
74	C3	304	PEE	C39-C38	3.94	1.54	1.31
74	N5	702	PEE	C39-C38	3.94	1.54	1.31
74	AL	203	PEE	C39-C38	3.94	1.54	1.31
74	S2	501	PEE	C39-C38	3.94	1.54	1.31
74	N5	701	PEE	C39-C38	3.93	1.54	1.31
74	N3	201	PEE	C39-C38	3.93	1.54	1.31
74	QJ	101	PEE	C39-C38	3.92	1.54	1.31
74	N5	705	PEE	C39-C38	3.91	1.54	1.31
78	C1	602	HEA	C4B-NB	-3.89	1.33	1.40
81	QC	402	HEM	C4D-ND	-3.89	1.33	1.40
78	C1	602	HEA	C3D-C2D	3.89	1.45	1.36
74	A9	402	PEE	C39-C38	3.87	1.54	1.28
81	Qc	404	HEM	C4D-ND	-3.87	1.33	1.40
78	C1	601	HEA	C3D-C2D	3.85	1.44	1.36
78	C1	602	HEA	CHC-C4B	3.85	1.46	1.38
81	QC	401	HEM	C4D-ND	-3.71	1.33	1.40
81	Qc	403	HEM	C4D-ND	-3.68	1.34	1.40
78	C1	601	HEA	C4C-NC	-3.49	1.33	1.39
78	C1	602	HEA	CHA-C1A	3.49	1.45	1.38
78	C1	602	HEA	C4C-NC	-3.46	1.33	1.39
78	C1	601	HEA	CHA-C1A	3.36	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	QD	401	HEC	CBC-CAC	-3.31	1.36	1.51
78	C1	601	HEA	CHD-C1D	3.29	1.45	1.38
82	Qd	401	HEC	CBC-CAC	-3.28	1.36	1.51
74	N1	404	PEE	O3-C30	3.26	1.42	1.33
74	C3	304	PEE	O3-C30	3.26	1.42	1.33
78	C1	601	HEA	CHC-C1C	3.25	1.46	1.39
74	QJ	101	PEE	O3-C30	3.25	1.42	1.33
74	A9	402	PEE	O3-C30	3.25	1.42	1.33
74	QB	502	PEE	O3-C30	3.25	1.42	1.33
74	N5	705	PEE	O3-C30	3.24	1.42	1.33
74	N3	201	PEE	O3-C30	3.24	1.42	1.33
74	S8	303	PEE	O3-C30	3.24	1.42	1.33
74	QC	403	PEE	O3-C30	3.23	1.42	1.33
74	Qc	402	PEE	O3-C30	3.23	1.42	1.33
74	N5	702	PEE	O3-C30	3.22	1.42	1.33
81	QC	402	HEM	C1B-NB	-3.21	1.34	1.40
74	S2	501	PEE	O3-C30	3.21	1.42	1.33
81	Qc	404	HEM	C1B-NB	-3.20	1.34	1.40
74	Qd	402	PEE	O3-C30	3.16	1.42	1.33
74	N5	701	PEE	O3-C30	3.13	1.42	1.33
74	AL	203	PEE	O3-C30	3.10	1.42	1.33
81	QC	401	HEM	C1B-NB	-3.09	1.35	1.40
74	QE	301	PEE	O3-C30	3.08	1.42	1.33
72	QB	504	PLX	O6-C4	-3.06	1.40	1.44
72	S7	302	PLX	O6-C4	-3.05	1.40	1.44
72	N4	501	PLX	O6-C4	-3.05	1.40	1.44
78	C1	602	HEA	CHB-C1B	3.04	1.46	1.39
72	6C	101	PLX	O6-C4	-3.03	1.40	1.44
81	Qc	403	HEM	C1B-NB	-3.03	1.35	1.40
78	C1	602	HEA	CHC-C1C	3.02	1.46	1.39
78	C1	602	HEA	CHD-C1D	3.02	1.44	1.38
72	CB	201	PLX	O6-C4	-3.00	1.40	1.44
72	B5	201	PLX	O6-C4	-2.97	1.40	1.44
78	C1	602	HEA	C1C-NC	-2.94	1.34	1.39
78	C1	601	HEA	C1B-NB	-2.93	1.32	1.38
81	QC	402	HEM	C1C-C2C	-2.90	1.39	1.45
78	C1	601	HEA	C1C-NC	-2.89	1.34	1.39
72	AM	201	PLX	O6-C4	-2.89	1.40	1.44
72	QI	301	PLX	O6-C4	-2.84	1.40	1.44
74	A9	402	PEE	O2-C10	2.84	1.42	1.34
81	Qc	404	HEM	C1C-C2C	-2.83	1.39	1.45
72	AL	204	PLX	O6-C4	-2.82	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	C1	602	HEA	CHD-C4C	2.80	1.45	1.39
72	N3	202	PLX	O6-C4	-2.80	1.40	1.44
78	C1	602	HEA	CHB-C4A	2.78	1.43	1.38
82	QD	401	HEC	CAC-C3C	2.75	1.58	1.51
74	N5	701	PEE	O2-C10	2.75	1.42	1.34
76	AK	401	ADP	C5-C6	2.73	1.48	1.41
74	QE	301	PEE	O2-C10	2.72	1.42	1.34
82	Qd	401	HEC	CAC-C3C	2.72	1.58	1.51
74	S8	303	PEE	O2-C10	2.71	1.42	1.34
74	QJ	101	PEE	O2-C10	2.70	1.41	1.34
78	C1	602	HEA	CHA-C4D	2.69	1.45	1.39
74	N5	702	PEE	O2-C10	2.69	1.41	1.34
74	QB	502	PEE	O2-C10	2.67	1.41	1.34
75	AB	201	ZMP	C9-C10	-2.67	1.48	1.50
78	C1	601	HEA	C4D-ND	-2.66	1.33	1.38
74	N1	404	PEE	O2-C10	2.66	1.41	1.34
74	Qd	402	PEE	O2-C10	2.65	1.41	1.34
81	QC	401	HEM	C1C-C2C	-2.65	1.40	1.45
78	C1	602	HEA	C4D-ND	-2.63	1.33	1.38
78	C1	602	HEA	C1B-NB	-2.63	1.33	1.38
78	C1	601	HEA	CHD-C4C	2.63	1.45	1.39
81	Qc	403	HEM	C1C-C2C	-2.62	1.40	1.45
74	N5	705	PEE	O2-C10	2.62	1.41	1.34
74	N3	201	PEE	O2-C10	2.62	1.41	1.34
78	C1	601	HEA	CHB-C4A	2.62	1.43	1.38
78	C1	601	HEA	CHA-C4D	2.61	1.45	1.39
74	AL	203	PEE	O2-C10	2.60	1.41	1.34
74	C3	304	PEE	O2-C10	2.60	1.41	1.34
74	Qc	402	PEE	O2-C2	-2.58	1.40	1.46
74	AL	203	PEE	O2-C2	-2.58	1.40	1.46
74	S2	501	PEE	O2-C10	2.57	1.41	1.34
81	QC	401	HEM	C1D-ND	-2.57	1.33	1.38
74	QC	403	PEE	O2-C10	2.57	1.41	1.34
81	Qc	404	HEM	C1D-ND	-2.56	1.33	1.38
81	Qc	403	HEM	FE-NB	2.54	2.02	1.94
74	QC	403	PEE	O2-C2	-2.54	1.40	1.46
78	C1	601	HEA	CHB-C1B	2.54	1.45	1.39
81	QC	402	HEM	C1D-ND	-2.53	1.33	1.38
81	QC	401	HEM	FE-NB	2.51	2.02	1.94
74	N5	705	PEE	O2-C2	-2.51	1.40	1.46
74	S2	501	PEE	O2-C2	-2.50	1.40	1.46
81	Qc	403	HEM	C1D-ND	-2.49	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	Qd	402	PEE	O2-C2	-2.49	1.40	1.46
81	Qc	404	HEM	FE-NB	2.48	2.02	1.94
74	C3	304	PEE	O2-C2	-2.48	1.40	1.46
74	N3	201	PEE	O2-C2	-2.47	1.40	1.46
74	Qc	402	PEE	O2-C10	2.47	1.41	1.34
74	QB	502	PEE	O2-C2	-2.45	1.40	1.46
82	Qd	401	HEC	CBB-CAB	-2.45	1.40	1.51
75	AC	201	ZMP	C9-C10	-2.44	1.48	1.50
78	C1	601	HEA	C4A-NA	2.44	1.44	1.39
74	QE	301	PEE	O2-C2	-2.44	1.40	1.46
74	QJ	101	PEE	O2-C2	-2.43	1.40	1.46
74	N5	702	PEE	O2-C2	-2.42	1.40	1.46
74	N1	404	PEE	O2-C2	-2.41	1.40	1.46
78	C1	601	HEA	O2D-CGD	-2.40	1.22	1.30
82	QD	401	HEC	CBB-CAB	-2.40	1.40	1.51
78	C1	601	HEA	O2A-CGA	-2.39	1.22	1.30
76	AK	401	ADP	C8-N7	2.38	1.36	1.31
78	C1	602	HEA	O2D-CGD	-2.37	1.22	1.30
78	C1	602	HEA	C4A-NA	2.36	1.44	1.39
81	QC	402	HEM	FE-NB	2.35	2.02	1.94
78	C1	602	HEA	O2A-CGA	-2.31	1.23	1.30
78	C1	601	HEA	C4B-C3B	2.31	1.48	1.44
82	Qd	401	HEC	CAB-C3B	2.27	1.56	1.51
72	QB	504	PLX	C1B-N1	-2.27	1.43	1.50
78	C1	601	HEA	C1A-NA	2.26	1.44	1.39
74	S8	303	PEE	O2-C2	-2.25	1.41	1.46
82	QD	401	HEC	CAB-C3B	2.25	1.56	1.51
78	C1	602	HEA	C1A-NA	2.24	1.44	1.39
76	AK	401	ADP	C5-N7	-2.23	1.34	1.39
81	Qc	403	HEM	FE-ND	2.18	2.01	1.94
72	QI	301	PLX	C1B-N1	-2.18	1.43	1.50
72	N4	501	PLX	C1B-N1	-2.17	1.43	1.50
81	QC	401	HEM	FE-ND	2.17	2.01	1.94
72	AL	204	PLX	C1B-N1	-2.15	1.43	1.50
72	CB	201	PLX	C1B-N1	-2.15	1.43	1.50
72	B5	201	PLX	C1B-N1	-2.14	1.43	1.50
72	QI	301	PLX	C1C-N1	-2.13	1.43	1.50
82	QD	401	HEC	FE-ND	2.13	2.01	1.94
72	QB	504	PLX	C1C-N1	-2.13	1.43	1.50
78	C1	602	HEA	C4B-C3B	2.12	1.48	1.44
74	N5	701	PEE	O2-C2	-2.12	1.41	1.46
72	6C	101	PLX	C1B-N1	-2.12	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	N3	202	PLX	C1B-N1	-2.11	1.43	1.50
82	Qd	401	HEC	FE-ND	2.10	2.01	1.94
74	A9	402	PEE	O2-C2	-2.09	1.41	1.46
72	S7	302	PLX	C1B-N1	-2.08	1.43	1.50
72	S7	302	PLX	C1C-N1	-2.08	1.43	1.50
72	AL	204	PLX	C1C-N1	-2.07	1.44	1.50
72	N3	202	PLX	P1-O4	2.07	1.67	1.59
72	AM	201	PLX	C1B-N1	-2.07	1.44	1.50
82	QD	401	HEC	CMD-C2D	2.07	1.55	1.50
72	AM	201	PLX	P1-O4	2.06	1.67	1.59
72	CB	201	PLX	C1C-N1	-2.05	1.44	1.50
72	N3	202	PLX	C7-C6	2.05	1.55	1.50
72	AL	204	PLX	C7-C6	2.04	1.55	1.50
72	QI	301	PLX	C7-C6	2.04	1.55	1.50
82	Qd	401	HEC	CMD-C2D	2.03	1.55	1.50
72	AL	204	PLX	P1-O4	2.03	1.67	1.59
72	B5	201	PLX	P1-O4	2.02	1.67	1.59
72	QB	504	PLX	P1-O4	2.02	1.67	1.59
74	N5	701	PEE	C11-C10	2.02	1.56	1.50
81	QC	402	HEM	C4B-NB	-2.02	1.34	1.38
72	AM	201	PLX	C1C-N1	-2.02	1.44	1.50
72	CB	201	PLX	P1-O4	2.02	1.67	1.59
72	6C	101	PLX	C1C-N1	-2.02	1.44	1.50
72	N4	501	PLX	C1C-N1	-2.02	1.44	1.50
74	A9	402	PEE	C11-C10	2.02	1.56	1.50
72	QI	301	PLX	P1-O4	2.00	1.67	1.59
72	6C	101	PLX	P1-O4	2.00	1.67	1.59

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	N3	202	PLX	C1A-N1-C1B	-11.48	79.45	108.97
72	N3	202	PLX	C1B-N1-C1C	-11.33	79.84	108.97
72	N3	202	PLX	C1A-N1-C1C	8.60	131.09	108.97
78	C1	601	HEA	CAD-CBD-CGD	-7.71	97.01	113.60
78	C1	602	HEA	CAD-CBD-CGD	-7.68	97.07	113.60
78	C1	601	HEA	C3C-C4C-NC	7.68	114.97	110.25
78	C1	602	HEA	CAA-CBA-CGA	-7.63	97.19	113.60
72	N3	202	PLX	C1A-N1-C1	-7.10	80.86	109.92
72	N3	202	PLX	C1C-N1-C1	-7.02	81.19	109.92
78	C1	602	HEA	C3C-C4C-NC	6.38	114.17	110.25
78	C1	602	HEA	C3D-C4D-ND	6.35	116.51	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	AK	401	ADP	C5-C4-N3	-6.16	118.72	126.75
78	C1	601	HEA	C3D-C4D-ND	6.05	116.22	110.36
78	C1	601	HEA	CAA-CBA-CGA	-6.02	100.65	113.60
78	C1	601	HEA	C3C-C2C-C1C	-5.65	100.34	107.16
78	C1	602	HEA	C3C-C2C-C1C	-5.46	100.57	107.16
72	N3	202	PLX	C1B-N1-C1	5.43	132.13	109.92
78	C1	601	HEA	C13-C12-C11	-5.24	106.48	114.35
78	C1	602	HEA	C13-C12-C11	-5.16	106.60	114.35
78	C1	601	HEA	C2B-C1B-NB	5.11	116.01	109.88
78	C1	601	HEA	CHB-C1B-C2B	-5.02	117.14	124.98
78	C1	602	HEA	C2D-C1D-ND	4.89	115.63	109.84
76	AK	401	ADP	N3-C4-N9	4.80	135.00	127.08
78	C1	601	HEA	C2D-C1D-ND	4.72	115.44	109.84
81	Qc	403	HEM	CHC-C4B-NB	4.65	129.47	124.42
78	C1	602	HEA	C1D-C2D-C3D	-4.63	102.09	106.96
78	C1	602	HEA	C2B-C1B-NB	4.59	115.38	109.88
81	QC	401	HEM	CHC-C4B-NB	4.58	129.40	124.42
78	C1	601	HEA	C1D-C2D-C3D	-4.56	102.17	106.96
81	Qc	403	HEM	CHD-C4C-NC	4.51	129.31	124.44
81	QC	402	HEM	C4D-ND-C1D	4.42	109.64	105.07
81	Qc	404	HEM	CHC-C4B-NB	4.41	129.21	124.42
78	C1	602	HEA	CHB-C1B-C2B	-4.38	118.13	124.98
81	QC	401	HEM	CHD-C4C-NC	4.36	129.16	124.44
74	QJ	101	PEE	O2-C10-C11	4.36	120.90	111.50
74	C3	304	PEE	O2-C10-C11	4.35	120.87	111.50
74	N5	701	PEE	O2-C10-C11	4.32	120.82	111.50
74	Qd	402	PEE	O2-C10-C11	4.26	120.67	111.50
74	N1	404	PEE	O2-C10-C11	4.21	120.57	111.50
74	N5	702	PEE	O2-C10-C11	4.13	120.40	111.50
81	Qc	404	HEM	CHD-C4C-NC	4.12	128.90	124.44
74	QB	502	PEE	O2-C10-C11	4.07	120.27	111.50
74	N5	705	PEE	O2-C10-C11	4.04	120.20	111.50
78	C1	602	HEA	C3B-C4B-NB	4.01	114.60	109.84
81	Qc	403	HEM	CHB-C1B-NB	4.01	129.32	124.37
74	N3	201	PEE	O2-C10-C11	3.99	120.10	111.50
74	QC	403	PEE	O2-C10-C11	3.98	120.08	111.50
74	AL	203	PEE	O2-C10-C11	3.96	120.05	111.50
74	S8	303	PEE	O2-C10-C11	3.94	119.99	111.50
78	C1	602	HEA	CHA-C4D-C3D	-3.92	119.08	124.84
74	S2	501	PEE	O2-C10-C11	3.91	119.92	111.50
81	QC	401	HEM	CHB-C1B-NB	3.91	129.19	124.37
78	C1	601	HEA	C2C-C1C-NC	3.89	116.01	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	QE	301	PEE	O2-C10-C11	3.88	119.85	111.50
81	QC	402	HEM	CHC-C4B-NB	3.87	128.62	124.42
76	AK	401	ADP	C2-N3-C4	3.84	120.83	111.75
81	Qc	404	HEM	C4D-ND-C1D	3.82	109.02	105.07
78	C1	601	HEA	CHA-C4D-C3D	-3.79	119.27	124.84
74	Qc	402	PEE	O2-C10-C11	3.77	119.63	111.50
81	Qc	404	HEM	CHB-C1B-NB	3.75	129.00	124.37
76	AK	401	ADP	PA-O3A-PB	-3.74	120.00	132.83
81	QC	402	HEM	CHB-C1B-NB	3.72	128.96	124.37
81	QC	402	HEM	CHD-C4C-NC	3.66	128.40	124.44
81	QC	402	HEM	C1B-NB-C4B	3.61	108.80	105.07
78	C1	602	HEA	C2C-C1C-NC	3.58	115.53	110.08
78	C1	602	HEA	C4B-C3B-C2B	-3.58	101.30	107.41
78	C1	601	HEA	C3B-C4B-NB	3.48	113.97	109.84
74	A9	402	PEE	O2-C10-C11	3.43	118.90	111.50
81	Qc	403	HEM	C4D-ND-C1D	3.36	108.54	105.07
78	C1	601	HEA	C4B-C3B-C2B	-3.35	101.68	107.41
81	QC	402	HEM	C4C-NC-C1C	3.34	108.62	105.35
76	AK	401	ADP	C4-C5-N7	-3.33	106.56	110.62
74	Qd	402	PEE	O3-C30-C31	3.31	120.07	111.38
81	QC	401	HEM	C4D-ND-C1D	3.31	108.49	105.07
81	Qc	403	HEM	C1B-NB-C4B	3.09	108.27	105.07
76	AK	401	ADP	N3-C2-N1	-3.06	123.82	128.60
81	Qc	404	HEM	C1B-NB-C4B	3.06	108.23	105.07
78	C1	601	HEA	C27-C19-C20	3.01	120.33	115.27
81	Qc	403	HEM	CHA-C4D-ND	3.00	128.07	124.37
81	QC	401	HEM	CHA-C4D-ND	2.97	128.04	124.37
81	QC	401	HEM	C1B-NB-C4B	2.91	108.08	105.07
82	Qd	401	HEC	O1D-CGD-CBD	-2.89	113.79	123.08
81	QC	402	HEM	C4A-NA-C1A	2.89	108.18	105.35
76	AK	401	ADP	C5-N7-C8	2.88	107.60	103.51
82	QD	401	HEC	O1D-CGD-CBD	-2.81	114.05	123.08
78	C1	601	HEA	C13-C14-C15	-2.81	120.90	127.66
81	QC	401	HEM	CHA-C1A-NA	2.80	129.00	123.85
78	C1	602	HEA	C17-C18-C19	-2.80	120.92	127.66
78	C1	602	HEA	C13-C14-C15	-2.76	121.00	127.66
81	Qc	404	HEM	CHD-C1D-ND	2.74	127.40	124.42
81	Qc	403	HEM	CHA-C1A-NA	2.74	128.89	123.85
81	Qc	404	HEM	CHA-C4D-ND	2.73	127.74	124.37
78	C1	601	HEA	C17-C18-C19	-2.70	121.17	127.66
74	QJ	101	PEE	O3-C30-C31	2.69	120.35	111.91
74	Qc	402	PEE	O3-C30-C31	2.68	120.32	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	C1	602	HEA	C4D-C3D-C2D	-2.68	102.99	106.90
78	C1	601	HEA	CMB-C2B-C1B	-2.66	120.98	125.04
74	N5	705	PEE	O3-C30-C31	2.66	120.24	111.91
81	Qc	403	HEM	CHD-C1D-ND	2.64	127.29	124.42
76	AK	401	ADP	C4-N9-C8	2.63	108.58	105.73
74	N5	702	PEE	O3-C30-C31	2.63	120.17	111.91
78	C1	602	HEA	C27-C19-C20	2.63	119.70	115.27
81	QC	401	HEM	CHD-C1D-ND	2.63	127.28	124.42
74	S8	303	PEE	O3-C30-C31	2.62	120.14	111.91
78	C1	601	HEA	CMB-C2B-C3B	2.62	135.34	130.34
74	A9	402	PEE	O3-C30-C31	2.61	120.11	111.91
81	QC	402	HEM	CHA-C4D-ND	2.61	127.59	124.37
78	C1	601	HEA	C1B-C2B-C3B	-2.61	103.68	106.80
74	S2	501	PEE	O3-C30-C31	2.61	120.09	111.91
74	N5	701	PEE	O3-C30-C31	2.59	120.04	111.91
78	C1	601	HEA	C26-C15-C16	2.59	119.63	115.27
74	AL	203	PEE	O3-C30-C31	2.58	120.02	111.91
81	Qc	404	HEM	C4C-NC-C1C	2.58	107.88	105.35
78	C1	602	HEA	CHC-C4B-NB	-2.58	121.19	124.37
74	C3	304	PEE	O3-C30-C31	2.58	120.00	111.91
74	A9	402	PEE	C37-C38-C39	-2.56	109.42	126.84
74	QC	403	PEE	O3-C30-C31	2.55	119.91	111.91
74	N3	201	PEE	O3-C30-C31	2.54	119.86	111.91
78	C1	601	HEA	C4D-C3D-C2D	-2.53	103.22	106.90
78	C1	602	HEA	CMB-C2B-C1B	-2.52	121.20	125.04
78	C1	602	HEA	OMA-CMA-C3A	-2.52	119.99	125.69
74	N1	404	PEE	O3-C30-C31	2.52	119.80	111.91
81	Qc	404	HEM	C4A-NA-C1A	2.51	107.81	105.35
74	QB	502	PEE	O3-C30-C31	2.51	119.78	111.91
81	Qc	404	HEM	CAD-CBD-CGD	-2.51	108.21	113.60
74	QE	301	PEE	O3-C30-C31	2.47	119.65	111.91
81	QC	402	HEM	CHD-C1D-ND	2.44	127.07	124.42
81	QC	402	HEM	C1C-CHC-C4B	-2.42	120.84	126.06
81	QC	402	HEM	C4A-CHB-C1B	-2.39	120.67	126.34
82	QD	401	HEC	O1A-CGA-CBA	-2.39	115.41	123.08
69	Qh	102	CDL	OA8-CA6-CA4	2.39	115.38	108.43
81	Qc	403	HEM	C4C-NC-C1C	2.37	107.67	105.35
81	QC	401	HEM	CHB-C1B-C2B	-2.35	120.19	126.73
81	QC	401	HEM	C4C-NC-C1C	2.35	107.65	105.35
81	Qc	403	HEM	CHB-C1B-C2B	-2.34	120.22	126.73
81	QC	401	HEM	CAD-CBD-CGD	-2.32	108.61	113.60
81	QC	402	HEM	C2A-C1A-NA	-2.29	107.58	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	QC	402	HEM	CHA-C1A-NA	2.29	128.06	123.85
81	Qc	404	HEM	CHB-C1B-C2B	-2.29	120.38	126.73
72	AM	201	PLX	O3-P1-O2	-2.27	101.03	112.24
72	QI	301	PLX	O3-P1-O2	-2.27	101.03	112.24
81	Qc	404	HEM	C1C-CHC-C4B	-2.27	121.17	126.06
72	6C	101	PLX	O3-P1-O2	-2.25	101.10	112.24
81	QC	402	HEM	CAD-CBD-CGD	-2.25	108.76	113.60
81	QC	401	HEM	C4A-NA-C1A	2.25	107.55	105.35
78	C1	601	HEA	C27-C19-C18	-2.25	117.91	123.68
78	C1	601	HEA	OMA-CMA-C3A	-2.24	120.62	125.69
78	C1	601	HEA	CHB-C1B-NB	2.24	126.85	124.42
78	C1	602	HEA	C1D-ND-C4D	-2.22	102.78	105.07
72	CB	201	PLX	O3-P1-O2	-2.22	101.28	112.24
72	QB	504	PLX	O3-P1-O2	-2.22	101.28	112.24
72	AL	204	PLX	O3-P1-O2	-2.21	101.29	112.24
76	AK	401	ADP	C6-C5-N7	2.21	136.13	132.02
72	N4	501	PLX	O3-P1-O2	-2.21	101.33	112.24
81	QC	402	HEM	CHB-C1B-C2B	-2.20	120.63	126.73
81	Qc	403	HEM	CAD-CBD-CGD	-2.19	108.88	113.60
72	N3	202	PLX	O3-P1-O2	-2.19	101.40	112.24
72	B5	201	PLX	O3-P1-O2	-2.19	101.42	112.24
72	S7	302	PLX	O3-P1-O2	-2.18	101.46	112.24
78	C1	601	HEA	CHC-C4B-NB	-2.18	121.69	124.37
82	QD	401	HEC	O2A-CGA-O1A	2.18	128.73	123.30
81	Qc	404	HEM	C4A-CHB-C1B	-2.18	121.17	126.34
81	QC	402	HEM	C4C-CHD-C1D	-2.17	121.38	126.06
78	C1	602	HEA	CHA-C1A-C2A	-2.17	121.42	124.94
76	AK	401	ADP	N9-C8-N7	-2.15	110.97	113.91
78	C1	602	HEA	CMB-C2B-C3B	2.15	134.43	130.34
82	Qd	401	HEC	O2A-CGA-O1A	2.14	128.64	123.30
78	C1	601	HEA	O1D-CGD-CBD	-2.14	116.21	123.08
72	6C	101	PLX	C8-C7-C6	-2.13	108.45	113.38
78	C1	601	HEA	CMC-C2C-C1C	2.13	128.61	125.37
82	Qd	401	HEC	C1D-ND-C4D	2.12	107.27	105.07
78	C1	602	HEA	C26-C15-C16	2.10	118.81	115.27
82	QD	401	HEC	C1D-ND-C4D	2.10	107.25	105.07
74	Qd	402	PEE	C2-O2-C10	-2.10	112.63	117.79
78	C1	602	HEA	C27-C19-C18	-2.10	118.30	123.68
81	QC	401	HEM	C1C-CHC-C4B	-2.09	121.55	126.06
74	S8	303	PEE	C17-C18-C19	-2.08	108.73	124.73
81	Qc	404	HEM	C2A-C1A-NA	-2.08	107.82	110.15
81	Qc	403	HEM	C4A-NA-C1A	2.08	107.38	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	C1	602	HEA	CMD-C2D-C1D	2.08	128.20	125.04
74	QE	301	PEE	C40-C39-C38	-2.07	108.81	124.73
78	C1	602	HEA	C2A-C1A-NA	2.07	112.34	110.32
81	Qc	403	HEM	C1C-CHC-C4B	-2.07	121.59	126.06
74	QC	403	PEE	C17-C18-C19	-2.07	108.86	124.73
78	C1	602	HEA	O1D-CGD-CBD	-2.07	116.44	123.08
81	Qc	404	HEM	O2A-CGA-CBA	2.07	120.67	114.03
85	V1	502	FMN	P-O5'-C5'	2.06	123.98	118.30
81	Qc	404	HEM	CHA-C1A-NA	2.06	127.63	123.85
74	QJ	101	PEE	C20-C19-C18	-2.05	108.96	124.73
81	Qc	403	HEM	C4A-CHB-C1B	-2.05	121.48	126.34
74	QE	301	PEE	C20-C19-C18	-2.04	109.04	124.73
74	N5	705	PEE	C37-C38-C39	-2.04	109.05	124.73
78	C1	601	HEA	C1D-ND-C4D	-2.04	102.96	105.07
78	C1	602	HEA	CAD-C3D-C2D	2.04	131.68	127.88
78	C1	602	HEA	C1B-C2B-C3B	-2.04	104.36	106.80
82	QD	401	HEC	CHC-C4B-NB	2.04	126.89	124.37
74	C3	304	PEE	C20-C19-C18	-2.03	109.13	124.73
74	C3	304	PEE	C40-C39-C38	-2.03	109.14	124.73
74	Qc	402	PEE	C17-C18-C19	-2.03	109.15	124.73
74	N5	705	PEE	C40-C39-C38	-2.03	109.15	124.73
78	C1	602	HEA	O1A-CGA-CBA	-2.03	116.57	123.08
72	S7	302	PLX	C8-C7-C6	-2.03	108.70	113.38
74	QJ	101	PEE	C17-C18-C19	-2.02	109.20	124.73
81	QC	401	HEM	C2A-C1A-NA	-2.02	107.89	110.15
74	Qc	402	PEE	C20-C19-C18	-2.02	109.22	124.73
81	QC	401	HEM	C4A-CHB-C1B	-2.02	121.55	126.34
82	Qd	401	HEC	O1A-CGA-CBA	-2.02	116.59	123.08
74	N5	705	PEE	C20-C19-C18	-2.01	109.28	124.73
74	S2	501	PEE	C37-C38-C39	-2.01	109.31	124.73
81	Qc	404	HEM	C4C-CHD-C1D	-2.01	121.73	126.06
76	AK	401	ADP	C3'-C2'-C1'	2.00	105.23	101.43
74	N3	201	PEE	C20-C19-C18	-2.00	109.34	124.73
74	N5	701	PEE	C40-C39-C38	-2.00	109.34	124.73
81	Qc	404	HEM	CAA-C2A-C1A	2.00	128.83	124.89
74	N3	201	PEE	C37-C38-C39	-2.00	109.36	124.73

All (2) chirality outliers are listed below:

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

All (1382) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	4L	201	CDL	CA2-OA2-PA1-OA3
69	4L	201	CDL	CB2-OB2-PB2-OB4
69	6A	102	CDL	CA3-OA5-PA1-OA2
69	6A	102	CDL	CA3-OA5-PA1-OA3
69	6A	102	CDL	CA3-OA5-PA1-OA4
69	6A	102	CDL	CB2-OB2-PB2-OB3
69	6A	102	CDL	CB2-OB2-PB2-OB4
69	6A	102	CDL	OB5-CB3-CB4-OB6
69	A7	201	CDL	CB2-OB2-PB2-OB3
69	A7	201	CDL	CB3-OB5-PB2-OB4
69	AK	402	CDL	CA2-OA2-PA1-OA3
69	AK	402	CDL	CA2-OA2-PA1-OA4
69	AK	402	CDL	CA2-OA2-PA1-OA5
69	AK	402	CDL	CA3-OA5-PA1-OA3
69	AK	402	CDL	CB2-OB2-PB2-OB3
69	AK	402	CDL	CB2-OB2-PB2-OB4
69	AK	402	CDL	CB2-OB2-PB2-OB5
69	AL	201	CDL	CB2-OB2-PB2-OB3
69	AL	201	CDL	CB2-OB2-PB2-OB4
69	AL	201	CDL	CB2-OB2-PB2-OB5
69	AL	201	CDL	CB3-OB5-PB2-OB4
69	AL	202	CDL	CA3-OA5-PA1-OA3
69	AL	202	CDL	CB2-OB2-PB2-OB3
69	AL	202	CDL	CB3-OB5-PB2-OB4
69	AL	202	CDL	OB6-CB4-CB6-OB8
69	B5	202	CDL	CB2-OB2-PB2-OB3
69	B5	202	CDL	CB2-OB2-PB2-OB4
69	B5	202	CDL	CB2-OB2-PB2-OB5
69	CB	203	CDL	CA2-OA2-PA1-OA3
69	CB	203	CDL	CA2-OA2-PA1-OA4
69	CB	203	CDL	CA2-OA2-PA1-OA5
69	CB	203	CDL	CA3-OA5-PA1-OA3
69	CB	203	CDL	CA3-OA5-PA1-OA4
69	N1	401	CDL	CA3-OA5-PA1-OA3
69	N1	401	CDL	CA3-OA5-PA1-OA4
69	N1	401	CDL	CB2-OB2-PB2-OB3
69	N1	401	CDL	CB3-OB5-PB2-OB3
69	N4	503	CDL	CA2-OA2-PA1-OA3
69	N4	503	CDL	CA3-OA5-PA1-OA2
69	N4	503	CDL	OB5-CB3-CB4-OB6
69	N5	703	CDL	O1-C1-CB2-OB2
69	N5	703	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
69	N5	703	CDL	CA3-OA5-PA1-OA3
69	N5	703	CDL	CB3-OB5-PB2-OB3
69	N5	703	CDL	CB3-OB5-PB2-OB4
69	QB	501	CDL	CA2-OA2-PA1-OA3
69	QB	501	CDL	CA3-OA5-PA1-OA3
69	QB	501	CDL	CA3-OA5-PA1-OA4
69	QB	501	CDL	CB3-OB5-PB2-OB3
69	QB	501	CDL	CB3-OB5-PB2-OB4
69	QD	402	CDL	CB2-C1-CA2-OA2
69	QD	402	CDL	CA3-OA5-PA1-OA3
69	QH	401	CDL	CA3-OA5-PA1-OA3
69	QH	401	CDL	CB2-OB2-PB2-OB3
69	QH	401	CDL	CB3-OB5-PB2-OB3
69	QH	401	CDL	CB3-OB5-PB2-OB4
69	Qb	501	CDL	CA2-OA2-PA1-OA3
69	Qb	501	CDL	CA3-OA5-PA1-OA3
69	Qb	501	CDL	CB2-OB2-PB2-OB5
69	Qb	501	CDL	CB3-OB5-PB2-OB3
69	Qc	401	CDL	CA2-OA2-PA1-OA3
69	Qc	401	CDL	CA2-OA2-PA1-OA4
69	Qc	401	CDL	CA3-OA5-PA1-OA3
69	Qc	401	CDL	CB2-OB2-PB2-OB3
69	Qc	401	CDL	CB2-OB2-PB2-OB4
69	Qh	102	CDL	CB2-OB2-PB2-OB3
71	6A	101	PC1	C11-O13-P-O12
71	6A	101	PC1	C1-O11-P-O12
71	6A	101	PC1	O13-C11-C12-N
71	6A	103	PC1	C1-O11-P-O14
71	C1	605	PC1	C11-O13-P-O12
71	C1	605	PC1	C1-O11-P-O12
71	C1	605	PC1	C1-O11-P-O14
71	C1	605	PC1	C1-O11-P-O13
71	C1	605	PC1	C2-C1-O11-P
71	C1	606	PC1	O13-C11-C12-N
71	C1	607	PC1	C11-O13-P-O14
71	C1	607	PC1	C1-O11-P-O13
71	C3	301	PC1	C11-O13-P-O12
71	C3	301	PC1	C11-O13-P-O14
71	C3	301	PC1	C11-O13-P-O11
71	C3	302	PC1	C11-O13-P-O14
71	C3	302	PC1	C1-O11-P-O12
71	C3	302	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
71	C3	302	PC1	C1-O11-P-O13
71	C3	303	PC1	C11-O13-P-O14
71	N1	402	PC1	C1-O11-P-O14
71	N1	403	PC1	C11-O13-P-O14
71	N1	403	PC1	C11-O13-P-O11
71	N1	403	PC1	C1-O11-P-O12
71	N1	403	PC1	C1-O11-P-O14
71	N1	403	PC1	C1-O11-P-O13
71	N3	203	PC1	C11-O13-P-O12
71	N3	203	PC1	C1-O11-P-O12
71	N3	203	PC1	C1-O11-P-O14
71	N3	203	PC1	C1-O11-P-O13
71	QB	503	PC1	C11-O13-P-O12
71	QB	503	PC1	C11-O13-P-O14
71	QB	503	PC1	C11-O13-P-O11
71	QB	503	PC1	C1-O11-P-O12
71	QB	503	PC1	C1-O11-P-O14
71	QB	503	PC1	O13-C11-C12-N
71	Qc	406	PC1	C12-C11-O13-P
71	Qh	101	PC1	C11-O13-P-O12
71	Qh	101	PC1	C11-O13-P-O14
71	Qh	101	PC1	C11-O13-P-O11
71	Qh	101	PC1	C1-O11-P-O12
71	Qh	101	PC1	C1-O11-P-O14
71	Qh	101	PC1	C1-O11-P-O13
72	6C	101	PLX	O7-C6-O6-C4
72	6C	101	PLX	O6-C4-C5-O8
72	6C	101	PLX	N1-C1-C2-O1
72	6C	101	PLX	O9-C24-O8-C5
72	AL	204	PLX	O7-C6-C7-C8
72	AL	204	PLX	O7-C6-O6-C4
72	AL	204	PLX	O6-C4-C5-O8
72	AL	204	PLX	C2-O1-P1-O2
72	AM	201	PLX	O7-C6-C7-C8
72	AM	201	PLX	O7-C6-O6-C4
72	AM	201	PLX	N1-C1-C2-O1
72	B5	201	PLX	O7-C6-O6-C4
72	CB	201	PLX	O7-C6-C7-C8
72	CB	201	PLX	O7-C6-O6-C4
72	CB	201	PLX	C2-O1-P1-O2
72	CB	201	PLX	C2-O1-P1-O3
72	N3	202	PLX	O7-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
72	N3	202	PLX	C7-C6-O6-C4
72	N3	202	PLX	C2-O1-P1-O2
72	N3	202	PLX	O9-C24-O8-C5
72	N3	202	PLX	O9-C24-C25-C26
72	N4	501	PLX	O7-C6-O6-C4
72	N4	501	PLX	C25-C24-O8-C5
72	QB	504	PLX	O7-C6-C7-C8
72	QB	504	PLX	O7-C6-O6-C4
72	QI	301	PLX	C2-O1-P1-O4
72	QI	301	PLX	C2-O1-P1-O2
72	QI	301	PLX	C2-O1-P1-O3
72	S7	302	PLX	O7-C6-C7-C8
72	S7	302	PLX	O6-C6-C7-C8
72	S7	302	PLX	C3-O4-P1-O1
72	S7	302	PLX	C3-O4-P1-O2
72	S7	302	PLX	C3-O4-P1-O3
72	S7	302	PLX	C2-O1-P1-O2
72	S7	302	PLX	O9-C24-C25-C26
73	A9	401	NDP	C5B-O5B-PA-O3
74	A9	402	PEE	C1-O3P-P-O4P
74	A9	402	PEE	O4P-C4-C5-N
74	AL	203	PEE	C4-O4P-P-O2P
74	C3	304	PEE	C4-O4P-P-O2P
74	C3	304	PEE	C4-O4P-P-O1P
74	C3	304	PEE	O4P-C4-C5-N
74	N1	404	PEE	C1-O3P-P-O2P
74	N1	404	PEE	C1-O3P-P-O1P
74	N1	404	PEE	C4-O4P-P-O3P
74	N1	404	PEE	C4-O4P-P-O2P
74	N1	404	PEE	C4-O4P-P-O1P
74	N3	201	PEE	C17-C18-C19-C20
74	N5	701	PEE	C11-C10-O2-C2
74	N5	701	PEE	C4-O4P-P-O2P
74	N5	701	PEE	O4P-C4-C5-N
74	N5	702	PEE	O4-C10-O2-C2
74	N5	702	PEE	C1-O3P-P-O1P
74	N5	702	PEE	C1-O3P-P-O4P
74	N5	702	PEE	C4-O4P-P-O2P
74	N5	702	PEE	C4-O4P-P-O1P
74	N5	702	PEE	O5-C30-O3-C3
74	N5	702	PEE	C31-C30-O3-C3
74	N5	702	PEE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
74	N5	705	PEE	C11-C10-O2-C2
74	N5	705	PEE	C1-O3P-P-O1P
74	N5	705	PEE	C4-O4P-P-O3P
74	N5	705	PEE	C4-O4P-P-O2P
74	N5	705	PEE	C4-O4P-P-O1P
74	QB	502	PEE	C11-C10-O2-C2
74	QB	502	PEE	O4-C10-O2-C2
74	QB	502	PEE	C1-O3P-P-O2P
74	QC	403	PEE	O2-C2-C3-O3
74	QC	403	PEE	C1-O3P-P-O1P
74	QC	403	PEE	O4P-C4-C5-N
74	QE	301	PEE	C1-O3P-P-O1P
74	QE	301	PEE	O4P-C4-C5-N
74	QJ	101	PEE	O4-C10-O2-C2
74	QJ	101	PEE	C1-O3P-P-O2P
74	QJ	101	PEE	C4-O4P-P-O3P
74	QJ	101	PEE	C4-O4P-P-O2P
74	QJ	101	PEE	C4-O4P-P-O1P
74	QJ	101	PEE	O5-C30-O3-C3
74	QJ	101	PEE	C31-C30-O3-C3
74	Qc	402	PEE	C1-O3P-P-O1P
74	Qc	402	PEE	O4P-C4-C5-N
74	Qd	402	PEE	O3P-C1-C2-O2
74	S2	501	PEE	C18-C19-C20-C21
74	S2	501	PEE	C2-C1-O3P-P
74	S2	501	PEE	C1-O3P-P-O1P
74	S2	501	PEE	C1-O3P-P-O4P
74	S8	303	PEE	C37-C38-C39-C40
75	AC	201	ZMP	C17-C18-C21-O5
75	AC	201	ZMP	S1-C11-C12-N1
75	AC	201	ZMP	O1-C10-S1-C11
75	AC	201	ZMP	C9-C10-S1-C11
77	B8	201	3PE	C1-O11-P-O13
77	B8	201	3PE	C1-O11-P-O14
77	B8	201	3PE	C11-O13-P-O11
77	B8	201	3PE	C11-O13-P-O12
77	B8	201	3PE	C11-O13-P-O14
77	C1	609	3PE	O13-C11-C12-N
77	CA	101	3PE	O13-C11-C12-N
77	CB	202	3PE	C11-O13-P-O12
77	CB	202	3PE	C12-C11-O13-P
77	CB	202	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
77	N5	706	3PE	C1-O11-P-O14
77	N5	706	3PE	C11-O13-P-O14
77	N5	706	3PE	O13-C11-C12-N
77	QE	302	3PE	C1-O11-P-O12
77	QE	302	3PE	C1-O11-P-O13
77	QE	302	3PE	C11-O13-P-O11
77	QE	302	3PE	C11-O13-P-O12
77	QE	302	3PE	C11-O13-P-O14
77	Qc	405	3PE	C11-O13-P-O14
77	Qj	101	3PE	C11-O13-P-O11
77	S7	303	3PE	C11-O13-P-O11
77	S7	303	3PE	C11-O13-P-O12
77	S7	303	3PE	C11-O13-P-O14
77	S7	303	3PE	O13-C11-C12-N
78	C1	601	HEA	C1A-C2A-CAA-CBA
78	C1	601	HEA	C2A-C3A-CMA-OMA
78	C1	601	HEA	C4A-C3A-CMA-OMA
78	C1	601	HEA	C17-C18-C19-C20
78	C1	601	HEA	C17-C18-C19-C27
78	C1	601	HEA	C18-C19-C20-C21
78	C1	601	HEA	C27-C19-C20-C21
78	C1	602	HEA	C3A-C2A-CAA-CBA
78	C1	602	HEA	C2A-C3A-CMA-OMA
78	C1	602	HEA	C4A-C3A-CMA-OMA
78	C1	602	HEA	C17-C18-C19-C20
78	C1	602	HEA	C17-C18-C19-C27
81	QC	402	HEM	C2B-C3B-CAB-CBB
81	QC	402	HEM	C4B-C3B-CAB-CBB
81	Qc	403	HEM	C2B-C3B-CAB-CBB
81	Qc	403	HEM	C4B-C3B-CAB-CBB
81	Qc	404	HEM	C1A-C2A-CAA-CBA
81	Qc	404	HEM	C2B-C3B-CAB-CBB
81	Qc	404	HEM	C4B-C3B-CAB-CBB
85	V1	502	FMN	C5'-O5'-P-O2P
85	V1	502	FMN	C5'-O5'-P-O3P
74	C3	304	PEE	O5-C30-O3-C3
74	N1	404	PEE	O5-C30-O3-C3
74	QB	502	PEE	O5-C30-O3-C3
74	C3	304	PEE	C31-C30-O3-C3
74	N1	404	PEE	C31-C30-O3-C3
74	QB	502	PEE	C31-C30-O3-C3
74	N3	201	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
74	Qc	402	PEE	O5-C30-O3-C3
74	N5	701	PEE	O4-C10-O2-C2
74	N5	705	PEE	O4-C10-O2-C2
74	S8	303	PEE	O4-C10-O2-C2
74	N3	201	PEE	C31-C30-O3-C3
74	Qc	402	PEE	C31-C30-O3-C3
74	N5	702	PEE	C11-C10-O2-C2
74	QJ	101	PEE	C11-C10-O2-C2
74	S8	303	PEE	C11-C10-O2-C2
78	C1	601	HEA	C3A-C2A-CAA-CBA
78	C1	602	HEA	C27-C19-C20-C21
74	AL	203	PEE	C37-C38-C39-C40
74	N5	701	PEE	C37-C38-C39-C40
74	N5	705	PEE	C17-C18-C19-C20
74	QJ	101	PEE	C17-C18-C19-C20
78	C1	602	HEA	C1A-C2A-CAA-CBA
69	A7	201	CDL	O1-C1-CA2-OA2
69	QD	402	CDL	O1-C1-CA2-OA2
74	AL	203	PEE	C31-C30-O3-C3
74	AL	203	PEE	O5-C30-O3-C3
78	C1	602	HEA	C19-C20-C21-C22
75	AC	201	ZMP	C14-C15-N2-C16
69	N5	703	CDL	CA2-C1-CB2-OB2
71	C1	606	PC1	C11-C12-N-C15
71	Qc	406	PC1	C11-C12-N-C14
72	N3	202	PLX	C2-C1-N1-C1C
74	QE	301	PEE	O2-C2-C3-O3
77	QE	302	3PE	O21-C2-C3-O31
69	6A	102	CDL	CB5-C51-C52-C53
69	N5	704	CDL	CB7-C71-C72-C73
74	QE	301	PEE	C31-C30-O3-C3
74	QC	403	PEE	C10-C11-C12-C13
74	Qd	402	PEE	C10-C11-C12-C13
77	B8	201	3PE	C21-C22-C23-C24
74	N5	705	PEE	C37-C38-C39-C40
74	QB	502	PEE	C37-C38-C39-C40
69	AL	202	CDL	CA5-C11-C12-C13
69	CB	203	CDL	CB7-C71-C72-C73
71	C3	301	PC1	C21-C22-C23-C24
71	Qb	502	PC1	C21-C22-C23-C24
74	AL	203	PEE	C10-C11-C12-C13
74	N5	702	PEE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
74	QB	502	PEE	C10-C11-C12-C13
69	AL	202	CDL	C72-C73-C74-C75
71	6A	101	PC1	C11-C12-N-C13
71	C1	606	PC1	C11-C12-N-C13
71	Qh	101	PC1	C11-C12-N-C15
74	QE	301	PEE	C33-C34-C35-C36
78	C1	601	HEA	C15-C16-C17-C18
78	C1	601	HEA	C19-C20-C21-C22
69	N5	704	CDL	CB5-C51-C52-C53
69	AL	202	CDL	O1-C1-CB2-OB2
69	CB	203	CDL	O1-C1-CB2-OB2
74	QE	301	PEE	O5-C30-O3-C3
74	AL	203	PEE	C11-C10-O2-C2
69	4L	201	CDL	CA2-OA2-PA1-OA5
69	4L	201	CDL	CA3-OA5-PA1-OA2
69	4L	201	CDL	CB2-OB2-PB2-OB5
69	6A	102	CDL	CB2-OB2-PB2-OB5
69	A7	201	CDL	CB3-OB5-PB2-OB2
69	AL	202	CDL	CA2-OA2-PA1-OA5
69	AL	202	CDL	CB2-OB2-PB2-OB5
69	AL	202	CDL	CB3-OB5-PB2-OB2
69	B5	202	CDL	CA3-OA5-PA1-OA2
69	B5	202	CDL	CB3-OB5-PB2-OB2
69	CB	203	CDL	CA3-OA5-PA1-OA2
69	N1	401	CDL	CA3-OA5-PA1-OA2
69	N4	503	CDL	CB2-OB2-PB2-OB5
69	N4	503	CDL	CB3-OB5-PB2-OB2
69	N5	703	CDL	CA2-OA2-PA1-OA5
69	N5	703	CDL	CA3-OA5-PA1-OA2
69	N5	703	CDL	CB3-OB5-PB2-OB2
69	N5	704	CDL	CB3-OB5-PB2-OB2
69	QB	501	CDL	CA2-OA2-PA1-OA5
69	QB	501	CDL	CA3-OA5-PA1-OA2
69	QB	501	CDL	CB3-OB5-PB2-OB2
69	QD	402	CDL	CA3-OA5-PA1-OA2
69	QD	402	CDL	CB2-OB2-PB2-OB5
69	QD	402	CDL	CB3-OB5-PB2-OB2
69	QH	401	CDL	CB3-OB5-PB2-OB2
69	Qb	501	CDL	CA2-OA2-PA1-OA5
69	Qb	501	CDL	CA3-OA5-PA1-OA2
69	Qc	401	CDL	CA2-OA2-PA1-OA5
69	Qc	401	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
69	Qh	102	CDL	CB2-OB2-PB2-OB5
71	6A	101	PC1	C11-O13-P-O11
71	6A	101	PC1	C1-O11-P-O13
71	6A	103	PC1	C11-O13-P-O11
71	6A	103	PC1	C1-O11-P-O13
71	C1	605	PC1	C11-O13-P-O11
71	C1	606	PC1	C11-O13-P-O11
71	C3	302	PC1	C11-O13-P-O11
71	C3	303	PC1	C11-O13-P-O11
71	N3	203	PC1	C11-O13-P-O11
71	QB	503	PC1	C1-O11-P-O13
71	Qc	406	PC1	C11-O13-P-O11
72	6C	101	PLX	C2-O1-P1-O4
72	AM	201	PLX	C2-O1-P1-O4
72	CB	201	PLX	C2-O1-P1-O4
72	N3	202	PLX	C2-O1-P1-O4
72	N4	501	PLX	C2-O1-P1-O4
72	S7	302	PLX	C2-O1-P1-O4
74	A9	402	PEE	C4-O4P-P-O3P
74	AL	203	PEE	C4-O4P-P-O3P
74	C3	304	PEE	C4-O4P-P-O3P
74	N1	404	PEE	C1-O3P-P-O4P
74	N3	201	PEE	C1-O3P-P-O4P
74	N3	201	PEE	C4-O4P-P-O3P
74	N5	701	PEE	C1-O3P-P-O4P
74	N5	701	PEE	C4-O4P-P-O3P
74	N5	702	PEE	C4-O4P-P-O3P
74	N5	705	PEE	C1-O3P-P-O4P
74	QB	502	PEE	C1-O3P-P-O4P
74	QB	502	PEE	C4-O4P-P-O3P
74	QC	403	PEE	C1-O3P-P-O4P
74	QE	301	PEE	C1-O3P-P-O4P
74	QJ	101	PEE	C1-O3P-P-O4P
74	Qc	402	PEE	C1-O3P-P-O4P
77	CB	202	3PE	C11-O13-P-O11
77	N5	706	3PE	C11-O13-P-O11
77	Qc	405	3PE	C11-O13-P-O11
72	QB	504	PLX	C15-C16-C17-C18
74	N3	201	PEE	C10-C11-C12-C13
74	Qc	402	PEE	C30-C31-C32-C33
69	A7	201	CDL	CB2-C1-CA2-OA2
69	AL	202	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
69	CB	203	CDL	CA2-C1-CB2-OB2
74	AL	203	PEE	O4-C10-O2-C2
74	Qc	402	PEE	C11-C12-C13-C14
71	6A	101	PC1	C11-C12-N-C14
71	C1	607	PC1	C11-C12-N-C13
71	C1	607	PC1	C11-C12-N-C15
71	N1	402	PC1	C11-C12-N-C13
71	N1	402	PC1	C11-C12-N-C14
71	N1	402	PC1	C11-C12-N-C15
71	N3	203	PC1	C11-C12-N-C15
71	Qc	406	PC1	C11-C12-N-C13
71	Qc	406	PC1	C11-C12-N-C15
71	Qh	101	PC1	C11-C12-N-C13
72	AL	204	PLX	O8-C24-C25-C26
72	CB	201	PLX	O6-C6-C7-C8
72	QB	504	PLX	O6-C6-C7-C8
72	S7	302	PLX	O8-C24-C25-C26
74	A9	402	PEE	C35-C36-C37-C38
74	N3	201	PEE	C35-C36-C37-C38
74	QB	502	PEE	C35-C36-C37-C38
74	QJ	101	PEE	C30-C31-C32-C33
72	N3	202	PLX	C27-C28-C29-C30
74	Qc	402	PEE	C20-C21-C22-C23
77	CB	202	3PE	C32-C33-C34-C35
74	C3	304	PEE	C14-C15-C16-C17
74	QC	403	PEE	C12-C13-C14-C15
69	6A	102	CDL	C51-C52-C53-C54
74	QB	502	PEE	C33-C34-C35-C36
74	QC	403	PEE	C21-C22-C23-C24
74	QC	403	PEE	C14-C15-C16-C17
74	QJ	101	PEE	C21-C22-C23-C24
77	C1	608	3PE	C37-C38-C39-C3A
77	S7	303	3PE	C38-C39-C3A-C3B
74	N5	701	PEE	C1-C2-O2-C10
72	B5	201	PLX	C13-C14-C15-C16
74	Qd	402	PEE	C11-C12-C13-C14
74	QJ	101	PEE	C2-C1-O3P-P
74	AL	203	PEE	C17-C18-C19-C20
69	N4	503	CDL	C36-C37-C38-C39
72	AM	201	PLX	C11-C10-C9-C8
72	N3	202	PLX	C25-C26-C27-C28
72	N3	202	PLX	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
74	N5	701	PEE	C14-C15-C16-C17
72	N4	501	PLX	C31-C32-C33-C34
74	QJ	101	PEE	C41-C42-C43-C44
71	Qh	101	PC1	C31-C32-C33-C34
72	B5	201	PLX	C16-C17-C18-C19
74	S8	303	PEE	C33-C34-C35-C36
75	AB	201	ZMP	C22-C1-C2-C3
72	QI	301	PLX	C11-C10-C9-C8
74	AL	203	PEE	C31-C32-C33-C34
74	N5	702	PEE	C14-C15-C16-C17
69	AK	402	CDL	C33-C34-C35-C36
69	AL	202	CDL	C75-C76-C77-C78
69	CB	203	CDL	C32-C33-C34-C35
71	6A	101	PC1	C32-C33-C34-C35
72	N3	202	PLX	C18-C19-C20-C21
74	A9	402	PEE	C31-C32-C33-C34
74	N5	705	PEE	C14-C15-C16-C17
74	QE	301	PEE	C32-C33-C34-C35
74	C3	304	PEE	C31-C32-C33-C34
74	S8	303	PEE	C12-C13-C14-C15
75	AC	201	ZMP	C3-C4-C5-C6
74	S2	501	PEE	C11-C10-O2-C2
69	B5	202	CDL	C38-C39-C40-C41
72	N4	501	PLX	C11-C10-C9-C8
74	N3	201	PEE	C32-C33-C34-C35
77	C1	609	3PE	C39-C3A-C3B-C3C
74	N5	701	PEE	C15-C16-C17-C18
74	S2	501	PEE	C35-C36-C37-C38
74	S8	303	PEE	C35-C36-C37-C38
69	4L	201	CDL	CA5-C11-C12-C13
71	Qb	502	PC1	C31-C32-C33-C34
71	N3	203	PC1	C2A-C2B-C2C-C2D
72	QI	301	PLX	C9-C10-C11-C12
74	AL	203	PEE	C11-C12-C13-C14
74	N5	701	PEE	C20-C21-C22-C23
74	N5	702	PEE	C12-C13-C14-C15
74	Qc	402	PEE	C23-C24-C25-C26
74	Qc	402	PEE	C31-C32-C33-C34
74	S2	501	PEE	C11-C12-C13-C14
71	C1	606	PC1	C11-C12-N-C14
71	C1	607	PC1	C11-C12-N-C14
72	N3	202	PLX	C2-C1-N1-C1A

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Mol	Chain	Res	Type	Atoms
74	N5	705	PEE	C21-C22-C23-C24
75	AC	201	ZMP	C1-C22-C23-C24
74	N5	705	PEE	O4P-C4-C5-N
74	QB	502	PEE	O4P-C4-C5-N
74	S2	501	PEE	O4P-C4-C5-N
77	B8	201	3PE	O13-C11-C12-N
71	N1	403	PC1	C36-C37-C38-C39
74	N3	201	PEE	C22-C23-C24-C25
69	QB	501	CDL	C51-C52-C53-C54
72	N4	501	PLX	C26-C27-C28-C29
77	QJ	102	3PE	C33-C34-C35-C36
72	S7	302	PLX	C35-C36-C37-C38
74	QE	301	PEE	C12-C13-C14-C15
72	AL	204	PLX	C9-C10-C11-C12
74	QJ	101	PEE	C23-C24-C25-C26
71	Qh	101	PC1	C1-C2-C3-O31
74	S8	303	PEE	C17-C18-C19-C20
75	AB	201	ZMP	C6-C7-C8-C9
74	Qc	402	PEE	C11-C10-O2-C2
74	N5	701	PEE	C34-C35-C36-C37
72	AL	204	PLX	O9-C24-C25-C26
72	B5	201	PLX	O9-C24-C25-C26
72	CB	201	PLX	O9-C24-C25-C26
72	QI	301	PLX	O9-C24-C25-C26
69	AK	402	CDL	C13-C14-C15-C16
69	QH	401	CDL	C51-C52-C53-C54
72	B5	201	PLX	C35-C36-C37-C38
74	AL	203	PEE	C14-C15-C16-C17
74	N5	701	PEE	C32-C33-C34-C35
74	QE	301	PEE	C19-C20-C21-C22
74	QE	301	PEE	C35-C36-C37-C38
74	QE	301	PEE	C39-C40-C41-C42
71	N1	403	PC1	C31-C32-C33-C34
72	S7	302	PLX	C7-C8-C9-C10
69	N4	502	CDL	C58-C59-C60-C61
74	N3	201	PEE	C33-C34-C35-C36
69	4L	201	CDL	C38-C39-C40-C41
72	6C	101	PLX	C16-C17-C18-C19
75	AC	201	ZMP	C2-C3-C4-C5
69	N4	503	CDL	C34-C35-C36-C37
74	S2	501	PEE	O4-C10-O2-C2
71	N1	403	PC1	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
72	N4	501	PLX	C19-C20-C21-C22
74	QE	301	PEE	C14-C15-C16-C17
71	N3	203	PC1	C32-C33-C34-C35
72	6C	101	PLX	C11-C10-C9-C8
74	Qc	402	PEE	C33-C34-C35-C36
71	6A	101	PC1	C11-C12-N-C15
71	6A	103	PC1	C11-C12-N-C14
71	C3	301	PC1	C11-C12-N-C14
71	N3	203	PC1	C11-C12-N-C13
71	N3	203	PC1	C11-C12-N-C14
74	N3	201	PEE	C11-C10-O2-C2
69	AL	202	CDL	C11-C12-C13-C14
69	B5	202	CDL	C22-C23-C24-C25
74	N1	404	PEE	C11-C12-C13-C14
74	N5	701	PEE	C33-C34-C35-C36
69	AL	201	CDL	C33-C34-C35-C36
74	C3	304	PEE	C12-C13-C14-C15
69	AL	202	CDL	C76-C77-C78-C79
71	N3	203	PC1	C3B-C3C-C3D-C3E
75	AB	201	ZMP	C4-C5-C6-C7
75	AC	201	ZMP	C22-C23-C24-C25
74	N5	705	PEE	C35-C36-C37-C38
74	Qc	402	PEE	O4-C10-O2-C2
69	6A	102	CDL	CA7-C31-C32-C33
71	N1	402	PC1	C31-C32-C33-C34
71	Qb	502	PC1	C22-C23-C24-C25
74	QJ	101	PEE	C22-C23-C24-C25
69	AL	201	CDL	C52-C53-C54-C55
74	Qc	402	PEE	C10-C11-C12-C13
69	4L	201	CDL	C15-C16-C17-C18
72	QI	301	PLX	C16-C17-C18-C19
74	QC	403	PEE	C11-C12-C13-C14
81	QC	401	HEM	C2B-C3B-CAB-CBB
69	B5	202	CDL	C42-C43-C44-C45
74	S2	501	PEE	C31-C30-O3-C3
69	6A	102	CDL	C32-C33-C34-C35
69	Qb	501	CDL	C71-C72-C73-C74
71	Qb	502	PC1	C36-C37-C38-C39
72	QI	301	PLX	C31-C32-C33-C34
74	N3	201	PEE	C21-C22-C23-C24
75	AC	201	ZMP	C1-C2-C3-C4
74	S2	501	PEE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
74	A9	402	PEE	C11-C10-O2-C2
74	Qd	402	PEE	C11-C10-O2-C2
72	QB	504	PLX	O4-C3-C4-O6
72	S7	302	PLX	O4-C3-C4-O6
74	AL	203	PEE	O3P-C1-C2-O2
74	A9	402	PEE	C14-C15-C16-C17
74	N3	201	PEE	C31-C32-C33-C34
74	QJ	101	PEE	C12-C13-C14-C15
74	S2	501	PEE	C16-C17-C18-C19
74	N3	201	PEE	O4-C10-O2-C2
71	N1	402	PC1	C2C-C2D-C2E-C2F
69	Qh	102	CDL	OA6-CA4-CA6-OA8
71	6A	101	PC1	O21-C2-C3-O31
74	C3	304	PEE	C43-C44-C45-C46
71	Qh	101	PC1	C11-C12-N-C14
72	N3	202	PLX	C14-C15-C16-C17
74	AL	203	PEE	C19-C20-C21-C22
77	QJ	102	3PE	C23-C24-C25-C26
81	Qc	404	HEM	C3A-C2A-CAA-CBA
71	C1	605	PC1	C22-C23-C24-C25
74	AL	203	PEE	C12-C13-C14-C15
74	QJ	101	PEE	C14-C15-C16-C17
74	C3	304	PEE	C37-C38-C39-C40
74	QJ	101	PEE	C37-C38-C39-C40
69	N4	503	CDL	C18-C19-C20-C21
72	AL	204	PLX	C10-C11-C12-C13
78	C1	602	HEA	C4D-C3D-CAD-CBD
74	Qd	402	PEE	O4-C10-O2-C2
69	Qc	401	CDL	C54-C55-C56-C57
72	B5	201	PLX	C17-C18-C19-C20
72	CB	201	PLX	C33-C34-C35-C36
72	QI	301	PLX	C30-C31-C32-C33
69	N4	503	CDL	CA2-OA2-PA1-OA5
69	QH	401	CDL	CB2-OB2-PB2-OB5
69	Qb	501	CDL	CB3-OB5-PB2-OB2
72	AL	204	PLX	C2-O1-P1-O4
72	N3	202	PLX	C3-O4-P1-O1
69	6A	102	CDL	C11-C12-C13-C14
71	N1	403	PC1	C29-C2A-C2B-C2C
69	B5	202	CDL	CB7-C71-C72-C73
74	N5	702	PEE	C13-C14-C15-C16
74	S8	303	PEE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
69	N4	503	CDL	OB5-CB3-CB4-CB6
69	QB	501	CDL	OB5-CB3-CB4-CB6
72	6C	101	PLX	O4-C3-C4-C5
72	S7	302	PLX	O4-C3-C4-C5
74	AL	203	PEE	O3P-C1-C2-C3
74	C3	304	PEE	O3P-C1-C2-C3
74	QC	403	PEE	O3P-C1-C2-C3
74	S2	501	PEE	C34-C35-C36-C37
77	S7	303	3PE	C31-C32-C33-C34
71	C3	301	PC1	C29-C2A-C2B-C2C
72	N4	501	PLX	C32-C33-C34-C35
74	AL	203	PEE	C39-C40-C41-C42
71	N1	402	PC1	C28-C29-C2A-C2B
74	QC	403	PEE	C31-C32-C33-C34
74	S2	501	PEE	C42-C43-C44-C45
74	QC	403	PEE	C31-C30-O3-C3
74	A9	402	PEE	O4-C10-O2-C2
71	N3	203	PC1	C3D-C3E-C3F-C3G
72	AL	204	PLX	C30-C31-C32-C33
72	QB	504	PLX	C7-C8-C9-C10
75	AB	201	ZMP	C2-C3-C4-C5
74	C3	304	PEE	C32-C33-C34-C35
71	N1	403	PC1	C35-C36-C37-C38
72	AM	201	PLX	C27-C28-C29-C30
69	AL	202	CDL	CB3-CB4-CB6-OB8
69	N4	503	CDL	CA3-CA4-CA6-OA8
69	N4	503	CDL	CB3-CB4-CB6-OB8
69	Qh	102	CDL	CA3-CA4-CA6-OA8
72	AL	204	PLX	C3-C4-C5-O8
72	N3	202	PLX	C34-C35-C36-C37
74	QB	502	PEE	C12-C13-C14-C15
74	Qc	402	PEE	C1-C2-C3-O3
74	Qd	402	PEE	C1-C2-C3-O3
74	N5	702	PEE	C17-C18-C19-C20
72	QI	301	PLX	C12-C13-C14-C15
75	AC	201	ZMP	C22-C1-C2-C3
74	Qc	402	PEE	C13-C14-C15-C16
74	S8	303	PEE	C21-C22-C23-C24
69	N1	401	CDL	C78-C79-C80-C81
69	QH	401	CDL	C73-C74-C75-C76
72	AL	204	PLX	C31-C32-C33-C34
74	AL	203	PEE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
74	QE	301	PEE	C15-C16-C17-C18
74	S8	303	PEE	C15-C16-C17-C18
74	S2	501	PEE	O5-C30-O3-C3
69	Qc	401	CDL	CA7-C31-C32-C33
69	AK	402	CDL	C31-C32-C33-C34
75	AB	201	ZMP	C5-C6-C7-C8
74	QJ	101	PEE	C3-C2-O2-C10
71	N1	403	PC1	C38-C39-C3A-C3B
71	Qb	502	PC1	C32-C33-C34-C35
74	QB	502	PEE	C38-C39-C40-C41
85	V1	502	FMN	C5'-O5'-P-O1P
72	QB	504	PLX	C25-C26-C27-C28
69	QD	402	CDL	OA5-CA3-CA4-OA6
69	QH	401	CDL	OB5-CB3-CB4-OB6
71	6A	103	PC1	C11-C12-N-C15
71	C3	301	PC1	C11-C12-N-C13
72	S7	302	PLX	C15-C16-C17-C18
74	N5	705	PEE	C22-C23-C24-C25
72	N4	501	PLX	C16-C17-C18-C19
69	QD	402	CDL	C52-C51-CB5-OB6
69	N5	703	CDL	C39-C40-C41-C42
77	S7	303	3PE	C34-C35-C36-C37
78	C1	602	HEA	C2D-C3D-CAD-CBD
71	C1	606	PC1	O31-C31-C32-C33
74	QC	403	PEE	O5-C30-O3-C3
69	N5	704	CDL	C81-C82-C83-C84
69	B5	202	CDL	C13-C14-C15-C16
72	6C	101	PLX	C12-C13-C14-C15
75	AB	201	ZMP	C1-C22-C23-C24
77	C1	608	3PE	C23-C24-C25-C26
69	B5	202	CDL	C54-C55-C56-C57
74	N5	701	PEE	C11-C12-C13-C14
72	QB	504	PLX	C16-C17-C18-C19
74	QJ	101	PEE	C20-C21-C22-C23
77	S7	303	3PE	C39-C3A-C3B-C3C
71	Qb	502	PC1	C39-C3A-C3B-C3C
77	S7	303	3PE	C3E-C3F-C3G-C3H
69	B5	202	CDL	C19-C20-C21-C22
72	N4	501	PLX	C14-C15-C16-C17
74	N5	705	PEE	C11-C12-C13-C14
82	Qd	401	HEC	C1A-C2A-CAA-CBA
69	AL	201	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
69	CB	203	CDL	OA5-CA3-CA4-CA6
69	QD	402	CDL	OA5-CA3-CA4-CA6
72	QB	504	PLX	O4-C3-C4-C5
74	QB	502	PEE	O3P-C1-C2-C3
74	Qd	402	PEE	O3P-C1-C2-C3
74	QB	502	PEE	C34-C35-C36-C37
75	AB	201	ZMP	C22-C23-C24-C25
77	C1	608	3PE	C2A-C2B-C2C-C2D
69	Qb	501	CDL	CA5-C11-C12-C13
71	Qb	502	PC1	C3A-C3B-C3C-C3D
74	N5	705	PEE	C33-C34-C35-C36
74	C3	304	PEE	C33-C34-C35-C36
74	Qc	402	PEE	C35-C36-C37-C38
69	N1	401	CDL	C76-C77-C78-C79
69	N5	703	CDL	C60-C61-C62-C63
69	AK	402	CDL	C52-C51-CB5-OB6
77	CB	202	3PE	C29-C2A-C2B-C2C
69	QH	401	CDL	CA4-CA3-OA5-PA1
69	Qc	401	CDL	CB4-CB3-OB5-PB2
77	C1	609	3PE	C2-C1-O11-P
74	QE	301	PEE	C16-C17-C18-C19
71	C1	607	PC1	C27-C28-C29-C2A
69	6A	102	CDL	C12-C13-C14-C15
69	Qc	401	CDL	C32-C33-C34-C35
72	N3	202	PLX	C11-C10-C9-C8
77	CB	202	3PE	C31-C32-C33-C34
71	6A	101	PC1	C33-C34-C35-C36
81	QC	401	HEM	C3D-CAD-CBD-CGD
81	Qc	403	HEM	C3D-CAD-CBD-CGD
69	6A	102	CDL	CA3-CA4-CA6-OA8
69	QH	401	CDL	CA3-CA4-CA6-OA8
71	6A	101	PC1	C1-C2-C3-O31
72	AM	201	PLX	C3-C4-C5-O8
72	N4	501	PLX	C3-C4-C5-O8
74	QE	301	PEE	C1-C2-C3-O3
77	QE	302	3PE	C1-C2-C3-O31
71	N1	402	PC1	C33-C34-C35-C36
74	QE	301	PEE	C40-C41-C42-C43
74	N5	702	PEE	C37-C38-C39-C40
74	AL	203	PEE	C24-C25-C26-C27
74	N3	201	PEE	C40-C41-C42-C43
75	AB	201	ZMP	N2-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
74	S8	303	PEE	C11-C12-C13-C14
71	C3	301	PC1	C1-O11-P-O13
72	AL	204	PLX	C5-C4-O6-C6
72	B5	201	PLX	C5-C4-O6-C6
72	CB	201	PLX	C5-C4-O6-C6
72	N4	501	PLX	C5-C4-O6-C6
74	N5	705	PEE	C30-C31-C32-C33
74	N1	404	PEE	C14-C15-C16-C17
72	6C	101	PLX	O7-C6-C7-C8
72	6C	101	PLX	O9-C24-C25-C26
69	AL	201	CDL	OA5-CA3-CA4-OA6
69	AL	201	CDL	OB5-CB3-CB4-OB6
69	B5	202	CDL	OB5-CB3-CB4-OB6
71	C3	303	PC1	O11-C1-C2-O21
77	QE	302	3PE	O11-C1-C2-O21
69	N5	703	CDL	C14-C15-C16-C17
69	Qc	401	CDL	OA6-CA4-CA6-OA8
74	N5	702	PEE	O2-C2-C3-O3
77	B8	201	3PE	O21-C2-C3-O31
72	N4	501	PLX	C18-C19-C20-C21
74	N3	201	PEE	C14-C15-C16-C17
77	C1	608	3PE	C25-C26-C27-C28
74	S8	303	PEE	C13-C14-C15-C16
72	N4	501	PLX	C25-C26-C27-C28
77	QE	302	3PE	C22-C23-C24-C25
72	S7	302	PLX	C11-C10-C9-C8
69	AK	402	CDL	C1-CA2-OA2-PA1
69	N4	502	CDL	C1-CB2-OB2-PB2
69	N4	502	CDL	CB4-CB3-OB5-PB2
69	N5	704	CDL	C1-CB2-OB2-PB2
71	Qb	502	PC1	C2-C1-O11-P
71	Qc	406	PC1	C2-C1-O11-P
74	N5	702	PEE	C2-C1-O3P-P
69	CB	203	CDL	C19-C20-C21-C22
69	N4	502	CDL	C81-C82-C83-C84
74	S8	303	PEE	C34-C35-C36-C37
74	N5	701	PEE	C31-C32-C33-C34
77	CA	101	3PE	C35-C36-C37-C38
72	AM	201	PLX	C12-C13-C14-C15
74	Qc	402	PEE	C22-C23-C24-C25
72	AM	201	PLX	O6-C6-C7-C8
72	CB	201	PLX	O8-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
72	QI	301	PLX	O8-C24-C25-C26
69	6A	102	CDL	OB5-CB3-CB4-CB6
69	B5	202	CDL	OB5-CB3-CB4-CB6
69	N5	704	CDL	OB5-CB3-CB4-CB6
69	QH	401	CDL	OB5-CB3-CB4-CB6
69	Qh	102	CDL	OA5-CA3-CA4-CA6
71	C3	303	PC1	O11-C1-C2-C3
71	QB	503	PC1	O11-C1-C2-C3
74	QC	403	PEE	C16-C17-C18-C19
74	Qc	402	PEE	C16-C17-C18-C19
74	N5	705	PEE	C19-C20-C21-C22
71	N1	403	PC1	C22-C23-C24-C25
69	N5	704	CDL	CA5-C11-C12-C13
72	N4	501	PLX	C29-C30-C31-C32
72	QB	504	PLX	C11-C10-C9-C8
72	QB	504	PLX	C27-C28-C29-C30
69	N4	502	CDL	C75-C76-C77-C78
71	6A	103	PC1	C11-C12-N-C13
69	N4	502	CDL	C18-C19-C20-C21
74	S8	303	PEE	C3-C2-O2-C10
81	QC	402	HEM	C2C-C3C-CAC-CBC
74	N5	705	PEE	C13-C14-C15-C16
71	C3	301	PC1	C2-C1-O11-P
72	6C	101	PLX	C3-C4-C5-O8
72	AM	201	PLX	C7-C6-O6-C4
72	B5	201	PLX	C3-C4-C5-O8
74	QC	403	PEE	C1-C2-C3-O3
77	CB	202	3PE	C1-C2-C3-O31
77	QJ	102	3PE	C1-C2-C3-O31
74	N3	201	PEE	C42-C43-C44-C45
69	AL	202	CDL	OB5-CB3-CB4-OB6
69	CB	203	CDL	OA5-CA3-CA4-OA6
69	N5	704	CDL	OB5-CB3-CB4-OB6
69	QB	501	CDL	OB5-CB3-CB4-OB6
69	QD	402	CDL	OB5-CB3-CB4-OB6
71	N1	402	PC1	O11-C1-C2-O21
72	CB	201	PLX	O4-C3-C4-O6
72	N3	202	PLX	O4-C3-C4-O6
74	C3	304	PEE	O3P-C1-C2-O2
74	N1	404	PEE	O3P-C1-C2-O2
74	N5	702	PEE	O3P-C1-C2-O2
74	QB	502	PEE	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
74	QC	403	PEE	O3P-C1-C2-O2
81	QC	401	HEM	C4B-C3B-CAB-CBB
69	CB	203	CDL	C13-C14-C15-C16
72	N3	202	PLX	C9-C10-C11-C12
74	QJ	101	PEE	C32-C33-C34-C35
69	6A	102	CDL	OA6-CA4-CA6-OA8
69	N4	503	CDL	OB6-CB4-CB6-OB8
69	QH	401	CDL	OA6-CA4-CA6-OA8
72	AM	201	PLX	O6-C4-C5-O8
72	N3	202	PLX	O6-C4-C5-O8
74	AL	203	PEE	O2-C2-C3-O3
74	Qc	402	PEE	O2-C2-C3-O3
69	N5	704	CDL	C18-C19-C20-C21
72	6C	101	PLX	C11-C12-C13-C14
69	AL	201	CDL	C77-C78-C79-C80
71	C1	605	PC1	C11-C12-N-C15
71	N3	203	PC1	C23-C24-C25-C26
72	N3	202	PLX	C30-C31-C32-C33
74	AL	203	PEE	C33-C34-C35-C36
74	QB	502	PEE	C30-C31-C32-C33
74	QE	301	PEE	C37-C38-C39-C40
77	C1	608	3PE	O21-C21-C22-C23
82	Qd	401	HEC	C3A-C2A-CAA-CBA
72	S7	302	PLX	C14-C15-C16-C17
74	QC	403	PEE	C33-C34-C35-C36
71	C1	605	PC1	C23-C24-C25-C26
74	N5	701	PEE	C22-C23-C24-C25
69	N4	502	CDL	C21-C22-C23-C24
72	B5	201	PLX	C24-C25-C26-C27
72	S7	302	PLX	C6-C7-C8-C9
74	A9	402	PEE	C19-C20-C21-C22
69	AK	402	CDL	CA3-OA5-PA1-OA2
69	AL	201	CDL	CB3-OB5-PB2-OB2
69	N1	401	CDL	CB3-OB5-PB2-OB2
69	N5	704	CDL	CA2-OA2-PA1-OA5
71	C1	607	PC1	C11-O13-P-O11
72	AL	204	PLX	C3-O4-P1-O1
72	CB	201	PLX	C3-O4-P1-O1
72	QI	301	PLX	C3-O4-P1-O1
77	N5	706	3PE	C1-O11-P-O13
72	AL	204	PLX	C33-C34-C35-C36
69	N5	704	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
69	N5	703	CDL	C38-C39-C40-C41
74	Qc	402	PEE	C12-C13-C14-C15
69	AK	402	CDL	CA4-CA3-OA5-PA1
69	AK	402	CDL	CB4-CB3-OB5-PB2
69	AL	201	CDL	CA4-CA3-OA5-PA1
69	QD	402	CDL	CA4-CA3-OA5-PA1
74	AL	203	PEE	C2-C1-O3P-P
74	Qc	402	PEE	C2-C1-O3P-P
77	Qj	101	3PE	C2-C1-O11-P
69	4L	201	CDL	CA2-OA2-PA1-OA4
69	4L	201	CDL	CA3-OA5-PA1-OA3
69	4L	201	CDL	CA3-OA5-PA1-OA4
69	AL	202	CDL	CA2-OA2-PA1-OA3
69	AL	202	CDL	CB2-OB2-PB2-OB4
69	AL	202	CDL	CB3-OB5-PB2-OB3
69	B5	202	CDL	CA3-OA5-PA1-OA3
69	B5	202	CDL	CA3-OA5-PA1-OA4
69	B5	202	CDL	CB3-OB5-PB2-OB3
69	N4	503	CDL	CA3-OA5-PA1-OA4
69	N4	503	CDL	CB2-OB2-PB2-OB3
69	N4	503	CDL	CB3-OB5-PB2-OB3
69	N4	503	CDL	CB3-OB5-PB2-OB4
69	N5	703	CDL	CA2-OA2-PA1-OA3
69	N5	703	CDL	CA3-OA5-PA1-OA4
69	N5	704	CDL	CB3-OB5-PB2-OB4
69	QB	501	CDL	CA2-OA2-PA1-OA4
69	QD	402	CDL	CA3-OA5-PA1-OA4
69	QD	402	CDL	CB2-OB2-PB2-OB3
69	QD	402	CDL	CB3-OB5-PB2-OB3
69	QH	401	CDL	CB2-OB2-PB2-OB4
69	Qb	501	CDL	CA2-OA2-PA1-OA4
69	Qb	501	CDL	CA3-OA5-PA1-OA4
69	Qb	501	CDL	CB2-OB2-PB2-OB4
69	Qb	501	CDL	CB3-OB5-PB2-OB4
69	Qh	102	CDL	CB2-OB2-PB2-OB4
71	6A	101	PC1	C11-O13-P-O14
71	6A	103	PC1	C11-O13-P-O14
71	6A	103	PC1	C1-O11-P-O12
71	C1	605	PC1	C11-C12-N-C14
71	C1	606	PC1	C11-O13-P-O12
71	C1	607	PC1	C1-O11-P-O12
71	C3	302	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
71	C3	303	PC1	C11-O13-P-O12
71	Qc	406	PC1	C11-O13-P-O14
72	6C	101	PLX	C2-O1-P1-O3
72	AM	201	PLX	C2-O1-P1-O3
72	N3	202	PLX	C3-O4-P1-O3
72	N4	501	PLX	C2-O1-P1-O3
72	QB	504	PLX	C2-O1-P1-O2
72	QI	301	PLX	C3-O4-P1-O2
72	S7	302	PLX	C2-O1-P1-O3
74	A9	402	PEE	C1-O3P-P-O2P
74	A9	402	PEE	C4-O4P-P-O2P
74	AL	203	PEE	C4-O4P-P-O1P
74	N3	201	PEE	C1-O3P-P-O2P
74	N3	201	PEE	C4-O4P-P-O2P
74	N5	701	PEE	C1-O3P-P-O2P
74	N5	701	PEE	C1-O3P-P-O1P
74	N5	701	PEE	C4-O4P-P-O1P
74	N5	705	PEE	C1-O3P-P-O2P
74	QB	502	PEE	C1-O3P-P-O1P
74	QB	502	PEE	C4-O4P-P-O1P
74	QE	301	PEE	C1-O3P-P-O2P
77	N5	706	3PE	C1-O11-P-O12
77	N5	706	3PE	C11-O13-P-O12
77	QE	302	3PE	C1-O11-P-O14
77	Qc	405	3PE	C11-O13-P-O12
77	Qj	101	3PE	C11-O13-P-O12
72	CB	201	PLX	C16-C17-C18-C19
69	AL	202	CDL	OB5-CB3-CB4-CB6
69	N4	502	CDL	OB5-CB3-CB4-CB6
69	N5	704	CDL	OA5-CA3-CA4-CA6
69	QD	402	CDL	OB5-CB3-CB4-CB6
71	N1	402	PC1	O11-C1-C2-C3
72	CB	201	PLX	O4-C3-C4-C5
72	N3	202	PLX	O4-C3-C4-C5
72	N4	501	PLX	O4-C3-C4-C5
74	N1	404	PEE	O3P-C1-C2-C3
69	N5	703	CDL	C52-C53-C54-C55
72	B5	201	PLX	C29-C30-C31-C32
71	6A	101	PC1	C12-C11-O13-P
71	N1	403	PC1	C12-C11-O13-P
71	QB	503	PC1	C12-C11-O13-P
72	6C	101	PLX	C1-C2-O1-P1

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Mol	Chain	Res	Type	Atoms
72	AL	204	PLX	C25-C24-O8-C5
72	CB	201	PLX	C1-C2-O1-P1
72	CB	201	PLX	C25-C24-O8-C5
72	S7	302	PLX	C25-C24-O8-C5
74	S2	501	PEE	C5-C4-O4P-P
71	6A	103	PC1	C23-C24-C25-C26
72	QB	504	PLX	C12-C13-C14-C15
72	N3	202	PLX	C28-C29-C30-C31
72	QB	504	PLX	C28-C29-C30-C31
69	N4	502	CDL	OB5-CB3-CB4-OB6
69	Qh	102	CDL	OA5-CA3-CA4-OA6
71	C3	301	PC1	O11-C1-C2-O21
72	N4	501	PLX	O4-C3-C4-O6
74	A9	402	PEE	O3P-C1-C2-O2
85	V1	502	FMN	N10-C1'-C2'-O2'
69	AL	201	CDL	C54-C55-C56-C57
72	AM	201	PLX	C25-C26-C27-C28
71	Qc	406	PC1	C39-C3A-C3B-C3C
72	QI	301	PLX	C32-C33-C34-C35
77	S7	303	3PE	C21-C22-C23-C24
74	QC	403	PEE	C11-C10-O2-C2
74	Qc	402	PEE	C32-C33-C34-C35
71	C3	301	PC1	C11-C12-N-C15
71	N1	403	PC1	C11-C12-N-C14
71	Qb	502	PC1	C11-C12-N-C15
69	Qc	401	CDL	CA3-CA4-CA6-OA8
71	C1	607	PC1	O13-C11-C12-N
71	C3	302	PC1	O13-C11-C12-N
71	N1	402	PC1	O13-C11-C12-N
71	N1	403	PC1	O13-C11-C12-N
71	Qc	406	PC1	O13-C11-C12-N
72	AL	204	PLX	N1-C1-C2-O1
72	QB	504	PLX	N1-C1-C2-O1
72	QI	301	PLX	N1-C1-C2-O1
74	AL	203	PEE	C1-C2-C3-O3
74	N5	701	PEE	C13-C14-C15-C16
74	N5	702	PEE	C1-C2-C3-O3
74	N5	705	PEE	C1-C2-C3-O3
69	N4	503	CDL	OA6-CA4-CA6-OA8
71	Qh	101	PC1	O21-C2-C3-O31
72	N4	501	PLX	O6-C4-C5-O8
74	N5	705	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
74	Qd	402	PEE	O2-C2-C3-O3
69	4L	201	CDL	C32-C33-C34-C35
71	QB	503	PC1	C28-C29-C2A-C2B
69	Qh	102	CDL	CA7-C31-C32-C33
72	6C	101	PLX	C18-C19-C20-C21
77	CB	202	3PE	C36-C37-C38-C39
69	CB	203	CDL	C1-CB2-OB2-PB2
71	N1	402	PC1	C2-C1-O11-P
72	6C	101	PLX	C4-C3-O4-P1
77	Qc	405	3PE	C2-C1-O11-P
74	QB	502	PEE	C32-C33-C34-C35
74	S8	303	PEE	C32-C33-C34-C35
75	AB	201	ZMP	O3-C16-C17-O4
75	AC	201	ZMP	O3-C16-C17-O4
74	S8	303	PEE	C14-C15-C16-C17
72	S7	302	PLX	C17-C18-C19-C20
77	S7	303	3PE	C32-C33-C34-C35
72	CB	201	PLX	C7-C8-C9-C10
75	AC	201	ZMP	C19-C18-C21-O5
75	AC	201	ZMP	C20-C18-C21-O5
72	S7	302	PLX	C29-C30-C31-C32
74	S8	303	PEE	C31-C32-C33-C34
77	S7	303	3PE	C27-C28-C29-C2A
71	C1	607	PC1	C32-C33-C34-C35
77	Qj	101	3PE	O31-C31-C32-C33
75	AC	201	ZMP	C6-C7-C8-C9
74	A9	402	PEE	C3-C2-O2-C10
74	AL	203	PEE	C3-C2-O2-C10
69	AL	201	CDL	OA5-CA3-CA4-CA6
71	C3	301	PC1	O11-C1-C2-C3
74	QC	403	PEE	O4-C10-O2-C2
72	AM	201	PLX	C26-C27-C28-C29
74	N5	702	PEE	C31-C32-C33-C34
72	N3	202	PLX	C4-C3-O4-P1
74	C3	304	PEE	C21-C22-C23-C24
74	QJ	101	PEE	C24-C25-C26-C27
69	N5	704	CDL	OA5-CA3-CA4-OA6
72	6C	101	PLX	O4-C3-C4-O6
72	AM	201	PLX	O4-C3-C4-O6
77	Qc	405	3PE	O11-C1-C2-O21
72	QI	301	PLX	C7-C8-C9-C10
71	Qb	502	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
69	AL	201	CDL	C52-C51-CB5-OB6
69	N1	401	CDL	C58-C59-C60-C61
72	CB	201	PLX	O6-C4-C5-O8
77	QJ	102	3PE	O21-C2-C3-O31
74	QE	301	PEE	C22-C23-C24-C25
69	6A	102	CDL	CA2-OA2-PA1-OA5
69	A7	201	CDL	CA2-OA2-PA1-OA5
69	A7	201	CDL	CB2-OB2-PB2-OB5
69	AL	202	CDL	CA3-OA5-PA1-OA2
69	CB	203	CDL	CB2-OB2-PB2-OB5
69	N4	502	CDL	CA3-OA5-PA1-OA2
69	N4	502	CDL	CB3-OB5-PB2-OB2
69	QH	401	CDL	CA3-OA5-PA1-OA2
69	Qc	401	CDL	CA3-OA5-PA1-OA2
71	N1	402	PC1	C1-O11-P-O13
72	B5	201	PLX	C2-O1-P1-O4
74	S8	303	PEE	C4-O4P-P-O3P
77	C1	608	3PE	C11-O13-P-O11
77	Qc	405	3PE	C1-O11-P-O13
69	QB	501	CDL	CA5-C11-C12-C13
71	Qh	101	PC1	C2B-C2C-C2D-C2E
74	N5	702	PEE	C18-C19-C20-C21
69	N5	704	CDL	C12-C11-CA5-OA6
69	CB	203	CDL	CA3-CA4-CA6-OA8
72	QI	301	PLX	C3-C4-C5-O8
74	S8	303	PEE	C1-C2-C3-O3
69	4L	201	CDL	C81-C82-C83-C84
69	N4	502	CDL	C39-C40-C41-C42
69	CB	203	CDL	CA5-C11-C12-C13
72	QB	504	PLX	C6-C7-C8-C9
74	N1	404	PEE	C31-C32-C33-C34
74	QE	301	PEE	C21-C22-C23-C24
71	QB	503	PC1	C11-C12-N-C14
73	A9	401	NDP	PN-O3-PA-O2A
74	N5	702	PEE	C34-C35-C36-C37
71	C3	302	PC1	C2-C1-O11-P
74	QC	403	PEE	C2-C1-O3P-P
85	V1	502	FMN	C4'-C5'-O5'-P
74	QE	301	PEE	O3-C30-C31-C32
72	N4	501	PLX	C10-C11-C12-C13
74	N5	701	PEE	C35-C36-C37-C38
69	AL	201	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
73	A9	401	NDP	O4D-C1D-N1N-C6N
69	CB	203	CDL	CB5-C51-C52-C53
74	Qd	402	PEE	O4P-C4-C5-N
69	N4	503	CDL	OA5-CA3-CA4-OA6
71	QB	503	PC1	O11-C1-C2-O21
72	B5	201	PLX	O4-C3-C4-O6
69	AK	402	CDL	C32-C33-C34-C35
77	Qc	405	3PE	C29-C2A-C2B-C2C
69	B5	202	CDL	C40-C41-C42-C43
74	QB	502	PEE	C11-C12-C13-C14
74	QJ	101	PEE	C42-C43-C44-C45
77	C1	609	3PE	C3A-C3B-C3C-C3D
81	Qc	403	HEM	CAA-CBA-CGA-O1A
72	N3	202	PLX	C35-C36-C37-C38
69	N5	703	CDL	C71-C72-C73-C74
72	AL	204	PLX	O6-C6-C7-C8
72	N3	202	PLX	O6-C6-C7-C8
72	N3	202	PLX	O8-C24-C25-C26
74	QB	502	PEE	O2-C2-C3-O3
69	N4	503	CDL	C1-CA2-OA2-PA1
71	C3	303	PC1	C2-C1-O11-P
71	N1	403	PC1	C3A-C3B-C3C-C3D
75	AB	201	ZMP	S1-C11-C12-N1
81	QC	401	HEM	CAA-CBA-CGA-O1A
81	Qc	403	HEM	CAD-CBD-CGD-O2D
71	C1	605	PC1	C11-C12-N-C13
74	AL	203	PEE	C18-C19-C20-C21
72	AM	201	PLX	C18-C19-C20-C21
72	QI	301	PLX	C6-C7-C8-C9
71	Qc	406	PC1	C1-C2-C3-O31
72	CB	201	PLX	C3-C4-C5-O8
81	Qc	403	HEM	CAD-CBD-CGD-O1D
72	S7	302	PLX	C25-C26-C27-C28
69	4L	201	CDL	C23-C24-C25-C26
81	Qc	404	HEM	CAD-CBD-CGD-O1D
69	6A	102	CDL	C72-C71-CB7-OB8
69	CB	203	CDL	C16-C17-C18-C19
81	QC	402	HEM	CAA-CBA-CGA-O1A
69	4L	201	CDL	CA6-CA4-OA6-CA5
69	AL	201	CDL	CA6-CA4-OA6-CA5
69	QB	501	CDL	CA6-CA4-OA6-CA5
69	Qb	501	CDL	CA3-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
71	QB	503	PC1	C1-C2-O21-C21
77	C1	608	3PE	C1-C2-O21-C21
71	Qb	502	PC1	C11-C12-N-C13
78	C1	602	HEA	CAD-CBD-CGD-O1D
81	QC	401	HEM	CAA-CBA-CGA-O2A
81	Qc	403	HEM	CAA-CBA-CGA-O2A
81	Qc	404	HEM	CAA-CBA-CGA-O1A
81	Qc	404	HEM	CAA-CBA-CGA-O2A
69	QD	402	CDL	C52-C51-CB5-OB7
74	AL	203	PEE	C40-C41-C42-C43
69	N4	502	CDL	C60-C61-C62-C63
73	A9	401	NDP	C2D-C1D-N1N-C6N
69	6A	102	CDL	C55-C56-C57-C58
74	A9	402	PEE	C33-C34-C35-C36
74	QJ	101	PEE	O3P-C1-C2-O2
78	C1	601	HEA	CAD-CBD-CGD-O2D
74	S2	501	PEE	C31-C32-C33-C34
74	S2	501	PEE	C40-C41-C42-C43
69	Qh	102	CDL	C31-CA7-OA8-CA6
74	N5	705	PEE	C31-C30-O3-C3
72	AM	201	PLX	O4-C3-C4-C5
74	Qc	402	PEE	O3P-C1-C2-C3
72	B5	201	PLX	C25-C26-C27-C28
72	N4	501	PLX	C11-C12-C13-C14
74	N3	201	PEE	C12-C13-C14-C15
78	C1	601	HEA	CAD-CBD-CGD-O1D
71	C3	301	PC1	C24-C25-C26-C27
71	C3	302	PC1	C34-C35-C36-C37
69	Qh	102	CDL	O1-C1-CA2-OA2
74	QJ	101	PEE	C34-C35-C36-C37
71	N1	403	PC1	C11-C12-N-C15
69	N4	502	CDL	C37-C38-C39-C40
72	AM	201	PLX	C32-C33-C34-C35
75	AB	201	ZMP	C12-C11-S1-C10
69	AL	201	CDL	OB6-CB4-CB6-OB8
69	CB	203	CDL	OA6-CA4-CA6-OA8
71	C1	605	PC1	O21-C2-C3-O31
72	B5	201	PLX	O6-C4-C5-O8
74	N1	404	PEE	O2-C2-C3-O3
71	Qb	502	PC1	C3E-C3F-C3G-C3H
74	QJ	101	PEE	C40-C41-C42-C43
71	QB	503	PC1	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
74	N3	201	PEE	C44-C45-C46-C47
69	AK	402	CDL	C71-C72-C73-C74
74	C3	304	PEE	C17-C18-C19-C20
74	N5	701	PEE	C17-C18-C19-C20
74	N5	705	PEE	O5-C30-O3-C3
69	4L	201	CDL	C55-C56-C57-C58
69	N5	703	CDL	C57-C58-C59-C60
78	C1	602	HEA	CAD-CBD-CGD-O2D
71	C3	303	PC1	C3E-C3F-C3G-C3H
69	AL	202	CDL	C52-C51-CB5-OB6
69	B5	202	CDL	C36-C37-C38-C39
74	QB	502	PEE	C1-C2-C3-O3
76	AK	401	ADP	O4'-C4'-C5'-O5'
71	C1	605	PC1	C39-C3A-C3B-C3C
71	N3	203	PC1	C2B-C2C-C2D-C2E
69	AK	402	CDL	C52-C51-CB5-OB7
71	C1	606	PC1	O32-C31-C32-C33
71	Qh	101	PC1	C32-C33-C34-C35
74	N5	705	PEE	C42-C43-C44-C45
71	N1	403	PC1	O21-C21-C22-C23
77	CA	101	3PE	O31-C31-C32-C33
72	6C	101	PLX	O6-C6-C7-C8
82	Qd	401	HEC	CAD-CBD-CGD-O1D
71	C3	302	PC1	C39-C3A-C3B-C3C
72	CB	201	PLX	C31-C32-C33-C34
81	QC	402	HEM	CAA-CBA-CGA-O2A
75	AC	201	ZMP	C7-C8-C9-C10
71	C3	301	PC1	O21-C2-C3-O31
74	S2	501	PEE	O2-C2-C3-O3
71	C3	303	PC1	C22-C23-C24-C25
82	QD	401	HEC	CAD-CBD-CGD-O2D
69	B5	202	CDL	C21-C22-C23-C24
71	QB	503	PC1	C3A-C3B-C3C-C3D
75	AC	201	ZMP	N2-C16-C17-O4
77	C1	608	3PE	C28-C29-C2A-C2B
81	QC	401	HEM	CAD-CBD-CGD-O1D
71	N1	403	PC1	C11-C12-N-C13
72	S7	302	PLX	C28-C29-C30-C31
74	Qc	402	PEE	C15-C16-C17-C18
69	AL	202	CDL	C81-C82-C83-C84
74	C3	304	PEE	C18-C19-C20-C21
77	C1	608	3PE	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
81	Qc	404	HEM	CAD-CBD-CGD-O2D
69	QD	402	CDL	CB3-CB4-OB6-CB5
71	C3	302	PC1	C3-C2-O21-C21
71	Qb	502	PC1	C3-C2-O21-C21
77	Qc	405	3PE	C1-C2-O21-C21
77	S7	303	3PE	C3-C2-O21-C21
69	N1	401	CDL	C54-C55-C56-C57
71	C1	605	PC1	C3C-C3D-C3E-C3F
69	4L	201	CDL	C12-C11-CA5-OA6
69	CB	203	CDL	C72-C71-CB7-OB8
69	N5	703	CDL	C12-C11-CA5-OA6
69	N5	704	CDL	C72-C71-CB7-OB8
69	Qb	501	CDL	C72-C71-CB7-OB8
69	N1	401	CDL	C77-C78-C79-C80
72	CB	201	PLX	C32-C33-C34-C35
77	CA	101	3PE	C26-C27-C28-C29
77	S7	303	3PE	C2A-C2B-C2C-C2D
69	AK	402	CDL	C32-C31-CA7-OA8
69	N1	401	CDL	C12-C11-CA5-OA6
74	S8	303	PEE	O2-C10-C11-C12
77	CB	202	3PE	O31-C31-C32-C33
77	QE	302	3PE	C23-C24-C25-C26
74	N5	701	PEE	C18-C19-C20-C21
74	N5	705	PEE	C15-C16-C17-C18
69	N1	401	CDL	C73-C74-C75-C76
72	CB	201	PLX	C7-C6-O6-C4
72	N3	202	PLX	C3-C4-C5-O8
77	B8	201	3PE	C1-C2-C3-O31
72	N4	501	PLX	C28-C29-C30-C31
71	C1	607	PC1	O11-C1-C2-O21
77	CA	101	3PE	O11-C1-C2-O21
71	C3	301	PC1	O31-C31-C32-C33
74	N3	201	PEE	O3-C30-C31-C32
69	N4	503	CDL	C12-C13-C14-C15
69	AL	202	CDL	CB7-C71-C72-C73
72	N4	501	PLX	C33-C34-C35-C36
81	QC	402	HEM	C4C-C3C-CAC-CBC
69	CB	203	CDL	C12-C11-CA5-OA6
69	N4	503	CDL	C32-C31-CA7-OA8
74	N5	702	PEE	C36-C37-C38-C39
74	N3	201	PEE	C43-C44-C45-C46
74	N5	705	PEE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
77	C1	609	3PE	C33-C34-C35-C36
69	B5	202	CDL	C37-C38-C39-C40
71	N1	402	PC1	C25-C26-C27-C28
69	AL	201	CDL	C32-C31-CA7-OA8
71	Qb	502	PC1	O31-C31-C32-C33
71	Qh	101	PC1	O31-C31-C32-C33
69	4L	201	CDL	C53-C54-C55-C56
72	B5	201	PLX	O4-C3-C4-C5
74	N5	702	PEE	O3P-C1-C2-C3
77	CA	101	3PE	O11-C1-C2-C3
77	QE	302	3PE	O11-C1-C2-C3
69	AL	202	CDL	C78-C79-C80-C81
69	QD	402	CDL	C74-C75-C76-C77
71	N1	402	PC1	C37-C38-C39-C3A
69	A7	201	CDL	C72-C71-CB7-OB8
77	C1	609	3PE	O31-C31-C32-C33
77	QE	302	3PE	O21-C21-C22-C23
71	Qh	101	PC1	C3B-C3C-C3D-C3E
72	CB	201	PLX	C11-C10-C9-C8
74	S8	303	PEE	C16-C17-C18-C19
69	CB	203	CDL	C52-C51-CB5-OB6
69	QB	501	CDL	C72-C71-CB7-OB8
77	Qc	405	3PE	O21-C21-C22-C23
69	N5	704	CDL	C53-C54-C55-C56
72	N3	202	PLX	C16-C17-C18-C19
69	A7	201	CDL	C12-C11-CA5-OA6
72	B5	201	PLX	C33-C34-C35-C36
77	B8	201	3PE	C33-C34-C35-C36
81	QC	401	HEM	CAD-CBD-CGD-O2D
72	QB	504	PLX	C26-C27-C28-C29
72	QB	504	PLX	C24-C25-C26-C27
74	QE	301	PEE	C13-C14-C15-C16
69	N4	503	CDL	C72-C71-CB7-OB8
74	AL	203	PEE	C34-C35-C36-C37
74	N5	701	PEE	C30-C31-C32-C33
69	AK	402	CDL	C72-C71-CB7-OB8
73	A9	401	NDP	PN-O3-PA-O1A
77	Qj	101	3PE	C23-C24-C25-C26
82	QD	401	HEC	CAD-CBD-CGD-O1D
69	N5	703	CDL	CB7-C71-C72-C73
74	N3	201	PEE	O2-C10-C11-C12
74	C3	304	PEE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
72	N3	202	PLX	C24-C25-C26-C27
72	N4	501	PLX	C6-C7-C8-C9
69	6A	102	CDL	C38-C39-C40-C41
82	Qd	401	HEC	CAD-CBD-CGD-O2D
74	N3	201	PEE	O5-C30-C31-C32
74	S8	303	PEE	O4-C10-C11-C12
77	QJ	102	3PE	C27-C28-C29-C2A
69	N4	503	CDL	CA2-C1-CB2-OB2
69	AL	201	CDL	C59-C60-C61-C62
74	N1	404	PEE	C34-C35-C36-C37
71	C1	605	PC1	C3B-C3C-C3D-C3E
69	AL	201	CDL	C32-C31-CA7-OA9
69	N5	703	CDL	C12-C11-CA5-OA7
71	C3	301	PC1	O32-C31-C32-C33
77	CB	202	3PE	O32-C31-C32-C33
71	C1	605	PC1	C1-C2-C3-O31
71	C1	607	PC1	O21-C21-C22-C23
77	C1	609	3PE	C38-C39-C3A-C3B
72	B5	201	PLX	C32-C33-C34-C35
74	S2	501	PEE	C14-C15-C16-C17
71	Qh	101	PC1	C22-C23-C24-C25
69	A7	201	CDL	C1-CA2-OA2-PA1
69	N4	503	CDL	C1-CB2-OB2-PB2
74	C3	304	PEE	C2-C1-O3P-P
72	N3	202	PLX	C26-C27-C28-C29
69	CB	203	CDL	C12-C11-CA5-OA7
69	CB	203	CDL	C52-C51-CB5-OB7
69	Qb	501	CDL	C72-C71-CB7-OB9
69	AK	402	CDL	CB3-OB5-PB2-OB3
69	AL	201	CDL	CB3-OB5-PB2-OB3
69	B5	202	CDL	CA2-OA2-PA1-OA3
69	CB	203	CDL	CB2-OB2-PB2-OB3
69	N4	503	CDL	CA2-OA2-PA1-OA4
69	QD	402	CDL	CB3-OB5-PB2-OB4
69	Qc	401	CDL	CA3-OA5-PA1-OA4
71	C3	301	PC1	C1-O11-P-O12
72	6C	101	PLX	C3-O4-P1-O2
72	AM	201	PLX	C3-O4-P1-O2
72	B5	201	PLX	C3-O4-P1-O3
72	CB	201	PLX	C3-O4-P1-O2
72	N4	501	PLX	C3-O4-P1-O3
74	A9	402	PEE	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
74	AL	203	PEE	C1-O3P-P-O1P
74	C3	304	PEE	C1-O3P-P-O1P
74	N3	201	PEE	C4-O4P-P-O1P
74	QC	403	PEE	C4-O4P-P-O1P
77	C1	608	3PE	C11-O13-P-O14
77	Qc	405	3PE	C1-O11-P-O14
69	4L	201	CDL	C12-C11-CA5-OA7
69	AK	402	CDL	C32-C31-CA7-OA9
69	N5	704	CDL	C72-C71-CB7-OB9
69	QB	501	CDL	C72-C71-CB7-OB9
71	Qh	101	PC1	O32-C31-C32-C33
74	N3	201	PEE	O4-C10-C11-C12
77	QE	302	3PE	O22-C21-C22-C23
77	Qc	405	3PE	O22-C21-C22-C23
69	CB	203	CDL	C59-C60-C61-C62
74	N5	702	PEE	O4P-C4-C5-N
74	QJ	101	PEE	C43-C44-C45-C46
69	N1	401	CDL	C32-C31-CA7-OA8
69	N4	503	CDL	C32-C31-CA7-OA9
69	QB	501	CDL	C12-C13-C14-C15
69	B5	202	CDL	C73-C74-C75-C76
69	AK	402	CDL	CA3-CA4-OA6-CA5
69	AK	402	CDL	CA6-CA4-OA6-CA5
69	QD	402	CDL	CB6-CB4-OB6-CB5
69	QH	401	CDL	CA3-CA4-OA6-CA5
69	QH	401	CDL	CA6-CA4-OA6-CA5
69	Qc	401	CDL	CA3-CA4-OA6-CA5
69	Qc	401	CDL	CA6-CA4-OA6-CA5
71	C1	605	PC1	C12-C11-O13-P
71	C3	302	PC1	C12-C11-O13-P
71	C3	302	PC1	C1-C2-O21-C21
71	QB	503	PC1	C3-C2-O21-C21
72	N3	202	PLX	C25-C24-O8-C5
74	AL	203	PEE	C1-C2-O2-C10
74	N3	201	PEE	C5-C4-O4P-P
74	N5	702	PEE	C5-C4-O4P-P
74	Qc	402	PEE	C5-C4-O4P-P
75	AB	201	ZMP	O3-C16-C17-C18
77	C1	608	3PE	C3-C2-O21-C21
77	C1	609	3PE	C12-C11-O13-P
77	S7	303	3PE	C1-C2-O21-C21
69	Qh	102	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
69	N1	401	CDL	C12-C11-CA5-OA7
71	C1	607	PC1	O22-C21-C22-C23
71	N1	402	PC1	C2A-C2B-C2C-C2D
74	N5	701	PEE	C39-C40-C41-C42
71	QB	503	PC1	C11-C12-N-C13
71	QB	503	PC1	C11-C12-N-C15
71	C3	301	PC1	O21-C21-C22-C23
72	B5	201	PLX	C34-C35-C36-C37
69	N1	401	CDL	C57-C58-C59-C60
69	N5	703	CDL	C33-C34-C35-C36
71	Qb	502	PC1	C37-C38-C39-C3A
74	N3	201	PEE	C23-C24-C25-C26
78	C1	602	HEA	CAA-CBA-CGA-O1A
72	CB	201	PLX	C36-C37-C38-C39
69	A7	201	CDL	C72-C71-CB7-OB9
69	AL	201	CDL	C57-C58-C59-C60
72	S7	302	PLX	C33-C34-C35-C36
69	N4	503	CDL	CA4-CA3-OA5-PA1
77	QE	302	3PE	C2-C1-O11-P
85	V1	502	FMN	N10-C1'-C2'-C3'
77	QE	302	3PE	C32-C33-C34-C35
74	QC	403	PEE	O2-C10-C11-C12
71	Qc	406	PC1	O31-C31-C32-C33
74	Qc	402	PEE	O2-C10-C11-C12
74	A9	402	PEE	C15-C16-C17-C18
74	QC	403	PEE	O4-C10-C11-C12
71	N1	403	PC1	C3C-C3D-C3E-C3F
69	N4	502	CDL	C35-C36-C37-C38
69	Qc	401	CDL	C52-C51-CB5-OB6
69	Qh	102	CDL	C32-C31-CA7-OA8
74	AL	203	PEE	O2-C10-C11-C12
69	AK	402	CDL	C72-C71-CB7-OB9
77	C1	609	3PE	O32-C31-C32-C33
71	C1	606	PC1	C33-C34-C35-C36
74	N5	705	PEE	C16-C17-C18-C19
74	N5	705	PEE	C31-C32-C33-C34
69	6A	102	CDL	C58-C59-C60-C61
74	A9	402	PEE	O2-C10-C11-C12

There are no ring outliers.

78 monomers are involved in 239 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	Qc	402	PEE	1	0
74	C3	304	PEE	6	0
69	Qc	401	CDL	1	0
71	QB	503	PC1	4	0
71	Qc	406	PC1	1	0
69	A7	201	CDL	1	0
69	AK	402	CDL	4	0
72	N4	501	PLX	3	0
77	C1	609	3PE	1	0
84	V1	501	SF4	1	0
69	4L	201	CDL	7	0
77	QJ	102	3PE	1	0
71	6A	101	PC1	6	0
71	C1	607	PC1	1	0
77	Qc	405	3PE	3	0
72	AL	204	PLX	1	0
81	Qc	404	HEM	7	0
71	N3	203	PC1	1	0
69	6A	102	CDL	5	0
81	QC	401	HEM	1	0
78	C1	602	HEA	3	0
69	N5	703	CDL	6	0
74	QE	301	PEE	1	0
77	N5	706	3PE	1	0
72	QB	504	PLX	3	0
76	AK	401	ADP	2	0
69	QD	402	CDL	1	0
74	N5	702	PEE	1	0
69	N5	704	CDL	3	0
74	N5	705	PEE	2	0
74	N3	201	PEE	2	0
71	C3	303	PC1	13	0
69	Qh	102	CDL	3	0
72	6C	101	PLX	1	0
69	AL	201	CDL	5	0
77	Qj	101	3PE	1	0
72	B5	201	PLX	1	0
77	C1	608	3PE	3	0
71	Qh	101	PC1	3	0
72	QI	301	PLX	5	0
82	QD	401	HEC	2	0
75	AC	201	ZMP	3	0
69	N1	401	CDL	6	0

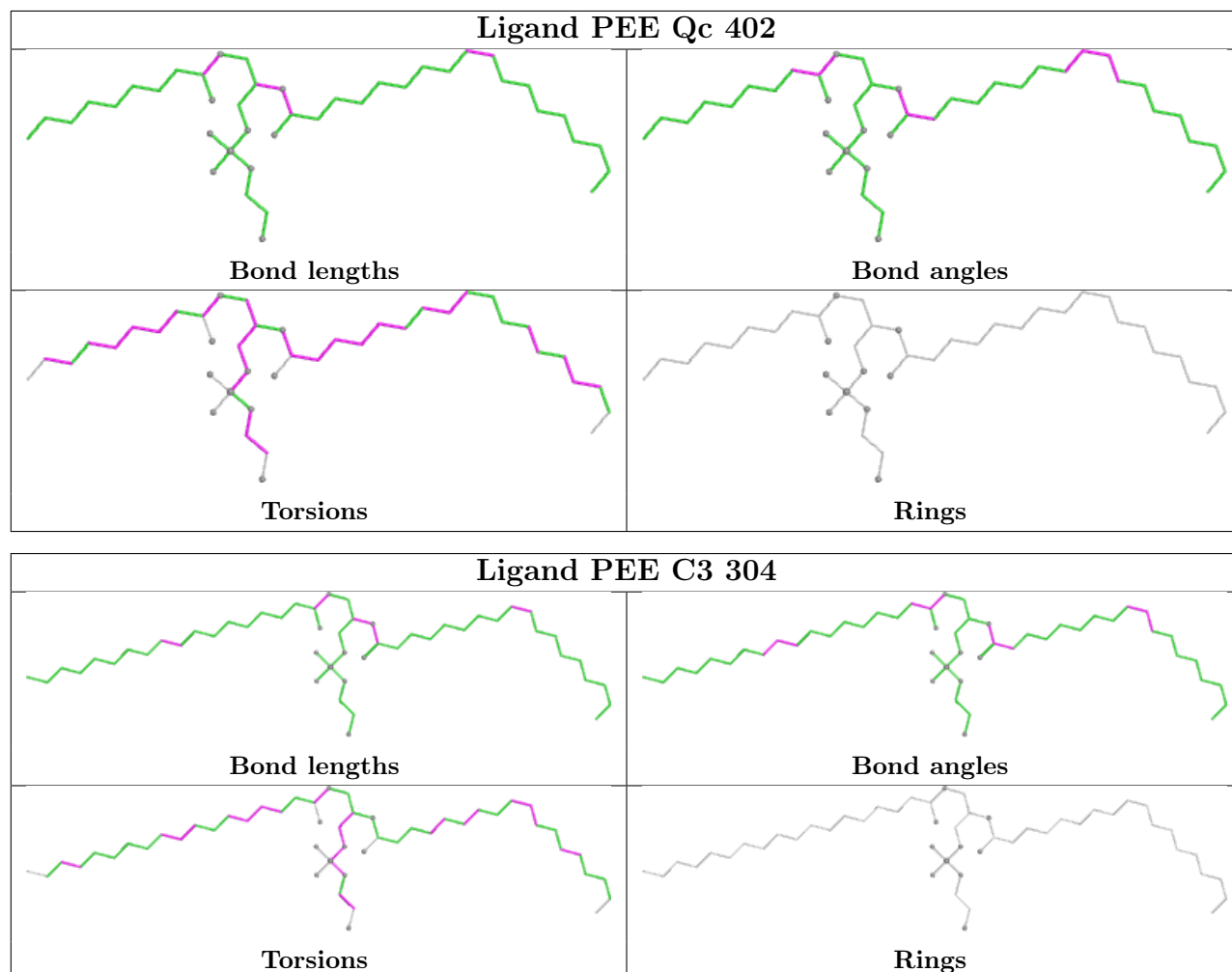
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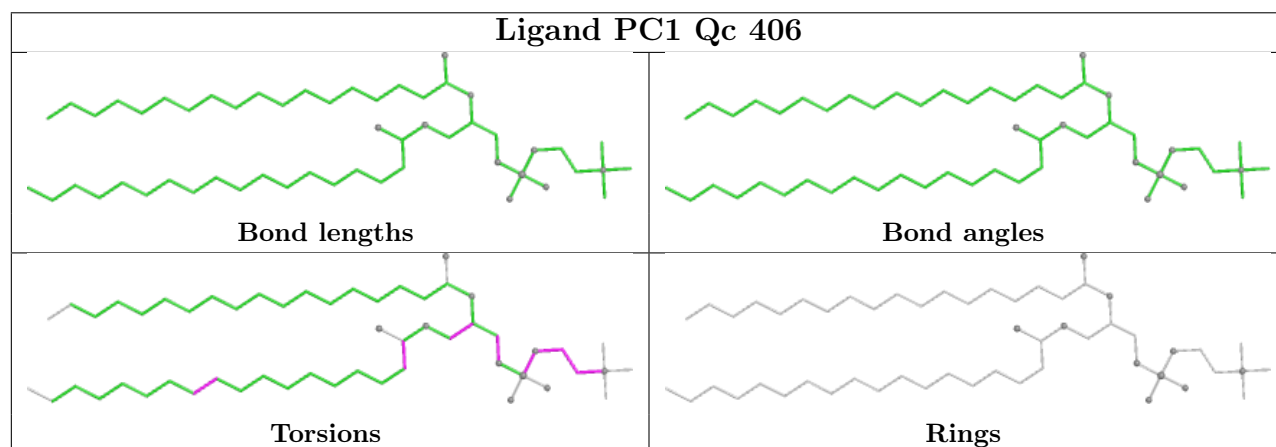
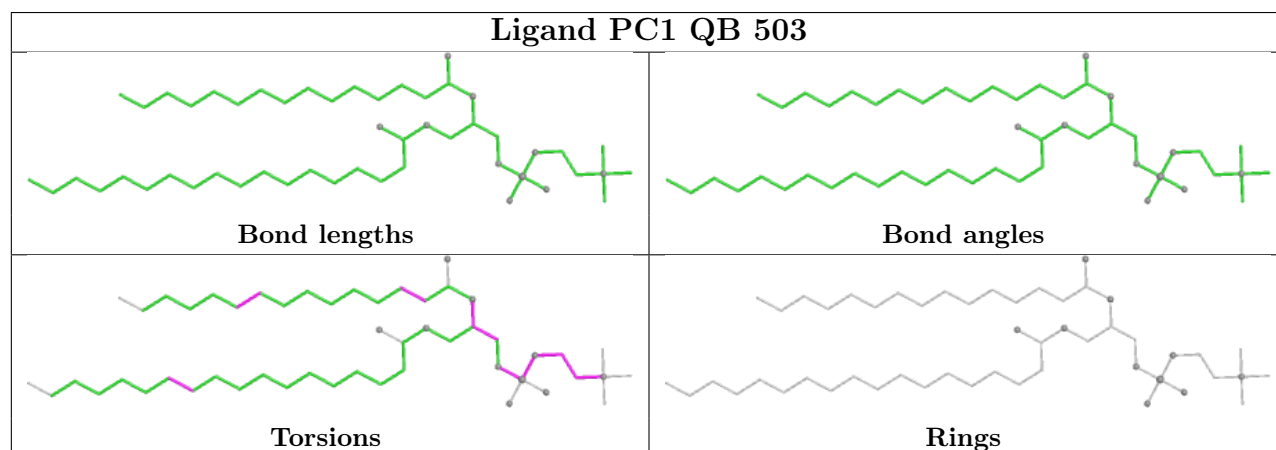
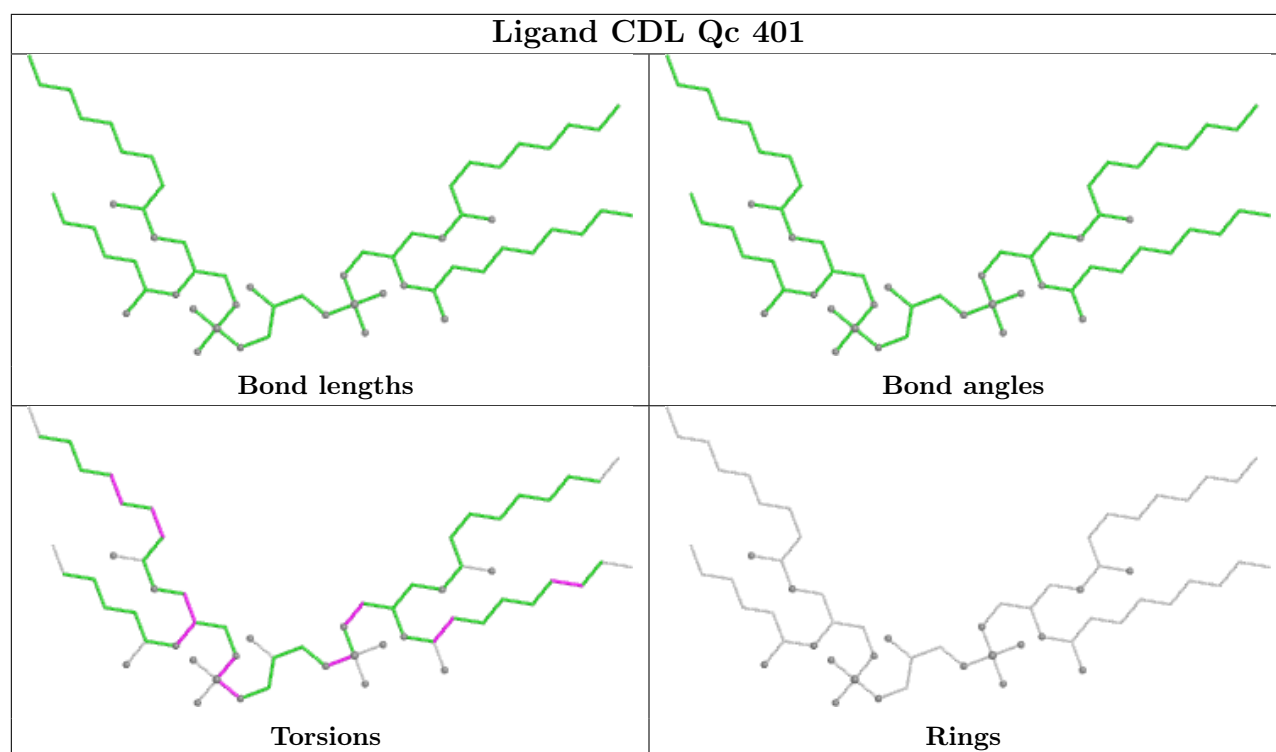
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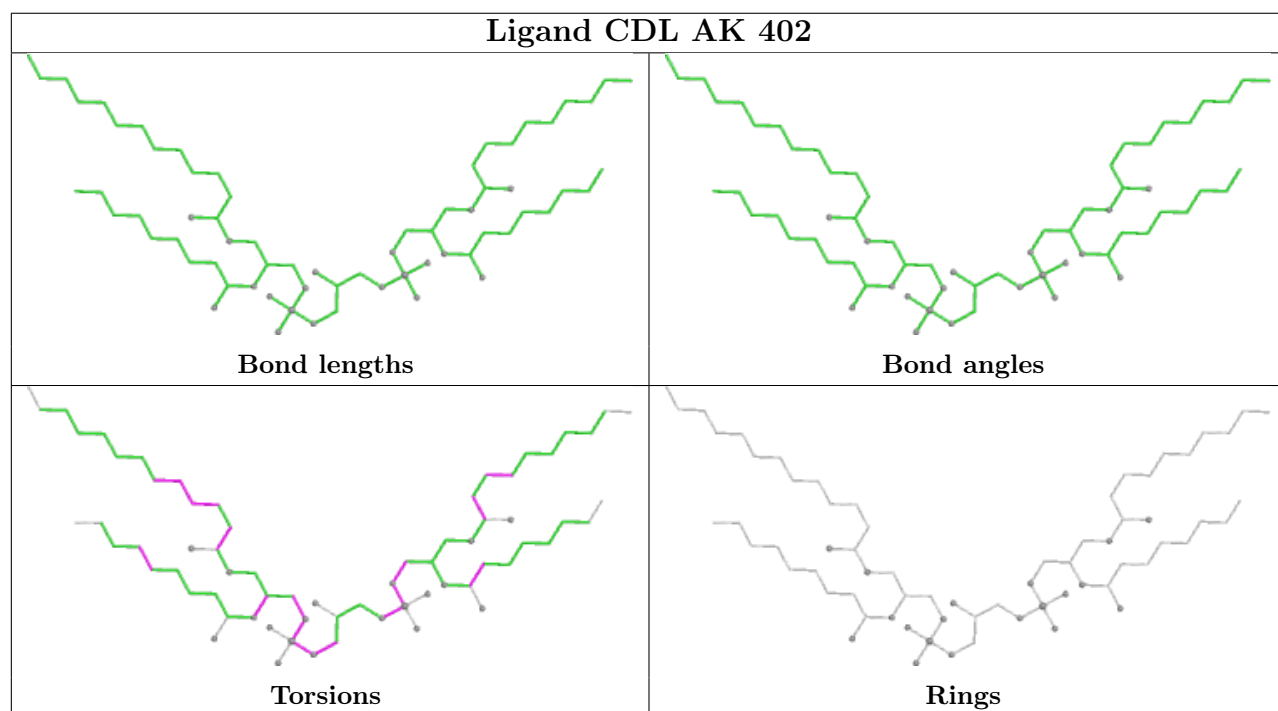
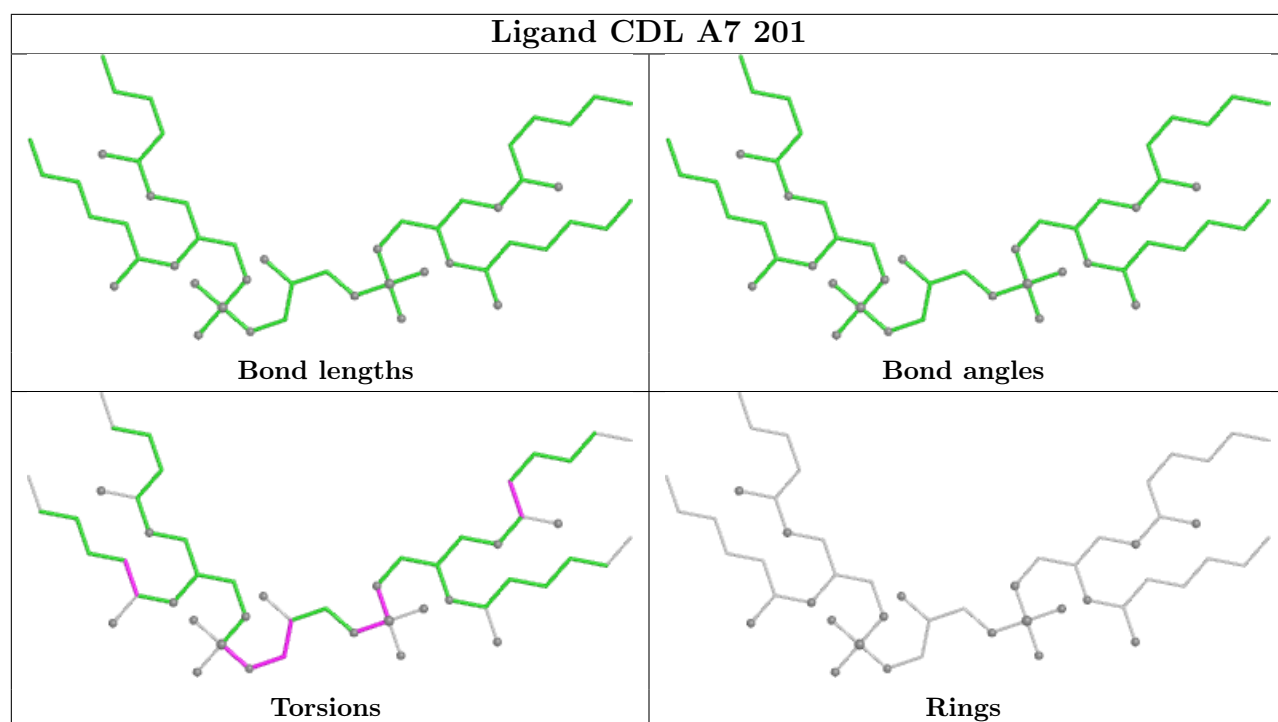
Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	QB	502	PEE	3	0
77	CB	202	3PE	5	0
84	S1	802	SF4	1	0
69	QH	401	CDL	4	0
74	N1	404	PEE	1	0
74	QJ	101	PEE	3	0
83	Qe	301	FES	1	0
71	N1	402	PC1	3	0
71	C3	301	PC1	2	0
74	S2	501	PEE	1	0
69	QB	501	CDL	2	0
69	AL	202	CDL	5	0
74	A9	402	PEE	1	0
71	Qb	502	PC1	5	0
72	AM	201	PLX	5	0
74	AL	203	PEE	4	0
77	S7	303	3PE	4	0
81	Qc	403	HEM	3	0
72	S7	302	PLX	4	0
78	C1	601	HEA	10	0
71	N1	403	PC1	6	0
72	CB	201	PLX	7	0
83	S1	803	FES	1	0
71	6A	103	PC1	2	0
72	N3	202	PLX	3	0
81	QC	402	HEM	5	0
69	CB	203	CDL	4	0
82	Qd	401	HEC	3	0
71	C3	302	PC1	9	0
74	S8	303	PEE	2	0
69	N4	502	CDL	6	0
74	N5	701	PEE	2	0
69	N4	503	CDL	4	0
69	Qb	501	CDL	3	0
69	B5	202	CDL	3	0

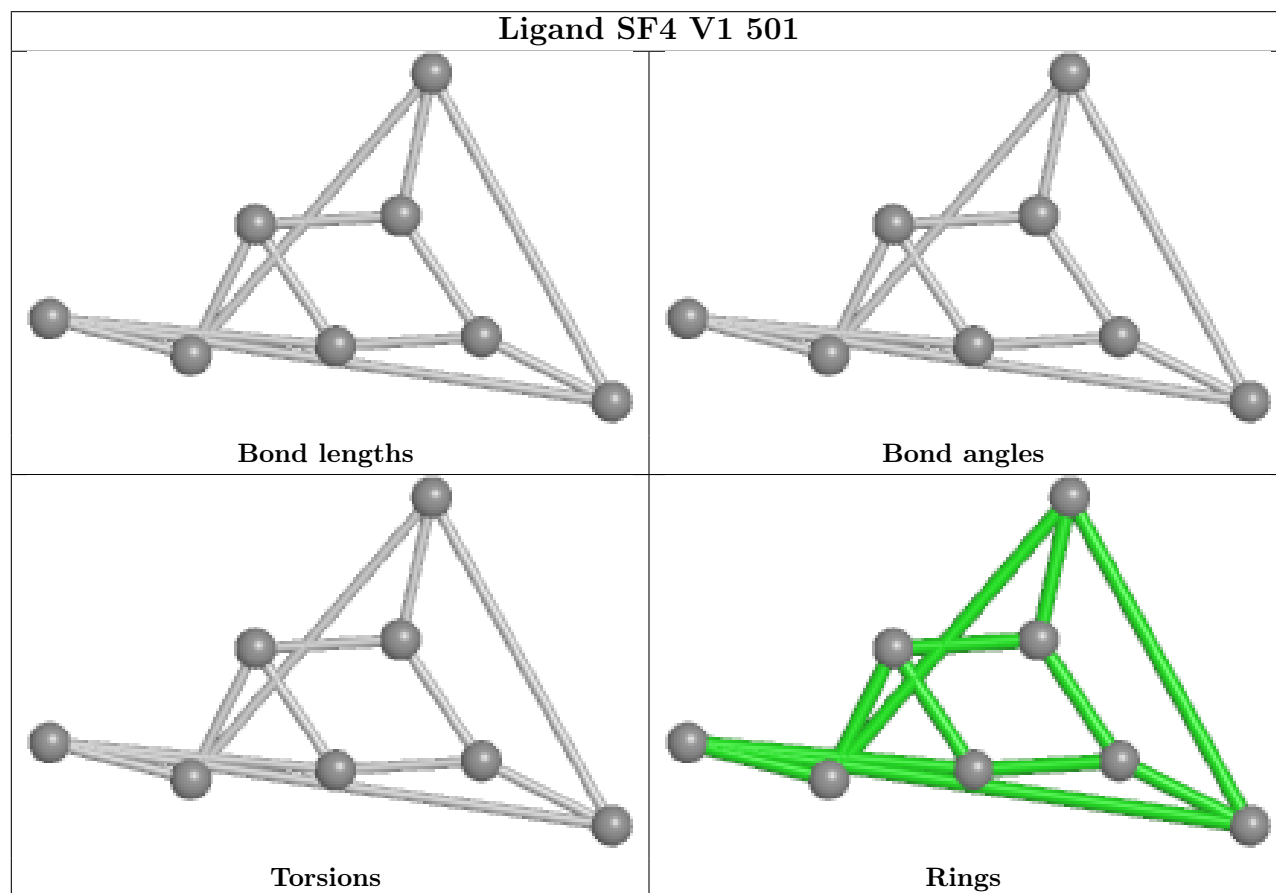
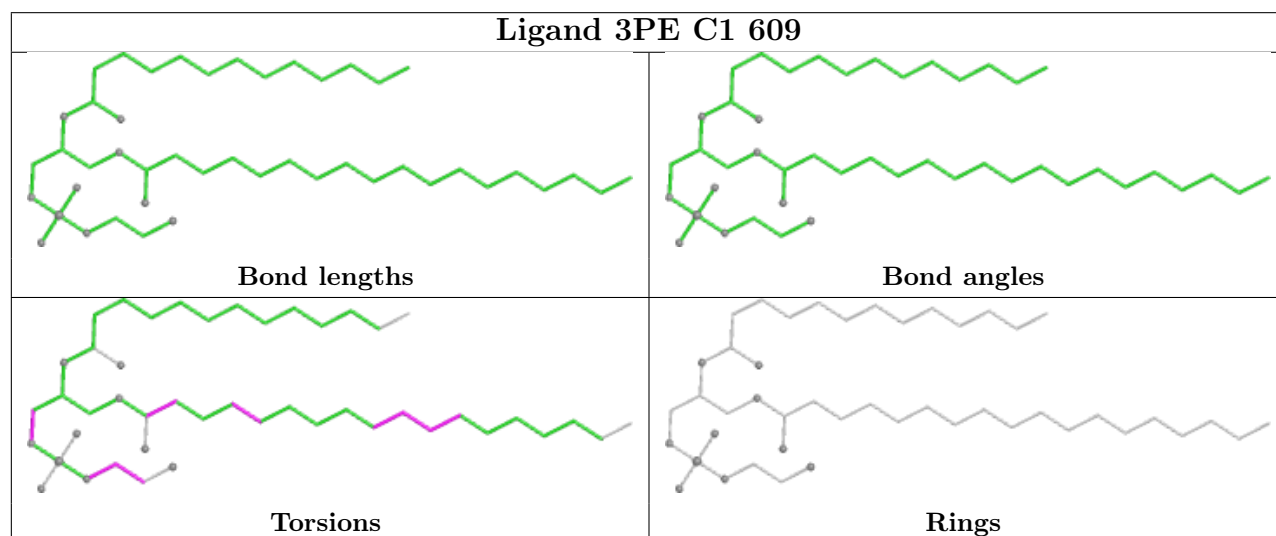
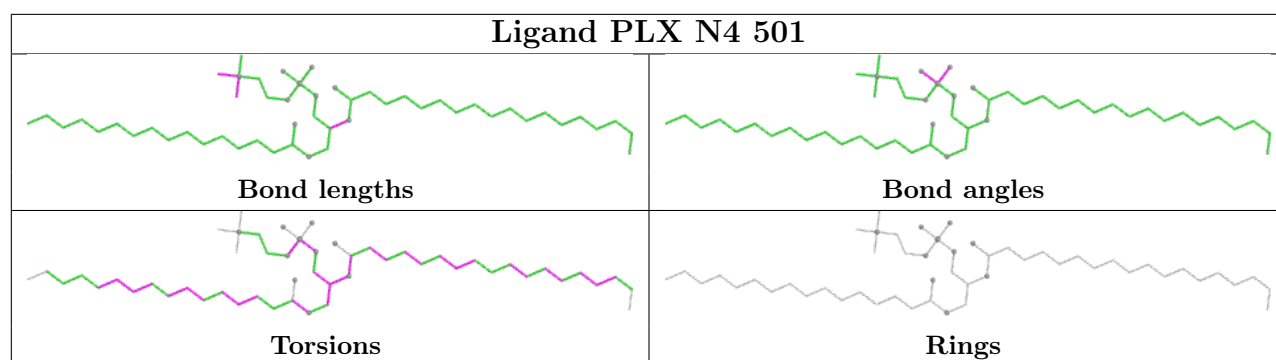
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

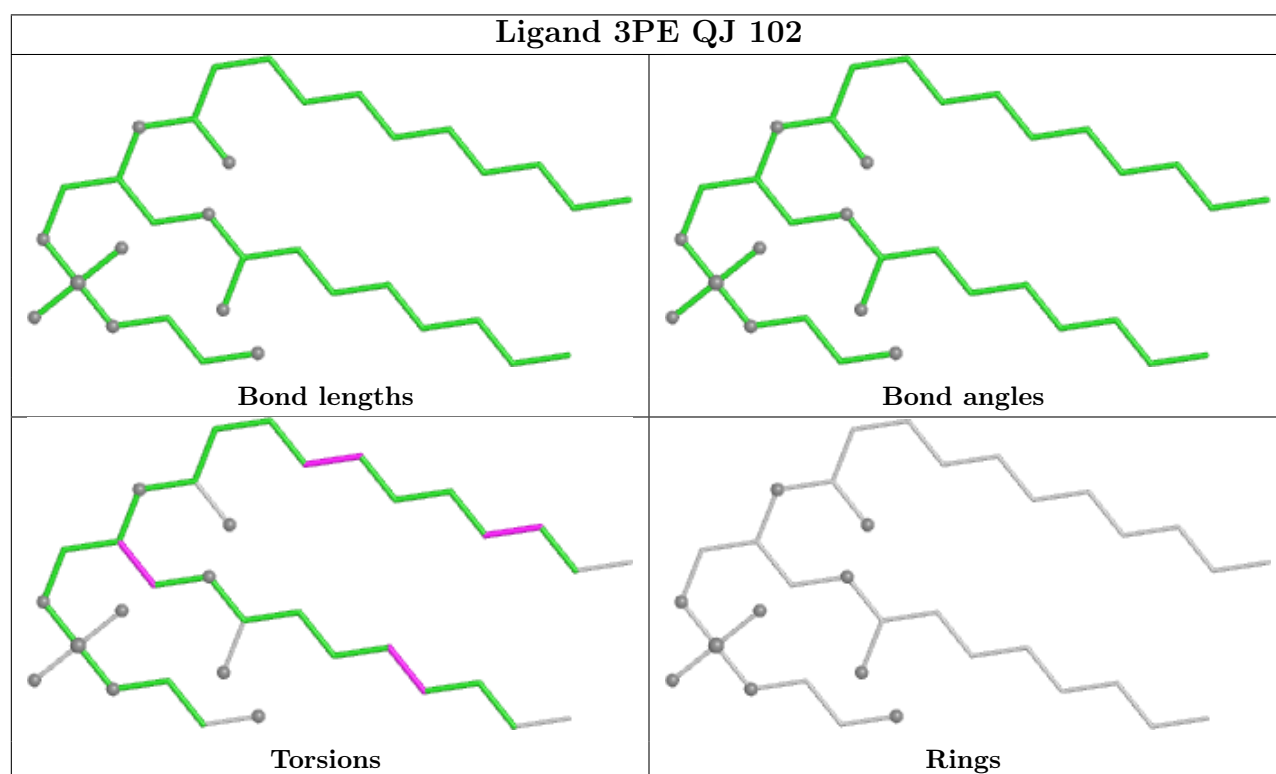
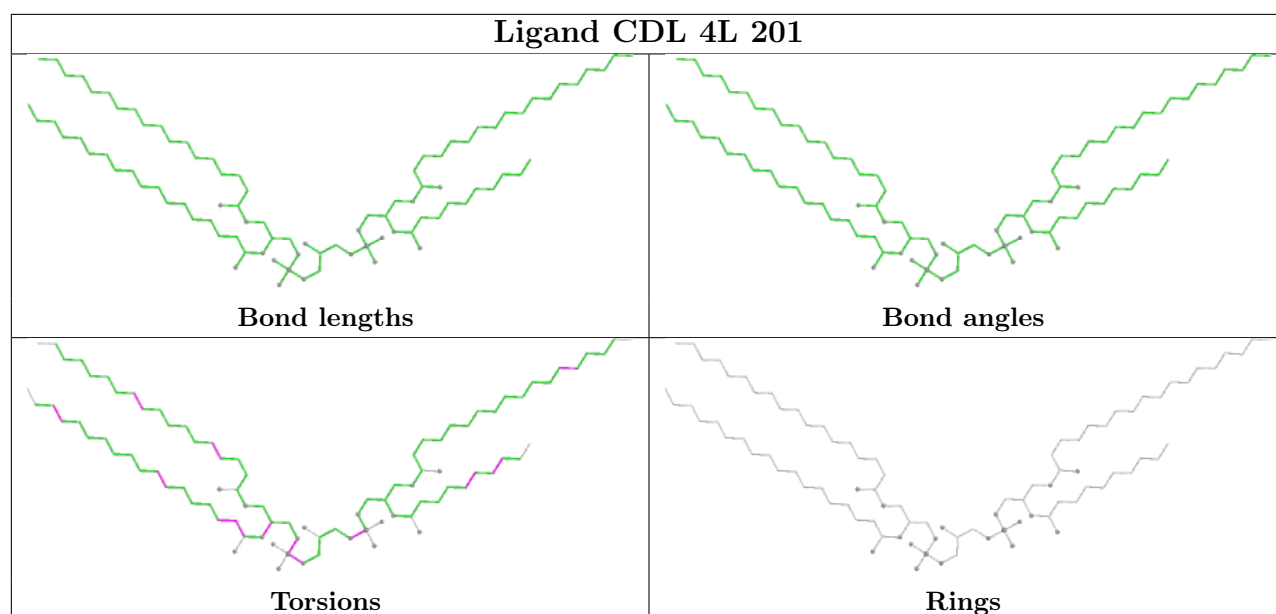
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

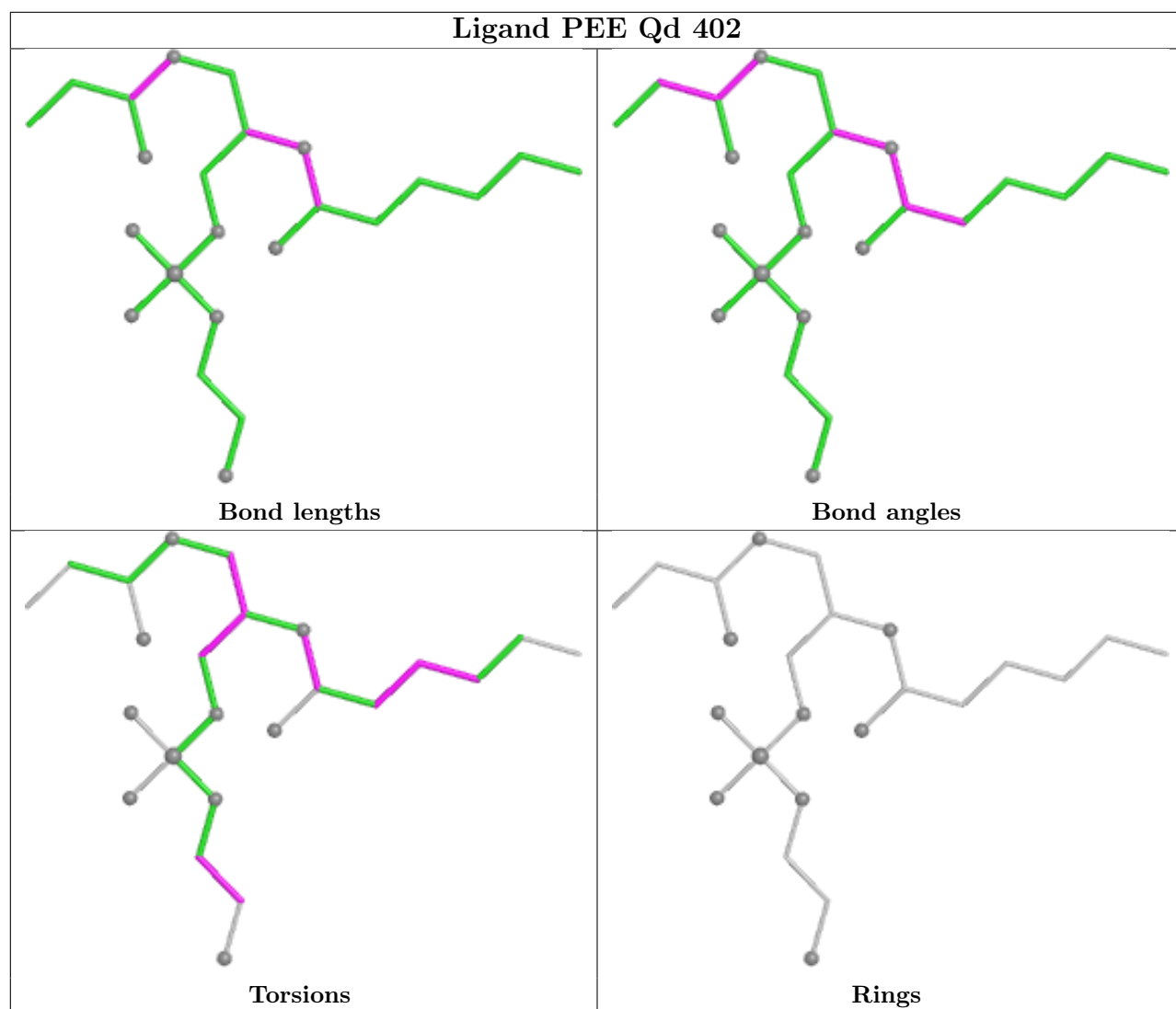
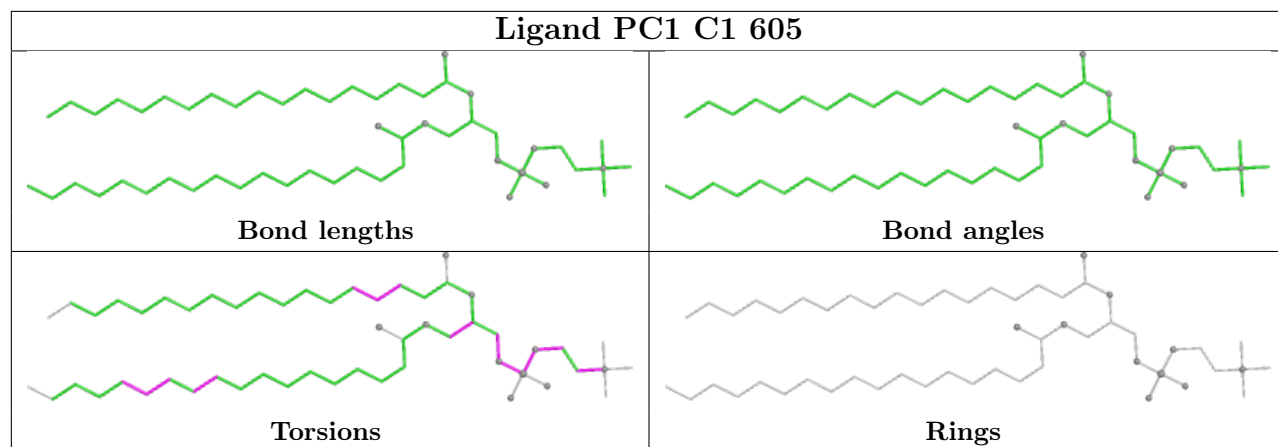


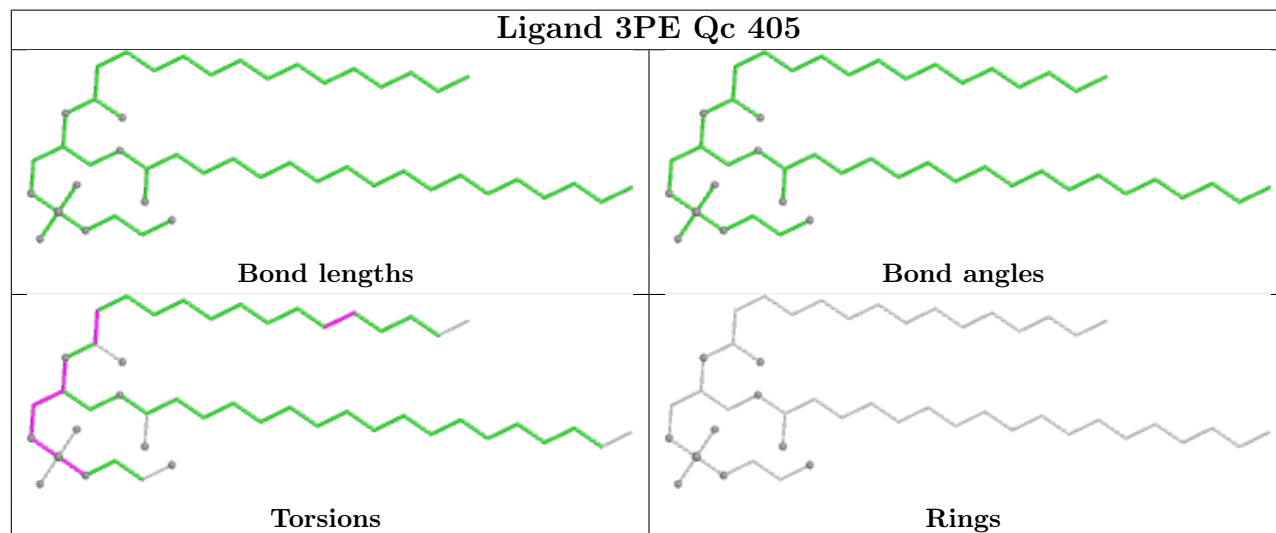
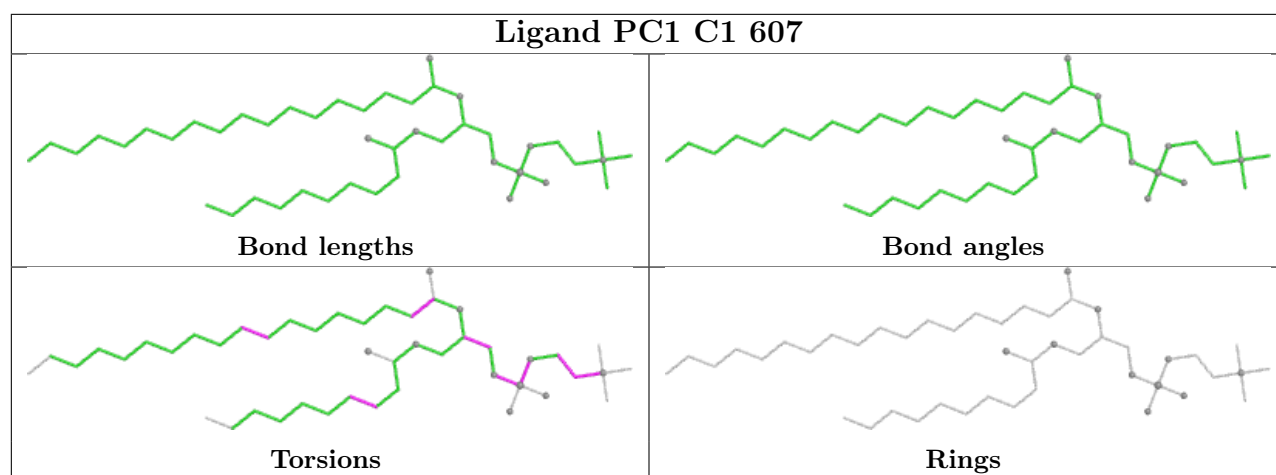
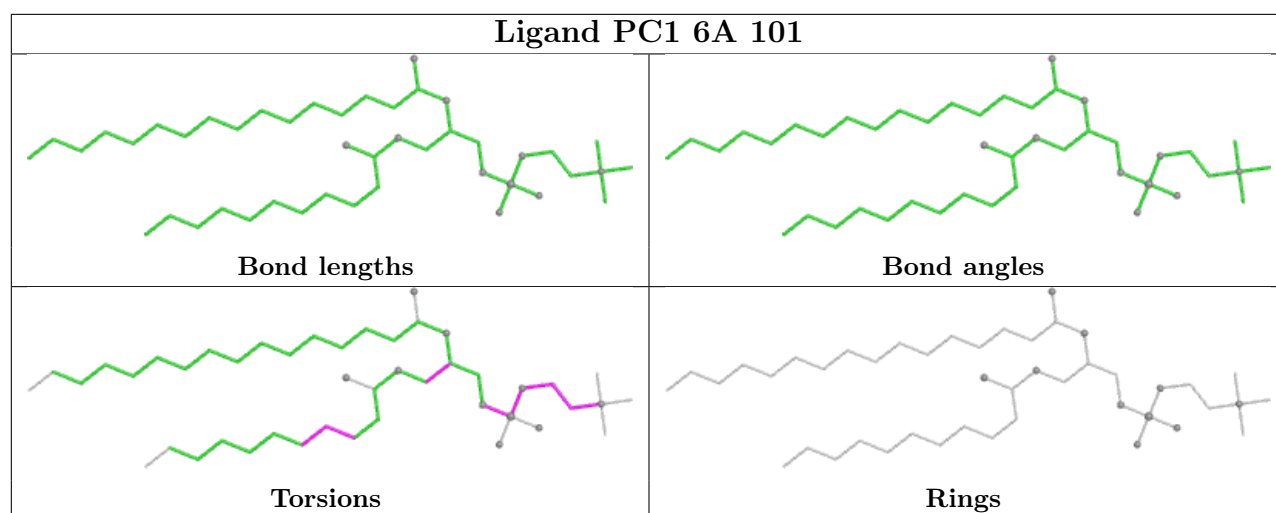


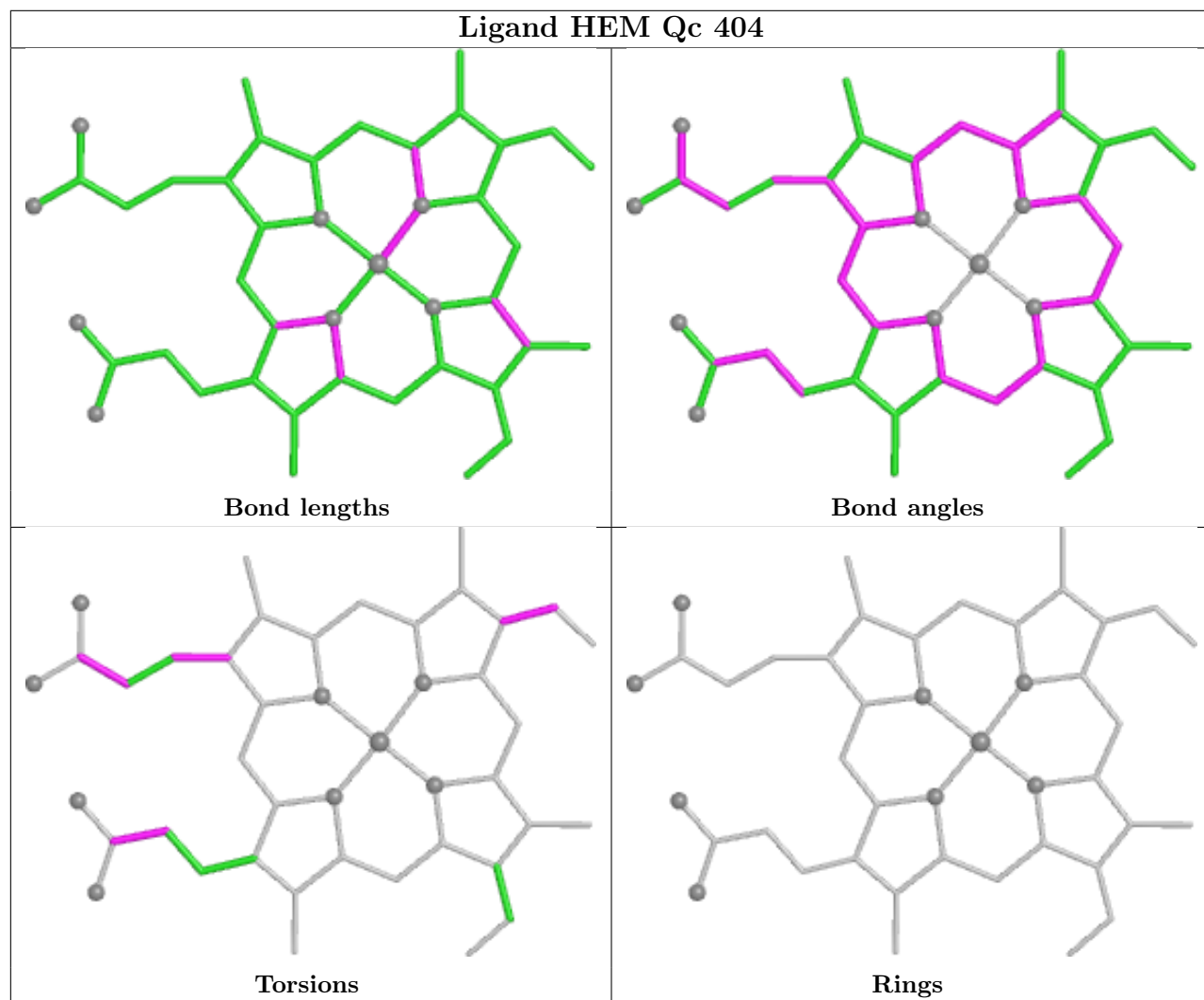
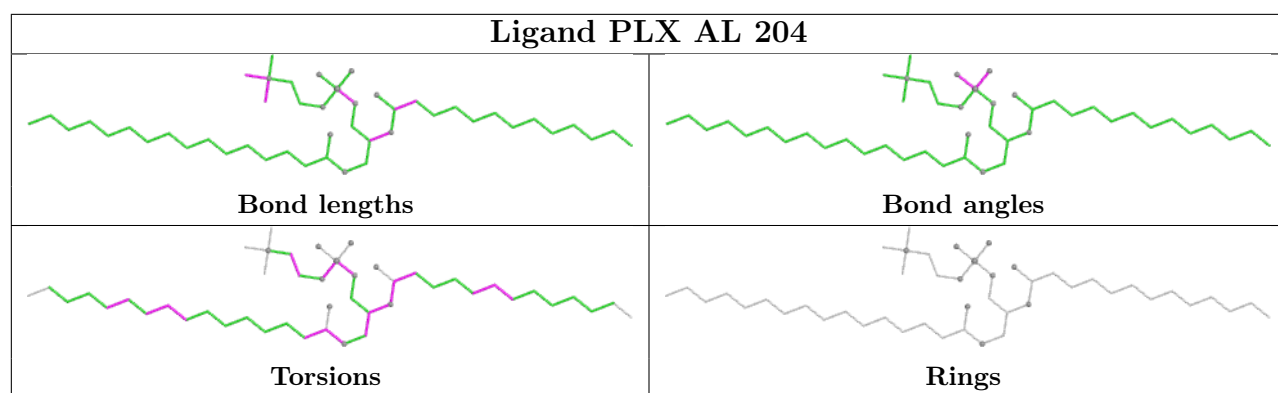


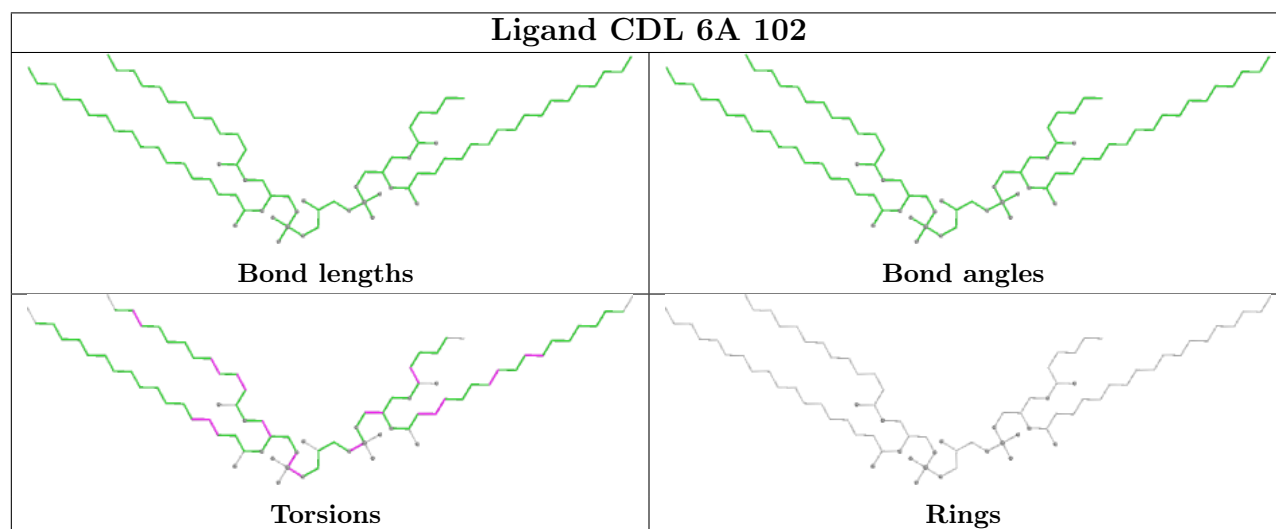
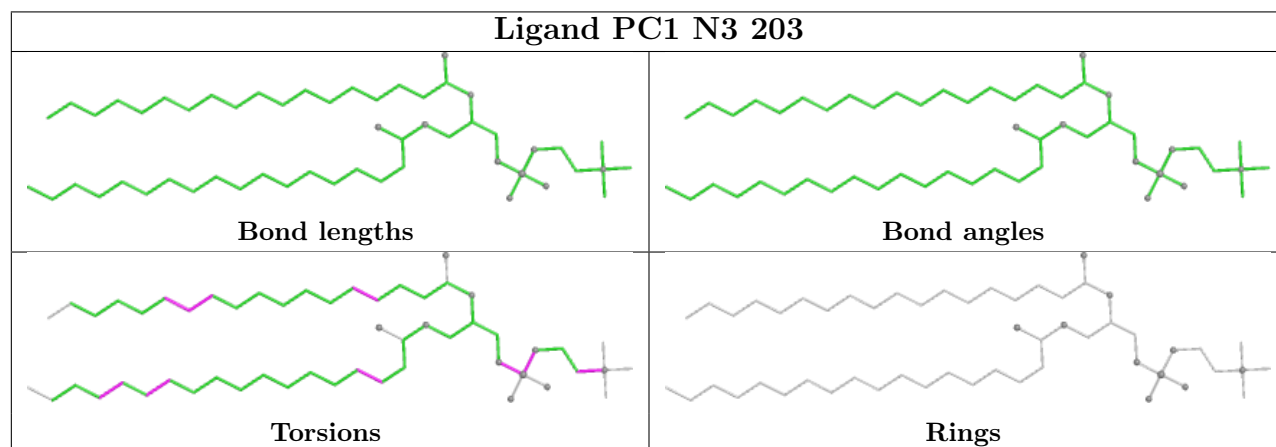
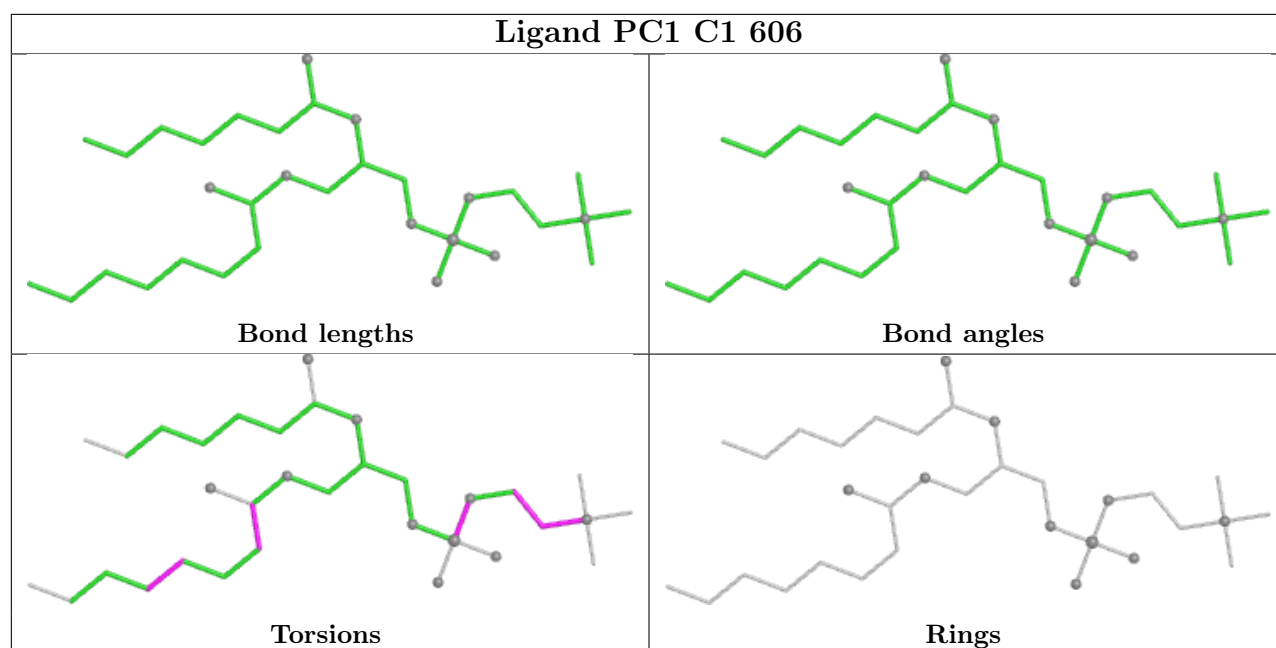




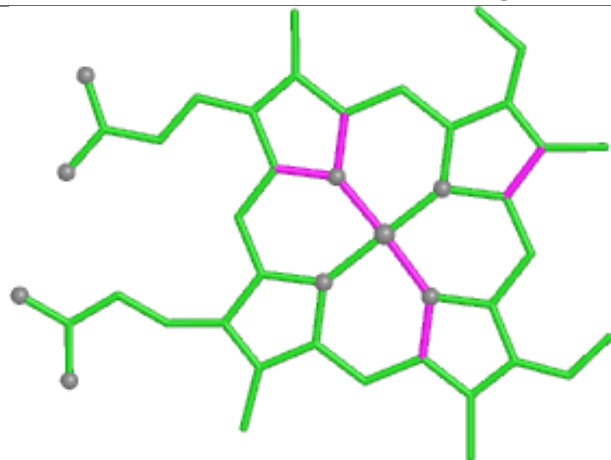




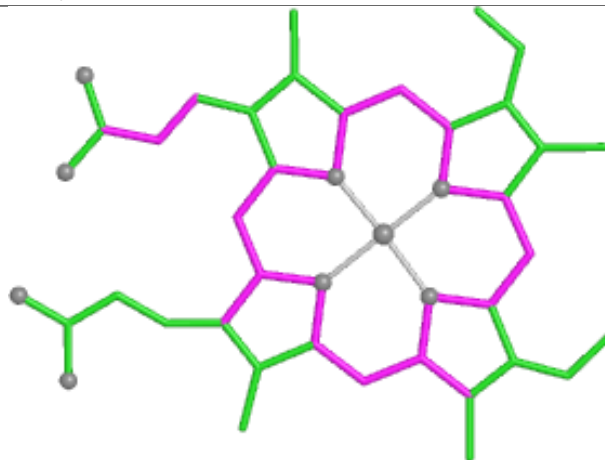




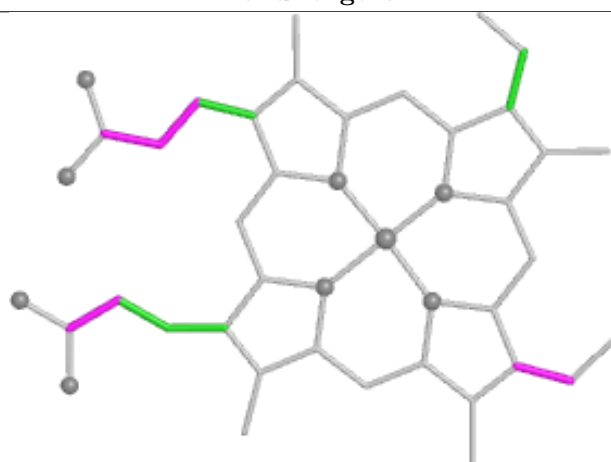
Ligand HEM QC 401



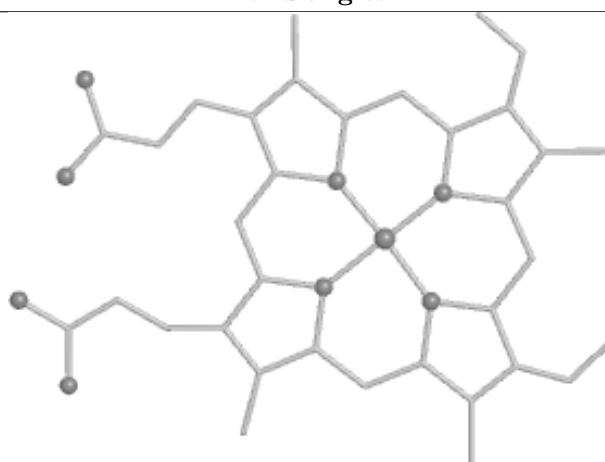
Bond lengths



Bond angles

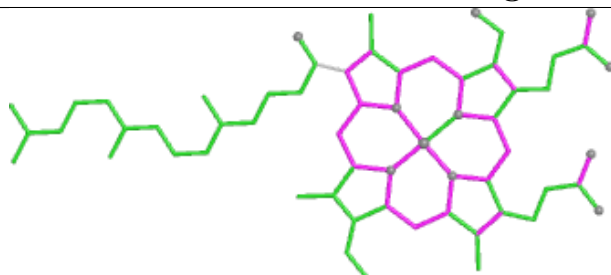


Torsions

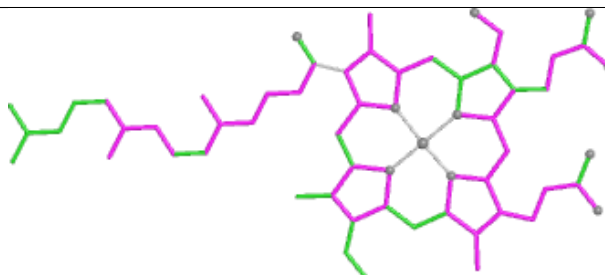


Rings

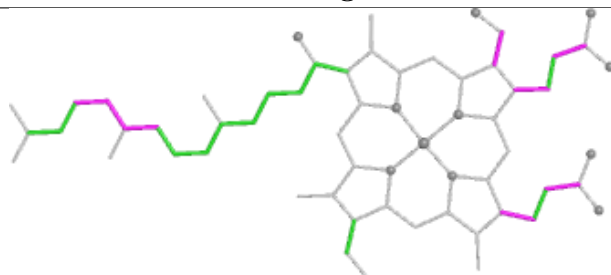
Ligand HEA C1 602



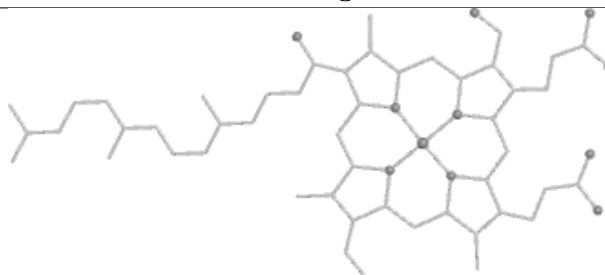
Bond lengths



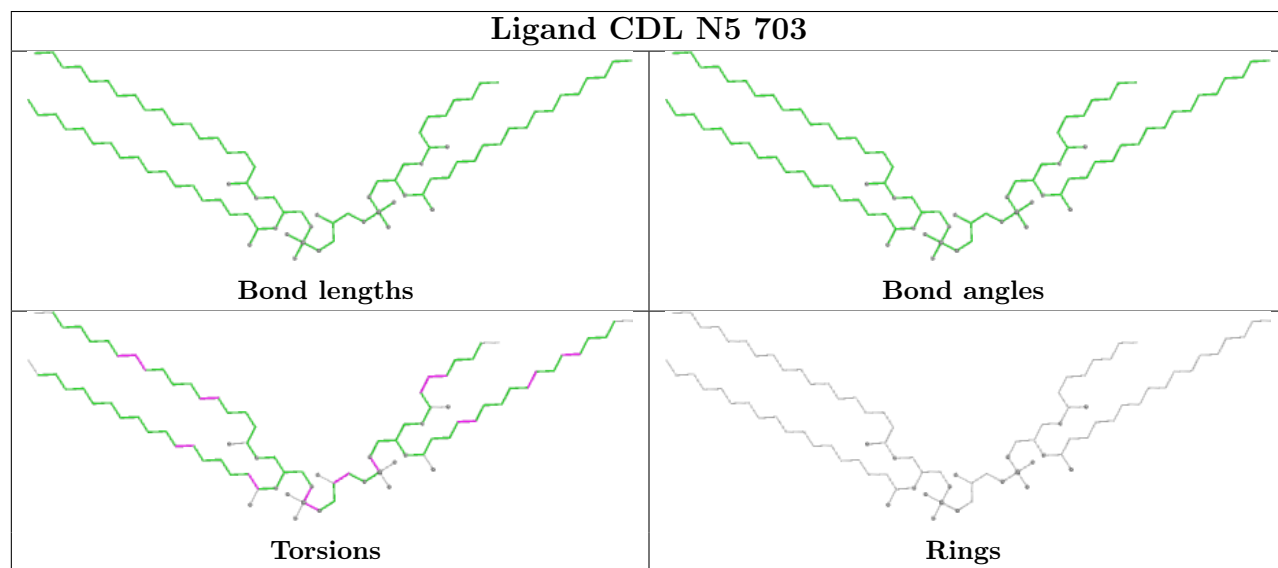
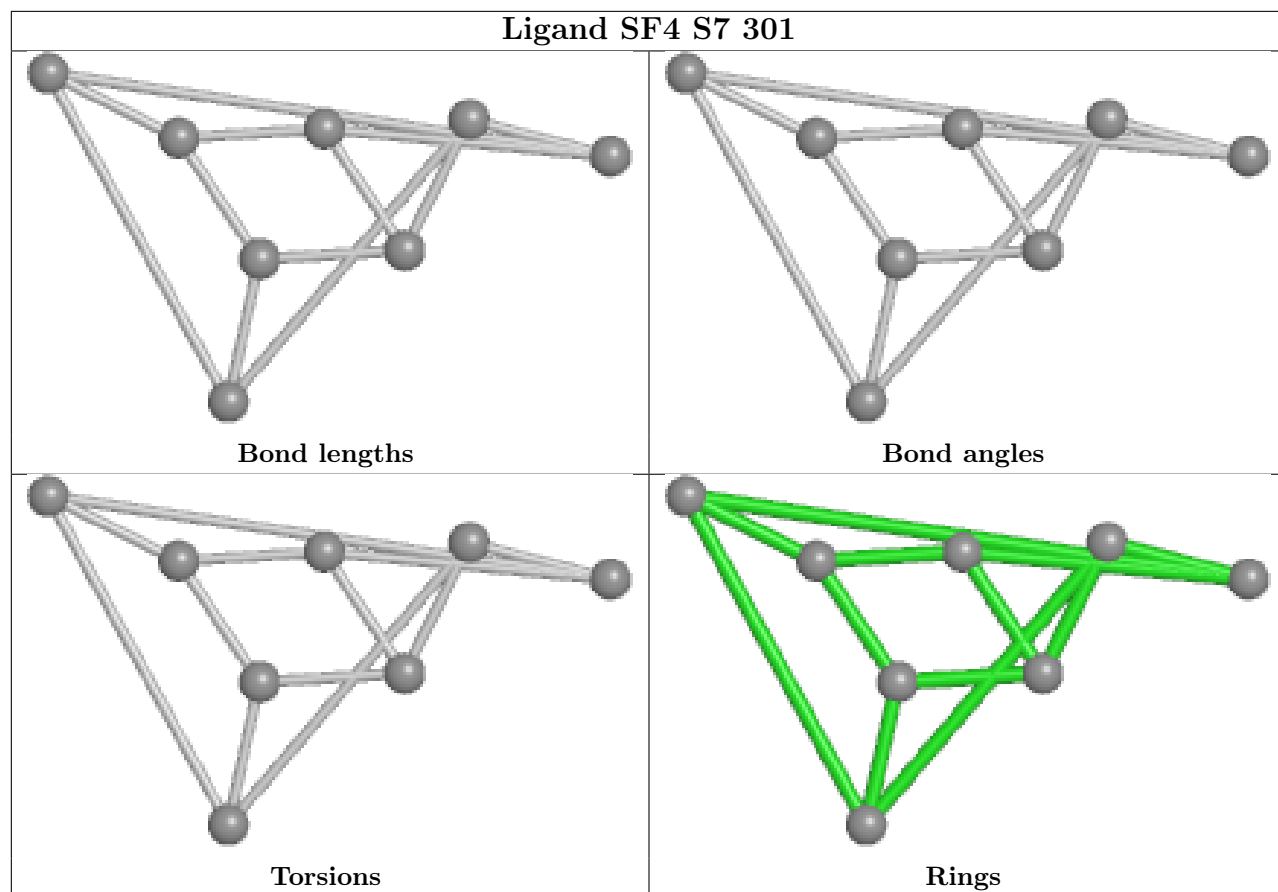
Bond angles

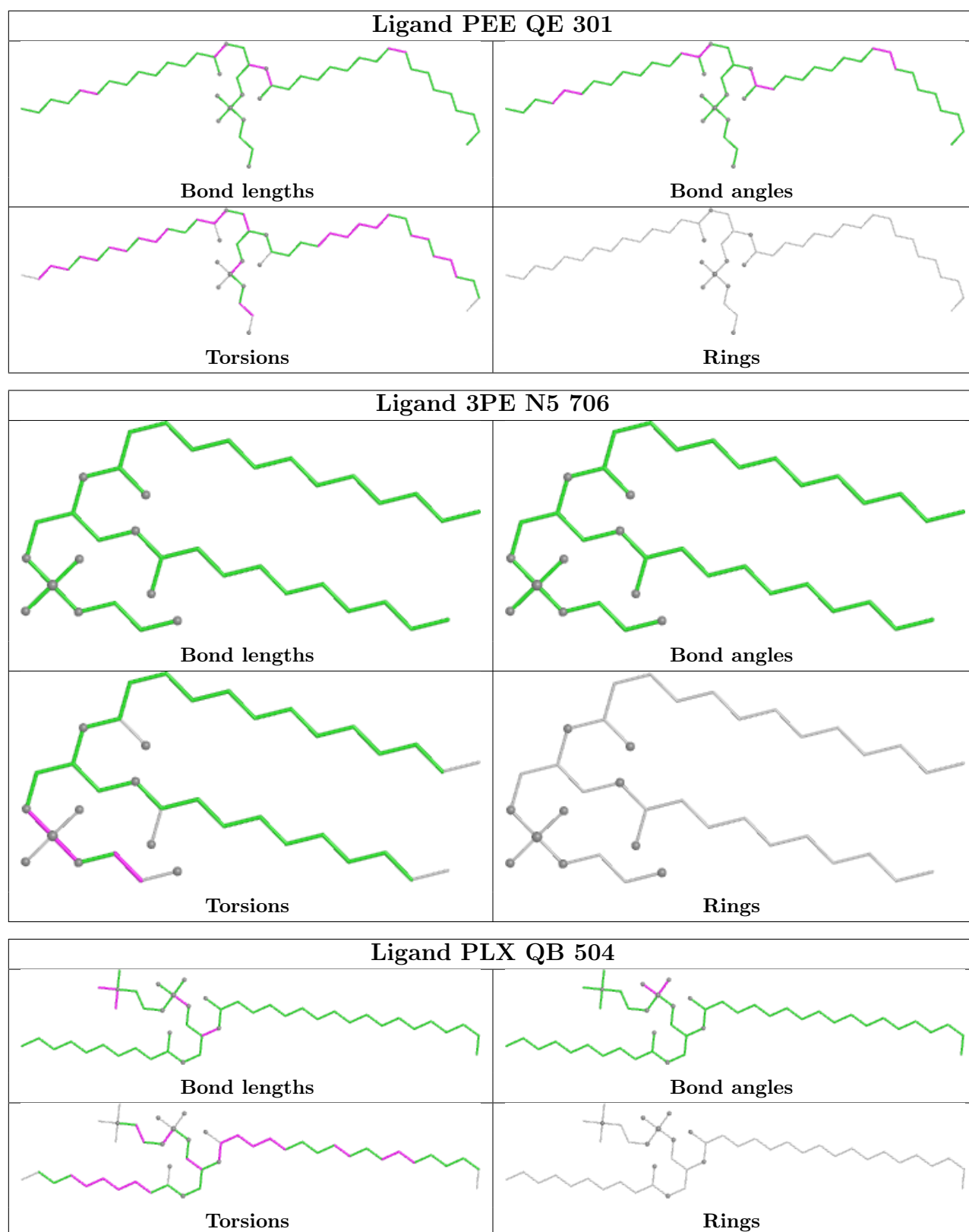


Torsions

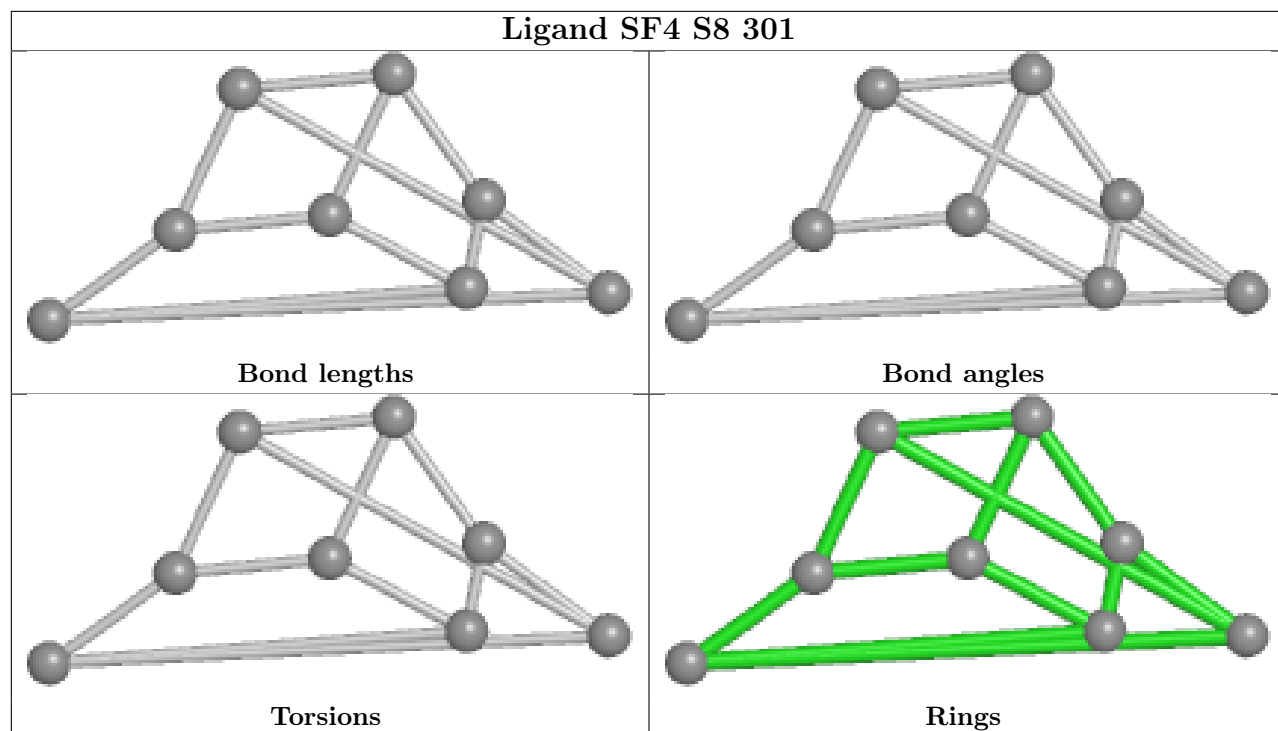


Rings

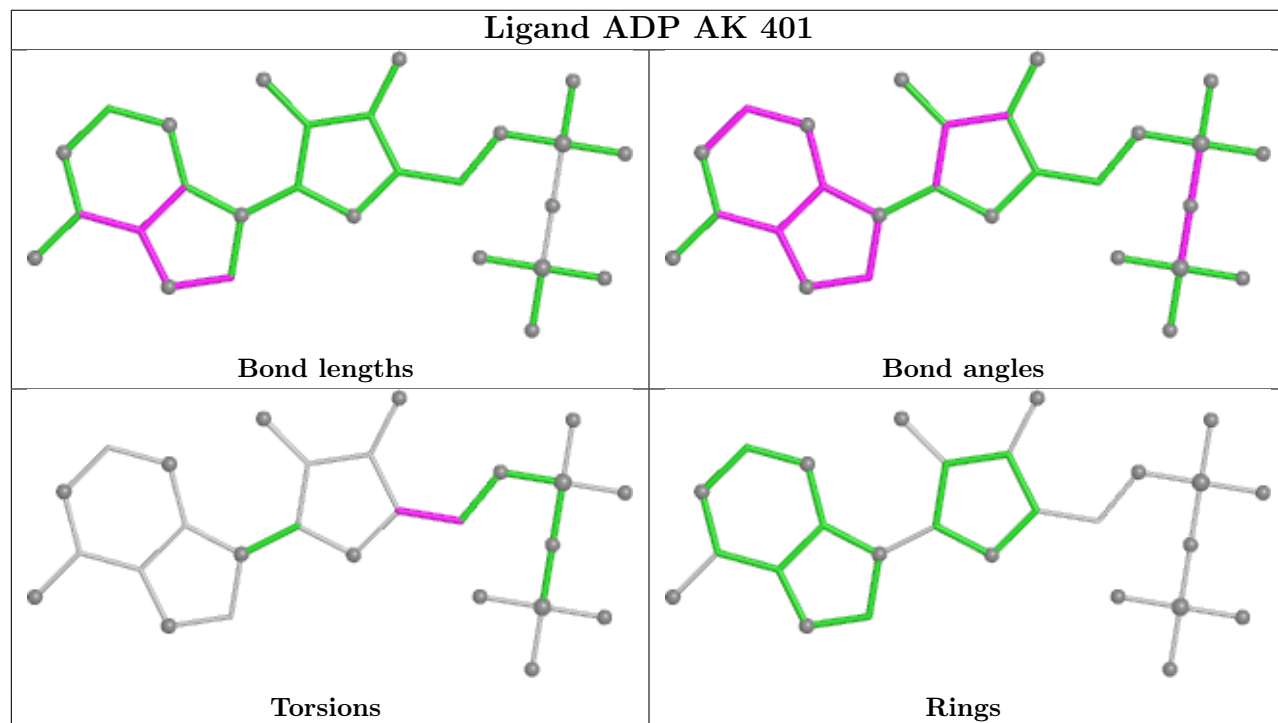


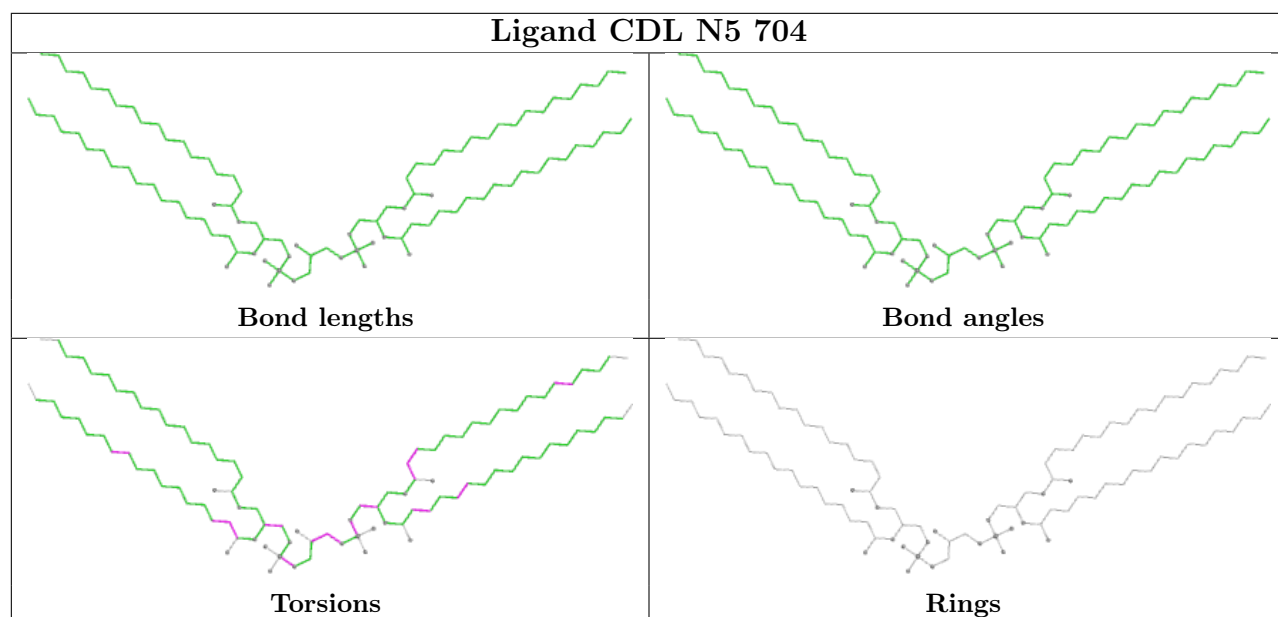
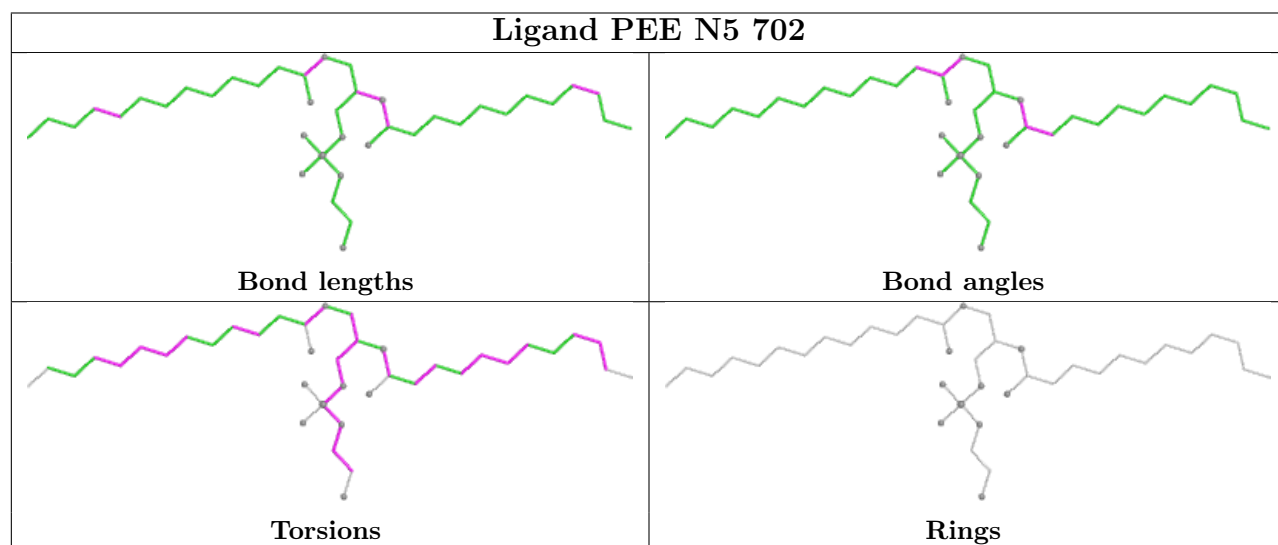
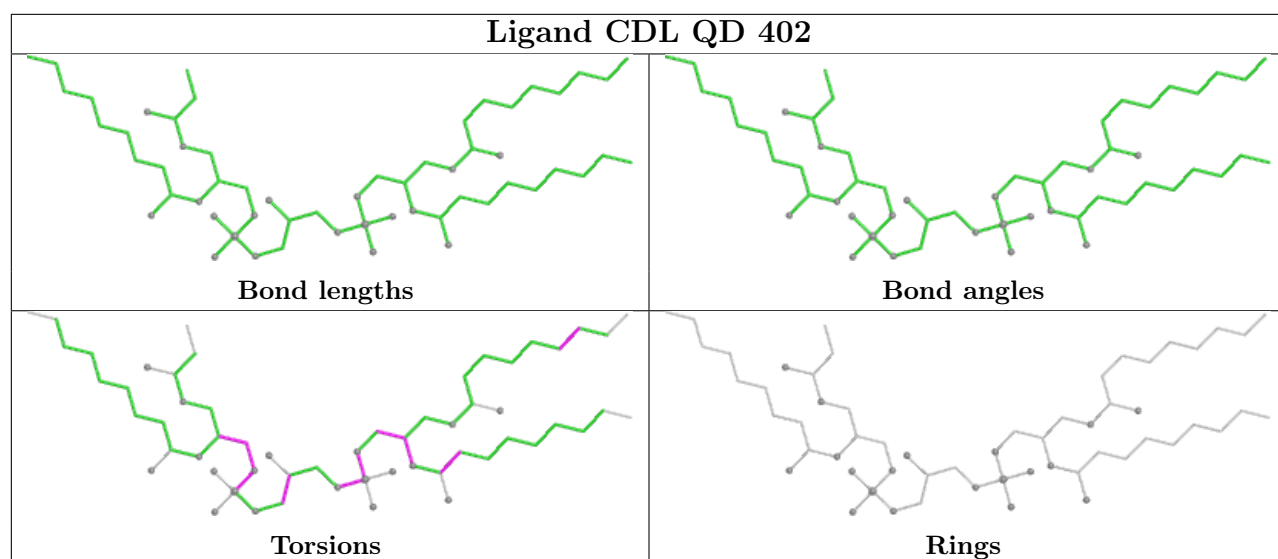


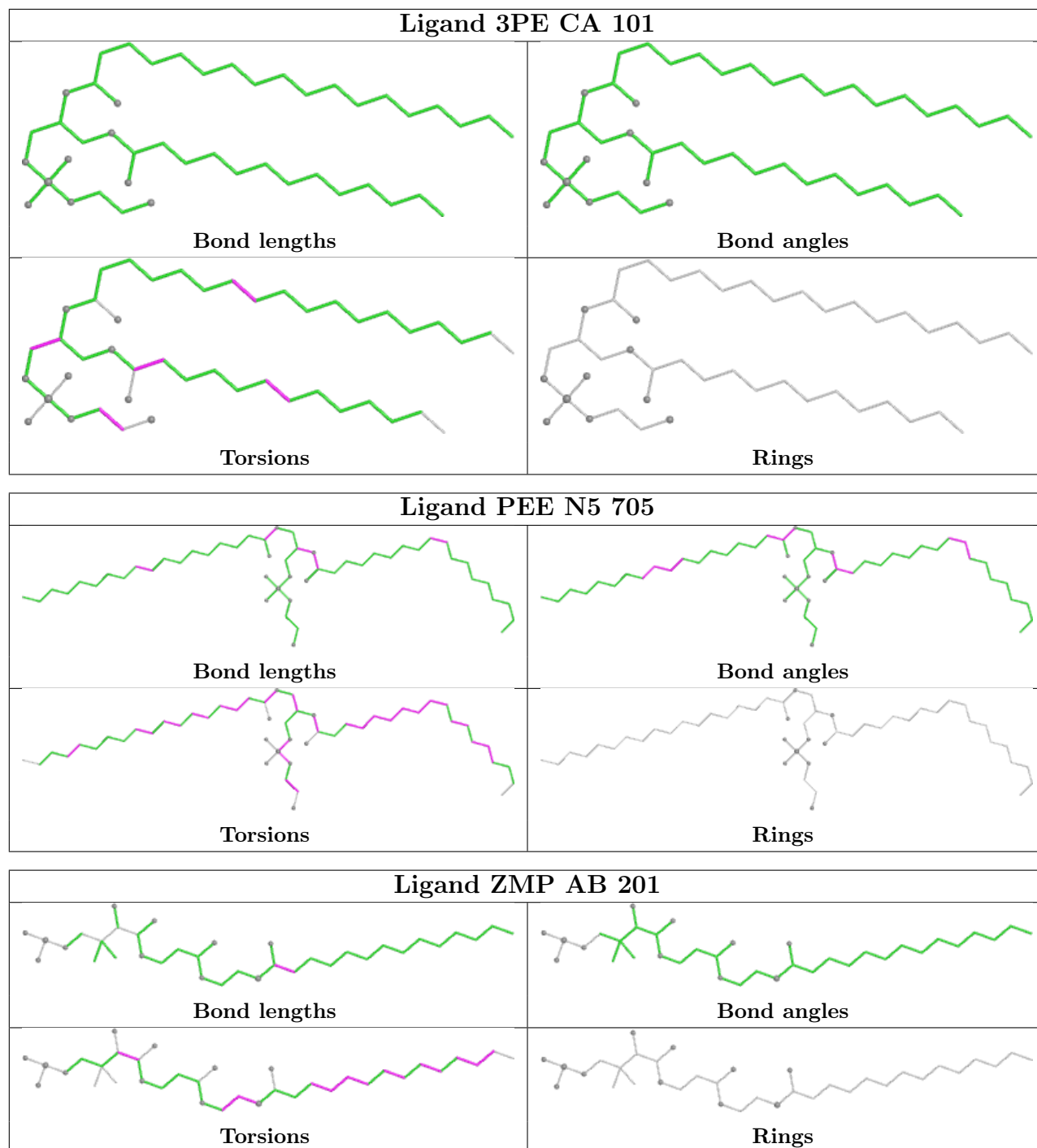
Ligand SF4 S8 301

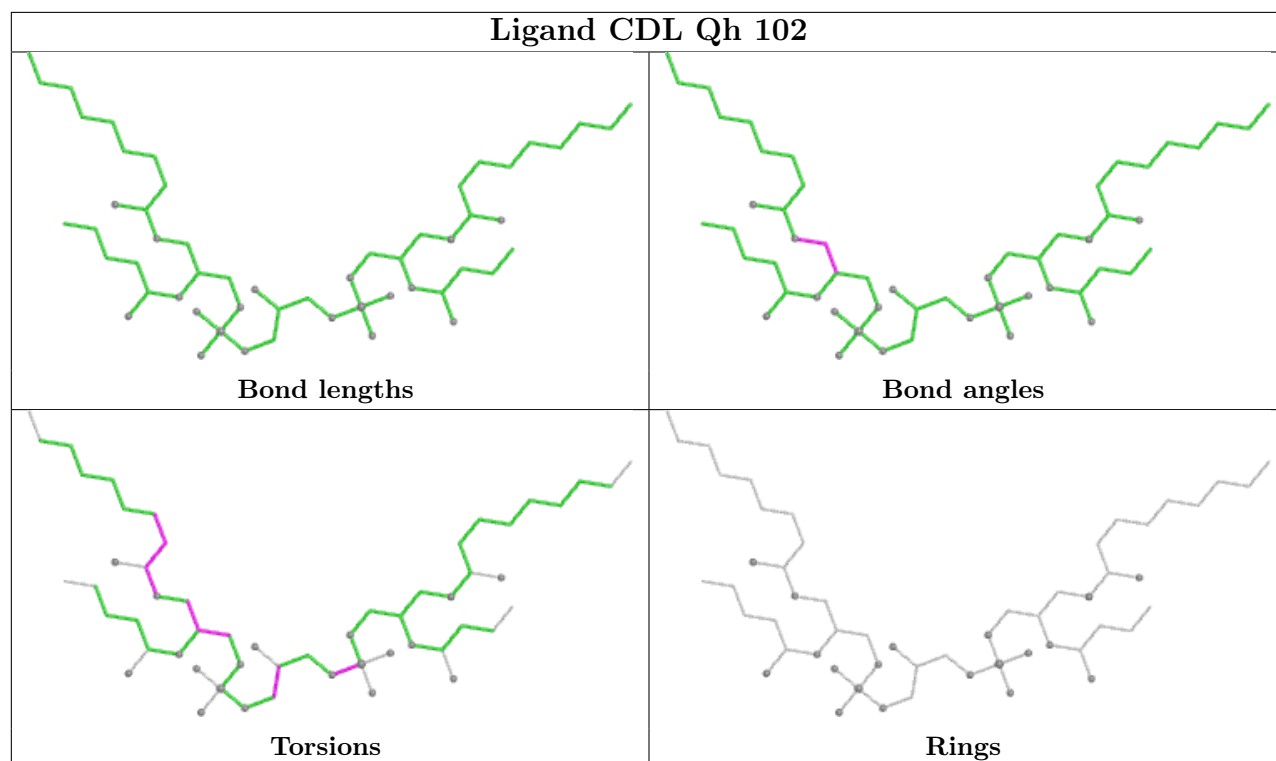
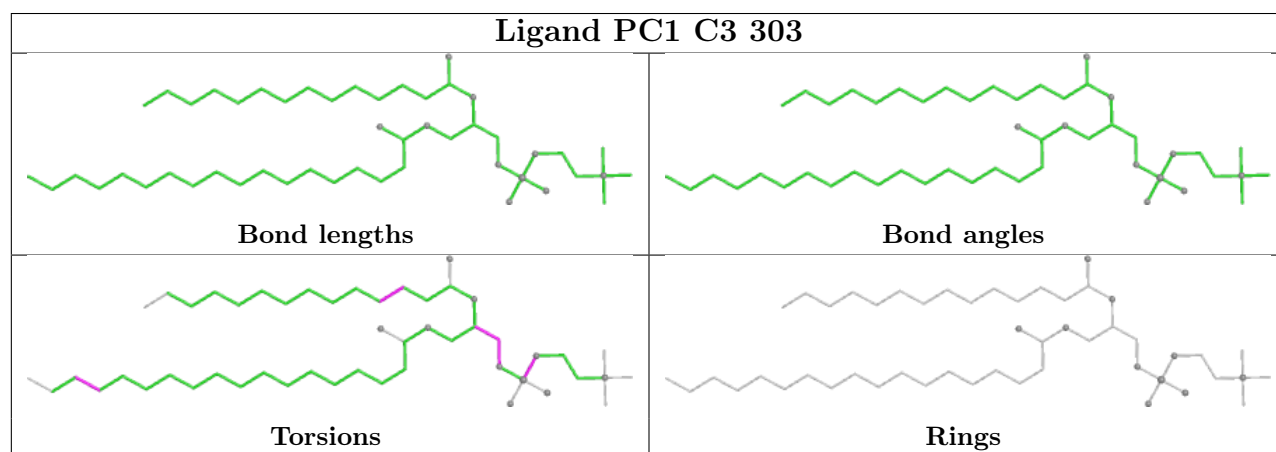
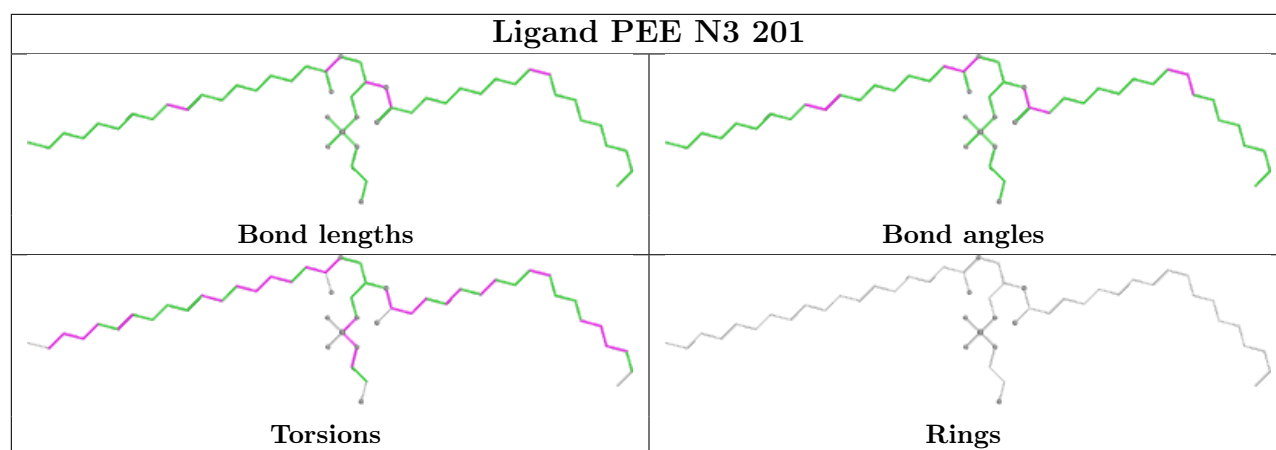


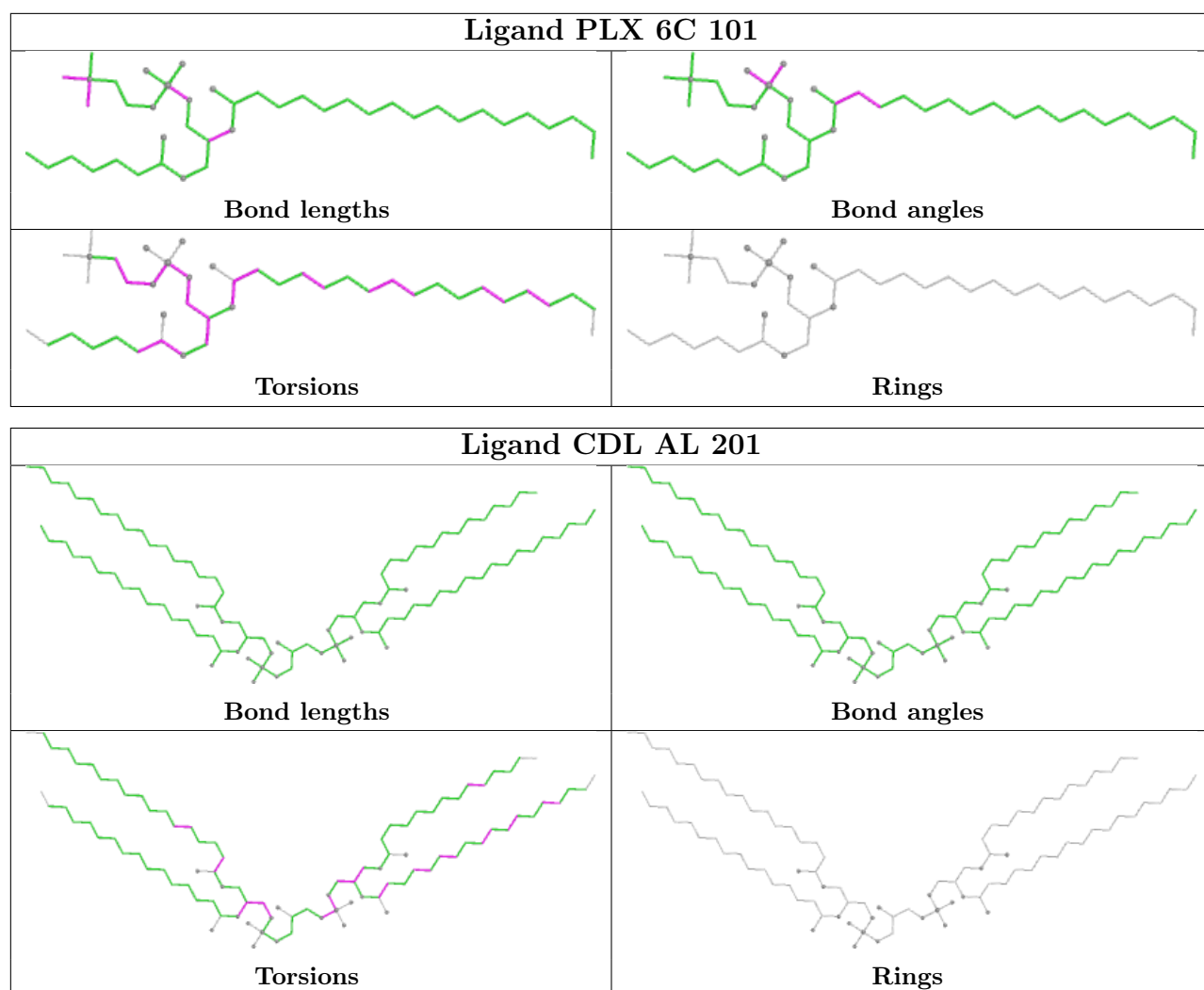
Ligand ADP AK 401

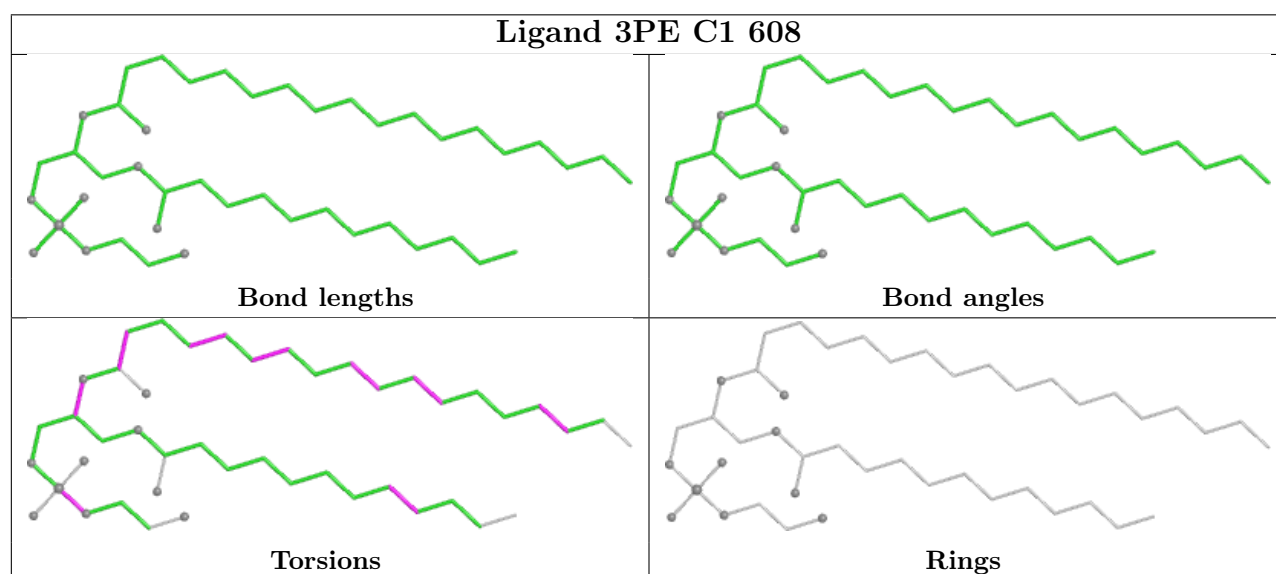
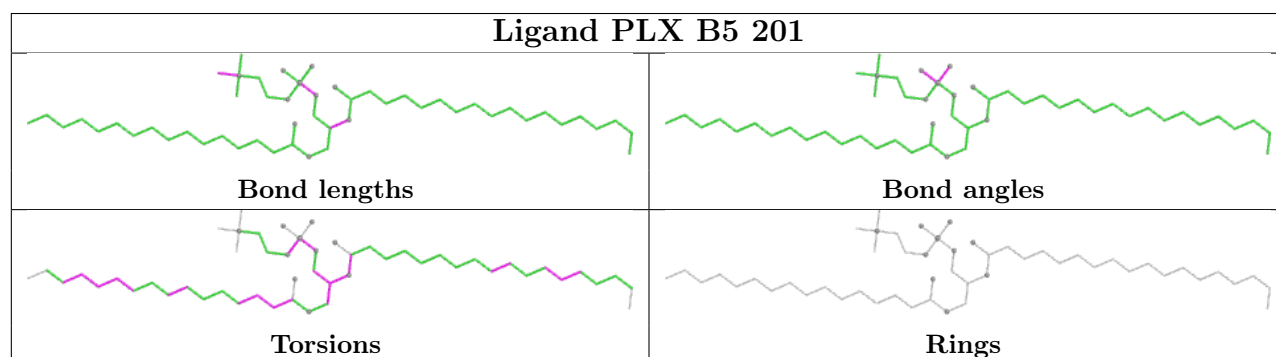
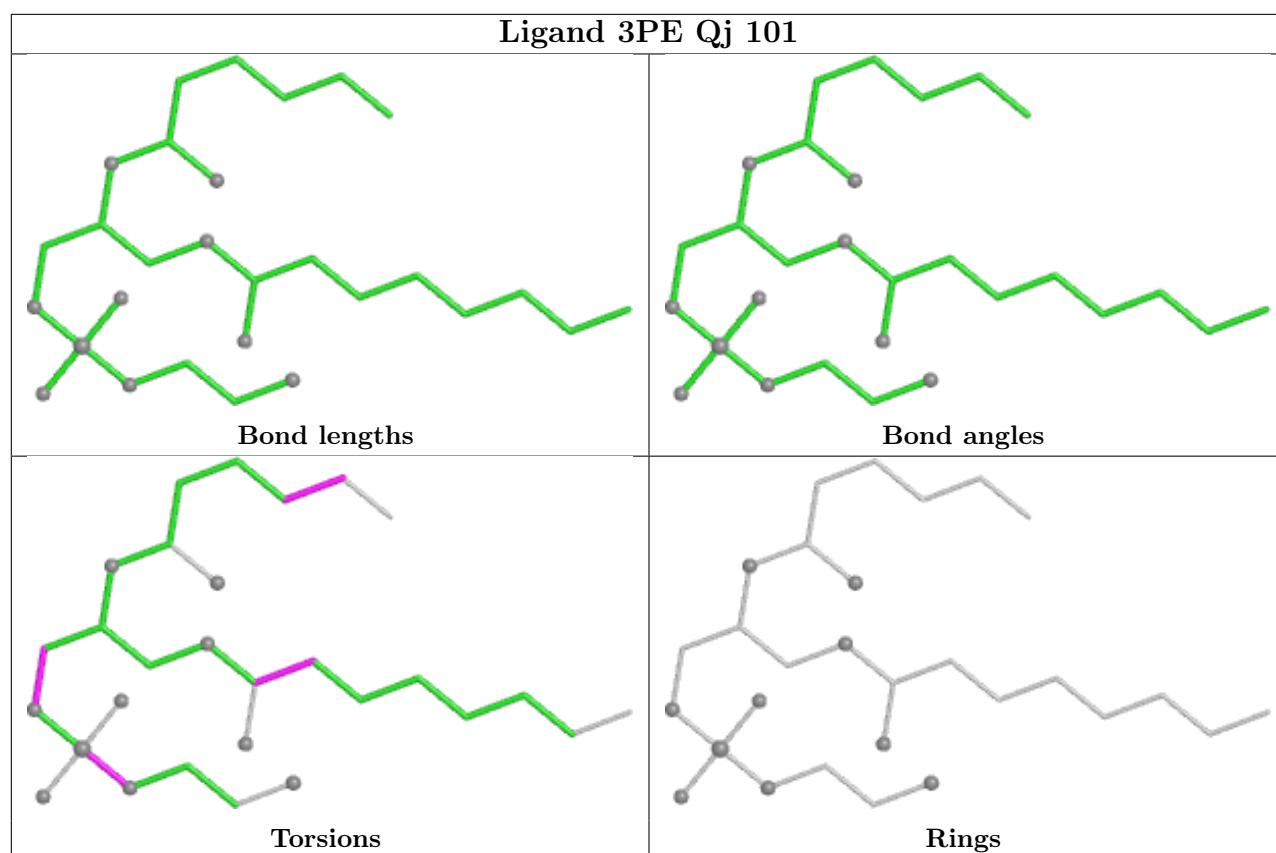


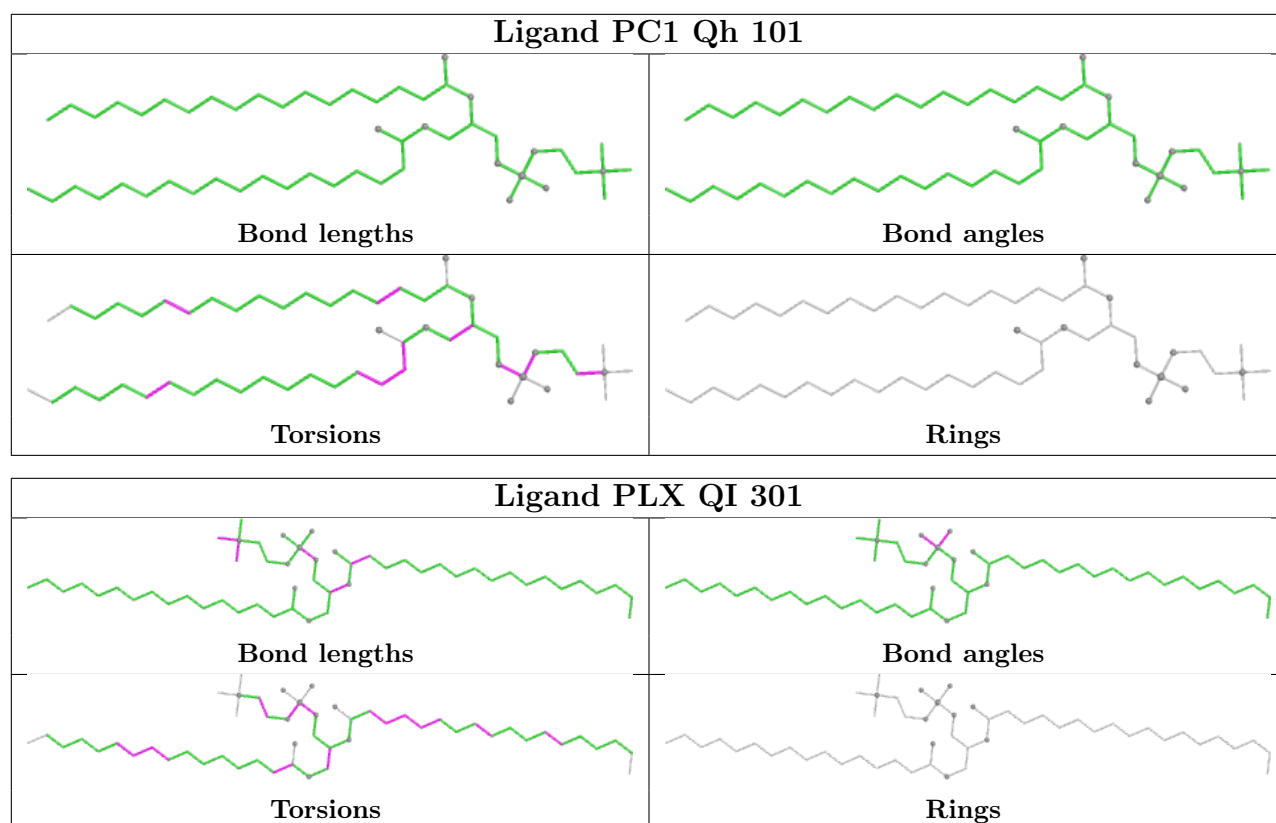


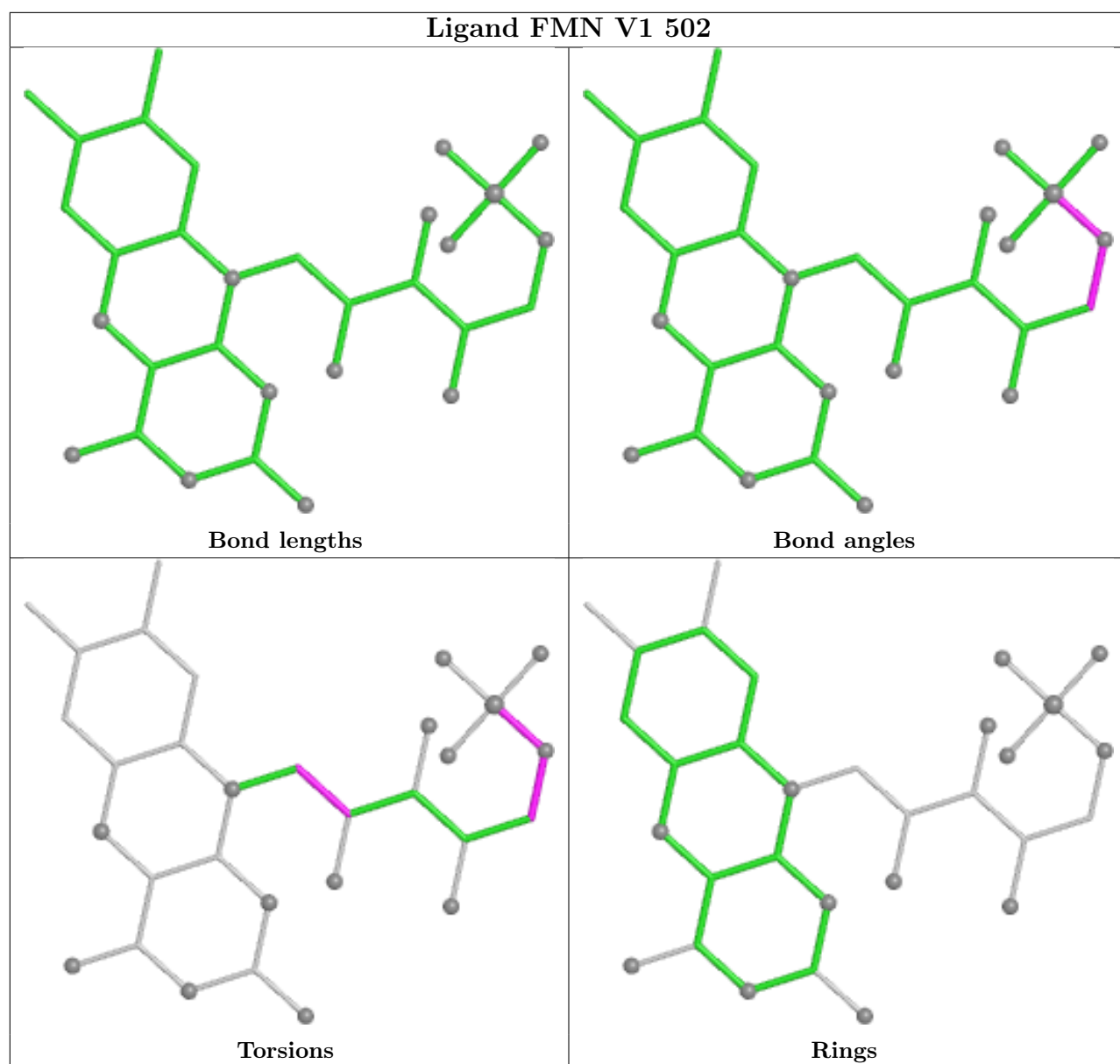




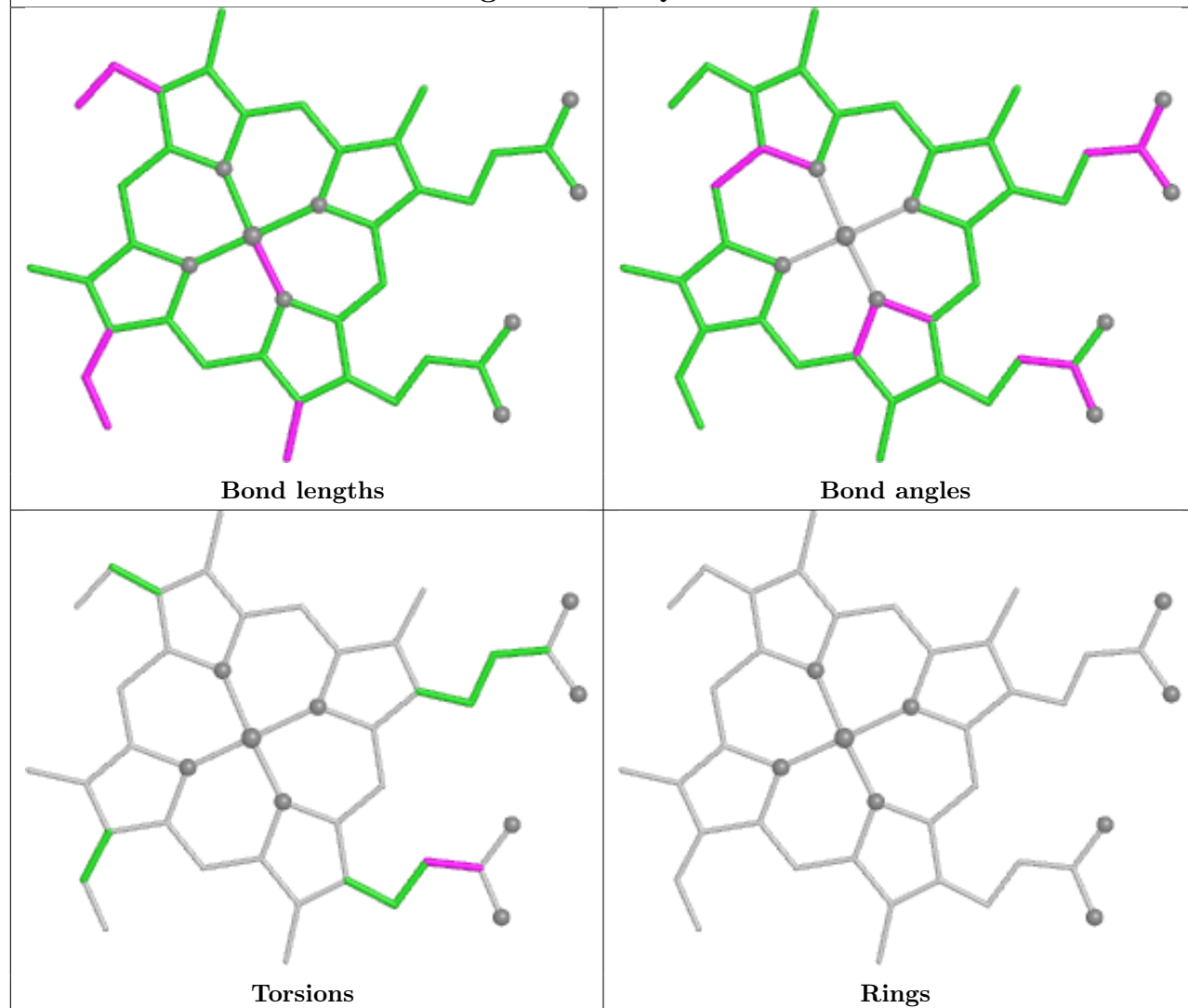




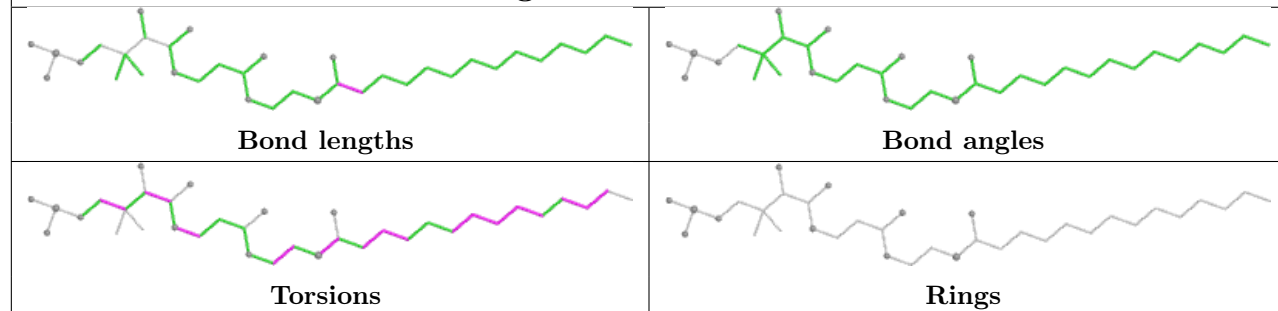


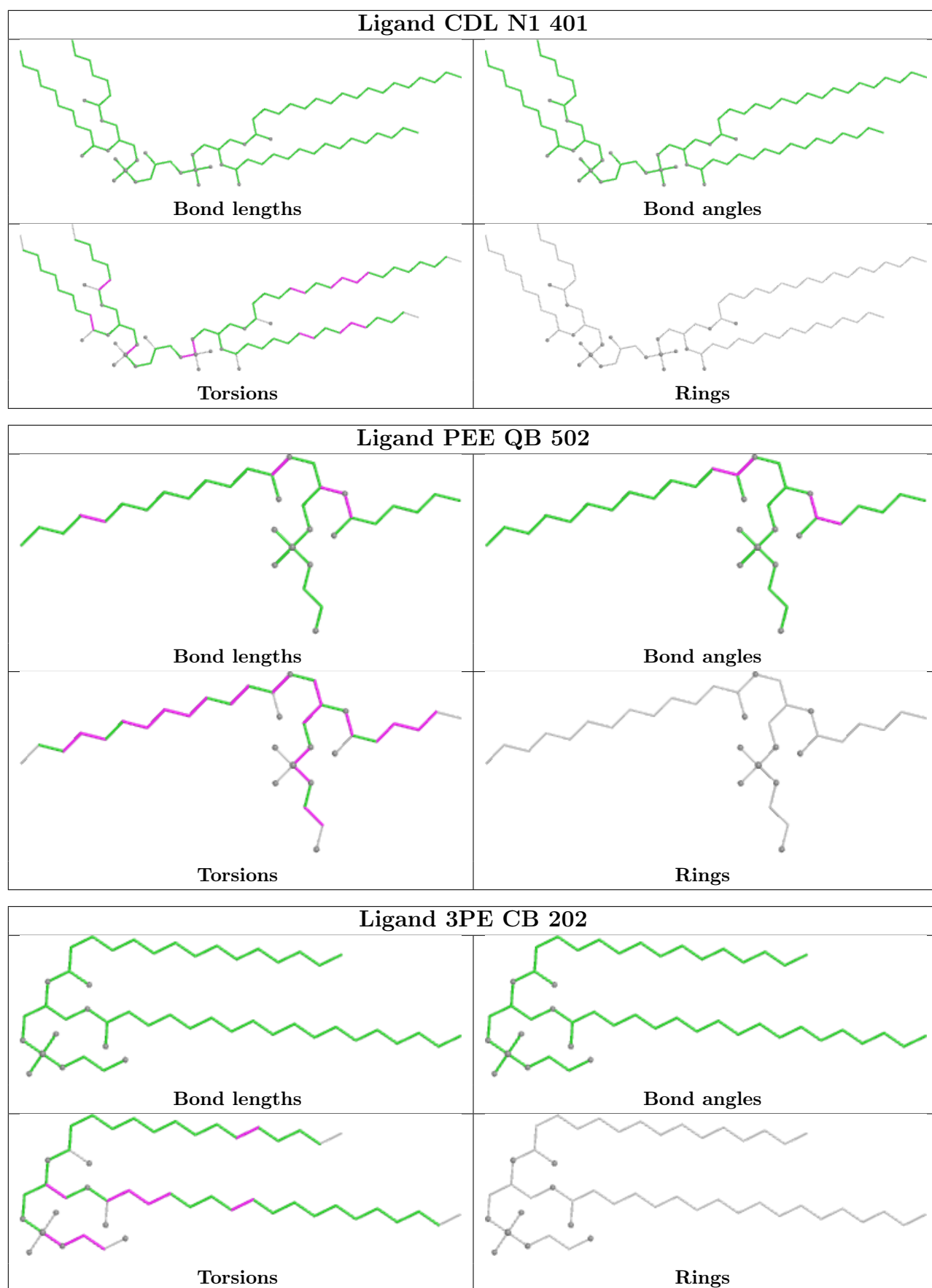


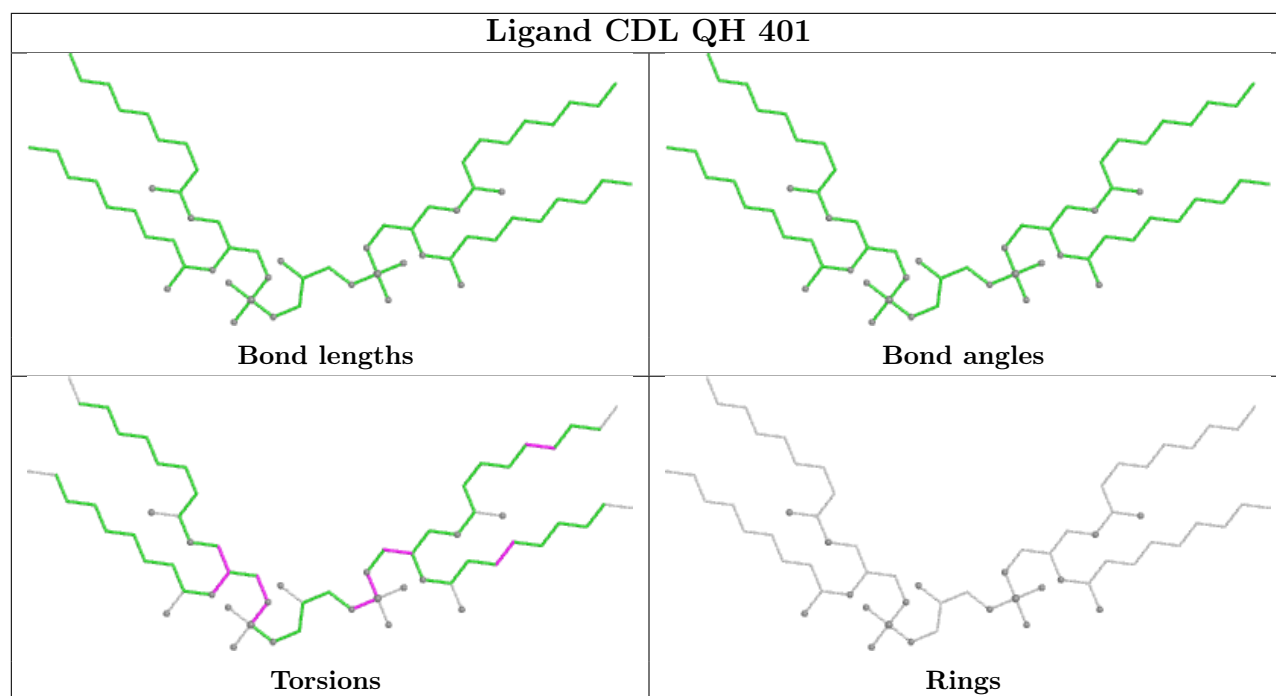
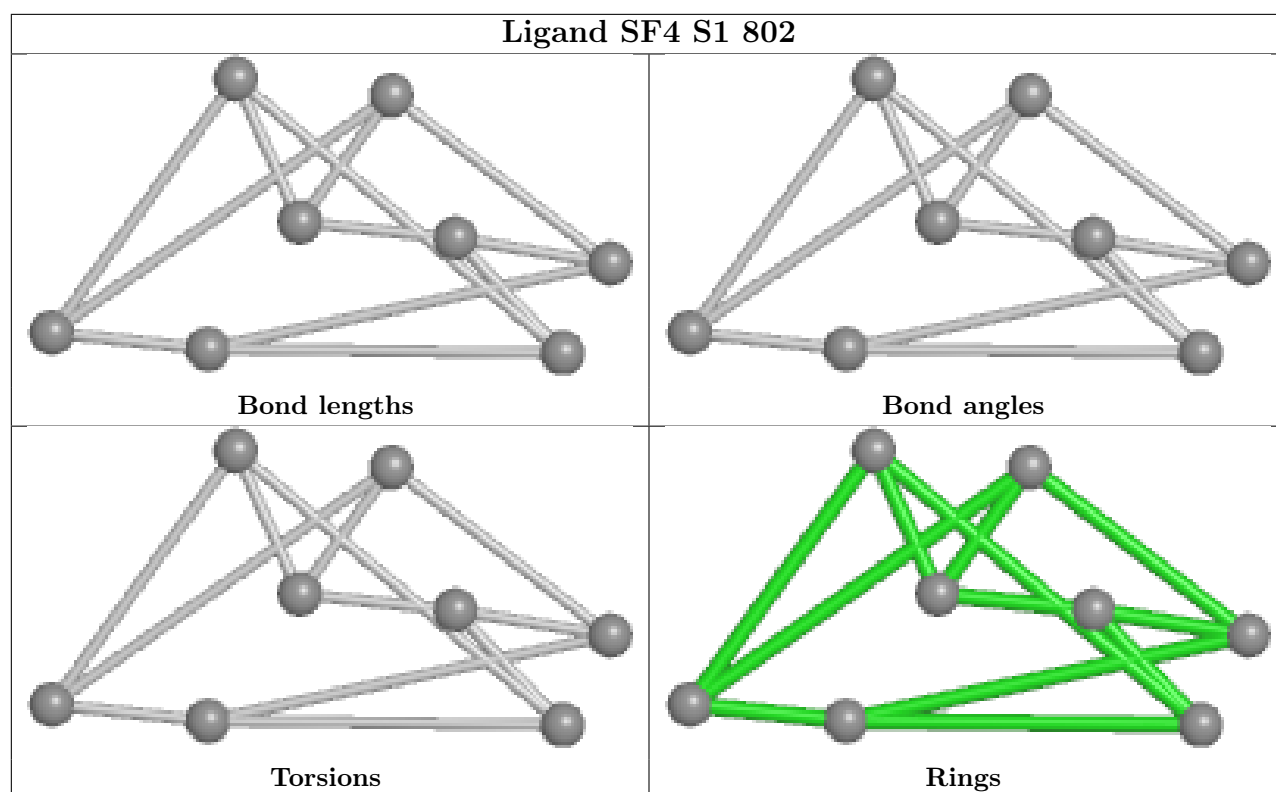
Ligand HEC QD 401

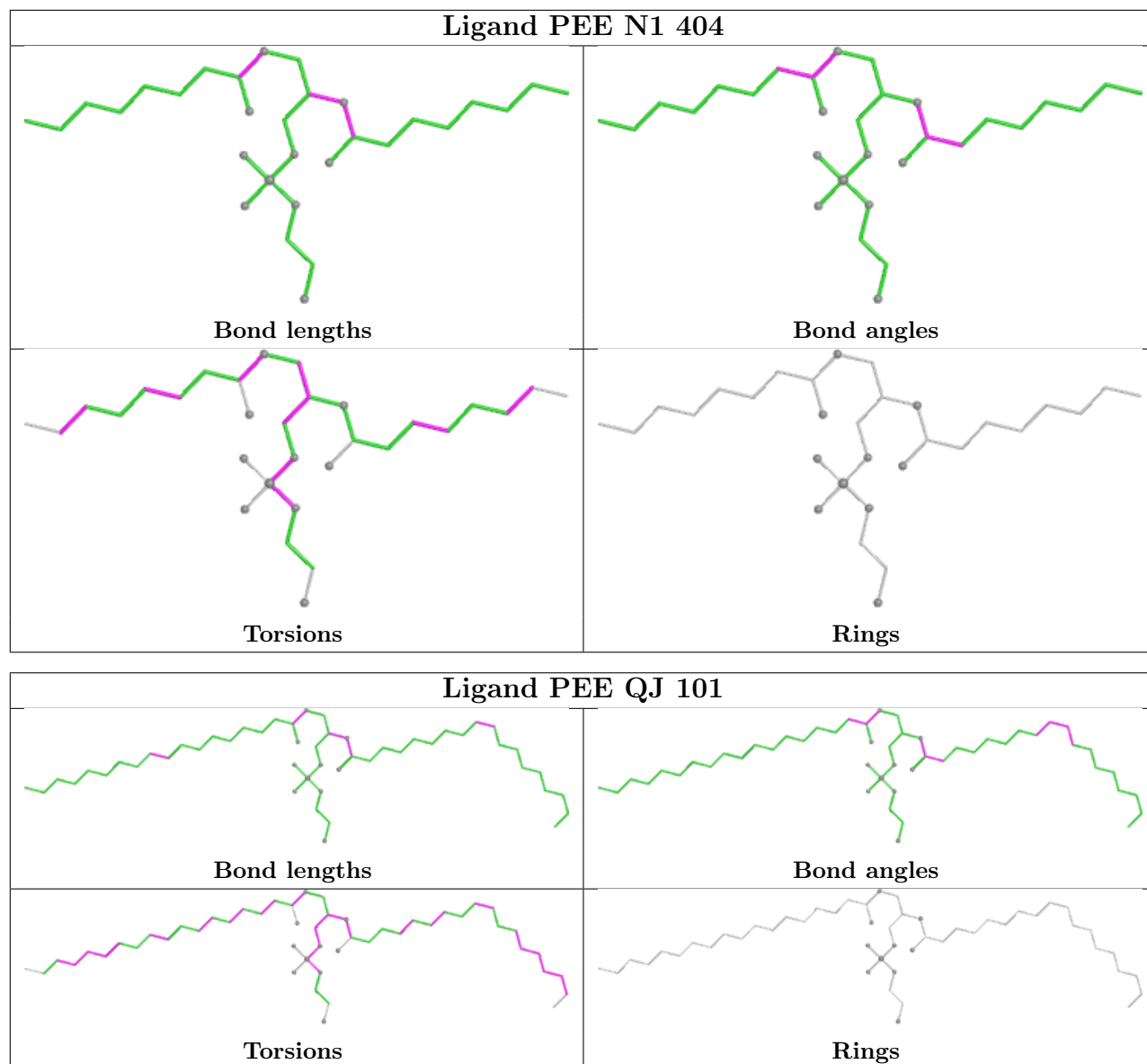


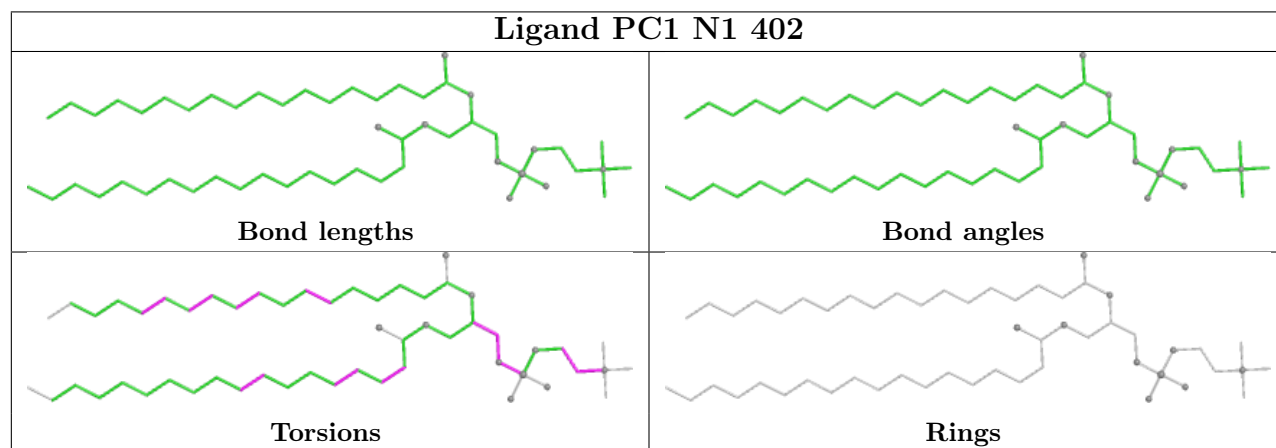
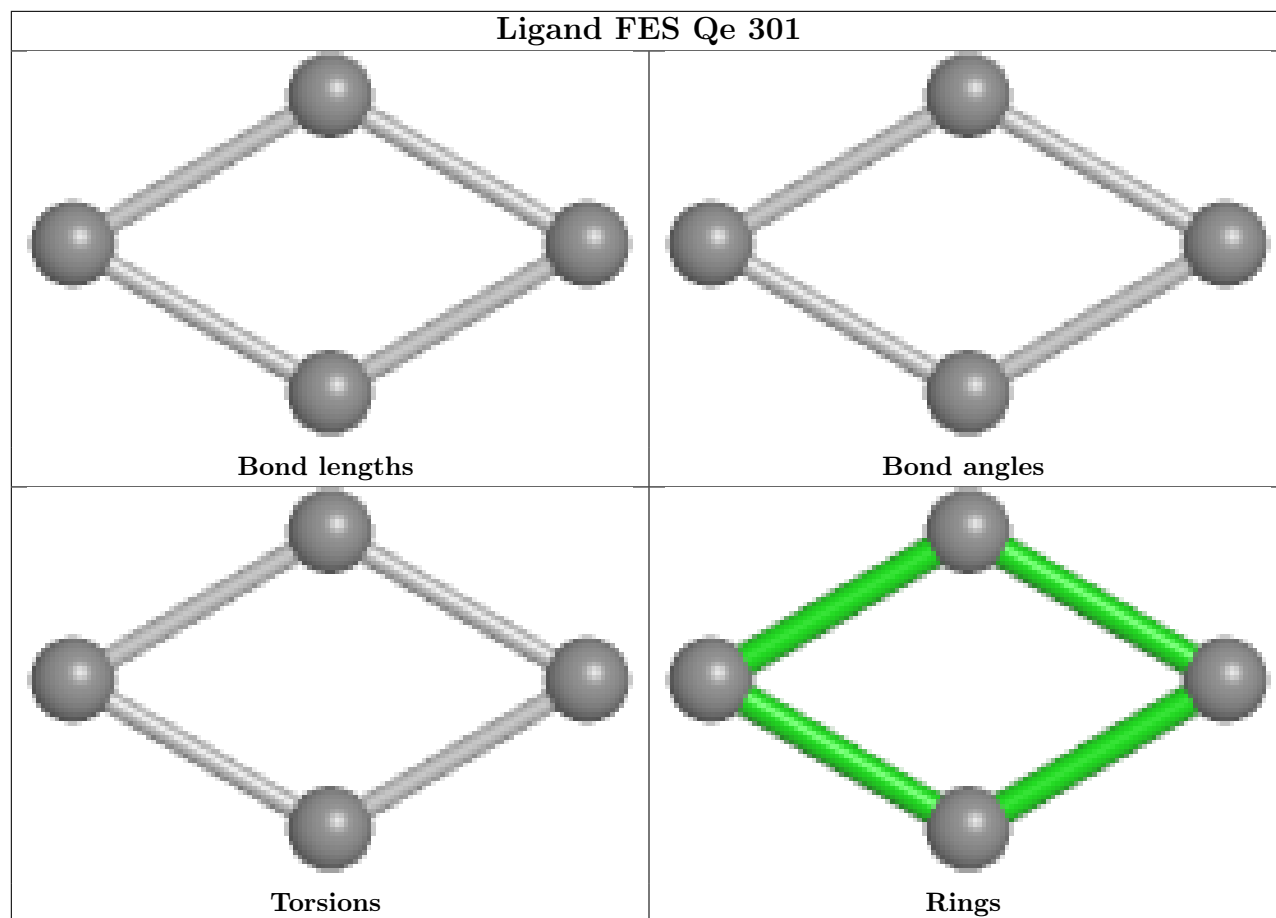
Ligand ZMP AC 201

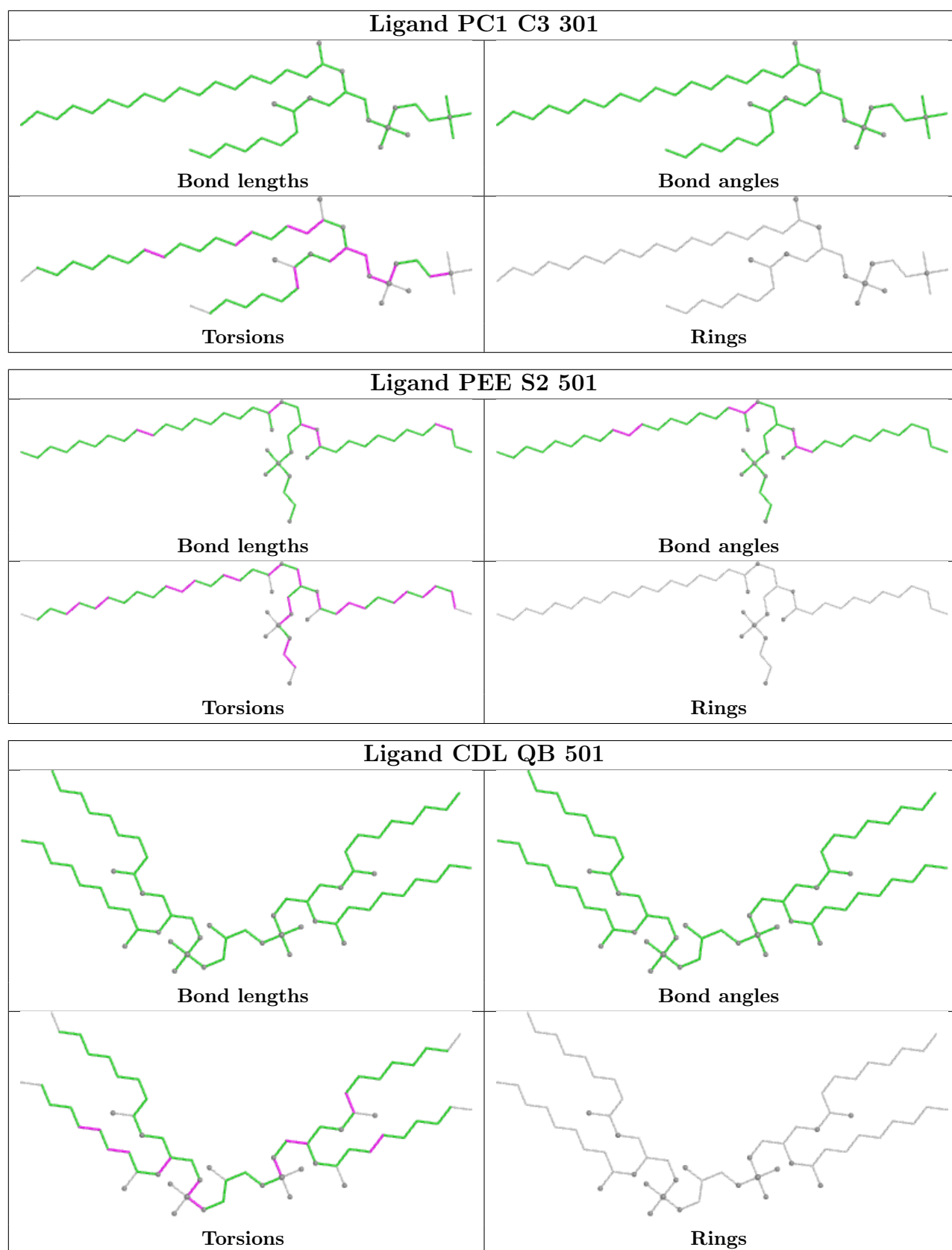


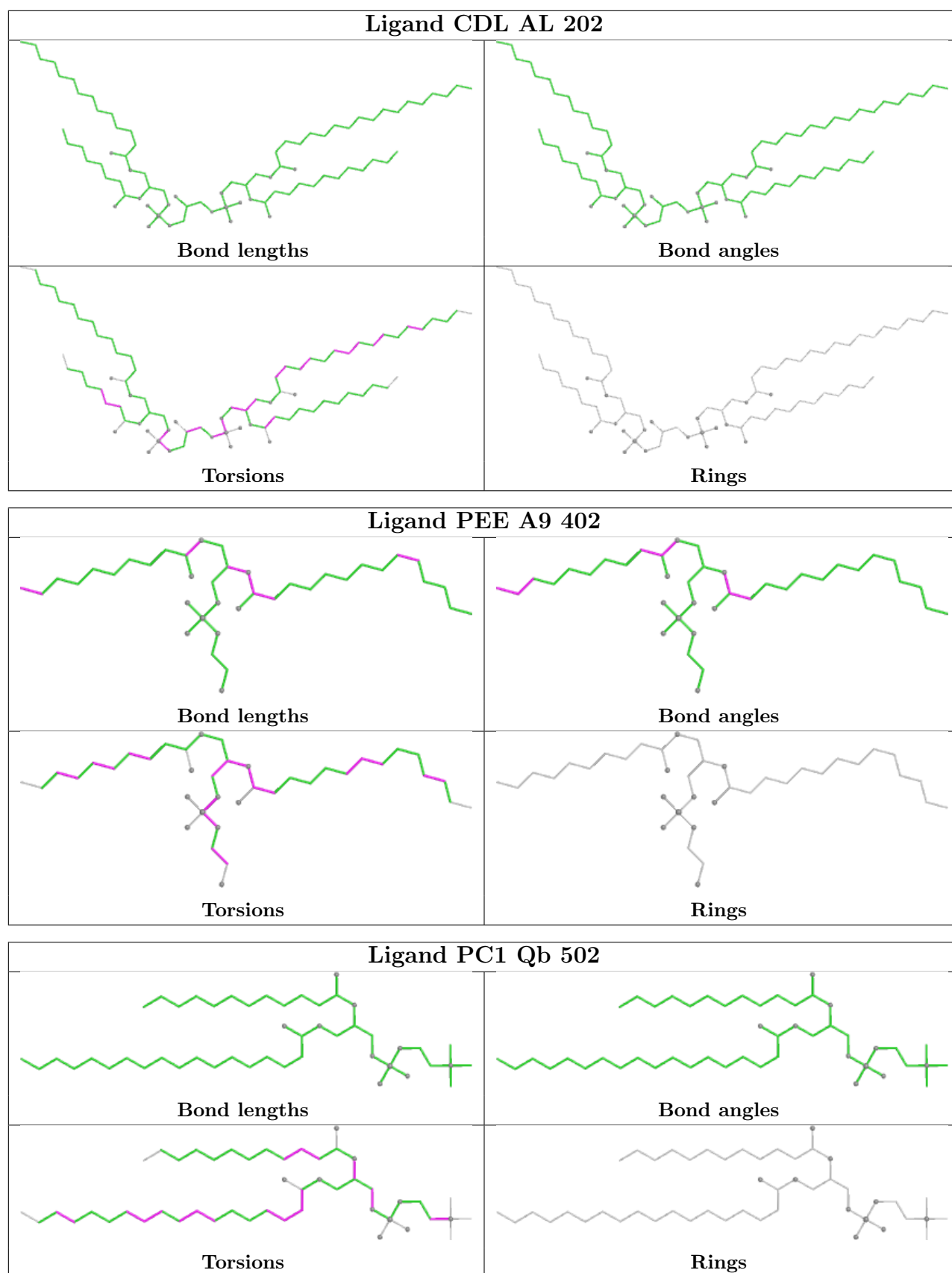


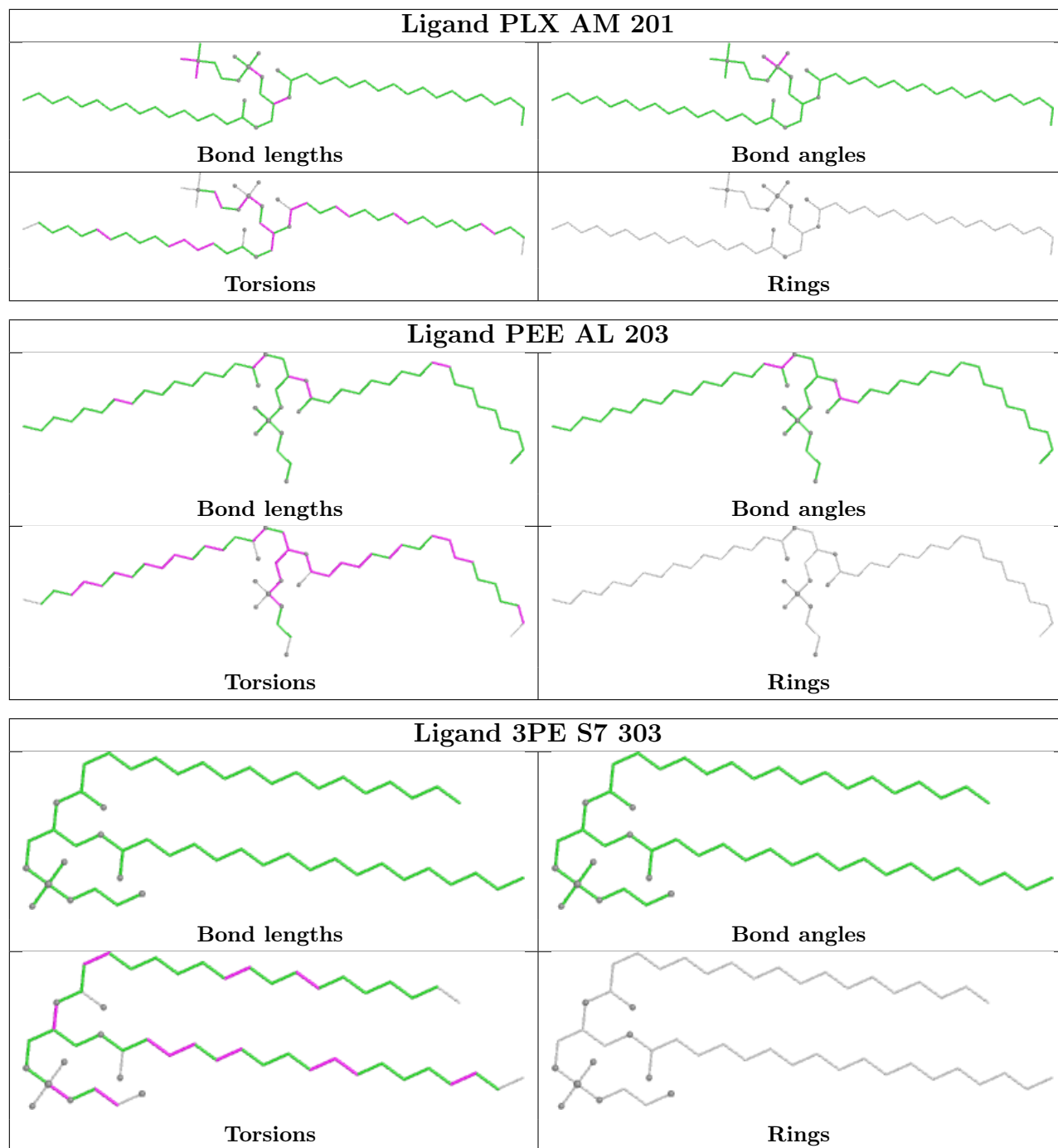


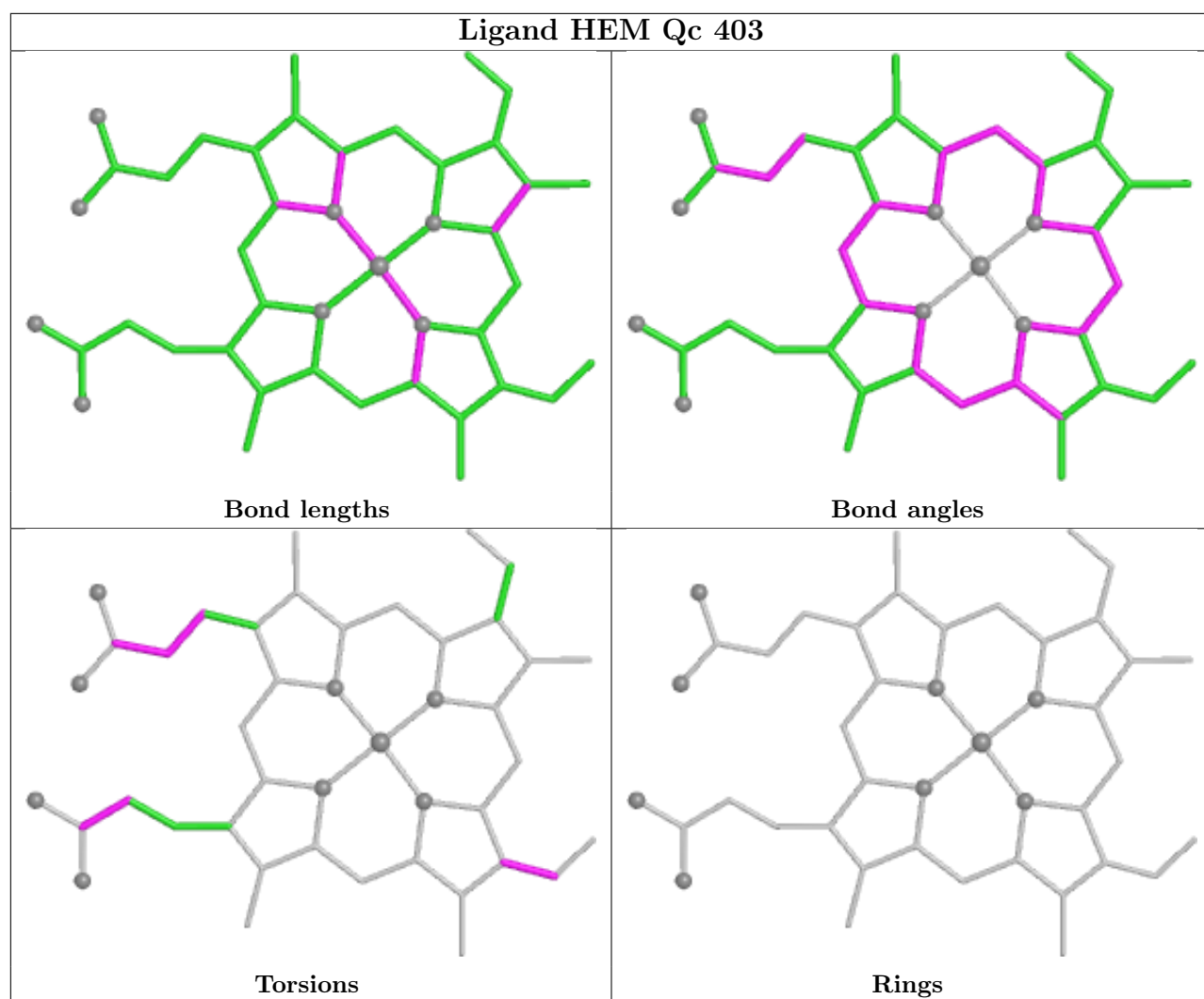


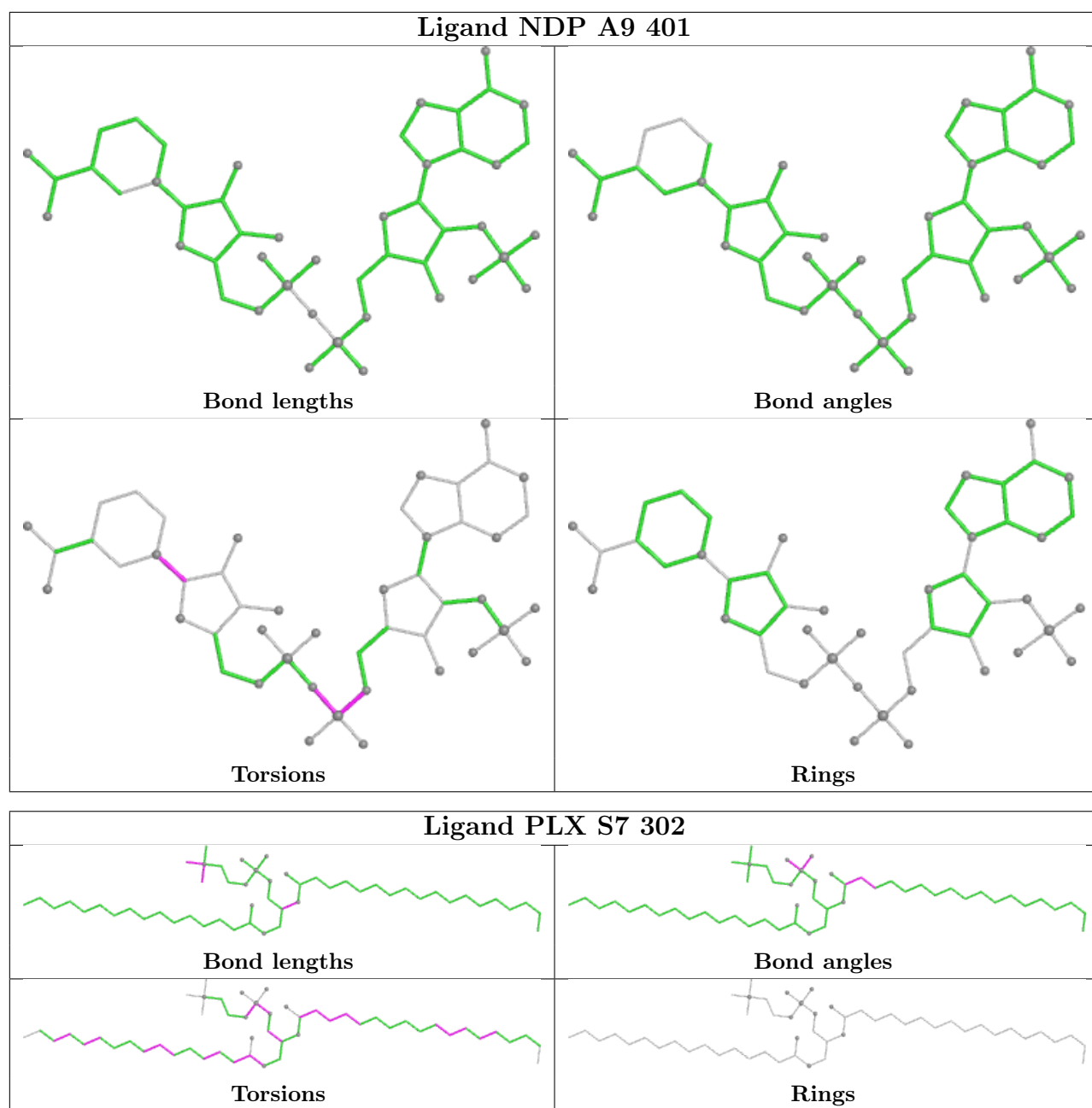


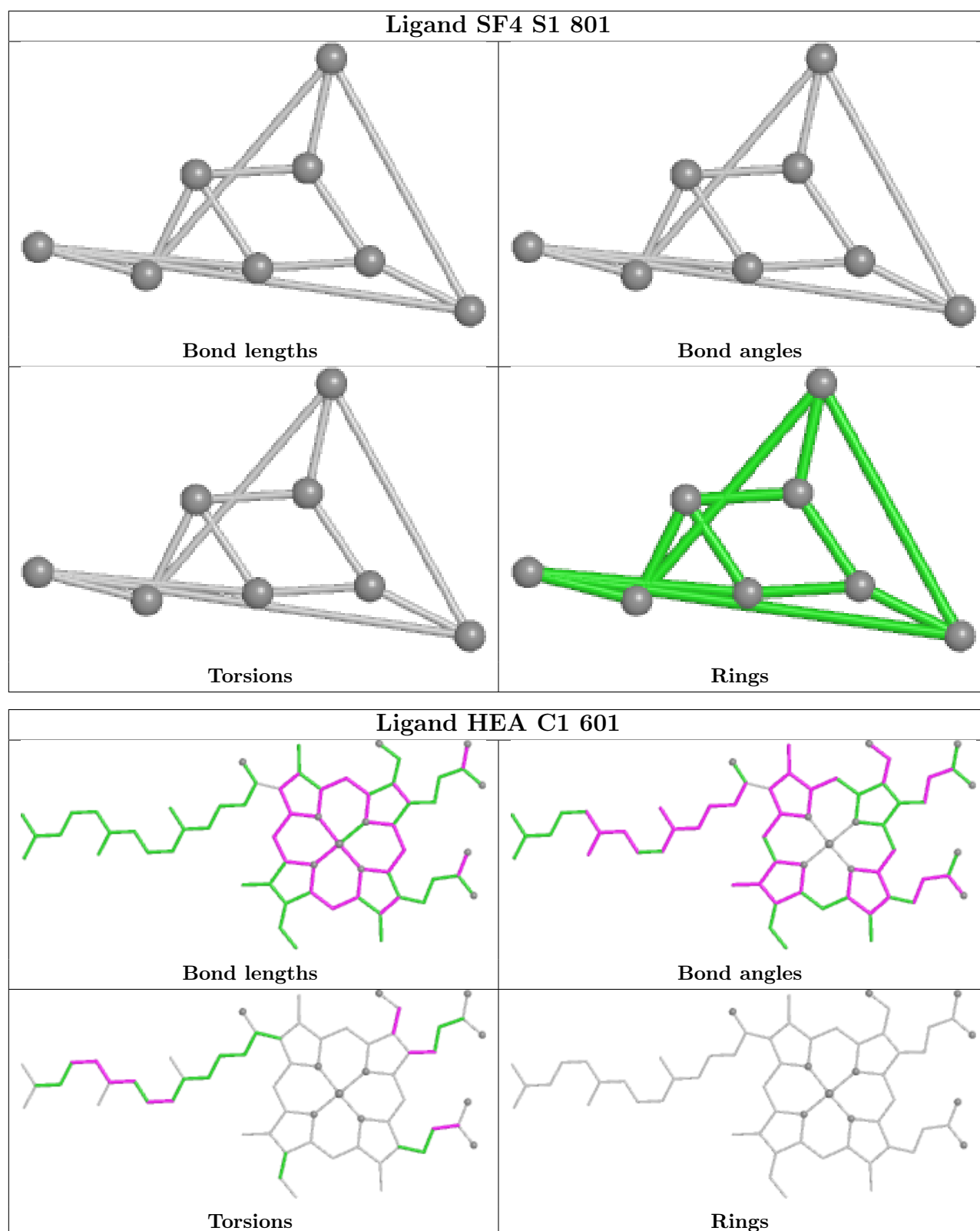


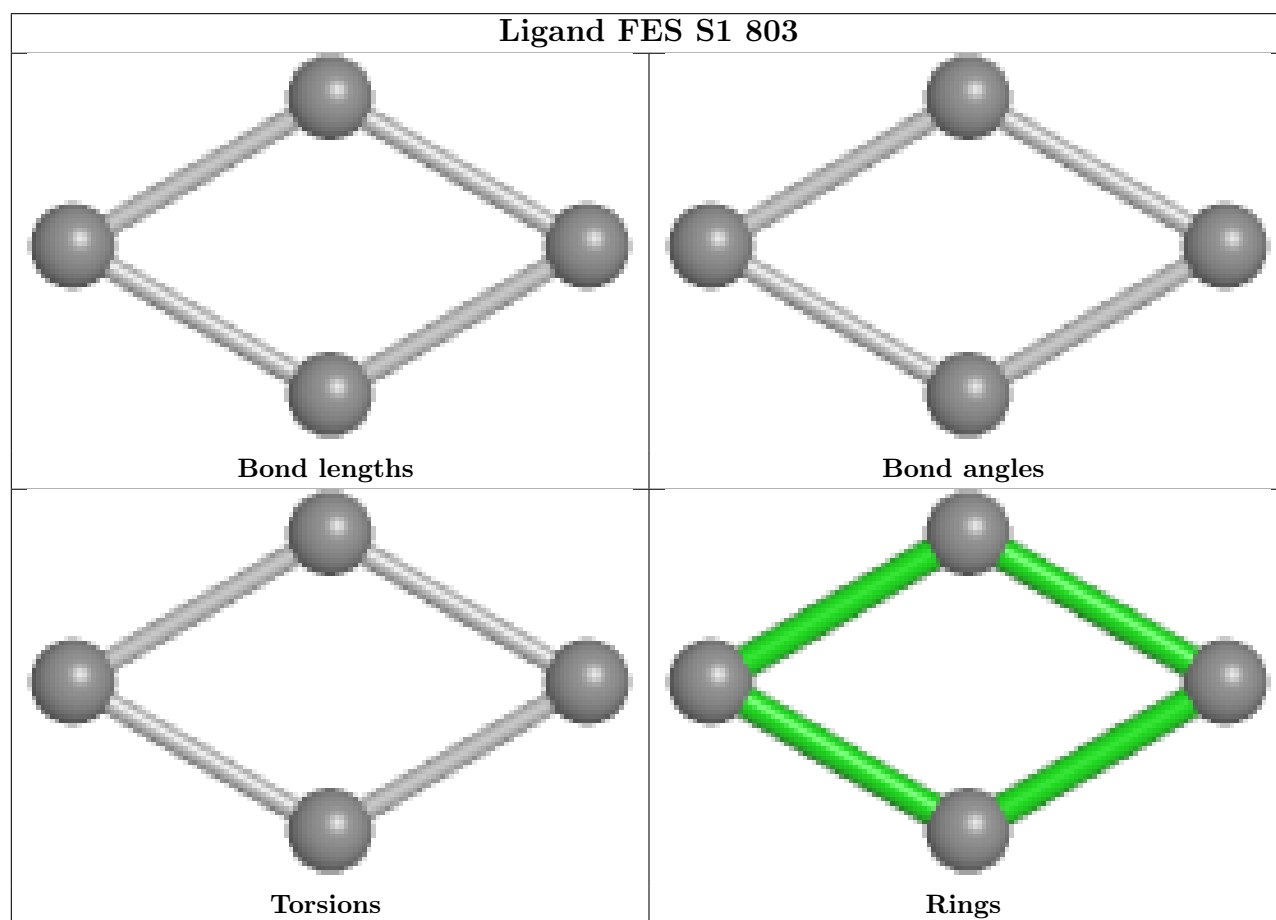
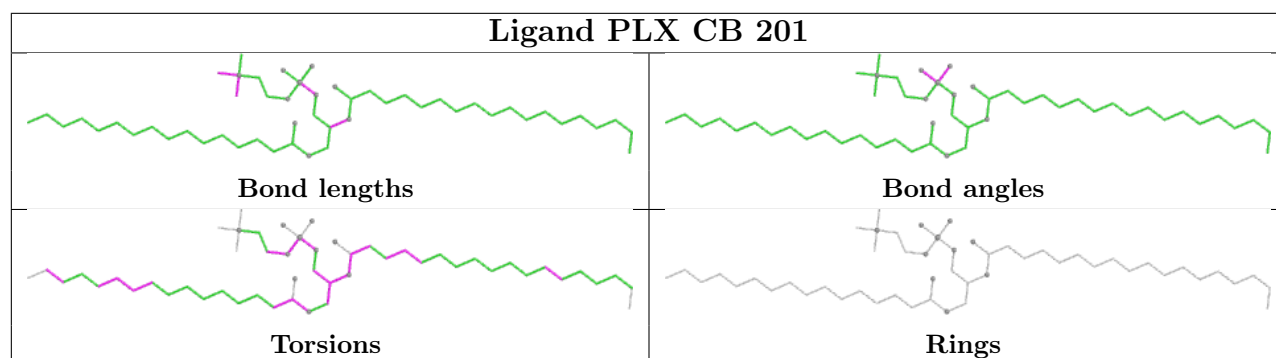
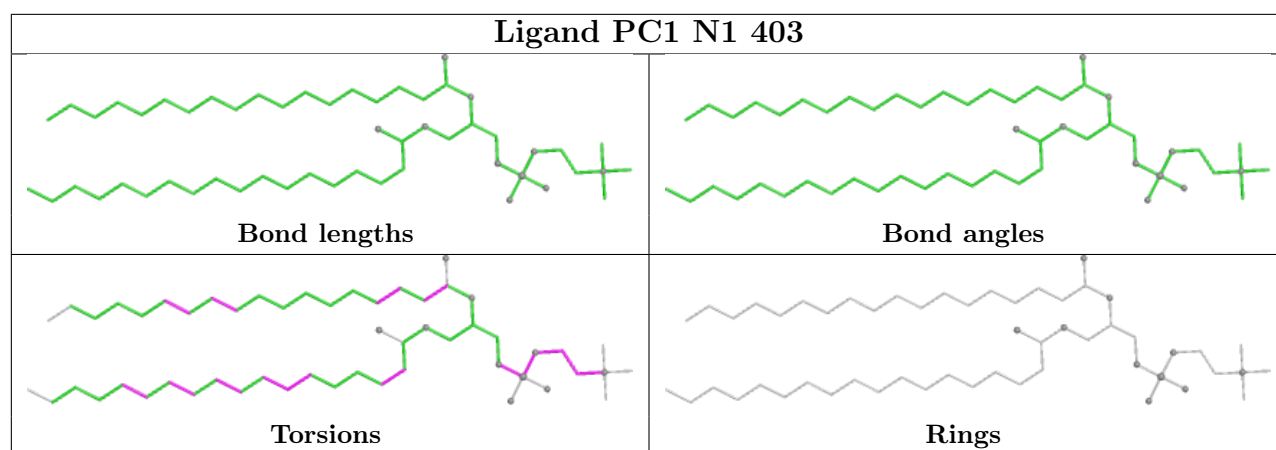


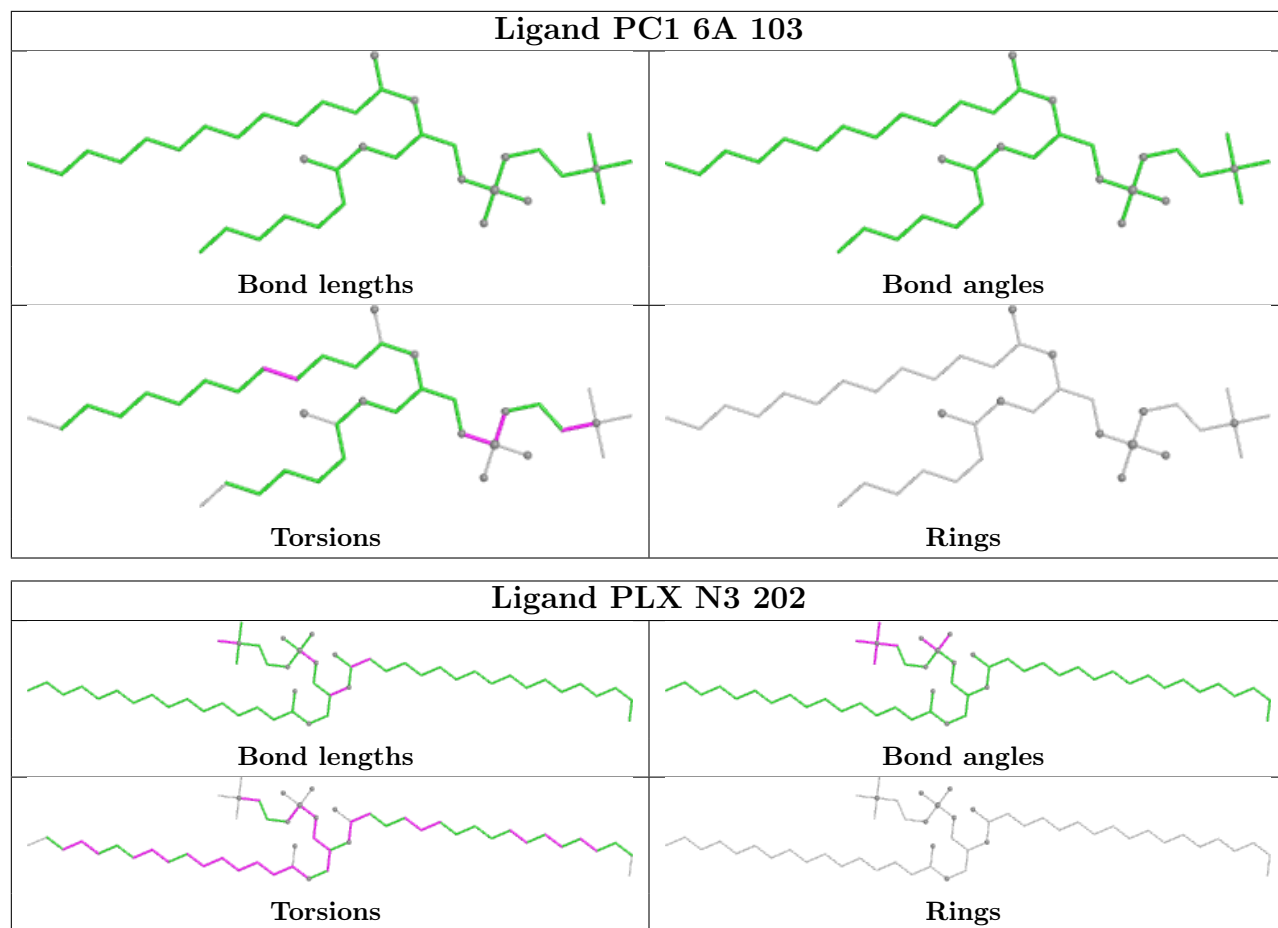




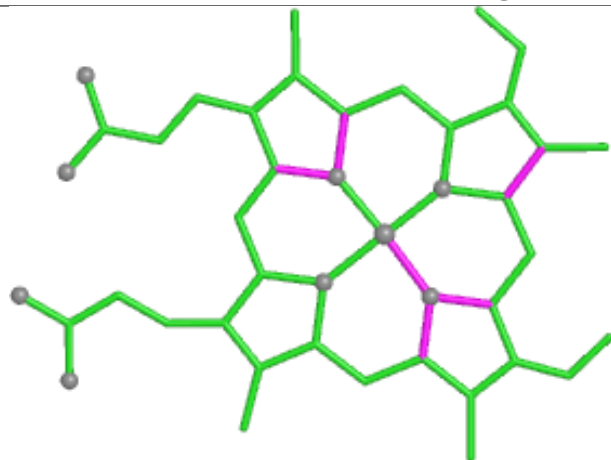




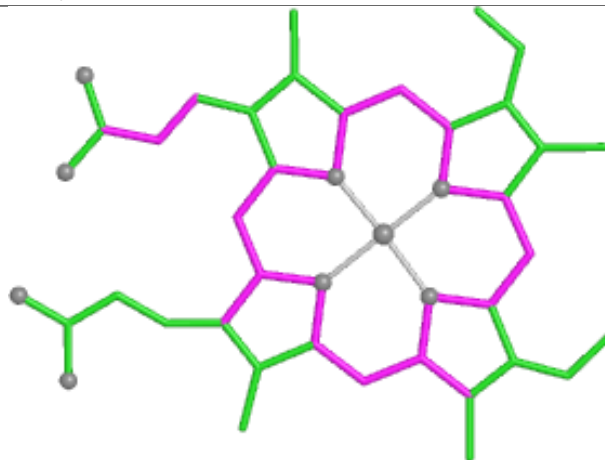




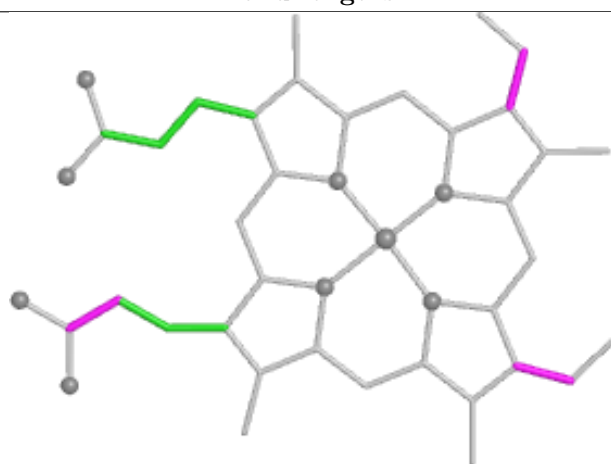
Ligand HEM QC 402



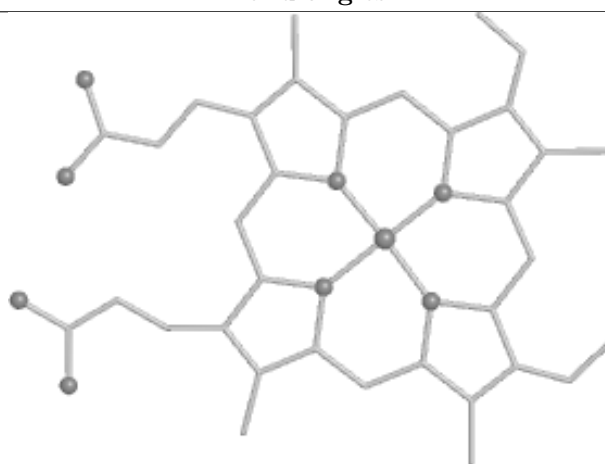
Bond lengths



Bond angles

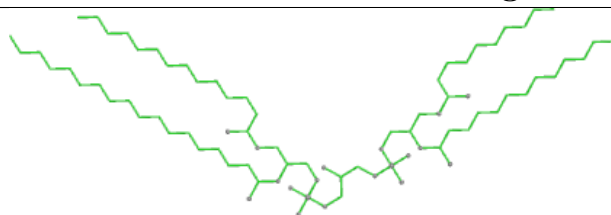


Torsions

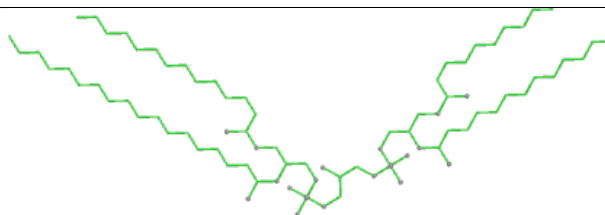


Rings

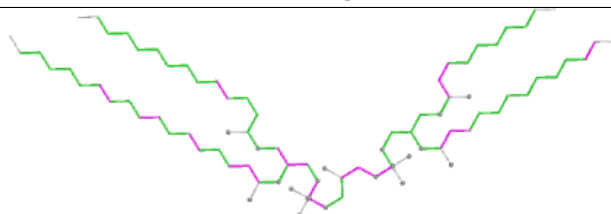
Ligand CDL CB 203



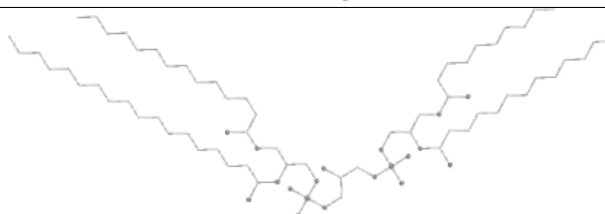
Bond lengths



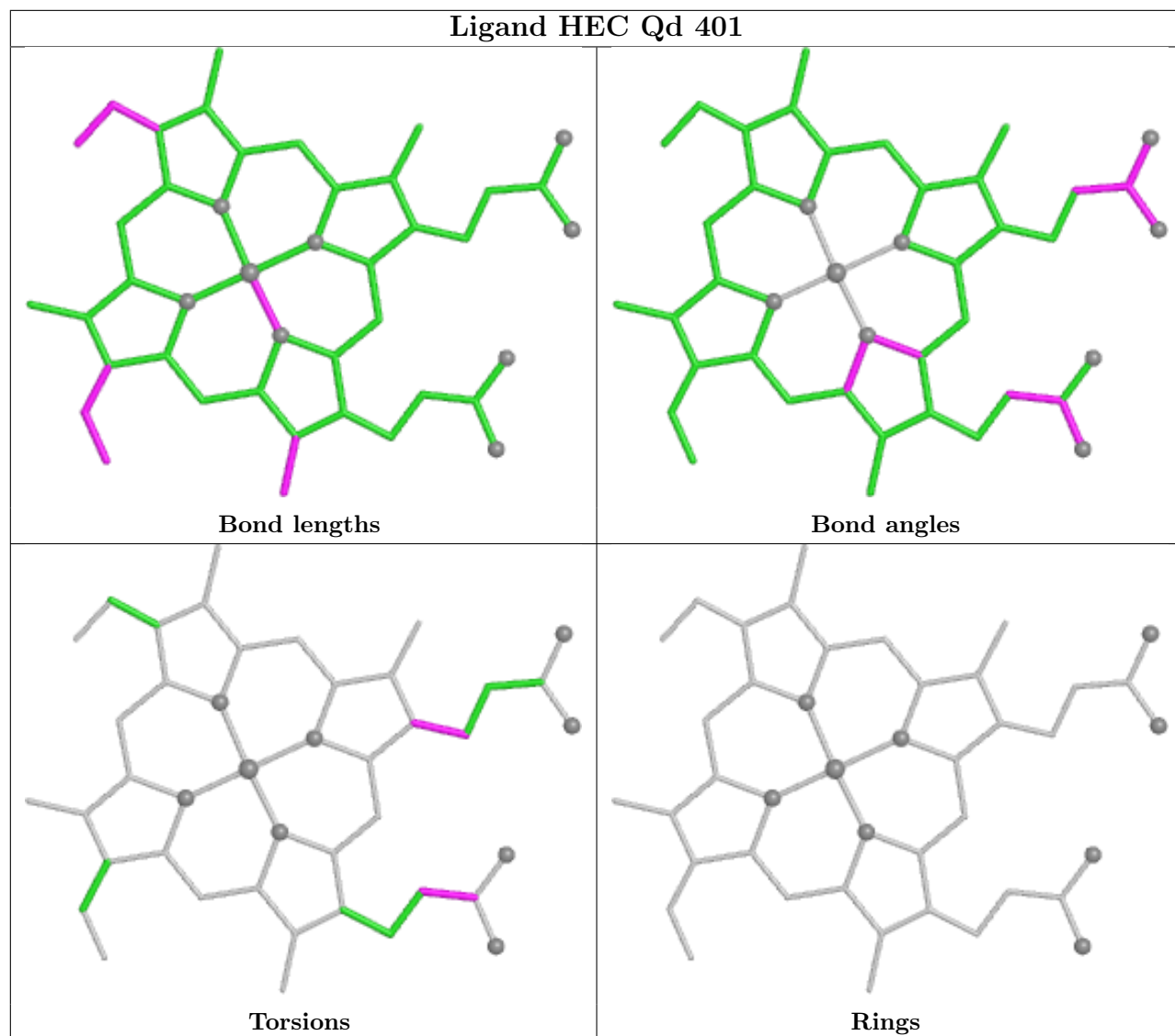
Bond angles

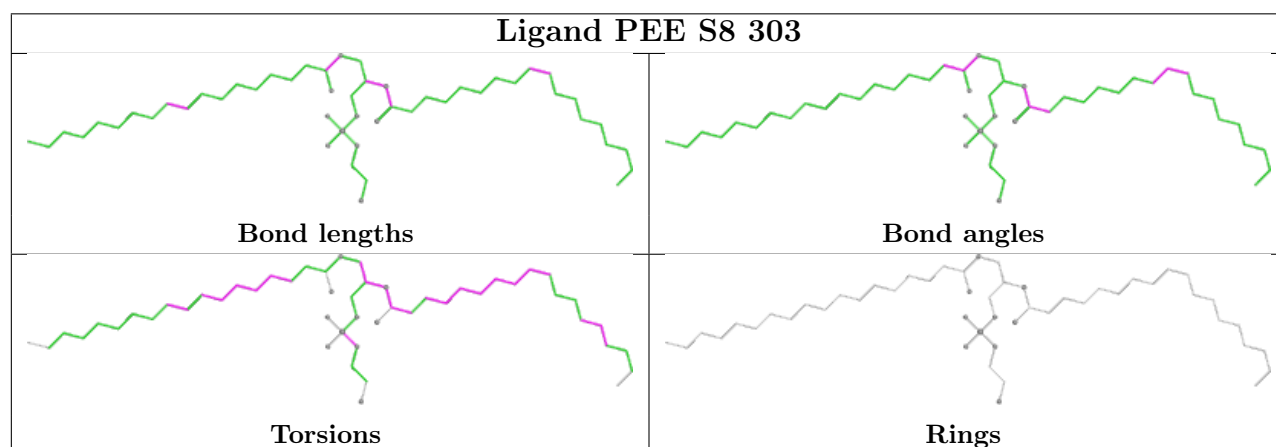
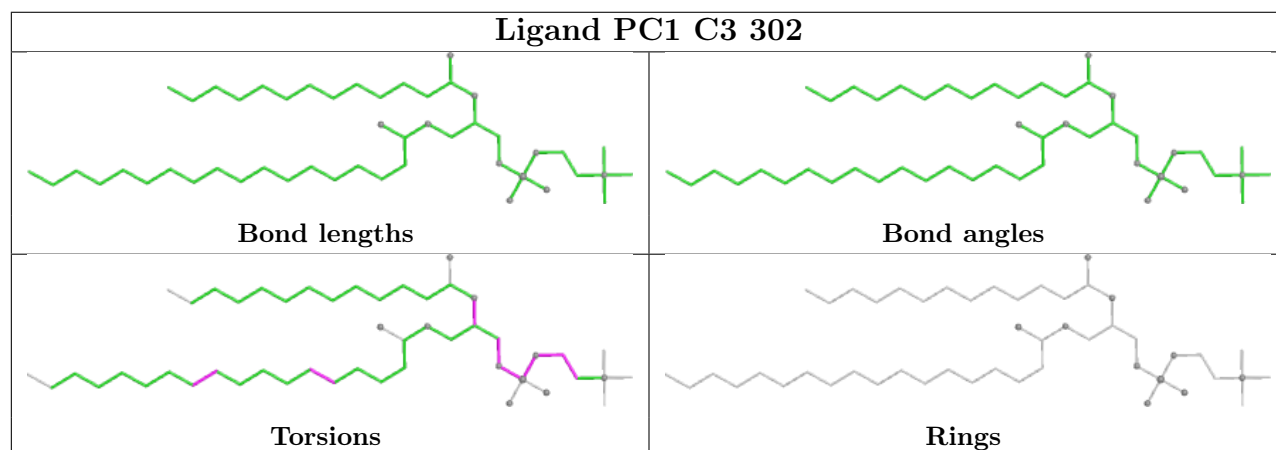
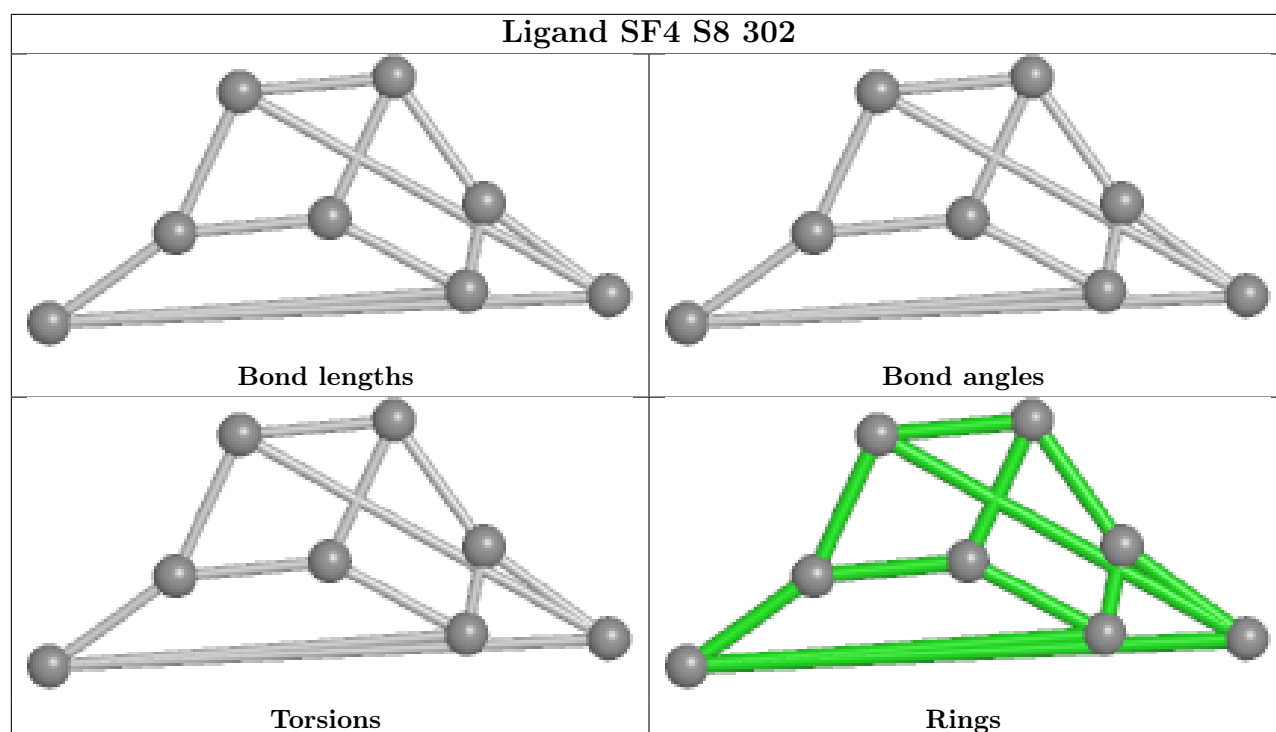


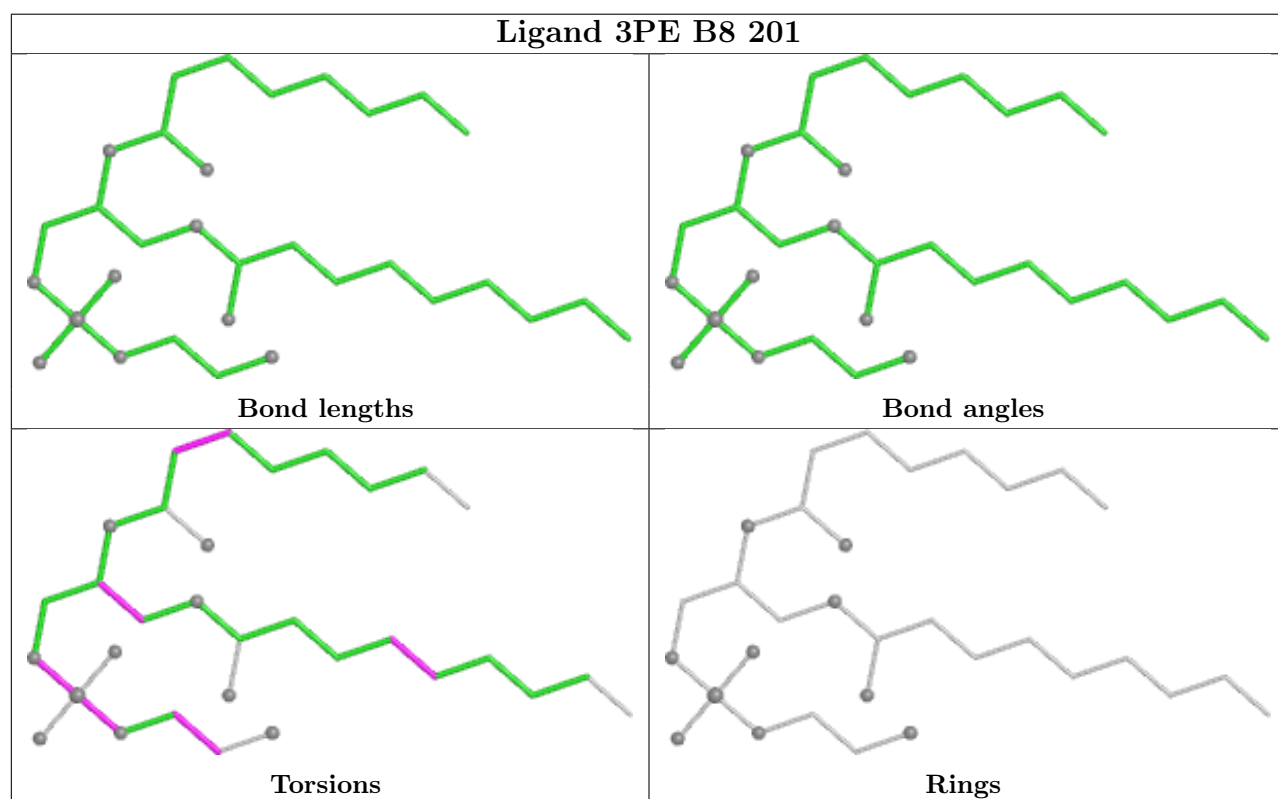
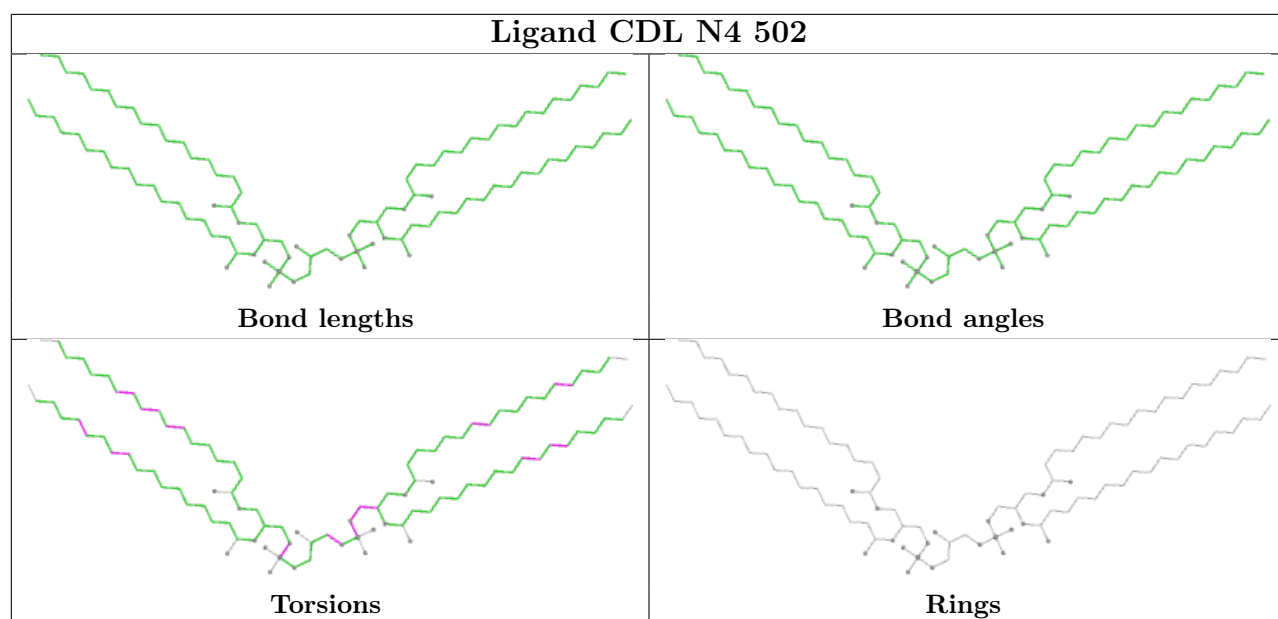
Torsions

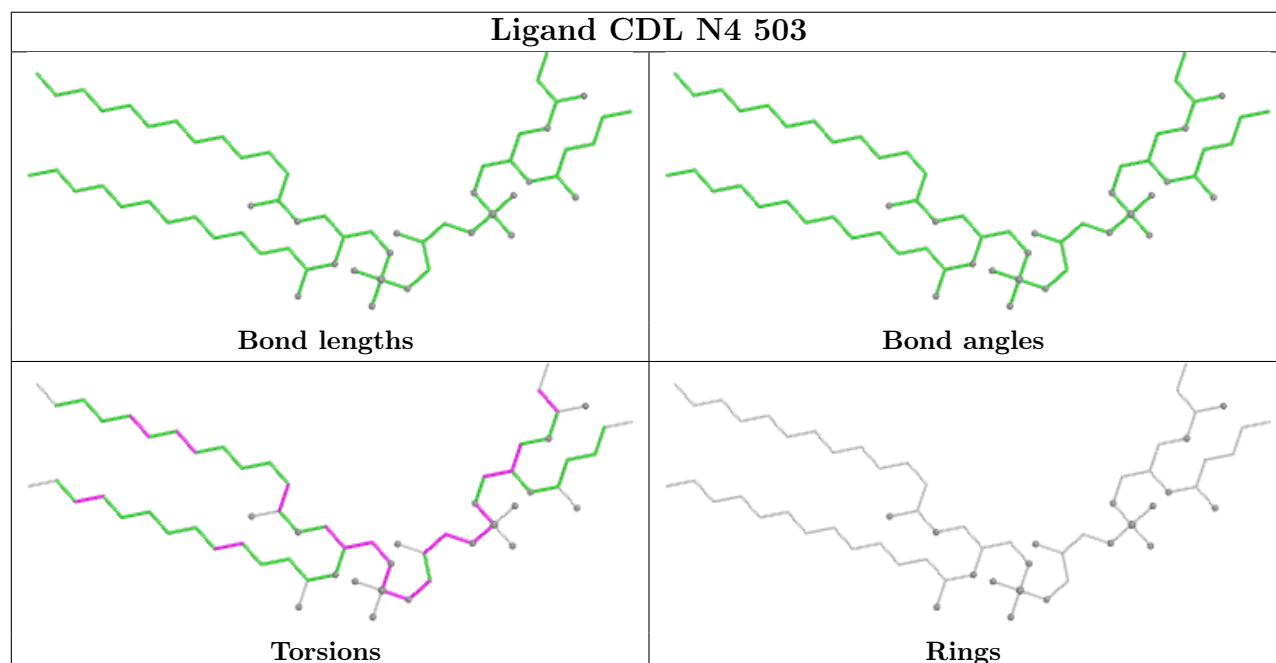
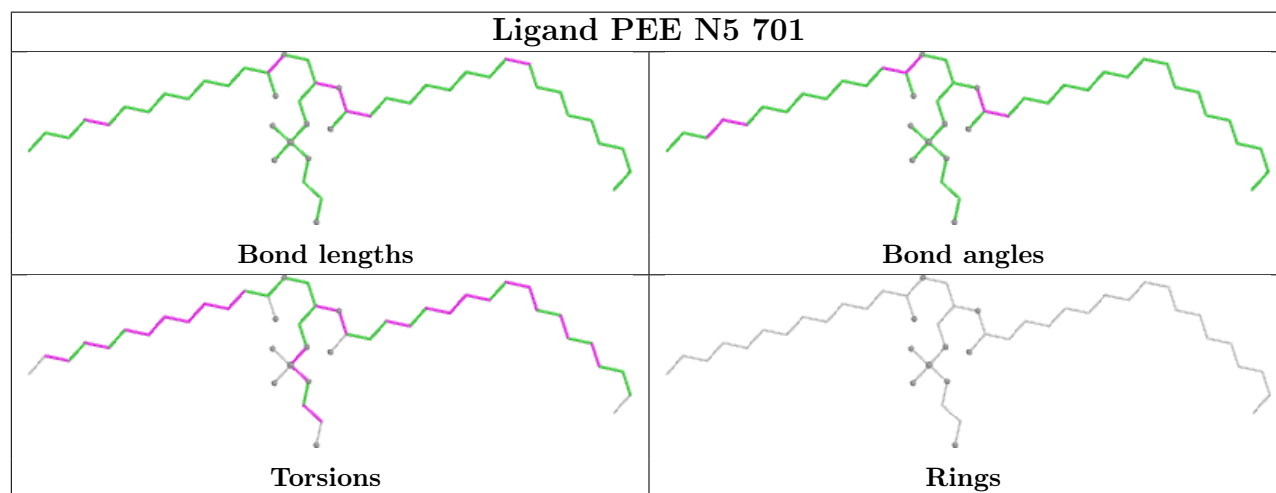
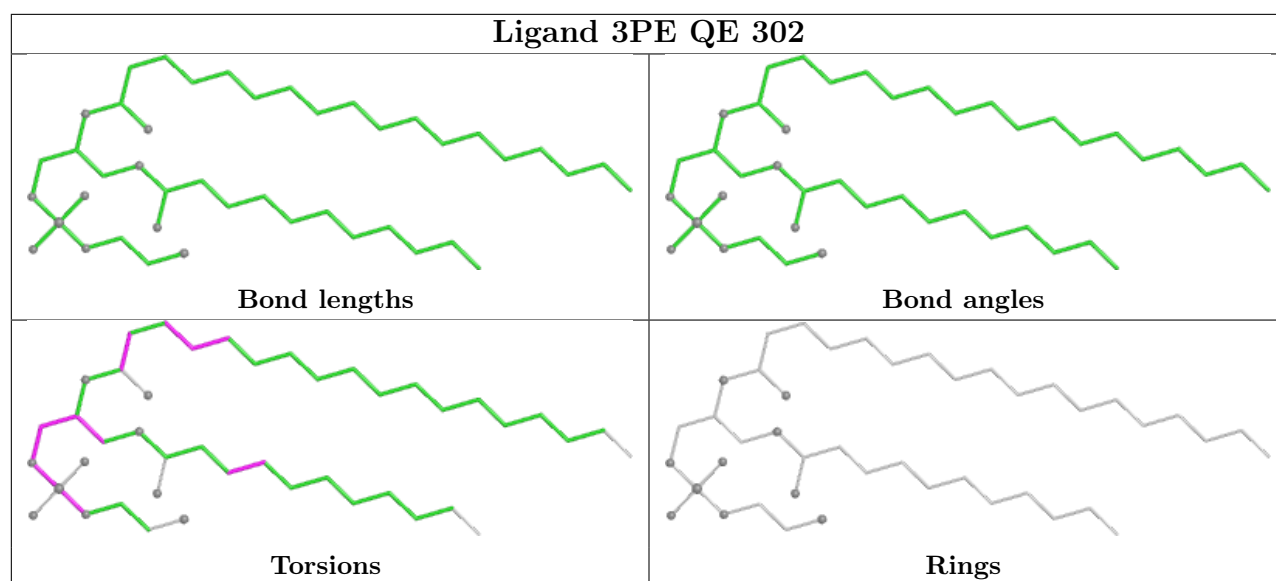


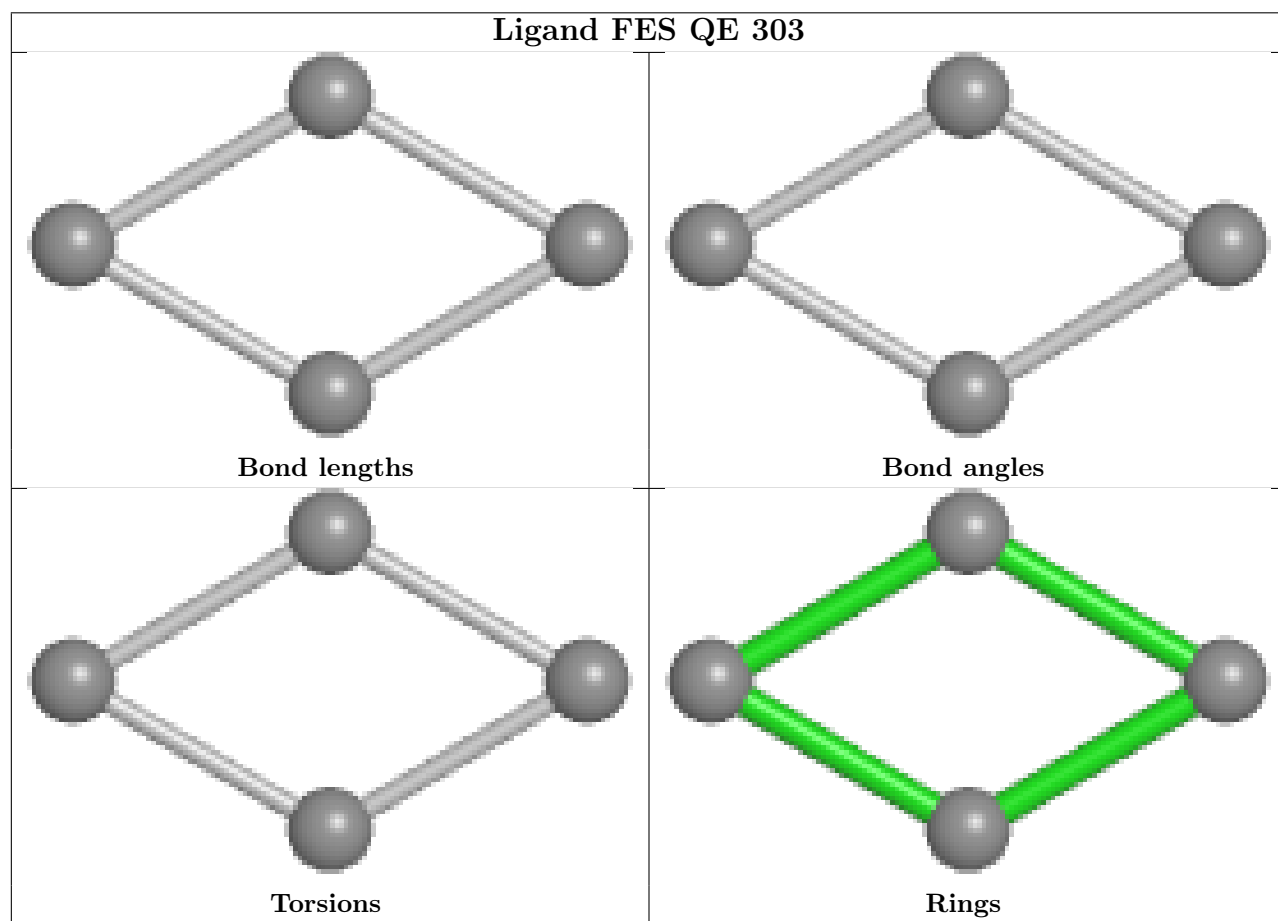
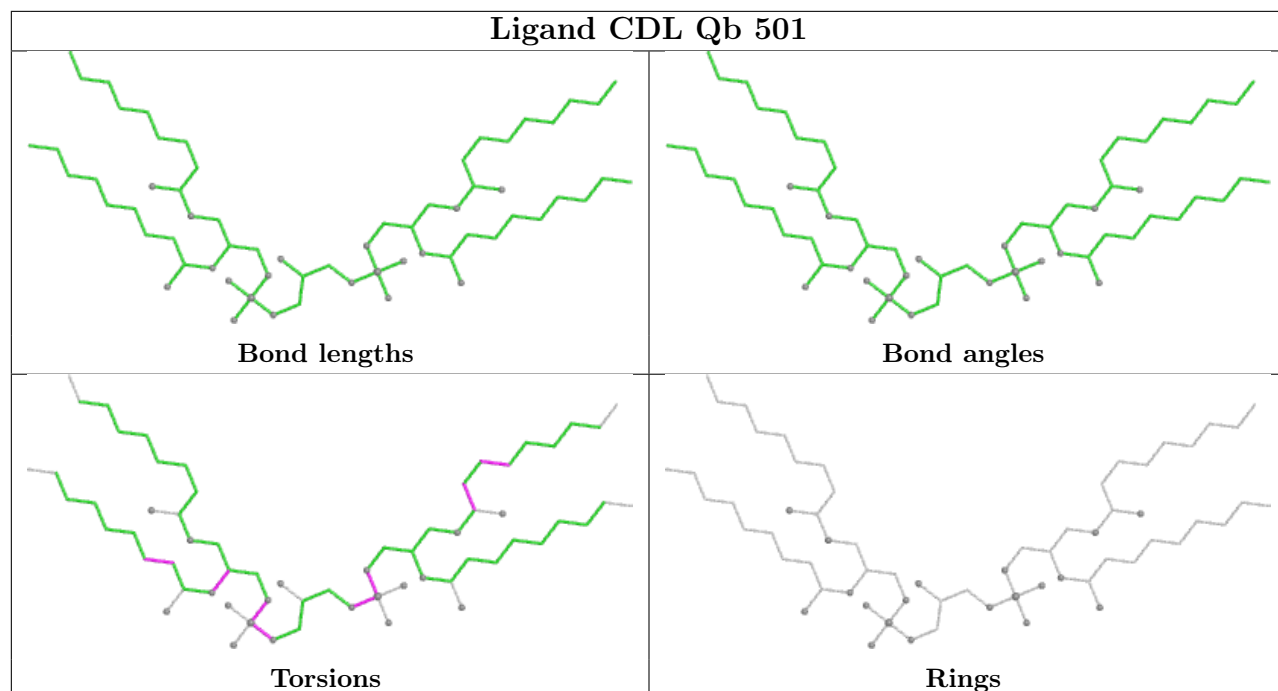
Rings

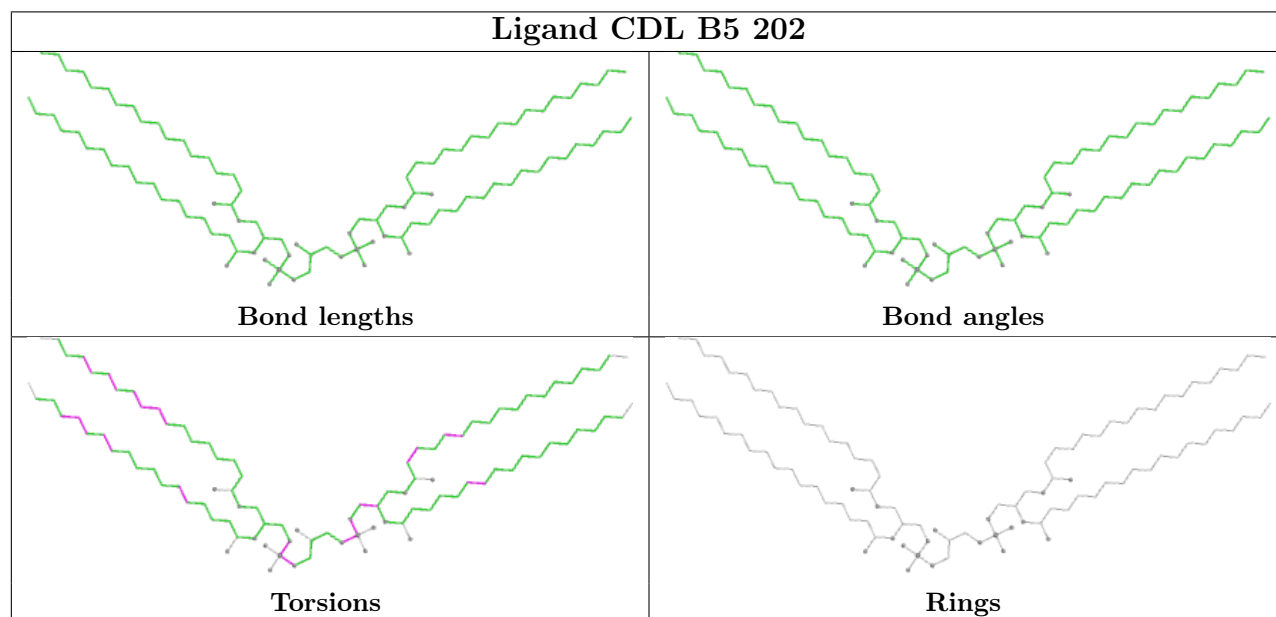
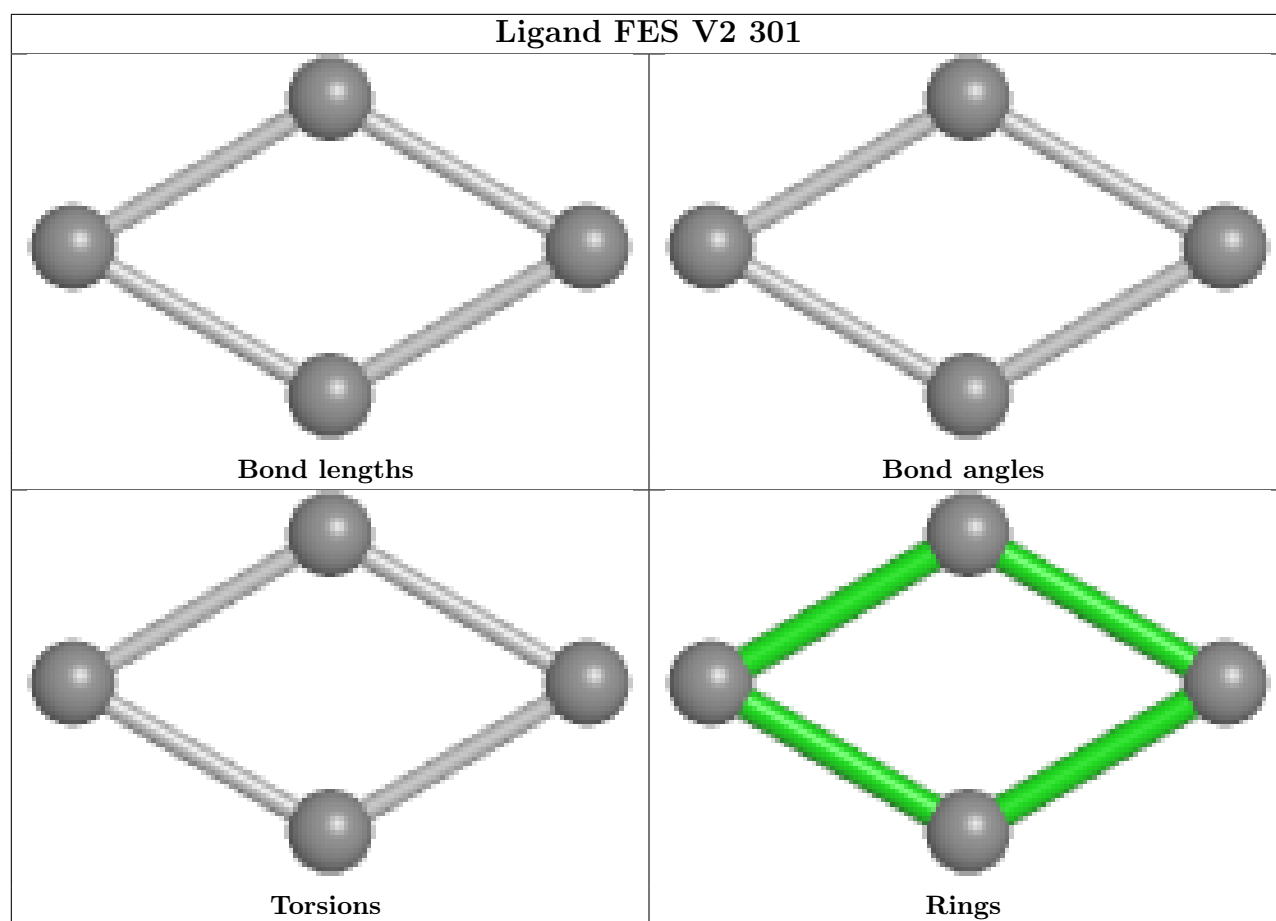


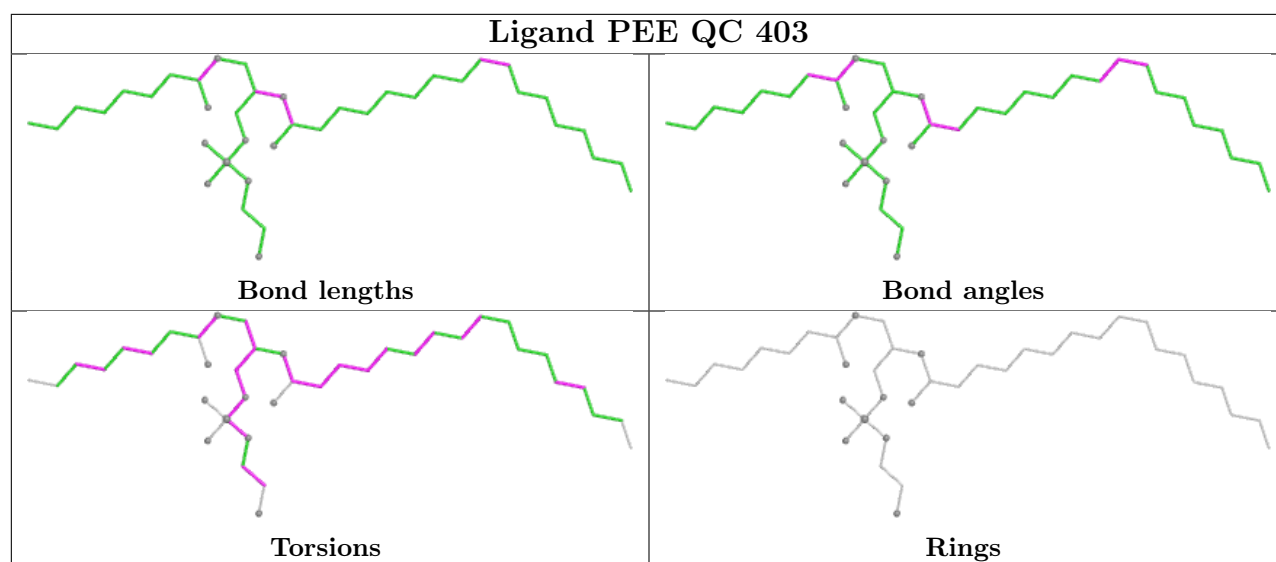












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

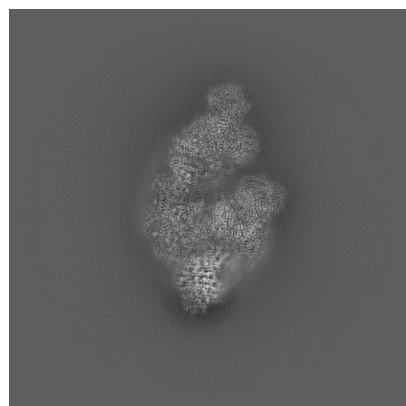
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60421. These allow visual inspection of the internal detail of the map and identification of artifacts.

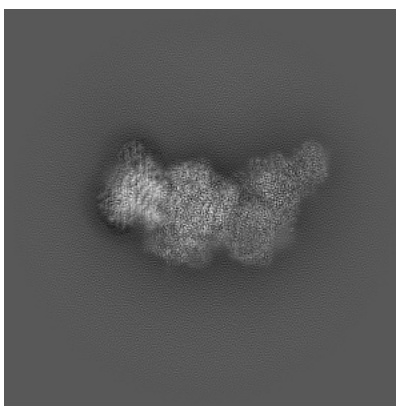
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

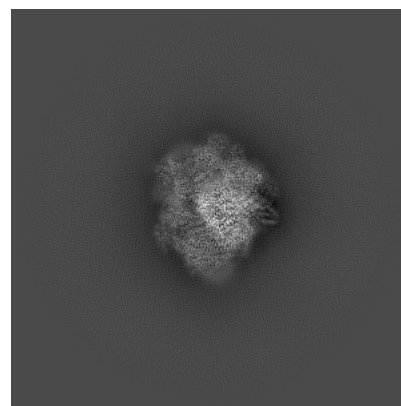
6.1.1 Primary map



X

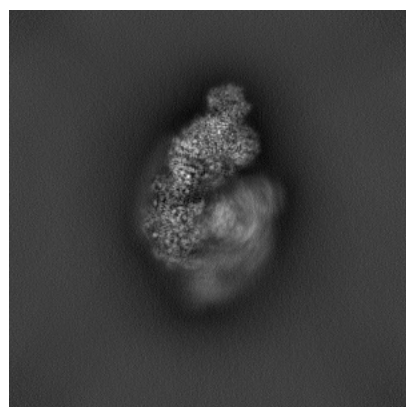


Y

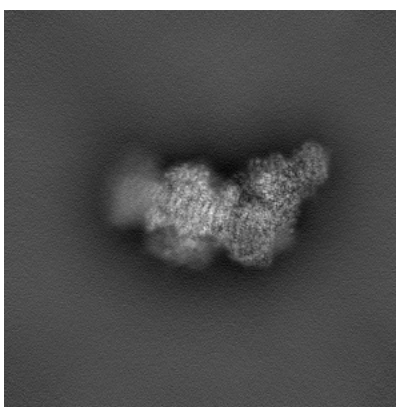


Z

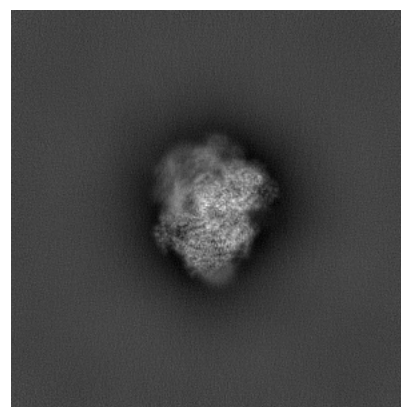
6.1.2 Raw map



X



Y

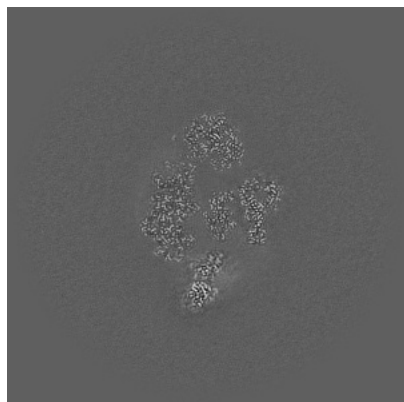


Z

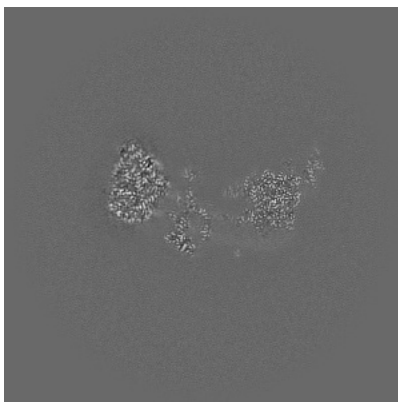
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

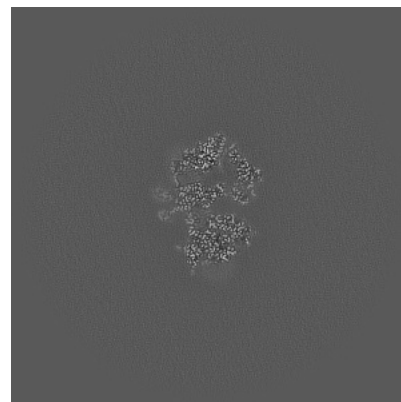
6.2.1 Primary map



X Index: 240

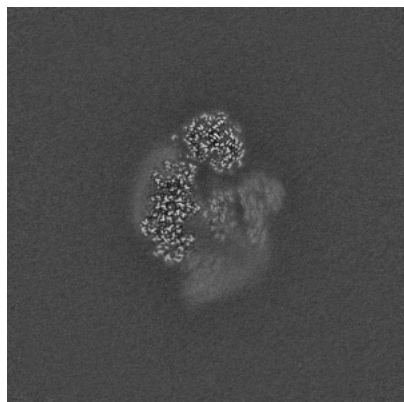


Y Index: 240

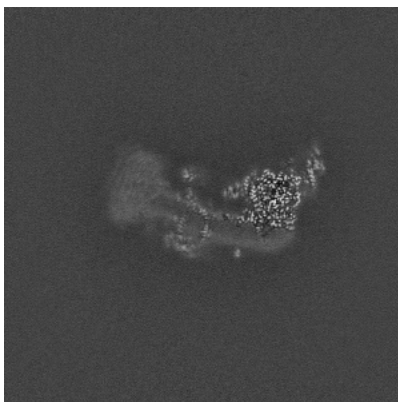


Z Index: 240

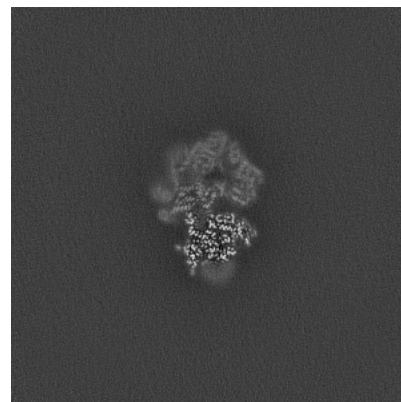
6.2.2 Raw map



X Index: 240



Y Index: 240

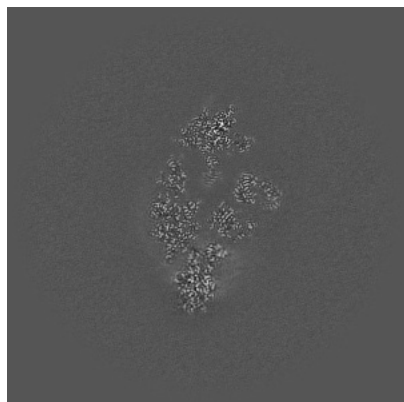


Z Index: 240

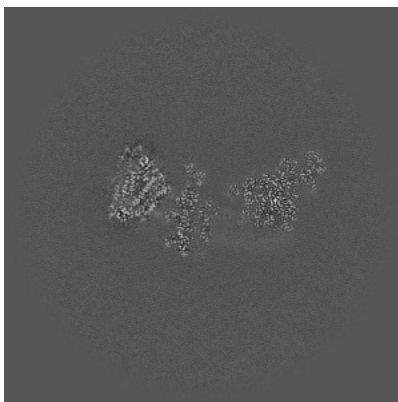
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

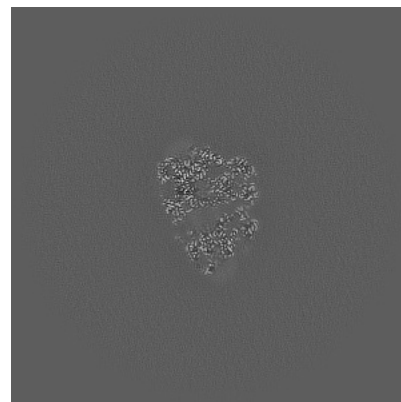
6.3.1 Primary map



X Index: 256

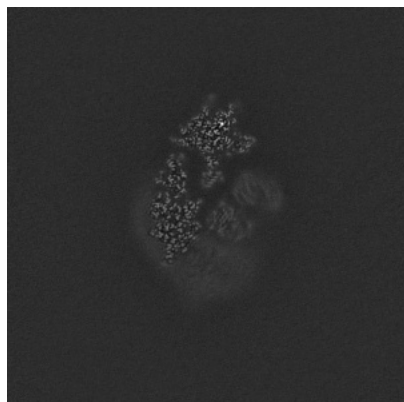


Y Index: 244

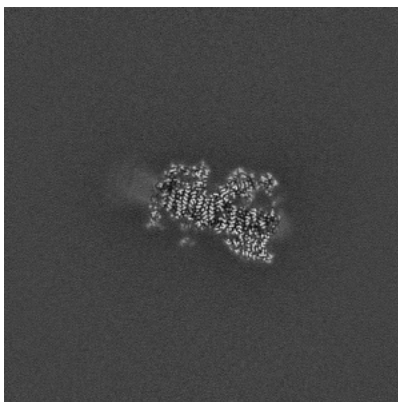


Z Index: 217

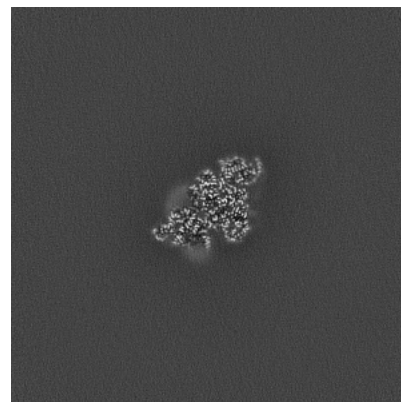
6.3.2 Raw map



X Index: 256



Y Index: 205

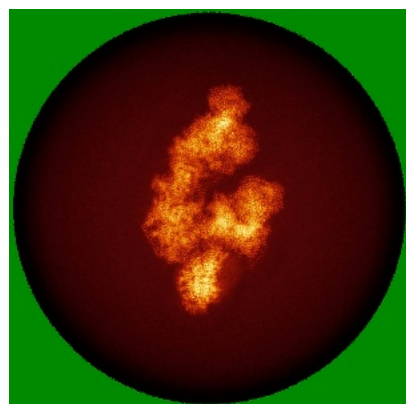


Z Index: 315

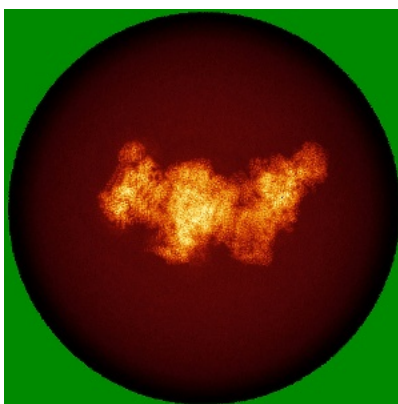
The images above show the largest variance slices of the map in three orthogonal directions.

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

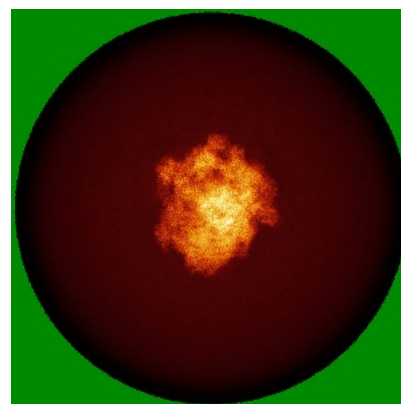
6.4.1 Primary map



X

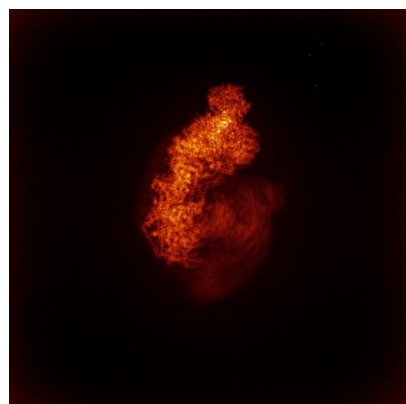


Y

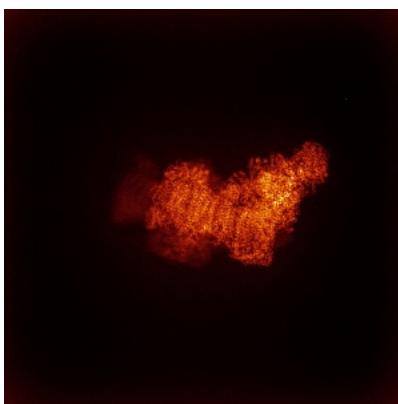


Z

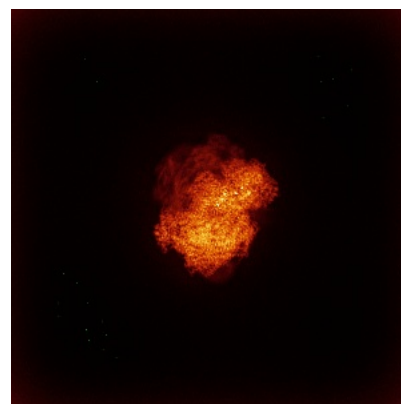
6.4.2 Raw map



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](#)

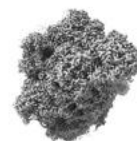
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

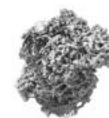
6.5.2 Raw map



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.

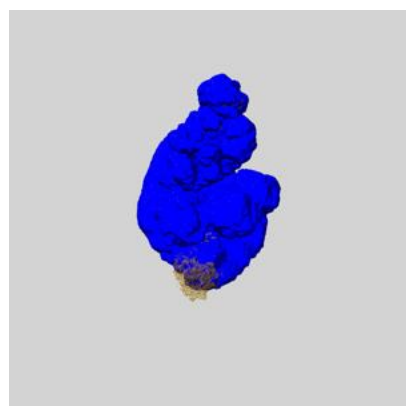
6.6 Mask visualisation [i](#)

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

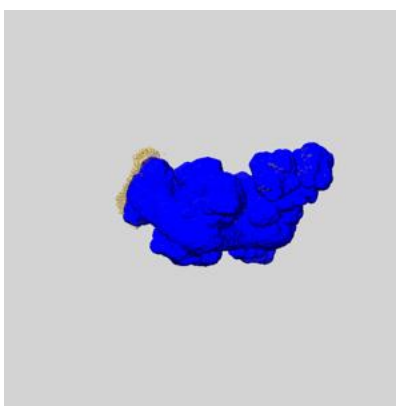
A mask typically either:

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

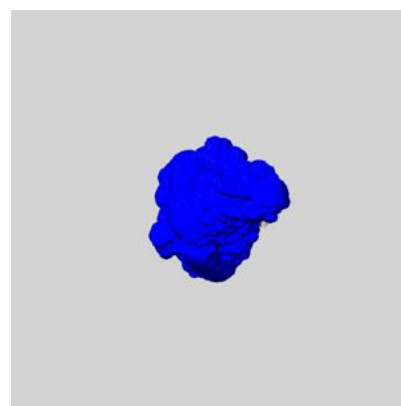
6.6.1 emd_60421_msk_1.map [i](#)



X



Y

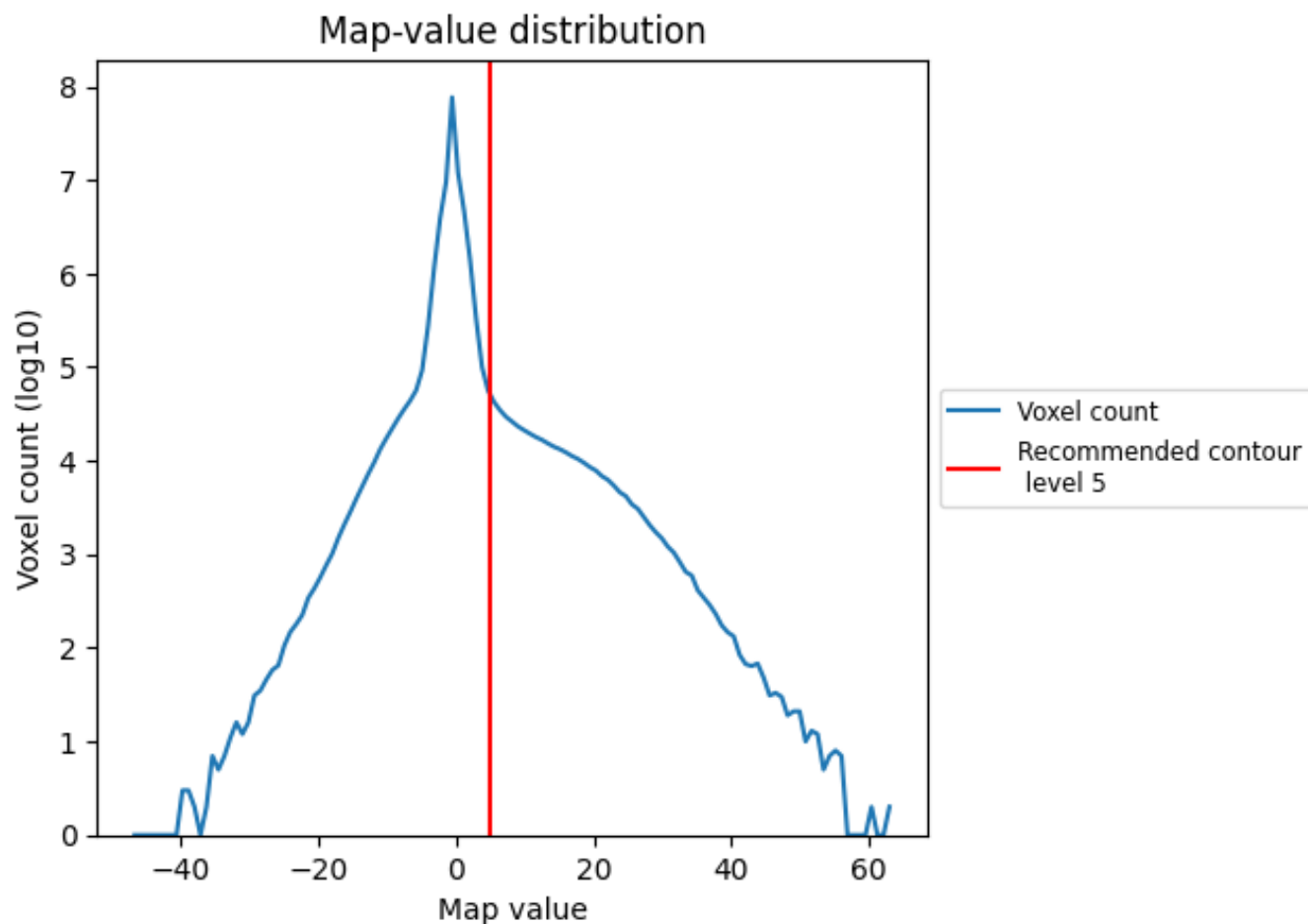


Z

7 Map analysis [i](#)

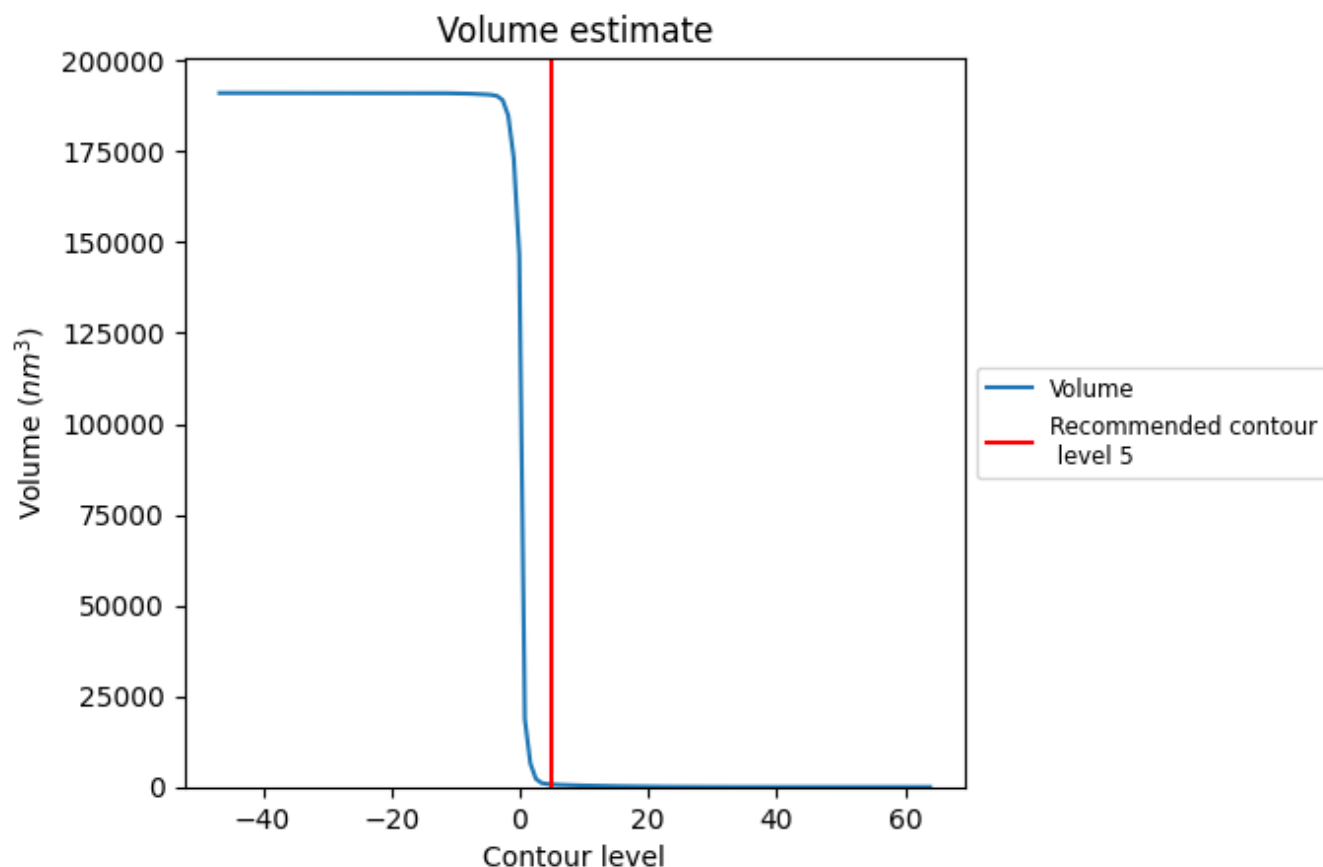
This section contains the results of statistical analysis of the map.

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.

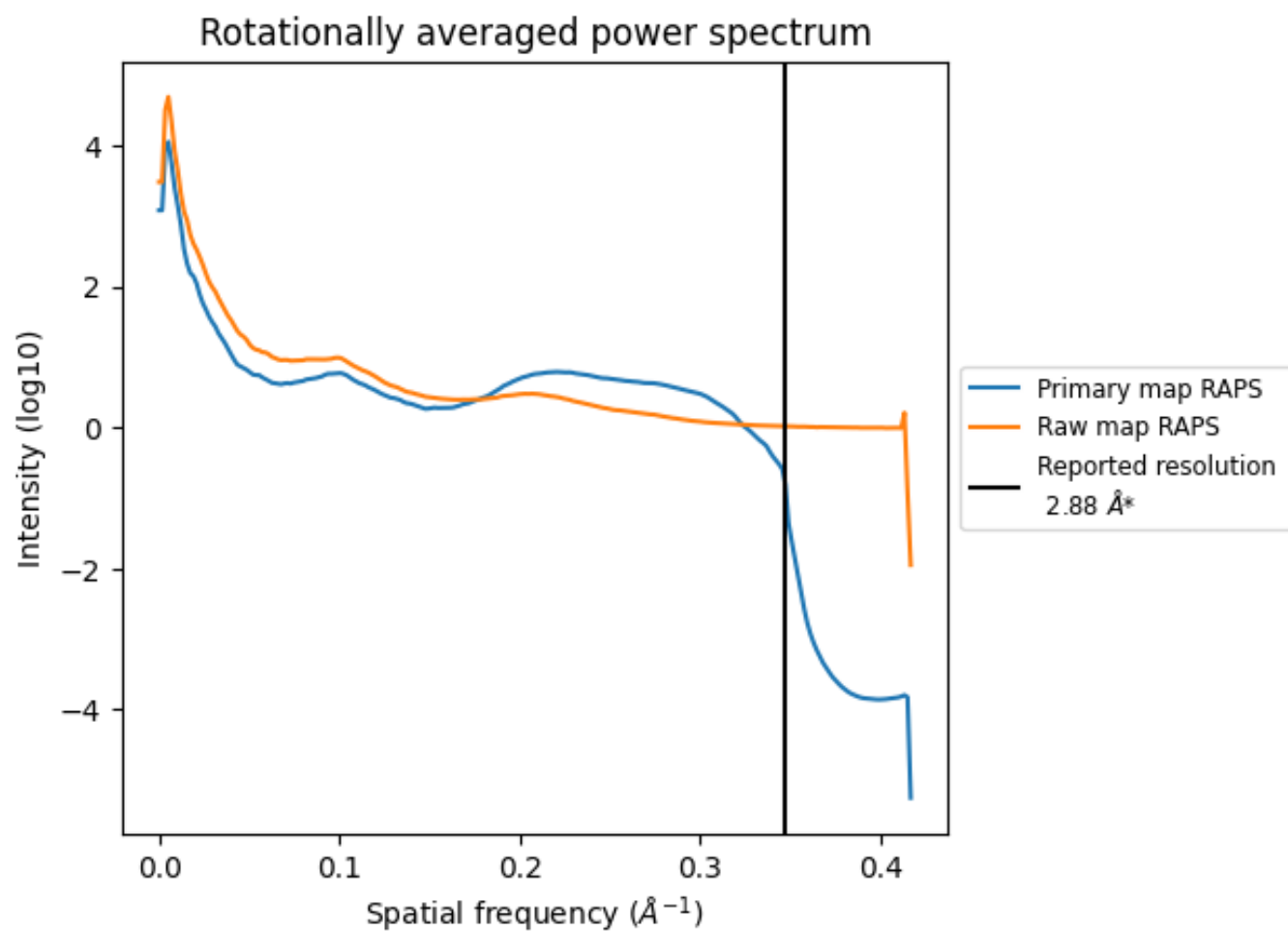
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 716 nm³; this corresponds to an approximate mass of 647 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 ⓘ

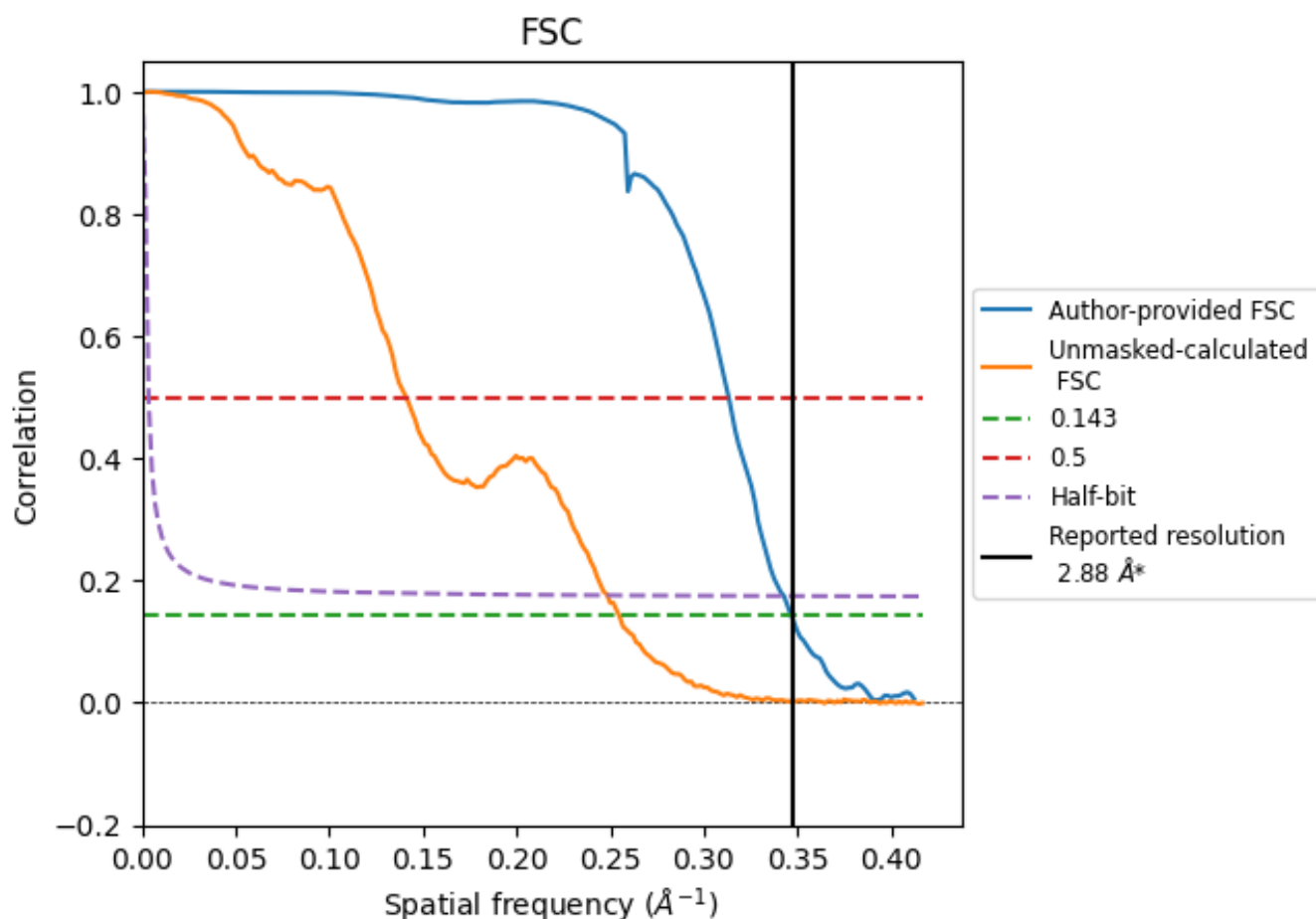


*Reported resolution corresponds to spatial frequency of 0.347 $\text{\AA}^{-1}$

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 0.347 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

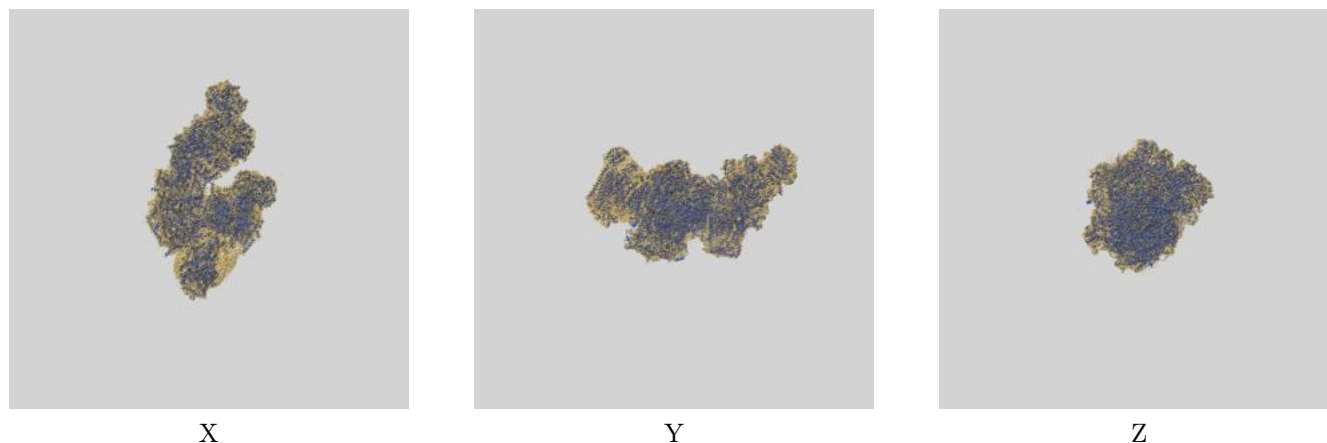
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.89	3.19	2.92
Unmasked-calculated*	3.93	7.10	4.03

*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 3.93 differs from the reported value 2.88 by more than 10 %

9 Map-model fit [i](#)

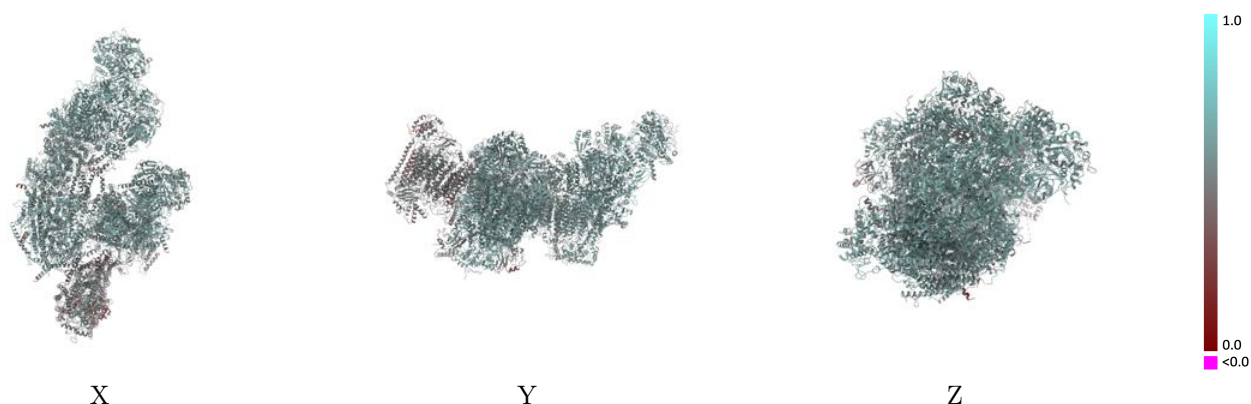
This section contains information regarding the fit between EMDB map EMD-60421 and PDB model 8ZSN. Per-residue inclusion information can be found in section [3](#) on page [31](#).

9.1 Map-model overlay [i](#)



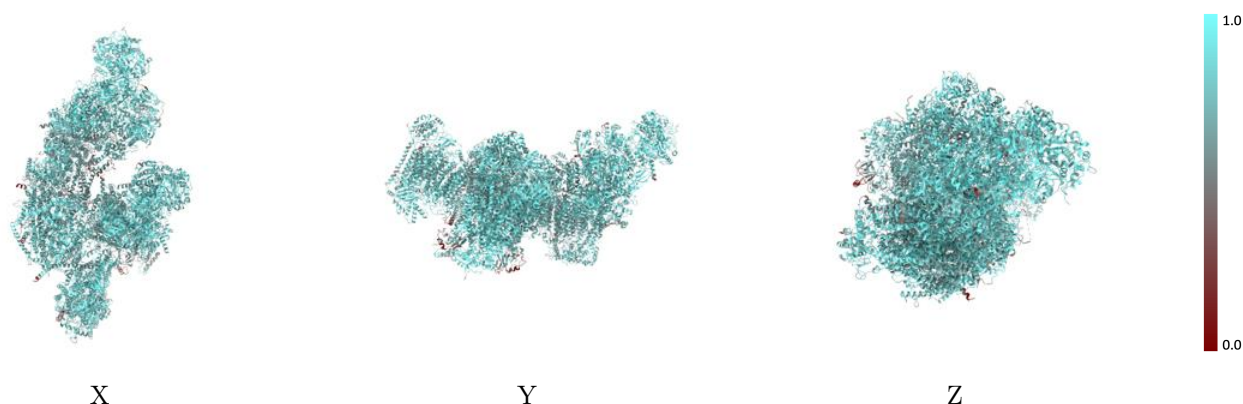
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



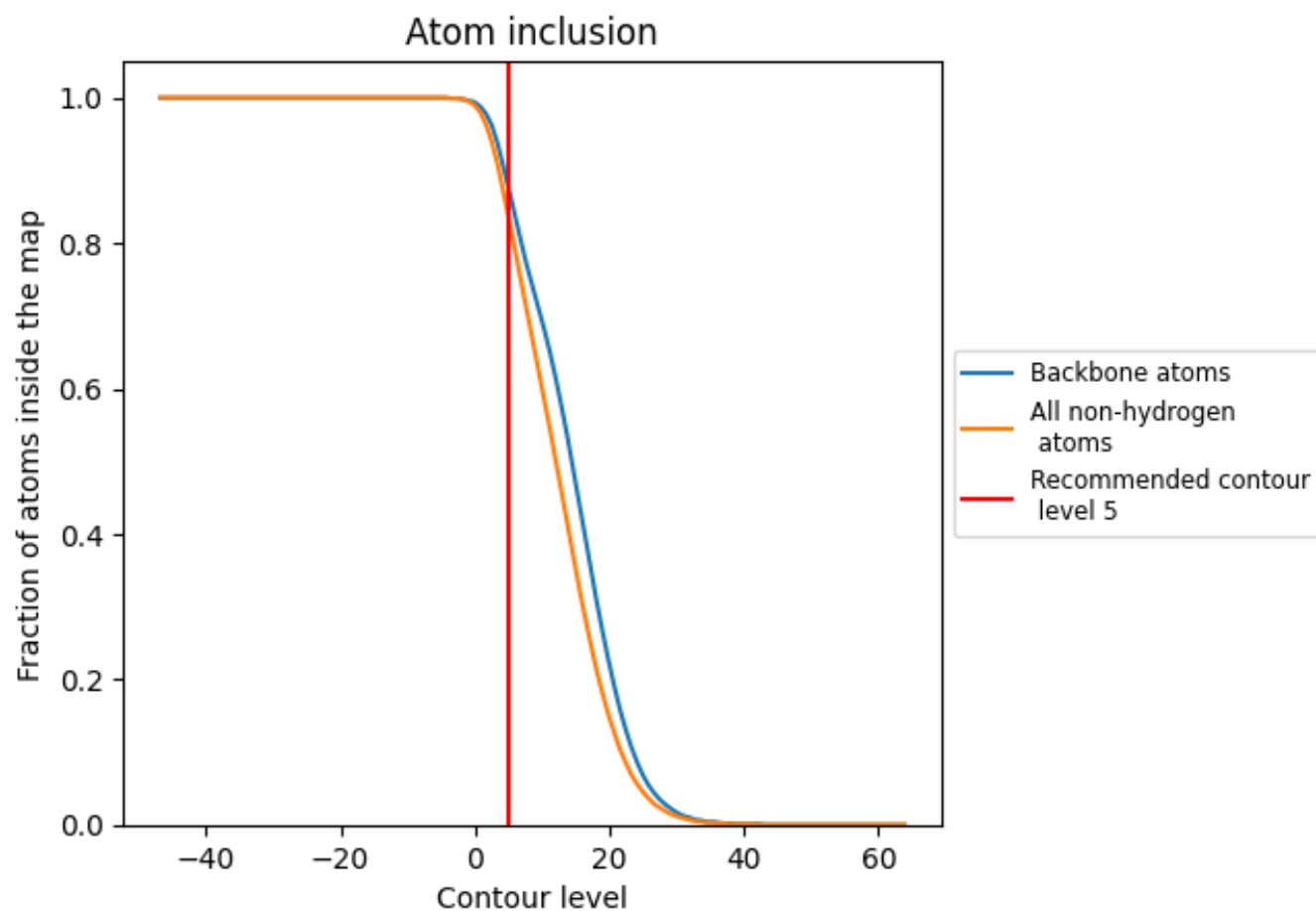
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8360	 0.5670
4L	 0.8320	 0.5910
5A	 0.7580	 0.4290
5B	 0.8440	 0.4410
6A	 0.8670	 0.4580
6B	 0.8750	 0.4400
6C	 0.7060	 0.4420
7A	 0.7560	 0.4210
7B	 0.5610	 0.4390
7C	 0.8920	 0.4830
8B	 0.8250	 0.4710
A1	 0.8580	 0.5950
A2	 0.7710	 0.5700
A3	 0.8110	 0.5750
A5	 0.8060	 0.5810
A6	 0.8090	 0.5860
A7	 0.7690	 0.5660
A8	 0.8270	 0.5880
A9	 0.8570	 0.5960
AB	 0.5740	 0.4850
AC	 0.8440	 0.5780
AK	 0.7820	 0.5590
AL	 0.7140	 0.5670
AM	 0.8010	 0.5860
AN	 0.8170	 0.5810
B1	 0.7260	 0.5310
B2	 0.8140	 0.5720
B3	 0.7570	 0.5410
B4	 0.8350	 0.5810
B5	 0.8620	 0.5980
B6	 0.7710	 0.5350
B7	 0.8020	 0.5510
B8	 0.8410	 0.5850
B9	 0.8460	 0.5860
BK	 0.8310	 0.5800



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Chain	Atom inclusion	Q-score
BL	 0.8290	 0.5720
C1	 0.8910	 0.5040
C2	 0.8580	 0.4780
C3	 0.8700	 0.4750
C4	 0.7870	 0.4500
CA	 0.7320	 0.5710
CB	 0.8510	 0.5870
N1	 0.8470	 0.5940
N2	 0.8870	 0.5990
N3	 0.7770	 0.5890
N4	 0.8770	 0.5940
N5	 0.8600	 0.5910
N6	 0.7830	 0.5590
QA	 0.8670	 0.5770
QB	 0.8530	 0.5800
QC	 0.8900	 0.5960
QD	 0.8740	 0.5850
QE	 0.6060	 0.5110
QF	 0.7330	 0.5180
QG	 0.8490	 0.5810
QH	 0.8350	 0.5740
QI	 0.8390	 0.5780
QJ	 0.7340	 0.5490
QK	 0.7470	 0.5590
Qa	 0.8610	 0.5790
Qb	 0.8690	 0.5830
Qc	 0.8800	 0.5900
Qd	 0.8940	 0.5950
Qe	 0.6060	 0.4870
Qf	 0.7540	 0.5370
Qg	 0.8190	 0.5740
Qh	 0.7890	 0.5740
Qi	 0.8320	 0.5720
Qj	 0.7970	 0.5620
S1	 0.8530	 0.5890
S2	 0.8800	 0.6060
S3	 0.9200	 0.6210
S4	 0.8470	 0.6040
S5	 0.7870	 0.5730
S6	 0.8280	 0.5920
S7	 0.8920	 0.6080
S8	 0.9180	 0.6170

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Chain	Atom inclusion	Q-score
V1	 0.8480	 0.5840
V2	 0.8290	 0.5760
V3	 0.7990	 0.5690