



## Full wwPDB EM Validation Report ⓘ

Dec 8, 2025 – 03:03 PM JST

PDB ID : 8ZP8 / pdb\_00008zp8  
EMDB ID : EMD-60329  
Title : Respirasome open state 1 in presence of metformin(SC-MetO1)  
Authors : Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.  
Deposited on : 2024-05-29  
Resolution : 2.97 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](mailto: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>.

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

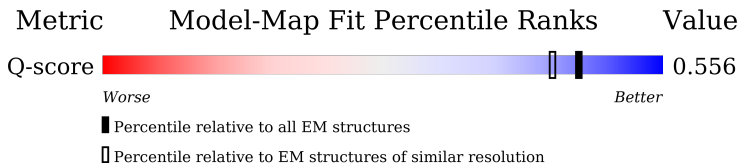
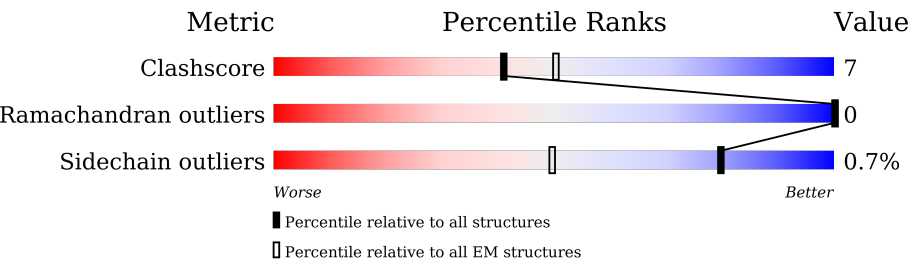
EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the 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) : 2.47

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.97 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.









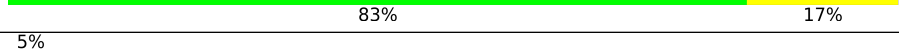
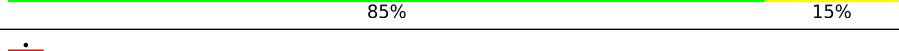
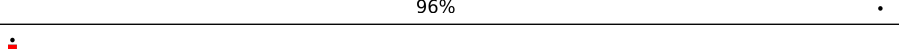
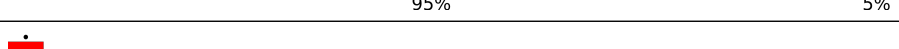
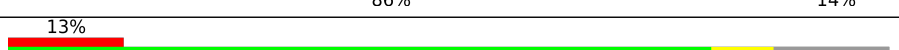

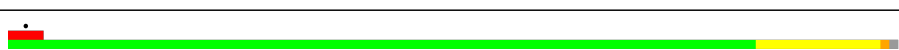
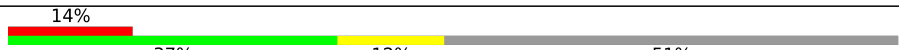
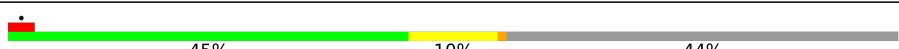





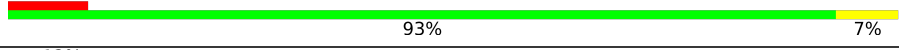
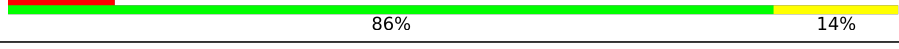

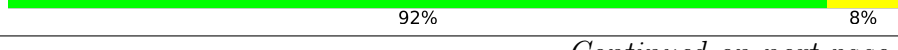

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13205 ( 2.47 - 3.47 )

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  $\geq 3$ , 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	<div><div></div><div>83%</div><div>17%</div></div>
2	5A	102	<div><div></div><div>84%</div><div>16%</div></div>
3	5B	95	<div><div>6%</div><div>85%</div><div>14%</div></div>
4	6A	76	<div><div>9%</div><div>89%</div><div>11%</div></div>

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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	156	
19	AC	156	
20	AK	320	
21	AL	140	
22	AM	144	
23	AN	142	
24	B1	56	
25	B2	67	
26	B3	80	
27	B4	128	
28	B5	138	



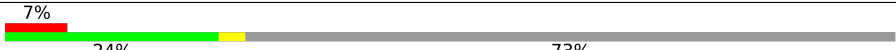
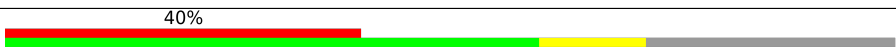

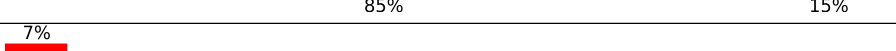
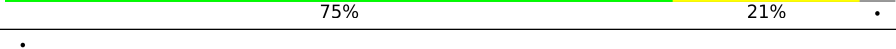





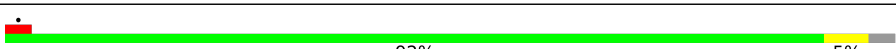


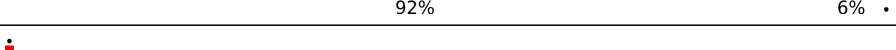








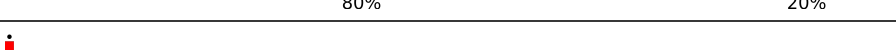
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Mol	Chain	Length	Quality of chain
29	B6	126	
30	B7	125	
31	B8	156	
32	B9	178	
33	BK	176	
34	BL	154	
35	C1	514	
36	C2	228	
37	C3	260	
38	C4	138	
39	CA	49	
40	CB	121	
41	N1	318	
42	N2	347	
43	N3	115	
44	N4	459	
45	N5	603	
46	N6	174	
47	QA	419	
47	Qa	419	
48	QB	446	
48	Qb	446	
49	QC	379	
49	Qc	379	
50	QD	326	

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Mol	Chain	Length	Quality of chain
50	Qd	326	
51	QE	274	
51	QK	274	
51	Qe	274	
52	QF	67	
52	Qf	67	
53	QG	101	
53	Qg	101	
54	QH	81	
54	Qh	81	
55	QI	62	
55	Qi	62	
56	QJ	52	
56	Qj	52	
57	S1	689	
58	S2	430	
59	S3	208	
60	S4	124	
61	S5	105	
62	S6	96	
63	S7	156	
64	S8	176	
65	V1	431	
66	V2	217	
67	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	FES	QE	303	-	-	X	-
82	FES	Qe	301	-	-	X	-
83	SF4	S1	801	-	-	X	-

## 2 Entry composition

There are 84 unique types of molecules in this entry. The entry contains 117250 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	76	Total	C	N	O	S	0	0
			624	403	119	101	1		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A9	337	Total	C	N	O	S	0	0
			2703	1750	472	472	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	320	Total	C	N	O	S	0	0
			2590	1649	440	491	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 Complex I-B17.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B6	102	Total	C	N	O	S	0	0
			870	568	155	146	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	305	Total	C	N	O	S	0	0
			2411	1619	371	400	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	96	Total	C	N	O	S	0	0
			770	525	111	129	5		

- 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	166	Total	C	N	O	S	0	0
			1259	844	180	224	11		

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

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

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

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

- Molecule 49 is a protein called Cytochrome b.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	S1	685	Total	C	N	O	S	0	0
			5266	3303	918	1006	39		

- Molecule 58 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	S2	429	Total	C	N	O	S	0	0
			3452	2208	593	627	24		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

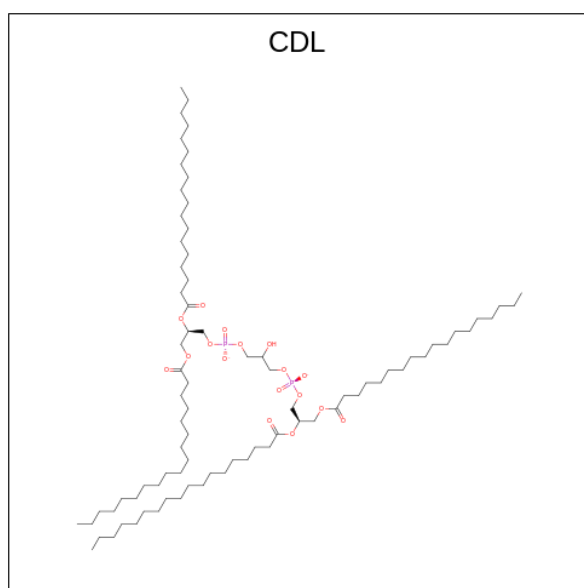
- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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

- Molecule 67 is a protein called Complex I-9kD.

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

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

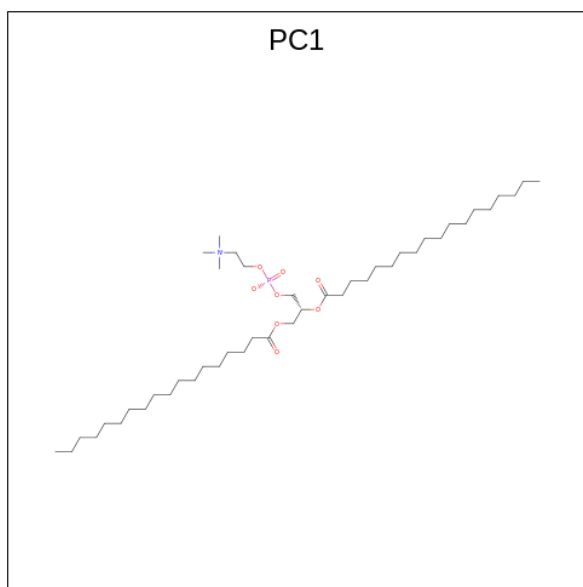


Mol	Chain	Residues	Atoms				AltConf
68	4L	1	Total	C	O	P	0
			92	73	17	2	
68	A1	1	Total	C	O	P	0
			94	75	17	2	
68	A8	1	Total	C	O	P	0
			77	58	17	2	
68	AL	1	Total	C	O	P	0
			94	75	17	2	
68	AL	1	Total	C	O	P	0
			90	71	17	2	
68	B4	1	Total	C	O	P	0
			62	43	17	2	
68	B5	1	Total	C	O	P	0
			98	79	17	2	
68	C1	1	Total	C	O	P	0
			77	58	17	2	
68	N2	1	Total	C	O	P	0
			68	49	17	2	
68	N2	1	Total	C	O	P	0
			100	81	17	2	
68	N5	1	Total	C	O	P	0
			82	63	17	2	
68	N5	1	Total	C	O	P	0
			100	81	17	2	
68	QB	1	Total	C	O	P	0
			61	42	17	2	
68	QC	1	Total	C	O	P	0
			55	36	17	2	
68	QD	1	Total	C	O	P	0
			64	45	17	2	
68	QE	1	Total	C	O	P	0
			100	81	17	2	
68	QH	1	Total	C	O	P	0
			61	42	17	2	
68	QH	1	Total	C	O	P	0
			64	45	17	2	
68	Qb	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 69 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 70 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).



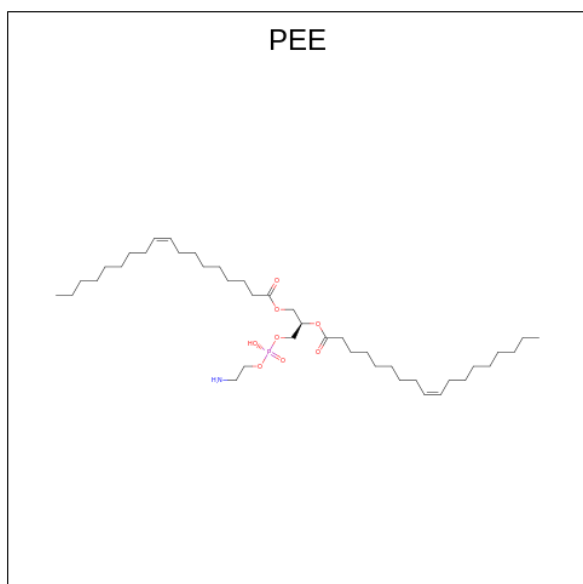
Mol	Chain	Residues	Atoms					AltConf
70	6A	1	Total	C	N	O	P	0
			45	35	1	8	1	
70	7C	1	Total	C	N	O	P	0
			52	42	1	8	1	
70	B5	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	B7	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	C1	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	C1	1	Total	C	N	O	P	0
			33	23	1	8	1	
70	C1	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	C1	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	C1	1	Total	C	N	O	P	0
			50	40	1	8	1	

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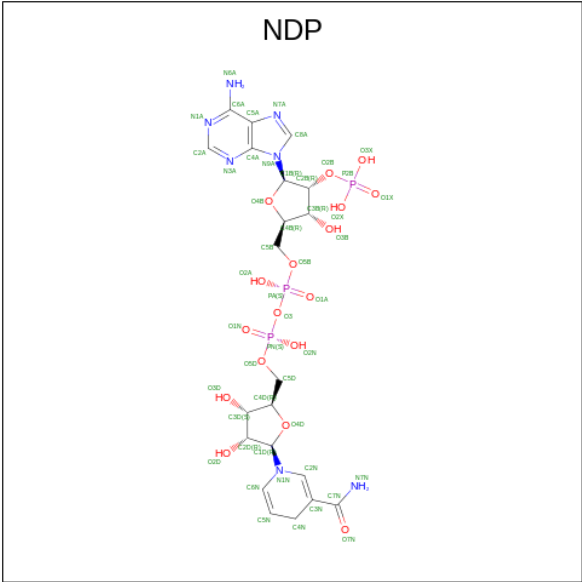
Mol	Chain	Residues	Atoms					AltConf
70	C3	1	Total	C	N	O	P	0
			44	34	1	8	1	
70	C3	1	Total	C	N	O	P	0
			49	39	1	8	1	
70	N1	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	N1	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	N3	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	N5	1	Total	C	N	O	P	0
			31	21	1	8	1	
70	QJ	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	Qb	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	Qc	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	Qc	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	Qd	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	Qh	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 71 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:  $C_{41}H_{78}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
71	6A	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	6A	1	Total	C	N	O	P	0
			36	26	1	8	1	
71	8B	1	Total	C	N	O	P	0
			42	32	1	8	1	
71	A3	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	AL	1	Total	C	N	O	P	0
			40	30	1	8	1	
71	B4	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	C3	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	N4	1	Total	C	N	O	P	0
			49	39	1	8	1	
71	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
71	N5	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	QB	1	Total	C	N	O	P	0
			34	24	1	8	1	
71	QB	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	QC	1	Total	C	N	O	P	0
			40	30	1	8	1	
71	QE	1	Total	C	N	O	P	0
			47	37	1	8	1	
71	Qc	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	Qc	1	Total	C	N	O	P	0
			42	32	1	8	1	
71	Qd	1	Total	C	N	O	P	0
			24	14	1	8	1	
71	S2	1	Total	C	N	O	P	0
			48	38	1	8	1	
71	S8	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 72 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).



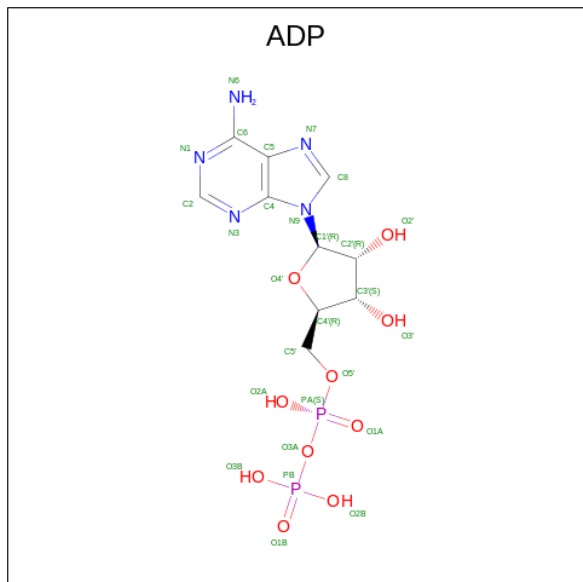
Mol	Chain	Residues	Atoms					AltConf
72	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 73 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>8</sub>PS) (labeled as "Ligand of Interest" by depositor).



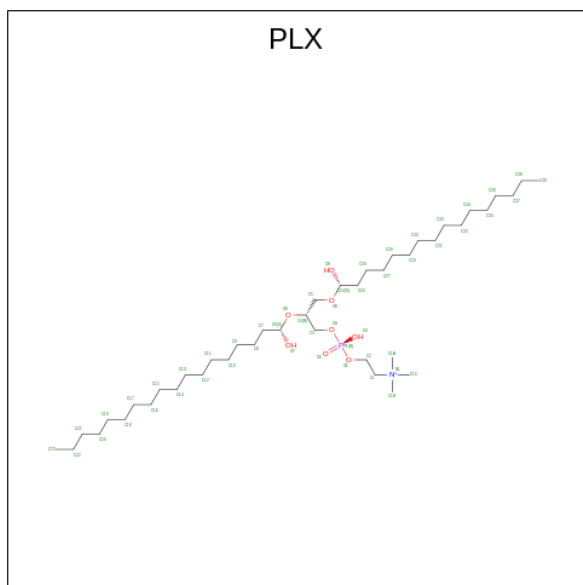
Mol	Chain	Residues	Atoms						AltConf
73	AB	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	
73	AC	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 74 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



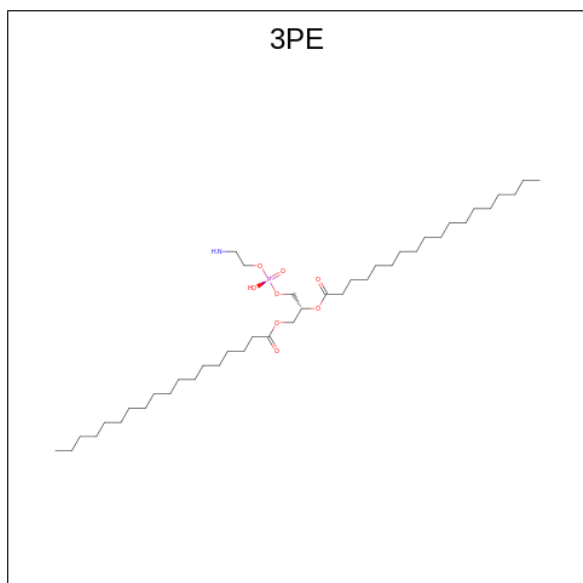
Mol	Chain	Residues	Atoms					AltConf
74	AK	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 75 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:  $C_{42}H_{89}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
75	AM	1	Total	C	N	O	P	0
			52	42	1	8	1	
75	AM	1	Total	C	N	O	P	0
			52	42	1	8	1	
75	B5	1	Total	C	N	O	P	0
			52	42	1	8	1	
75	C2	1	Total	C	N	O	P	0
			43	33	1	8	1	
75	CB	1	Total	C	N	O	P	0
			52	42	1	8	1	
75	N3	1	Total	C	N	O	P	0
			52	42	1	8	1	
75	N4	1	Total	C	N	O	P	0
			47	37	1	8	1	
75	N4	1	Total	C	N	O	P	0
			52	42	1	8	1	
75	QB	1	Total	C	N	O	P	0
			46	36	1	8	1	
75	QI	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 76 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



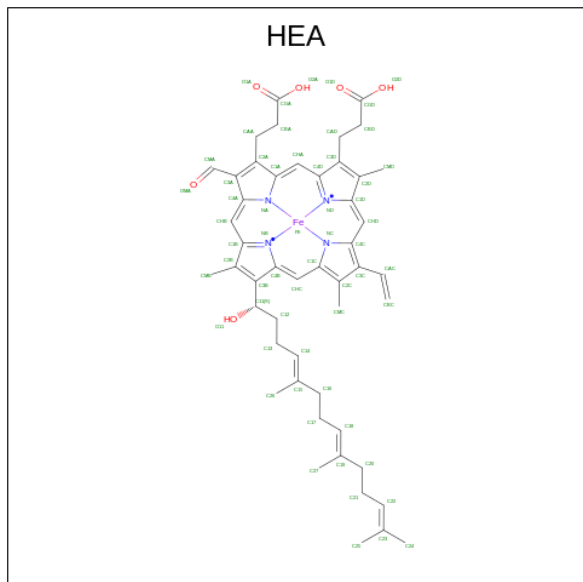
Mol	Chain	Residues	Atoms					AltConf
76	B4	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
76	B8	1	Total	C	N	O	P	0
			32	22	1	8	1	
76	C1	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	C2	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	CA	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	QE	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 77 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
77	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
77	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

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

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

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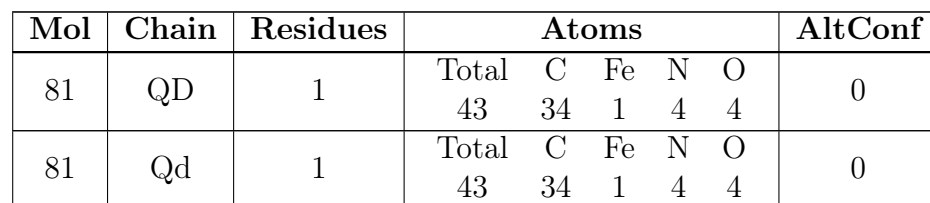
Mol	Chain	Residues	Atoms	AltConf
78	C2	2	Total Cu 2 2	0

- | Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 79  | C1    | 1        | Total Mg<br>1 1 | 0       |
| 79  | S1    | 1        | Total Mg<br>1 1 | 0       |

- # HEM

Mol	Chain	Residues	Atoms					AltConf
80	QC	1	Total 43	C 34	Fe 1	N 4	O 4	0
80	QC	1	Total 43	C 34	Fe 1	N 4	O 4	0
80	Qc	1	Total 43	C 34	Fe 1	N 4	O 4	0
80	Qc	1	Total 43	C 34	Fe 1	N 4	O 4	0

- WORLDWIDE  
**PDB**  
PROTEIN DATA BANK



- 
- Diagram illustrating the structure of a ferredoxin (FES) molecule, showing a square arrangement of four atoms: two Sulfur (S) atoms in yellow and two Iron (Fe) atoms in purple. The atoms are connected by lines forming a square. Labels S1, S2, FE1, and FE2 are placed around the square in green text.

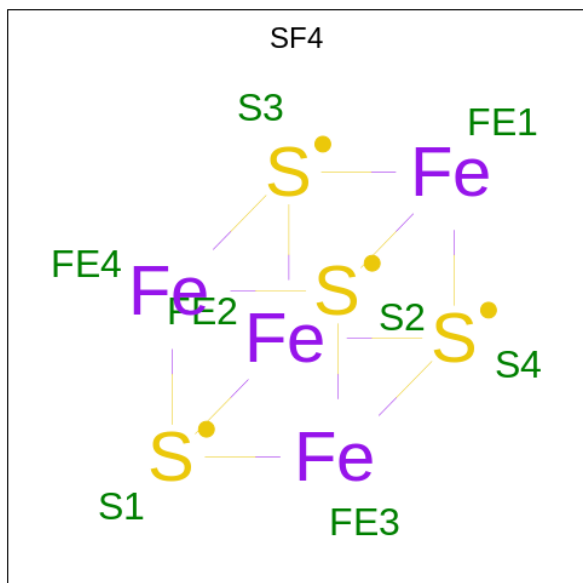
Mol	Chain	Residues	Atoms			AltConf
82	QE	1	Total 4	Fe 2	S 2	0
82	Qe	1	Total 4	Fe 2	S 2	0

WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

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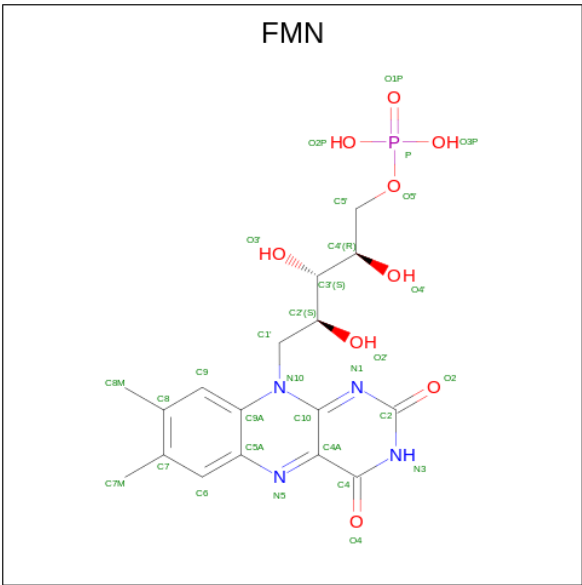
Mol	Chain	Residues	Atoms			AltConf
82	S1	1	Total	Fe	S	0
			4	2	2	
82	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 83 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 84 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ) (labeled as "Ligand of Interest" by depositor).




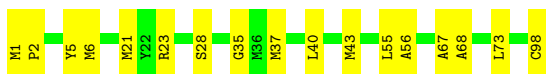
Mol	Chain	Residues	Atoms					AltConf
84	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

### 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.

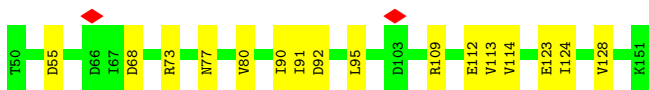
- Molecule 1: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L:  83% 17%




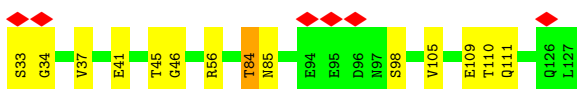
- Molecule 2: Cytochrome c oxidase subunit 5A, mitochondrial

Chain 5A:  84% 16%




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

Chain 5B:  6% 85% 14%




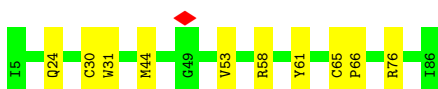
- Molecule 4: Cytochrome c oxidase subunit

Chain 6A:  9% 89% 11%




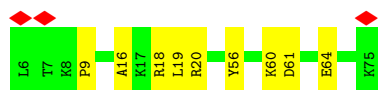
- Molecule 5: Cytochrome c oxidase subunit

Chain 6B:  88% 12%



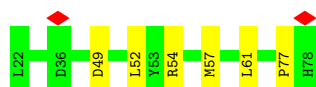
- Molecule 6: Cytochrome c oxidase subunit 6C

Chain 6C:  87% 13%




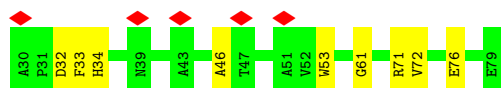
- Molecule 7: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain 7A:  89% 11%




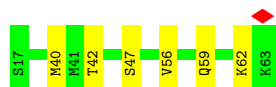
- Molecule 8: Cytochrome c oxidase subunit 7B, mitochondrial

Chain 7B:  10% 82% 18%




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

Chain 7C:  87% 13%




- Molecule 10: Cytochrome c oxidase subunit 8

Chain 8B:  86% 14%




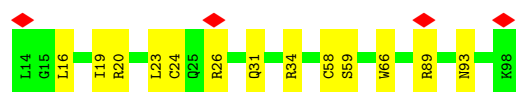
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain A1:  83% 17%

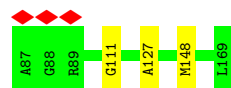


- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

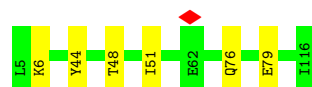
Chain A2:  5% 85% 15%



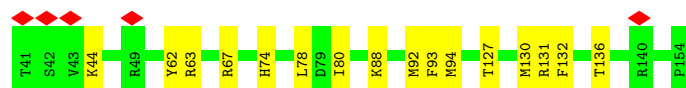
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



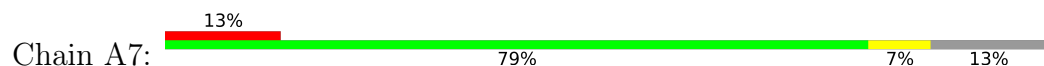
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



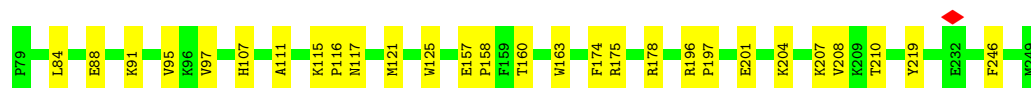
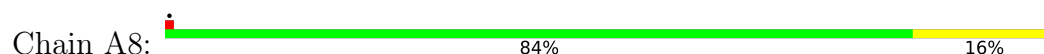
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



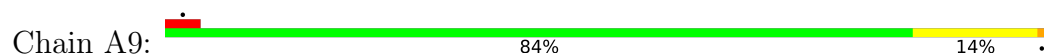
- Molecule 16: Complex I-B14.5a

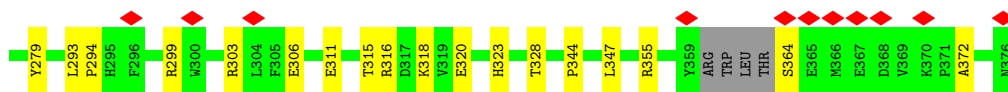


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

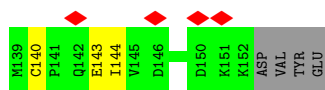
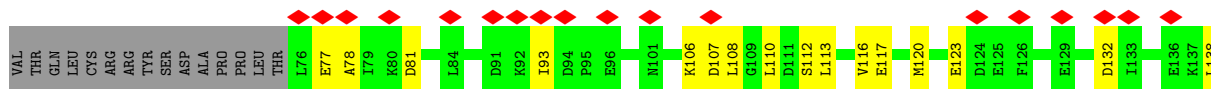
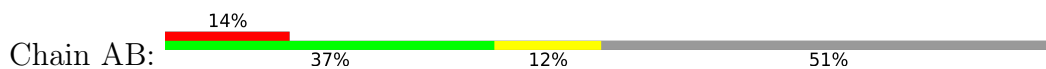


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

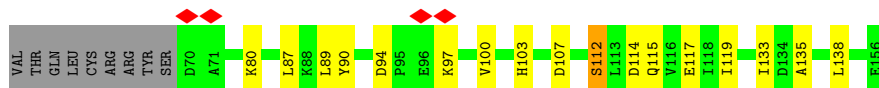




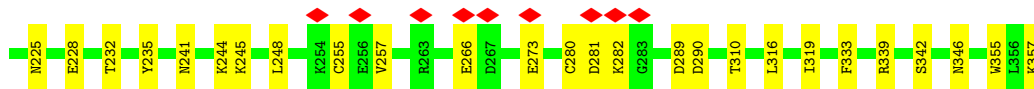
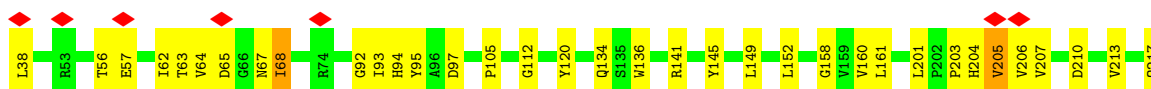
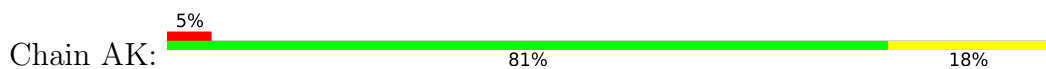
- Molecule 19: Acyl carrier protein



- Molecule 19: Acyl carrier protein



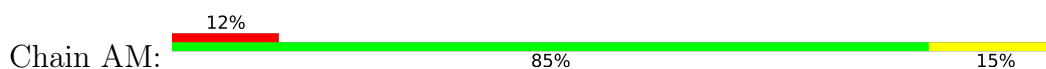
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

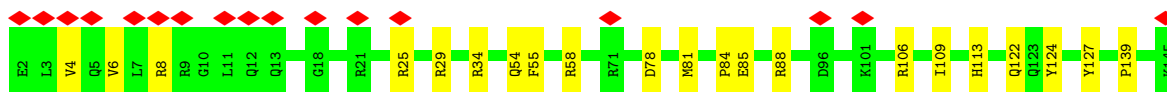


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

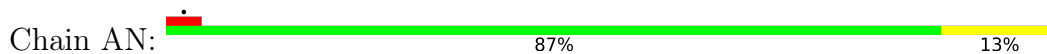


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

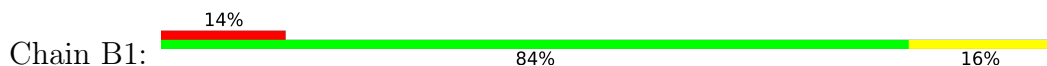




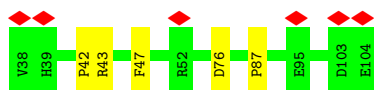
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



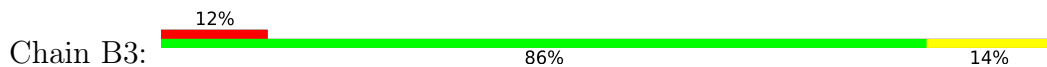
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



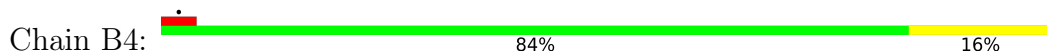
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



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



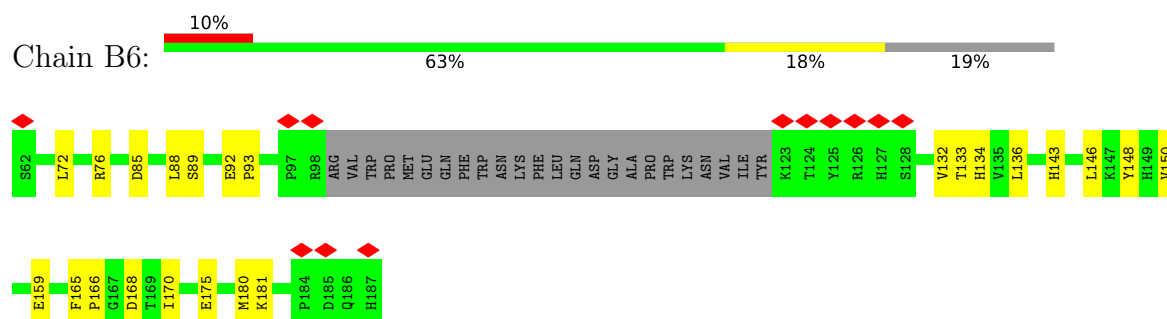
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



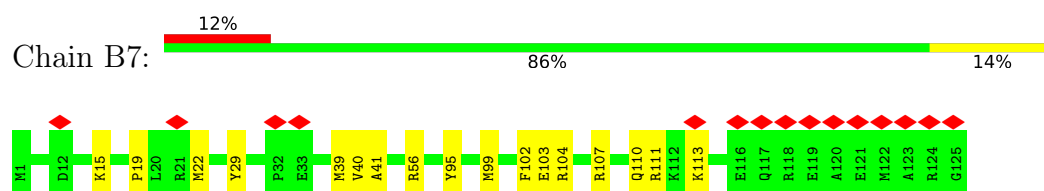
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



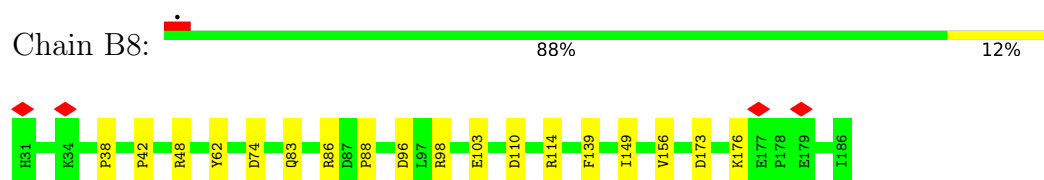
- Molecule 29: Complex I-B17



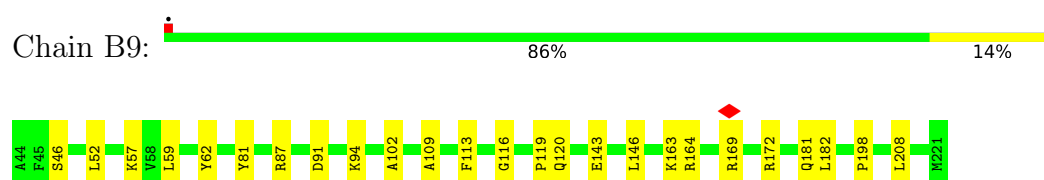
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



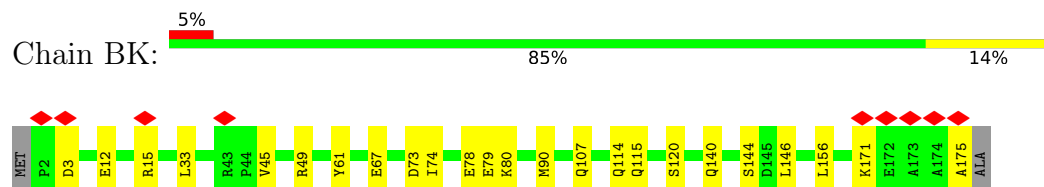
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



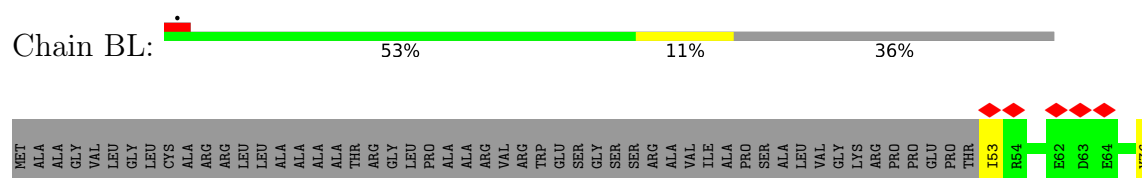
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



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



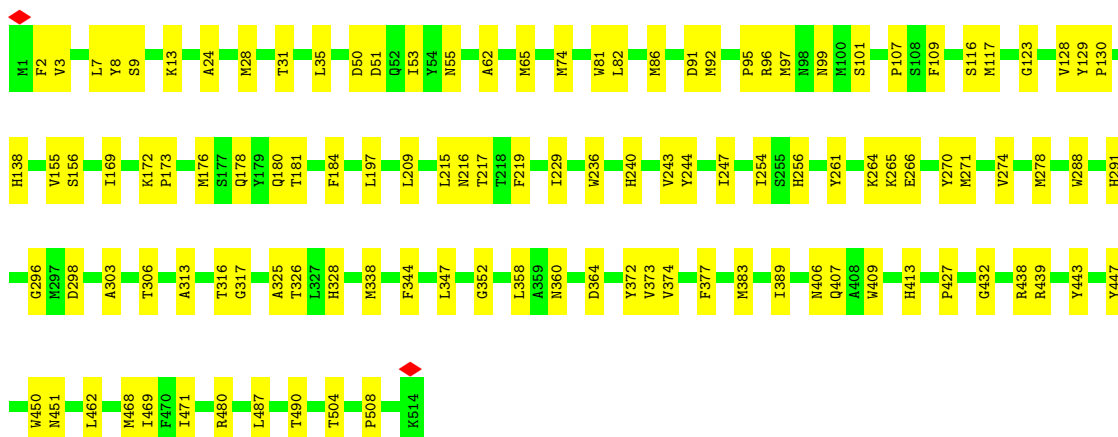
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial





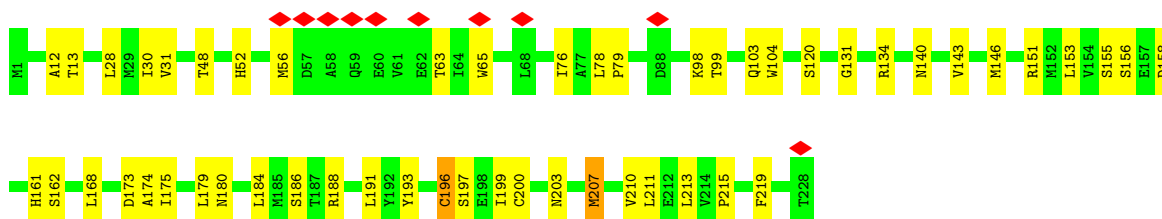
• Molecule 35: Cytochrome c oxidase subunit 1

Chain C1: 78% 22%



• Molecule 36: Cytochrome c oxidase subunit 2

Chain C2: 77% 22%



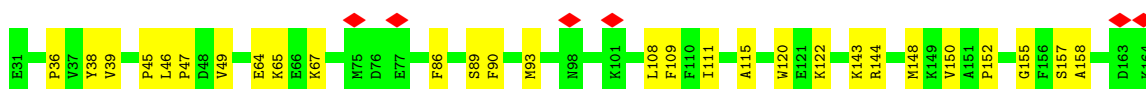
• Molecule 37: Cytochrome c oxidase subunit 3

Chain C3: 82% 18%



• Molecule 38: Cytochrome c oxidase subunit 4

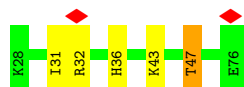
Chain C4: 80% 20%





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

Chain CA: 90% 8%



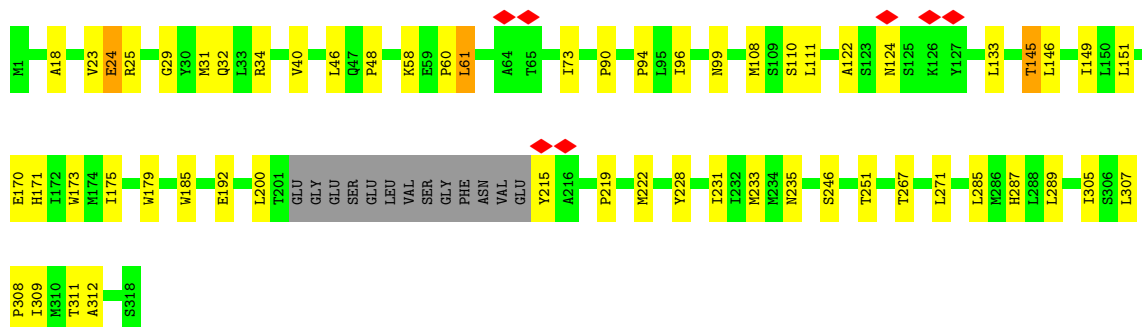
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain CB: 89% 11%



- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain N1: 78% 17%



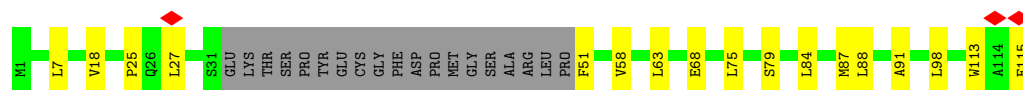
- Molecule 42: NADH-ubiquinone oxidoreductase chain 2

Chain N2: 78% 22%



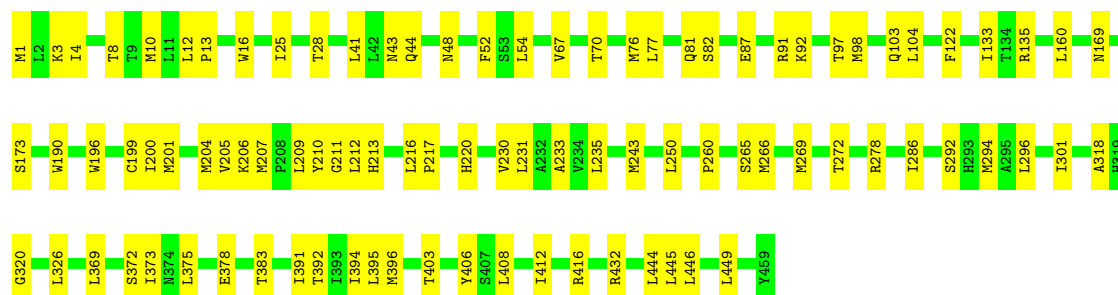
- Molecule 43: NADH-ubiquinone oxidoreductase chain 3

Chain N3: 69% 15% 17%



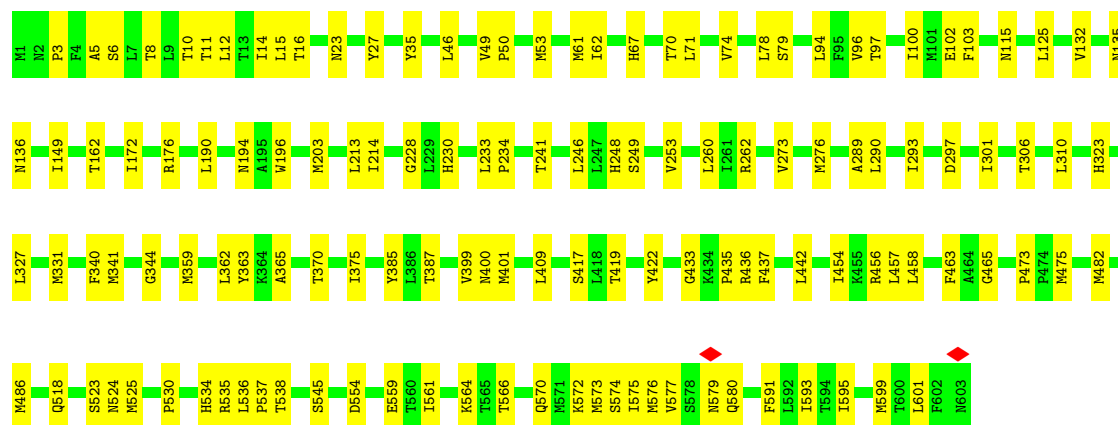
- Molecule 44: NADH-ubiquinone oxidoreductase chain 4

Chain N4: 80% 20%



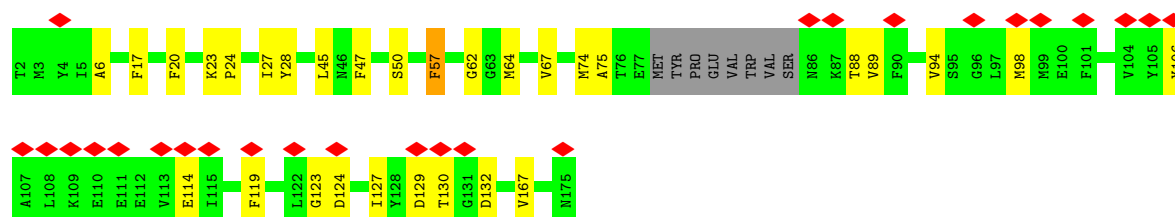
- Molecule 45: NADH-ubiquinone oxidoreductase chain 5

Chain N5: 78% 22%



- Molecule 46: NADH-ubiquinone oxidoreductase chain 6

Chain N6: 15% 78% 17% 5%



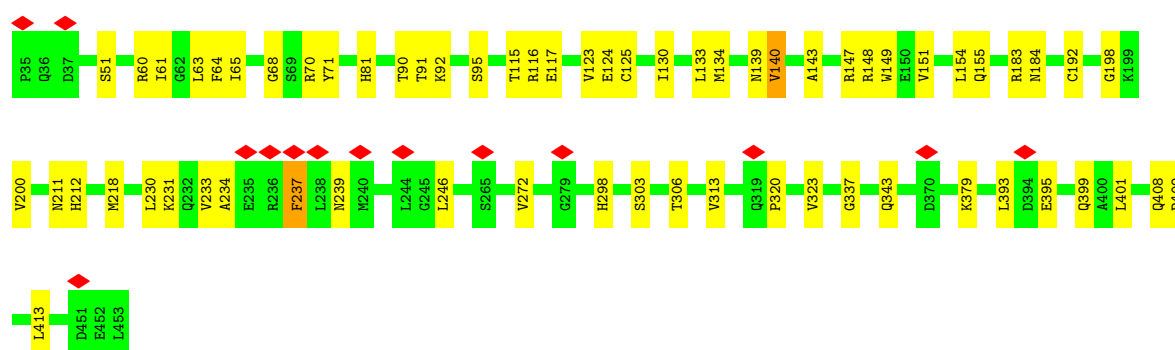
- Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain QA: 85% 15%



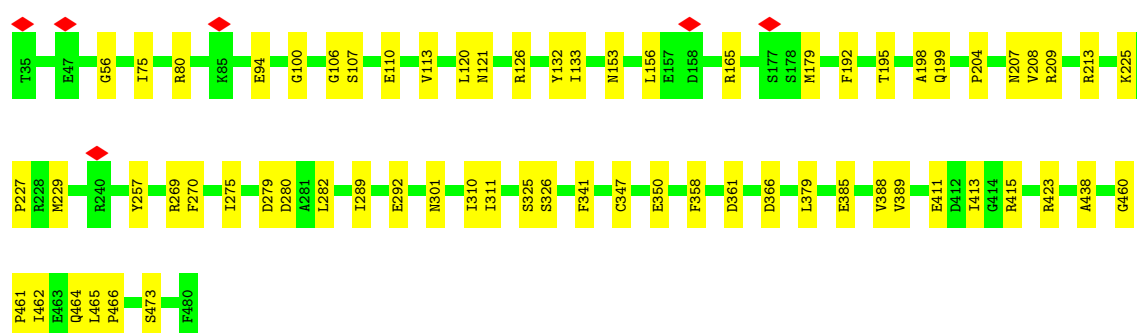
- Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain Qa: 85% 15%



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

Chain QB: 85% 15%




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

Chain Qb: 86% 11%




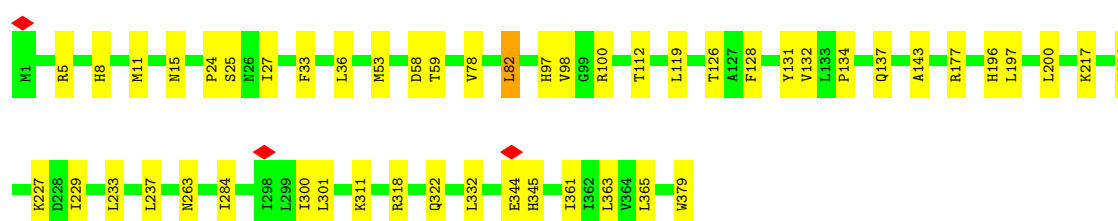
- Molecule 49: Cytochrome b

Chain QC:  87% 13%



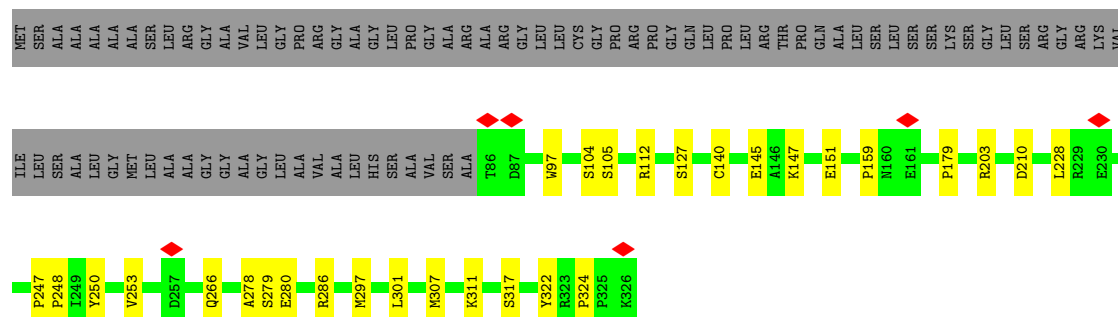
- Molecule 49: Cytochrome b

Chain Qc:  87% 13%



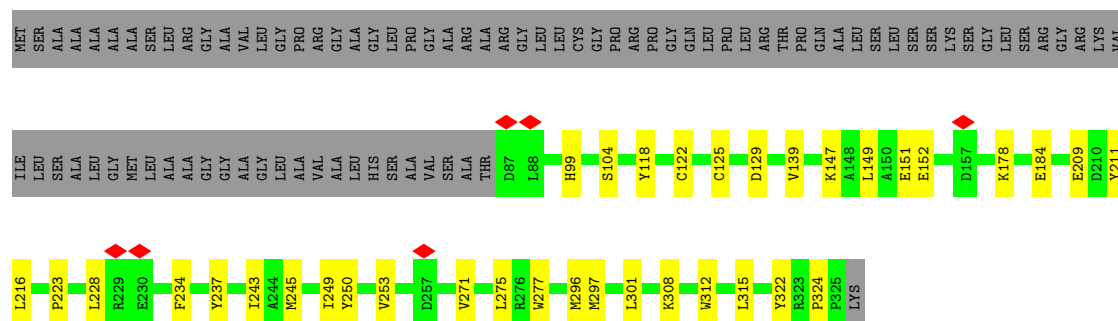
- Molecule 50: Cytochrome c1, heme protein, mitochondrial

Chain QD:  64% 10% 26%

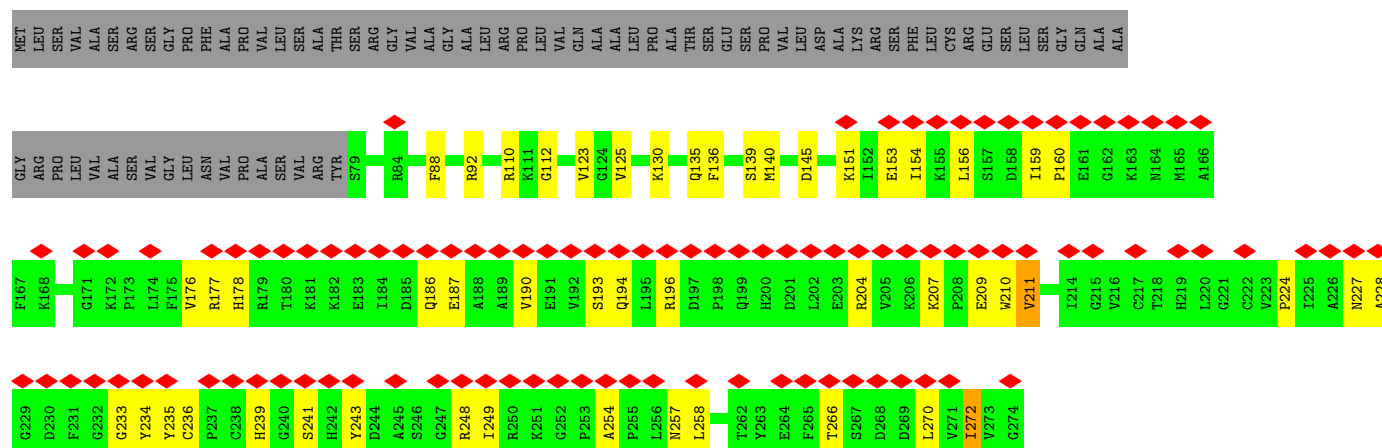
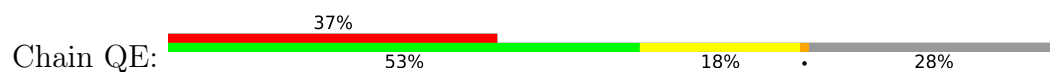


- Molecule 50: Cytochrome c1, heme protein, mitochondrial

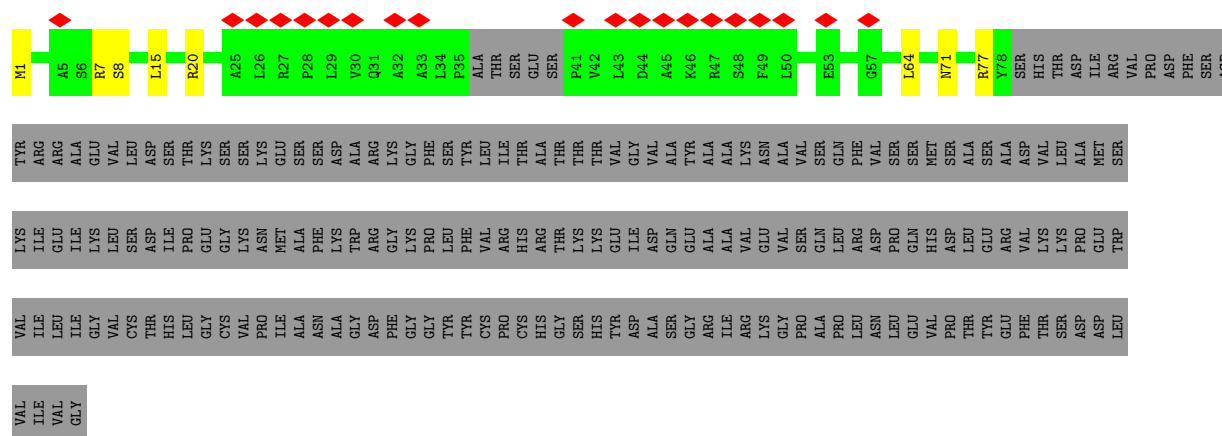
Chain Qd:  62% 11% 27%



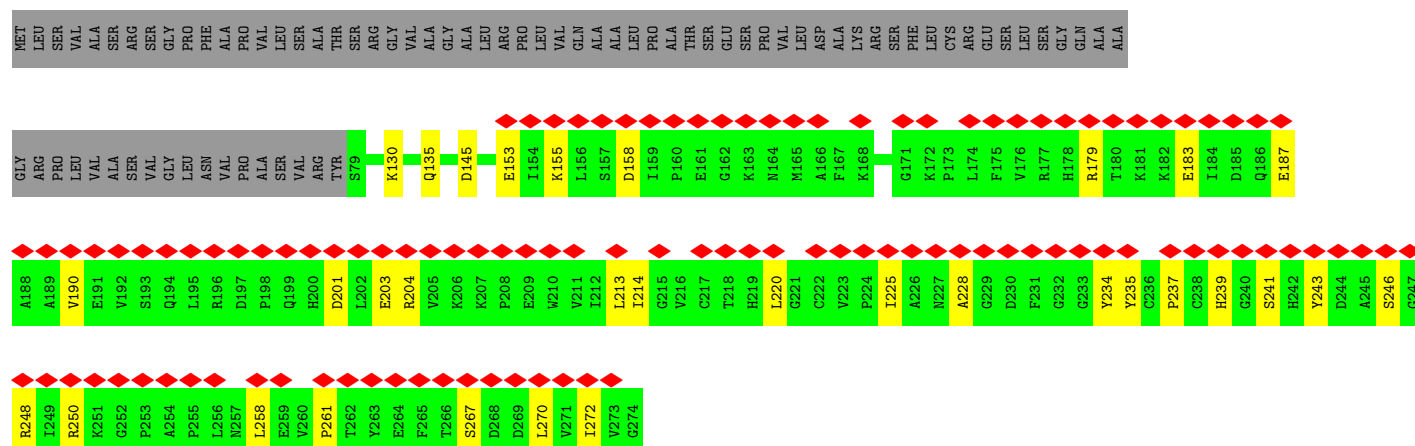
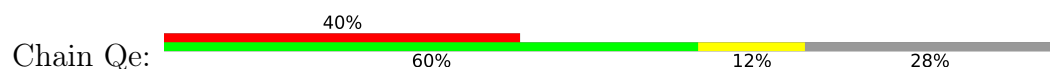
- Molecule 51: Cytochrome b-c1 complex subunit Rieske, mitochondrial



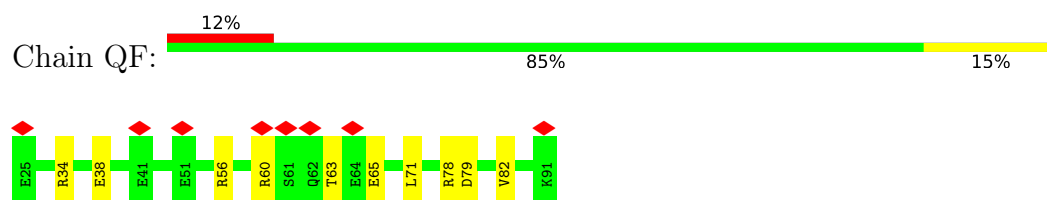
- Molecule 51: Cytochrome b-c1 complex subunit Rieske, mitochondrial



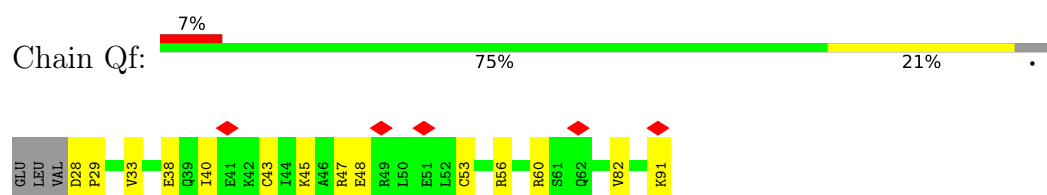
- Molecule 51: Cytochrome b-c1 complex subunit Rieske, mitochondrial



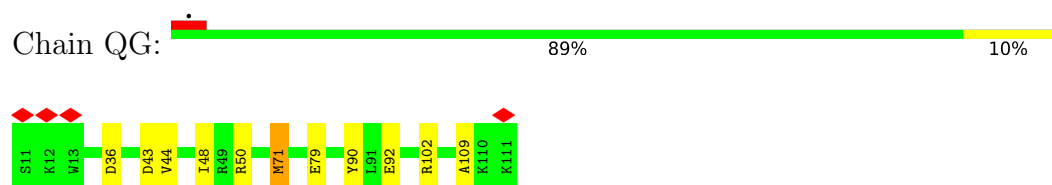
- Molecule 52: Cytochrome b-c1 complex subunit 6



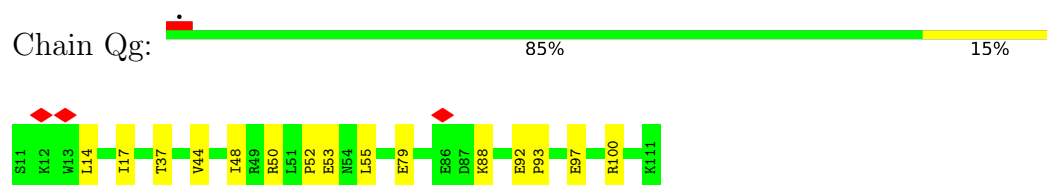
- Molecule 52: Cytochrome b-c1 complex subunit 6



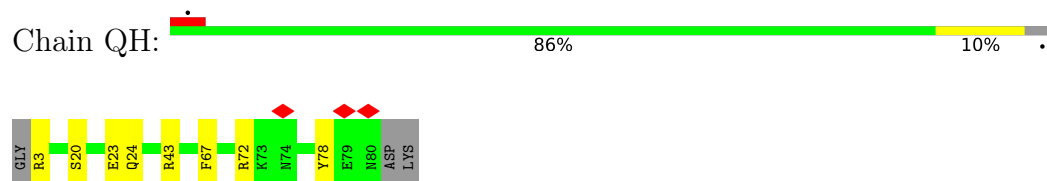
- Molecule 53: Cytochrome b-c1 complex subunit 7



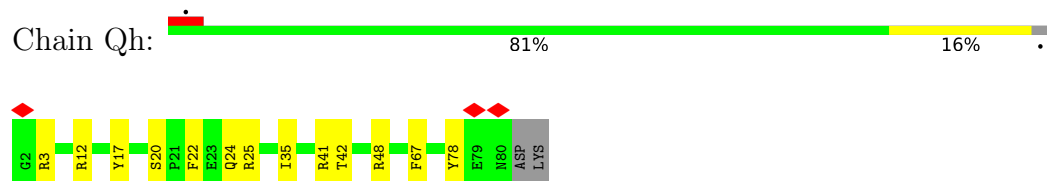
- Molecule 53: Cytochrome b-c1 complex subunit 7



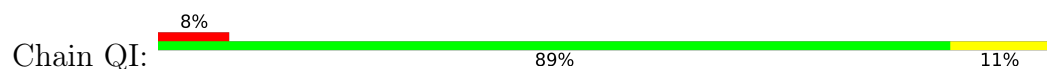
- Molecule 54: Cytochrome b-c1 complex subunit 8

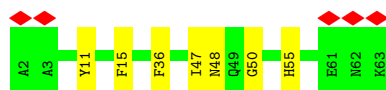


- Molecule 54: Cytochrome b-c1 complex subunit 8

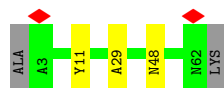


- Molecule 55: Complex III subunit 9

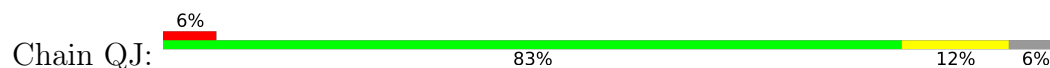




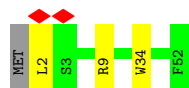
- Molecule 55: Complex III subunit 9



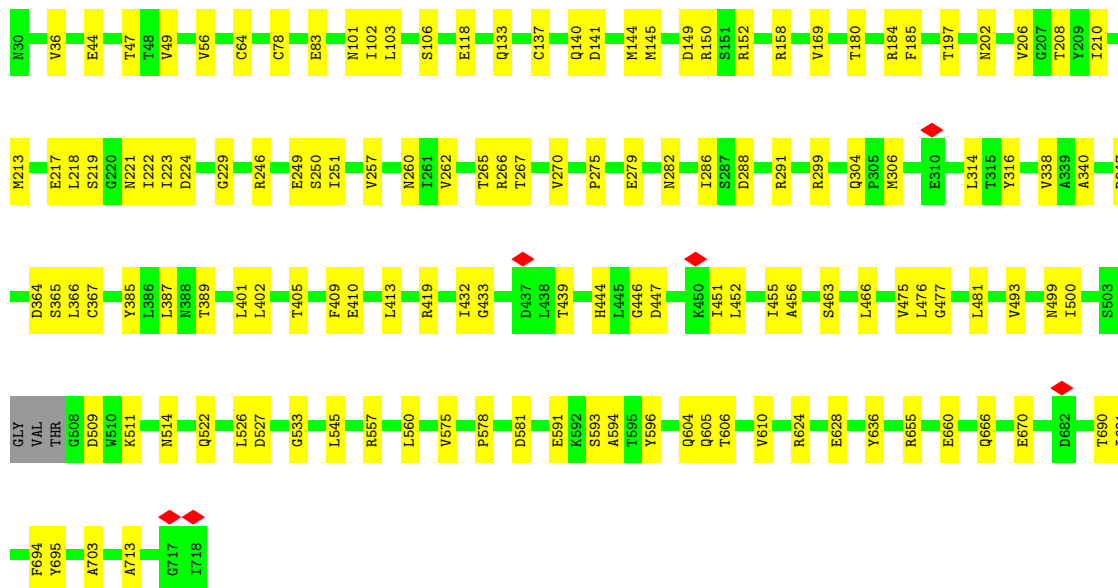
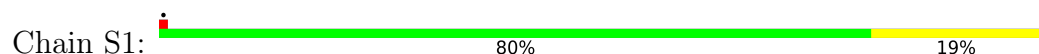
- Molecule 56: Cytochrome b-c1 complex subunit 10



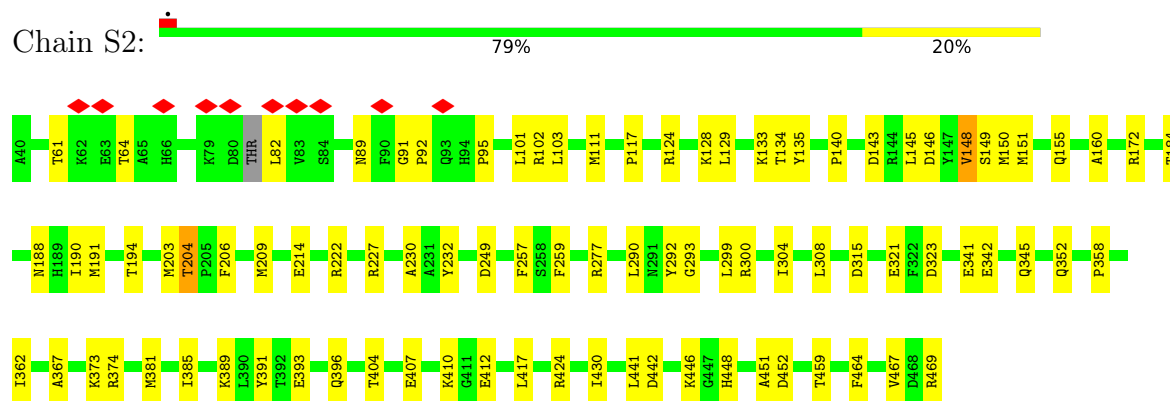
- Molecule 56: Cytochrome b-c1 complex subunit 10



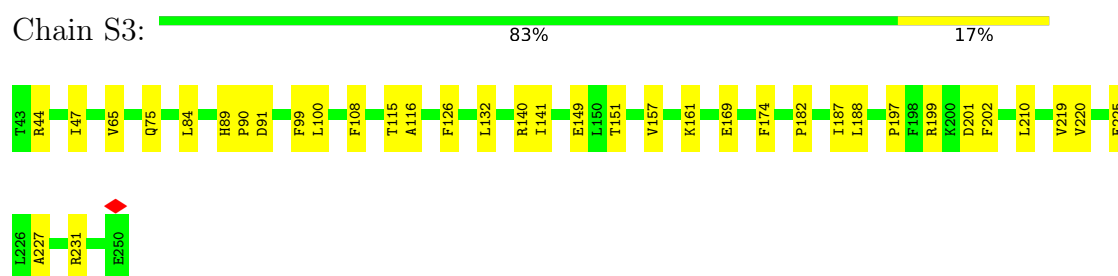
- Molecule 57: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



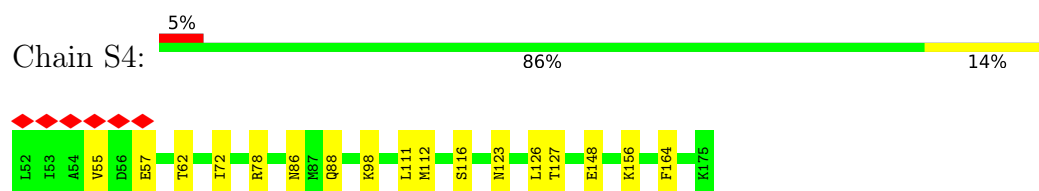
- Molecule 58: Complex I-49kD



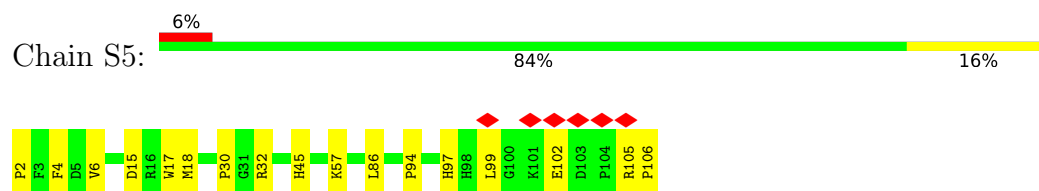
- Molecule 59: Complex I-30kD



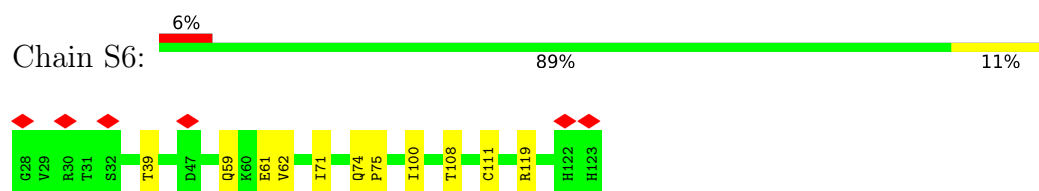
- Molecule 60: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



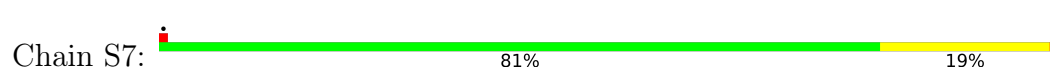
- Molecule 61: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

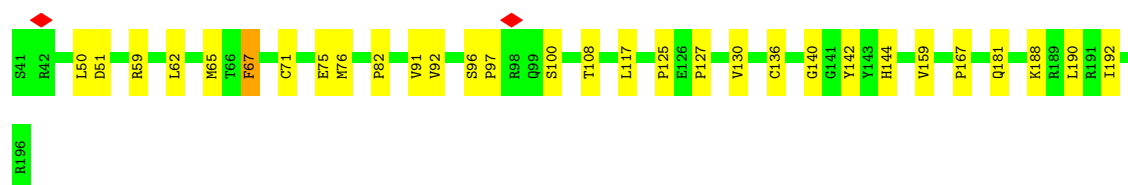


- Molecule 62: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

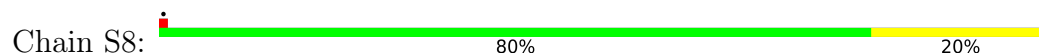


- Molecule 63: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

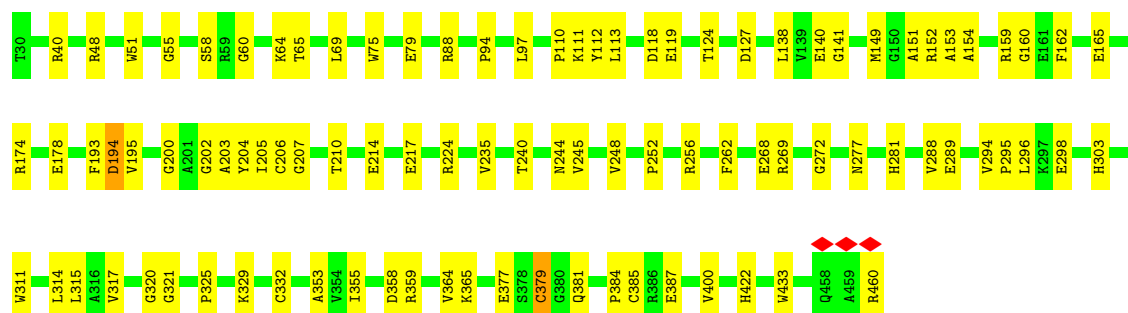
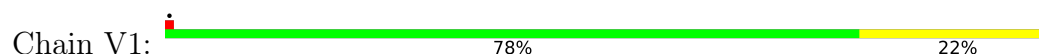




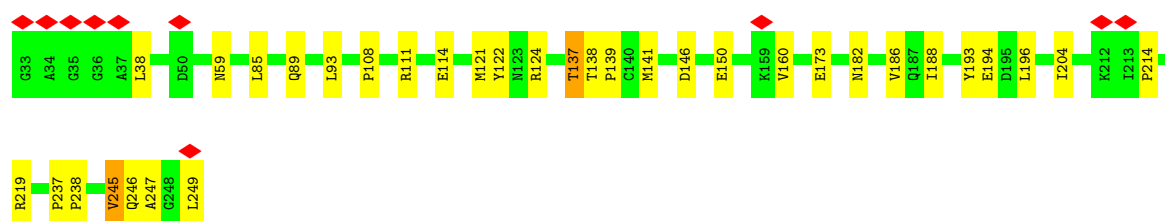
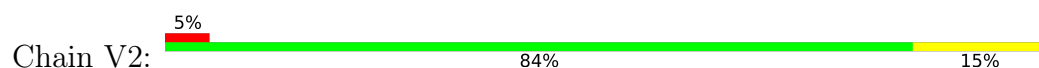
- Molecule 64: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



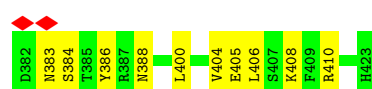
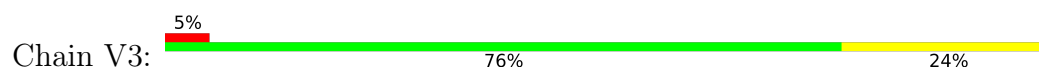
- Molecule 65: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



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



- Molecule 67: Complex I-9kD



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	217871	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	51.9	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	47.979	Depositor
Minimum map value	-21.464	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	1.073	Depositor
Recommended contour level	6	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: PC1, HEC, PEE, HEA, 2MR, HEM, FES, 3PE, MG, PLX, CDL, SF4, NDP, CU, ADP, FMN, ZMP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	4L	0.23	0/759	0.27	0/1029
2	5A	0.17	0/843	0.25	0/1145
3	5B	0.21	0/739	0.32	0/1002
4	6A	0.16	0/652	0.26	0/893
5	6B	0.20	0/704	0.25	0/951
6	6C	0.17	0/587	0.27	0/781
7	7A	0.17	0/457	0.27	0/620
8	7B	0.16	0/405	0.24	0/555
9	7C	0.23	0/400	0.26	0/536
10	8B	0.21	0/349	0.26	0/477
11	A1	0.20	0/577	0.28	0/777
12	A2	0.15	0/697	0.25	0/938
13	A3	0.17	0/664	0.24	0/912
14	A5	0.18	0/929	0.24	0/1258
15	A6	0.18	0/991	0.25	0/1335
16	A7	0.16	0/798	0.23	0/1079
17	A8	0.19	0/1436	0.26	0/1938
18	A9	0.18	0/2777	0.26	0/3762
19	AB	0.12	0/633	0.22	0/851
19	AC	0.21	0/714	0.25	0/965
20	AK	0.20	0/2650	0.36	2/3588 (0.1%)
21	AL	0.17	0/1042	0.22	0/1411
22	AM	0.16	0/1245	0.23	0/1694
23	AN	0.20	0/1204	0.25	0/1624
24	B1	0.18	0/491	0.24	0/663
25	B2	0.18	0/610	0.26	0/836
26	B3	0.17	0/660	0.27	0/892
27	B4	0.20	0/1092	0.26	0/1481
28	B5	0.22	0/1184	0.27	0/1603
29	B6	0.20	0/897	0.31	0/1219
30	B7	0.17	0/1092	0.25	0/1459

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	B8	0.20	0/1371	0.25	0/1875
32	B9	0.20	0/1590	0.28	0/2155
33	BK	0.20	0/1489	0.25	0/2008
34	BL	0.21	0/851	0.31	0/1155
35	C1	0.27	0/4164	0.34	0/5689
36	C2	0.24	0/1880	0.32	0/2564
37	C3	0.23	0/2186	0.29	0/2991
38	C4	0.18	0/1187	0.25	0/1606
39	CA	0.17	0/430	0.23	0/581
40	CB	0.22	0/1031	0.27	0/1394
41	N1	0.24	0/2482	0.36	0/3394
42	N2	0.26	0/2773	0.35	0/3768
43	N3	0.21	0/788	0.26	0/1076
44	N4	0.25	0/3723	0.34	0/5078
45	N5	0.23	0/4914	0.35	0/6683
46	N6	0.20	0/1289	0.31	0/1744
47	QA	0.21	0/3200	0.29	0/4333
47	Qa	0.21	0/3200	0.29	0/4333
48	QB	0.22	0/3531	0.31	0/4793
48	Qb	0.21	0/3436	0.28	0/4659
49	QC	0.24	0/3123	0.31	0/4269
49	Qc	0.24	0/3123	0.32	0/4269
50	QD	0.21	0/1979	0.27	0/2684
50	Qd	0.21	0/1962	0.28	0/2663
51	QE	0.16	0/1550	0.25	0/2098
51	QK	0.16	0/528	0.27	0/716
51	Qe	0.15	0/1550	0.28	0/2098
52	QF	0.16	0/558	0.23	0/747
52	Qf	0.17	0/534	0.25	0/714
53	QG	0.21	0/913	0.27	0/1223
53	Qg	0.21	0/913	0.28	0/1223
54	QH	0.20	0/684	0.32	0/926
54	Qh	0.20	0/688	0.29	0/931
55	QI	0.18	0/520	0.21	0/701
55	Qi	0.20	0/506	0.25	0/683
56	QJ	0.16	0/420	0.24	0/576
56	Qj	0.19	0/437	0.30	0/598
57	S1	0.22	0/5353	0.32	2/7251 (0.0%)
58	S2	0.25	0/3530	0.31	0/4783
59	S3	0.23	0/1789	0.29	0/2436
60	S4	0.22	0/1030	0.28	0/1391
61	S5	0.19	0/889	0.27	0/1190
62	S6	0.17	0/755	0.26	0/1018

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
63	S7	0.23	0/1279	0.27	0/1730
64	S8	0.24	0/1443	0.29	0/1952
65	V1	0.19	0/3391	0.30	0/4583
66	V2	0.17	0/1711	0.28	0/2328
67	V3	0.14	0/365	0.19	0/493
All	All	0.21	0/115316	0.29	4/156427 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AK	204	HIS	CA-C-N	-5.99	114.71	123.10
20	AK	204	HIS	C-N-CA	-5.99	114.71	123.10
57	S1	364	ASP	CA-C-N	-5.66	113.83	122.21
57	S1	364	ASP	C-N-CA	-5.66	113.83	122.21

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4L	748	0	799	16	0
2	5A	825	0	823	12	0
3	5B	724	0	705	10	0
4	6A	624	0	592	7	0
5	6B	684	0	649	8	0
6	6C	574	0	590	7	0
7	7A	447	0	443	5	0
8	7B	392	0	372	9	0
9	7C	387	0	385	7	0
10	8B	338	0	342	6	0
11	A1	562	0	557	9	0
12	A2	686	0	699	8	0
13	A3	643	0	642	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A5	910	0	950	4	0
15	A6	967	0	972	18	0
16	A7	780	0	808	7	0
17	A8	1398	0	1372	20	0
18	A9	2703	0	2720	30	0
19	AB	624	0	625	15	0
19	AC	702	0	694	12	0
20	AK	2590	0	2553	44	0
21	AL	1021	0	1025	7	0
22	AM	1204	0	1162	16	0
23	AN	1173	0	1166	16	0
24	B1	479	0	486	6	0
25	B2	584	0	529	4	0
26	B3	641	0	620	9	0
27	B4	1062	0	1072	16	0
28	B5	1151	0	1164	11	0
29	B6	870	0	890	18	0
30	B7	1068	0	1041	13	0
31	B8	1315	0	1208	14	0
32	B9	1534	0	1470	19	0
33	BK	1456	0	1426	22	0
34	BL	828	0	788	12	0
35	C1	4024	0	4005	91	0
36	C2	1833	0	1843	38	0
37	C3	2103	0	2034	48	0
38	C4	1153	0	1130	24	0
39	CA	417	0	422	4	0
40	CB	1000	0	994	15	0
41	N1	2411	0	2522	49	0
42	N2	2710	0	2874	57	0
43	N3	770	0	816	17	0
44	N4	3631	0	3839	68	0
45	N5	4785	0	4933	99	0
46	N6	1259	0	1261	28	0
47	QA	3147	0	3129	40	0
47	Qa	3147	0	3129	40	0
48	QB	3459	0	3350	41	0
48	Qb	3367	0	3262	33	0
49	QC	3025	0	3090	36	0
49	Qc	3025	0	3090	39	0
50	QD	1921	0	1867	22	0
50	Qd	1904	0	1849	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	QE	1517	0	1500	37	0
51	QK	520	0	554	5	0
51	Qe	1517	0	1500	23	0
52	QF	552	0	536	9	0
52	Qf	528	0	510	8	0
53	QG	893	0	888	7	0
53	Qg	893	0	888	8	0
54	QH	662	0	660	7	0
54	Qh	666	0	663	12	0
55	QI	507	0	509	5	0
55	Qi	493	0	491	4	0
56	QJ	405	0	405	6	0
56	Qj	421	0	418	2	0
57	S1	5266	0	5296	81	0
58	S2	3452	0	3388	65	0
59	S3	1738	0	1693	26	0
60	S4	1007	0	1008	14	0
61	S5	867	0	871	16	0
62	S6	741	0	701	9	0
63	S7	1248	0	1254	19	0
64	S8	1412	0	1363	29	0
65	V1	3316	0	3272	60	0
66	V2	1671	0	1673	21	0
67	V3	355	0	329	9	0
68	4L	92	0	137	3	0
68	A1	94	0	141	5	0
68	A8	77	0	98	10	0
68	AL	184	0	268	9	0
68	B4	62	0	68	3	0
68	B5	98	0	149	3	0
68	C1	77	0	98	7	0
68	N2	168	0	236	13	0
68	N5	182	0	270	12	0
68	QB	61	0	66	1	0
68	QC	55	0	54	4	0
68	QD	64	0	72	1	0
68	QE	100	0	156	2	0
68	QH	125	0	138	4	0
68	Qb	64	0	72	6	0
69	5B	1	0	0	0	0
69	S6	1	0	0	0	0
70	6A	45	0	64	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	7C	52	0	81	4	0
70	B5	54	0	88	2	0
70	B7	54	0	88	1	0
70	C1	237	0	362	22	0
70	C3	93	0	140	9	0
70	N1	108	0	176	11	0
70	N3	54	0	88	3	0
70	N5	31	0	36	2	0
70	QJ	54	0	88	3	0
70	Qb	54	0	88	5	0
70	Qc	108	0	176	3	0
70	Qd	54	0	88	2	0
70	Qh	54	0	88	1	0
71	6A	87	0	131	5	0
71	8B	42	0	61	2	0
71	A3	51	0	82	3	0
71	AL	40	0	54	4	0
71	B4	51	0	82	4	0
71	C3	51	0	82	4	0
71	N4	49	0	75	3	0
71	N5	97	0	151	7	0
71	QB	85	0	124	3	0
71	QC	40	0	54	0	0
71	QE	47	0	71	1	0
71	Qc	93	0	143	6	0
71	Qd	24	0	22	1	0
71	S2	48	0	73	1	0
71	S8	51	0	82	0	0
72	A9	48	0	26	1	0
73	AB	36	0	47	1	0
73	AC	36	0	47	4	0
74	AK	27	0	12	4	0
75	AM	104	0	176	3	0
75	B5	52	0	88	0	0
75	C2	43	0	67	2	0
75	CB	52	0	88	3	0
75	N3	52	0	88	1	0
75	N4	99	0	163	16	0
75	QB	46	0	73	4	0
75	QI	52	0	88	5	0
76	B4	51	0	82	8	0
76	B8	32	0	38	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
76	C1	51	0	82	5	0
76	C2	51	0	82	2	0
76	CA	51	0	82	5	0
76	QE	44	0	65	0	0
77	C1	120	0	108	21	0
78	C1	1	0	0	0	0
78	C2	2	0	0	0	0
79	C1	1	0	0	0	0
79	S1	1	0	0	0	0
80	QC	86	0	60	9	0
80	Qc	86	0	60	10	0
81	QD	43	0	30	0	0
81	Qd	43	0	32	3	0
82	QE	4	0	0	2	0
82	Qe	4	0	0	2	0
82	S1	4	0	0	1	0
82	V2	4	0	0	0	0
83	S1	16	0	0	3	0
83	S7	8	0	0	0	0
83	S8	16	0	0	2	0
83	V1	8	0	0	1	0
84	V1	31	0	19	2	0
All	All	117250	0	118812	1573	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1573) 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)
29:B6:88:LEU:HD22	29:B6:92:GLU:HG2	1.59	0.85
36:C2:196:CYS:HB3	36:C2:207:MET:SD	2.18	0.82
42:N2:88:LYS:HG3	42:N2:148:SER:HB3	1.61	0.82
36:C2:196:CYS:CB	36:C2:207:MET:SD	2.68	0.82
7:7A:77:PRO:HG3	9:7C:62:LYS:HG3	1.61	0.80
49:QC:237:LEU:HB2	50:QD:297:MET:HE2	1.62	0.80
76:CA:101:3PE:H3F1	42:N2:325:LEU:HD21	1.65	0.78
47:QA:70:ARG:HD2	47:QA:117:GLU:HG2	1.67	0.76
51:Qe:190:VAL:HG21	51:Qe:250:ARG:HH22	1.51	0.75
35:C1:468:MET:HE1	77:C1:602:HEA:H211	1.68	0.75
68:A1:101:CDL:HA31	22:AM:6:VAL:HG21	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:V1:110:PRO:HB3	65:V1:152:ARG:HD3	1.68	0.74
4:6A:63:HIS:HB2	5:6B:76:ARG:HH12	1.52	0.74
58:S2:222:ARG:NH1	58:S2:249:ASP:OD2	2.20	0.74
4:6A:81:LEU:HB3	70:6A:101:PC1:H12	1.70	0.74
18:A9:129:LEU:HD23	18:A9:167:ILE:HG13	1.70	0.73
68:A8:301:CDL:H381	42:N2:256:PRO:HB2	1.69	0.73
48:QB:100:GLY:HA2	48:QB:106:GLY:H	1.54	0.73
49:Qc:98:VAL:HG22	80:Qc:404:HEM:HBC2	1.68	0.73
51:QK:1:MET:O	51:QK:7:ARG:NH1	2.22	0.72
70:C1:611:PC1:H2A1	70:C3:302:PC1:H3C1	1.70	0.72
68:N2:402:CDL:H821	68:N2:402:CDL:H451	1.70	0.72
47:Qa:81:HIS:HD2	47:Qa:192:CYS:H	1.37	0.72
57:S1:246:ARG:HH22	60:S4:123:ASN:HD21	1.35	0.72
50:QD:280:GLU:OE2	50:QD:286:ARG:NH1	2.23	0.72
33:BK:140:GLN:O	33:BK:144:SER:HB2	1.90	0.71
60:S4:62:THR:HG23	60:S4:72:ILE:HD13	1.72	0.71
49:QC:97:HIS:HE1	80:QC:402:HEM:ND	1.89	0.70
12:A2:24:CYS:N	12:A2:58:CYS:SG	2.64	0.70
51:Qe:204:ARG:NH2	51:Qe:258:LEU:O	2.23	0.70
57:S1:149:ASP:HB2	58:S2:367:ALA:HB3	1.73	0.70
41:N1:246:SER:HB2	70:N1:402:PC1:H132	1.73	0.70
8:7B:53:TRP:HE1	38:C4:111:ILE:HG22	1.55	0.70
35:C1:51:ASP:OD1	35:C1:55:ASN:ND2	2.23	0.70
65:V1:235:VAL:HG12	65:V1:240:THR:HG21	1.73	0.70
41:N1:99:ASN:HB2	70:N1:401:PC1:H111	1.72	0.69
75:AM:201:PLX:H291	75:AM:202:PLX:H132	1.72	0.69
58:S2:190:ILE:HG23	58:S2:209:MET:HB3	1.73	0.69
35:C1:184:PHE:H	35:C1:256:HIS:HE1	1.39	0.69
50:Qd:125:CYS:SG	81:Qd:401:HEC:HAC	2.33	0.69
49:Qc:284:ILE:HD11	70:Qc:405:PC1:H252	1.74	0.69
44:N4:391:ILE:HG23	44:N4:394:ILE:HD12	1.75	0.69
47:Qa:155:GLN:HE22	47:Qa:200:VAL:HB	1.57	0.69
42:N2:93:VAL:HG13	45:N5:599:MET:HE1	1.75	0.68
58:S2:290:LEU:O	58:S2:293:GLY:N	2.27	0.68
37:C3:253:TYR:HA	37:C3:257:TYR:HD2	1.59	0.68
28:B5:186:THR:HG22	61:S5:30:PRO:HG3	1.74	0.68
41:N1:60:PRO:HD3	43:N3:25:PRO:HB2	1.73	0.68
49:QC:312:GLN:HG3	53:Qg:37:THR:HG22	1.75	0.68
20:AK:94:HIS:HB3	20:AK:105:PRO:HB3	1.74	0.68
41:N1:231:ILE:O	41:N1:235:ASN:ND2	2.28	0.67
35:C1:51:ASP:O	35:C1:55:ASN:ND2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:QC:71:ARG:NH2	50:QD:278:ALA:O	2.27	0.67
75:QI:301:PLX:H141	70:Qb:502:PC1:H2C2	1.75	0.67
66:V2:59:ASN:ND2	66:V2:89:GLN:OE1	2.28	0.67
57:S1:338:VAL:O	57:S1:365:SER:HB2	1.95	0.67
42:N2:108:LEU:HD11	42:N2:191:THR:HG21	1.77	0.67
20:AK:62:ILE:O	20:AK:160:VAL:HA	1.94	0.67
57:S1:275:PRO:HG3	57:S1:286:ILE:HG12	1.77	0.67
57:S1:387:LEU:HD12	57:S1:514:ASN:HB3	1.76	0.67
66:V2:182:ASN:HB3	66:V2:194:GLU:HB3	1.77	0.66
23:AN:51:MET:HE2	41:N1:311:THR:HB	1.77	0.66
65:V1:112:TYR:HB2	65:V1:240:THR:HG22	1.76	0.66
58:S2:412:GLU:OE2	59:S3:140:ARG:NH2	2.27	0.66
49:QC:98:VAL:HG22	80:QC:402:HEM:HBC2	1.76	0.66
19:AC:94:ASP:HB3	19:AC:97:LYS:HG2	1.78	0.66
35:C1:508:PRO:HG3	37:C3:6:HIS:HB3	1.78	0.66
48:QB:280:ASP:HA	48:QB:461:PRO:HB3	1.76	0.66
58:S2:300:ARG:NH1	58:S2:342:GLU:OE2	2.28	0.66
51:QE:110:ARG:NH1	54:Qh:22:PHE:O	2.26	0.66
70:7C:101:PC1:H352	70:7C:101:PC1:H241	1.78	0.66
35:C1:229:ILE:HD11	36:C2:175:ILE:HG12	1.78	0.66
75:N4:503:PLX:H112	71:N5:701:PEE:H23	1.77	0.66
48:QB:473:SER:HB3	71:QB:502:PEE:H9	1.78	0.66
9:7C:59:GLN:NE2	35:C1:116:SER:O	2.28	0.66
35:C1:439:ARG:NH2	77:C1:602:HEA:O1D	2.28	0.65
49:QC:319:PRO:HB3	54:Qh:48:ARG:HH21	1.60	0.65
1:4L:98:CYS:HB3	45:N5:580:GLN:HB2	1.78	0.65
35:C1:169:ILE:O	35:C1:172:LYS:NZ	2.30	0.65
2:5A:114:VAL:HG11	2:5A:128:VAL:HG11	1.77	0.65
26:B3:27:THR:HG22	26:B3:29:LEU:H	1.60	0.65
20:AK:92:GLY:H	20:AK:95:TYR:HB3	1.61	0.65
43:N3:27:LEU:HD21	70:N3:202:PC1:H252	1.80	0.64
35:C1:352:GLY:HA3	77:C1:603:HEA:H162	1.80	0.64
36:C2:52:HIS:HD2	36:C2:56:MET:HE2	1.60	0.64
58:S2:155:GLN:NE2	58:S2:315:ASP:OD2	2.29	0.64
25:B2:76:ASP:O	45:N5:385:TYR:OH	2.13	0.64
9:7C:62:LYS:NZ	35:C1:117:MET:O	2.29	0.64
19:AB:93:ILE:HD11	19:AB:110:LEU:HD11	1.80	0.64
68:N2:402:CDL:H841	68:N2:402:CDL:H471	1.80	0.64
60:S4:112:MET:O	64:S8:144:ARG:NH1	2.29	0.64
51:Qe:145:ASP:N	51:Qe:145:ASP:OD1	2.31	0.64
65:V1:48:ARG:HH21	67:V3:384:SER:HA	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5B:105:VAL:HA	3:5B:111:GLN:HG3	1.79	0.63
30:B7:56:ARG:HH22	33:BK:120:SER:HB3	1.63	0.63
35:C1:184:PHE:H	35:C1:256:HIS:CE1	2.17	0.63
47:QA:235:GLU:O	47:QA:239:ASN:ND2	2.30	0.63
53:Qg:53:GLU:OE2	54:Qh:12:ARG:NH1	2.32	0.63
20:AK:134:GLN:HE22	74:AK:401:ADP:HN62	1.44	0.63
17:A8:107:HIS:HB3	17:A8:197:PRO:HD2	1.80	0.63
47:Qa:70:ARG:HD2	47:Qa:117:GLU:HG2	1.80	0.63
41:N1:32:GLN:HE22	58:S2:203:MET:HE2	1.64	0.63
49:Qc:311:LYS:NZ	49:Qc:379:TRP:OXT	2.32	0.63
58:S2:393:GLU:OE2	58:S2:396:GLN:NE2	2.32	0.63
1:4L:56:ALA:HA	61:S5:18:MET:HE3	1.81	0.63
35:C1:91:ASP:OD1	35:C1:92:MET:N	2.29	0.63
65:V1:214:GLU:OE2	65:V1:224:ARG:NE	2.25	0.63
41:N1:73:ILE:HG23	70:N1:401:PC1:H2I1	1.81	0.63
47:QA:116:ARG:NH1	47:QA:188:ASN:O	2.32	0.62
41:N1:173:TRP:HB3	41:N1:175:ILE:HG22	1.81	0.62
45:N5:575:ILE:O	45:N5:579:ASN:HB2	1.98	0.62
57:S1:224:ASP:OD2	57:S1:291:ARG:NH2	2.29	0.62
66:V2:108:PRO:HB2	66:V2:111:ARG:HG2	1.80	0.62
12:A2:89:ARG:O	12:A2:93:ASN:ND2	2.31	0.62
14:A5:6:LYS:NZ	14:A5:76:GLN:OE1	2.32	0.62
68:AL:201:CDL:H761	68:AL:202:CDL:H211	1.81	0.62
50:QD:147:LYS:NZ	50:QD:151:GLU:OE2	2.31	0.62
20:AK:120:TYR:OH	74:AK:401:ADP:O2'	2.14	0.62
70:C1:606:PC1:H2G1	70:C1:606:PC1:H3I3	1.80	0.62
47:QA:233:VAL:HG22	47:QA:236:ARG:HH12	1.64	0.62
57:S1:141:ASP:OD2	60:S4:88:GLN:NE2	2.30	0.62
59:S3:89:HIS:ND1	59:S3:91:ASP:OD1	2.31	0.62
65:V1:60:GLY:O	65:V1:256:ARG:NH2	2.33	0.62
25:B2:87:PRO:HD2	30:B7:99:MET:HE1	1.82	0.62
57:S1:275:PRO:O	60:S4:86:ASN:ND2	2.32	0.62
6:6C:56:TYR:OH	6:6C:61:ASP:OD2	2.16	0.61
36:C2:12:ALA:O	36:C2:188:ARG:NH2	2.33	0.61
62:S6:74:GLN:HG3	64:S8:108:SER:HB2	1.82	0.61
31:B8:173:ASP:OD2	31:B8:176:LYS:NZ	2.32	0.61
48:QB:301:ASN:ND2	48:QB:347:CYS:SG	2.73	0.61
47:Qa:313:VAL:HG21	47:Qa:323:VAL:HG11	1.83	0.61
7:7A:54:ARG:NH2	68:C1:610:CDL:OB3	2.33	0.61
20:AK:206:VAL:HB	20:AK:257:VAL:HG13	1.82	0.61
33:BK:171:LYS:O	33:BK:175:ALA:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:V1:195:VAL:O	67:V3:410:ARG:NH1	2.32	0.61
23:AN:98:MET:HE3	23:AN:101:VAL:HG21	1.83	0.61
41:N1:110:SER:HB2	46:N6:62:GLY:HA3	1.82	0.61
42:N2:142:LEU:HB3	42:N2:194:LEU:HD21	1.82	0.61
49:QC:100:ARG:NH2	80:QC:402:HEM:O1A	2.34	0.61
49:QC:246:SER:HB2	49:QC:249:LEU:HB2	1.82	0.61
64:S8:205:ILE:O	64:S8:209:TYR:HB3	2.01	0.61
45:N5:3:PRO:HB2	45:N5:53:MET:HE1	1.82	0.61
19:AC:114:ASP:OD1	32:B9:87:ARG:NH2	2.33	0.60
65:V1:40:ARG:NH1	65:V1:289:GLU:O	2.34	0.60
45:N5:362:LEU:HA	45:N5:365:ALA:HB3	1.83	0.60
47:QA:184:ASN:HD21	47:QA:252:LYS:H	1.49	0.60
17:A8:219:TYR:OH	28:B5:189:ASN:ND2	2.33	0.60
35:C1:155:VAL:HG11	70:C1:611:PC1:H3B1	1.82	0.60
54:QH:3:ARG:HH22	49:Qc:217:LYS:HE2	1.66	0.60
50:Qd:147:LYS:NZ	50:Qd:151:GLU:OE2	2.34	0.60
20:AK:97:ASP:OD1	42:N2:316:GLN:NE2	2.32	0.60
29:B6:132:VAL:O	29:B6:136:LEU:HB3	2.01	0.60
30:B7:29:TYR:O	30:B7:104:ARG:NH2	2.34	0.60
47:QA:77:LEU:O	47:QA:196:ARG:NH1	2.26	0.60
63:S7:51:ASP:HB3	63:S7:190:LEU:HB2	1.84	0.60
65:V1:194:ASP:OD1	65:V1:194:ASP:N	2.32	0.60
37:C3:16:TRP:NE1	37:C3:60:ASP:OD2	2.29	0.60
48:QB:195:THR:HG21	48:QB:269:ARG:H	1.66	0.60
47:Qa:81:HIS:CD2	47:Qa:192:CYS:H	2.20	0.60
65:V1:205:ILE:HG12	65:V1:379:CYS:HB3	1.82	0.60
11:A1:46:ASN:ND2	46:N6:132:ASP:OD2	2.34	0.60
68:N2:401:CDL:H741	68:N2:401:CDL:H522	1.82	0.60
45:N5:400:ASN:HB3	45:N5:486:MET:HE3	1.83	0.60
45:N5:530:PRO:O	45:N5:534:HIS:HB2	2.01	0.60
57:S1:64:CYS:O	57:S1:184:ARG:NH2	2.32	0.60
53:QG:36:ASP:OD1	53:QG:90:TYR:OH	2.10	0.60
15:A6:74:HIS:HE1	18:A9:364:SER:HA	1.67	0.60
57:S1:405:THR:HB	57:S1:477:GLY:HA3	1.82	0.60
68:B5:202:CDL:H671	45:N5:12:LEU:HB3	1.83	0.59
50:Qd:211:TYR:OH	81:Qd:401:HEC:O1A	2.20	0.59
66:V2:38:LEU:O	66:V2:124:ARG:NH2	2.33	0.59
6:6C:60:LYS:NZ	6:6C:64:GLU:OE2	2.35	0.59
30:B7:29:TYR:OH	30:B7:111:ARG:NH2	2.35	0.59
76:C2:302:3PE:H2C1	76:C2:302:3PE:H272	1.84	0.59
70:C1:611:PC1:H341	70:C1:611:PC1:H292	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:C2:161:HIS:HB2	36:C2:174:ALA:HB3	1.84	0.59
51:Qe:187:GLU:OE1	51:Qe:248:ARG:NH2	2.34	0.59
59:S3:115:THR:OG1	59:S3:116:ALA:N	2.35	0.59
18:A9:212:ARG:NH1	18:A9:311:GLU:OE2	2.34	0.59
73:AC:201:ZMP:H1	32:B9:113:PHE:HA	1.84	0.59
20:AK:255:CYS:HA	20:AK:282:LYS:HG3	1.84	0.59
35:C1:28:MET:HE3	35:C1:469:ILE:HD11	1.84	0.59
57:S1:266:ARG:HG2	57:S1:267:THR:HG23	1.84	0.59
70:C1:611:PC1:H371	37:C3:50:ASN:HD21	1.66	0.59
42:N2:100:MET:HE3	45:N5:595:ILE:HG12	1.84	0.59
65:V1:119:GLU:O	65:V1:159:ARG:NH1	2.35	0.59
41:N1:99:ASN:N	70:N1:401:PC1:O12	2.35	0.59
50:QD:159:PRO:HB2	50:Qd:184:GLU:HG3	1.85	0.59
50:QD:266:GLN:HE22	52:Qf:91:LYS:H	1.50	0.59
50:Qd:243:ILE:HG12	50:Qd:245:MET:H	1.66	0.59
27:B4:11:LEU:O	45:N5:535:ARG:NH1	2.35	0.59
71:B4:202:PEE:H51	54:Qh:35:ILE:HD12	1.85	0.59
49:Qc:78:VAL:O	49:Qc:82:LEU:HB2	2.03	0.59
57:S1:433:GLY:O	57:S1:444:HIS:NE2	2.33	0.59
17:A8:174:PHE:HB3	17:A8:178:ARG:HH12	1.67	0.59
18:A9:299:ARG:NH2	18:A9:320:GLU:OE2	2.33	0.59
44:N4:200:ILE:O	44:N4:204:MET:HG2	2.02	0.59
45:N5:103:PHE:HB2	45:N5:341:MET:HE3	1.85	0.59
48:Qb:388:VAL:HG21	48:Qb:438:ALA:HA	1.84	0.59
22:AM:88:ARG:HD3	64:S8:200:GLU:HG3	1.85	0.58
76:C1:601:3PE:H3A2	76:C1:601:3PE:H2C2	1.84	0.58
76:CA:101:3PE:H381	42:N2:324:LYS:HA	1.85	0.58
42:N2:289:ASN:HA	42:N2:292:PHE:CE2	2.38	0.58
70:N1:401:PC1:H132	70:N1:401:PC1:H12	1.83	0.58
47:Qa:92:LYS:HD3	47:Qa:143:ALA:HB1	1.85	0.58
58:S2:188:ASN:OD1	58:S2:410:LYS:NZ	2.37	0.58
65:V1:111:LYS:HB2	65:V1:151:ALA:HA	1.85	0.58
36:C2:173:ASP:O	36:C2:180:ASN:ND2	2.37	0.58
47:QA:151:VAL:O	47:QA:155:GLN:HG2	2.04	0.58
52:QF:56:ARG:NH2	52:QF:65:GLU:OE2	2.36	0.58
47:Qa:65:ILE:HG12	47:Qa:218:MET:HG2	1.84	0.58
16:A7:40:LYS:HB3	23:AN:7:LYS:H	1.69	0.58
71:QB:503:PEE:H40	75:QB:504:PLX:H302	1.86	0.58
51:Qe:204:ARG:NE	51:Qe:246:SER:O	2.34	0.58
57:S1:545:LEU:HD22	57:S1:560:LEU:HD11	1.86	0.58
15:A6:67:ARG:NH2	19:AB:123:GLU:OE1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:QC:214:ASP:OD1	54:Qh:3:ARG:NH2	2.36	0.58
63:S7:65:MET:HE3	63:S7:97:PRO:HB3	1.84	0.58
36:C2:151:ARG:HD3	36:C2:153:LEU:HD21	1.85	0.58
42:N2:42:PRO:HG2	46:N6:167:VAL:HG22	1.86	0.58
48:Qb:195:THR:HG21	48:Qb:269:ARG:H	1.68	0.58
68:B4:203:CDL:HB22	44:N4:260:PRO:HG3	1.86	0.58
49:Qc:24:PRO:HB2	49:Qc:27:ILE:HG23	1.84	0.58
1:4L:28:SER:HB3	46:N6:23:LYS:HD2	1.84	0.57
70:Qh:101:PC1:H3I3	70:Qh:101:PC1:H2F1	1.86	0.57
65:V1:281:HIS:ND1	65:V1:358:ASP:OD1	2.37	0.57
17:A8:84:LEU:O	23:AN:88:ARG:NH1	2.38	0.57
20:AK:64:VAL:HG13	20:AK:207:VAL:HB	1.87	0.57
42:N2:242:SER:HB2	68:N2:402:CDL:H3I2	1.86	0.57
68:QC:404:CDL:HA31	54:Qh:41:ARG:HB3	1.85	0.57
68:QC:404:CDL:H322	68:QD:402:CDL:HB61	1.86	0.57
9:7C:42:THR:OG1	10:8B:49:SER:HB3	2.03	0.57
34:BL:89:VAL:HG21	44:N4:25:ILE:HG23	1.86	0.57
34:BL:128:TYR:O	34:BL:132:ASN:ND2	2.37	0.57
45:N5:100:ILE:HG21	45:N5:246:LEU:HB2	1.86	0.57
49:QC:138:MET:HB2	49:QC:255:ASN:HD22	1.69	0.57
15:A6:88:LYS:NZ	15:A6:132:PHE:O	2.37	0.57
73:AC:201:ZMP:H14	32:B9:102:ALA:HB1	1.86	0.57
71:AL:203:PEE:H10	71:AL:203:PEE:H8	1.85	0.57
37:C3:213:THR:HG21	71:C3:303:PEE:H43	1.86	0.57
75:N4:502:PLX:H311	75:N4:502:PLX:H262	1.86	0.57
19:AB:116:VAL:HG12	19:AB:120:MET:HE2	1.86	0.57
41:N1:18:ALA:HB1	41:N1:48:PRO:HB3	1.86	0.57
57:S1:158:ARG:NH1	57:S1:202:ASN:OD1	2.37	0.57
70:7C:101:PC1:H12	68:C1:610:CDL:H352	1.85	0.57
67:V3:405:GLU:O	67:V3:408:LYS:NZ	2.37	0.57
18:A9:293:LEU:HD12	18:A9:294:PRO:HD2	1.87	0.57
20:AK:357:LYS:O	40:CB:62:ARG:NH1	2.30	0.57
50:QD:104:SER:HA	55:Qi:48:ASN:HD21	1.69	0.57
55:QI:48:ASN:HD21	50:Qd:104:SER:HA	1.70	0.57
58:S2:194:THR:HB	58:S2:206:PHE:HA	1.86	0.57
36:C2:199:ILE:HD12	36:C2:199:ILE:H	1.69	0.57
48:QB:80:ARG:NH2	48:QB:350:GLU:OE1	2.36	0.57
37:C3:112:LEU:HD13	37:C3:118:PRO:HG3	1.85	0.57
40:CB:52:ARG:NH1	42:N2:318:GLU:OE1	2.38	0.57
45:N5:375:ILE:HD12	45:N5:458:LEU:HD11	1.87	0.57
53:Qg:14:LEU:HD12	53:Qg:17:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:CA:101:3PE:H321	42:N2:322:GLN:HE22	1.69	0.57
18:A9:206:ILE:HG13	72:A9:401:NDP:H42N	1.86	0.56
18:A9:344:PRO:HG2	18:A9:347:LEU:HD13	1.86	0.56
19:AB:143:GLU:OE1	19:AB:143:GLU:N	2.38	0.56
75:CB:201:PLX:H332	42:N2:342:ALA:HB3	1.86	0.56
70:QJ:101:PC1:H2E2	70:QJ:101:PC1:H2A2	1.86	0.56
45:N5:399:VAL:HG12	45:N5:409:LEU:HD13	1.87	0.56
48:QB:204:PRO:HG2	48:QB:207:ASN:HB2	1.87	0.56
57:S1:83:GLU:HB2	57:S1:101:ASN:HB3	1.87	0.56
57:S1:140:GLN:NE2	83:S1:801:SF4:S3	2.79	0.56
57:S1:419:ARG:NH1	57:S1:439:THR:O	2.37	0.56
3:5B:98:SER:OG	35:C1:266:GLU:OE1	2.22	0.56
48:QB:411:GLU:OE2	48:QB:415:ARG:NH2	2.38	0.56
49:Qc:300:ILE:HD11	49:Qc:363:LEU:HD21	1.88	0.56
62:S6:100:ILE:HD11	62:S6:111:CYS:HB2	1.88	0.56
70:6A:101:PC1:H231	35:C1:215:LEU:HD21	1.88	0.56
17:A8:246:PHE:HE1	68:A8:301:CDL:H341	1.70	0.56
28:B5:74:TYR:O	34:BL:96:SER:OG	2.21	0.56
35:C1:409:TRP:HB3	35:C1:471:ILE:HG12	1.86	0.56
26:B3:60:ASN:HD22	45:N5:433:GLY:H	1.54	0.56
71:6A:102:PEE:H38	70:C1:611:PC1:H3I1	1.87	0.56
39:CA:43:LYS:O	39:CA:47:THR:OG1	2.21	0.56
47:Qa:155:GLN:NE2	47:Qa:200:VAL:O	2.38	0.56
58:S2:61:THR:N	58:S2:64:THR:OG1	2.33	0.56
1:4L:2:PRO:HG3	46:N6:127:ILE:HD13	1.88	0.56
73:AC:201:ZMP:H5A	32:B9:109:ALA:HB1	1.88	0.56
8:7B:71:ARG:HG3	8:7B:72:VAL:HG23	1.87	0.56
36:C2:161:HIS:CE1	36:C2:207:MET:HE1	2.41	0.56
40:CB:13:LEU:HD11	61:S5:6:VAL:HG12	1.88	0.56
4:6A:83:HIS:HA	70:6A:101:PC1:H132	1.88	0.56
18:A9:201:ILE:HG22	18:A9:203:PRO:HD3	1.87	0.56
35:C1:197:LEU:HA	37:C3:92:LEU:HD13	1.86	0.56
51:QE:204:ARG:NH2	51:QE:258:LEU:O	2.31	0.56
52:QF:34:ARG:O	52:QF:38:GLU:HG2	2.06	0.56
18:A9:198:ALA:O	18:A9:260:GLY:HA2	2.06	0.55
33:BK:114:GLN:HG3	45:N5:203:MET:HG2	1.88	0.55
65:V1:94:PRO:HB2	65:V1:97:LEU:HB2	1.88	0.55
65:V1:365:LYS:NZ	66:V2:141:MET:SD	2.79	0.55
48:Qb:422:ARG:NH2	48:Qb:428:GLU:OE1	2.37	0.55
44:N4:403:THR:HA	44:N4:406:TYR:CE2	2.42	0.55
45:N5:97:THR:HG21	45:N5:125:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:QH:67:PHE:HE1	49:Qc:344:GLU:HG3	1.71	0.55
49:Qc:237:LEU:HD13	50:Qd:297:MET:HG2	1.87	0.55
66:V2:111:ARG:NH1	66:V2:114:GLU:OE2	2.39	0.55
14:A5:44:TYR:O	14:A5:48:THR:HG22	2.06	0.55
34:BL:76:TYR:HD1	44:N4:81:GLN:HE22	1.53	0.55
44:N4:446:LEU:HB3	75:N4:503:PLX:H272	1.88	0.55
57:S1:433:GLY:HA2	57:S1:447:ASP:HA	1.87	0.55
18:A9:49:SER:HB2	59:S3:225:GLU:HG2	1.87	0.55
35:C1:24:ALA:HA	77:C1:602:HEA:H22	1.87	0.55
47:QA:148:ARG:NH2	53:QG:50:ARG:O	2.38	0.55
47:Qa:151:VAL:O	47:Qa:155:GLN:HG2	2.06	0.55
70:Qc:406:PC1:H381	70:Qc:406:PC1:H2B1	1.87	0.55
65:V1:119:GLU:HA	84:V1:502:FMN:HM71	1.89	0.55
22:AM:106:ARG:HB2	22:AM:109:ILE:HG13	1.87	0.55
27:B4:127:ILE:HG22	33:BK:140:GLN:HB2	1.88	0.55
35:C1:82:LEU:HB3	35:C1:86:MET:HE3	1.87	0.55
42:N2:91:ASN:HD22	42:N2:94:ALA:H	1.54	0.55
20:AK:241:ASN:HB3	20:AK:245:LYS:HE2	1.89	0.55
27:B4:15:PRO:HG2	27:B4:18:LEU:HB2	1.89	0.55
65:V1:295:PRO:HG2	65:V1:298:GLU:HB3	1.89	0.55
66:V2:204:ILE:HG23	66:V2:214:PRO:HG2	1.88	0.55
20:AK:210:ASP:OD2	20:AK:244:LYS:NZ	2.34	0.55
36:C2:104:TRP:CG	36:C2:203:ASN:HB2	2.42	0.55
45:N5:249:SER:HA	45:N5:306:THR:HG21	1.88	0.55
68:A1:101:CDL:H722	68:A1:101:CDL:H781	1.88	0.55
44:N4:392:THR:O	44:N4:396:MET:HG2	2.07	0.55
45:N5:417:SER:HB2	68:N5:703:CDL:H572	1.88	0.55
47:QA:304:ASN:O	47:QA:311:GLN:NE2	2.37	0.55
51:Qe:241:SER:OG	82:Qe:301:FES:S2	2.56	0.55
58:S2:308:LEU:HB2	58:S2:407:GLU:HB2	1.88	0.55
70:C1:606:PC1:H3E2	70:C1:606:PC1:H3A2	1.88	0.55
42:N2:298:TYR:O	42:N2:303:THR:OG1	2.22	0.55
65:V1:113:LEU:O	65:V1:154:ALA:HA	2.06	0.55
65:V1:203:ALA:HB3	65:V1:206:CYS:HB2	1.89	0.55
3:5B:33:SER:OG	3:5B:34:GLY:N	2.40	0.54
18:A9:173:ASP:HB3	18:A9:176:SER:HB2	1.88	0.54
29:B6:134:HIS:NE2	45:N5:35:TYR:OH	2.29	0.54
48:Qb:183:VAL:HG21	48:Qb:286:HIS:HB3	1.87	0.54
48:Qb:276:ARG:NH2	48:Qb:466:PRO:O	2.40	0.54
65:V1:113:LEU:HD13	65:V1:149:MET:HE1	1.90	0.54
14:A5:76:GLN:HB2	14:A5:79:GLU:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AK:244:LYS:HA	20:AK:248:LEU:HD12	1.89	0.54
70:B7:201:PC1:H291	45:N5:49:VAL:HG22	1.88	0.54
47:QA:301:ARG:NH2	48:QB:94:GLU:OE2	2.29	0.54
53:Qg:97:GLU:OE1	53:Qg:100:ARG:NH1	2.41	0.54
58:S2:146:ASP:OD2	58:S2:149:SER:OG	2.25	0.54
68:C1:610:CDL:H382	68:C1:610:CDL:H191	1.89	0.54
38:C4:152:PRO:HA	38:C4:157:SER:HB2	1.90	0.54
58:S2:91:GLY:HA3	58:S2:102:ARG:HA	1.90	0.54
65:V1:311:TRP:O	65:V1:329:LYS:NZ	2.40	0.54
30:B7:15:LYS:HG2	30:B7:113:LYS:HG3	1.89	0.54
8:7B:32:ASP:OD1	8:7B:33:PHE:N	2.40	0.54
29:B6:143:HIS:CD2	33:BK:45:VAL:HG21	2.42	0.54
35:C1:347:LEU:HD13	35:C1:383:MET:HE2	1.87	0.54
49:QC:197:LEU:HD11	80:QC:402:HEM:HMA3	1.90	0.54
50:QD:228:LEU:HD11	50:QD:234:PHE:HB2	1.88	0.54
48:Qb:87:ASN:HD22	48:Qb:204:PRO:HD3	1.73	0.54
50:Qd:216:LEU:HB3	50:Qd:249:ILE:HD11	1.90	0.54
50:Qd:228:LEU:HD11	50:Qd:234:PHE:HB2	1.90	0.54
58:S2:194:THR:HG21	58:S2:209:MET:HB2	1.90	0.54
77:C1:602:HEA:HMA	77:C1:602:HEA:HBA2	1.90	0.54
37:C3:58:TRP:CD2	70:C3:302:PC1:H262	2.42	0.54
42:N2:26:TRP:HB3	42:N2:74:ILE:HD13	1.90	0.54
44:N4:373:ILE:HD11	44:N4:444:LEU:HD23	1.90	0.54
50:Qd:118:TYR:HA	50:Qd:122:CYS:SG	2.47	0.54
48:QB:165:ARG:HD3	48:QB:209:ARG:HA	1.89	0.54
57:S1:149:ASP:OD2	57:S1:150:ARG:NH2	2.41	0.54
65:V1:325:PRO:HG3	65:V1:433:TRP:HB3	1.90	0.54
49:QC:97:HIS:HE1	80:QC:402:HEM:C1D	2.25	0.54
35:C1:107:PRO:HB3	37:C3:25:LEU:HB2	1.89	0.53
35:C1:443:TYR:O	36:C2:134:ARG:NH2	2.41	0.53
43:N3:79:SER:HA	43:N3:87:MET:HE2	1.90	0.53
53:QG:43:ASP:OD2	53:QG:102:ARG:NH1	2.40	0.53
48:Qb:121:ASN:ND2	48:Qb:132:TYR:OH	2.41	0.53
58:S2:140:PRO:HA	58:S2:143:ASP:HB2	1.90	0.53
20:AK:63:THR:HG23	20:AK:203:PRO:HB3	1.90	0.53
35:C1:13:LYS:NZ	35:C1:504:THR:OG1	2.39	0.53
65:V1:321:GLY:H	65:V1:353:ALA:HB3	1.73	0.53
68:A8:301:CDL:H582	68:A8:301:CDL:H531	1.89	0.53
24:B1:57:TRP:NE1	28:B5:134:GLU:OE1	2.31	0.53
41:N1:24:GLU:HA	41:N1:271:LEU:HD13	1.89	0.53
75:N4:503:PLX:H1C3	71:N5:701:PEE:H3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:QB:107:SER:HA	48:QB:110:GLU:HG2	1.91	0.53
47:Qa:233:VAL:HA	47:Qa:237:PHE:HE1	1.74	0.53
52:Qf:60:ARG:NH1	54:Qh:78:TYR:O	2.36	0.53
3:5B:84:THR:OG1	3:5B:85:ASN:N	2.40	0.53
34:BL:77:ASP:OD1	34:BL:78:LYS:N	2.41	0.53
70:C1:611:PC1:H3A1	37:C3:24:ALA:HB2	1.89	0.53
45:N5:253:VAL:HG23	45:N5:310:LEU:HD21	1.91	0.53
48:Qb:479:ARG:HH21	68:Qb:501:CDL:HB21	1.74	0.53
51:Qe:153:GLU:HG2	51:Qe:272:ILE:HG12	1.91	0.53
51:Qe:179:ARG:NH1	51:Qe:246:SER:OG	2.42	0.53
35:C1:62:ALA:HB2	77:C1:602:HEA:HBD1	1.91	0.53
44:N4:449:LEU:HG	68:N5:702:CDL:H441	1.91	0.53
51:QE:151:LYS:HB3	51:QE:272:ILE:HD11	1.89	0.53
65:V1:162:PHE:HB3	65:V1:165:GLU:HB2	1.90	0.53
58:S2:381:MET:HE2	58:S2:385:ILE:HG13	1.90	0.53
3:5B:45:THR:OG1	3:5B:46:GLY:N	2.42	0.53
45:N5:536:LEU:HB3	45:N5:537:PRO:HD3	1.91	0.53
50:QD:97:TRP:NE1	50:QD:210:ASP:OD1	2.38	0.53
47:Qa:234:ALA:O	47:Qa:239:ASN:HB2	2.08	0.53
47:Qa:51:SER:HB3	47:Qa:230:LEU:HD12	1.89	0.53
58:S2:321:GLU:O	58:S2:352:GLN:NE2	2.41	0.53
21:AL:129:GLN:HG2	68:AL:202:CDL:HB32	1.91	0.53
43:N3:68:GLU:HG3	43:N3:98:LEU:HD13	1.91	0.53
3:5B:41:GLU:HG2	3:5B:56:ARG:HH22	1.74	0.53
38:C4:90:PHE:HA	38:C4:93:MET:HG2	1.91	0.53
48:QB:126:ARG:NH1	48:QB:199:GLN:O	2.42	0.53
57:S1:666:GLN:NE2	57:S1:670:GLU:OE2	2.42	0.53
70:6A:101:PC1:H32	37:C3:188:ILE:HD12	1.91	0.52
20:AK:225:ASN:HB3	20:AK:228:GLU:HG2	1.91	0.52
45:N5:248:HIS:O	45:N5:253:VAL:HG22	2.09	0.52
45:N5:387:THR:HG22	45:N5:465:GLY:H	1.74	0.52
68:Qb:501:CDL:H511	71:Qc:401:PEE:H26	1.90	0.52
58:S2:230:ALA:O	64:S8:98:ARG:NH2	2.43	0.52
66:V2:146:ASP:O	66:V2:150:GLU:HG2	2.09	0.52
77:C1:602:HEA:HBD2	77:C1:602:HEA:HHA	1.91	0.52
42:N2:17:THR:HG23	42:N2:137:ALA:HB2	1.90	0.52
49:QC:165:TRP:O	49:QC:174:THR:OG1	2.23	0.52
47:Qa:71:TYR:HB3	47:Qa:212:HIS:CE1	2.44	0.52
32:B9:52:LEU:O	32:B9:57:LYS:NZ	2.42	0.52
35:C1:240:HIS:HB2	35:C1:291:HIS:HE1	1.74	0.52
41:N1:170:GLU:HG2	41:N1:171:HIS:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:S1:250:SER:HB2	57:S1:606:THR:HG23	1.89	0.52
68:AL:201:CDL:H162	68:AL:201:CDL:H372	1.91	0.52
33:BK:12:GLU:OE2	33:BK:15:ARG:NH2	2.42	0.52
36:C2:28:LEU:HA	36:C2:31:VAL:HG22	1.91	0.52
36:C2:155:SER:HB2	36:C2:179:LEU:HD23	1.91	0.52
38:C4:155:GLY:H	38:C4:158:ALA:HB3	1.73	0.52
47:QA:84:ARG:NH2	47:QA:190:LEU:O	2.42	0.52
48:QB:121:ASN:ND2	48:QB:132:TYR:OH	2.40	0.52
75:QI:301:PLX:H161	70:Qb:502:PC1:H2E2	1.91	0.52
50:Qd:122:CYS:SG	81:Qd:401:HEC:HAB	2.49	0.52
5:6B:30:CYS:HB2	5:6B:65:CYS:SG	2.49	0.52
11:A1:49:GLU:OE1	11:A1:52:ARG:NH2	2.39	0.52
27:B4:84:PRO:HD3	76:B4:201:3PE:H122	1.89	0.52
34:BL:95:PHE:O	34:BL:99:LEU:HB2	2.10	0.52
41:N1:200:LEU:HD11	41:N1:285:LEU:HD21	1.90	0.52
45:N5:149:ILE:HD11	68:N5:702:CDL:H161	1.92	0.52
45:N5:566:THR:O	45:N5:570:GLN:HG2	2.10	0.52
46:N6:45:LEU:HD23	46:N6:50:SER:HA	1.91	0.52
59:S3:132:LEU:HB2	59:S3:141:ILE:HG22	1.91	0.52
47:QA:138:LEU:O	47:QA:142:ALA:HB3	2.10	0.52
47:Qa:320:PRO:HG2	47:Qa:343:GLN:HE21	1.74	0.52
51:Qe:225:ILE:HG12	51:Qe:237:PRO:HD3	1.92	0.52
58:S2:469:ARG:NH2	59:S3:169:GLU:OE2	2.43	0.52
1:4L:68:ALA:HB2	46:N6:64:MET:HE2	1.92	0.52
3:5B:37:VAL:HB	37:C3:154:GLY:HA2	1.91	0.52
4:6A:70:LYS:O	35:C1:216:ASN:ND2	2.42	0.52
4:6A:88:ASN:CG	70:6A:101:PC1:H131	2.35	0.52
44:N4:82:SER:HB2	44:N4:432:ARG:NH1	2.24	0.52
51:QE:177:ARG:HB3	51:QE:211:VAL:HG13	1.92	0.52
57:S1:251:ILE:HD13	57:S1:604:GLN:HB2	1.91	0.52
58:S2:430:ILE:HB	58:S2:469:ARG:HD2	1.92	0.52
59:S3:157:VAL:HG21	59:S3:182:PRO:HD3	1.92	0.52
70:6A:101:PC1:H112	37:C3:198:PHE:CZ	2.44	0.52
33:BK:67:GLU:OE2	34:BL:124:ARG:NH1	2.41	0.52
68:N2:402:CDL:H792	68:N2:402:CDL:H381	1.92	0.52
47:QA:272:VAL:HA	47:QA:337:GLY:HA3	1.92	0.52
51:QE:151:LYS:HE2	51:QE:272:ILE:HD11	1.92	0.52
52:QF:71:LEU:HD22	50:Qd:223:PRO:HG3	1.91	0.52
64:S8:119:CYS:SG	64:S8:145:TYR:OH	2.63	0.52
5:6B:65:CYS:O	36:C2:98:LYS:NZ	2.40	0.52
44:N4:12:LEU:HB2	44:N4:13:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AL:202:CDL:H461	68:AL:202:CDL:H201	1.91	0.52
68:B4:203:CDL:HA21	75:N4:502:PLX:H91	1.90	0.52
35:C1:96:ARG:NH2	37:C3:64:GLU:OE1	2.41	0.52
44:N4:383:THR:HG21	45:N5:190:LEU:HD22	1.92	0.52
48:QB:192:PHE:O	48:QB:198:ALA:HB2	2.10	0.52
47:Qa:68:GLY:H	47:Qa:71:TYR:HD2	1.58	0.52
62:S6:108:THR:HG22	62:S6:119:ARG:HD3	1.91	0.52
7:7A:49:ASP:OD2	37:C3:63:ARG:NH2	2.40	0.51
68:A8:301:CDL:H331	68:A8:301:CDL:H171	1.92	0.51
18:A9:279:TYR:HB2	18:A9:372:ALA:HB2	1.93	0.51
20:AK:67:ASN:OD1	20:AK:68:ILE:N	2.36	0.51
47:QA:177:LEU:HD11	47:QA:272:VAL:HG22	1.92	0.51
48:Qb:152:GLN:HE22	48:Qb:250:PHE:HA	1.75	0.51
60:S4:55:VAL:HG22	60:S4:57:GLU:HG2	1.93	0.51
57:S1:144:MET:HG3	58:S2:389:LYS:HG3	1.93	0.51
2:5A:77:ASN:HD21	38:C4:46:LEU:H	1.56	0.51
14:A5:48:THR:HA	14:A5:51:ILE:HG12	1.93	0.51
21:AL:2:ALA:HB2	45:N5:601:LEU:HD23	1.92	0.51
22:AM:78:ASP:HB2	22:AM:81:MET:HG3	1.92	0.51
35:C1:123:GLY:H	35:C1:138:HIS:CE1	2.28	0.51
41:N1:32:GLN:HG2	58:S2:204:THR:HG23	1.92	0.51
52:Qf:53:CYS:SG	52:Qf:56:ARG:NH2	2.83	0.51
44:N4:196:TRP:CD1	44:N4:250:LEU:HB3	2.45	0.51
50:QD:112:ARG:NH2	50:QD:145:GLU:OE1	2.42	0.51
57:S1:385:TYR:OH	57:S1:527:ASP:OD1	2.20	0.51
65:V1:288:VAL:HG21	65:V1:303:HIS:CD2	2.45	0.51
48:QB:100:GLY:HA2	48:QB:106:GLY:N	2.24	0.51
47:Qa:272:VAL:HA	47:Qa:337:GLY:HA3	1.93	0.51
57:S1:466:LEU:HD13	57:S1:500:ILE:HD11	1.92	0.51
60:S4:78:ARG:NH2	60:S4:148:GLU:OE1	2.44	0.51
68:A1:101:CDL:H121	68:A1:101:CDL:H532	1.93	0.51
21:AL:108:TYR:HB2	76:B4:201:3PE:H11	1.92	0.51
23:AN:103:ASP:OD1	23:AN:103:ASP:N	2.43	0.51
37:C3:58:TRP:HE1	70:C3:302:PC1:H351	1.74	0.51
47:QA:399:GLN:HA	47:QA:402:VAL:HG22	1.91	0.51
22:AM:55:PHE:CZ	22:AM:58:ARG:HG3	2.46	0.51
35:C1:374:VAL:HA	35:C1:377:PHE:CE2	2.45	0.51
47:Qa:91:THR:HG21	47:Qa:140:VAL:HA	1.92	0.51
57:S1:257:VAL:HG11	57:S1:413:LEU:HB2	1.92	0.51
20:AK:213:VAL:HG12	20:AK:217:GLN:HE21	1.76	0.51
30:B7:103:GLU:O	30:B7:107:ARG:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:QA:367:SER:OG	47:QA:370:ASP:OD1	2.29	0.51
57:S1:591:GLU:HG2	57:S1:610:VAL:HG23	1.92	0.51
22:AM:34:ARG:HH21	22:AM:54:GLN:HG3	1.75	0.51
27:B4:9:SER:OG	27:B4:10:ARG:N	2.43	0.51
42:N2:276:ILE:HG13	71:N4:501:PEE:H3	1.93	0.51
45:N5:228:GLY:H	45:N5:230:HIS:HD2	1.59	0.51
57:S1:299:ARG:NH1	57:S1:703:ALA:O	2.43	0.51
58:S2:95:PRO:HG2	63:S7:65:MET:HE2	1.93	0.51
58:S2:140:PRO:HB2	63:S7:142:TYR:CE2	2.46	0.51
1:4L:23:ARG:NH1	46:N6:23:LYS:O	2.44	0.51
19:AC:103:HIS:N	19:AC:107:ASP:OD1	2.44	0.51
57:S1:347:ASP:OD1	57:S1:347:ASP:N	2.37	0.51
65:V1:55:GLY:O	65:V1:58:SER:OG	2.23	0.51
8:7B:76:GLU:OE2	38:C4:143:LYS:NZ	2.45	0.50
27:B4:14:LEU:HD12	27:B4:15:PRO:HD2	1.93	0.50
35:C1:74:MET:HE3	35:C1:389:ILE:HG13	1.93	0.50
45:N5:573:MET:HE2	70:N5:705:PC1:H11	1.93	0.50
70:Qd:402:PC1:H2A1	70:Qd:402:PC1:H392	1.93	0.50
58:S2:148:VAL:HG11	58:S2:191:MET:HG2	1.93	0.50
35:C1:2:PHE:N	68:C1:610:CDL:OA3	2.44	0.50
35:C1:31:THR:OG1	77:C1:602:HEA:H14	2.10	0.50
41:N1:58:LYS:HD2	63:S7:127:PRO:HD2	1.93	0.50
52:QF:79:ASP:OD2	50:Qd:237:TYR:OH	2.26	0.50
58:S2:145:LEU:HD13	58:S2:430:ILE:HG21	1.93	0.50
63:S7:96:SER:O	63:S7:100:SER:OG	2.25	0.50
29:B6:181:LYS:HB2	30:B7:40:VAL:HG13	1.94	0.50
35:C1:178:GLN:HG2	70:C1:608:PC1:H32	1.94	0.50
48:QB:465:LEU:HD12	48:QB:466:PRO:HD2	1.93	0.50
47:Qa:61:ILE:HG12	47:Qa:130:ILE:HD11	1.93	0.50
70:Qc:406:PC1:H381	70:Qc:406:PC1:H281	1.92	0.50
68:4L:201:CDL:H181	45:N5:593:ILE:HG12	1.93	0.50
42:N2:112:HIS:O	42:N2:116:PRO:HD2	2.12	0.50
75:N4:503:PLX:H182	68:N5:702:CDL:H432	1.93	0.50
47:QA:104:GLU:OE1	48:QB:325:SER:OG	2.27	0.50
3:5B:109:GLU:OE1	3:5B:110:THR:N	2.45	0.50
76:C1:601:3PE:H391	76:C1:601:3PE:H2A1	1.94	0.50
37:C3:54:MET:HB3	37:C3:58:TRP:CZ3	2.46	0.50
37:C3:148:HIS:HE1	37:C3:152:MET:HE3	1.76	0.50
38:C4:148:MET:HG3	38:C4:150:VAL:HG23	1.94	0.50
44:N4:216:LEU:HB3	44:N4:217:PRO:HD3	1.94	0.50
48:QB:120:LEU:HD13	48:QB:133:ILE:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:QE:177:ARG:HH12	51:QE:233:GLY:HA2	1.76	0.50
68:QH:102:CDL:HA32	50:Qd:308:LYS:HE3	1.94	0.50
67:V3:386:TYR:CZ	67:V3:388:ASN:HB3	2.47	0.50
35:C1:50:ASP:OD1	35:C1:51:ASP:N	2.45	0.50
35:C1:219:PHE:HZ	37:C3:199:VAL:HG21	1.76	0.50
41:N1:222:MET:HG3	43:N3:18:VAL:HG22	1.94	0.50
45:N5:49:VAL:HB	45:N5:50:PRO:HD3	1.93	0.50
1:4L:37:MET:HG3	1:4L:67:ALA:CB	2.42	0.50
19:AB:106:LYS:NZ	19:AB:107:ASP:OD1	2.44	0.50
23:AN:144:THR:HB	41:N1:96:ILE:HG23	1.93	0.50
29:B6:165:PHE:O	29:B6:168:ASP:HB2	2.12	0.50
35:C1:2:PHE:CZ	68:C1:610:CDL:H351	2.47	0.50
56:QJ:14:ALA:O	56:QJ:18:ILE:HG12	2.12	0.50
57:S1:265:THR:HG22	57:S1:270:VAL:HA	1.94	0.50
64:S8:128:ILE:HG12	64:S8:147:ILE:HG12	1.94	0.50
62:S6:39:THR:HG22	62:S6:62:VAL:HG22	1.93	0.50
10:8B:52:ILE:HA	71:8B:201:PEE:H19	1.93	0.50
68:A8:301:CDL:H112	40:CB:32:ARG:HG2	1.94	0.50
19:AC:80:LYS:HD2	19:AC:100:VAL:HG11	1.94	0.50
42:N2:77:ASN:O	42:N2:81:SER:OG	2.30	0.50
45:N5:6:SER:O	45:N5:10:THR:OG1	2.20	0.50
48:Qb:192:PHE:O	48:Qb:195:THR:OG1	2.27	0.50
51:Qe:155:LYS:HG3	51:Qe:158:ASP:H	1.77	0.50
58:S2:214:GLU:OE2	58:S2:227:ARG:NH2	2.41	0.50
17:A8:88:GLU:HA	17:A8:91:LYS:HE2	1.94	0.49
18:A9:303:ARG:HB2	18:A9:316:ARG:HD3	1.94	0.49
28:B5:152:LYS:HD3	40:CB:96:VAL:HG21	1.93	0.49
35:C1:65:MET:HB3	77:C1:602:HEA:CAC	2.42	0.49
41:N1:122:ALA:O	41:N1:124:ASN:ND2	2.45	0.49
48:Qb:152:GLN:NE2	48:Qb:250:PHE:HA	2.27	0.49
49:Qc:24:PRO:O	49:Qc:224:TYR:OH	2.19	0.49
65:V1:140:GLU:OE2	65:V1:256:ARG:NH1	2.45	0.49
47:Qa:148:ARG:NH2	53:Qg:50:ARG:O	2.44	0.49
57:S1:133:GLN:O	57:S1:137:CYS:HB2	2.13	0.49
67:V3:383:ASN:O	67:V3:383:ASN:ND2	2.45	0.49
11:A1:40:HIS:N	11:A1:44:GLN:OE1	2.42	0.49
15:A6:44:LYS:HD3	59:S3:151:THR:HG23	1.94	0.49
20:AK:65:ASP:HB2	20:AK:206:VAL:HA	1.94	0.49
47:Qa:70:ARG:NH1	47:Qa:117:GLU:OE2	2.45	0.49
47:Qa:90:THR:HG23	47:Qa:95:SER:HA	1.94	0.49
58:S2:149:SER:HA	58:S2:184:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A3:148:MET:O	17:A8:207:LYS:NZ	2.42	0.49
20:AK:357:LYS:HD3	39:CA:36:HIS:O	2.12	0.49
23:AN:124:LEU:HD12	46:N6:130:THR:HG21	1.94	0.49
25:B2:43:ARG:NH1	25:B2:47:PHE:O	2.45	0.49
68:B5:202:CDL:H771	34:BL:103:SER:HB2	1.93	0.49
33:BK:73:ASP:OD1	33:BK:73:ASP:N	2.39	0.49
68:N2:402:CDL:H232	44:N4:97:THR:HG21	1.93	0.49
44:N4:212:LEU:HD22	71:N4:501:PEE:H46	1.93	0.49
48:Qb:360:CYS:SG	48:Qb:368:MET:HG3	2.52	0.49
58:S2:300:ARG:NH2	58:S2:407:GLU:OE2	2.40	0.49
58:S2:374:ARG:NH2	64:S8:162:CYS:O	2.39	0.49
59:S3:227:ALA:O	60:S4:116:SER:OG	2.27	0.49
65:V1:320:GLY:HA2	65:V1:353:ALA:H	1.77	0.49
9:7C:56:VAL:HG13	35:C1:53:ILE:HD11	1.95	0.49
24:B1:3:ASN:ND2	24:B1:5:LEU:H	2.11	0.49
36:C2:103:GLN:N	36:C2:158:ASP:OD2	2.44	0.49
37:C3:253:TYR:HA	37:C3:257:TYR:CD2	2.43	0.49
51:QE:207:LYS:HE3	51:QE:210:TRP:HD1	1.77	0.49
42:N2:137:ALA:HB3	42:N2:138:PRO:HD3	1.94	0.49
42:N2:186:HIS:O	42:N2:190:MET:HG3	2.13	0.49
48:QB:56:GLY:HA3	48:QB:227:PRO:HB3	1.94	0.49
51:Qe:228:ALA:HB3	51:Qe:235:TYR:HB3	1.95	0.49
57:S1:340:ALA:HB3	57:S1:366:LEU:HD23	1.95	0.49
65:V1:296:LEU:HD21	65:V1:317:VAL:HG11	1.94	0.49
8:7B:53:TRP:NE1	38:C4:111:ILE:HG22	2.25	0.49
16:A7:112:TYR:HE2	64:S8:43:MET:HE2	1.77	0.49
42:N2:149:ILE:HD13	42:N2:154:MET:HE3	1.95	0.49
45:N5:419:THR:HA	45:N5:422:TYR:CE2	2.48	0.49
52:QF:56:ARG:NH1	52:QF:65:GLU:OE1	2.45	0.49
58:S2:160:ALA:HA	58:S2:404:THR:HG21	1.95	0.49
68:Qb:501:CDL:H112	70:Qb:502:PC1:H11	1.95	0.49
57:S1:401:LEU:HD11	57:S1:432:ILE:HG13	1.93	0.49
63:S7:67:PHE:HE2	63:S7:117:LEU:HA	1.77	0.49
64:S8:162:CYS:HA	83:S8:301:SF4:S3	2.53	0.49
65:V1:118:ASP:HB3	65:V1:207:GLY:HA2	1.94	0.49
12:A2:59:SER:HB2	57:S1:655:ARG:HD3	1.94	0.49
68:A8:301:CDL:H512	40:CB:34:VAL:HG11	1.94	0.49
19:AC:119:ILE:HG21	19:AC:135:ALA:HB1	1.93	0.49
68:B5:202:CDL:H662	45:N5:16:THR:HG21	1.94	0.49
48:QB:460:GLY:HA2	48:QB:462:ILE:HG12	1.94	0.49
66:V2:204:ILE:HD11	66:V2:219:ARG:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:4L:201:CDL:H511	46:N6:88:THR:HG23	1.94	0.49
2:5A:55:ASP:HA	2:5A:90:ILE:HD11	1.95	0.49
20:AK:289:ASP:OD1	20:AK:290:ASP:N	2.45	0.49
24:B1:30:ARG:O	24:B1:33:GLU:HG2	2.13	0.49
33:BK:171:LYS:O	33:BK:175:ALA:CB	2.61	0.49
35:C1:3:VAL:HG13	35:C1:7:LEU:HD12	1.95	0.49
35:C1:358:LEU:HB3	77:C1:603:HEA:HMA	1.94	0.49
45:N5:359:MET:O	45:N5:436:ARG:NH2	2.45	0.49
47:QA:70:ARG:HA	47:QA:185:ALA:O	2.13	0.49
47:QA:82:LEU:HD23	47:QA:205:LEU:HD11	1.94	0.49
48:QB:310:ILE:HD11	48:QB:388:VAL:HA	1.94	0.49
51:QK:20:ARG:HD2	48:Qb:318:TYR:CE1	2.48	0.49
51:Qe:214:ILE:HD11	51:Qe:261:PRO:HB3	1.95	0.49
35:C1:360:ASN:O	35:C1:364:ASP:N	2.42	0.48
76:C1:601:3PE:H2D2	38:C4:109:PHE:HB3	1.94	0.48
37:C3:140:SER:HB2	37:C3:242:TRP:HE1	1.78	0.48
44:N4:211:GLY:H	44:N4:213:HIS:HD2	1.60	0.48
51:QK:64:LEU:HA	51:QK:77:ARG:O	2.13	0.48
66:V2:93:LEU:HD12	66:V2:122:TYR:HB3	1.93	0.48
1:4L:6:MET:HB2	46:N6:119:PHE:CD1	2.49	0.48
18:A9:258:ALA:HA	18:A9:261:LYS:HD2	1.95	0.48
44:N4:201:MET:HE1	44:N4:212:LEU:HD11	1.94	0.48
48:QB:110:GLU:HA	48:QB:113:VAL:HG22	1.95	0.48
49:QC:233:LEU:HG	50:QD:297:MET:HE1	1.95	0.48
49:Qc:126:THR:HG21	80:Qc:403:HEM:HBB2	1.95	0.48
49:Qc:301:LEU:HD21	71:Qc:402:PEE:H47	1.94	0.48
16:A7:46:SER:O	16:A7:52:ASN:ND2	2.46	0.48
17:A8:95:VAL:HG12	17:A8:97:VAL:HG22	1.95	0.48
71:AL:203:PEE:H63	45:N5:561:ILE:HG23	1.94	0.48
30:B7:39:MET:HE2	30:B7:41:ALA:H	1.78	0.48
31:B8:149:ILE:HD12	76:B8:201:3PE:H11	1.95	0.48
47:QA:155:GLN:HE21	47:QA:198:GLY:H	1.61	0.48
50:QD:322:TYR:CE2	50:QD:324:PRO:HG3	2.48	0.48
63:S7:59:ARG:HG3	63:S7:181:GLN:HB3	1.95	0.48
36:C2:131:GLY:O	38:C4:144:ARG:HD3	2.13	0.48
47:QA:90:THR:HG23	47:QA:95:SER:HA	1.94	0.48
51:QE:224:PRO:HA	51:QE:236:CYS:HA	1.95	0.48
49:Qc:227:LYS:HG2	50:Qd:308:LYS:HE2	1.95	0.48
57:S1:49:VAL:HG13	57:S1:102:ILE:HD13	1.94	0.48
62:S6:61:GLU:OE2	64:S8:192:ASN:ND2	2.47	0.48
65:V1:112:TYR:CD1	65:V1:153:ALA:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:QE:234:TYR:HB2	51:QE:243:TYR:HB2	1.94	0.48
47:Qa:211:ASN:HB3	47:Qa:246:LEU:HG	1.96	0.48
58:S2:299:LEU:HD22	58:S2:304:ILE:HD12	1.95	0.48
58:S2:374:ARG:NH2	64:S8:165:ASP:OD1	2.41	0.48
60:S4:111:LEU:HG	60:S4:112:MET:HG2	1.95	0.48
65:V1:160:GLY:N	65:V1:200:GLY:O	2.46	0.48
10:8B:52:ILE:HB	10:8B:53:PRO:HD3	1.95	0.48
31:B8:42:PRO:HB2	31:B8:48:ARG:HG2	1.94	0.48
35:C1:95:PRO:HD2	70:C1:611:PC1:H111	1.94	0.48
35:C1:101:SER:O	35:C1:156:SER:OG	2.24	0.48
47:QA:125:CYS:HB3	47:QA:133:LEU:HD22	1.94	0.48
58:S2:89:ASN:HD22	58:S2:102:ARG:HH21	1.61	0.48
65:V1:174:ARG:HA	67:V3:406:LEU:HD21	1.95	0.48
66:V2:160:VAL:HG21	66:V2:173:GLU:HG3	1.95	0.48
33:BK:107:GLN:HE22	45:N5:194:ASN:ND2	2.10	0.48
35:C1:372:TYR:N	35:C1:432:GLY:HA3	2.29	0.48
77:C1:602:HEA:HBA2	77:C1:602:HEA:CMA	2.44	0.48
42:N2:17:THR:HG22	42:N2:21:MET:HE2	1.96	0.48
44:N4:76:MET:SD	44:N4:230:VAL:HB	2.53	0.48
45:N5:401:MET:SD	45:N5:482:MET:HB3	2.53	0.48
75:QB:504:PLX:H111	51:QE:125:VAL:HG21	1.95	0.48
21:AL:118:MET:HA	21:AL:121:THR:HG22	1.96	0.48
34:BL:90:VAL:HG22	44:N4:28:THR:HG21	1.95	0.48
36:C2:143:VAL:HG12	36:C2:219:PHE:HD1	1.78	0.48
42:N2:170:LEU:HD11	42:N2:288:LEU:HD22	1.95	0.48
44:N4:318:ALA:HB2	44:N4:373:ILE:HG13	1.94	0.48
45:N5:214:ILE:HG12	45:N5:276:MET:HE1	1.95	0.48
47:Qa:63:LEU:HD21	47:Qa:218:MET:HE3	1.96	0.48
48:Qb:302:VAL:HB	48:Qb:303:PRO:HD3	1.96	0.48
5:6B:58:ARG:HA	5:6B:61:TYR:CE2	2.48	0.48
20:AK:316:LEU:HB2	20:AK:319:ILE:HG12	1.96	0.48
28:B5:139:ILE:HG23	44:N4:54:LEU:HD23	1.95	0.48
35:C1:261:TYR:HB2	35:C1:338:MET:HE2	1.94	0.48
48:QB:156:LEU:O	48:QB:213:ARG:NH1	2.43	0.48
68:QC:404:CDL:H111	54:Qh:42:THR:HG23	1.96	0.48
58:S2:391:TYR:HD1	64:S8:122:VAL:HG21	1.79	0.48
65:V1:202:GLY:H	66:V2:121:MET:HG3	1.79	0.48
65:V1:244:ASN:OD1	65:V1:245:VAL:N	2.47	0.48
18:A9:61:ALA:HB3	18:A9:82:VAL:HG13	1.94	0.48
19:AB:140:CYS:HB2	19:AB:143:GLU:OE1	2.14	0.48
75:C2:301:PLX:H1C3	75:C2:301:PLX:H22	1.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:CB:13:LEU:HD21	61:S5:4:PHE:HB3	1.94	0.48
75:N4:503:PLX:H1C3	75:N4:503:PLX:H22	1.64	0.48
51:QE:239:HIS:HB2	82:QE:303:FES:S1	2.53	0.48
48:Qb:315:ASP:OD1	48:Qb:316:SER:N	2.46	0.48
47:QA:85:LEU:HD12	47:QA:158:LEU:HD23	1.96	0.47
49:Qc:332:LEU:HD11	71:Qc:402:PEE:H44	1.95	0.47
41:N1:24:GLU:OE2	41:N1:228:TYR:OH	2.26	0.47
41:N1:31:MET:HG2	64:S8:77:LEU:HB2	1.96	0.47
41:N1:108:MET:HE1	70:N1:401:PC1:H291	1.96	0.47
41:N1:219:PRO:HA	41:N1:222:MET:HG2	1.96	0.47
48:QB:366:ASP:H	48:QB:464:GLN:HE21	1.62	0.47
49:QC:31:TRP:NE1	80:QC:402:HEM:O2D	2.47	0.47
49:Qc:361:ILE:HG12	49:Qc:365:LEU:HD12	1.95	0.47
58:S2:448:HIS:HB3	58:S2:452:ASP:HB2	1.96	0.47
27:B4:98:LEU:HD11	76:B4:201:3PE:H3H2	1.96	0.47
37:C3:204:HIS:NE2	37:C3:249:TRP:HB2	2.30	0.47
48:QB:270:PHE:CG	48:QB:292:GLU:HB2	2.50	0.47
53:QG:109:ALA:O	56:Qj:9:ARG:HD3	2.14	0.47
68:QH:101:CDL:HB62	68:QH:102:CDL:OA9	2.15	0.47
47:Qa:409:PRO:O	47:Qa:413:LEU:HG	2.14	0.47
15:A6:63:ARG:NH2	19:AB:132:ASP:OD2	2.46	0.47
32:B9:120:GLN:HB2	45:N5:524:ASN:HD21	1.79	0.47
33:BK:3:ASP:N	33:BK:3:ASP:OD1	2.47	0.47
35:C1:254:ILE:HG13	35:C1:344:PHE:CD2	2.49	0.47
51:QE:209:GLU:HG3	51:QE:210:TRP:CD1	2.49	0.47
52:Qf:38:GLU:OE1	52:Qf:47:ARG:NH2	2.46	0.47
5:6B:44:MET:HE3	5:6B:53:VAL:HG11	1.97	0.47
20:AK:93:ILE:HG23	20:AK:136:TRP:NE1	2.29	0.47
32:B9:181:GLN:NE2	32:B9:198:PRO:O	2.46	0.47
35:C1:274:VAL:HG12	35:C1:278:MET:HE2	1.97	0.47
37:C3:58:TRP:NE1	70:C3:302:PC1:H351	2.29	0.47
44:N4:408:LEU:HD12	45:N5:172:ILE:HG21	1.95	0.47
50:Qd:99:HIS:HE2	50:Qd:209:GLU:CD	2.22	0.47
57:S1:446:GLY:HA3	57:S1:451:ILE:HD12	1.96	0.47
65:V1:112:TYR:O	65:V1:240:THR:HA	2.14	0.47
35:C1:130:PRO:HG3	35:C1:209:LEU:HD13	1.96	0.47
68:4L:201:CDL:H161	45:N5:593:ILE:HD11	1.97	0.47
70:6A:101:PC1:H3A1	37:C3:206:LEU:HD22	1.97	0.47
17:A8:196:ARG:NH2	23:AN:63:GLU:OE2	2.48	0.47
23:AN:43:LEU:HG	41:N1:179:TRP:HE1	1.79	0.47
31:B8:110:ASP:HB3	44:N4:278:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C1:447:TYR:O	35:C1:451:ASN:ND2	2.47	0.47
37:C3:133:ASN:HB3	37:C3:173:PHE:CE1	2.50	0.47
71:C3:303:PEE:H49	71:C3:303:PEE:H55	1.53	0.47
43:N3:115:GLU:HA	58:S2:111:MET:HG2	1.96	0.47
56:QJ:35:ALA:HB1	70:Qb:502:PC1:H3H2	1.96	0.47
49:Qc:137:GLN:NE2	49:Qc:263:ASN:O	2.48	0.47
53:Qg:44:VAL:O	53:Qg:48:ILE:HG12	2.14	0.47
57:S1:36:VAL:HG11	57:S1:56:VAL:HG21	1.97	0.47
57:S1:208:THR:O	57:S1:210:ILE:N	2.48	0.47
57:S1:557:ARG:NH2	57:S1:581:ASP:OD1	2.47	0.47
57:S1:593:SER:HA	57:S1:606:THR:O	2.14	0.47
65:V1:204:TYR:HB3	65:V1:377:GLU:HB3	1.97	0.47
66:V2:85:LEU:HD13	67:V3:400:LEU:HD22	1.96	0.47
10:8B:26:TYR:HE2	38:C4:39:VAL:HG23	1.80	0.47
10:8B:46:THR:O	10:8B:49:SER:OG	2.31	0.47
68:AL:201:CDL:H532	45:N5:577:VAL:HA	1.96	0.47
22:AM:139:PRO:HG3	57:S1:306:MET:HE1	1.96	0.47
36:C2:162:SER:HB3	36:C2:197:SER:H	1.79	0.47
59:S3:174:PHE:O	59:S3:199:ARG:NE	2.45	0.47
1:4L:73:LEU:HD21	42:N2:41:ILE:HG13	1.97	0.47
6:6C:18:ARG:CZ	36:C2:48:THR:HB	2.45	0.47
15:A6:93:PHE:CE1	73:AB:201:ZMP:H7	2.50	0.47
76:CA:101:3PE:H381	42:N2:325:LEU:H	1.80	0.47
71:6A:102:PEE:H39	71:6A:102:PEE:H46	1.66	0.47
20:AK:64:VAL:HA	20:AK:205:VAL:O	2.15	0.47
30:B7:19:PRO:HA	30:B7:22:MET:HE3	1.97	0.47
35:C1:97:MET:HE1	70:C1:611:PC1:H251	1.96	0.47
35:C1:264:LYS:NZ	35:C1:326:THR:O	2.40	0.47
42:N2:139:LEU:HD13	42:N2:190:MET:HE1	1.97	0.47
48:QB:179:MET:HE1	48:QB:282:LEU:HD13	1.96	0.47
49:QC:102:LEU:HD22	49:QC:304:MET:HE2	1.97	0.47
49:Qc:8:HIS:HB3	49:Qc:11:MET:HB2	1.96	0.47
49:Qc:197:LEU:HD11	80:Qc:404:HEM:HMA2	1.96	0.47
57:S1:180:THR:O	57:S1:184:ARG:NE	2.47	0.47
57:S1:522:GLN:O	57:S1:526:LEU:HG	2.15	0.47
1:4L:40:LEU:HD13	42:N2:71:MET:HG3	1.97	0.46
20:AK:141:ARG:NH2	74:AK:401:ADP:N7	2.63	0.46
20:AK:205:VAL:O	20:AK:207:VAL:HG23	2.15	0.46
20:AK:205:VAL:HG12	20:AK:207:VAL:HG22	1.97	0.46
41:N1:24:GLU:HB2	41:N1:271:LEU:HD22	1.98	0.46
75:N3:201:PLX:H1A2	75:N3:201:PLX:H22	1.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:N5:27:TYR:O	45:N5:115:ASN:ND2	2.48	0.46
49:Qc:233:LEU:HD23	50:Qd:301:LEU:HD23	1.96	0.46
57:S1:367:CYS:HB3	57:S1:533:GLY:O	2.16	0.46
58:S2:117:PRO:HG3	58:S2:441:LEU:HD23	1.97	0.46
58:S2:145:LEU:HD11	58:S2:430:ILE:HD13	1.97	0.46
27:B4:6:TYR:OH	27:B4:12:ALA:O	2.27	0.46
35:C1:439:ARG:HD3	36:C2:199:ILE:HD11	1.97	0.46
70:C1:611:PC1:H361	70:C1:611:PC1:H2B1	1.96	0.46
45:N5:570:GLN:HB2	71:S2:501:PEE:H50	1.97	0.46
51:QE:187:GLU:OE1	51:QE:248:ARG:NH2	2.45	0.46
68:QH:102:CDL:HB32	68:QH:102:CDL:HA21	1.95	0.46
57:S1:594:ALA:O	57:S1:605:GLN:HA	2.16	0.46
63:S7:108:THR:HA	63:S7:136:CYS:HB3	1.98	0.46
20:AK:63:THR:CG2	20:AK:203:PRO:HB3	2.45	0.46
20:AK:232:THR:HG23	20:AK:235:TYR:H	1.80	0.46
21:AL:66:ILE:HD11	21:AL:101:LEU:HB2	1.96	0.46
70:C1:606:PC1:H2F2	70:C1:606:PC1:H2B2	1.96	0.46
68:C1:610:CDL:H802	68:C1:610:CDL:H552	1.96	0.46
37:C3:58:TRP:CD1	37:C3:61:ILE:HD12	2.49	0.46
41:N1:24:GLU:HG3	41:N1:25:ARG:N	2.30	0.46
41:N1:151:LEU:HD21	43:N3:75:LEU:HD12	1.97	0.46
42:N2:132:THR:HG23	42:N2:209:ILE:HG12	1.97	0.46
44:N4:67:VAL:HG12	75:N4:503:PLX:H362	1.97	0.46
50:QD:127:SER:HB3	50:QD:179:PRO:HD2	1.97	0.46
49:Qc:132:VAL:HG22	49:Qc:143:ALA:HB2	1.97	0.46
51:Qe:234:TYR:HB2	51:Qe:243:TYR:HB2	1.97	0.46
16:A7:39:PRO:HG3	64:S8:211:TYR:CZ	2.51	0.46
45:N5:176:ARG:HA	45:N5:176:ARG:HD3	1.66	0.46
47:QA:121:TYR:HB3	47:QA:137:LEU:HD11	1.96	0.46
47:Qa:123:VAL:HB	47:Qa:133:LEU:HD23	1.97	0.46
29:B6:148:TYR:CE1	33:BK:49:ARG:HG2	2.51	0.46
37:C3:95:THR:HG23	70:C3:301:PC1:H2A2	1.97	0.46
44:N4:265:SER:O	44:N4:269:MET:HG3	2.16	0.46
45:N5:136:ASN:HD21	71:N5:701:PEE:H46	1.81	0.46
47:Qa:298:HIS:HB2	48:Qb:114:GLU:HG2	1.98	0.46
48:Qb:274:GLU:CD	48:Qb:276:ARG:HE	2.24	0.46
48:Qb:422:ARG:HH22	48:Qb:428:GLU:CD	2.24	0.46
64:S8:117:LYS:NZ	64:S8:130:ILE:O	2.48	0.46
65:V1:51:TRP:CD1	67:V3:388:ASN:HD22	2.34	0.46
28:B5:57:ILE:HG23	32:B9:146:LEU:HD13	1.97	0.46
35:C1:7:LEU:HD13	68:C1:610:CDL:H521	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:N5:11:THR:HG22	45:N5:46:LEU:HB3	1.97	0.46
45:N5:71:LEU:N	45:N5:74:VAL:O	2.46	0.46
47:QA:451:ASP:OD2	47:Qa:183:ARG:NH2	2.48	0.46
57:S1:575:VAL:C	57:S1:578:PRO:HD2	2.41	0.46
20:AK:63:THR:HG22	20:AK:161:LEU:HD12	1.97	0.46
31:B8:96:ASP:OD1	31:B8:96:ASP:N	2.48	0.46
33:BK:78:GLU:HA	40:CB:110:THR:HA	1.97	0.46
35:C1:236:TRP:O	35:C1:288:TRP:HB2	2.16	0.46
41:N1:146:LEU:HD11	41:N1:192:GLU:HG3	1.97	0.46
45:N5:78:LEU:HD11	68:N5:702:CDL:H261	1.97	0.46
45:N5:341:MET:HE2	45:N5:454:ILE:HG12	1.98	0.46
70:Qb:502:PC1:H282	49:Qc:229:ILE:HD11	1.97	0.46
57:S1:44:GLU:O	57:S1:47:THR:OG1	2.30	0.46
20:AK:355:TRP:H	20:AK:355:TRP:CD1	2.33	0.46
37:C3:77:LYS:NZ	37:C3:81:TYR:OH	2.44	0.46
45:N5:241:THR:HG21	45:N5:344:GLY:HA3	1.98	0.46
46:N6:129:ASP:HB2	61:S5:32:ARG:NH1	2.31	0.46
49:QC:119:LEU:HD22	80:QC:402:HEM:HBB2	1.97	0.46
55:QI:47:ILE:HG23	70:Qd:402:PC1:H152	1.97	0.46
75:QI:301:PLX:H342	75:QI:301:PLX:H312	1.77	0.46
51:Qe:220:LEU:HD12	51:Qe:239:HIS:CE1	2.50	0.46
30:B7:107:ARG:HA	30:B7:110:GLN:HG2	1.98	0.46
37:C3:210:ILE:HD13	70:C3:302:PC1:H3D1	1.98	0.46
40:CB:38:PHE:HZ	68:N2:402:CDL:H832	1.80	0.46
41:N1:111:LEU:HD23	70:N1:401:PC1:H3I1	1.98	0.46
41:N1:305:ILE:HD13	43:N3:91:ALA:HB1	1.98	0.46
42:N2:42:PRO:HG3	46:N6:167:VAL:HG13	1.98	0.46
45:N5:435:PRO:HB3	45:N5:437:PHE:CZ	2.51	0.46
46:N6:17:PHE:HA	46:N6:20:PHE:CD2	2.50	0.46
47:QA:259:ARG:HB3	47:QA:444:LEU:HD13	1.98	0.46
48:QB:413:ILE:HG12	48:QB:423:ARG:HD2	1.98	0.46
75:QI:301:PLX:H341	56:QJ:31:GLY:HA3	1.97	0.46
65:V1:384:PRO:HG2	65:V1:422:HIS:O	2.16	0.46
22:AM:127:TYR:OH	62:S6:61:GLU:O	2.23	0.46
38:C4:64:GLU:HA	38:C4:67:LYS:HZ2	1.80	0.46
70:N3:202:PC1:H262	70:N3:202:PC1:H291	1.73	0.46
49:QC:131:TYR:O	49:QC:134:PRO:HD2	2.15	0.46
49:QC:141:TRP:CD1	49:QC:265:PRO:HD3	2.51	0.46
51:QE:153:GLU:HB3	51:QE:270:LEU:HD11	1.98	0.46
52:Qf:28:ASP:HB3	52:Qf:29:PRO:HD3	1.98	0.46
57:S1:260:ASN:N	57:S1:282:ASN:HD21	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:V1:124:THR:HA	65:V1:277:ASN:HD22	1.81	0.46
2:5A:91:ILE:O	2:5A:95:LEU:HG	2.16	0.45
8:7B:46:ALA:HA	38:C4:108:LEU:HD13	1.98	0.45
18:A9:204:SER:HB2	18:A9:266:VAL:HG12	1.97	0.45
18:A9:215:ASN:HD21	18:A9:355:ARG:HH22	1.63	0.45
29:B6:159:GLU:HG2	45:N5:61:MET:HG2	1.98	0.45
44:N4:266:MET:HB3	44:N4:395:LEU:HD13	1.98	0.45
44:N4:412:ILE:HG12	44:N4:416:ARG:HD2	1.97	0.45
44:N4:445:LEU:HB3	68:N5:702:CDL:H452	1.98	0.45
45:N5:190:LEU:HB2	45:N5:196:TRP:NE1	2.31	0.45
47:QA:155:GLN:HB3	47:QA:198:GLY:HA2	1.97	0.45
49:QC:37:LEU:HD12	49:QC:97:HIS:HD2	1.81	0.45
49:QC:138:MET:HE1	49:QC:269:LYS:H	1.81	0.45
50:Qd:209:GLU:H	50:Qd:209:GLU:HG2	1.53	0.45
57:S1:169:VAL:HG22	57:S1:223:ILE:HD11	1.98	0.45
57:S1:455:ILE:O	57:S1:463:SER:OG	2.32	0.45
58:S2:128:LYS:NZ	59:S3:202:PHE:O	2.44	0.45
58:S2:134:THR:HA	58:S2:424:ARG:HG2	1.98	0.45
1:4L:37:MET:HE1	46:N6:64:MET:HE1	1.99	0.45
70:6A:101:PC1:H111	37:C3:187:THR:HA	1.98	0.45
71:6A:102:PEE:H43	70:C3:302:PC1:H3H1	1.97	0.45
20:AK:145:TYR:OH	20:AK:201:LEU:O	2.25	0.45
70:B5:203:PC1:H232	70:B5:203:PC1:H352	1.97	0.45
29:B6:85:ASP:O	32:B9:163:LYS:NZ	2.49	0.45
33:BK:115:GLN:HG2	45:N5:62:ILE:HG12	1.97	0.45
35:C1:35:LEU:HD13	35:C1:462:LEU:HD22	1.98	0.45
36:C2:155:SER:OG	36:C2:156:SER:N	2.47	0.45
37:C3:231:HIS:HB3	70:C3:302:PC1:H133	1.98	0.45
41:N1:233:MET:HE3	41:N1:233:MET:HB3	1.88	0.45
75:N4:502:PLX:H4	75:N4:502:PLX:H72	1.38	0.45
49:QC:30:TRP:HE1	68:QC:404:CDL:H1	1.81	0.45
50:QD:203:ARG:HB2	50:QD:279:SER:HB2	1.97	0.45
47:Qa:125:CYS:HB3	47:Qa:133:LEU:HD22	1.98	0.45
48:Qb:74:TRP:CZ2	48:Qb:411:GLU:HA	2.52	0.45
49:Qc:112:THR:HG22	49:Qc:196:HIS:CE1	2.52	0.45
17:A8:201:GLU:HA	17:A8:204:LYS:HD3	1.98	0.45
75:AM:202:PLX:H311	75:AM:202:PLX:H341	1.72	0.45
37:C3:133:ASN:HB3	37:C3:173:PHE:HE1	1.82	0.45
76:CA:101:3PE:H2H2	75:CB:201:PLX:H182	1.98	0.45
41:N1:151:LEU:HD11	43:N3:75:LEU:HB2	1.98	0.45
57:S1:456:ALA:O	57:S1:499:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A1:64:LYS:HB3	11:A1:68:ASN:HD22	1.82	0.45
18:A9:229:ILE:HB	18:A9:323:HIS:CD2	2.51	0.45
20:AK:112:GLY:HA2	20:AK:136:TRP:CD2	2.52	0.45
30:B7:22:MET:HE1	30:B7:102:PHE:CD2	2.51	0.45
35:C1:173:PRO:HD2	35:C1:176:MET:HE2	1.99	0.45
35:C1:288:TRP:HZ3	70:C1:607:PC1:H362	1.82	0.45
42:N2:197:ASN:HB2	42:N2:269:GLU:HG2	1.97	0.45
42:N2:216:PHE:O	42:N2:220:ILE:HG13	2.16	0.45
43:N3:58:VAL:HG21	43:N3:113:TRP:HZ2	1.82	0.45
71:N4:501:PEE:H25	71:N4:501:PEE:H31	1.73	0.45
51:QE:130:LYS:HD2	56:Qj:34:TRP:CE2	2.51	0.45
51:QE:196:ARG:NH1	51:QE:254:ALA:O	2.49	0.45
53:QG:44:VAL:O	53:QG:48:ILE:HG12	2.17	0.45
51:Qe:201:ASP:C	51:Qe:203:GLU:H	2.24	0.45
52:Qf:33:VAL:HG12	52:Qf:82:VAL:HG22	1.96	0.45
57:S1:219:SER:O	57:S1:222:ILE:HG12	2.17	0.45
59:S3:126:PHE:HE2	59:S3:149:GLU:HG3	1.82	0.45
71:A3:201:PEE:H27	71:A3:201:PEE:H22	1.55	0.45
35:C1:240:HIS:O	35:C1:243:VAL:HG22	2.16	0.45
35:C1:313:ALA:HA	77:C1:603:HEA:H262	1.99	0.45
49:QC:137:GLN:NE2	49:QC:263:ASN:O	2.49	0.45
51:QE:227:ASN:N	51:QE:233:GLY:O	2.40	0.45
58:S2:129:LEU:O	58:S2:133:LYS:HG2	2.17	0.45
27:B4:77:TYR:CZ	45:N5:564:LYS:HG2	2.52	0.45
37:C3:58:TRP:HD1	37:C3:61:ILE:HD12	1.81	0.45
44:N4:207:MET:HE3	44:N4:294:MET:HE3	1.98	0.45
45:N5:5:ALA:HB2	45:N5:61:MET:HE1	1.98	0.45
63:S7:62:LEU:O	63:S7:91:VAL:HA	2.15	0.45
65:V1:364:VAL:HG12	65:V1:400:VAL:HG12	1.97	0.45
71:8B:201:PEE:H56	38:C4:120:TRP:HD1	1.81	0.45
13:A3:111:GLY:HA3	71:A3:201:PEE:H37	1.99	0.45
70:C1:606:PC1:H2H2	70:C1:606:PC1:H261	1.98	0.45
75:CB:201:PLX:H72	75:CB:201:PLX:H4	1.65	0.45
44:N4:233:ALA:HA	44:N4:320:GLY:HA2	1.99	0.45
44:N4:243:MET:HB3	44:N4:301:ILE:HG21	1.98	0.45
45:N5:230:HIS:H	45:N5:230:HIS:CD2	2.35	0.45
45:N5:327:LEU:O	45:N5:331:MET:HG2	2.16	0.45
49:QC:27:ILE:HA	49:QC:208:PRO:HD3	1.98	0.45
53:QG:71:MET:HE2	50:Qd:312:TRP:HZ3	1.80	0.45
48:Qb:190:THR:HB	48:Qb:275:ILE:HG13	1.99	0.45
58:S2:442:ASP:OD1	58:S2:446:LYS:NZ	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4L:5:TYR:HB3	1:4L:43:MET:HE1	1.99	0.45
71:6A:103:PEE:H21	71:6A:103:PEE:H28	1.55	0.45
15:A6:88:LYS:HD2	15:A6:88:LYS:HA	1.79	0.45
22:AM:109:ILE:HG12	64:S8:198:GLU:HB3	1.98	0.45
28:B5:147:ALA:HB2	44:N4:173:SER:HB2	1.99	0.45
38:C4:36:PRO:HB2	38:C4:49:VAL:HG13	1.98	0.45
44:N4:122:PHE:CZ	44:N4:206:LYS:HE3	2.51	0.45
44:N4:231:LEU:HA	44:N4:235:LEU:HB2	1.99	0.45
49:QC:155:TYR:CZ	70:QJ:101:PC1:H143	2.52	0.45
51:QE:123:VAL:HG13	55:Qi:29:ALA:HA	1.99	0.45
68:QH:101:CDL:H751	68:QH:101:CDL:H562	1.97	0.45
65:V1:75:TRP:O	65:V1:79:GLU:HG2	2.15	0.45
2:5A:68:ASP:OD1	2:5A:68:ASP:N	2.45	0.45
17:A8:111:ALA:HB2	17:A8:197:PRO:HG3	1.98	0.45
26:B3:47:ARG:HA	26:B3:50:ALA:HB3	1.98	0.45
32:B9:169:ARG:HG2	32:B9:172:ARG:HH22	1.82	0.45
35:C1:407:GLN:N	76:C1:601:3PE:O12	2.49	0.45
41:N1:133:LEU:HD21	46:N6:74:MET:HB3	1.99	0.45
48:QB:366:ASP:HB2	48:QB:464:GLN:HG2	1.97	0.45
49:Qc:200:LEU:CD2	80:Qc:404:HEM:HAA1	2.47	0.45
63:S7:75:GLU:HG3	63:S7:167:PRO:HB2	1.98	0.45
65:V1:217:GLU:OE2	65:V1:224:ARG:NH2	2.50	0.45
66:V2:246:GLN:HG2	66:V2:247:ALA:H	1.82	0.45
9:7C:40:MET:SD	70:7C:101:PC1:H32	2.57	0.45
19:AC:112:SER:HB3	32:B9:59:LEU:HD11	1.99	0.45
19:AC:117:GLU:OE2	32:B9:62:TYR:OH	2.34	0.45
70:B5:203:PC1:H272	70:B5:203:PC1:H2D1	1.99	0.45
31:B8:110:ASP:HB3	44:N4:278:ARG:NH1	2.32	0.45
35:C1:352:GLY:HA3	77:C1:603:HEA:C14	2.47	0.45
42:N2:168:GLY:O	42:N2:172:GLN:HG2	2.16	0.45
47:Qa:154:LEU:HD23	47:Qa:154:LEU:HA	1.83	0.45
15:A6:74:HIS:CE1	18:A9:364:SER:HA	2.50	0.44
15:A6:88:LYS:HE2	15:A6:92:MET:HE2	1.98	0.44
17:A8:121:MET:HE3	17:A8:125:TRP:HZ3	1.82	0.44
17:A8:175:ARG:NH1	41:N1:170:GLU:OE1	2.50	0.44
20:AK:56:THR:OG1	20:AK:57:GLU:N	2.48	0.44
22:AM:124:TYR:OH	64:S8:184:LEU:O	2.33	0.44
44:N4:70:THR:HA	44:N4:103:GLN:HE21	1.82	0.44
45:N5:341:MET:SD	45:N5:457:LEU:HD12	2.57	0.44
51:QE:228:ALA:HB3	51:QE:235:TYR:HB3	1.99	0.44
48:Qb:81:TYR:HB3	48:Qb:223:HIS:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Qe:214:ILE:HG13	51:Qe:261:PRO:HD3	1.99	0.44
70:6A:101:PC1:H121	37:C3:181:TYR:O	2.17	0.44
30:B7:95:TYR:CZ	31:B8:156:VAL:HG11	2.52	0.44
32:B9:182:LEU:HD11	32:B9:208:LEU:HG	1.98	0.44
70:C1:611:PC1:H362	37:C3:54:MET:HG2	1.99	0.44
42:N2:271:THR:HG23	44:N4:169:ASN:ND2	2.31	0.44
45:N5:518:GLN:HB2	68:N5:703:CDL:H262	2.00	0.44
68:QB:501:CDL:H721	49:QC:4:ILE:HD11	1.99	0.44
58:S2:277:ARG:NH2	58:S2:451:ALA:HB1	2.32	0.44
76:B4:201:3PE:H3B2	76:B4:201:3PE:H3E1	1.66	0.44
35:C1:325:ALA:HB2	36:C2:65:TRP:HH2	1.83	0.44
37:C3:55:TYR:HA	71:C3:303:PEE:H65	1.99	0.44
41:N1:215:TYR:HD2	41:N1:219:PRO:HB2	1.82	0.44
71:N5:701:PEE:H30	68:N5:702:CDL:H251	1.99	0.44
46:N6:6:ALA:HB3	46:N6:124:ASP:OD2	2.16	0.44
55:QI:50:GLY:H	55:QI:55:HIS:CD2	2.36	0.44
47:Qa:231:LYS:HB3	47:Qa:231:LYS:HE2	1.74	0.44
27:B4:99:PHE:CZ	76:B4:201:3PE:H2I3	2.52	0.44
28:B5:176:LYS:H	61:S5:45:HIS:CD2	2.35	0.44
44:N4:133:ILE:HD11	44:N4:231:LEU:HD11	1.99	0.44
44:N4:205:VAL:HG22	44:N4:212:LEU:HD13	1.99	0.44
47:QA:175:GLU:HG3	47:QA:189:SER:HB3	1.99	0.44
58:S2:190:ILE:HD11	58:S2:257:PHE:CZ	2.53	0.44
1:4L:55:LEU:HD13	61:S5:17:TRP:HE3	1.83	0.44
16:A7:23:LYS:HG3	58:S2:259:PHE:CD1	2.53	0.44
19:AB:77:GLU:CD	19:AB:77:GLU:H	2.26	0.44
35:C1:219:PHE:CZ	37:C3:199:VAL:HG21	2.52	0.44
45:N5:289:ALA:O	45:N5:293:ILE:HG23	2.18	0.44
45:N5:297:ASP:O	45:N5:301:ILE:HG13	2.17	0.44
48:QB:388:VAL:HG21	48:QB:438:ALA:HA	2.00	0.44
80:QC:401:HEM:HMC1	80:QC:401:HEM:HBC2	2.00	0.44
58:S2:292:TYR:HA	59:S3:161:LYS:HB2	1.98	0.44
66:V2:186:VAL:HG22	66:V2:196:LEU:HD11	2.00	0.44
2:5A:73:ARG:HA	38:C4:46:LEU:HD12	2.00	0.44
71:A3:201:PEE:H67	71:A3:201:PEE:H72	1.75	0.44
18:A9:169:HIS:HB2	18:A9:184:LYS:HD3	1.99	0.44
76:B4:201:3PE:H3H1	44:N4:210:TYR:CE2	2.53	0.44
41:N1:309:ILE:HD11	43:N3:87:MET:HE1	1.99	0.44
41:N1:309:ILE:HD12	43:N3:88:LEU:HD13	1.99	0.44
51:QE:234:TYR:N	51:QE:243:TYR:O	2.47	0.44
71:Qc:402:PEE:H35	71:Qc:402:PEE:H30	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:V2:245:VAL:HG13	66:V2:249:LEU:HD22	2.00	0.44
11:A1:12:MET:HE2	41:N1:23:VAL:HG21	2.00	0.44
17:A8:115:LYS:HB3	17:A8:116:PRO:HD3	1.99	0.44
73:AC:201:ZMP:H24	32:B9:116:GLY:O	2.17	0.44
29:B6:166:PRO:HG2	29:B6:180:MET:HG3	2.00	0.44
35:C1:265:LYS:HE2	35:C1:487:LEU:HD22	1.99	0.44
35:C1:438:ARG:NH2	77:C1:603:HEA:O2D	2.47	0.44
48:QB:80:ARG:HH22	48:QB:350:GLU:CD	2.26	0.44
51:QE:193:SER:OG	51:QE:194:GLN:OE1	2.34	0.44
47:Qa:230:LEU:HD23	47:Qa:230:LEU:HA	1.87	0.44
49:Qc:100:ARG:NH2	80:Qc:404:HEM:O1A	2.51	0.44
15:A6:62:TYR:OH	19:AB:117:GLU:OE2	2.25	0.44
15:A6:127:THR:O	15:A6:131:ARG:HG3	2.17	0.44
19:AC:87:LEU:HD23	19:AC:87:LEU:HA	1.85	0.44
21:AL:9:TYR:CZ	21:AL:21:LYS:HE3	2.52	0.44
27:B4:71:ALA:HB2	31:B8:38:PRO:HG2	2.00	0.44
31:B8:86:ARG:NH1	31:B8:103:GLU:OE2	2.40	0.44
37:C3:163:LEU:HD23	37:C3:163:LEU:HA	1.83	0.44
41:N1:29:GLY:O	41:N1:34:ARG:N	2.47	0.44
44:N4:211:GLY:H	44:N4:213:HIS:CD2	2.35	0.44
50:Qd:271:VAL:O	50:Qd:275:LEU:HG	2.17	0.44
57:S1:624:ARG:NH1	57:S1:628:GLU:OE1	2.37	0.44
58:S2:150:MET:SD	58:S2:150:MET:N	2.89	0.44
64:S8:63:TRP:HB3	64:S8:66:LEU:HD12	1.98	0.44
18:A9:180:TYR:CE1	18:A9:184:LYS:HD2	2.53	0.44
19:AB:117:GLU:HA	19:AB:120:MET:HE3	1.99	0.44
26:B3:27:THR:O	26:B3:30:GLU:HG2	2.17	0.44
33:BK:74:ILE:HG23	33:BK:156:LEU:HD22	1.98	0.44
42:N2:140:SER:HB3	61:S5:2:PRO:HA	2.00	0.44
42:N2:167:TRP:HB3	45:N5:574:SER:HA	1.99	0.44
42:N2:235:ASN:O	42:N2:315:TRP:NE1	2.49	0.44
75:QI:301:PLX:H22	75:QI:301:PLX:H1C3	1.56	0.44
51:Qe:239:HIS:HB2	82:Qe:301:FES:S2	2.58	0.44
57:S1:246:ARG:HH22	60:S4:123:ASN:ND2	2.10	0.44
65:V1:210:THR:HB	65:V1:224:ARG:H	1.83	0.44
2:5A:112:GLU:OE2	38:C4:89:SER:HB2	2.18	0.43
28:B5:71:MET:HE3	68:N5:702:CDL:H551	2.00	0.43
35:C1:244:TYR:HA	35:C1:247:ILE:HG22	2.00	0.43
70:C1:609:PC1:H282	70:C1:609:PC1:H391	2.00	0.43
36:C2:200:CYS:SG	36:C2:207:MET:CE	3.06	0.43
40:CB:35:TYR:OH	42:N2:335:LEU:O	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:N2:337:LEU:O	42:N2:340:THR:OG1	2.31	0.43
44:N4:369:LEU:O	44:N4:372:SER:OG	2.26	0.43
48:Qb:165:ARG:NH1	48:Qb:208:VAL:O	2.50	0.43
80:Qc:403:HEM:HMC1	80:Qc:403:HEM:HBC2	1.99	0.43
50:Qd:139:VAL:HG21	50:Qd:277:TRP:CZ2	2.53	0.43
57:S1:219:SER:OG	57:S1:288:ASP:OD2	2.23	0.43
57:S1:229:GLY:N	83:S1:801:SF4:S2	2.85	0.43
63:S7:140:GLY:HA3	63:S7:144:HIS:HA	1.99	0.43
65:V1:315:LEU:HB2	65:V1:359:ARG:HA	1.99	0.43
18:A9:270:ARG:NH1	18:A9:328:THR:OG1	2.51	0.43
19:AB:93:ILE:HD12	19:AB:108:LEU:HD13	2.00	0.43
25:B2:42:PRO:HB3	45:N5:442:LEU:HD23	2.00	0.43
26:B3:52:ARG:HD3	45:N5:435:PRO:O	2.18	0.43
34:BL:116:GLU:OE2	34:BL:120:ARG:NH1	2.50	0.43
34:BL:150:PRO:HG3	40:CB:115:LEU:HD22	2.00	0.43
36:C2:30:ILE:HG21	36:C2:76:ILE:HD11	2.00	0.43
45:N5:132:VAL:O	45:N5:262:ARG:NH2	2.49	0.43
50:QD:311:LYS:HD3	50:QD:311:LYS:HA	1.87	0.43
51:QE:241:SER:OG	82:QE:303:FES:S1	2.61	0.43
51:QE:266:THR:OG1	51:QE:270:LEU:O	2.28	0.43
47:Qa:408:GLN:HE21	47:Qa:409:PRO:HD2	1.82	0.43
50:Qd:129:ASP:OD1	50:Qd:178:LYS:NZ	2.51	0.43
58:S2:464:PHE:HA	58:S2:467:VAL:HB	2.00	0.43
61:S5:94:PRO:HB2	61:S5:99:LEU:HG	2.00	0.43
12:A2:20:ARG:HB2	12:A2:66:TRP:HB2	1.99	0.43
20:AK:67:ASN:CG	20:AK:68:ILE:H	2.21	0.43
23:AN:85:GLN:CD	61:S5:105:ARG:HD2	2.43	0.43
27:B4:105:PHE:CE1	44:N4:391:ILE:HB	2.54	0.43
36:C2:186:SER:OG	36:C2:213:LEU:HD13	2.17	0.43
42:N2:2:ASN:HD22	42:N2:4:ILE:H	1.65	0.43
43:N3:63:LEU:HD22	46:N6:67:VAL:HG21	1.99	0.43
51:Qe:183:GLU:O	51:Qe:187:GLU:HG2	2.18	0.43
57:S1:452:LEU:HD11	57:S1:493:VAL:HG12	1.99	0.43
60:S4:98:LYS:NZ	60:S4:127:THR:OG1	2.40	0.43
65:V1:138:LEU:HD13	65:V1:245:VAL:HG13	2.00	0.43
2:5A:123:GLU:OE1	2:5A:123:GLU:N	2.50	0.43
2:5A:124:ILE:HG12	6:6C:9:PRO:HG2	2.00	0.43
22:AM:4:VAL:O	22:AM:8:ARG:HG2	2.18	0.43
22:AM:122:GLN:HA	62:S6:59:GLN:HG2	1.99	0.43
35:C1:317:GLY:HA3	77:C1:603:HEA:H201	1.99	0.43
36:C2:13:THR:HB	36:C2:168:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:N1:401:PC1:H291	46:N6:57:PHE:HE2	1.83	0.43
44:N4:41:LEU:O	44:N4:44:GLN:NE2	2.49	0.43
48:QB:192:PHE:HB3	48:QB:195:THR:OG1	2.17	0.43
58:S2:151:MET:HE2	58:S2:232:TYR:HB3	2.00	0.43
59:S3:84:LEU:HD23	59:S3:141:ILE:HG13	2.00	0.43
65:V1:381:GLN:N	83:V1:501:SF4:S4	2.91	0.43
71:B4:202:PEE:H24	71:B4:202:PEE:H18	1.89	0.43
35:C1:406:ASN:HB3	35:C1:409:TRP:HB2	2.00	0.43
51:QE:140:MET:O	49:Qc:177:ARG:NH2	2.52	0.43
47:Qa:379:LYS:HG2	47:Qa:413:LEU:HD22	1.99	0.43
51:Qe:267:SER:HB3	51:Qe:270:LEU:HB3	2.00	0.43
53:Qg:52:PRO:HD2	53:Qg:55:LEU:HD12	2.01	0.43
57:S1:197:THR:HG22	57:S1:206:VAL:HG22	2.01	0.43
58:S2:341:GLU:O	58:S2:345:GLN:HG2	2.19	0.43
61:S5:15:ASP:OD1	61:S5:15:ASP:N	2.50	0.43
65:V1:64:LYS:HD2	66:V2:249:LEU:HD21	2.00	0.43
2:5A:109:ARG:HD2	38:C4:86:PHE:CE1	2.54	0.43
68:A1:101:CDL:H112	68:A1:101:CDL:H521	2.01	0.43
18:A9:109:ASN:HB3	18:A9:112:ASP:HB2	1.99	0.43
20:AK:94:HIS:HA	20:AK:97:ASP:HB2	1.99	0.43
20:AK:280:CYS:SG	20:AK:281:ASP:N	2.91	0.43
36:C2:78:LEU:HB2	36:C2:79:PRO:HD3	2.00	0.43
36:C2:193:TYR:CD2	36:C2:210:VAL:HG22	2.54	0.43
44:N4:220:HIS:NE2	44:N4:231:LEU:HB3	2.34	0.43
49:Qc:58:ASP:OD1	49:Qc:59:THR:N	2.51	0.43
49:Qc:318:ARG:O	49:Qc:322:GLN:HG3	2.19	0.43
59:S3:231:ARG:NH2	64:S8:128:ILE:O	2.52	0.43
66:V2:237:PRO:HA	66:V2:238:PRO:HD3	1.91	0.43
13:A3:127:ALA:HB2	41:N1:312:ALA:HA	2.00	0.43
68:A8:301:CDL:HB61	40:CB:29:THR:O	2.19	0.43
29:B6:92:GLU:HB3	29:B6:93:PRO:HD3	1.99	0.43
35:C1:439:ARG:HH11	36:C2:199:ILE:HD11	1.83	0.43
42:N2:49:ASN:ND2	42:N2:52:ALA:H	2.17	0.43
68:N2:402:CDL:H511	44:N4:16:TRP:HB3	1.99	0.43
45:N5:323:HIS:CE1	45:N5:475:MET:HG2	2.54	0.43
49:QC:181:PHE:CE1	49:Qc:53:MET:HE2	2.54	0.43
51:QE:249:ILE:HG22	51:QE:257:ASN:HD22	1.83	0.43
49:Qc:128:PHE:O	49:Qc:132:VAL:HG23	2.19	0.43
57:S1:279:GLU:OE2	60:S4:156:LYS:NZ	2.48	0.43
64:S8:153:ILE:HG12	83:S8:302:SF4:S1	2.59	0.43
65:V1:235:VAL:H	65:V1:240:THR:HG21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:8B:30:ALA:HB2	35:C1:480:ARG:HG3	2.01	0.43
23:AN:97:ILE:HG23	61:S5:86:LEU:HD12	2.01	0.43
26:B3:32:VAL:HG13	32:B9:81:TYR:HB2	2.01	0.43
33:BK:144:SER:O	33:BK:146:LEU:N	2.50	0.43
38:C4:45:PRO:O	38:C4:47:PRO:HD3	2.19	0.43
41:N1:149:ILE:HG21	41:N1:185:TRP:HB2	2.01	0.43
68:N5:703:CDL:H251	68:N5:703:CDL:H212	2.01	0.43
49:QC:344:GLU:HG3	54:Qh:67:PHE:HE1	1.83	0.43
51:QE:112:GLY:HA2	55:Qi:11:TYR:HB2	2.01	0.43
54:QH:20:SER:HB3	54:QH:23:GLU:HG2	2.01	0.43
47:Qa:184:ASN:OD1	47:Qa:184:ASN:N	2.47	0.43
49:Qc:97:HIS:HD2	80:Qc:404:HEM:C1C	2.36	0.43
5:6B:30:CYS:SG	5:6B:31:TRP:N	2.92	0.43
15:A6:127:THR:HG23	59:S3:219:VAL:O	2.18	0.43
68:A8:301:CDL:H561	44:N4:10:MET:HE3	2.01	0.43
68:A8:301:CDL:H542	24:B1:23:PHE:CE2	2.53	0.43
35:C1:288:TRP:CH2	70:C1:607:PC1:H232	2.53	0.43
70:N1:401:PC1:H261	43:N3:7:LEU:HD11	1.99	0.43
75:N4:503:PLX:H22	71:N5:701:PEE:H3	1.99	0.43
56:QJ:38:TRP:CD2	70:QJ:101:PC1:H322	2.53	0.43
51:QK:71:ASN:OD1	51:QK:71:ASN:N	2.52	0.43
57:S1:347:ASP:HB3	57:S1:594:ALA:HB1	2.00	0.43
57:S1:691:ILE:HG13	57:S1:695:TYR:CE2	2.53	0.43
62:S6:71:ILE:HD12	62:S6:71:ILE:HA	1.91	0.43
64:S8:153:ILE:HG13	64:S8:155:CYS:HB3	2.01	0.43
70:6A:101:PC1:O14	37:C3:187:THR:OG1	2.37	0.43
15:A6:80:ILE:HG23	15:A6:130:MET:HE1	2.01	0.43
17:A8:208:VAL:HG12	17:A8:210:THR:HG23	2.00	0.43
18:A9:299:ARG:NH1	18:A9:316:ARG:HD2	2.34	0.43
23:AN:89:GLU:OE1	23:AN:128:ARG:NH2	2.39	0.43
31:B8:83:GLN:HA	31:B8:86:ARG:HG3	2.01	0.43
33:BK:33:LEU:HD13	45:N5:49:VAL:HG13	2.00	0.43
45:N5:293:ILE:HD12	68:N5:703:CDL:H521	2.00	0.43
47:Qa:64:PHE:HB3	47:Qa:401:LEU:HD11	2.00	0.43
49:Qc:200:LEU:HD22	80:Qc:404:HEM:HAA1	2.00	0.43
59:S3:44:ARG:HD2	59:S3:47:ILE:HD12	2.00	0.43
59:S3:65:VAL:HG12	59:S3:99:PHE:HE2	1.84	0.43
62:S6:74:GLN:NE2	62:S6:75:PRO:HD2	2.34	0.43
67:V3:400:LEU:O	67:V3:404:VAL:HG23	2.19	0.43
7:7A:52:LEU:HD23	7:7A:52:LEU:HA	1.91	0.42
20:AK:149:LEU:HD23	20:AK:149:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B4:82:PRO:O	76:B4:201:3PE:H2	2.18	0.42
29:B6:170:ILE:HB	29:B6:175:GLU:HB3	2.01	0.42
37:C3:204:HIS:CE1	37:C3:249:TRP:HB2	2.53	0.42
40:CB:38:PHE:CZ	68:N2:402:CDL:H832	2.54	0.42
45:N5:8:THR:O	45:N5:11:THR:OG1	2.30	0.42
45:N5:102:GLU:OE1	45:N5:456:ARG:NH2	2.34	0.42
45:N5:401:MET:SD	45:N5:482:MET:HE2	2.59	0.42
48:Qb:109:LEU:HD21	48:Qb:150:ILE:HD11	2.01	0.42
58:S2:172:ARG:NH1	58:S2:358:PRO:O	2.46	0.42
15:A6:136:THR:HG21	59:S3:220:VAL:HG11	2.01	0.42
17:A8:246:PHE:CE1	68:A8:301:CDL:H341	2.53	0.42
71:B4:202:PEE:H69	71:B4:202:PEE:H62	1.90	0.42
33:BK:90:MET:SD	44:N4:48:ASN:HB3	2.60	0.42
70:C1:609:PC1:H3D2	70:C1:609:PC1:H3G1	1.84	0.42
37:C3:65:SER:HB3	37:C3:71:HIS:CE1	2.54	0.42
41:N1:61:LEU:HD23	63:S7:125:PRO:HB3	2.02	0.42
45:N5:457:LEU:HD23	45:N5:457:LEU:HA	1.80	0.42
48:QB:165:ARG:NH1	48:QB:208:VAL:O	2.52	0.42
50:QD:105:SER:H	55:Qi:48:ASN:ND2	2.17	0.42
50:QD:250:TYR:CZ	50:QD:253:VAL:HG23	2.54	0.42
49:Qc:5:ARG:HH11	49:Qc:15:ASN:ND2	2.17	0.42
49:Qc:131:TYR:O	49:Qc:134:PRO:HD2	2.19	0.42
71:Qc:402:PEE:H30	71:Qc:402:PEE:H23	1.73	0.42
59:S3:187:ILE:HG23	59:S3:188:LEU:HG	2.00	0.42
60:S4:112:MET:HG3	64:S8:184:LEU:HD23	2.01	0.42
61:S5:97:HIS:HA	61:S5:102:GLU:HB3	2.00	0.42
65:V1:268:GLU:OE1	65:V1:269:ARG:NE	2.48	0.42
8:7B:34:HIS:NE2	76:C1:601:3PE:O22	2.49	0.42
18:A9:315:THR:H	18:A9:318:LYS:HB3	1.84	0.42
19:AC:133:ILE:HG13	32:B9:46:SER:HB2	2.00	0.42
23:AN:88:ARG:O	23:AN:92:GLU:HG2	2.19	0.42
32:B9:91:ASP:HA	32:B9:94:LYS:HB2	2.01	0.42
35:C1:129:TYR:OH	35:C1:236:TRP:NE1	2.34	0.42
70:N1:402:PC1:H391	70:N1:402:PC1:H3C2	1.86	0.42
44:N4:200:ILE:HD13	44:N4:200:ILE:HA	1.90	0.42
75:N4:502:PLX:H1A2	75:N4:502:PLX:H21	1.55	0.42
45:N5:15:LEU:HD11	45:N5:94:LEU:HD21	2.02	0.42
68:QE:304:CDL:H541	68:QE:304:CDL:H511	1.93	0.42
68:Qb:501:CDL:H761	68:Qb:501:CDL:H732	1.83	0.42
58:S2:91:GLY:HA2	58:S2:92:PRO:HA	1.88	0.42
58:S2:190:ILE:HD11	58:S2:257:PHE:HZ	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:S3:100:LEU:O	59:S3:108:PHE:HB2	2.19	0.42
64:S8:53:VAL:HG22	64:S8:56:ARG:HH21	1.84	0.42
15:A6:44:LYS:HE3	15:A6:44:LYS:HB2	1.87	0.42
68:AL:201:CDL:HB21	45:N5:576:MET:HE2	2.01	0.42
71:AL:203:PEE:H58	71:AL:203:PEE:H52	1.64	0.42
22:AM:85:GLU:CD	22:AM:85:GLU:H	2.27	0.42
39:CA:31:ILE:HG13	39:CA:32:ARG:H	1.83	0.42
41:N1:90:PRO:HB3	41:N1:94:PRO:HD3	2.02	0.42
42:N2:111:PHE:HA	45:N5:591:PHE:CE1	2.54	0.42
44:N4:1:MET:HG2	44:N4:52:PHE:CD2	2.54	0.42
49:QC:215:MET:HE2	49:QC:215:MET:HB3	1.94	0.42
50:QD:247:PRO:HA	50:QD:248:PRO:HD3	1.86	0.42
55:QL:36:PHE:CZ	50:Qd:296:MET:HG2	2.54	0.42
48:Qb:183:VAL:HG21	48:Qb:286:HIS:CB	2.49	0.42
58:S2:101:LEU:HB2	58:S2:464:PHE:CZ	2.54	0.42
23:AN:82:ARG:NH1	61:S5:106:PRO:O	2.52	0.42
44:N4:3:LYS:HG3	44:N4:4:ILE:HD12	2.01	0.42
44:N4:160:LEU:HD13	44:N4:199:CYS:HA	2.00	0.42
44:N4:190:TRP:HH2	75:N4:502:PLX:H51	1.84	0.42
45:N5:233:LEU:HB3	45:N5:234:PRO:HD3	2.01	0.42
48:QB:225:LYS:HD2	48:QB:257:TYR:CE2	2.55	0.42
71:QB:502:PEE:H48	71:QB:502:PEE:H7	1.86	0.42
51:QE:154:ILE:HD13	51:QE:176:VAL:HG21	2.00	0.42
48:Qb:396:ARG:NE	48:Qb:430:GLU:OE2	2.53	0.42
49:Qc:33:PHE:HA	49:Qc:36:LEU:HB2	2.01	0.42
52:Qf:40:ILE:HG13	52:Qf:43:CYS:H	1.84	0.42
64:S8:142:THR:O	64:S8:187:LYS:NZ	2.51	0.42
65:V1:65:THR:O	65:V1:69:LEU:HG	2.19	0.42
1:4L:1:MET:SD	42:N2:80:TYR:OH	2.71	0.42
1:4L:21:MET:O	46:N6:23:LYS:NZ	2.51	0.42
6:6C:19:LEU:HD13	35:C1:328:HIS:CE1	2.54	0.42
12:A2:31:GLN:O	12:A2:31:GLN:NE2	2.52	0.42
15:A6:94:MET:HE2	19:AB:113:LEU:HD12	2.02	0.42
29:B6:146:LEU:HD23	29:B6:150:VAL:HG21	2.01	0.42
44:N4:204:MET:HE3	44:N4:209:LEU:HD13	2.00	0.42
45:N5:228:GLY:H	45:N5:230:HIS:CD2	2.37	0.42
45:N5:572:LYS:HG2	70:N5:705:PC1:H142	2.02	0.42
46:N6:24:PRO:HA	46:N6:89:VAL:HG21	2.01	0.42
68:QE:304:CDL:HB21	54:Qh:25:ARG:HG2	2.00	0.42
47:Qa:155:GLN:HB3	47:Qa:198:GLY:HA2	2.01	0.42
50:Qd:149:LEU:O	50:Qd:152:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:S1:402:LEU:HD23	57:S1:475:VAL:HB	2.02	0.42
65:V1:262:PHE:CZ	65:V1:272:GLY:HA3	2.54	0.42
3:5B:45:THR:O	37:C3:69:GLY:HA3	2.20	0.42
11:A1:69:ILE:HD12	11:A1:70:ASP:HB2	2.01	0.42
12:A2:26:ARG:HH22	57:S1:660:GLU:HG2	1.85	0.42
15:A6:78:LEU:HD22	15:A6:130:MET:HE2	2.02	0.42
20:AK:342:SER:O	20:AK:346:ASN:ND2	2.52	0.42
68:AL:201:CDL:H352	71:AL:203:PEE:H26	2.01	0.42
75:AM:202:PLX:H112	75:AM:202:PLX:H142	1.83	0.42
68:B4:203:CDL:OA8	75:N4:502:PLX:O7	2.37	0.42
35:C1:9:SER:OG	35:C1:99:ASN:ND2	2.53	0.42
68:N2:402:CDL:HB62	44:N4:16:TRP:CZ3	2.55	0.42
44:N4:77:LEU:O	44:N4:81:GLN:HG3	2.20	0.42
45:N5:67:HIS:NE2	45:N5:70:THR:OG1	2.53	0.42
45:N5:559:GLU:O	45:N5:564:LYS:HB2	2.20	0.42
53:QG:71:MET:HE1	50:Qd:315:LEU:HD13	2.02	0.42
47:Qa:395:GLU:O	47:Qa:399:GLN:HG2	2.20	0.42
49:Qc:119:LEU:HD22	80:Qc:404:HEM:HBB2	2.00	0.42
57:S1:36:VAL:HG22	57:S1:102:ILE:HD12	2.02	0.42
57:S1:217:GLU:HG2	57:S1:218:LEU:HG	2.02	0.42
61:S5:57:LYS:HE2	61:S5:57:LYS:HB3	1.90	0.42
1:4L:35:GLY:HA3	46:N6:20:PHE:HZ	1.83	0.42
16:A7:57:ARG:HH12	57:S1:150:ARG:HH21	1.66	0.42
16:A7:68:ILE:HD12	59:S3:75:GLN:HE21	1.85	0.42
29:B6:89:SER:HB2	29:B6:92:GLU:HB2	2.00	0.42
35:C1:427:PRO:HB3	35:C1:450:TRP:HB3	2.01	0.42
77:C1:603:HEA:H271	77:C1:603:HEA:H211	1.83	0.42
48:QB:361:ASP:OD1	48:QB:361:ASP:N	2.52	0.42
49:QC:128:PHE:O	49:QC:132:VAL:HG23	2.20	0.42
52:QF:65:GLU:HB2	54:QH:78:TYR:CD1	2.55	0.42
47:Qa:115:THR:OG1	47:Qa:116:ARG:N	2.53	0.42
57:S1:251:ILE:HD11	57:S1:596:TYR:HB2	2.01	0.42
65:V1:317:VAL:HB	65:V1:332:CYS:SG	2.60	0.42
84:V1:502:FMN:H9	84:V1:502:FMN:H4'	2.02	0.42
17:A8:157:GLU:HB3	17:A8:158:PRO:HD3	2.01	0.42
29:B6:132:VAL:O	29:B6:136:LEU:CB	2.68	0.42
31:B8:62:TYR:OH	31:B8:74:ASP:O	2.24	0.42
35:C1:109:PHE:HB3	70:C1:609:PC1:H241	2.00	0.42
38:C4:65:LYS:HE2	38:C4:65:LYS:HB3	1.77	0.42
42:N2:265:MET:HE3	42:N2:340:THR:HG21	2.01	0.42
45:N5:213:LEU:HD23	45:N5:213:LEU:HA	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:QA:49:ILE:HD13	47:QA:220:LEU:HB3	2.02	0.42
51:QE:156:LEU:HB3	51:QE:210:TRP:CZ2	2.54	0.42
51:QE:178:HIS:HB2	51:QE:210:TRP:CZ3	2.54	0.42
53:Qg:92:GLU:HB3	53:Qg:93:PRO:HD3	2.02	0.42
59:S3:89:HIS:CG	59:S3:90:PRO:HD2	2.55	0.42
59:S3:197:PRO:HA	59:S3:202:PHE:CD2	2.55	0.42
63:S7:62:LEU:HD23	63:S7:62:LEU:HA	1.90	0.42
6:6C:16:ALA:O	6:6C:20:ARG:HG3	2.19	0.42
19:AB:138:LEU:HD23	19:AB:144:ILE:HG12	2.01	0.42
20:AK:152:LEU:HD12	20:AK:158:GLY:HA2	2.02	0.42
68:N2:402:CDL:H712	68:N2:402:CDL:OA9	2.20	0.42
43:N3:51:PHE:CZ	46:N6:75:ALA:HB2	2.55	0.42
44:N4:272:THR:OG1	44:N4:292:SER:OG	2.31	0.42
45:N5:363:TYR:CD1	45:N5:370:THR:HG21	2.55	0.42
47:QA:178:HIS:NE2	47:QA:330:TYR:OH	2.38	0.42
48:Qb:102:LYS:HG2	48:Qb:153:ASN:HB3	2.00	0.42
80:Qc:404:HEM:HHA	80:Qc:404:HEM:HBA1	2.02	0.42
66:V2:137:THR:HG22	66:V2:138:THR:H	1.85	0.42
18:A9:218:ALA:O	18:A9:221:ARG:NH1	2.52	0.41
18:A9:306:GLU:HG2	18:A9:315:THR:HG22	2.02	0.41
22:AM:8:ARG:HA	22:AM:8:ARG:HH11	1.84	0.41
23:AN:48:TRP:CZ2	23:AN:52:LYS:HD2	2.55	0.41
29:B6:72:LEU:O	29:B6:76:ARG:HG3	2.20	0.41
42:N2:335:LEU:HD21	68:N2:402:CDL:H402	2.02	0.41
46:N6:94:VAL:HG12	46:N6:98:MET:HE2	2.02	0.41
48:QB:279:ASP:H	48:QB:460:GLY:HA3	1.85	0.41
75:QB:504:PLX:H152	75:QB:504:PLX:H182	1.62	0.41
49:QC:63:PHE:O	49:QC:67:THR:HG23	2.21	0.41
51:QE:145:ASP:OD1	51:QE:145:ASP:N	2.53	0.41
56:QJ:34:TRP:CE2	51:Qe:130:LYS:HD2	2.55	0.41
64:S8:150:THR:HG21	64:S8:180:HIS:CD2	2.55	0.41
65:V1:154:ALA:HB2	65:V1:193:PHE:HZ	1.85	0.41
11:A1:50:ARG:NH2	17:A8:95:VAL:O	2.52	0.41
22:AM:84:PRO:HD3	22:AM:113:HIS:CD2	2.55	0.41
27:B4:63:PRO:O	27:B4:67:ARG:HG3	2.19	0.41
35:C1:181:THR:O	35:C1:270:TYR:OH	2.32	0.41
35:C1:373:VAL:HG13	77:C1:603:HEA:HBA1	2.00	0.41
77:C1:602:HEA:HHB	77:C1:602:HEA:HMB1	1.84	0.41
41:N1:307:LEU:HB3	41:N1:308:PRO:HD3	2.02	0.41
68:N2:402:CDL:H202	44:N4:98:MET:HE1	2.02	0.41
44:N4:91:ARG:HD3	44:N4:135:ARG:HH21	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:N4:296:LEU:HD21	44:N4:378:GLU:HG3	2.02	0.41
45:N5:96:VAL:O	45:N5:100:ILE:HG12	2.19	0.41
45:N5:290:LEU:O	45:N5:523:SER:OG	2.37	0.41
46:N6:106:TYR:HE2	46:N6:114:GLU:HG2	1.85	0.41
49:QC:314:SER:O	49:QC:318:ARG:HD3	2.20	0.41
48:Qb:99:LYS:NZ	48:Qb:164:GLU:OE2	2.48	0.41
48:Qb:310:ILE:HD11	48:Qb:388:VAL:HA	2.01	0.41
68:Qb:501:CDL:OA9	68:Qb:501:CDL:H132	2.20	0.41
58:S2:149:SER:HA	58:S2:184:THR:CG2	2.49	0.41
65:V1:355:ILE:HD13	66:V2:139:PRO:HG3	2.01	0.41
8:7B:61:GLY:O	38:C4:122:LYS:NZ	2.53	0.41
11:A1:3:PHE:HE2	68:A1:101:CDL:HA21	1.85	0.41
15:A6:131:ARG:NH2	59:S3:210:LEU:HD21	2.35	0.41
29:B6:143:HIS:HD2	33:BK:45:VAL:HG21	1.86	0.41
77:C1:602:HEA:H212	77:C1:602:HEA:H271	1.54	0.41
36:C2:28:LEU:HD11	75:C2:301:PLX:H71	2.02	0.41
41:N1:40:VAL:HG12	41:N1:46:LEU:HB2	2.02	0.41
49:QC:37:LEU:HD12	49:QC:97:HIS:CD2	2.55	0.41
49:QC:237:LEU:HD22	50:QD:301:LEU:HD11	2.02	0.41
54:QH:20:SER:O	54:QH:24:GLN:HG2	2.20	0.41
47:Qa:60:ARG:NH2	47:Qa:124:GLU:OE1	2.52	0.41
48:Qb:40:GLN:HA	48:Qb:43:GLN:HG2	2.02	0.41
48:Qb:140:LEU:HD22	48:Qb:237:VAL:HG22	2.01	0.41
71:Qd:403:PEE:H16	51:Qe:135:GLN:HE22	1.85	0.41
65:V1:88:ARG:C	65:V1:244:ASN:HD22	2.29	0.41
17:A8:117:ASN:O	17:A8:121:MET:HG2	2.19	0.41
24:B1:54:GLU:N	24:B1:54:GLU:OE1	2.53	0.41
30:B7:113:LYS:HA	30:B7:113:LYS:HD3	1.90	0.41
32:B9:119:PRO:HB3	45:N5:525:MET:HE1	2.02	0.41
35:C1:316:THR:HG21	77:C1:603:HEA:C14	2.51	0.41
36:C2:120:SER:OG	36:C2:140:ASN:O	2.37	0.41
36:C2:191:LEU:HA	36:C2:211:LEU:O	2.21	0.41
48:QB:385:GLU:O	48:QB:389:VAL:HG13	2.20	0.41
4:6A:36:ALA:HB2	37:C3:142:VAL:HG21	2.01	0.41
8:7B:53:TRP:CE2	38:C4:115:ALA:HB2	2.54	0.41
76:B4:201:3PE:H3I2	76:B4:201:3PE:H3F2	1.91	0.41
31:B8:114:ARG:HB2	45:N5:162:THR:HG21	2.02	0.41
31:B8:139:PHE:CD2	68:N5:703:CDL:H851	2.56	0.41
36:C2:98:LYS:HG2	36:C2:153:LEU:HB2	2.02	0.41
37:C3:226:HIS:HE1	71:C3:303:PEE:H48	1.84	0.41
45:N5:538:THR:HG21	71:N5:704:PEE:H7	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:S1:304:GLN:HB2	57:S1:316:TYR:CD1	2.55	0.41
65:V1:119:GLU:OE2	65:V1:127:ASP:N	2.48	0.41
65:V1:244:ASN:O	65:V1:248:VAL:HG22	2.21	0.41
2:5A:80:VAL:HG11	2:5A:113:VAL:HG21	2.02	0.41
4:6A:66:ARG:NE	4:6A:89:PRO:HG2	2.36	0.41
71:6A:102:PEE:H22	71:6A:102:PEE:H27	1.56	0.41
35:C1:298:ASP:OD2	70:C1:607:PC1:H121	2.20	0.41
38:C4:38:TYR:CE1	38:C4:47:PRO:HG2	2.55	0.41
41:N1:145:THR:HG21	41:N1:289:LEU:HD11	2.03	0.41
41:N1:267:THR:O	41:N1:271:LEU:HG	2.21	0.41
42:N2:135:LYS:O	42:N2:139:LEU:HD12	2.20	0.41
42:N2:218:LEU:HD21	42:N2:330:ILE:HD11	2.03	0.41
42:N2:276:ILE:C	42:N2:279:PRO:HD2	2.45	0.41
44:N4:8:THR:HB	44:N4:104:LEU:HD13	2.02	0.41
47:QA:138:LEU:HD13	47:QA:237:PHE:HB2	2.02	0.41
48:QB:75:ILE:HG12	48:QB:229:MET:HG2	2.02	0.41
48:QB:275:ILE:HG22	54:Qh:17:TYR:CD1	2.56	0.41
48:QB:311:ILE:O	48:QB:326:SER:OG	2.31	0.41
51:QE:88:PHE:O	51:QE:92:ARG:HG3	2.20	0.41
51:QE:135:GLN:HE22	71:QE:301:PEE:H16	1.86	0.41
50:Qd:322:TYR:CZ	50:Qd:324:PRO:HG3	2.55	0.41
57:S1:249:GLU:HG2	57:S1:262:VAL:HG22	2.03	0.41
6:6C:19:LEU:HD13	35:C1:328:HIS:HE1	1.85	0.41
19:AB:78:ALA:HA	19:AB:81:ASP:OD2	2.20	0.41
19:AC:115:GLN:NE2	19:AC:138:LEU:O	2.52	0.41
28:B5:94:GLY:O	33:BK:61:TYR:OH	2.36	0.41
31:B8:88:PRO:HB3	31:B8:98:ARG:NH2	2.35	0.41
35:C1:2:PHE:CZ	70:C1:609:PC1:H153	2.55	0.41
35:C1:358:LEU:HD13	77:C1:603:HEA:HBA2	2.02	0.41
36:C2:146:MET:HE2	36:C2:215:PRO:HG3	2.03	0.41
75:N4:502:PLX:H392	75:N4:502:PLX:H362	1.80	0.41
46:N6:24:PRO:HG2	46:N6:28:TYR:HB2	2.02	0.41
47:QA:77:LEU:O	47:QA:196:ARG:HD3	2.21	0.41
47:QA:117:GLU:CD	47:QA:330:TYR:HB3	2.46	0.41
51:QE:159:ILE:HA	51:QE:160:PRO:HD3	1.92	0.41
54:QH:72:ARG:HA	54:QH:72:ARG:HD3	1.84	0.41
57:S1:118:GLU:OE2	57:S1:152:ARG:NE	2.50	0.41
57:S1:476:LEU:HD21	57:S1:481:LEU:HD21	2.03	0.41
58:S2:101:LEU:HD11	58:S2:103:LEU:HD13	2.03	0.41
63:S7:188:LYS:O	63:S7:192:ILE:HG12	2.21	0.41
5:6B:24:GLN:NE2	35:C1:296:GLY:HA2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A1:64:LYS:CB	11:A1:68:ASN:HD22	2.33	0.41
12:A2:16:LEU:HD21	12:A2:19:ILE:HD11	2.02	0.41
19:AB:93:ILE:HD13	19:AB:93:ILE:HA	1.92	0.41
19:AC:90:TYR:HE1	26:B3:44:PRO:HB2	1.85	0.41
23:AN:85:GLN:OE1	61:S5:105:ARG:NH1	2.53	0.41
71:B4:202:PEE:H81	71:B4:202:PEE:H75	1.78	0.41
33:BK:79:GLU:HG2	33:BK:80:LYS:HG2	2.03	0.41
42:N2:112:HIS:HB2	42:N2:184:ILE:HD13	2.03	0.41
56:QJ:34:TRP:CZ2	51:Qe:130:LYS:HD2	2.56	0.41
47:Qa:147:ARG:HD3	47:Qa:149:TRP:CZ2	2.55	0.41
57:S1:213:MET:HE1	57:S1:713:ALA:HB1	2.03	0.41
3:5B:105:VAL:HG22	3:5B:111:GLN:HB2	2.02	0.41
18:A9:65:LEU:HG	18:A9:129:LEU:HD22	2.03	0.41
20:AK:93:ILE:HA	20:AK:136:TRP:HE1	1.86	0.41
68:AL:201:CDL:H612	42:N2:160:LEU:HD11	2.03	0.41
29:B6:133:THR:OG1	29:B6:134:HIS:N	2.54	0.41
35:C1:439:ARG:NH1	36:C2:199:ILE:HD11	2.36	0.41
36:C2:184:LEU:HD11	36:C2:211:LEU:HD21	2.02	0.41
41:N1:34:ARG:HG2	63:S7:82:PRO:HA	2.03	0.41
70:N1:401:PC1:H291	46:N6:57:PHE:CE2	2.55	0.41
42:N2:250:SER:O	42:N2:259:GLY:HA3	2.20	0.41
43:N3:84:LEU:HD23	43:N3:84:LEU:HA	1.94	0.41
44:N4:278:ARG:HG3	45:N5:545:SER:HB2	2.02	0.41
45:N5:213:LEU:HB3	45:N5:273:VAL:HG11	2.03	0.41
47:QA:66:LYS:O	47:QA:217:ARG:NH2	2.51	0.41
47:QA:257:GLU:OE2	47:QA:259:ARG:HD3	2.21	0.41
47:QA:282:GLU:OE2	47:QA:430:LYS:NZ	2.46	0.41
75:QB:504:PLX:H22	75:QB:504:PLX:H1C3	1.68	0.41
49:QC:112:THR:HG22	49:QC:196:HIS:CE1	2.55	0.41
49:QC:116:GLY:HA3	80:QC:402:HEM:C3C	2.55	0.41
54:QH:3:ARG:NH2	49:Qc:217:LYS:HE2	2.34	0.41
55:QI:11:TYR:HA	55:QI:15:PHE:HB2	2.02	0.41
49:Qc:36:LEU:HD23	49:Qc:36:LEU:HA	1.90	0.41
52:Qf:45:LYS:O	52:Qf:48:GLU:HG2	2.21	0.41
54:Qh:20:SER:O	54:Qh:24:GLN:HG2	2.21	0.41
57:S1:141:ASP:O	57:S1:145:MET:HG2	2.20	0.41
58:S2:135:TYR:HE1	58:S2:417:LEU:HD21	1.86	0.41
58:S2:140:PRO:HB2	63:S7:142:TYR:HE2	1.85	0.41
65:V1:141:GLY:HA2	65:V1:252:PRO:HD3	2.03	0.41
2:5A:77:ASN:HD22	38:C4:45:PRO:HD2	1.86	0.41
18:A9:64:PHE:CD1	18:A9:210:GLU:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AK:333:PHE:CZ	20:AK:339:ARG:HD3	2.55	0.41
32:B9:143:GLU:O	32:B9:164:ARG:NH2	2.54	0.41
40:CB:105:GLU:H	40:CB:105:GLU:CD	2.29	0.41
42:N2:190:MET:HB3	42:N2:190:MET:HE2	1.73	0.41
44:N4:375:LEU:O	44:N4:375:LEU:HG	2.20	0.41
45:N5:10:THR:O	45:N5:14:ILE:HG23	2.21	0.41
45:N5:260:LEU:HD23	45:N5:260:LEU:HA	1.91	0.41
46:N6:123:GLY:O	46:N6:127:ILE:HG23	2.20	0.41
50:QD:112:ARG:HB2	50:QD:140:CYS:HB2	2.02	0.41
50:QD:307:MET:HE2	50:QD:307:MET:HB3	1.96	0.41
51:QE:136:PHE:O	51:QE:139:SER:OG	2.32	0.41
51:QK:8:SER:OG	51:QK:15:LEU:HD12	2.20	0.41
48:Qb:81:TYR:HB3	48:Qb:223:HIS:CE1	2.56	0.41
57:S1:78:CYS:HB3	82:S1:803:FES:S1	2.60	0.41
57:S1:389:THR:OG1	57:S1:511:LYS:O	2.39	0.41
57:S1:405:THR:OG1	57:S1:410:GLU:OE1	2.33	0.41
58:S2:323:ASP:OD1	64:S8:37:THR:OG1	2.32	0.41
63:S7:130:VAL:HB	63:S7:159:VAL:HA	2.03	0.41
66:V2:188:ILE:HB	66:V2:193:TYR:HE2	1.85	0.41
12:A2:23:LEU:HD13	12:A2:34:ARG:HG2	2.03	0.40
17:A8:160:THR:HA	17:A8:163:TRP:CD1	2.56	0.40
19:AC:89:LEU:HD13	26:B3:48:ASN:HA	2.02	0.40
26:B3:59:ASN:OD1	26:B3:59:ASN:N	2.54	0.40
35:C1:413:HIS:CE1	35:C1:468:MET:HB2	2.57	0.40
44:N4:87:GLU:HB3	44:N4:92:LYS:HG3	2.02	0.40
75:N4:502:PLX:H362	75:N4:502:PLX:H331	1.87	0.40
45:N5:473:PRO:HG2	45:N5:475:MET:SD	2.60	0.40
71:N5:701:PEE:H29	71:N5:701:PEE:H35	1.77	0.40
47:QA:278:THR:HG22	47:QA:331:SER:HA	2.03	0.40
52:QF:56:ARG:O	52:QF:60:ARG:HG3	2.21	0.40
57:S1:103:LEU:HB3	57:S1:106:SER:HB2	2.02	0.40
57:S1:409:PHE:CD1	57:S1:694:PHE:HB2	2.56	0.40
7:7A:57:MET:O	7:7A:61:LEU:HG	2.22	0.40
20:AK:134:GLN:HE22	74:AK:401:ADP:N6	2.17	0.40
76:C2:302:3PE:H2A2	76:C2:302:3PE:H2D1	1.86	0.40
37:C3:129:VAL:HG21	37:C3:180:GLU:OE2	2.21	0.40
37:C3:140:SER:CB	37:C3:242:TRP:HE1	2.33	0.40
47:QA:337:GLY:HA2	47:QA:431:PHE:CE1	2.56	0.40
51:QE:140:MET:HE3	49:Qc:177:ARG:HE	1.86	0.40
57:S1:306:MET:HE2	57:S1:314:LEU:HB3	2.03	0.40
58:S2:290:LEU:O	58:S2:293:GLY:CA	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AL:101:LEU:HD21	68:AL:201:CDL:H321	2.02	0.40
35:C1:265:LYS:HD2	35:C1:490:THR:HG21	2.02	0.40
37:C3:234:GLY:N	70:C3:302:PC1:O12	2.39	0.40
42:N2:36:ASN:OD1	42:N2:134:GLN:NE2	2.31	0.40
45:N5:79:SER:HB2	45:N5:135:ASN:HD22	1.86	0.40
48:QB:341:PHE:HB2	48:QB:358:PHE:HB3	2.03	0.40
48:QB:379:LEU:HD23	48:QB:379:LEU:HA	1.91	0.40
48:Qb:99:LYS:HA	48:Qb:99:LYS:HD3	1.92	0.40
50:Qd:250:TYR:H	50:Qd:253:VAL:CG2	2.35	0.40
57:S1:185:PHE:CZ	57:S1:221:ASN:HB2	2.56	0.40
58:S2:203:MET:O	58:S2:206:PHE:HB3	2.21	0.40
65:V1:314:LEU:HD11	65:V1:317:VAL:HG23	2.04	0.40
9:7C:47:SER:HB2	70:7C:101:PC1:H3F1	2.04	0.40
18:A9:168:SER:O	18:A9:203:PRO:HD2	2.21	0.40
20:AK:65:ASP:HB2	20:AK:206:VAL:HG13	2.03	0.40
20:AK:310:THR:O	42:N2:310:ASN:ND2	2.43	0.40
24:B1:42:SER:O	24:B1:46:LYS:HB2	2.22	0.40
34:BL:109:LEU:HD22	44:N4:43:ASN:HB2	2.02	0.40
35:C1:8:TYR:CZ	37:C3:15:PRO:HB3	2.57	0.40
39:CA:31:ILE:HG13	39:CA:32:ARG:N	2.36	0.40
47:QA:153:ALA:O	47:QA:156:SER:OG	2.27	0.40
52:QF:60:ARG:HD3	52:QF:63:THR:HG21	2.02	0.40
48:Qb:465:LEU:HD12	48:Qb:466:PRO:HD2	2.04	0.40
68:Qb:501:CDL:H171	71:Qc:401:PEE:H37	2.03	0.40
64:S8:49:ASP:OD1	64:S8:49:ASP:N	2.55	0.40
64:S8:75:SER:O	64:S8:79:ARG:HG3	2.21	0.40
5:6B:66:PRO:HD3	36:C2:179:LEU:HD11	2.02	0.40
22:AM:25:ARG:O	22:AM:29:ARG:HG2	2.20	0.40
27:B4:81:ARG:HA	27:B4:82:PRO:HD3	1.97	0.40
27:B4:109:ARG:HH22	40:CB:122:ARG:C	2.29	0.40
35:C1:303:ALA:O	35:C1:306:THR:OG1	2.34	0.40
41:N1:287:HIS:HE1	43:N3:113:TRP:HD1	1.68	0.40
70:N3:202:PC1:H371	63:S7:50:LEU:HD22	2.04	0.40
44:N4:286:ILE:HD13	44:N4:326:LEU:HB3	2.03	0.40
75:N4:502:PLX:H331	75:N4:502:PLX:H302	1.40	0.40
47:QA:313:VAL:HG11	47:QA:350:VAL:HG13	2.04	0.40
50:QD:317:SER:O	50:QD:317:SER:OG	2.37	0.40
51:QE:186:GLN:O	51:QE:190:VAL:HG23	2.21	0.40
51:QE:207:LYS:HG2	51:QE:209:GLU:HG2	2.02	0.40
52:QF:78:ARG:O	52:QF:82:VAL:HG23	2.21	0.40
49:Qc:237:LEU:HB2	50:Qd:297:MET:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Qe:213:LEU:HD13	51:Qe:258:LEU:HD12	2.03	0.40
57:S1:180:THR:N	83:S1:802:SF4:S4	2.93	0.40
58:S2:373:LYS:HE3	58:S2:373:LYS:HB2	1.94	0.40
59:S3:201:ASP:HB3	60:S4:126:LEU:HD21	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%)	93 (97%)	3 (3%)	0	100	100
2	5A	100/102 (98%)	100 (100%)	0	0	100	100
3	5B	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
4	6A	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
5	6B	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
6	6C	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
7	7A	55/57 (96%)	54 (98%)	1 (2%)	0	100	100
8	7B	48/50 (96%)	45 (94%)	3 (6%)	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%)	66 (97%)	2 (3%)	0	100	100
12	A2	83/85 (98%)	79 (95%)	4 (5%)	0	100	100
13	A3	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
14	A5	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
15	A6	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
16	A7	93/112 (83%)	92 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	A8	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
18	A9	333/341 (98%)	324 (97%)	9 (3%)	0	100	100
19	AB	75/156 (48%)	69 (92%)	6 (8%)	0	100	100
19	AC	85/156 (54%)	85 (100%)	0	0	100	100
20	AK	318/320 (99%)	306 (96%)	12 (4%)	0	100	100
21	AL	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
22	AM	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
23	AN	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
24	B1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
25	B2	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
26	B3	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
27	B4	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
28	B5	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
29	B6	98/126 (78%)	95 (97%)	3 (3%)	0	100	100
30	B7	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
31	B8	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
32	B9	176/178 (99%)	173 (98%)	3 (2%)	0	100	100
33	BK	172/176 (98%)	166 (96%)	6 (4%)	0	100	100
34	BL	97/154 (63%)	91 (94%)	6 (6%)	0	100	100
35	C1	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
36	C2	226/228 (99%)	216 (96%)	10 (4%)	0	100	100
37	C3	258/260 (99%)	248 (96%)	10 (4%)	0	100	100
38	C4	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
39	CA	47/49 (96%)	47 (100%)	0	0	100	100
40	CB	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
41	N1	301/318 (95%)	287 (95%)	14 (5%)	0	100	100
42	N2	345/347 (99%)	336 (97%)	9 (3%)	0	100	100
43	N3	92/115 (80%)	89 (97%)	3 (3%)	0	100	100
44	N4	457/459 (100%)	452 (99%)	5 (1%)	0	100	100
45	N5	601/603 (100%)	567 (94%)	34 (6%)	0	100	100
46	N6	162/174 (93%)	148 (91%)	14 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	QA	417/419 (100%)	405 (97%)	12 (3%)	0	100	100
47	Qa	417/419 (100%)	406 (97%)	11 (3%)	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%)	372 (99%)	5 (1%)	0	100	100
49	Qc	377/379 (100%)	369 (98%)	8 (2%)	0	100	100
50	QD	239/326 (73%)	231 (97%)	8 (3%)	0	100	100
50	Qd	237/326 (73%)	232 (98%)	5 (2%)	0	100	100
51	QE	194/274 (71%)	189 (97%)	5 (3%)	0	100	100
51	QK	69/274 (25%)	69 (100%)	0	0	100	100
51	Qe	194/274 (71%)	187 (96%)	7 (4%)	0	100	100
52	QF	65/67 (97%)	65 (100%)	0	0	100	100
52	Qf	62/67 (92%)	60 (97%)	2 (3%)	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	76/81 (94%)	73 (96%)	3 (4%)	0	100	100
54	Qh	77/81 (95%)	77 (100%)	0	0	100	100
55	QI	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
55	Qi	58/62 (94%)	58 (100%)	0	0	100	100
56	QJ	47/52 (90%)	46 (98%)	1 (2%)	0	100	100
56	Qj	49/52 (94%)	47 (96%)	2 (4%)	0	100	100
57	S1	681/689 (99%)	650 (95%)	31 (5%)	0	100	100
58	S2	424/430 (99%)	399 (94%)	25 (6%)	0	100	100
59	S3	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
60	S4	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
61	S5	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
62	S6	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
63	S7	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
64	S8	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
65	V1	429/431 (100%)	413 (96%)	16 (4%)	0	100	100
66	V2	215/217 (99%)	207 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	V3	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
All	All	13910/14938 (93%)	13480 (97%)	430 (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%)	88 (99%)	1 (1%)	70	86
3	5B	80/80 (100%)	79 (99%)	1 (1%)	65	84
4	6A	66/66 (100%)	66 (100%)	0	100	100
5	6B	73/73 (100%)	73 (100%)	0	100	100
6	6C	57/57 (100%)	57 (100%)	0	100	100
7	7A	48/48 (100%)	48 (100%)	0	100	100
8	7B	39/39 (100%)	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%)	87 (100%)	0	100	100
17	A8	153/153 (100%)	153 (100%)	0	100	100
18	A9	291/295 (99%)	289 (99%)	2 (1%)	81	91
19	AB	71/132 (54%)	70 (99%)	1 (1%)	62	83
19	AC	80/132 (61%)	79 (99%)	1 (1%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AK	283/283 (100%)	278 (98%)	5 (2%)	54	79
21	AL	101/101 (100%)	99 (98%)	2 (2%)	50	76
22	AM	130/130 (100%)	130 (100%)	0	100	100
23	AN	123/123 (100%)	123 (100%)	0	100	100
24	B1	53/53 (100%)	53 (100%)	0	100	100
25	B2	62/62 (100%)	62 (100%)	0	100	100
26	B3	62/62 (100%)	62 (100%)	0	100	100
27	B4	113/113 (100%)	113 (100%)	0	100	100
28	B5	121/121 (100%)	121 (100%)	0	100	100
29	B6	97/119 (82%)	97 (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	155/156 (99%)	155 (100%)	0	100	100
34	BL	91/129 (70%)	90 (99%)	1 (1%)	70	86
35	C1	425/425 (100%)	420 (99%)	5 (1%)	67	85
36	C2	212/212 (100%)	208 (98%)	4 (2%)	52	77
37	C3	224/224 (100%)	224 (100%)	0	100	100
38	C4	123/123 (100%)	123 (100%)	0	100	100
39	CA	45/45 (100%)	44 (98%)	1 (2%)	47	74
40	CB	108/108 (100%)	108 (100%)	0	100	100
41	N1	264/275 (96%)	260 (98%)	4 (2%)	60	82
42	N2	311/311 (100%)	311 (100%)	0	100	100
43	N3	84/100 (84%)	84 (100%)	0	100	100
44	N4	410/410 (100%)	410 (100%)	0	100	100
45	N5	537/537 (100%)	533 (99%)	4 (1%)	81	91
46	N6	132/140 (94%)	129 (98%)	3 (2%)	45	73
47	QA	330/330 (100%)	330 (100%)	0	100	100
47	Qa	330/330 (100%)	323 (98%)	7 (2%)	48	75
48	QB	372/372 (100%)	370 (100%)	2 (0%)	86	94
48	Qb	362/372 (97%)	361 (100%)	1 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	QC	332/332 (100%)	327 (98%)	5 (2%)	60	82
49	Qc	332/332 (100%)	329 (99%)	3 (1%)	75	88
50	QD	206/259 (80%)	206 (100%)	0	100	100
50	Qd	204/259 (79%)	204 (100%)	0	100	100
51	QE	166/225 (74%)	164 (99%)	2 (1%)	67	85
51	QK	55/225 (24%)	55 (100%)	0	100	100
51	Qe	166/225 (74%)	166 (100%)	0	100	100
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%)	90 (97%)	3 (3%)	34	65
53	Qg	93/93 (100%)	91 (98%)	2 (2%)	47	74
54	QH	70/72 (97%)	69 (99%)	1 (1%)	62	83
54	Qh	70/72 (97%)	70 (100%)	0	100	100
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%)	44	72
57	S1	576/579 (100%)	573 (100%)	3 (0%)	86	94
58	S2	369/370 (100%)	364 (99%)	5 (1%)	62	83
59	S3	190/190 (100%)	190 (100%)	0	100	100
60	S4	112/112 (100%)	111 (99%)	1 (1%)	75	88
61	S5	93/93 (100%)	93 (100%)	0	100	100
62	S6	79/79 (100%)	79 (100%)	0	100	100
63	S7	132/132 (100%)	128 (97%)	4 (3%)	36	67
64	S8	151/151 (100%)	151 (100%)	0	100	100
65	V1	344/344 (100%)	337 (98%)	7 (2%)	50	76
66	V2	183/183 (100%)	181 (99%)	2 (1%)	70	86
67	V3	41/41 (100%)	41 (100%)	0	100	100
All	All	12139/12783 (95%)	12055 (99%)	84 (1%)	80	91

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	5A	92	ASP
3	5B	84	THR
18	A9	129	LEU
18	A9	201	ILE
19	AB	112	SER
19	AC	112	SER
20	AK	38	LEU
20	AK	68	ILE
20	AK	205	VAL
20	AK	266	GLU
20	AK	273	GLU
21	AL	106	ARG
21	AL	115	CYS
34	BL	53	ILE
35	C1	81	TRP
35	C1	128	VAL
35	C1	180	GLN
35	C1	217	THR
35	C1	271	MET
36	C2	63	THR
36	C2	99	THR
36	C2	196	CYS
36	C2	207	MET
39	CA	47	THR
41	N1	24	GLU
41	N1	61	LEU
41	N1	145	THR
41	N1	251	THR
45	N5	23	ASN
45	N5	340	PHE
45	N5	463	PHE
45	N5	554	ASP
46	N6	27	ILE
46	N6	47	PHE
46	N6	57	PHE
48	QB	153	ASN
48	QB	289	ILE
49	QC	122	THR
49	QC	158	THR
49	QC	215	MET
49	QC	281	LEU
49	QC	343	VAL
51	QE	211	VAL

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Mol	Chain	Res	Type
51	QE	272	ILE
53	QG	71	MET
53	QG	79	GLU
53	QG	92	GLU
54	QH	43	ARG
47	Qa	134	MET
47	Qa	139	ASN
47	Qa	140	VAL
47	Qa	237	PHE
47	Qa	303	SER
47	Qa	306	THR
47	Qa	393	LEU
48	Qb	104	ARG
49	Qc	25	SER
49	Qc	82	LEU
49	Qc	345	HIS
53	Qg	79	GLU
53	Qg	88	LYS
56	Qj	2	LEU
57	S1	509	ASP
57	S1	636	TYR
57	S1	690	THR
58	S2	82	LEU
58	S2	148	VAL
58	S2	204	THR
58	S2	362	ILE
58	S2	459	THR
60	S4	164	PHE
63	S7	67	PHE
63	S7	71	CYS
63	S7	76	MET
63	S7	92	VAL
65	V1	178	GLU
65	V1	194	ASP
65	V1	294	VAL
65	V1	379	CYS
65	V1	385	CYS
65	V1	387	GLU
65	V1	460	ARG
66	V2	137	THR
66	V2	245	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (260)

such sidechains are listed below:

Mol	Chain	Res	Type
1	4L	7	ASN
2	5A	77	ASN
3	5B	43	GLN
3	5B	97	ASN
4	6A	64	HIS
4	6A	83	HIS
5	6B	11	ASN
5	6B	26	GLN
7	7A	50	ASN
8	7B	59	GLN
11	A1	68	ASN
12	A2	86	GLN
13	A3	137	ASN
13	A3	168	ASN
14	A5	21	HIS
14	A5	86	ASN
14	A5	110	ASN
15	A6	74	HIS
15	A6	84	GLN
16	A7	9	GLN
17	A8	93	GLN
17	A8	108	HIS
17	A8	112	GLN
17	A8	141	ASN
17	A8	142	GLN
18	A9	37	HIS
18	A9	154	GLN
18	A9	215	ASN
20	AK	134	GLN
20	AK	151	HIS
20	AK	217	GLN
20	AK	221	GLN
20	AK	325	GLN
21	AL	79	GLN
21	AL	89	ASN
22	AM	52	ASN
22	AM	113	HIS
23	AN	61	GLN
23	AN	90	ASN
24	B1	3	ASN
24	B1	6	GLN
25	B2	49	GLN

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Mol	Chain	Res	Type
25	B2	57	GLN
26	B3	21	GLN
27	B4	50	GLN
27	B4	55	ASN
27	B4	79	ASN
27	B4	123	GLN
28	B5	181	HIS
29	B6	127	HIS
30	B7	110	GLN
31	B8	56	ASN
31	B8	115	ASN
31	B8	127	ASN
31	B8	154	GLN
32	B9	93	HIS
32	B9	104	GLN
32	B9	108	GLN
32	B9	117	GLN
33	BK	28	ASN
33	BK	59	ASN
33	BK	107	GLN
34	BL	148	GLN
35	C1	12	HIS
35	C1	43	GLN
35	C1	80	ASN
35	C1	138	HIS
35	C1	151	HIS
35	C1	170	ASN
35	C1	256	HIS
35	C1	328	HIS
35	C1	360	ASN
35	C1	407	GLN
35	C1	413	HIS
35	C1	422	ASN
35	C1	451	ASN
35	C1	496	HIS
36	C2	26	HIS
36	C2	52	HIS
36	C2	59	GLN
37	C3	38	ASN
37	C3	50	ASN
37	C3	76	GLN
37	C3	103	HIS

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Mol	Chain	Res	Type
37	C3	125	ASN
37	C3	148	HIS
37	C3	161	GLN
37	C3	204	HIS
37	C3	226	HIS
37	C3	231	HIS
37	C3	232	HIS
38	C4	51	HIS
38	C4	141	GLN
38	C4	154	GLN
39	CA	62	HIS
41	N1	124	ASN
41	N1	138	GLN
41	N1	171	HIS
41	N1	287	HIS
41	N1	317	GLN
42	N2	49	ASN
42	N2	77	ASN
42	N2	83	GLN
42	N2	91	ASN
42	N2	112	HIS
42	N2	186	HIS
42	N2	322	GLN
43	N3	26	GLN
44	N4	48	ASN
44	N4	81	GLN
44	N4	188	ASN
44	N4	213	HIS
44	N4	251	ASN
44	N4	279	GLN
44	N4	304	GLN
45	N5	2	ASN
45	N5	59	GLN
45	N5	72	GLN
45	N5	135	ASN
45	N5	136	ASN
45	N5	139	GLN
45	N5	159	HIS
45	N5	199	GLN
45	N5	230	HIS
45	N5	248	HIS
45	N5	323	HIS

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Mol	Chain	Res	Type
45	N5	332	HIS
45	N5	471	ASN
45	N5	524	ASN
45	N5	580	GLN
46	N6	175	ASN
47	QA	167	GLN
47	QA	176	ASN
47	QA	184	ASN
47	QA	284	ASN
47	QA	291	HIS
47	QA	365	ASN
47	QA	399	GLN
47	QA	415	GLN
47	QA	426	ASN
48	QB	49	GLN
48	QB	66	GLN
48	QB	95	HIS
48	QB	152	GLN
48	QB	173	GLN
48	QB	188	HIS
48	QB	223	HIS
48	QB	301	ASN
48	QB	373	GLN
48	QB	402	HIS
48	QB	464	GLN
49	QC	54	HIS
49	QC	68	HIS
49	QC	97	HIS
49	QC	255	ASN
49	QC	260	ASN
49	QC	267	HIS
49	QC	308	HIS
49	QC	322	GLN
50	QD	206	HIS
50	QD	251	ASN
50	QD	266	GLN
50	QD	283	HIS
51	QE	135	GLN
51	QE	186	GLN
51	QE	239	HIS
51	QE	257	ASN
52	QF	88	ASN

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Mol	Chain	Res	Type
55	QI	38	GLN
55	QI	48	ASN
55	QI	55	HIS
56	QJ	16	ASN
51	QK	58	GLN
47	Qa	81	HIS
47	Qa	167	GLN
47	Qa	172	GLN
47	Qa	178	HIS
47	Qa	239	ASN
47	Qa	290	GLN
47	Qa	304	ASN
47	Qa	343	GLN
47	Qa	365	ASN
47	Qa	376	ASN
47	Qa	408	GLN
48	Qb	43	GLN
48	Qb	66	GLN
48	Qb	83	ASN
48	Qb	87	ASN
48	Qb	95	HIS
48	Qb	152	GLN
48	Qb	153	ASN
48	Qb	160	GLN
48	Qb	170	GLN
48	Qb	188	HIS
48	Qb	223	HIS
48	Qb	239	HIS
48	Qb	313	HIS
48	Qb	323	HIS
48	Qb	357	HIS
49	Qc	8	HIS
49	Qc	15	ASN
49	Qc	54	HIS
49	Qc	341	GLN
50	Qd	190	ASN
50	Qd	206	HIS
50	Qd	251	ASN
50	Qd	283	HIS
50	Qd	310	HIS
51	Qe	135	GLN
51	Qe	186	GLN

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Mol	Chain	Res	Type
51	Qe	199	GLN
51	Qe	200	HIS
52	Qf	36	GLN
52	Qf	55	GLN
52	Qf	80	HIS
53	Qg	23	ASN
54	Qh	13	HIS
54	Qh	65	GLN
55	Qi	38	GLN
55	Qi	48	ASN
57	S1	30	ASN
57	S1	39	GLN
57	S1	278	HIS
57	S1	331	GLN
57	S1	453	GLN
57	S1	498	GLN
57	S1	652	ASN
57	S1	677	GLN
57	S1	688	GLN
58	S2	98	HIS
58	S2	153	ASN
58	S2	229	HIS
58	S2	240	GLN
58	S2	460	GLN
59	S3	75	GLN
59	S3	82	ASN
59	S3	107	GLN
59	S3	123	GLN
59	S3	196	HIS
59	S3	228	GLN
60	S4	123	ASN
60	S4	163	ASN
61	S5	25	GLN
62	S6	59	GLN
62	S6	74	GLN
62	S6	117	GLN
63	S7	123	GLN
63	S7	144	HIS
65	V1	133	HIS
65	V1	270	ASN
65	V1	303	HIS
65	V1	376	HIS

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Mol	Chain	Res	Type
65	V1	381	GLN
65	V1	393	ASN
66	V2	90	ASN
66	V2	123	ASN
66	V2	153	GLN
66	V2	246	GLN
67	V3	388	ASN
67	V3	419	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
58	2MR	S2	124	58	10,12,13	2.39	3 (30%)	5,13,15	1.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	2MR	S2	124	58	-	3/10/13/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	S2	124	2MR	CZ-NE	5.05	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	S2	124	2MR	CZ-NH2	4.89	1.44	1.33
58	S2	124	2MR	CQ1-NH1	-2.09	1.42	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	S2	124	2MR	NE-CD-CG-CB
58	S2	124	2MR	CA-CB-CG-CD
58	S2	124	2MR	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 105 ligands modelled in this entry, 7 are monoatomic - leaving 98 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
75	PLX	C2	301	-	42,42,51	1.16	2 (4%)	46,50,59	0.88	1 (2%)
76	3PE	C2	302	-	50,50,50	0.30	0	53,55,55	0.33	0
81	HEC	Qd	401	50	32,50,50	2.08	4 (12%)	24,82,82	2.25	12 (50%)
70	PC1	C1	609	-	53,53,53	0.29	0	59,61,61	0.29	0
71	PEE	QB	503	-	50,50,50	1.32	5 (10%)	53,55,55	1.19	4 (7%)
70	PC1	N1	402	-	53,53,53	0.29	0	59,61,61	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
73	ZMP	AB	201	19	29,35,36	0.68	1 (3%)	34,42,45	0.73	0
82	FES	QE	303	51	0,4,4	-	-	-		
68	CDL	N5	702	-	81,81,99	0.32	0	87,93,111	0.36	0
70	PC1	6A	101	-	44,44,53	0.33	0	50,52,61	0.33	0
83	SF4	S7	301	63	0,12,12	-	-	-		
68	CDL	QH	102	-	63,63,99	0.37	0	69,75,111	0.41	0
83	SF4	V1	501	65	0,12,12	-	-	-		
70	PC1	Qc	406	-	53,53,53	0.29	0	59,61,61	0.28	0
68	CDL	N5	703	-	99,99,99	0.30	0	105,111,111	0.29	0
82	FES	Qe	301	51	0,4,4	-	-	-		
75	PLX	AM	201	-	51,51,51	1.11	4 (7%)	55,59,59	0.84	1 (1%)
83	SF4	S1	802	57	0,12,12	-	-	-		
76	3PE	B4	201	-	50,50,50	0.30	0	53,55,55	0.37	0
81	HEC	QD	401	50	32,50,50	2.08	4 (12%)	24,82,82	2.42	15 (62%)
70	PC1	N3	202	-	53,53,53	0.29	0	59,61,61	0.35	0
73	ZMP	AC	201	19	29,35,36	0.70	1 (3%)	34,42,45	0.68	0
70	PC1	B7	201	-	53,53,53	0.30	0	59,61,61	0.29	0
70	PC1	C1	606	-	53,53,53	0.30	0	59,61,61	0.28	0
68	CDL	AL	201	-	93,93,99	0.30	0	99,105,111	0.34	0
82	FES	V2	301	66	0,4,4	-	-	-		
68	CDL	QE	304	-	99,99,99	0.31	0	105,111,111	0.32	0
75	PLX	CB	201	-	51,51,51	1.11	4 (7%)	55,59,59	0.89	1 (1%)
75	PLX	N4	502	-	46,46,51	1.15	5 (10%)	50,54,59	0.89	1 (2%)
70	PC1	Qd	402	-	53,53,53	0.29	0	59,61,61	0.28	0
68	CDL	C1	610	-	76,76,99	0.34	0	82,88,111	0.35	0
75	PLX	N4	503	-	51,51,51	1.12	3 (5%)	55,59,59	0.89	1 (1%)
70	PC1	Qc	405	-	53,53,53	0.29	0	59,61,61	0.29	0
75	PLX	AM	202	-	51,51,51	1.11	3 (5%)	55,59,59	0.92	1 (1%)
68	CDL	QB	501	-	60,60,99	0.39	0	66,72,111	0.43	0
70	PC1	C3	302	-	48,48,53	0.30	0	54,56,61	0.36	0
71	PEE	Qd	403	-	23,23,50	1.41	3 (13%)	26,28,55	1.41	2 (7%)
68	CDL	B4	203	-	61,61,99	0.38	0	67,73,111	0.37	0
72	NDP	A9	401	-	45,52,52	0.56	0	53,80,80	0.52	1 (1%)
80	HEM	QC	402	49	41,50,50	1.26	4 (9%)	45,82,82	1.73	8 (17%)
70	PC1	N1	401	-	53,53,53	0.29	0	59,61,61	0.32	0
70	PC1	Qh	101	-	53,53,53	0.30	0	59,61,61	0.29	0
68	CDL	N2	402	-	99,99,99	0.30	0	105,111,111	0.32	0
70	PC1	C1	611	-	49,49,53	0.31	0	55,57,61	0.33	0
68	CDL	AL	202	-	89,89,99	0.32	0	95,101,111	0.43	0
71	PEE	N5	704	-	50,50,50	1.31	5 (10%)	53,55,55	1.22	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
80	HEM	Qc	404	49	41,50,50	1.27	4 (9%)	45,82,82	1.73	8 (17%)
77	HEA	C1	602	35	57,67,67	2.01	15 (26%)	61,103,103	2.67	26 (42%)
70	PC1	7C	101	-	51,51,53	0.30	0	57,59,61	0.30	0
70	PC1	B5	203	-	53,53,53	0.29	0	59,61,61	0.28	0
71	PEE	Qc	402	-	41,41,50	1.28	4 (9%)	44,46,55	1.16	3 (6%)
80	HEM	Qc	403	49	41,50,50	1.24	4 (9%)	45,82,82	1.67	8 (17%)
71	PEE	B4	202	-	50,50,50	1.32	5 (10%)	53,55,55	1.17	3 (5%)
68	CDL	4L	201	-	91,91,99	0.32	0	97,103,111	0.31	0
76	3PE	B8	201	-	31,31,50	0.38	0	34,36,55	0.35	0
77	HEA	C1	603	35	57,67,67	2.00	15 (26%)	61,103,103	2.63	26 (42%)
71	PEE	C3	303	-	50,50,50	1.32	6 (12%)	53,55,55	1.21	3 (5%)
71	PEE	S2	501	-	47,47,50	1.33	5 (10%)	50,52,55	1.24	4 (8%)
68	CDL	A1	101	-	93,93,99	0.31	0	99,105,111	0.29	0
84	FMN	V1	502	-	33,33,33	0.32	0	48,50,50	0.47	0
71	PEE	6A	103	-	35,35,50	1.37	4 (11%)	38,40,55	1.24	3 (7%)
70	PC1	C1	608	-	45,45,53	0.31	0	51,53,61	0.36	0
68	CDL	Qb	501	-	63,63,99	0.38	0	69,75,111	0.51	0
68	CDL	A8	301	-	76,76,99	0.34	0	82,88,111	0.43	0
68	CDL	N2	401	-	67,67,99	0.35	0	73,79,111	0.37	0
76	3PE	C1	601	-	50,50,50	0.30	0	53,55,55	0.35	0
75	PLX	B5	201	-	51,51,51	1.11	4 (7%)	55,59,59	0.88	1 (1%)
82	FES	S1	803	57	0,4,4	-	-	-	-	-
70	PC1	N5	705	-	30,30,53	0.37	0	36,38,61	0.44	0
71	PEE	QB	502	-	33,33,50	1.40	4 (12%)	36,38,55	1.14	3 (8%)
71	PEE	AL	203	-	39,39,50	1.48	5 (12%)	41,44,55	1.17	3 (7%)
70	PC1	C3	301	-	43,43,53	0.31	0	49,51,61	0.32	0
71	PEE	QE	301	-	46,46,50	1.35	5 (10%)	49,51,55	1.30	5 (10%)
71	PEE	A3	201	-	50,50,50	1.30	5 (10%)	53,55,55	1.18	4 (7%)
76	3PE	CA	101	-	50,50,50	0.31	0	53,55,55	0.32	0
83	SF4	S8	301	64	0,12,12	-	-	-	-	-
80	HEM	QC	401	49	41,50,50	1.25	4 (9%)	45,82,82	1.71	9 (20%)
71	PEE	QC	403	-	39,39,50	1.30	4 (10%)	42,44,55	1.20	3 (7%)
70	PC1	QJ	101	-	53,53,53	0.30	0	59,61,61	0.36	0
71	PEE	6A	102	-	50,50,50	1.31	5 (10%)	53,55,55	1.20	5 (9%)
71	PEE	Qc	401	-	50,50,50	1.32	5 (10%)	53,55,55	1.09	3 (5%)
71	PEE	S8	303	-	50,50,50	1.30	5 (10%)	53,55,55	1.20	3 (5%)
75	PLX	N3	201	-	51,51,51	1.11	5 (9%)	55,59,59	0.89	2 (3%)
71	PEE	N5	701	-	45,45,50	1.37	5 (11%)	48,50,55	1.20	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
83	SF4	S1	801	57	0,12,12	-	-	-		
71	PEE	8B	201	-	41,41,50	1.29	4 (9%)	44,46,55	1.13	2 (4%)
68	CDL	QH	101	-	60,60,99	0.38	0	66,72,111	0.40	0
75	PLX	QB	504	-	45,45,51	1.17	3 (6%)	49,53,59	0.92	2 (4%)
68	CDL	B5	202	-	97,97,99	0.30	0	103,109,111	0.29	0
68	CDL	QC	404	-	54,54,99	0.40	0	60,66,111	0.42	0
74	ADP	AK	401	-	24,29,29	0.92	1 (4%)	29,45,45	1.40	4 (13%)
75	PLX	QI	301	-	51,51,51	1.12	3 (5%)	55,59,59	0.89	1 (1%)
71	PEE	N4	501	-	48,48,50	1.34	5 (10%)	51,53,55	1.18	4 (7%)
70	PC1	C1	607	-	32,32,53	0.36	0	38,40,61	0.33	0
70	PC1	Qb	502	-	53,53,53	0.30	0	59,61,61	0.39	0
68	CDL	QD	402	-	63,63,99	0.38	0	69,75,111	0.63	2 (2%)
76	3PE	QE	302	-	43,43,50	0.32	0	46,48,55	0.31	0
83	SF4	S8	302	64	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	PLX	C2	301	-	-	17/46/46/55	-
76	3PE	C2	302	-	-	19/54/54/54	-
81	HEC	Qd	401	50	-	2/10/54/54	-
70	PC1	C1	609	-	-	15/57/57/57	-
71	PEE	QB	503	-	-	27/54/54/54	-
70	PC1	N1	402	-	-	15/57/57/57	-
73	ZMP	AB	201	19	-	19/40/42/43	-
82	FES	QE	303	51	-	-	0/1/1/1
68	CDL	N5	702	-	-	30/92/92/110	-
70	PC1	6A	101	-	-	13/48/48/57	-
83	SF4	S7	301	63	-	-	0/6/5/5
68	CDL	QH	102	-	-	22/74/74/110	-
83	SF4	V1	501	65	-	-	0/6/5/5
70	PC1	Qc	406	-	-	16/57/57/57	-
68	CDL	N5	703	-	-	25/110/110/110	-
82	FES	Qe	301	51	-	-	0/1/1/1
75	PLX	AM	201	-	-	24/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	SF4	S1	802	57	-	-	0/6/5/5
76	3PE	B4	201	-	-	11/54/54/54	-
81	HEC	QD	401	50	-	2/10/54/54	-
70	PC1	N3	202	-	-	12/57/57/57	-
73	ZMP	AC	201	19	-	14/40/42/43	-
70	PC1	B7	201	-	-	8/57/57/57	-
70	PC1	C1	606	-	-	14/57/57/57	-
68	CDL	AL	201	-	-	21/104/104/110	-
82	FES	V2	301	66	-	-	0/1/1/1
68	CDL	QE	304	-	-	30/110/110/110	-
75	PLX	CB	201	-	-	23/55/55/55	-
75	PLX	N4	502	-	-	33/50/50/55	-
70	PC1	Qd	402	-	-	10/57/57/57	-
68	CDL	C1	610	-	-	23/87/87/110	-
75	PLX	N4	503	-	-	22/55/55/55	-
70	PC1	Qc	405	-	-	10/57/57/57	-
75	PLX	AM	202	-	-	19/55/55/55	-
68	CDL	QB	501	-	-	17/71/71/110	-
70	PC1	C3	302	-	-	10/52/52/57	-
71	PEE	Qd	403	-	-	8/27/27/54	-
68	CDL	B4	203	-	-	12/72/72/110	-
72	NDP	A9	401	-	-	10/30/77/77	0/5/5/5
80	HEM	QC	402	49	-	4/12/54/54	-
70	PC1	N1	401	-	-	19/57/57/57	-
70	PC1	Qh	101	-	-	20/57/57/57	-
68	CDL	N2	402	-	-	22/110/110/110	-
70	PC1	C1	611	-	-	8/53/53/57	-
68	CDL	AL	202	-	-	17/100/100/110	-
71	PEE	N5	704	-	-	27/54/54/54	-
80	HEM	Qc	404	49	-	9/12/54/54	-
77	HEA	C1	602	35	-	11/32/76/76	-
70	PC1	7C	101	-	-	10/55/55/57	-
70	PC1	B5	203	-	-	18/57/57/57	-
71	PEE	Qc	402	-	-	19/45/45/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
80	HEM	Qc	403	49	-	7/12/54/54	-
71	PEE	B4	202	-	-	28/54/54/54	-
68	CDL	4L	201	-	-	25/102/102/110	-
76	3PE	B8	201	-	-	6/35/35/54	-
77	HEA	C1	603	35	-	12/32/76/76	-
71	PEE	C3	303	-	-	27/54/54/54	-
71	PEE	S2	501	-	-	17/51/51/54	-
68	CDL	A1	101	-	-	30/104/104/110	-
84	FMN	V1	502	-	-	5/18/18/18	0/3/3/3
71	PEE	6A	103	-	-	17/39/39/54	-
70	PC1	C1	608	-	-	9/49/49/57	-
68	CDL	Qb	501	-	-	14/74/74/110	-
68	CDL	A8	301	-	-	29/87/87/110	-
68	CDL	N2	401	-	-	25/78/78/110	-
76	3PE	C1	601	-	-	8/54/54/54	-
75	PLX	B5	201	-	-	22/55/55/55	-
82	FES	S1	803	57	-	-	0/1/1/1
70	PC1	N5	705	-	-	8/34/34/57	-
71	PEE	QB	502	-	-	22/37/37/54	-
71	PEE	AL	203	-	-	26/43/43/54	-
70	PC1	C3	301	-	-	13/47/47/57	-
71	PEE	QE	301	-	-	21/50/50/54	-
71	PEE	A3	201	-	-	27/54/54/54	-
76	3PE	CA	101	-	-	18/54/54/54	-
83	SF4	S8	301	64	-	-	0/6/5/5
80	HEM	QC	401	49	-	7/12/54/54	-
71	PEE	QC	403	-	-	23/43/43/54	-
70	PC1	QJ	101	-	-	22/57/57/57	-
71	PEE	6A	102	-	-	27/54/54/54	-
71	PEE	Qc	401	-	-	39/54/54/54	-
71	PEE	S8	303	-	-	25/54/54/54	-
75	PLX	N3	201	-	-	17/55/55/55	-
71	PEE	N5	701	-	-	23/49/49/54	-
83	SF4	S1	801	57	-	-	0/6/5/5
71	PEE	8B	201	-	-	27/45/45/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	CDL	QH	101	-	-	22/71/71/110	-
75	PLX	QB	504	-	-	17/49/49/55	-
68	CDL	B5	202	-	-	27/108/108/110	-
68	CDL	QC	404	-	-	12/65/65/110	-
74	ADP	AK	401	-	-	2/12/32/32	0/3/3/3
75	PLX	QI	301	-	-	24/55/55/55	-
71	PEE	N4	501	-	-	27/52/52/54	-
70	PC1	C1	607	-	-	16/36/36/57	-
70	PC1	Qb	502	-	-	11/57/57/57	-
68	CDL	QD	402	-	-	21/74/74/110	-
76	3PE	QE	302	-	-	9/47/47/54	-
83	SF4	S8	302	64	-	-	0/6/5/5

All (182) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	Qd	401	HEC	C3C-C2C	-6.88	1.33	1.40
81	QD	401	HEC	C3C-C2C	-6.78	1.33	1.40
81	QD	401	HEC	C2B-C3B	-6.49	1.34	1.40
81	Qd	401	HEC	C2B-C3B	-6.47	1.34	1.40
77	C1	602	HEA	C3B-C2B	5.19	1.46	1.34
77	C1	603	HEA	C3B-C2B	5.02	1.46	1.34
77	C1	602	HEA	CHC-C4B	4.47	1.46	1.35
77	C1	603	HEA	CHC-C4B	4.40	1.46	1.35
77	C1	602	HEA	C3A-C2A	4.31	1.46	1.40
77	C1	603	HEA	C3C-C2C	4.19	1.46	1.40
77	C1	603	HEA	C4B-NB	-4.11	1.33	1.40
71	QE	301	PEE	C18-C19	4.07	1.55	1.31
71	6A	103	PEE	C18-C19	4.07	1.55	1.31
77	C1	602	HEA	C4B-NB	-4.07	1.33	1.40
71	Qc	401	PEE	C18-C19	4.07	1.55	1.31
77	C1	603	HEA	CHD-C1D	4.07	1.45	1.35
71	QB	503	PEE	C18-C19	4.06	1.55	1.31
71	B4	202	PEE	C18-C19	4.06	1.55	1.31
71	N5	704	PEE	C18-C19	4.05	1.55	1.31
71	QC	403	PEE	C18-C19	4.04	1.55	1.31
71	C3	303	PEE	C18-C19	4.04	1.55	1.31
77	C1	602	HEA	C3C-C2C	4.03	1.46	1.40
71	Qc	402	PEE	C18-C19	4.03	1.55	1.31
71	N4	501	PEE	C18-C19	4.03	1.55	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	AL	203	PEE	C18-C19	4.03	1.55	1.31
77	C1	603	HEA	C3A-C2A	4.02	1.45	1.40
77	C1	603	HEA	C1D-ND	-4.01	1.33	1.40
71	6A	102	PEE	C18-C19	4.01	1.55	1.31
71	S8	303	PEE	C18-C19	4.01	1.55	1.31
71	N5	701	PEE	C18-C19	4.00	1.55	1.31
71	8B	201	PEE	C39-C38	3.99	1.54	1.31
71	S2	501	PEE	C18-C19	3.99	1.54	1.31
71	A3	201	PEE	C18-C19	3.98	1.54	1.31
71	N4	501	PEE	C39-C38	3.96	1.54	1.31
80	Qc	404	HEM	C4D-ND	-3.95	1.33	1.40
71	Qc	401	PEE	C39-C38	3.94	1.54	1.31
71	B4	202	PEE	C39-C38	3.94	1.54	1.31
71	S8	303	PEE	C39-C38	3.94	1.54	1.31
71	6A	102	PEE	C39-C38	3.93	1.54	1.31
71	QB	503	PEE	C39-C38	3.93	1.54	1.31
71	QE	301	PEE	C39-C38	3.92	1.54	1.31
71	N5	704	PEE	C39-C38	3.91	1.54	1.31
71	A3	201	PEE	C39-C38	3.91	1.54	1.31
71	N5	701	PEE	C39-C38	3.91	1.54	1.31
71	QB	502	PEE	C39-C38	3.91	1.54	1.31
71	AL	203	PEE	C39-C38	3.91	1.54	1.31
71	C3	303	PEE	C39-C38	3.90	1.54	1.31
77	C1	603	HEA	C3D-C2D	3.90	1.45	1.36
71	S2	501	PEE	C39-C38	3.89	1.54	1.31
77	C1	602	HEA	CHD-C1D	3.83	1.44	1.35
80	QC	402	HEM	C4D-ND	-3.78	1.33	1.40
80	QC	401	HEM	C4D-ND	-3.78	1.33	1.40
80	Qc	403	HEM	C4D-ND	-3.76	1.33	1.40
77	C1	602	HEA	C1D-ND	-3.76	1.33	1.40
77	C1	602	HEA	C3D-C2D	3.66	1.44	1.36
81	QD	401	HEC	CBC-CAC	-3.42	1.36	1.49
81	Qd	401	HEC	CBC-CAC	-3.39	1.36	1.49
80	QC	402	HEM	C1B-NB	-3.31	1.34	1.40
80	Qc	404	HEM	C1B-NB	-3.30	1.34	1.40
71	C3	303	PEE	O3-C30	3.24	1.42	1.33
71	QB	502	PEE	O3-C30	3.23	1.42	1.33
71	QC	403	PEE	O3-C30	3.23	1.42	1.33
71	QB	503	PEE	O3-C30	3.23	1.42	1.33
71	AL	203	PEE	O3-C30	3.22	1.42	1.33
71	6A	103	PEE	O3-C30	3.21	1.42	1.33
71	8B	201	PEE	O3-C30	3.21	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	N4	503	PLX	O6-C4	-3.21	1.40	1.44
71	Qc	402	PEE	O3-C30	3.21	1.42	1.33
71	Qc	401	PEE	O3-C30	3.19	1.42	1.33
71	N5	704	PEE	O3-C30	3.19	1.42	1.33
77	C1	602	HEA	C1B-NB	-3.19	1.32	1.38
71	B4	202	PEE	O3-C30	3.18	1.42	1.33
71	6A	102	PEE	O3-C30	3.18	1.42	1.33
75	AM	202	PLX	O6-C4	-3.17	1.40	1.44
80	QC	401	HEM	C1B-NB	-3.17	1.34	1.40
71	Qd	403	PEE	O3-C30	3.16	1.42	1.33
71	A3	201	PEE	O3-C30	3.16	1.42	1.33
71	S8	303	PEE	O3-C30	3.13	1.42	1.33
75	CB	201	PLX	O6-C4	-3.12	1.40	1.44
71	N4	501	PEE	O3-C30	3.09	1.42	1.33
71	QE	301	PEE	O3-C30	3.09	1.42	1.33
71	N5	701	PEE	O3-C30	3.08	1.42	1.33
71	S2	501	PEE	O3-C30	3.06	1.42	1.33
80	Qc	403	HEM	C1B-NB	-3.05	1.35	1.40
75	QI	301	PLX	O6-C4	-3.02	1.40	1.44
75	B5	201	PLX	O6-C4	-3.01	1.40	1.44
75	QB	504	PLX	O6-C4	-3.01	1.40	1.44
77	C1	603	HEA	C1B-NB	-2.96	1.32	1.38
75	AM	201	PLX	O6-C4	-2.95	1.40	1.44
75	C2	301	PLX	O6-C4	-2.93	1.40	1.44
77	C1	602	HEA	CAA-C2A	-2.85	1.47	1.52
71	Qc	401	PEE	O2-C10	2.85	1.42	1.34
71	AL	203	PEE	O2-C10	2.84	1.42	1.34
75	N4	502	PLX	O6-C4	-2.79	1.40	1.44
75	N3	201	PLX	O6-C4	-2.78	1.40	1.44
80	Qc	404	HEM	C1D-ND	-2.75	1.33	1.38
77	C1	602	HEA	C4D-ND	-2.74	1.33	1.38
77	C1	603	HEA	CAA-C2A	-2.73	1.47	1.52
71	Qd	403	PEE	O2-C2	-2.73	1.39	1.46
71	Qc	402	PEE	O2-C2	-2.72	1.39	1.46
71	N5	701	PEE	O2-C10	2.68	1.41	1.34
71	C3	303	PEE	O2-C10	2.66	1.41	1.34
71	QC	403	PEE	O2-C2	-2.66	1.40	1.46
80	QC	401	HEM	C1D-ND	-2.65	1.33	1.38
71	8B	201	PEE	O2-C2	-2.65	1.40	1.46
73	AC	201	ZMP	C9-C10	-2.64	1.48	1.50
71	B4	202	PEE	O2-C10	2.63	1.41	1.34
80	Qc	403	HEM	C1D-ND	-2.63	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	N4	501	PEE	O2-C2	-2.62	1.40	1.46
71	S8	303	PEE	O2-C10	2.61	1.41	1.34
71	QB	502	PEE	O2-C10	2.60	1.41	1.34
71	6A	103	PEE	O2-C2	-2.60	1.40	1.46
77	C1	603	HEA	C4D-ND	-2.59	1.33	1.38
71	N5	704	PEE	O2-C2	-2.59	1.40	1.46
80	QC	402	HEM	C1D-ND	-2.59	1.33	1.38
71	A3	201	PEE	O2-C2	-2.58	1.40	1.46
71	6A	102	PEE	O2-C10	2.57	1.41	1.34
71	S2	501	PEE	O2-C2	-2.57	1.40	1.46
71	S8	303	PEE	O2-C2	-2.57	1.40	1.46
71	A3	201	PEE	O2-C10	2.57	1.41	1.34
71	QE	301	PEE	O2-C10	2.55	1.41	1.34
71	S2	501	PEE	O2-C10	2.55	1.41	1.34
71	QE	301	PEE	O2-C2	-2.55	1.40	1.46
71	6A	102	PEE	O2-C2	-2.54	1.40	1.46
71	QB	503	PEE	O2-C2	-2.54	1.40	1.46
71	QB	503	PEE	O2-C10	2.54	1.41	1.34
71	Qd	403	PEE	O2-C10	2.53	1.41	1.34
77	C1	603	HEA	FE-ND	2.52	2.09	1.96
71	B4	202	PEE	O2-C2	-2.52	1.40	1.46
71	Qc	402	PEE	O2-C10	2.51	1.41	1.34
77	C1	602	HEA	O2D-CGD	-2.50	1.22	1.30
71	6A	103	PEE	O2-C10	2.50	1.41	1.34
71	N4	501	PEE	O2-C10	2.49	1.41	1.34
71	C3	303	PEE	O2-C2	-2.48	1.40	1.46
77	C1	602	HEA	FE-ND	2.48	2.09	1.96
77	C1	603	HEA	FE-NB	2.48	2.09	1.96
77	C1	602	HEA	FE-NB	2.46	2.09	1.96
71	N5	704	PEE	O2-C10	2.46	1.41	1.34
73	AB	201	ZMP	C9-C10	-2.45	1.48	1.50
77	C1	602	HEA	O2A-CGA	-2.45	1.22	1.30
71	QC	403	PEE	O2-C10	2.44	1.41	1.34
77	C1	603	HEA	O2D-CGD	-2.44	1.22	1.30
71	8B	201	PEE	O2-C10	2.44	1.41	1.34
77	C1	603	HEA	O2A-CGA	-2.43	1.22	1.30
71	N5	701	PEE	O2-C2	-2.40	1.40	1.46
71	QB	502	PEE	O2-C2	-2.39	1.40	1.46
81	QD	401	HEC	CBB-CAB	-2.36	1.40	1.49
81	Qd	401	HEC	CBB-CAB	-2.34	1.40	1.49
75	QB	504	PLX	C1B-N1	-2.32	1.43	1.50
75	QI	301	PLX	C1B-N1	-2.31	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	AK	401	ADP	C5-C4	2.31	1.47	1.40
75	QB	504	PLX	C1C-N1	-2.27	1.43	1.50
75	N4	502	PLX	C1B-N1	-2.25	1.43	1.50
75	N3	201	PLX	C7-C6	2.23	1.55	1.50
75	QI	301	PLX	C1C-N1	-2.22	1.43	1.50
75	CB	201	PLX	C1B-N1	-2.22	1.43	1.50
75	N4	503	PLX	C1B-N1	-2.22	1.43	1.50
75	N3	201	PLX	C1B-N1	-2.20	1.43	1.50
75	B5	201	PLX	C1B-N1	-2.19	1.43	1.50
75	AM	202	PLX	C1B-N1	-2.18	1.43	1.50
80	QC	401	HEM	C4B-NB	-2.16	1.34	1.38
71	AL	203	PEE	O2-C2	-2.15	1.41	1.46
75	C2	301	PLX	C1B-N1	-2.13	1.43	1.50
75	N4	502	PLX	C1C-N1	-2.13	1.43	1.50
75	AM	201	PLX	C1B-N1	-2.13	1.43	1.50
75	N4	502	PLX	C7-C6	2.11	1.55	1.50
75	CB	201	PLX	C1C-N1	-2.10	1.43	1.50
80	QC	402	HEM	C4B-NB	-2.10	1.34	1.38
75	AM	201	PLX	P1-O4	2.10	1.67	1.59
71	Qc	401	PEE	O2-C2	-2.08	1.41	1.46
75	N4	503	PLX	C1C-N1	-2.07	1.44	1.50
71	C3	303	PEE	C11-C10	2.07	1.56	1.50
75	N3	201	PLX	C1C-N1	-2.06	1.44	1.50
75	AM	202	PLX	C1C-N1	-2.06	1.44	1.50
75	B5	201	PLX	C1C-N1	-2.04	1.44	1.50
80	Qc	404	HEM	C4B-NB	-2.04	1.34	1.38
75	AM	201	PLX	C1C-N1	-2.02	1.44	1.50
75	B5	201	PLX	P1-O4	2.01	1.67	1.59
80	Qc	403	HEM	CHB-C1B	2.01	1.40	1.35
75	N3	201	PLX	P1-O4	2.01	1.67	1.59
75	N4	502	PLX	P1-O4	2.00	1.67	1.59
75	CB	201	PLX	P1-O4	2.00	1.67	1.59

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	C1	603	HEA	CAD-CBD-CGD	-7.97	96.44	113.60
77	C1	602	HEA	CAD-CBD-CGD	-7.50	97.46	113.60
77	C1	603	HEA	C3D-C4D-ND	5.82	115.99	110.36
77	C1	602	HEA	C3D-C4D-ND	5.73	115.91	110.36
77	C1	602	HEA	C13-C12-C11	-5.43	106.20	114.35
77	C1	602	HEA	C2B-C1B-NB	5.06	115.95	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	C1	602	HEA	CHB-C1B-C2B	-4.81	117.47	124.98
77	C1	603	HEA	C2D-C1D-ND	4.75	115.47	109.84
77	C1	602	HEA	C2D-C1D-ND	4.75	115.47	109.84
77	C1	603	HEA	CAA-CBA-CGA	-4.74	100.47	113.76
77	C1	602	HEA	CAA-CBA-CGA	-4.71	100.56	113.76
77	C1	603	HEA	C2B-C1B-NB	4.70	115.51	109.88
80	QC	401	HEM	CHC-C4B-NB	4.69	129.53	124.43
71	QE	301	PEE	O2-C10-C11	4.67	121.56	111.50
77	C1	602	HEA	C1D-C2D-C3D	-4.64	102.08	106.96
77	C1	603	HEA	C13-C12-C11	-4.63	107.39	114.35
80	Qc	403	HEM	CHC-C4B-NB	4.57	129.39	124.43
77	C1	603	HEA	CHB-C1B-C2B	-4.56	117.85	124.98
77	C1	603	HEA	C1D-C2D-C3D	-4.56	102.17	106.96
80	Qc	404	HEM	CHC-C4B-NB	4.49	129.31	124.43
71	C3	303	PEE	O2-C10-C11	4.41	121.00	111.50
77	C1	602	HEA	C3C-C4C-NC	4.40	114.89	109.21
81	QD	401	HEC	CMD-C2D-C1D	-4.38	121.74	128.46
80	QC	402	HEM	C4D-ND-C1D	4.35	109.56	105.07
71	Qd	403	PEE	O2-C10-C11	4.29	120.74	111.50
71	S8	303	PEE	O2-C10-C11	4.21	120.58	111.50
71	N5	704	PEE	O2-C10-C11	4.18	120.50	111.50
71	QB	503	PEE	O2-C10-C11	4.16	120.48	111.50
77	C1	603	HEA	C3B-C4B-NB	4.16	114.77	109.84
80	QC	402	HEM	CHC-C4B-NB	4.11	128.89	124.43
71	6A	102	PEE	O2-C10-C11	4.05	120.23	111.50
71	QC	403	PEE	O2-C10-C11	4.04	120.20	111.50
81	Qd	401	HEC	CMD-C2D-C1D	-4.03	122.28	128.46
71	S2	501	PEE	O2-C10-C11	4.00	120.11	111.50
71	N5	701	PEE	O2-C10-C11	3.98	120.08	111.50
80	Qc	404	HEM	C4D-ND-C1D	3.97	109.18	105.07
77	C1	603	HEA	C3C-C4C-NC	3.92	114.27	109.21
80	Qc	403	HEM	CHB-C1B-NB	3.91	129.22	124.38
71	B4	202	PEE	O2-C10-C11	3.91	119.93	111.50
71	6A	103	PEE	O2-C10-C11	3.90	119.91	111.50
71	A3	201	PEE	O2-C10-C11	3.89	119.89	111.50
80	QC	401	HEM	CHB-C1B-NB	3.87	129.16	124.38
80	Qc	404	HEM	CHB-C1B-NB	3.84	129.12	124.38
71	AL	203	PEE	O2-C10-C11	3.80	119.69	111.50
77	C1	602	HEA	C3B-C4B-NB	3.80	114.34	109.84
71	N4	501	PEE	O2-C10-C11	3.72	119.53	111.50
77	C1	603	HEA	CHA-C4D-C3D	-3.67	119.44	124.84
77	C1	603	HEA	C4B-C3B-C2B	-3.67	101.14	107.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	QC	402	HEM	C1B-NB-C4B	3.66	108.85	105.07
71	Qc	402	PEE	O2-C10-C11	3.64	119.35	111.50
71	QB	502	PEE	O2-C10-C11	3.63	119.32	111.50
77	C1	603	HEA	CMC-C2C-C3C	3.58	131.38	124.68
81	QD	401	HEC	CMB-C2B-C3B	3.58	130.03	125.82
81	Qd	401	HEC	CMB-C2B-C1B	-3.57	122.97	128.46
80	QC	402	HEM	CHB-C1B-NB	3.55	128.77	124.38
71	8B	201	PEE	O2-C10-C11	3.53	119.11	111.50
81	QD	401	HEC	CMB-C2B-C1B	-3.53	123.04	128.46
77	C1	602	HEA	C4B-C3B-C2B	-3.53	101.39	107.41
74	AK	401	ADP	PA-O3A-PB	-3.52	120.76	132.83
77	C1	602	HEA	CHA-C4D-C3D	-3.49	119.71	124.84
71	Qd	403	PEE	O3-C30-C31	3.48	120.51	111.38
81	Qd	401	HEC	CMB-C2B-C3B	3.45	129.88	125.82
71	Qc	401	PEE	O2-C10-C11	3.42	118.87	111.50
80	Qc	404	HEM	C1B-NB-C4B	3.34	108.53	105.07
71	6A	103	PEE	O3-C30-C31	3.34	120.14	111.38
80	QC	401	HEM	C4D-ND-C1D	3.33	108.51	105.07
77	C1	602	HEA	C27-C19-C20	3.33	120.87	115.27
81	Qd	401	HEC	CMC-C2C-C3C	3.30	129.70	125.82
68	QD	402	CDL	OB6-CB4-CB3	3.23	120.11	108.40
74	AK	401	ADP	N3-C2-N1	-3.23	123.63	128.68
81	QD	401	HEC	CMC-C2C-C3C	3.22	129.60	125.82
77	C1	602	HEA	CMC-C2C-C3C	3.11	130.50	124.68
80	Qc	403	HEM	C1B-NB-C4B	3.10	108.27	105.07
81	Qd	401	HEC	C4C-C3C-C2C	3.09	109.69	106.35
80	QC	401	HEM	C1B-NB-C4B	3.06	108.23	105.07
81	QD	401	HEC	CBD-CAD-C3D	3.04	117.80	112.62
80	QC	401	HEM	CHA-C4D-ND	3.00	128.08	124.38
80	Qc	403	HEM	C4D-ND-C1D	2.98	108.15	105.07
81	QD	401	HEC	C4C-C3C-C2C	2.98	109.57	106.35
77	C1	603	HEA	C27-C19-C20	2.95	120.24	115.27
71	N4	501	PEE	O3-C30-C31	2.90	121.02	111.91
80	QC	401	HEM	CHD-C1D-ND	2.88	127.56	124.43
71	N5	704	PEE	O3-C30-C31	2.84	120.81	111.91
71	Qc	402	PEE	O3-C30-C31	2.84	120.81	111.91
71	QE	301	PEE	O3-C30-C31	2.80	120.69	111.91
77	C1	602	HEA	C17-C18-C19	-2.79	120.94	127.66
77	C1	603	HEA	C13-C14-C15	-2.78	120.96	127.66
81	Qd	401	HEC	O1D-CGD-CBD	-2.77	114.17	123.08
81	QD	401	HEC	O1D-CGD-CBD	-2.75	114.23	123.08
80	QC	402	HEM	CAD-CBD-CGD	-2.75	107.67	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	Qc	403	HEM	CHA-C4D-ND	2.75	127.78	124.38
71	S8	303	PEE	O3-C30-C31	2.72	120.43	111.91
80	Qc	404	HEM	CHD-C1D-ND	2.71	127.38	124.43
80	Qc	404	HEM	CAD-CBD-CGD	-2.70	107.79	113.60
77	C1	602	HEA	C13-C14-C15	-2.69	121.18	127.66
71	8B	201	PEE	O3-C30-C31	2.68	120.32	111.91
71	S2	501	PEE	O3-C30-C31	2.68	120.30	111.91
71	QC	403	PEE	O3-C30-C31	2.67	120.30	111.91
71	QB	502	PEE	O3-C30-C31	2.64	120.21	111.91
68	QD	402	CDL	CB4-OB6-CB5	2.64	124.28	117.79
77	C1	602	HEA	CMB-C2B-C1B	-2.63	121.03	125.04
71	AL	203	PEE	O3-C30-C31	2.62	120.13	111.91
81	QD	401	HEC	CMC-C2C-C1C	-2.60	124.46	128.46
74	AK	401	ADP	C4-C5-N7	-2.59	106.70	109.40
71	A3	201	PEE	O3-C30-C31	2.59	120.03	111.91
71	QB	503	PEE	O3-C30-C31	2.59	120.02	111.91
71	6A	102	PEE	O3-C30-C31	2.58	120.02	111.91
80	Qc	403	HEM	CHD-C1D-ND	2.58	127.23	124.43
71	B4	202	PEE	O3-C30-C31	2.58	120.00	111.91
81	Qd	401	HEC	CMC-C2C-C1C	-2.56	124.53	128.46
80	Qc	403	HEM	CBA-CAA-C2A	-2.56	108.26	112.62
81	QD	401	HEC	CBA-CAA-C2A	2.55	116.90	112.60
80	QC	402	HEM	CHD-C1D-ND	2.53	127.19	124.43
81	QD	401	HEC	O1A-CGA-CBA	-2.53	114.95	123.08
81	Qd	401	HEC	CMA-C3A-C2A	2.53	129.70	124.94
71	N5	701	PEE	O3-C30-C31	2.52	119.83	111.91
71	Qc	401	PEE	O3-C30-C31	2.52	119.81	111.91
81	QD	401	HEC	CMA-C3A-C2A	2.52	129.68	124.94
81	QD	401	HEC	CMD-C2D-C3D	2.51	129.67	124.94
77	C1	603	HEA	C4D-C3D-C2D	-2.50	103.25	106.90
71	C3	303	PEE	O3-C30-C31	2.50	119.74	111.91
77	C1	602	HEA	CMB-C2B-C3B	2.49	135.09	130.34
80	Qc	404	HEM	CHA-C4D-ND	2.48	127.45	124.38
77	C1	602	HEA	C27-C19-C18	-2.46	117.37	123.68
77	C1	602	HEA	C1B-C2B-C3B	-2.45	103.88	106.80
77	C1	602	HEA	OMA-CMA-C3A	-2.43	119.62	124.91
77	C1	603	HEA	CMB-C2B-C1B	-2.41	121.37	125.04
77	C1	603	HEA	C17-C18-C19	-2.40	121.88	127.66
80	QC	401	HEM	CBA-CAA-C2A	-2.38	108.55	112.62
72	A9	401	NDP	C5A-C6A-N6A	2.37	123.95	120.35
77	C1	602	HEA	C26-C15-C16	2.37	119.25	115.27
80	QC	402	HEM	CHA-C4D-ND	2.36	127.29	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	Qd	401	HEC	CMD-C2D-C3D	2.33	129.33	124.94
75	QB	504	PLX	O3-P1-O2	-2.32	100.76	112.24
75	QI	301	PLX	O3-P1-O2	-2.32	100.77	112.24
80	Qc	403	HEM	CHB-C1B-C2B	-2.32	120.32	126.72
77	C1	602	HEA	C4D-C3D-C2D	-2.32	103.52	106.90
80	QC	401	HEM	CHB-C1B-C2B	-2.31	120.34	126.72
81	QD	401	HEC	O2A-CGA-O1A	2.30	129.04	123.30
80	QC	401	HEM	CAD-CBD-CGD	-2.29	108.67	113.60
81	QD	401	HEC	C1D-C2D-C3D	2.29	108.59	107.00
81	Qd	401	HEC	O2A-CGA-O1A	2.28	128.99	123.30
80	Qc	404	HEM	CHB-C1B-C2B	-2.25	120.49	126.72
77	C1	603	HEA	O1D-CGD-CBD	-2.25	115.84	123.08
75	AM	201	PLX	O3-P1-O2	-2.25	101.12	112.24
75	N3	201	PLX	O3-P1-O2	-2.24	101.17	112.24
81	Qd	401	HEC	O1A-CGA-CBA	-2.23	115.91	123.08
75	B5	201	PLX	O3-P1-O2	-2.22	101.25	112.24
71	QE	301	PEE	C2-O2-C10	-2.22	112.32	117.79
75	N4	503	PLX	O3-P1-O2	-2.22	101.28	112.24
75	C2	301	PLX	O3-P1-O2	-2.22	101.28	112.24
75	N4	502	PLX	O3-P1-O2	-2.19	101.42	112.24
81	QD	401	HEC	C2B-C3B-C4B	2.17	108.70	106.35
75	CB	201	PLX	O3-P1-O2	-2.15	101.63	112.24
71	C3	303	PEE	C40-C39-C38	-2.14	108.30	124.73
71	6A	103	PEE	C2-O2-C10	-2.14	112.53	117.79
75	AM	202	PLX	O3-P1-O2	-2.13	101.73	112.24
77	C1	603	HEA	O1A-CGA-CBA	-2.11	116.29	123.08
71	S2	501	PEE	C37-C38-C39	-2.11	108.50	124.73
71	A3	201	PEE	C17-C18-C19	-2.11	108.51	124.73
77	C1	603	HEA	CHC-C4B-NB	-2.10	121.79	124.38
77	C1	603	HEA	C1B-C2B-C3B	-2.10	104.30	106.80
71	QC	403	PEE	C17-C18-C19	-2.09	108.66	124.73
77	C1	603	HEA	CMB-C2B-C3B	2.09	134.33	130.34
71	QB	502	PEE	C37-C38-C39	-2.09	108.71	124.73
80	QC	402	HEM	CHB-C1B-C2B	-2.08	120.97	126.72
77	C1	602	HEA	CHC-C4B-NB	-2.08	121.81	124.38
71	Qc	402	PEE	C20-C19-C18	-2.07	108.81	124.73
75	QB	504	PLX	C26-C25-C24	-2.06	108.61	113.38
71	QE	301	PEE	C40-C39-C38	-2.06	108.93	124.73
77	C1	602	HEA	O1D-CGD-CBD	-2.06	116.48	123.08
77	C1	603	HEA	CHD-C1D-C2D	-2.05	121.04	126.72
71	QB	503	PEE	C37-C38-C39	-2.05	109.01	124.73
71	S2	501	PEE	C20-C19-C18	-2.05	109.02	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
71	6A	102	PEE	C37-C38-C39	-2.05	109.02	124.73
71	QE	301	PEE	C20-C19-C18	-2.05	109.03	124.73
71	N4	501	PEE	C37-C38-C39	-2.04	109.04	124.73
71	Qc	401	PEE	C40-C39-C38	-2.04	109.06	124.73
71	N4	501	PEE	C20-C19-C18	-2.04	109.07	124.73
71	6A	102	PEE	C20-C19-C18	-2.04	109.08	124.73
71	B4	202	PEE	C40-C39-C38	-2.04	109.11	124.73
77	C1	603	HEA	CHB-C1B-NB	2.04	126.64	124.43
71	N5	704	PEE	C20-C19-C18	-2.03	109.15	124.73
77	C1	602	HEA	CHD-C1D-C2D	-2.03	121.11	126.72
71	QB	503	PEE	C40-C39-C38	-2.03	109.15	124.73
71	N5	704	PEE	C40-C39-C38	-2.03	109.16	124.73
75	N3	201	PLX	C26-C25-C24	-2.03	108.69	113.38
77	C1	603	HEA	C26-C15-C14	-2.02	118.49	123.68
71	N5	701	PEE	C37-C38-C39	-2.02	109.24	124.73
71	6A	102	PEE	C17-C18-C19	-2.02	109.25	124.73
71	AL	203	PEE	C37-C38-C39	-2.01	109.27	124.73
81	Qd	401	HEC	C1D-C2D-C3D	2.01	108.40	107.00
71	A3	201	PEE	C40-C39-C38	-2.01	109.28	124.73
71	S8	303	PEE	C17-C18-C19	-2.01	109.30	124.73
71	N5	701	PEE	C20-C19-C18	-2.01	109.32	124.73
74	AK	401	ADP	C3'-C2'-C1'	2.01	104.00	100.98

There are no chirality outliers.

All (1551) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
68	4L	201	CDL	CA2-OA2-PA1-OA3
68	4L	201	CDL	CB2-OB2-PB2-OB3
68	4L	201	CDL	CB3-OB5-PB2-OB2
68	4L	201	CDL	CB3-OB5-PB2-OB3
68	4L	201	CDL	CB3-OB5-PB2-OB4
68	A1	101	CDL	CA2-OA2-PA1-OA3
68	A1	101	CDL	CA2-OA2-PA1-OA4
68	A1	101	CDL	CA3-OA5-PA1-OA3
68	A8	301	CDL	CA2-OA2-PA1-OA3
68	A8	301	CDL	CA2-OA2-PA1-OA4
68	A8	301	CDL	CA2-OA2-PA1-OA5
68	A8	301	CDL	CA3-OA5-PA1-OA2
68	A8	301	CDL	CA3-OA5-PA1-OA4
68	A8	301	CDL	CB2-OB2-PB2-OB3
68	A8	301	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
68	A8	301	CDL	CB3-OB5-PB2-OB4
68	A8	301	CDL	OB6-CB4-CB6-OB8
68	AL	201	CDL	CA2-OA2-PA1-OA4
68	AL	201	CDL	CB2-OB2-PB2-OB3
68	AL	202	CDL	CA3-OA5-PA1-OA4
68	B4	203	CDL	C1-CB2-OB2-PB2
68	B4	203	CDL	CB3-OB5-PB2-OB3
68	B4	203	CDL	CB3-OB5-PB2-OB4
68	B5	202	CDL	CA3-OA5-PA1-OA2
68	B5	202	CDL	CA3-OA5-PA1-OA3
68	B5	202	CDL	CA3-OA5-PA1-OA4
68	C1	610	CDL	CB2-OB2-PB2-OB3
68	C1	610	CDL	CB2-OB2-PB2-OB4
68	C1	610	CDL	CB2-OB2-PB2-OB5
68	N2	402	CDL	CA2-OA2-PA1-OA3
68	N2	402	CDL	CA2-OA2-PA1-OA5
68	N2	402	CDL	CA3-OA5-PA1-OA2
68	N2	402	CDL	CB3-OB5-PB2-OB2
68	N2	402	CDL	CB3-OB5-PB2-OB3
68	N2	402	CDL	CB3-OB5-PB2-OB4
68	N5	702	CDL	CA2-OA2-PA1-OA3
68	N5	702	CDL	CA3-OA5-PA1-OA3
68	N5	702	CDL	CA3-OA5-PA1-OA4
68	N5	702	CDL	CB2-OB2-PB2-OB3
68	N5	702	CDL	CB2-OB2-PB2-OB5
68	N5	703	CDL	CA2-OA2-PA1-OA3
68	N5	703	CDL	CA2-OA2-PA1-OA4
68	N5	703	CDL	CA3-OA5-PA1-OA3
68	N5	703	CDL	CB3-OB5-PB2-OB3
68	QB	501	CDL	CA2-OA2-PA1-OA3
68	QB	501	CDL	CB3-OB5-PB2-OB3
68	QB	501	CDL	CB3-OB5-PB2-OB4
68	QC	404	CDL	CA3-OA5-PA1-OA2
68	QC	404	CDL	CA3-OA5-PA1-OA3
68	QD	402	CDL	CA3-OA5-PA1-OA3
68	QD	402	CDL	CB2-OB2-PB2-OB4
68	QD	402	CDL	CB3-CB4-OB6-CB5
68	QE	304	CDL	CB2-C1-CA2-OA2
68	QE	304	CDL	CA2-OA2-PA1-OA3
68	QE	304	CDL	CA2-OA2-PA1-OA4
68	QH	101	CDL	CA2-OA2-PA1-OA3
68	QH	101	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
68	QH	102	CDL	CB2-OB2-PB2-OB3
68	QH	102	CDL	CB2-OB2-PB2-OB4
68	QH	102	CDL	CB3-OB5-PB2-OB2
68	QH	102	CDL	CB3-OB5-PB2-OB3
68	QH	102	CDL	CB3-OB5-PB2-OB4
68	Qb	501	CDL	CA3-OA5-PA1-OA4
68	Qb	501	CDL	CB2-OB2-PB2-OB3
68	Qb	501	CDL	CB2-OB2-PB2-OB4
68	Qb	501	CDL	CB2-OB2-PB2-OB5
70	6A	101	PC1	O21-C2-C3-O31
70	B5	203	PC1	C11-O13-P-O12
70	C1	606	PC1	C11-O13-P-O12
70	C1	606	PC1	C11-O13-P-O14
70	C1	606	PC1	O13-C11-C12-N
70	C1	607	PC1	C11-O13-P-O14
70	C1	607	PC1	C1-O11-P-O12
70	C1	608	PC1	C11-O13-P-O12
70	C1	608	PC1	C11-O13-P-O14
70	C1	609	PC1	C1-O11-P-O13
70	C1	611	PC1	C11-O13-P-O14
70	C3	301	PC1	C11-O13-P-O12
70	C3	301	PC1	C11-O13-P-O14
70	C3	301	PC1	C1-O11-P-O12
70	C3	301	PC1	C1-O11-P-O14
70	C3	302	PC1	C1-O11-P-O12
70	N1	401	PC1	C11-O13-P-O12
70	N1	401	PC1	C11-O13-P-O11
70	N1	401	PC1	C1-O11-P-O14
70	N1	402	PC1	C1-O11-P-O12
70	N1	402	PC1	C1-O11-P-O14
70	N1	402	PC1	O13-C11-C12-N
70	N3	202	PC1	C11-O13-P-O12
70	N3	202	PC1	C11-O13-P-O14
70	N3	202	PC1	C1-O11-P-O12
70	N5	705	PC1	C11-O13-P-O12
70	N5	705	PC1	C11-O13-P-O14
70	QJ	101	PC1	C11-O13-P-O12
70	QJ	101	PC1	C11-O13-P-O14
70	QJ	101	PC1	C11-O13-P-O11
70	QJ	101	PC1	C1-O11-P-O12
70	Qc	405	PC1	C11-O13-P-O14
70	Qc	405	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
70	Qc	405	PC1	C1-O11-P-O13
70	Qc	406	PC1	C11-O13-P-O14
70	Qd	402	PC1	C11-O13-P-O14
70	Qh	101	PC1	C11-O13-P-O14
70	Qh	101	PC1	C11-O13-P-O11
70	Qh	101	PC1	C1-O11-P-O12
70	Qh	101	PC1	C1-O11-P-O14
70	Qh	101	PC1	C1-O11-P-O13
70	Qh	101	PC1	O11-C1-C2-O21
71	6A	102	PEE	C17-C18-C19-C20
71	6A	102	PEE	C11-C10-O2-C2
71	6A	102	PEE	O4-C10-O2-C2
71	6A	102	PEE	C1-O3P-P-O4P
71	6A	102	PEE	C4-O4P-P-O1P
71	6A	103	PEE	C17-C18-C19-C20
71	6A	103	PEE	C11-C10-O2-C2
71	6A	103	PEE	O4P-C4-C5-N
71	8B	201	PEE	C11-C10-O2-C2
71	8B	201	PEE	C1-O3P-P-O2P
71	8B	201	PEE	C1-O3P-P-O1P
71	8B	201	PEE	C4-O4P-P-O3P
71	8B	201	PEE	C4-O4P-P-O2P
71	8B	201	PEE	C4-O4P-P-O1P
71	A3	201	PEE	O2-C2-C3-O3
71	A3	201	PEE	C1-O3P-P-O2P
71	A3	201	PEE	C1-O3P-P-O1P
71	A3	201	PEE	C1-O3P-P-O4P
71	AL	203	PEE	C1-O3P-P-O1P
71	AL	203	PEE	C37-C38-C39-C40
71	B4	202	PEE	O3P-C1-C2-O2
71	B4	202	PEE	C1-O3P-P-O2P
71	B4	202	PEE	C1-O3P-P-O1P
71	B4	202	PEE	C4-O4P-P-O3P
71	B4	202	PEE	C4-O4P-P-O2P
71	B4	202	PEE	C4-O4P-P-O1P
71	C3	303	PEE	O4-C10-O2-C2
71	C3	303	PEE	C1-O3P-P-O2P
71	C3	303	PEE	C1-O3P-P-O1P
71	C3	303	PEE	C1-O3P-P-O4P
71	C3	303	PEE	O4P-C4-C5-N
71	N4	501	PEE	C1-O3P-P-O4P
71	N4	501	PEE	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
71	N5	704	PEE	C11-C10-O2-C2
71	N5	704	PEE	C1-O3P-P-O1P
71	N5	704	PEE	C4-O4P-P-O2P
71	N5	704	PEE	C37-C38-C39-C40
71	QB	503	PEE	C1-O3P-P-O2P
71	QB	503	PEE	C1-O3P-P-O1P
71	QB	503	PEE	C1-O3P-P-O4P
71	QB	503	PEE	C4-O4P-P-O3P
71	QB	503	PEE	C4-O4P-P-O2P
71	QB	503	PEE	C4-O4P-P-O1P
71	QC	403	PEE	O2-C2-C3-O3
71	QC	403	PEE	C1-O3P-P-O1P
71	QC	403	PEE	C1-O3P-P-O4P
71	QC	403	PEE	C4-O4P-P-O1P
71	QC	403	PEE	O4P-C4-C5-N
71	Qc	401	PEE	C4-O4P-P-O3P
71	Qc	401	PEE	C4-O4P-P-O2P
71	Qc	401	PEE	C4-O4P-P-O1P
71	Qc	401	PEE	O4P-C4-C5-N
71	Qc	402	PEE	C1-O3P-P-O2P
71	Qc	402	PEE	C1-O3P-P-O1P
71	Qc	402	PEE	C1-O3P-P-O4P
71	Qc	402	PEE	C4-O4P-P-O1P
71	S2	501	PEE	C11-C10-O2-C2
71	S2	501	PEE	O4-C10-O2-C2
71	S2	501	PEE	C4-O4P-P-O2P
71	S2	501	PEE	C4-O4P-P-O1P
71	S2	501	PEE	O4P-C4-C5-N
71	S8	303	PEE	C11-C10-O2-C2
71	S8	303	PEE	O4-C10-O2-C2
71	S8	303	PEE	C37-C38-C39-C40
72	A9	401	NDP	C5D-O5D-PN-O1N
73	AB	201	ZMP	C17-C18-C21-O5
73	AB	201	ZMP	C16-C17-C18-C21
73	AB	201	ZMP	C16-C17-C18-C19
73	AB	201	ZMP	O4-C17-C18-C20
73	AB	201	ZMP	C16-C17-C18-C20
73	AB	201	ZMP	N2-C16-C17-O4
73	AB	201	ZMP	C13-C14-C15-N2
73	AB	201	ZMP	C7-C8-C9-C10
73	AC	201	ZMP	S1-C11-C12-N1
73	AC	201	ZMP	O1-C10-S1-C11

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Mol	Chain	Res	Type	Atoms
73	AC	201	ZMP	C9-C10-S1-C11
73	AC	201	ZMP	C7-C8-C9-C10
75	AM	201	PLX	O7-C6-C7-C8
75	AM	201	PLX	O7-C6-O6-C4
75	AM	201	PLX	C2-O1-P1-O2
75	AM	201	PLX	C2-O1-P1-O3
75	AM	201	PLX	C1-C2-O1-P1
75	AM	202	PLX	O9-C24-O8-C5
75	B5	201	PLX	O7-C6-O6-C4
75	B5	201	PLX	C3-O4-P1-O2
75	B5	201	PLX	C2-O1-P1-O4
75	B5	201	PLX	C2-O1-P1-O3
75	B5	201	PLX	C25-C24-O8-C5
75	B5	201	PLX	O9-C24-C25-C26
75	C2	301	PLX	C3-O4-P1-O2
75	C2	301	PLX	C3-O4-P1-O3
75	C2	301	PLX	O9-C24-O8-C5
75	C2	301	PLX	O9-C24-C25-C26
75	CB	201	PLX	O7-C6-C7-C8
75	CB	201	PLX	O7-C6-O6-C4
75	CB	201	PLX	C2-O1-P1-O2
75	CB	201	PLX	C2-O1-P1-O3
75	CB	201	PLX	O9-C24-O8-C5
75	N3	201	PLX	O7-C6-C7-C8
75	N3	201	PLX	C7-C6-O6-C4
75	N3	201	PLX	N1-C1-C2-O1
75	N3	201	PLX	O9-C24-O8-C5
75	N3	201	PLX	O9-C24-C25-C26
75	N4	502	PLX	O7-C6-C7-C8
75	N4	502	PLX	C7-C6-O6-C4
75	N4	502	PLX	O7-C6-O6-C4
75	N4	502	PLX	O4-C3-C4-O6
75	N4	502	PLX	C3-O4-P1-O2
75	N4	502	PLX	C3-O4-P1-O3
75	N4	502	PLX	C2-O1-P1-O2
75	N4	502	PLX	C2-O1-P1-O3
75	N4	502	PLX	N1-C1-C2-O1
75	N4	502	PLX	O9-C24-O8-C5
75	N4	503	PLX	O7-C6-O6-C4
75	N4	503	PLX	C2-O1-P1-O4
75	QB	504	PLX	O7-C6-C7-C8
75	QB	504	PLX	O7-C6-O6-C4

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Mol	Chain	Res	Type	Atoms
75	QB	504	PLX	O4-C3-C4-O6
75	QB	504	PLX	C2-O1-P1-O2
75	QB	504	PLX	C2-O1-P1-O3
75	QI	301	PLX	O7-C6-O6-C4
75	QI	301	PLX	C5-C4-O6-C6
75	QI	301	PLX	C3-O4-P1-O3
75	QI	301	PLX	C2-O1-P1-O2
75	QI	301	PLX	O9-C24-C25-C26
76	B4	201	3PE	O13-C11-C12-N
76	B4	201	3PE	O21-C2-C3-O31
76	B8	201	3PE	C11-O13-P-O11
76	B8	201	3PE	C11-O13-P-O14
76	B8	201	3PE	O13-C11-C12-N
76	C1	601	3PE	C1-O11-P-O12
76	C1	601	3PE	C1-O11-P-O14
76	C1	601	3PE	C11-O13-P-O12
76	C1	601	3PE	C11-O13-P-O14
76	C2	302	3PE	C1-O11-P-O14
76	C2	302	3PE	C11-O13-P-O14
76	C2	302	3PE	O13-C11-C12-N
76	CA	101	3PE	C1-O11-P-O12
76	CA	101	3PE	C1-O11-P-O14
76	CA	101	3PE	C11-O13-P-O11
76	CA	101	3PE	C11-O13-P-O12
76	CA	101	3PE	C11-O13-P-O14
76	QE	302	3PE	O13-C11-C12-N
77	C1	602	HEA	C1A-C2A-CAA-CBA
77	C1	602	HEA	C3A-C2A-CAA-CBA
77	C1	602	HEA	C17-C18-C19-C27
77	C1	602	HEA	C18-C19-C20-C21
77	C1	602	HEA	C27-C19-C20-C21
77	C1	603	HEA	C2D-C3D-CAD-CBD
77	C1	603	HEA	C4D-C3D-CAD-CBD
77	C1	603	HEA	C17-C18-C19-C20
77	C1	603	HEA	C17-C18-C19-C27
77	C1	603	HEA	C18-C19-C20-C21
77	C1	603	HEA	C19-C20-C21-C22
80	QC	401	HEM	C2B-C3B-CAB-CBB
80	QC	402	HEM	C2B-C3B-CAB-CBB
80	QC	402	HEM	C4B-C3B-CAB-CBB
80	Qc	403	HEM	C2B-C3B-CAB-CBB
80	Qc	403	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
80	Qc	404	HEM	C1A-C2A-CAA-CBA
80	Qc	404	HEM	C3A-C2A-CAA-CBA
80	Qc	404	HEM	C2B-C3B-CAB-CBB
80	Qc	404	HEM	C4B-C3B-CAB-CBB
84	V1	502	FMN	C5'-O5'-P-O1P
84	V1	502	FMN	C5'-O5'-P-O2P
84	V1	502	FMN	C5'-O5'-P-O3P
71	N4	501	PEE	O5-C30-O3-C3
71	N5	704	PEE	O5-C30-O3-C3
71	QB	502	PEE	O5-C30-O3-C3
71	QB	502	PEE	C31-C30-O3-C3
71	6A	103	PEE	O5-C30-O3-C3
71	8B	201	PEE	O5-C30-O3-C3
71	AL	203	PEE	O5-C30-O3-C3
71	8B	201	PEE	O4-C10-O2-C2
71	N5	704	PEE	O4-C10-O2-C2
71	A3	201	PEE	C31-C30-O3-C3
71	AL	203	PEE	C31-C30-O3-C3
71	N4	501	PEE	C31-C30-O3-C3
71	N5	704	PEE	C31-C30-O3-C3
71	C3	303	PEE	C11-C10-O2-C2
71	6A	103	PEE	C31-C30-O3-C3
71	8B	201	PEE	C31-C30-O3-C3
71	C3	303	PEE	C31-C30-O3-C3
71	A3	201	PEE	C17-C18-C19-C20
71	N5	701	PEE	C37-C38-C39-C40
71	S8	303	PEE	C17-C18-C19-C20
71	6A	103	PEE	O4-C10-O2-C2
77	C1	602	HEA	C17-C18-C19-C20
71	A3	201	PEE	O5-C30-O3-C3
68	B5	202	CDL	O1-C1-CA2-OA2
68	QC	404	CDL	O1-C1-CA2-OA2
68	QE	304	CDL	O1-C1-CA2-OA2
71	QB	502	PEE	C11-C10-O2-C2
71	C3	303	PEE	O5-C30-O3-C3
70	C3	302	PC1	C2-C1-O11-P
77	C1	602	HEA	C19-C20-C21-C22
68	N5	702	CDL	C51-C52-C53-C54
68	B5	202	CDL	CB2-C1-CA2-OA2
70	N1	401	PC1	C24-C25-C26-C27
70	C1	606	PC1	C11-C12-N-C14
70	Qc	406	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
73	AC	201	ZMP	C14-C15-N2-C16
71	Qc	402	PEE	C31-C30-O3-C3
73	AB	201	ZMP	C1-C22-C23-C24
70	B5	203	PC1	C21-C22-C23-C24
71	6A	102	PEE	C10-C11-C12-C13
68	N5	702	CDL	OA6-CA4-CA6-OA8
68	B5	202	CDL	C55-C56-C57-C58
68	QD	402	CDL	CB7-C71-C72-C73
68	QE	304	CDL	CA7-C31-C32-C33
71	AL	203	PEE	C10-C11-C12-C13
71	QE	301	PEE	C10-C11-C12-C13
71	Qc	402	PEE	O5-C30-O3-C3
75	N4	502	PLX	C30-C31-C32-C33
71	Qd	403	PEE	C10-C11-C12-C13
71	6A	102	PEE	C37-C38-C39-C40
71	B4	202	PEE	C17-C18-C19-C20
68	4L	201	CDL	CB5-C51-C52-C53
68	A1	101	CDL	CA5-C11-C12-C13
70	QJ	101	PC1	C21-C22-C23-C24
70	Qb	502	PC1	C31-C32-C33-C34
71	8B	201	PEE	C30-C31-C32-C33
71	C3	303	PEE	C10-C11-C12-C13
71	QB	503	PEE	C30-C31-C32-C33
71	S2	501	PEE	C10-C11-C12-C13
71	QB	502	PEE	O4-C10-O2-C2
70	N1	401	PC1	C11-C12-N-C14
70	N3	202	PC1	C11-C12-N-C15
70	Qc	406	PC1	C11-C12-N-C13
75	N4	502	PLX	C2-C1-N1-C1A
71	B4	202	PEE	C30-C31-C32-C33
71	N5	701	PEE	C31-C32-C33-C34
71	QE	301	PEE	C33-C34-C35-C36
68	QH	102	CDL	O1-C1-CA2-OA2
71	Qc	401	PEE	C35-C36-C37-C38
71	N5	704	PEE	C17-C18-C19-C20
68	4L	201	CDL	CA2-OA2-PA1-OA5
68	A1	101	CDL	CA2-OA2-PA1-OA5
68	A1	101	CDL	CB2-OB2-PB2-OB5
68	A8	301	CDL	CB2-OB2-PB2-OB5
68	A8	301	CDL	CB3-OB5-PB2-OB2
68	AL	202	CDL	CA3-OA5-PA1-OA2
68	B4	203	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
68	B4	203	CDL	CB3-OB5-PB2-OB2
68	B5	202	CDL	CB3-OB5-PB2-OB2
68	N2	401	CDL	CA2-OA2-PA1-OA5
68	N2	401	CDL	CB2-OB2-PB2-OB5
68	N2	401	CDL	CB3-OB5-PB2-OB2
68	N5	702	CDL	CA2-OA2-PA1-OA5
68	N5	702	CDL	CA3-OA5-PA1-OA2
68	N5	703	CDL	CA2-OA2-PA1-OA5
68	QB	501	CDL	CA2-OA2-PA1-OA5
68	QB	501	CDL	CA3-OA5-PA1-OA2
68	QB	501	CDL	CB3-OB5-PB2-OB2
68	QD	402	CDL	CB2-OB2-PB2-OB5
68	QD	402	CDL	CB3-OB5-PB2-OB2
68	QE	304	CDL	CA2-OA2-PA1-OA5
68	QE	304	CDL	CB2-OB2-PB2-OB5
68	QE	304	CDL	CB3-OB5-PB2-OB2
68	QH	101	CDL	CA2-OA2-PA1-OA5
68	QH	101	CDL	CB2-OB2-PB2-OB5
68	QH	102	CDL	CB2-OB2-PB2-OB5
70	B7	201	PC1	C11-O13-P-O11
70	C1	606	PC1	C11-O13-P-O11
70	C1	608	PC1	C11-O13-P-O11
70	C1	611	PC1	C11-O13-P-O11
70	C3	301	PC1	C11-O13-P-O11
70	C3	301	PC1	C1-O11-P-O13
70	C3	302	PC1	C1-O11-P-O13
70	N1	401	PC1	C1-O11-P-O13
70	N1	402	PC1	C11-O13-P-O11
70	N1	402	PC1	C1-O11-P-O13
70	N3	202	PC1	C11-O13-P-O11
70	N5	705	PC1	C11-O13-P-O11
71	6A	102	PEE	C4-O4P-P-O3P
71	6A	103	PEE	C4-O4P-P-O3P
71	8B	201	PEE	C1-O3P-P-O4P
71	B4	202	PEE	C1-O3P-P-O4P
71	N5	701	PEE	C1-O3P-P-O4P
71	N5	701	PEE	C4-O4P-P-O3P
71	N5	704	PEE	C4-O4P-P-O3P
71	QB	502	PEE	C1-O3P-P-O4P
71	QC	403	PEE	C4-O4P-P-O3P
71	QE	301	PEE	C1-O3P-P-O4P
71	Qc	401	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
71	Qc	402	PEE	C4-O4P-P-O3P
71	S2	501	PEE	C4-O4P-P-O3P
71	S8	303	PEE	C4-O4P-P-O3P
75	AM	201	PLX	C2-O1-P1-O4
75	C2	301	PLX	C3-O4-P1-O1
75	CB	201	PLX	C2-O1-P1-O4
75	N3	201	PLX	C3-O4-P1-O1
75	N4	502	PLX	C3-O4-P1-O1
75	N4	502	PLX	C2-O1-P1-O4
75	QB	504	PLX	C2-O1-P1-O4
75	QI	301	PLX	C3-O4-P1-O1
76	C1	601	3PE	C1-O11-P-O13
76	C1	601	3PE	C11-O13-P-O11
76	C2	302	3PE	C11-O13-P-O11
76	CA	101	3PE	C1-O11-P-O13
71	B4	202	PEE	C10-C11-C12-C13
71	S2	501	PEE	C31-C30-O3-C3
68	QH	101	CDL	CA5-C11-C12-C13
68	QH	102	CDL	CB2-C1-CA2-OA2
70	C1	606	PC1	C34-C35-C36-C37
70	B5	203	PC1	C11-C12-N-C13
70	B5	203	PC1	C11-C12-N-C14
70	B5	203	PC1	C11-C12-N-C15
70	C1	606	PC1	C11-C12-N-C13
70	C1	606	PC1	C11-C12-N-C15
70	N1	402	PC1	C11-C12-N-C13
70	N1	402	PC1	C11-C12-N-C14
70	N1	402	PC1	C11-C12-N-C15
70	Qh	101	PC1	C11-C12-N-C13
70	Qh	101	PC1	C11-C12-N-C15
71	6A	102	PEE	C31-C30-O3-C3
71	AL	203	PEE	C33-C34-C35-C36
75	C2	301	PLX	O8-C24-C25-C26
75	QI	301	PLX	O8-C24-C25-C26
71	N5	704	PEE	C35-C36-C37-C38
70	C3	301	PC1	C2B-C2C-C2D-C2E
70	Qh	101	PC1	C36-C37-C38-C39
71	AL	203	PEE	C11-C10-O2-C2
70	C1	609	PC1	C26-C27-C28-C29
71	6A	102	PEE	C23-C24-C25-C26
71	8B	201	PEE	C33-C34-C35-C36
71	QB	502	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
71	Qc	401	PEE	C33-C34-C35-C36
75	AM	201	PLX	C15-C16-C17-C18
75	AM	202	PLX	C29-C30-C31-C32
75	N4	503	PLX	C32-C33-C34-C35
76	QE	302	3PE	C34-C35-C36-C37
71	6A	102	PEE	C12-C13-C14-C15
71	8B	201	PEE	C32-C33-C34-C35
71	C3	303	PEE	C21-C22-C23-C24
71	C3	303	PEE	C34-C35-C36-C37
71	QC	403	PEE	C21-C22-C23-C24
75	AM	202	PLX	C25-C26-C27-C28
71	AL	203	PEE	O4-C10-O2-C2
71	QB	502	PEE	C10-C11-C12-C13
71	QB	502	PEE	C30-C31-C32-C33
68	A8	301	CDL	C54-C55-C56-C57
68	B4	203	CDL	C37-C38-C39-C40
71	QC	403	PEE	C14-C15-C16-C17
76	CA	101	3PE	C24-C25-C26-C27
71	A3	201	PEE	C37-C38-C39-C40
71	C3	303	PEE	C17-C18-C19-C20
71	QE	301	PEE	C37-C38-C39-C40
71	Qc	401	PEE	C17-C18-C19-C20
68	4L	201	CDL	C78-C79-C80-C81
68	C1	610	CDL	C77-C78-C79-C80
70	C1	609	PC1	C36-C37-C38-C39
70	Qc	406	PC1	C33-C34-C35-C36
71	C3	303	PEE	C33-C34-C35-C36
68	A1	101	CDL	O1-C1-CA2-OA2
70	C3	302	PC1	C23-C24-C25-C26
70	QJ	101	PC1	C38-C39-C3A-C3B
71	S8	303	PEE	C10-C11-C12-C13
68	AL	202	CDL	C36-C37-C38-C39
70	Qh	101	PC1	C2D-C2E-C2F-C2G
71	B4	202	PEE	C12-C13-C14-C15
71	QC	403	PEE	C12-C13-C14-C15
73	AC	201	ZMP	C1-C2-C3-C4
75	AM	201	PLX	C29-C30-C31-C32
71	6A	102	PEE	O5-C30-O3-C3
71	S2	501	PEE	O5-C30-O3-C3
71	6A	103	PEE	C11-C12-C13-C14
71	A3	201	PEE	C33-C34-C35-C36
71	N5	701	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
71	N5	704	PEE	C22-C23-C24-C25
75	AM	201	PLX	C31-C32-C33-C34
75	N3	201	PLX	C33-C34-C35-C36
68	QC	404	CDL	C72-C73-C74-C75
68	QD	402	CDL	C51-C52-C53-C54
70	C3	302	PC1	C36-C37-C38-C39
70	Qc	405	PC1	C2C-C2D-C2E-C2F
70	Qd	402	PC1	C3E-C3F-C3G-C3H
71	N5	704	PEE	C12-C13-C14-C15
73	AB	201	ZMP	C2-C3-C4-C5
75	N4	502	PLX	C13-C14-C15-C16
76	C1	601	3PE	C29-C2A-C2B-C2C
71	6A	103	PEE	C14-C15-C16-C17
71	B4	202	PEE	C11-C12-C13-C14
71	N4	501	PEE	C14-C15-C16-C17
71	N5	701	PEE	C12-C13-C14-C15
71	N5	704	PEE	C42-C43-C44-C45
71	QB	503	PEE	C22-C23-C24-C25
71	QB	503	PEE	C41-C42-C43-C44
75	CB	201	PLX	C9-C10-C11-C12
75	N4	503	PLX	C17-C18-C19-C20
68	A1	101	CDL	C20-C21-C22-C23
68	A8	301	CDL	C38-C39-C40-C41
71	N5	701	PEE	C21-C22-C23-C24
71	B4	202	PEE	C35-C36-C37-C38
71	Qc	401	PEE	C19-C20-C21-C22
68	A1	101	CDL	CB5-C51-C52-C53
71	A3	201	PEE	C10-C11-C12-C13
71	QB	503	PEE	C10-C11-C12-C13
68	A1	101	CDL	C14-C15-C16-C17
68	A8	301	CDL	C33-C34-C35-C36
68	QH	102	CDL	C51-C52-C53-C54
70	Qh	101	PC1	C2B-C2C-C2D-C2E
71	QB	503	PEE	C11-C12-C13-C14
71	Qc	401	PEE	C34-C35-C36-C37
71	Qd	403	PEE	C11-C12-C13-C14
73	AC	201	ZMP	C2-C3-C4-C5
75	N4	503	PLX	C31-C32-C33-C34
75	QB	504	PLX	C15-C16-C17-C18
75	QB	504	PLX	C11-C10-C9-C8
76	CA	101	3PE	C29-C2A-C2B-C2C
70	Qh	101	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
77	C1	602	HEA	C15-C16-C17-C18
68	N5	703	CDL	C61-C62-C63-C64
71	QE	301	PEE	C32-C33-C34-C35
75	N4	503	PLX	C10-C11-C12-C13
75	QI	301	PLX	C30-C31-C32-C33
76	B4	201	3PE	C3E-C3F-C3G-C3H
71	B4	202	PEE	O4P-C4-C5-N
71	N4	501	PEE	O4P-C4-C5-N
76	CA	101	3PE	O13-C11-C12-N
70	C1	611	PC1	C22-C23-C24-C25
71	8B	201	PEE	C43-C44-C45-C46
71	A3	201	PEE	C21-C22-C23-C24
71	N5	701	PEE	C23-C24-C25-C26
71	QB	503	PEE	C33-C34-C35-C36
68	C1	610	CDL	CA7-C31-C32-C33
70	C3	301	PC1	C21-C22-C23-C24
71	Qc	401	PEE	C30-C31-C32-C33
71	Qc	402	PEE	C30-C31-C32-C33
71	QC	403	PEE	C31-C30-O3-C3
70	N3	202	PC1	C2D-C2E-C2F-C2G
71	AL	203	PEE	C11-C12-C13-C14
75	QI	301	PLX	C15-C16-C17-C18
70	N1	401	PC1	C33-C34-C35-C36
70	Qc	406	PC1	C23-C24-C25-C26
71	N4	501	PEE	C13-C14-C15-C16
71	Qc	401	PEE	C41-C42-C43-C44
68	N5	703	CDL	C35-C36-C37-C38
68	QH	101	CDL	C32-C33-C34-C35
75	QB	504	PLX	C16-C17-C18-C19
68	B4	203	CDL	CA3-CA4-CA6-OA8
71	AL	203	PEE	C17-C18-C19-C20
68	N5	703	CDL	C16-C17-C18-C19
71	A3	201	PEE	C22-C23-C24-C25
71	C3	303	PEE	C12-C13-C14-C15
70	C3	301	PC1	C25-C26-C27-C28
75	N4	503	PLX	C30-C31-C32-C33
75	QI	301	PLX	C12-C13-C14-C15
76	B4	201	3PE	C3C-C3D-C3E-C3F
75	AM	201	PLX	O9-C24-C25-C26
75	AM	202	PLX	O7-C6-C7-C8
71	N4	501	PEE	C12-C13-C14-C15
75	AM	201	PLX	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
75	N4	502	PLX	C25-C26-C27-C28
71	A3	201	PEE	C35-C36-C37-C38
71	C3	303	PEE	C19-C20-C21-C22
71	N5	704	PEE	C19-C20-C21-C22
71	QC	403	PEE	C10-C11-C12-C13
68	N5	702	CDL	O1-C1-CB2-OB2
68	QE	304	CDL	C75-C76-C77-C78
71	B4	202	PEE	C21-C22-C23-C24
68	A1	101	CDL	CB2-C1-CA2-OA2
75	B5	201	PLX	C13-C14-C15-C16
70	C1	608	PC1	C23-C24-C25-C26
68	Qb	501	CDL	C54-C55-C56-C57
71	6A	102	PEE	C33-C34-C35-C36
75	AM	201	PLX	C28-C29-C30-C31
75	C2	301	PLX	C18-C19-C20-C21
76	C2	302	3PE	C3C-C3D-C3E-C3F
70	N1	401	PC1	C11-C12-N-C15
70	Qc	406	PC1	C11-C12-N-C15
70	Qd	402	PC1	C21-C22-C23-C24
71	N5	701	PEE	C13-C14-C15-C16
71	S2	501	PEE	C42-C43-C44-C45
80	QC	401	HEM	C3D-CAD-CBD-CGD
68	A1	101	CDL	C51-C52-C53-C54
76	B4	201	3PE	C21-C22-C23-C24
68	B5	202	CDL	C33-C34-C35-C36
71	B4	202	PEE	C22-C23-C24-C25
71	AL	203	PEE	C18-C19-C20-C21
73	AC	201	ZMP	C22-C23-C24-C25
75	QI	301	PLX	C16-C17-C18-C19
71	QC	403	PEE	O5-C30-O3-C3
71	A3	201	PEE	C19-C20-C21-C22
71	QE	301	PEE	C35-C36-C37-C38
71	N5	701	PEE	O4-C10-O2-C2
71	Qd	403	PEE	O4-C10-O2-C2
70	N1	402	PC1	C21-C22-C23-C24
71	AL	203	PEE	C30-C31-C32-C33
71	Qc	401	PEE	C42-C43-C44-C45
68	A1	101	CDL	C74-C75-C76-C77
68	C1	610	CDL	C73-C74-C75-C76
71	B4	202	PEE	C40-C41-C42-C43
71	N5	704	PEE	C33-C34-C35-C36
71	QB	503	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
71	Qc	401	PEE	C13-C14-C15-C16
75	QI	301	PLX	C29-C30-C31-C32
70	QJ	101	PC1	C27-C28-C29-C2A
71	QB	503	PEE	C43-C44-C45-C46
75	QB	504	PLX	C12-C13-C14-C15
75	QI	301	PLX	C9-C10-C11-C12
76	C1	601	3PE	C23-C24-C25-C26
70	B5	203	PC1	C24-C25-C26-C27
68	4L	201	CDL	C38-C39-C40-C41
75	QB	504	PLX	C7-C8-C9-C10
71	N5	701	PEE	C11-C10-O2-C2
71	Qd	403	PEE	C11-C10-O2-C2
75	AM	202	PLX	O4-C3-C4-O6
70	B7	201	PC1	C39-C3A-C3B-C3C
71	S2	501	PEE	C14-C15-C16-C17
71	S2	501	PEE	C31-C32-C33-C34
75	CB	201	PLX	C16-C17-C18-C19
80	QC	401	HEM	C4B-C3B-CAB-CBB
75	AM	202	PLX	C15-C16-C17-C18
68	N5	702	CDL	OB6-CB4-CB6-OB8
71	8B	201	PEE	O2-C2-C3-O3
71	Qc	402	PEE	C22-C23-C24-C25
76	CA	101	3PE	C36-C37-C38-C39
70	N1	401	PC1	C11-C12-N-C13
70	N3	202	PC1	C11-C12-N-C13
70	N3	202	PC1	C11-C12-N-C14
70	Qb	502	PC1	C11-C12-N-C13
75	N4	502	PLX	C2-C1-N1-C1C
75	N4	502	PLX	C2-C1-N1-C1B
76	CA	101	3PE	C2C-C2D-C2E-C2F
71	6A	102	PEE	C35-C36-C37-C38
71	N4	501	PEE	C19-C20-C21-C22
71	N5	704	PEE	C39-C40-C41-C42
71	QE	301	PEE	C39-C40-C41-C42
75	QB	504	PLX	C28-C29-C30-C31
70	C1	608	PC1	C34-C35-C36-C37
71	6A	102	PEE	C34-C35-C36-C37
75	AM	202	PLX	C16-C17-C18-C19
76	C2	302	3PE	C28-C29-C2A-C2B
70	B5	203	PC1	C39-C3A-C3B-C3C
70	N1	402	PC1	C22-C23-C24-C25
75	AM	201	PLX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
71	6A	103	PEE	C18-C19-C20-C21
71	QE	301	PEE	C16-C17-C18-C19
71	N5	704	PEE	C2-C3-O3-C30
68	A1	101	CDL	CA3-OA5-PA1-OA2
68	AL	201	CDL	CB2-OB2-PB2-OB5
68	AL	202	CDL	CB3-OB5-PB2-OB2
68	N5	703	CDL	CB2-OB2-PB2-OB5
68	N5	703	CDL	CB3-OB5-PB2-OB2
68	QD	402	CDL	CA3-OA5-PA1-OA2
70	B5	203	PC1	C11-O13-P-O11
70	C1	607	PC1	C11-O13-P-O11
71	N5	704	PEE	C1-O3P-P-O4P
68	QC	404	CDL	CA7-C31-C32-C33
70	C1	609	PC1	C31-C32-C33-C34
76	C2	302	3PE	C21-C22-C23-C24
70	B5	203	PC1	C28-C29-C2A-C2B
68	N2	401	CDL	OA5-CA3-CA4-CA6
68	N5	703	CDL	OA5-CA3-CA4-CA6
68	QB	501	CDL	OB5-CB3-CB4-CB6
68	QD	402	CDL	OA5-CA3-CA4-CA6
68	QE	304	CDL	OB5-CB3-CB4-CB6
71	B4	202	PEE	O3P-C1-C2-C3
71	QB	503	PEE	O3P-C1-C2-C3
71	QC	403	PEE	O3P-C1-C2-C3
75	N4	502	PLX	O4-C3-C4-C5
75	QB	504	PLX	O4-C3-C4-C5
70	QJ	101	PC1	C34-C35-C36-C37
75	N4	502	PLX	C27-C28-C29-C30
70	C1	607	PC1	C31-C32-C33-C34
71	Qc	402	PEE	C20-C21-C22-C23
71	C3	303	PEE	C39-C40-C41-C42
71	N4	501	PEE	C35-C36-C37-C38
75	AM	201	PLX	C13-C14-C15-C16
75	C2	301	PLX	C15-C16-C17-C18
75	N4	503	PLX	C11-C12-C13-C14
68	4L	201	CDL	C42-C43-C44-C45
71	S8	303	PEE	C32-C33-C34-C35
70	Qb	502	PC1	C29-C2A-C2B-C2C
71	N5	704	PEE	C40-C41-C42-C43
68	N2	402	CDL	CB3-CB4-CB6-OB8
68	N5	702	CDL	CB3-CB4-CB6-OB8
68	N5	703	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
68	QD	402	CDL	CA3-CA4-CA6-OA8
68	QH	101	CDL	CA3-CA4-CA6-OA8
70	6A	101	PC1	C1-C2-C3-O31
70	QJ	101	PC1	C1-C2-C3-O31
71	6A	103	PEE	C1-C2-C3-O3
71	A3	201	PEE	C1-C2-C3-O3
71	Qc	402	PEE	C1-C2-C3-O3
75	AM	202	PLX	C3-C4-C5-O8
75	N4	503	PLX	C3-C4-C5-O8
76	B4	201	3PE	C1-C2-C3-O31
75	N4	502	PLX	C4-C5-O8-C24
68	A1	101	CDL	C17-C18-C19-C20
73	AB	201	ZMP	C6-C7-C8-C9
73	AB	201	ZMP	C3-C4-C5-C6
75	C2	301	PLX	C17-C18-C19-C20
71	S2	501	PEE	C43-C44-C45-C46
75	N3	201	PLX	O6-C6-C7-C8
73	AB	201	ZMP	O3-C16-C17-O4
73	AC	201	ZMP	O3-C16-C17-O4
70	Qb	502	PC1	C2D-C2E-C2F-C2G
71	QC	403	PEE	C11-C12-C13-C14
71	Qc	401	PEE	C32-C33-C34-C35
71	Qc	401	PEE	C16-C17-C18-C19
71	Qc	402	PEE	C13-C14-C15-C16
71	S8	303	PEE	C22-C23-C24-C25
71	8B	201	PEE	C35-C36-C37-C38
71	QB	502	PEE	C35-C36-C37-C38
71	S8	303	PEE	C35-C36-C37-C38
71	S8	303	PEE	C39-C40-C41-C42
76	C2	302	3PE	C22-C23-C24-C25
71	QC	403	PEE	C11-C10-O2-C2
75	QI	301	PLX	C11-C10-C9-C8
68	Qb	501	CDL	C52-C53-C54-C55
75	AM	201	PLX	C7-C8-C9-C10
68	B5	202	CDL	CA5-C11-C12-C13
71	S2	501	PEE	C44-C45-C46-C47
75	CB	201	PLX	C34-C35-C36-C37
70	Qc	406	PC1	C2C-C2D-C2E-C2F
71	A3	201	PEE	C11-C12-C13-C14
71	C3	303	PEE	C3-C2-O2-C10
71	QB	502	PEE	C1-C2-O2-C10
71	N4	501	PEE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
71	Qc	401	PEE	C31-C32-C33-C34
71	S2	501	PEE	C11-C12-C13-C14
70	7C	101	PC1	C2A-C2B-C2C-C2D
70	Qd	402	PC1	C33-C34-C35-C36
71	S8	303	PEE	C13-C14-C15-C16
75	N4	503	PLX	C15-C16-C17-C18
71	Qc	402	PEE	C16-C17-C18-C19
71	S2	501	PEE	C38-C39-C40-C41
68	AL	201	CDL	C55-C56-C57-C58
71	6A	102	PEE	C11-C12-C13-C14
75	QI	301	PLX	C20-C21-C22-C23
68	4L	201	CDL	OB5-CB3-CB4-OB6
68	C1	610	CDL	OA5-CA3-CA4-OA6
68	QH	102	CDL	OB5-CB3-CB4-OB6
71	N4	501	PEE	O3P-C1-C2-O2
71	QB	502	PEE	O3P-C1-C2-O2
76	QE	302	3PE	O11-C1-C2-O21
71	8B	201	PEE	C37-C38-C39-C40
70	C3	302	PC1	C3D-C3E-C3F-C3G
68	AL	201	CDL	O1-C1-CA2-OA2
71	A3	201	PEE	C32-C33-C34-C35
71	C3	303	PEE	C30-C31-C32-C33
71	QB	502	PEE	C12-C13-C14-C15
71	S8	303	PEE	C31-C32-C33-C34
68	N2	402	CDL	C72-C71-CB7-OB8
68	N5	703	CDL	OB6-CB4-CB6-OB8
70	7C	101	PC1	O21-C2-C3-O31
71	6A	103	PEE	O2-C2-C3-O3
75	N4	502	PLX	C14-C15-C16-C17
73	AB	201	ZMP	O4-C17-C18-C19
76	C2	302	3PE	C29-C2A-C2B-C2C
68	A1	101	CDL	C73-C74-C75-C76
68	N5	703	CDL	C14-C15-C16-C17
68	QH	101	CDL	C33-C34-C35-C36
70	C3	301	PC1	C2A-C2B-C2C-C2D
70	B7	201	PC1	C38-C39-C3A-C3B
71	N5	701	PEE	C22-C23-C24-C25
75	CB	201	PLX	C32-C33-C34-C35
68	B5	202	CDL	C73-C74-C75-C76
71	QB	503	PEE	C21-C22-C23-C24
70	C1	606	PC1	C28-C29-C2A-C2B
71	N4	501	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
71	N4	501	PEE	C34-C35-C36-C37
71	QE	301	PEE	C31-C32-C33-C34
75	AM	201	PLX	C34-C35-C36-C37
71	Qc	401	PEE	C18-C19-C20-C21
71	Qc	401	PEE	C38-C39-C40-C41
70	Qb	502	PC1	C11-C12-N-C15
68	N5	702	CDL	OB5-CB3-CB4-CB6
75	AM	202	PLX	O4-C3-C4-C5
75	N4	502	PLX	C29-C30-C31-C32
76	C2	302	3PE	C26-C27-C28-C29
71	QB	503	PEE	O4P-C4-C5-N
71	S8	303	PEE	O4P-C4-C5-N
71	Qc	401	PEE	C21-C22-C23-C24
71	QB	502	PEE	C11-C12-C13-C14
71	6A	102	PEE	C43-C44-C45-C46
75	B5	201	PLX	C11-C10-C9-C8
68	A8	301	CDL	CA5-C11-C12-C13
70	6A	101	PC1	C33-C34-C35-C36
71	QB	503	PEE	C44-C45-C46-C47
75	N4	502	PLX	C31-C32-C33-C34
68	N2	401	CDL	C1-CA2-OA2-PA1
68	N2	401	CDL	CA4-CA3-OA5-PA1
70	7C	101	PC1	C2-C1-O11-P
75	AM	201	PLX	C4-C3-O4-P1
80	Qc	404	HEM	C2A-CAA-CBA-CGA
75	QI	301	PLX	C31-C32-C33-C34
75	N4	502	PLX	C15-C16-C17-C18
71	N5	704	PEE	C41-C42-C43-C44
71	Qc	402	PEE	C33-C34-C35-C36
80	Qc	403	HEM	C3D-CAD-CBD-CGD
68	QD	402	CDL	C33-C34-C35-C36
75	N4	503	PLX	C18-C19-C20-C21
68	A8	301	CDL	CB3-CB4-CB6-OB8
68	N5	702	CDL	CA3-CA4-CA6-OA8
70	C1	606	PC1	C1-C2-C3-O31
71	8B	201	PEE	C1-C2-C3-O3
71	QB	502	PEE	C1-C2-C3-O3
71	QE	301	PEE	C1-C2-C3-O3
71	Qd	403	PEE	C1-C2-C3-O3
75	B5	201	PLX	C3-C4-C5-O8
75	N4	502	PLX	C3-C4-C5-O8
68	A8	301	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
70	C3	302	PC1	C26-C27-C28-C29
71	QE	301	PEE	C40-C41-C42-C43
75	B5	201	PLX	C26-C27-C28-C29
71	S8	303	PEE	C44-C45-C46-C47
75	CB	201	PLX	C36-C37-C38-C39
68	4L	201	CDL	C14-C15-C16-C17
68	C1	610	CDL	C52-C53-C54-C55
71	6A	103	PEE	C22-C23-C24-C25
71	QE	301	PEE	C34-C35-C36-C37
68	4L	201	CDL	CA3-OA5-PA1-OA2
68	AL	201	CDL	CA2-OA2-PA1-OA5
68	N5	702	CDL	CB3-OB5-PB2-OB2
75	B5	201	PLX	C5-C4-O6-C6
75	C2	301	PLX	C3-C4-O6-C6
75	CB	201	PLX	C5-C4-O6-C6
75	CB	201	PLX	C3-O4-P1-O1
75	QI	301	PLX	C2-O1-P1-O4
75	CB	201	PLX	O9-C24-C25-C26
75	N4	503	PLX	O7-C6-C7-C8
75	QB	504	PLX	O9-C24-C25-C26
68	A1	101	CDL	C58-C59-C60-C61
70	N3	202	PC1	C25-C26-C27-C28
68	B5	202	CDL	OB5-CB3-CB4-OB6
68	C1	610	CDL	OB5-CB3-CB4-OB6
68	N2	401	CDL	OA5-CA3-CA4-OA6
68	N5	702	CDL	OB5-CB3-CB4-OB6
68	QD	402	CDL	OA5-CA3-CA4-OA6
70	C1	611	PC1	O11-C1-C2-O21
70	N1	402	PC1	O11-C1-C2-O21
70	Qc	405	PC1	O11-C1-C2-O21
71	QB	503	PEE	O3P-C1-C2-O2
71	S8	303	PEE	O3P-C1-C2-O2
70	7C	101	PC1	C29-C2A-C2B-C2C
71	N4	501	PEE	C11-C12-C13-C14
71	QE	301	PEE	C14-C15-C16-C17
71	8B	201	PEE	C10-C11-C12-C13
75	N3	201	PLX	C16-C17-C18-C19
71	8B	201	PEE	C44-C45-C46-C47
75	N3	201	PLX	C14-C15-C16-C17
71	AL	203	PEE	O2-C2-C3-O3
71	Qc	401	PEE	O2-C2-C3-O3
75	AM	202	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
75	C2	301	PLX	O6-C4-C5-O8
75	CB	201	PLX	O6-C4-C5-O8
70	B7	201	PC1	C2E-C2F-C2G-C2H
75	AM	202	PLX	C28-C29-C30-C31
75	CB	201	PLX	C33-C34-C35-C36
71	QC	403	PEE	O4-C10-O2-C2
71	Qc	401	PEE	O4-C10-O2-C2
70	C3	301	PC1	C31-C32-C33-C34
70	QJ	101	PC1	C2B-C2C-C2D-C2E
68	N5	703	CDL	CA4-CA3-OA5-PA1
68	QE	304	CDL	C1-CB2-OB2-PB2
76	CA	101	3PE	C2-C1-O11-P
76	QE	302	3PE	C33-C34-C35-C36
70	C1	607	PC1	C11-C12-N-C15
68	QC	404	CDL	C33-C34-C35-C36
71	A3	201	PEE	C23-C24-C25-C26
76	B4	201	3PE	C3B-C3C-C3D-C3E
70	B5	203	PC1	C36-C37-C38-C39
75	CB	201	PLX	C25-C26-C27-C28
76	C2	302	3PE	C31-C32-C33-C34
71	Qc	401	PEE	C11-C10-O2-C2
68	N2	401	CDL	C72-C73-C74-C75
68	N2	402	CDL	C40-C41-C42-C43
71	QB	503	PEE	C12-C13-C14-C15
71	6A	102	PEE	C24-C25-C26-C27
75	B5	201	PLX	C20-C21-C22-C23
75	AM	201	PLX	O6-C6-C7-C8
75	B5	201	PLX	O8-C24-C25-C26
68	B5	202	CDL	OB5-CB3-CB4-CB6
68	C1	610	CDL	OA5-CA3-CA4-CA6
68	N2	401	CDL	OB5-CB3-CB4-CB6
68	QH	102	CDL	OB5-CB3-CB4-CB6
68	Qb	501	CDL	OB5-CB3-CB4-CB6
70	C1	611	PC1	O11-C1-C2-C3
70	Qc	405	PC1	O11-C1-C2-C3
70	Qh	101	PC1	O11-C1-C2-C3
71	QB	502	PEE	O3P-C1-C2-C3
76	QE	302	3PE	O11-C1-C2-C3
71	N5	701	PEE	C34-C35-C36-C37
71	B4	202	PEE	C18-C19-C20-C21
68	AL	202	CDL	C43-C44-C45-C46
71	QC	403	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
71	A3	201	PEE	C40-C41-C42-C43
75	QI	301	PLX	C19-C20-C21-C22
68	QH	101	CDL	C31-C32-C33-C34
74	AK	401	ADP	O4'-C4'-C5'-O5'
68	AL	202	CDL	C72-C73-C74-C75
73	AC	201	ZMP	N2-C16-C17-O4
68	N5	702	CDL	CB5-C51-C52-C53
71	QB	502	PEE	C34-C35-C36-C37
73	AC	201	ZMP	C3-C4-C5-C6
68	QH	101	CDL	C72-C71-CB7-OB8
70	C1	606	PC1	C32-C33-C34-C35
70	N1	402	PC1	C3A-C3B-C3C-C3D
71	N4	501	PEE	C42-C43-C44-C45
71	QC	403	PEE	C16-C17-C18-C19
68	QB	501	CDL	CA6-CA4-OA6-CA5
71	Qc	401	PEE	C3-C2-O2-C10
68	A1	101	CDL	C56-C57-C58-C59
71	8B	201	PEE	C12-C13-C14-C15
70	C1	606	PC1	C2B-C2C-C2D-C2E
68	AL	201	CDL	C1-CA2-OA2-PA1
68	C1	610	CDL	CA4-CA3-OA5-PA1
70	7C	101	PC1	C1-C2-C3-O31
70	C1	607	PC1	C2-C1-O11-P
70	C1	611	PC1	C2-C1-O11-P
70	Qc	406	PC1	C2-C1-O11-P
71	8B	201	PEE	C2-C1-O3P-P
71	AL	203	PEE	C1-C2-C3-O3
71	N4	501	PEE	C1-C2-C3-O3
71	Qc	401	PEE	C1-C2-C3-O3
71	S8	303	PEE	C1-C2-C3-O3
75	N4	502	PLX	C4-C3-O4-P1
71	Qc	402	PEE	C14-C15-C16-C17
68	AL	202	CDL	OB5-CB3-CB4-OB6
68	N2	401	CDL	OB5-CB3-CB4-OB6
68	QB	501	CDL	OB5-CB3-CB4-OB6
68	QC	404	CDL	OA5-CA3-CA4-OA6
75	N3	201	PLX	O4-C3-C4-O6
76	C2	302	3PE	O11-C1-C2-O21
68	C1	610	CDL	C72-C71-CB7-OB8
68	AL	201	CDL	CB2-C1-CA2-OA2
68	N5	702	CDL	CA2-C1-CB2-OB2
68	B5	202	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
68	B5	202	CDL	C78-C79-C80-C81
68	QD	402	CDL	OA6-CA4-CA6-OA8
70	C1	606	PC1	O21-C2-C3-O31
70	QJ	101	PC1	O21-C2-C3-O31
71	QE	301	PEE	O2-C2-C3-O3
71	Qd	403	PEE	O2-C2-C3-O3
71	S8	303	PEE	O2-C2-C3-O3
75	N4	502	PLX	O6-C4-C5-O8
68	N2	401	CDL	C71-C72-C73-C74
71	QE	301	PEE	C22-C23-C24-C25
72	A9	401	NDP	C5D-O5D-PN-O3
71	Qc	401	PEE	C39-C40-C41-C42
76	B4	201	3PE	C35-C36-C37-C38
71	C3	303	PEE	C31-C32-C33-C34
70	QJ	101	PC1	C3D-C3E-C3F-C3G
68	N2	402	CDL	C21-C22-C23-C24
68	4L	201	CDL	C36-C37-C38-C39
70	C3	301	PC1	C24-C25-C26-C27
68	QE	304	CDL	C37-C38-C39-C40
71	C3	303	PEE	C23-C24-C25-C26
68	4L	201	CDL	CB2-OB2-PB2-OB5
68	QD	402	CDL	CA2-OA2-PA1-OA5
70	Qc	406	PC1	C11-O13-P-O11
70	Qd	402	PC1	C11-O13-P-O11
71	A3	201	PEE	C4-O4P-P-O3P
71	C3	303	PEE	C4-O4P-P-O3P
68	A1	101	CDL	CA4-CA3-OA5-PA1
68	C1	610	CDL	CB4-CB3-OB5-PB2
68	N5	702	CDL	CB4-CB3-OB5-PB2
68	QD	402	CDL	CA4-CA3-OA5-PA1
68	QD	402	CDL	CB4-CB3-OB5-PB2
68	QH	101	CDL	C1-CB2-OB2-PB2
70	C1	609	PC1	C2-C1-O11-P
70	N1	401	PC1	C2-C1-O11-P
70	Qc	405	PC1	C2-C1-O11-P
71	AL	203	PEE	C2-C1-O3P-P
75	N4	503	PLX	C4-C3-O4-P1
68	QE	304	CDL	C58-C59-C60-C61
71	Qc	402	PEE	C12-C13-C14-C15
68	4L	201	CDL	CA2-OA2-PA1-OA4
68	4L	201	CDL	CB2-OB2-PB2-OB4
68	A1	101	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
68	A1	101	CDL	CB2-OB2-PB2-OB3
68	A8	301	CDL	CA3-OA5-PA1-OA3
68	A8	301	CDL	CB3-OB5-PB2-OB3
68	AL	201	CDL	CA2-OA2-PA1-OA3
68	AL	201	CDL	CB2-OB2-PB2-OB4
68	AL	202	CDL	CA3-OA5-PA1-OA3
68	B4	203	CDL	CB2-OB2-PB2-OB3
68	B5	202	CDL	CB3-OB5-PB2-OB3
68	N2	401	CDL	CA2-OA2-PA1-OA3
68	N2	401	CDL	CB2-OB2-PB2-OB3
68	N2	401	CDL	CB3-OB5-PB2-OB3
68	N2	401	CDL	CB3-OB5-PB2-OB4
68	N2	402	CDL	CA3-OA5-PA1-OA4
68	N5	702	CDL	CA2-OA2-PA1-OA4
68	N5	703	CDL	CB3-OB5-PB2-OB4
68	QB	501	CDL	CA2-OA2-PA1-OA4
68	QB	501	CDL	CA3-OA5-PA1-OA3
68	QD	402	CDL	CA3-OA5-PA1-OA4
68	QD	402	CDL	CB3-OB5-PB2-OB3
68	QD	402	CDL	CB3-OB5-PB2-OB4
68	QE	304	CDL	CB2-OB2-PB2-OB3
68	QE	304	CDL	CB3-OB5-PB2-OB3
68	QH	101	CDL	CB2-OB2-PB2-OB3
70	B5	203	PC1	C11-O13-P-O14
70	B7	201	PC1	C11-O13-P-O14
70	C1	607	PC1	C11-O13-P-O12
70	C1	607	PC1	C11-C12-N-C14
70	C1	609	PC1	C1-O11-P-O12
70	C1	611	PC1	C11-O13-P-O12
70	N1	401	PC1	C11-O13-P-O14
70	N1	401	PC1	C1-O11-P-O12
70	N1	402	PC1	C11-O13-P-O14
71	6A	103	PEE	C4-O4P-P-O2P
71	A3	201	PEE	C4-O4P-P-O1P
71	AL	203	PEE	C4-O4P-P-O2P
71	N5	701	PEE	C1-O3P-P-O2P
71	N5	701	PEE	C1-O3P-P-O1P
71	N5	701	PEE	C4-O4P-P-O1P
71	N5	704	PEE	C1-O3P-P-O2P
71	QB	502	PEE	C1-O3P-P-O2P
71	QE	301	PEE	C1-O3P-P-O2P
71	Qc	401	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
71	S8	303	PEE	C4-O4P-P-O2P
72	A9	401	NDP	C5D-O5D-PN-O2N
75	B5	201	PLX	C2-O1-P1-O2
75	N3	201	PLX	C3-O4-P1-O2
75	N3	201	PLX	C3-O4-P1-O3
75	N4	503	PLX	C3-O4-P1-O3
75	QI	301	PLX	C3-O4-P1-O2
76	C2	302	3PE	C11-O13-P-O12
68	C1	610	CDL	OB5-CB3-CB4-CB6
70	N1	402	PC1	O11-C1-C2-C3
71	N4	501	PEE	O3P-C1-C2-C3
71	S8	303	PEE	O3P-C1-C2-C3
75	N3	201	PLX	O4-C3-C4-C5
75	N4	503	PLX	C7-C8-C9-C10
71	6A	102	PEE	C14-C15-C16-C17
75	B5	201	PLX	C1-C2-O1-P1
75	CB	201	PLX	C1-C2-O1-P1
75	N4	502	PLX	C25-C24-O8-C5
75	N4	503	PLX	C25-C24-O8-C5
76	CA	101	3PE	C12-C11-O13-P
70	C3	301	PC1	O21-C21-C22-C23
68	AL	201	CDL	C33-C34-C35-C36
70	6A	101	PC1	C32-C33-C34-C35
76	B4	201	3PE	C28-C29-C2A-C2B
68	A1	101	CDL	C72-C73-C74-C75
71	AL	203	PEE	C35-C36-C37-C38
68	QH	101	CDL	CB7-C71-C72-C73
68	4L	201	CDL	C79-C80-C81-C82
73	AB	201	ZMP	C4-C5-C6-C7
68	QC	404	CDL	CB2-C1-CA2-OA2
68	QE	304	CDL	OB5-CB3-CB4-OB6
68	Qb	501	CDL	OB5-CB3-CB4-OB6
70	6A	101	PC1	O11-C1-C2-O21
70	C1	608	PC1	O11-C1-C2-O21
71	6A	102	PEE	O3P-C1-C2-O2
71	AL	203	PEE	O3P-C1-C2-O2
71	N5	701	PEE	O3P-C1-C2-O2
71	QC	403	PEE	O3P-C1-C2-O2
74	AK	401	ADP	C3'-C4'-C5'-O5'
84	V1	502	FMN	N10-C1'-C2'-O2'
71	N5	701	PEE	C11-C12-C13-C14
71	B4	202	PEE	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
71	8B	201	PEE	C31-C32-C33-C34
68	AL	201	CDL	C34-C35-C36-C37
68	N2	402	CDL	C17-C18-C19-C20
71	QB	503	PEE	C34-C35-C36-C37
75	AM	201	PLX	C27-C28-C29-C30
70	Qc	406	PC1	C26-C27-C28-C29
70	6A	101	PC1	C11-C12-N-C15
68	C1	610	CDL	C54-C55-C56-C57
68	QE	304	CDL	CB5-C51-C52-C53
68	QE	304	CDL	CB7-C71-C72-C73
70	6A	101	PC1	O13-C11-C12-N
70	B7	201	PC1	O13-C11-C12-N
70	C1	608	PC1	O13-C11-C12-N
70	C3	302	PC1	O13-C11-C12-N
70	N5	705	PC1	O13-C11-C12-N
70	QJ	101	PC1	O13-C11-C12-N
70	Qc	405	PC1	O13-C11-C12-N
70	Qd	402	PC1	O13-C11-C12-N
70	Qh	101	PC1	O13-C11-C12-N
71	QC	403	PEE	C1-C2-C3-O3
73	AB	201	ZMP	O4-C17-C18-C21
75	AM	201	PLX	N1-C1-C2-O1
75	AM	202	PLX	N1-C1-C2-O1
75	B5	201	PLX	N1-C1-C2-O1
75	B5	201	PLX	C27-C28-C29-C30
75	C2	301	PLX	C3-C4-C5-O8
75	C2	301	PLX	N1-C1-C2-O1
68	B4	203	CDL	OA6-CA4-CA6-OA8
68	N2	402	CDL	OB6-CB4-CB6-OB8
68	QH	101	CDL	OA6-CA4-CA6-OA8
71	N4	501	PEE	O2-C2-C3-O3
71	QB	502	PEE	O2-C2-C3-O3
75	B5	201	PLX	O6-C4-C5-O8
75	N4	503	PLX	O6-C4-C5-O8
76	QE	302	3PE	O21-C2-C3-O31
68	N2	401	CDL	C33-C34-C35-C36
76	C2	302	3PE	C23-C24-C25-C26
71	Qc	401	PEE	C37-C38-C39-C40
71	S8	303	PEE	C16-C17-C18-C19
68	QH	102	CDL	C1-CA2-OA2-PA1
76	QE	302	3PE	C2-C1-O11-P
70	Qh	101	PC1	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
71	N5	704	PEE	C23-C24-C25-C26
75	B5	201	PLX	C14-C15-C16-C17
75	C2	301	PLX	C24-C25-C26-C27
71	Qc	401	PEE	C11-C12-C13-C14
75	N4	502	PLX	O6-C6-C7-C8
75	QB	504	PLX	O6-C6-C7-C8
71	B4	202	PEE	C33-C34-C35-C36
70	QJ	101	PC1	C3A-C3B-C3C-C3D
70	Qh	101	PC1	C33-C34-C35-C36
75	B5	201	PLX	O7-C6-C7-C8
72	A9	401	NDP	O4D-C1D-N1N-C6N
70	Qb	502	PC1	C11-C12-N-C14
68	N5	703	CDL	C76-C77-C78-C79
71	S8	303	PEE	C21-C22-C23-C24
68	N2	402	CDL	C77-C78-C79-C80
68	N5	702	CDL	C14-C15-C16-C17
70	Qc	406	PC1	C24-C25-C26-C27
68	N5	703	CDL	C21-C22-C23-C24
71	Qc	401	PEE	C40-C41-C42-C43
73	AB	201	ZMP	C19-C18-C21-O5
73	AB	201	ZMP	C20-C18-C21-O5
71	6A	102	PEE	C38-C39-C40-C41
71	C3	303	PEE	C24-C25-C26-C27
75	AM	202	PLX	C20-C21-C22-C23
68	N2	402	CDL	C13-C14-C15-C16
68	N2	402	CDL	C18-C19-C20-C21
75	QB	504	PLX	C25-C26-C27-C28
70	C1	609	PC1	C3C-C3D-C3E-C3F
70	Qc	406	PC1	C3D-C3E-C3F-C3G
71	N5	704	PEE	C11-C12-C13-C14
68	AL	202	CDL	CA3-CA4-OA6-CA5
70	Qb	502	PC1	C3-C2-O21-C21
71	AL	203	PEE	C1-C2-O2-C10
68	QC	404	CDL	OA5-CA3-CA4-CA6
70	6A	101	PC1	O11-C1-C2-C3
70	C1	608	PC1	O11-C1-C2-C3
71	6A	102	PEE	O3P-C1-C2-C3
71	N5	701	PEE	O3P-C1-C2-C3
71	B4	202	PEE	O4-C10-O2-C2
71	B4	202	PEE	C13-C14-C15-C16
68	B4	203	CDL	CB4-CB3-OB5-PB2
68	QH	101	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
75	N4	503	PLX	C35-C36-C37-C38
68	N5	703	CDL	OA5-CA3-CA4-OA6
68	AL	201	CDL	C54-C55-C56-C57
71	QB	503	PEE	C14-C15-C16-C17
75	QI	301	PLX	C13-C14-C15-C16
70	6A	101	PC1	C11-C12-N-C14
68	N2	401	CDL	CA5-C11-C12-C13
68	AL	201	CDL	C52-C51-CB5-OB6
68	C1	610	CDL	C32-C31-CA7-OA8
76	B8	201	3PE	O21-C21-C22-C23
68	A8	301	CDL	C11-CA5-OA6-CA4
71	B4	202	PEE	C11-C10-O2-C2
70	6A	101	PC1	O31-C31-C32-C33
71	Qc	402	PEE	O2-C2-C3-O3
70	B5	203	PC1	C3A-C3B-C3C-C3D
68	AL	201	CDL	CA3-OA5-PA1-OA2
68	AL	202	CDL	CA2-OA2-PA1-OA5
68	C1	610	CDL	CA3-OA5-PA1-OA2
68	QH	102	CDL	CA3-OA5-PA1-OA2
70	6A	101	PC1	C11-O13-P-O11
70	6A	101	PC1	C1-O11-P-O13
70	N5	705	PC1	C1-O11-P-O13
70	Qc	405	PC1	C11-O13-P-O11
70	Qd	402	PC1	C1-O11-P-O13
71	AL	203	PEE	C1-O3P-P-O4P
71	QB	502	PEE	C4-O4P-P-O3P
75	N3	201	PLX	C2-O1-P1-O4
76	B4	201	3PE	C1-O11-P-O13
76	B8	201	3PE	C1-O11-P-O13
76	QE	302	3PE	C11-O13-P-O11
71	N4	501	PEE	C22-C23-C24-C25
70	Qh	101	PC1	C35-C36-C37-C38
68	QE	304	CDL	C77-C78-C79-C80
70	B5	203	PC1	C22-C23-C24-C25
71	QB	503	PEE	C1-C2-C3-O3
68	N2	401	CDL	C34-C35-C36-C37
68	QE	304	CDL	C32-C33-C34-C35
68	AL	201	CDL	C38-C39-C40-C41
68	A1	101	CDL	C55-C56-C57-C58
71	6A	102	PEE	C21-C22-C23-C24
68	N2	402	CDL	C35-C36-C37-C38
75	N4	503	PLX	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
68	B5	202	CDL	C56-C57-C58-C59
68	QH	101	CDL	C71-C72-C73-C74
68	AL	202	CDL	C1-CB2-OB2-PB2
68	N2	402	CDL	CB4-CB3-OB5-PB2
70	B5	203	PC1	C2-C1-O11-P
70	Qb	502	PC1	C36-C37-C38-C39
71	B4	202	PEE	C36-C37-C38-C39
70	C1	611	PC1	C3E-C3F-C3G-C3H
71	B4	202	PEE	C19-C20-C21-C22
71	B4	202	PEE	C37-C38-C39-C40
72	A9	401	NDP	C2D-C1D-N1N-C6N
71	6A	103	PEE	C23-C24-C25-C26
71	C3	303	PEE	C44-C45-C46-C47
68	Qb	501	CDL	CA7-C31-C32-C33
70	Qc	406	PC1	C31-C32-C33-C34
70	C1	607	PC1	C11-C12-N-C13
75	AM	201	PLX	C24-C25-C26-C27
75	C2	301	PLX	C6-C7-C8-C9
71	AL	203	PEE	O4P-C4-C5-N
68	C1	610	CDL	C76-C77-C78-C79
68	QB	501	CDL	OA5-CA3-CA4-OA6
68	QH	101	CDL	OB5-CB3-CB4-OB6
71	N4	501	PEE	C33-C34-C35-C36
68	QE	304	CDL	C44-C45-C46-C47
80	QC	401	HEM	CAD-CBD-CGD-O1D
80	Qc	403	HEM	CAD-CBD-CGD-O1D
71	QB	503	PEE	C15-C16-C17-C18
71	N5	704	PEE	C14-C15-C16-C17
68	AL	201	CDL	C13-C14-C15-C16
75	N4	502	PLX	C6-C7-C8-C9
70	B7	201	PC1	C27-C28-C29-C2A
75	B5	201	PLX	C15-C16-C17-C18
80	QC	402	HEM	CAA-CBA-CGA-O1A
75	CB	201	PLX	O8-C24-C25-C26
71	Qc	402	PEE	C21-C22-C23-C24
68	QH	102	CDL	CA4-CA3-OA5-PA1
68	QH	102	CDL	C52-C53-C54-C55
77	C1	603	HEA	CAA-CBA-CGA-O2A
70	C1	609	PC1	C11-C12-N-C13
68	A8	301	CDL	C53-C54-C55-C56
68	N5	702	CDL	C33-C34-C35-C36
71	N5	704	PEE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
75	AM	201	PLX	C20-C21-C22-C23
80	Qc	403	HEM	CAA-CBA-CGA-O2A
70	7C	101	PC1	C3A-C3B-C3C-C3D
68	A1	101	CDL	C82-C83-C84-C85
75	AM	202	PLX	C24-C25-C26-C27
80	Qc	403	HEM	CAD-CBD-CGD-O2D
80	Qc	404	HEM	CAD-CBD-CGD-O1D
71	S8	303	PEE	C30-C31-C32-C33
68	N2	401	CDL	C31-C32-C33-C34
70	N1	401	PC1	C1-C2-C3-O31
68	AL	201	CDL	C43-C44-C45-C46
71	QB	502	PEE	C33-C34-C35-C36
73	AC	201	ZMP	C20-C18-C21-O5
71	Qc	401	PEE	C23-C24-C25-C26
77	C1	603	HEA	CAD-CBD-CGD-O1D
80	Qc	403	HEM	CAA-CBA-CGA-O1A
70	Qh	101	PC1	C39-C3A-C3B-C3C
75	N3	201	PLX	C15-C16-C17-C18
70	C1	609	PC1	C2B-C2C-C2D-C2E
80	QC	401	HEM	CAA-CBA-CGA-O1A
80	Qc	404	HEM	CAA-CBA-CGA-O1A
68	B4	203	CDL	CB6-CB4-OB6-CB5
68	QE	304	CDL	CA6-CA4-OA6-CA5
68	Qb	501	CDL	CA6-CA4-OA6-CA5
70	C3	302	PC1	C3-C2-O21-C21
70	QJ	101	PC1	C3-C2-O21-C21
71	S2	501	PEE	C1-C2-O2-C10
68	QE	304	CDL	C76-C77-C78-C79
80	Qc	404	HEM	CAA-CBA-CGA-O2A
70	7C	101	PC1	C34-C35-C36-C37
68	N5	703	CDL	CA3-OA5-PA1-OA2
70	QJ	101	PC1	C1-O11-P-O13
76	C2	302	3PE	C1-O11-P-O13
68	B5	202	CDL	C36-C37-C38-C39
71	6A	102	PEE	C13-C14-C15-C16
68	QC	404	CDL	CA4-CA3-OA5-PA1
68	QE	304	CDL	CA4-CA3-OA5-PA1
71	Qd	403	PEE	O3P-C1-C2-O2
80	QC	402	HEM	CAA-CBA-CGA-O2A
68	4L	201	CDL	C17-C18-C19-C20
68	AL	201	CDL	C52-C53-C54-C55
71	C3	303	PEE	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
68	AL	202	CDL	OB5-CB3-CB4-CB6
71	8B	201	PEE	O3P-C1-C2-C3
68	A8	301	CDL	C75-C76-C77-C78
80	Qc	404	HEM	CAD-CBD-CGD-O2D
68	QB	501	CDL	C32-C33-C34-C35
70	N1	401	PC1	C27-C28-C29-C2A
72	A9	401	NDP	O4B-C4B-C5B-O5B
81	Qd	401	HEC	CAA-CBA-CGA-O2A
70	7C	101	PC1	C35-C36-C37-C38
70	6A	101	PC1	C11-C12-N-C13
70	C1	609	PC1	C25-C26-C27-C28
71	A3	201	PEE	C43-C44-C45-C46
73	AB	201	ZMP	C12-C11-S1-C10
68	QH	102	CDL	OA6-CA4-CA6-OA8
71	6A	103	PEE	C21-C22-C23-C24
73	AC	201	ZMP	C6-C7-C8-C9
80	QC	401	HEM	CAA-CBA-CGA-O2A
71	8B	201	PEE	C15-C16-C17-C18
68	N2	402	CDL	C72-C71-CB7-OB9
68	QD	402	CDL	C32-C33-C34-C35
70	Qd	402	PC1	C34-C35-C36-C37
77	C1	602	HEA	CAD-CBD-CGD-O2D
80	QC	401	HEM	CAD-CBD-CGD-O2D
68	QE	304	CDL	C55-C56-C57-C58
68	B5	202	CDL	CA7-C31-C32-C33
68	A8	301	CDL	C55-C56-C57-C58
70	C1	609	PC1	C23-C24-C25-C26
68	AL	202	CDL	C11-C12-C13-C14
76	C2	302	3PE	C2A-C2B-C2C-C2D
68	4L	201	CDL	C13-C14-C15-C16
70	Qb	502	PC1	C27-C28-C29-C2A
76	CA	101	3PE	C25-C26-C27-C28
68	C1	610	CDL	C1-CB2-OB2-PB2
68	AL	202	CDL	C12-C11-CA5-OA6
75	C2	301	PLX	C14-C15-C16-C17
71	N5	704	PEE	C31-C32-C33-C34
70	N3	202	PC1	O31-C31-C32-C33
75	B5	201	PLX	C16-C17-C18-C19
75	N4	502	PLX	C12-C13-C14-C15
81	Qd	401	HEC	CAA-CBA-CGA-O1A
68	A8	301	CDL	C15-C16-C17-C18
75	QI	301	PLX	C4-C5-O8-C24

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Mol	Chain	Res	Type	Atoms
77	C1	603	HEA	CAD-CBD-CGD-O2D
75	AM	201	PLX	C11-C10-C9-C8
75	QI	301	PLX	C34-C35-C36-C37
71	AL	203	PEE	C16-C17-C18-C19
70	QJ	101	PC1	O11-C1-C2-O21
75	N4	503	PLX	O4-C3-C4-O6
70	Qh	101	PC1	C31-C32-C33-C34
71	Qc	401	PEE	C20-C21-C22-C23
68	A8	301	CDL	C72-C71-CB7-OB8
76	CA	101	3PE	C3B-C3C-C3D-C3E
70	N1	401	PC1	C21-C22-C23-C24
77	C1	603	HEA	CAA-CBA-CGA-O1A
75	AM	202	PLX	C11-C12-C13-C14
68	4L	201	CDL	OB5-CB3-CB4-CB6
68	QB	501	CDL	OA5-CA3-CA4-CA6
71	AL	203	PEE	O3P-C1-C2-C3
68	AL	202	CDL	O1-C1-CB2-OB2
68	4L	201	CDL	CA4-CA3-OA5-PA1
68	QH	101	CDL	CB4-CB3-OB5-PB2
71	6A	102	PEE	C19-C20-C21-C22
68	4L	201	CDL	CA2-C1-CB2-OB2
68	N5	702	CDL	C36-C37-C38-C39
70	Qc	406	PC1	C2D-C2E-C2F-C2G
77	C1	603	HEA	C21-C22-C23-C25
68	QH	102	CDL	C72-C71-CB7-OB8
70	Qb	502	PC1	O21-C21-C22-C23
70	Qc	405	PC1	O21-C21-C22-C23
71	A3	201	PEE	O3-C30-C31-C32
68	Qb	501	CDL	C31-C32-C33-C34
75	AM	202	PLX	C13-C14-C15-C16
71	N4	501	PEE	C18-C19-C20-C21
71	QB	503	PEE	C18-C19-C20-C21
71	QE	301	PEE	C18-C19-C20-C21
71	N5	701	PEE	O2-C10-C11-C12
77	C1	603	HEA	C27-C19-C20-C21
71	QE	301	PEE	C19-C20-C21-C22
68	B5	202	CDL	C12-C11-CA5-OA6
68	B5	202	CDL	C32-C31-CA7-OA8
70	C1	607	PC1	O31-C31-C32-C33
70	N5	705	PC1	O21-C21-C22-C23
71	Qc	401	PEE	O2-C10-C11-C12
76	C2	302	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
71	QB	502	PEE	C36-C37-C38-C39
71	Qc	402	PEE	C18-C19-C20-C21
70	Qc	406	PC1	C3B-C3C-C3D-C3E
77	C1	602	HEA	CAD-CBD-CGD-O1D
68	C1	610	CDL	CA6-CA4-OA6-CA5
68	QH	101	CDL	CA3-CA4-OA6-CA5
68	QH	101	CDL	CA6-CA4-OA6-CA5
68	QH	102	CDL	CA6-CA4-OA6-CA5
68	N5	702	CDL	C39-C40-C41-C42
68	A8	301	CDL	OA7-CA5-OA6-CA4
68	N5	702	CDL	C12-C11-CA5-OA6
70	C1	607	PC1	O21-C21-C22-C23
68	B5	202	CDL	C59-C60-C61-C62
71	QB	503	PEE	C42-C43-C44-C45
70	B7	201	PC1	C26-C27-C28-C29
68	N2	401	CDL	C32-C31-CA7-OA8
71	N5	701	PEE	C16-C17-C18-C19
75	C2	301	PLX	C11-C12-C13-C14
75	CB	201	PLX	C7-C6-O6-C4
68	QE	304	CDL	C62-C63-C64-C65
71	N5	704	PEE	C43-C44-C45-C46
68	QH	101	CDL	OA5-CA3-CA4-OA6
71	A3	201	PEE	O3P-C1-C2-O2
71	N4	501	PEE	O2-C10-C11-C12
68	QH	102	CDL	CA7-C31-C32-C33
75	AM	202	PLX	C31-C32-C33-C34
70	7C	101	PC1	C39-C3A-C3B-C3C
71	Qd	403	PEE	C12-C13-C14-C15
68	A1	101	CDL	C32-C31-CA7-OA8
68	B5	202	CDL	C31-C32-C33-C34
70	B5	203	PC1	C3F-C3G-C3H-C3I
71	B4	202	PEE	C32-C33-C34-C35
71	AL	203	PEE	O3-C30-C31-C32
71	N4	501	PEE	C15-C16-C17-C18
68	B4	203	CDL	C34-C35-C36-C37
70	N1	401	PC1	C29-C2A-C2B-C2C
68	A1	101	CDL	OB5-CB3-CB4-CB6
70	QJ	101	PC1	O11-C1-C2-C3
76	C2	302	3PE	O11-C1-C2-C3
76	CA	101	3PE	O31-C31-C32-C33
71	6A	102	PEE	C41-C42-C43-C44
68	B5	202	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
68	QB	501	CDL	OA6-CA4-CA6-OA8
70	N1	401	PC1	O21-C2-C3-O31
68	N5	702	CDL	C54-C55-C56-C57
70	QJ	101	PC1	C2E-C2F-C2G-C2H
71	8B	201	PEE	C38-C39-C40-C41
71	Qc	401	PEE	C36-C37-C38-C39
70	C1	609	PC1	C3B-C3C-C3D-C3E
68	N2	401	CDL	C52-C51-CB5-OB6
71	C3	303	PEE	O2-C10-C11-C12
71	S8	303	PEE	C33-C34-C35-C36
75	QI	301	PLX	C7-C8-C9-C10
72	A9	401	NDP	C2B-O2B-P2B-O2X
76	CA	101	3PE	C32-C33-C34-C35
71	6A	103	PEE	C15-C16-C17-C18
70	C1	609	PC1	C32-C33-C34-C35
68	4L	201	CDL	C39-C40-C41-C42
68	N2	402	CDL	C58-C59-C60-C61
71	S8	303	PEE	C18-C19-C20-C21
71	S8	303	PEE	C36-C37-C38-C39
68	QB	501	CDL	C72-C71-CB7-OB8
71	A3	201	PEE	O2-C10-C11-C12
68	B5	202	CDL	C32-C31-CA7-OA9
75	CB	201	PLX	C20-C21-C22-C23
70	C1	607	PC1	O22-C21-C22-C23
70	QJ	101	PC1	C29-C2A-C2B-C2C
68	QE	304	CDL	C72-C73-C74-C75
75	AM	201	PLX	C35-C36-C37-C38
68	N5	703	CDL	C73-C74-C75-C76
71	6A	102	PEE	C16-C17-C18-C19
76	B4	201	3PE	C3F-C3G-C3H-C3I
76	C2	302	3PE	O22-C21-C22-C23
71	Qc	401	PEE	C12-C13-C14-C15
75	AM	202	PLX	O6-C6-C7-C8
68	A1	101	CDL	C34-C35-C36-C37
70	N1	401	PC1	C28-C29-C2A-C2B
77	C1	602	HEA	CAA-CBA-CGA-O1A
68	N5	703	CDL	C39-C40-C41-C42
70	C1	607	PC1	C34-C35-C36-C37
71	A3	201	PEE	O5-C30-C31-C32
71	N5	701	PEE	O4-C10-C11-C12
68	A1	101	CDL	C32-C31-CA7-OA9
68	N2	401	CDL	C32-C31-CA7-OA9

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Mol	Chain	Res	Type	Atoms
68	QH	102	CDL	C72-C71-CB7-OB9
70	Qb	502	PC1	O22-C21-C22-C23
71	Qc	401	PEE	O4-C10-C11-C12
68	N2	401	CDL	CA3-CA4-CA6-OA8
75	CB	201	PLX	C3-C4-C5-O8
75	N4	502	PLX	C24-C25-C26-C27
68	Qb	501	CDL	C72-C73-C74-C75
68	N5	702	CDL	C12-C11-CA5-OA7
71	A3	201	PEE	O4-C10-C11-C12
70	Qd	402	PC1	C26-C27-C28-C29
71	C3	303	PEE	C2-C1-O3P-P
71	QC	403	PEE	C2-C1-O3P-P
70	C1	607	PC1	O32-C31-C32-C33
68	A1	101	CDL	C18-C19-C20-C21
68	AL	201	CDL	CB3-OB5-PB2-OB3
68	AL	202	CDL	CA2-OA2-PA1-OA3
68	C1	610	CDL	CA3-OA5-PA1-OA3
68	N2	401	CDL	CA3-OA5-PA1-OA3
68	N5	702	CDL	CB3-OB5-PB2-OB3
68	N5	703	CDL	CB2-OB2-PB2-OB3
68	QH	102	CDL	CA3-OA5-PA1-OA3
68	Qb	501	CDL	CA3-OA5-PA1-OA3
70	C1	607	PC1	C1-O11-P-O14
70	C1	609	PC1	C11-C12-N-C14
70	C1	609	PC1	C11-C12-N-C15
70	N3	202	PC1	C1-O11-P-O14
70	QJ	101	PC1	C1-O11-P-O14
70	Qd	402	PC1	C1-O11-P-O14
71	QB	502	PEE	C1-O3P-P-O1P
72	A9	401	NDP	C2N-C3N-C7N-N7N
75	CB	201	PLX	C3-O4-P1-O2
75	QI	301	PLX	C2-O1-P1-O3
71	N4	501	PEE	C32-C33-C34-C35
68	QB	501	CDL	C72-C71-CB7-OB9
68	B5	202	CDL	C12-C11-CA5-OA7
71	AL	203	PEE	O5-C30-C31-C32
68	QE	304	CDL	C43-C44-C45-C46
73	AC	201	ZMP	C19-C18-C21-O5
68	N5	702	CDL	C35-C36-C37-C38
75	N4	503	PLX	C9-C10-C11-C12
71	Qc	401	PEE	C22-C23-C24-C25
75	QB	504	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
81	QD	401	HEC	CAD-CBD-CGD-O2D
71	QE	301	PEE	O2-C10-C11-C12
68	QE	304	CDL	C34-C35-C36-C37
70	C1	606	PC1	C3A-C3B-C3C-C3D
68	C1	610	CDL	CA3-CA4-OA6-CA5
68	QE	304	CDL	CA3-CA4-OA6-CA5
68	QH	102	CDL	CA3-CA4-OA6-CA5
70	C1	607	PC1	C12-C11-O13-P
70	C3	302	PC1	C12-C11-O13-P
70	QJ	101	PC1	C1-C2-O21-C21
71	N4	501	PEE	C5-C4-O4P-P
71	QE	301	PEE	C5-C4-O4P-P
71	Qc	401	PEE	C5-C4-O4P-P
76	QE	302	3PE	C12-C11-O13-P
70	N5	705	PC1	O22-C21-C22-C23
71	C3	303	PEE	O4-C10-C11-C12
71	N4	501	PEE	O4-C10-C11-C12
76	CA	101	3PE	O32-C31-C32-C33
68	Qb	501	CDL	C32-C33-C34-C35
68	QC	404	CDL	C31-C32-C33-C34
68	QH	101	CDL	C72-C71-CB7-OB9
72	A9	401	NDP	C2D-C1D-N1N-C2N
70	C1	608	PC1	C11-C12-N-C14
68	B5	202	CDL	C52-C51-CB5-OB6
71	Qc	401	PEE	C43-C44-C45-C46
68	A1	101	CDL	C71-C72-C73-C74
68	N5	702	CDL	C21-C22-C23-C24
70	N1	402	PC1	C39-C3A-C3B-C3C
70	N3	202	PC1	C3E-C3F-C3G-C3H
68	N5	703	CDL	C12-C11-CA5-OA6
70	B5	203	PC1	O21-C21-C22-C23
68	N2	401	CDL	C52-C51-CB5-OB7
75	AM	202	PLX	C4-C3-O4-P1
75	N4	503	PLX	C24-C25-C26-C27
71	AL	203	PEE	C32-C33-C34-C35
68	A8	301	CDL	OB5-CB3-CB4-OB6
68	N2	402	CDL	OB5-CB3-CB4-OB6
71	QE	301	PEE	O3P-C1-C2-O2
84	V1	502	FMN	N10-C1'-C2'-C3'
68	B5	202	CDL	C52-C51-CB5-OB7
68	A8	301	CDL	C32-C31-CA7-OA8
68	AL	202	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
68	QC	404	CDL	C72-C71-CB7-OB8
71	QC	403	PEE	O2-C10-C11-C12
70	N1	401	PC1	C34-C35-C36-C37
68	A8	301	CDL	C32-C31-CA7-OA9
68	AL	201	CDL	C73-C74-C75-C76
76	B8	201	3PE	C35-C36-C37-C38
68	4L	201	CDL	C52-C51-CB5-OB6
70	B5	203	PC1	O31-C31-C32-C33
72	A9	401	NDP	O4D-C1D-N1N-C2N
81	QD	401	HEC	CAD-CBD-CGD-O1D
68	N5	703	CDL	C57-C58-C59-C60
75	N3	201	PLX	C19-C20-C21-C22
68	N2	402	CDL	C15-C16-C17-C18
70	Qh	101	PC1	C3C-C3D-C3E-C3F
68	QD	402	CDL	C72-C71-CB7-OB8
71	N5	701	PEE	O3-C30-C31-C32
70	B5	203	PC1	O22-C21-C22-C23
70	N5	705	PC1	C11-C12-N-C14
70	Qc	406	PC1	C34-C35-C36-C37
71	QB	503	PEE	C16-C17-C18-C19
71	8B	201	PEE	C34-C35-C36-C37
68	C1	610	CDL	C72-C71-CB7-OB9
71	QC	403	PEE	O4-C10-C11-C12
70	7C	101	PC1	O21-C21-C22-C23

There are no ring outliers.

91 monomers are involved in 306 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
75	C2	301	PLX	2	0
76	C2	302	3PE	2	0
81	Qd	401	HEC	3	0
70	C1	609	PC1	4	0
71	QB	503	PEE	1	0
70	N1	402	PC1	2	0
73	AB	201	ZMP	1	0
82	QE	303	FES	2	0
68	N5	702	CDL	7	0
70	6A	101	PC1	10	0
68	QH	102	CDL	3	0
83	V1	501	SF4	1	0
70	Qc	406	PC1	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
68	N5	703	CDL	5	0
82	Qe	301	FES	2	0
75	AM	201	PLX	1	0
83	S1	802	SF4	1	0
76	B4	201	3PE	8	0
70	N3	202	PC1	3	0
73	AC	201	ZMP	4	0
70	B7	201	PC1	1	0
70	C1	606	PC1	4	0
68	AL	201	CDL	7	0
68	QE	304	CDL	2	0
75	CB	201	PLX	3	0
75	N4	502	PLX	9	0
70	Qd	402	PC1	2	0
68	C1	610	CDL	7	0
75	N4	503	PLX	7	0
70	Qc	405	PC1	1	0
75	AM	202	PLX	3	0
68	QB	501	CDL	1	0
70	C3	302	PC1	8	0
71	Qd	403	PEE	1	0
68	B4	203	CDL	3	0
72	A9	401	NDP	1	0
80	QC	402	HEM	8	0
70	N1	401	PC1	9	0
70	Qh	101	PC1	1	0
68	N2	402	CDL	12	0
70	C1	611	PC1	10	0
68	AL	202	CDL	3	0
71	N5	704	PEE	1	0
80	Qc	404	HEM	8	0
77	C1	602	HEA	11	0
70	7C	101	PC1	4	0
70	B5	203	PC1	2	0
71	Qc	402	PEE	4	0
80	Qc	403	HEM	2	0
71	B4	202	PEE	4	0
68	4L	201	CDL	3	0
76	B8	201	3PE	1	0
77	C1	603	HEA	10	0
71	C3	303	PEE	4	0
71	S2	501	PEE	1	0

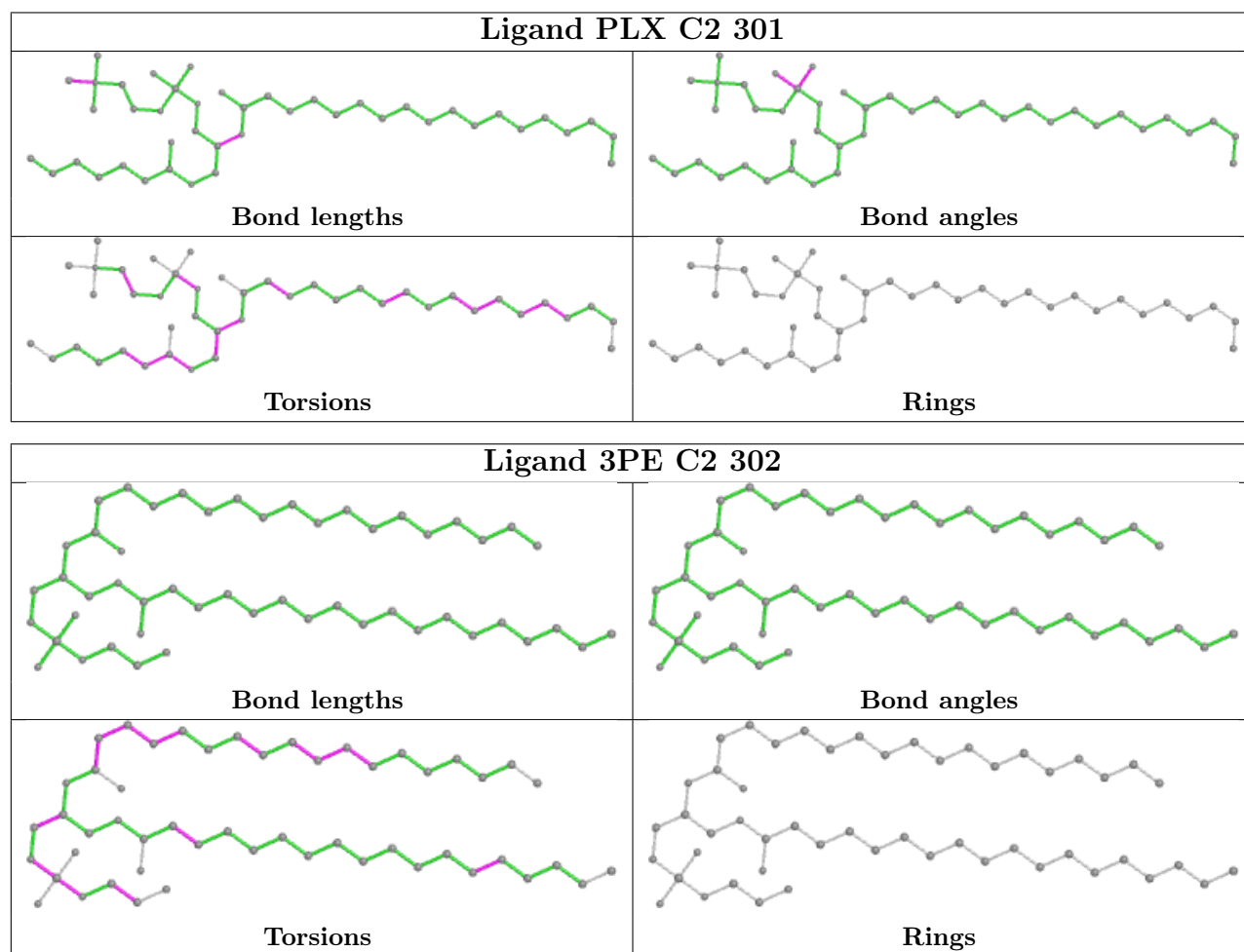
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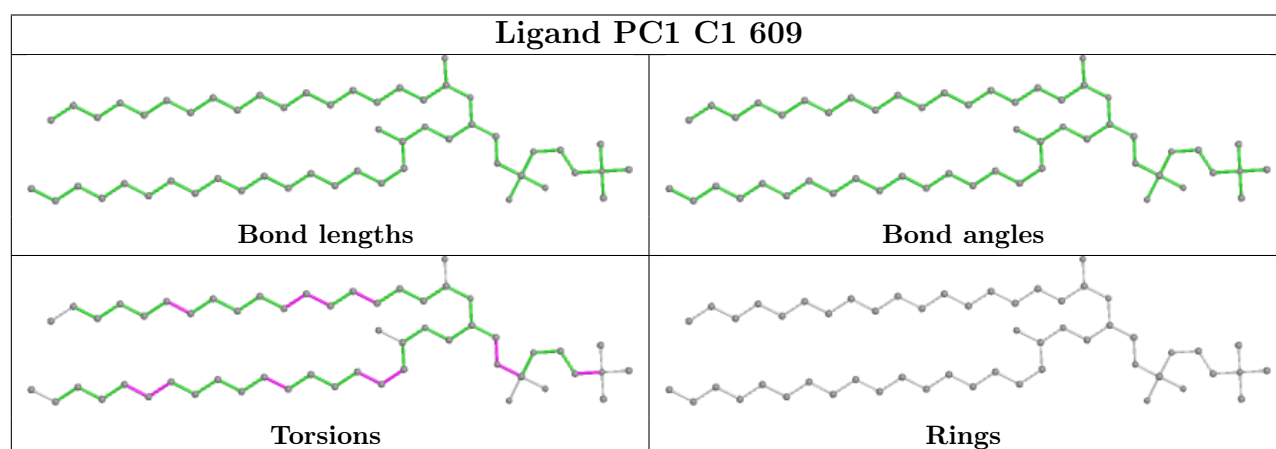
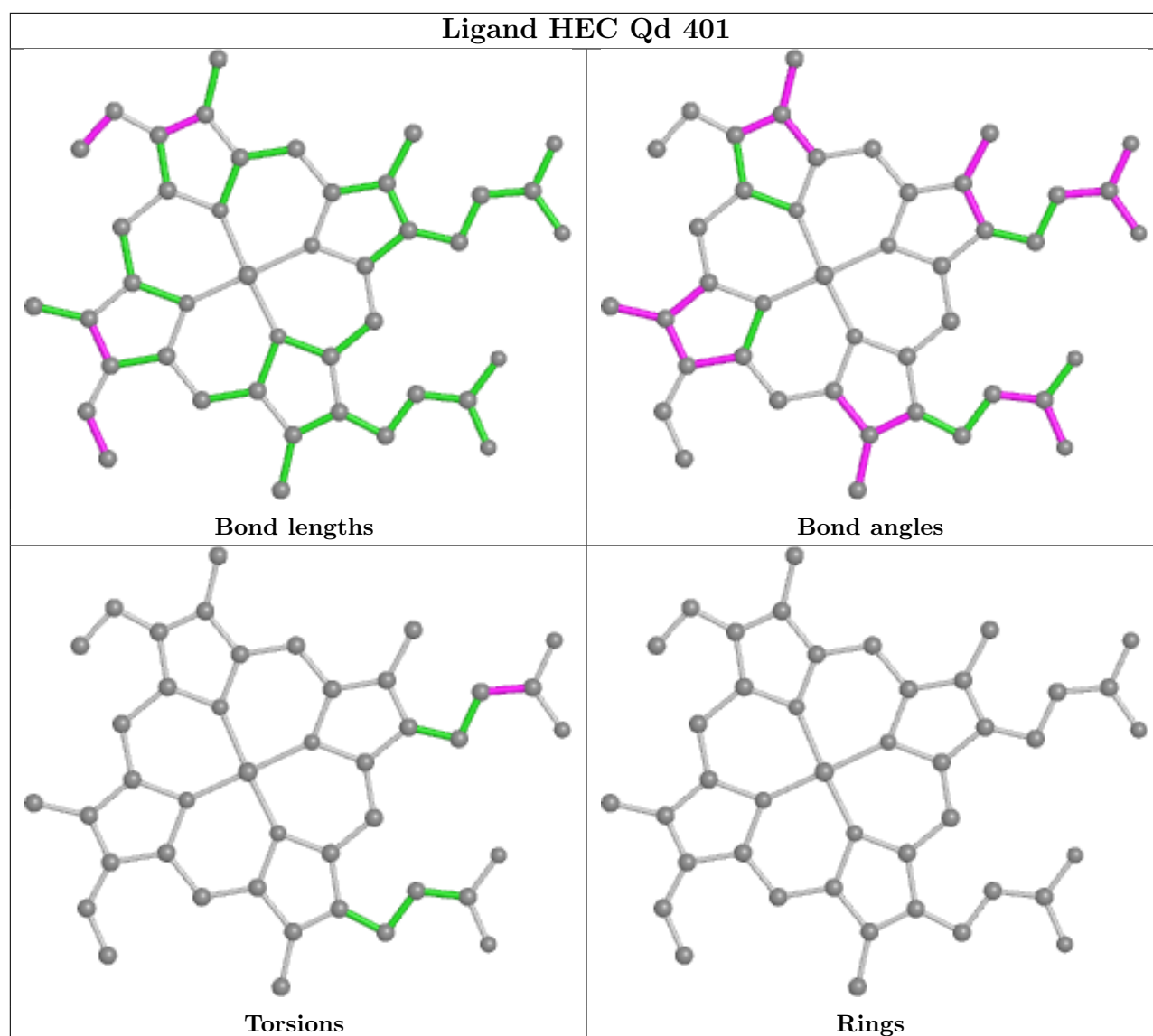
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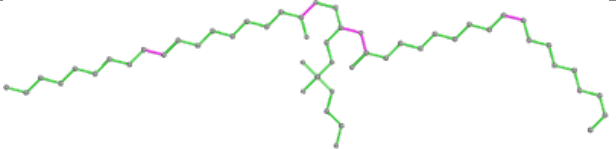
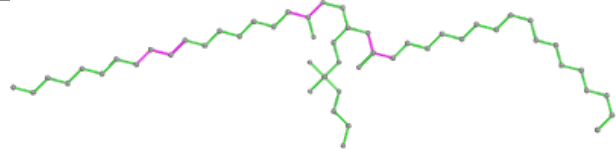
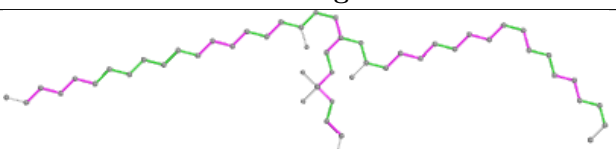
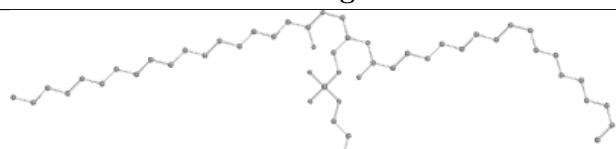
Mol	Chain	Res	Type	Clashes	Symm-Clashes
68	A1	101	CDL	5	0
84	V1	502	FMN	2	0
71	6A	103	PEE	1	0
70	C1	608	PC1	1	0
68	Qb	501	CDL	6	0
68	A8	301	CDL	10	0
68	N2	401	CDL	1	0
76	C1	601	3PE	5	0
82	S1	803	FES	1	0
70	N5	705	PC1	2	0
71	QB	502	PEE	2	0
71	AL	203	PEE	4	0
70	C3	301	PC1	1	0
71	QE	301	PEE	1	0
71	A3	201	PEE	3	0
76	CA	101	3PE	5	0
83	S8	301	SF4	1	0
80	QC	401	HEM	1	0
70	QJ	101	PC1	3	0
71	6A	102	PEE	4	0
71	Qc	401	PEE	2	0
75	N3	201	PLX	1	0
71	N5	701	PEE	6	0
83	S1	801	SF4	2	0
71	8B	201	PEE	2	0
68	QH	101	CDL	2	0
75	QB	504	PLX	4	0
68	B5	202	CDL	3	0
68	QC	404	CDL	4	0
74	AK	401	ADP	4	0
75	QI	301	PLX	5	0
71	N4	501	PEE	3	0
70	C1	607	PC1	3	0
70	Qb	502	PC1	5	0
68	QD	402	CDL	1	0
83	S8	302	SF4	1	0

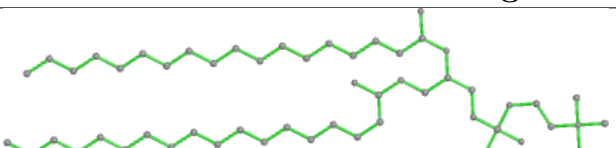
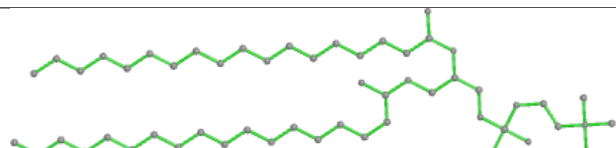
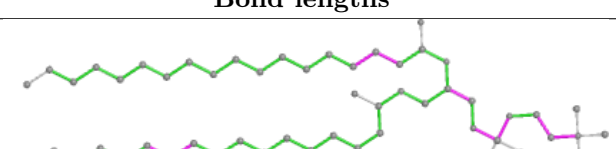
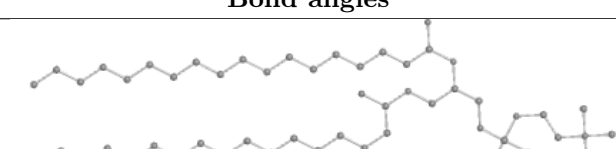
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

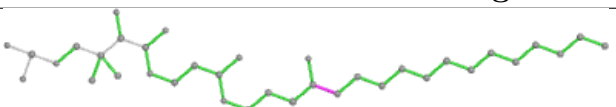

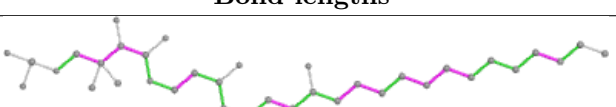
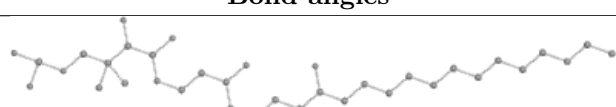
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

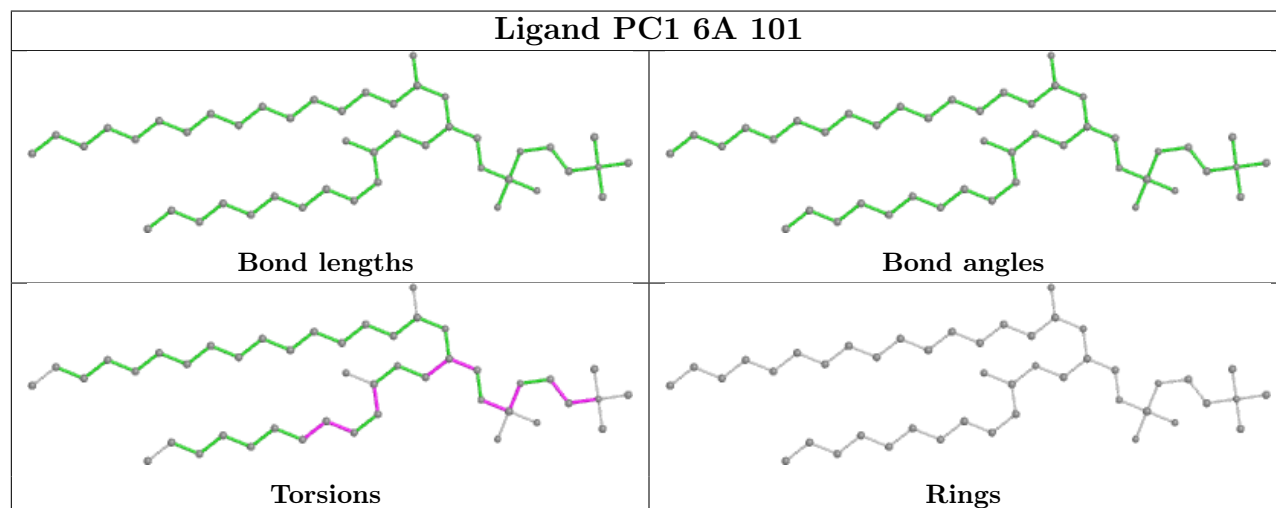
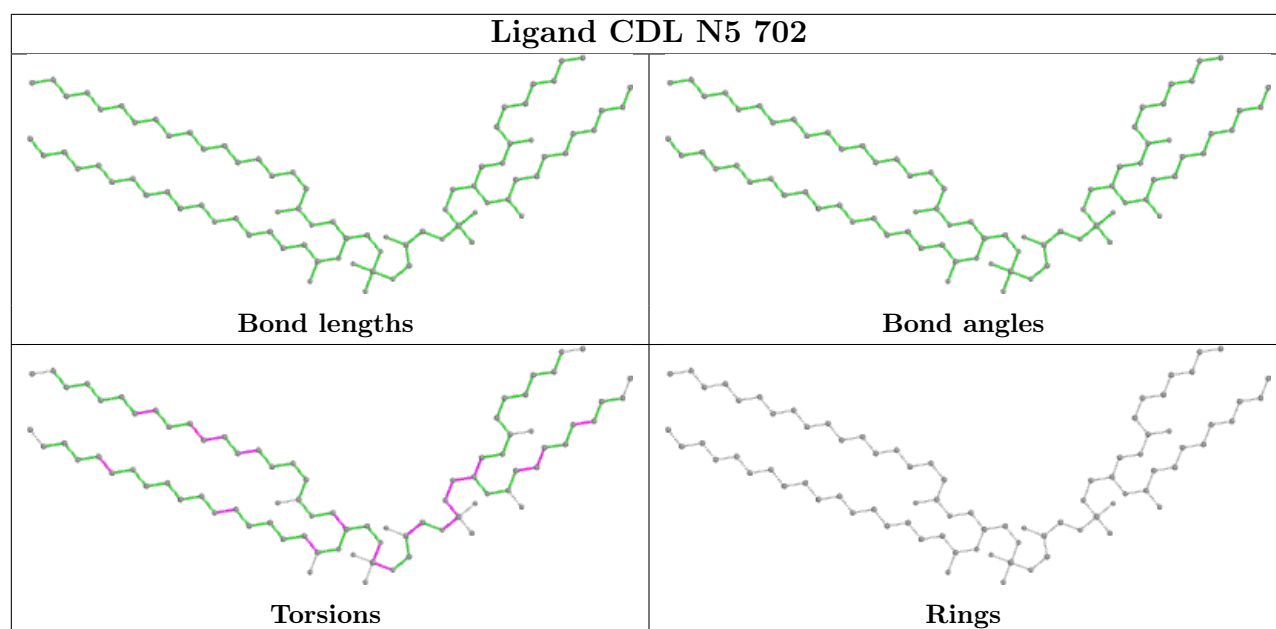


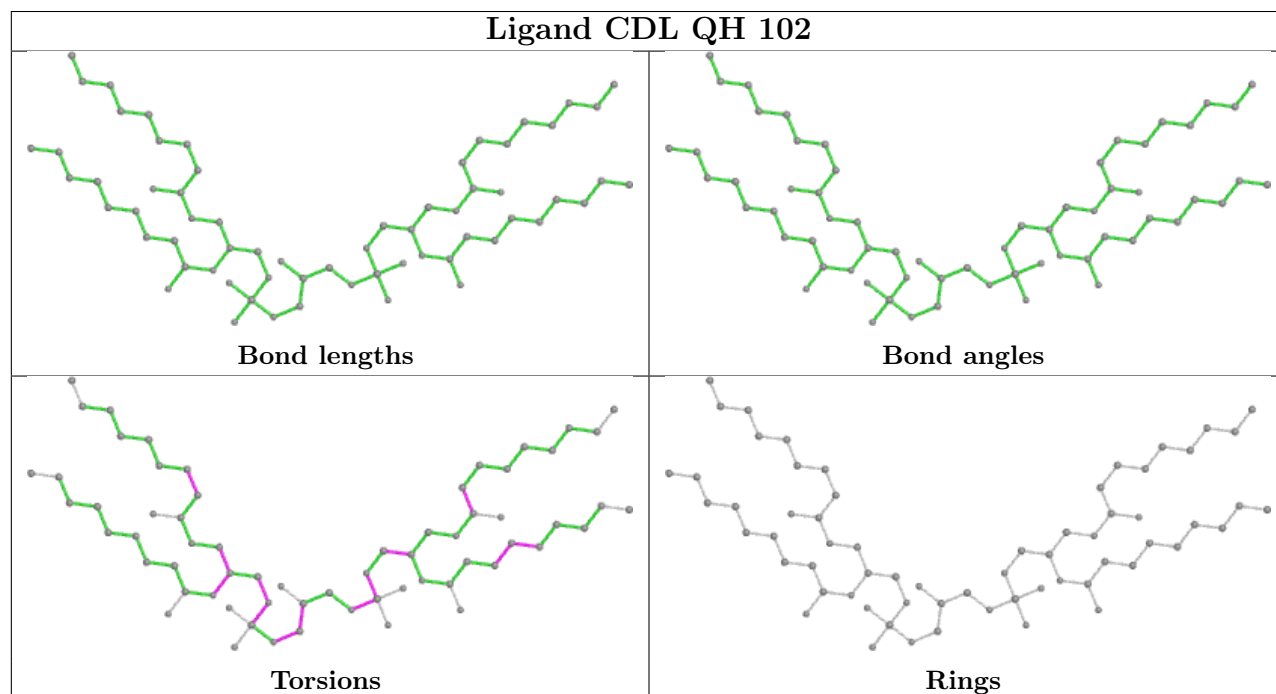
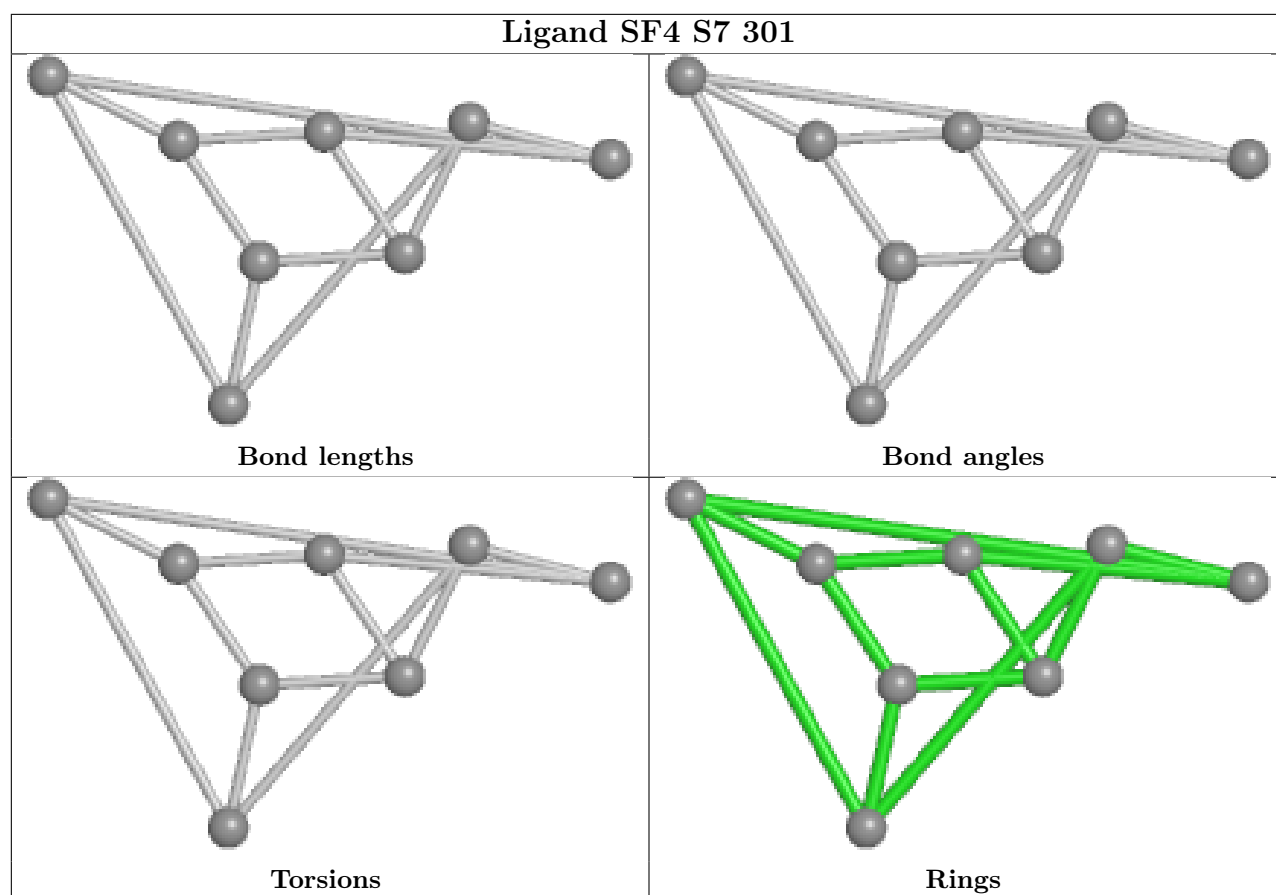


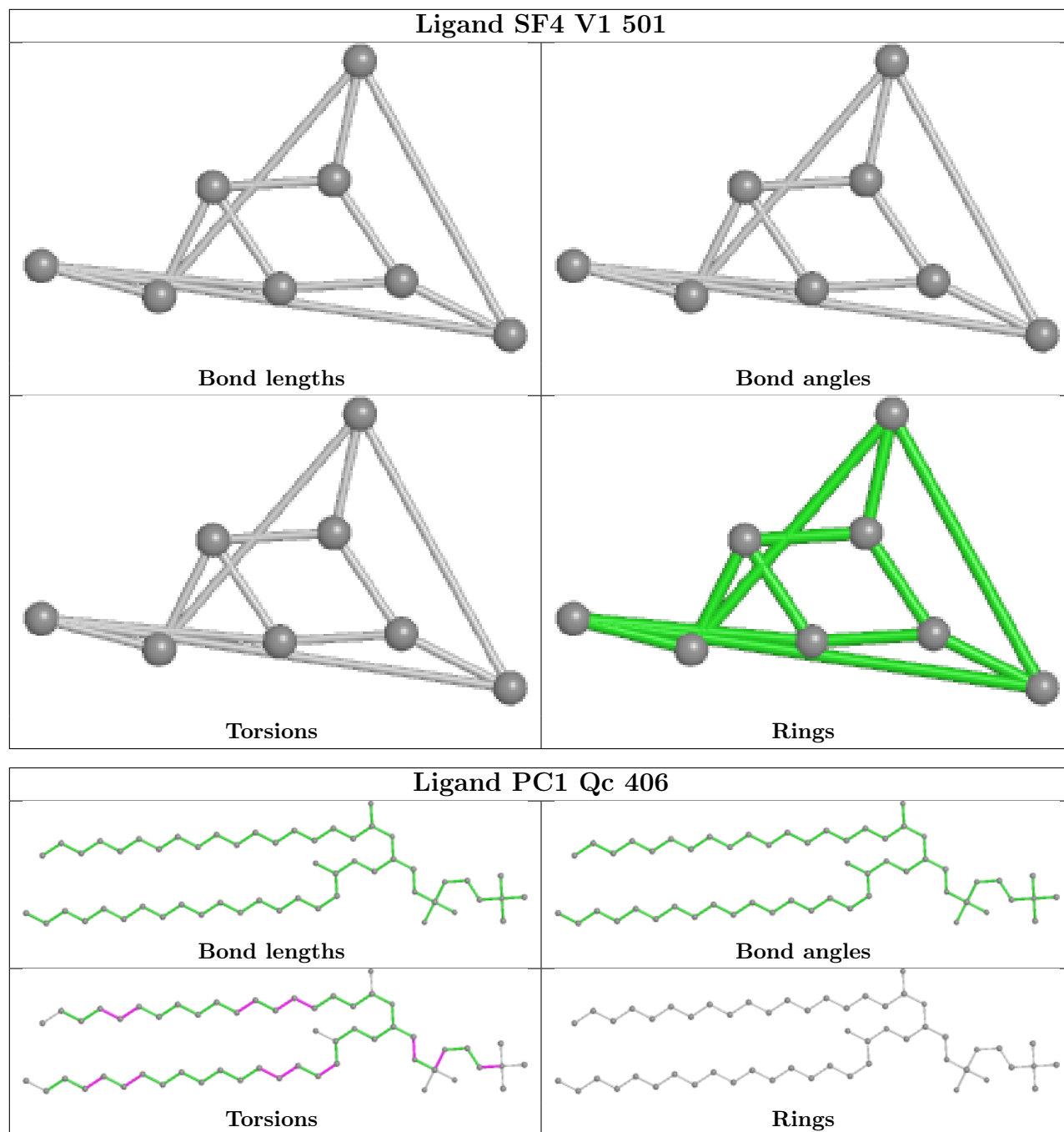
Ligand PEE QB 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

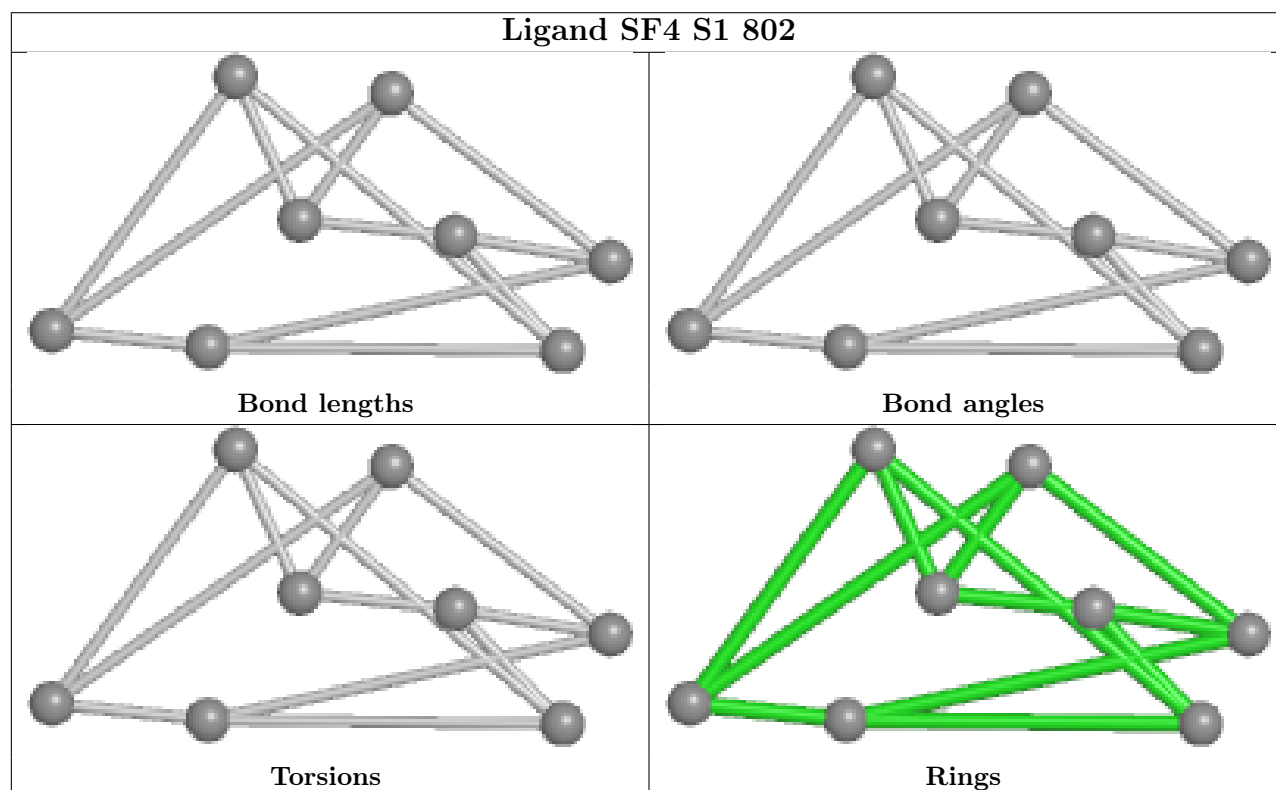
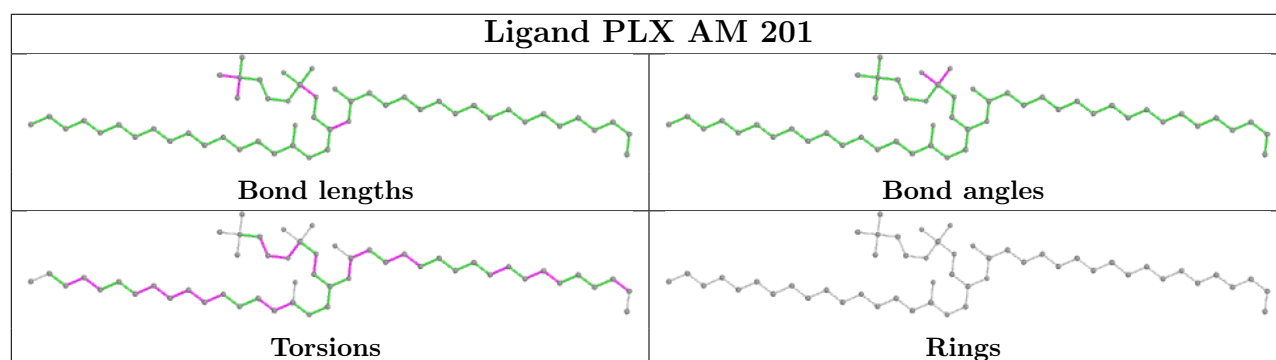
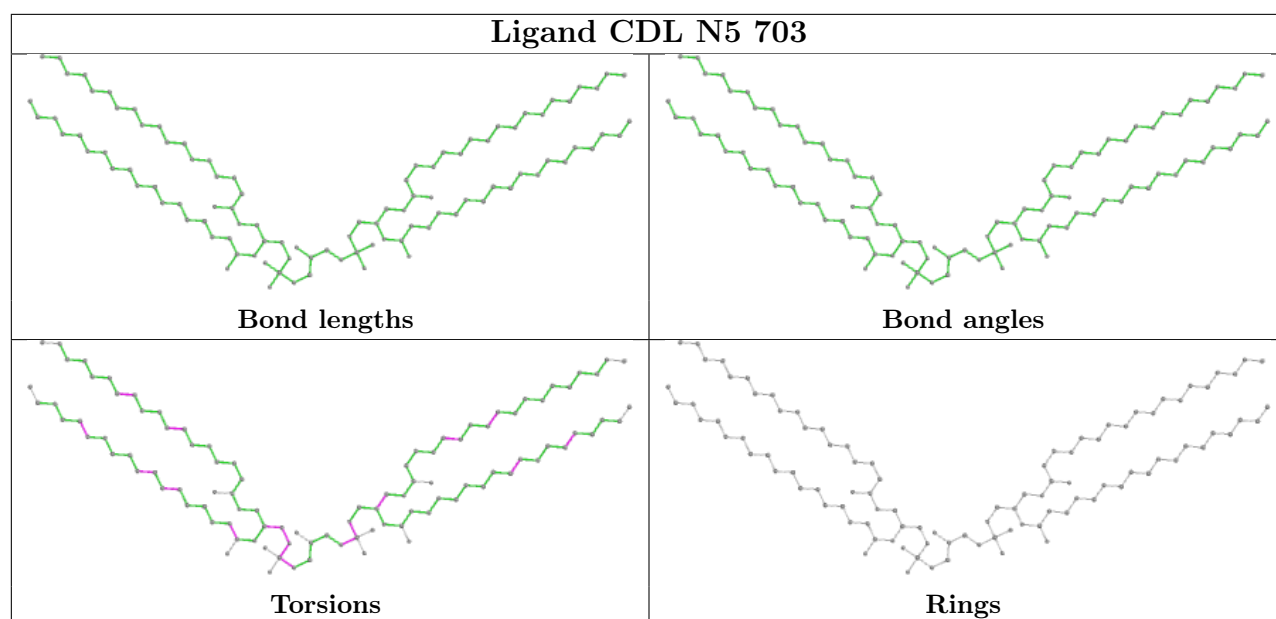
Ligand PC1 N1 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

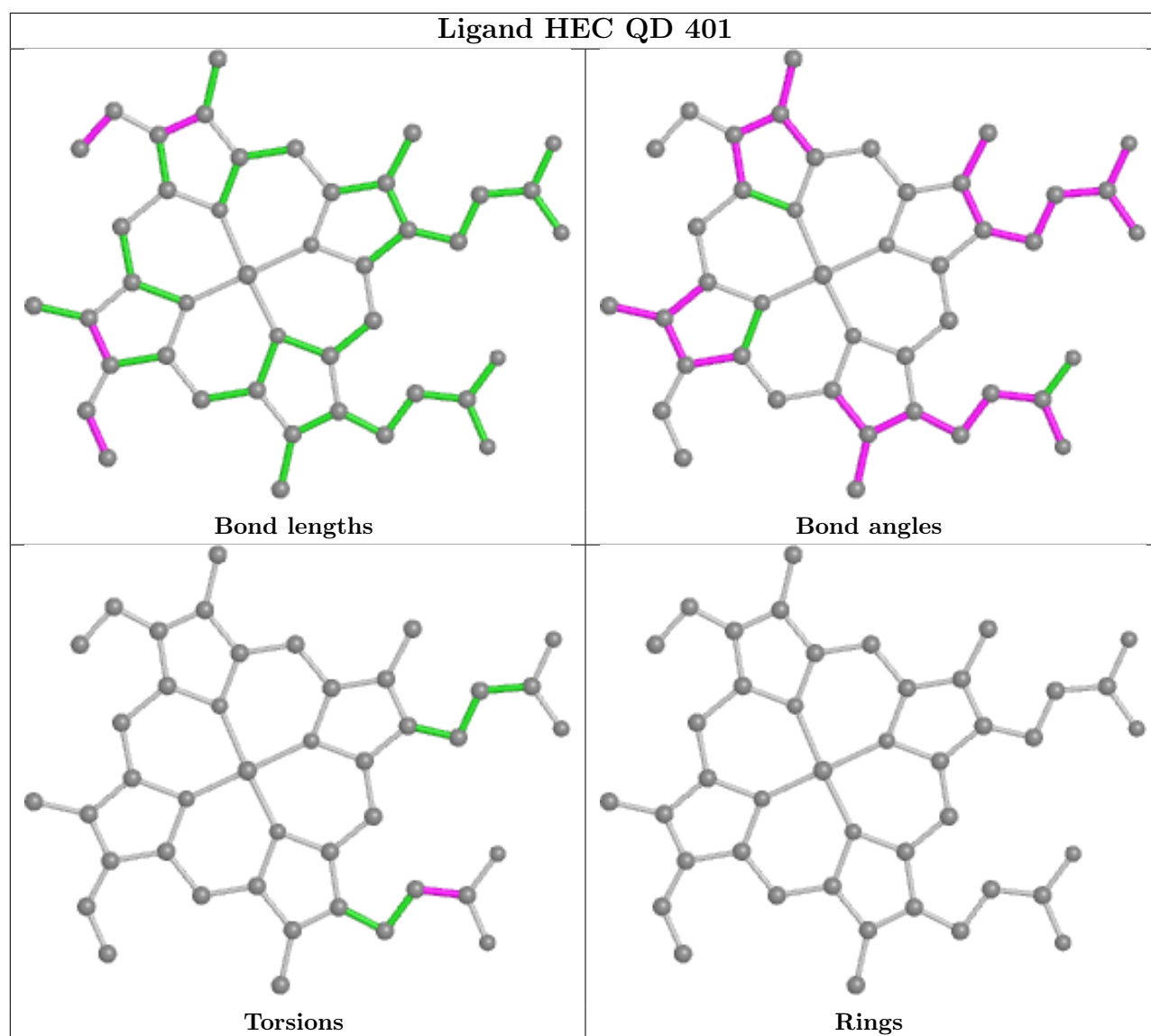
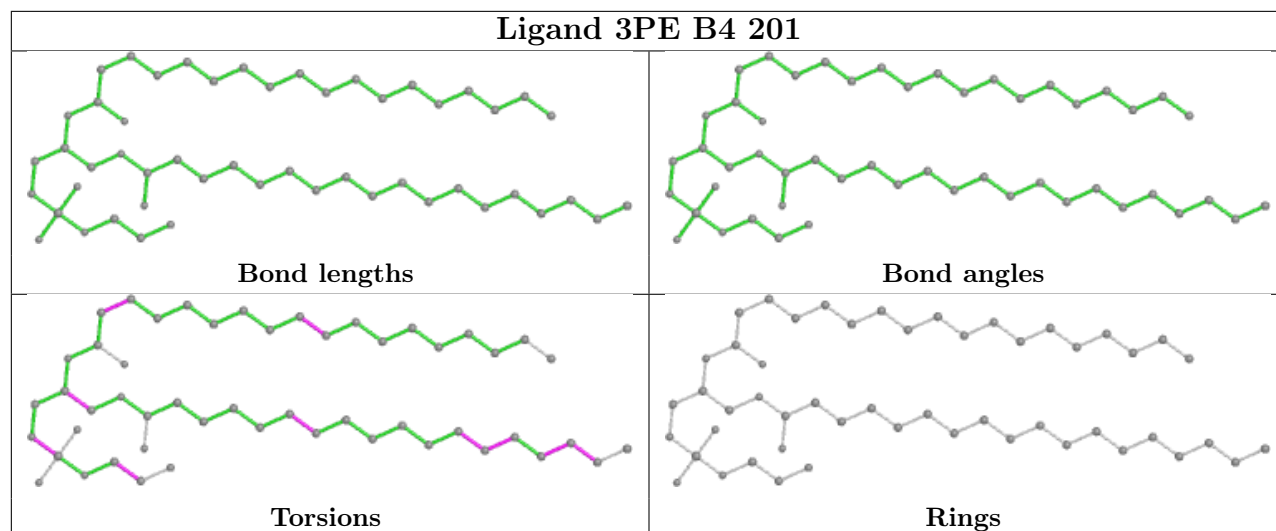
Ligand ZMP AB 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

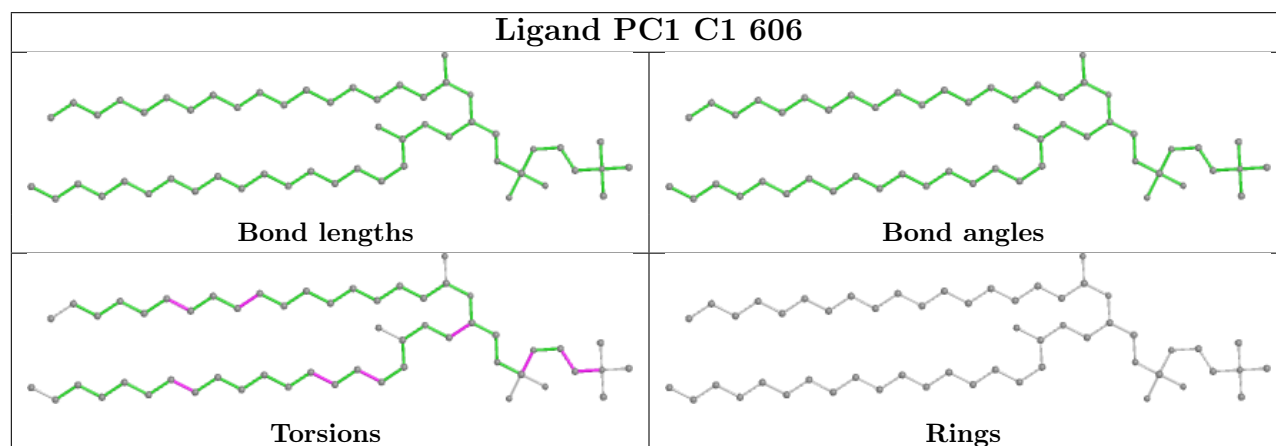
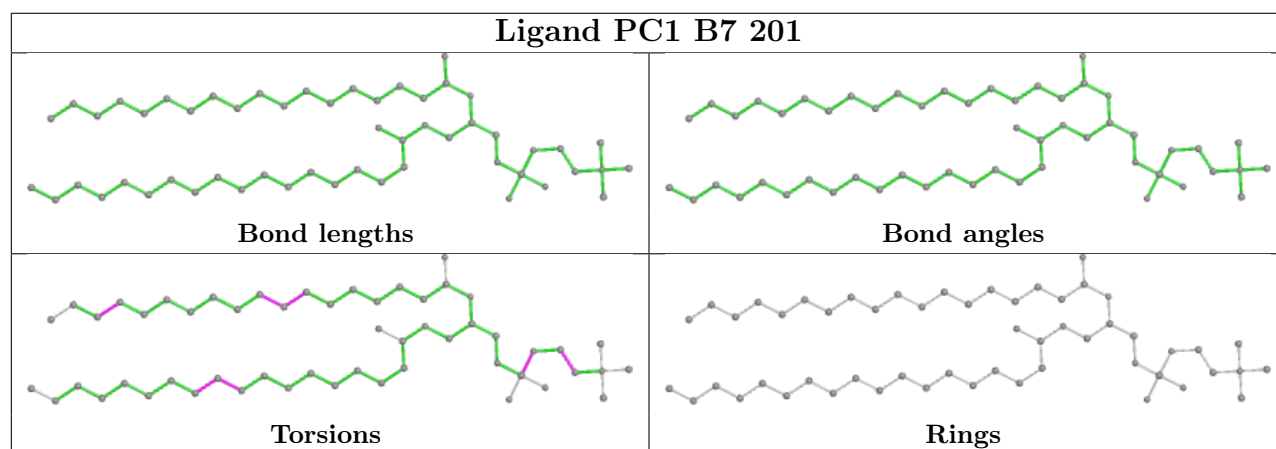
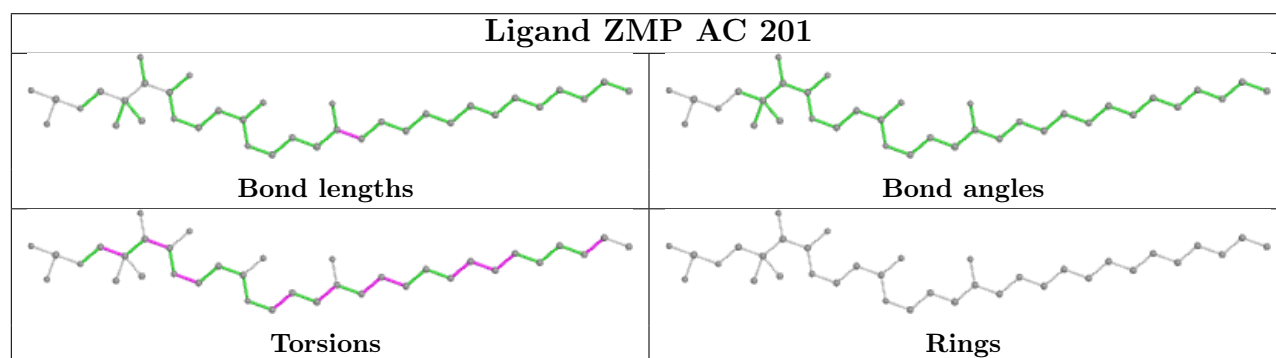
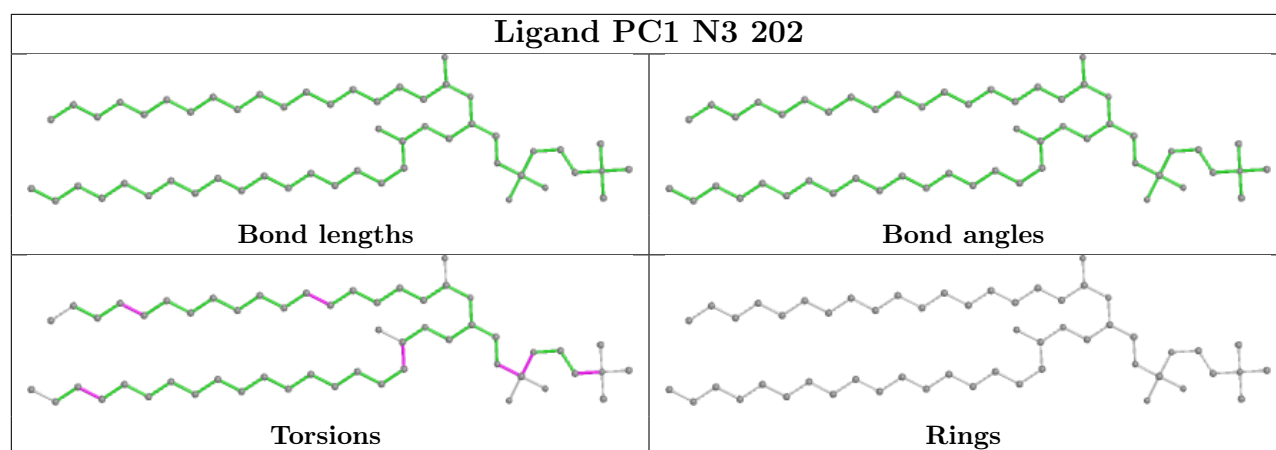


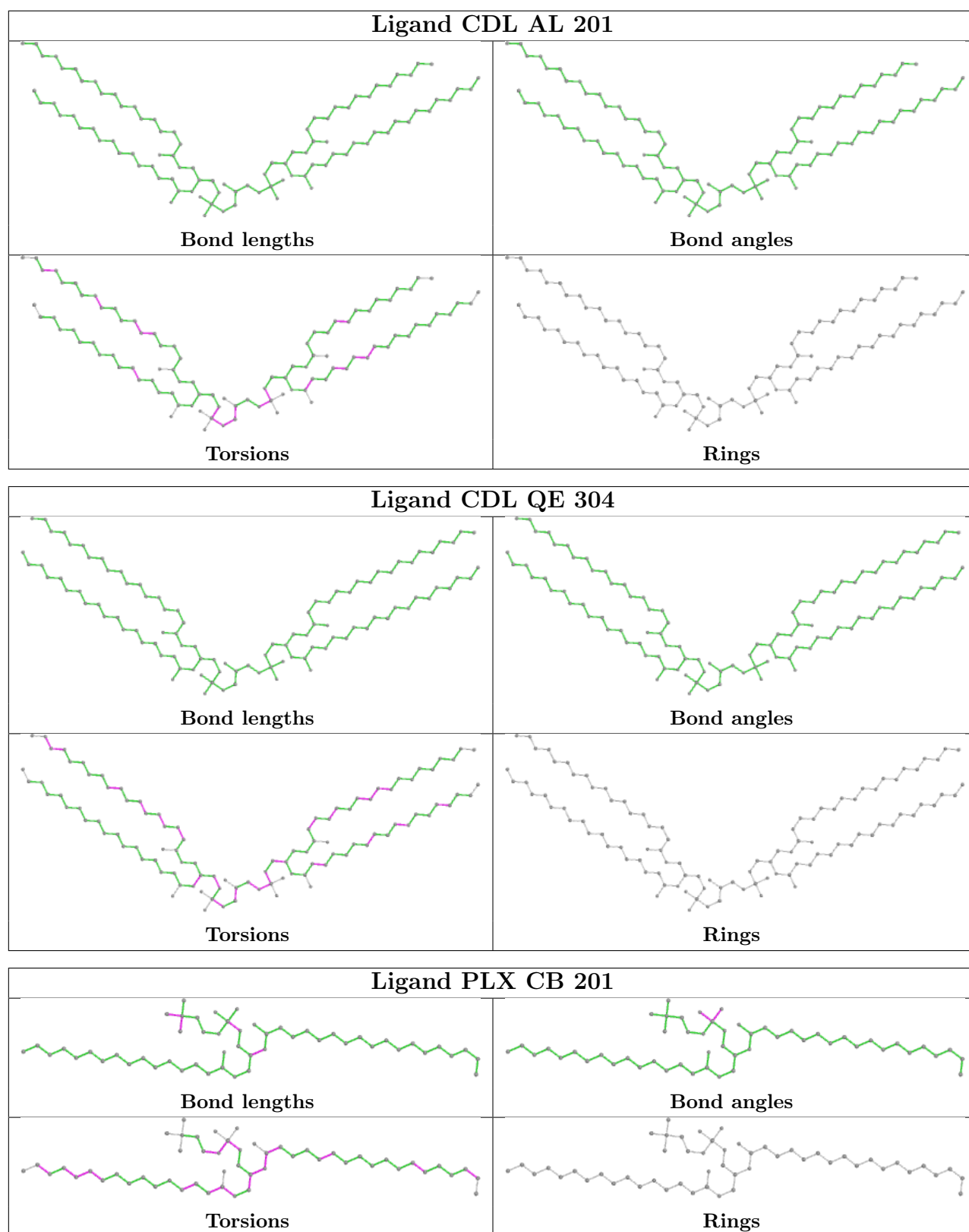


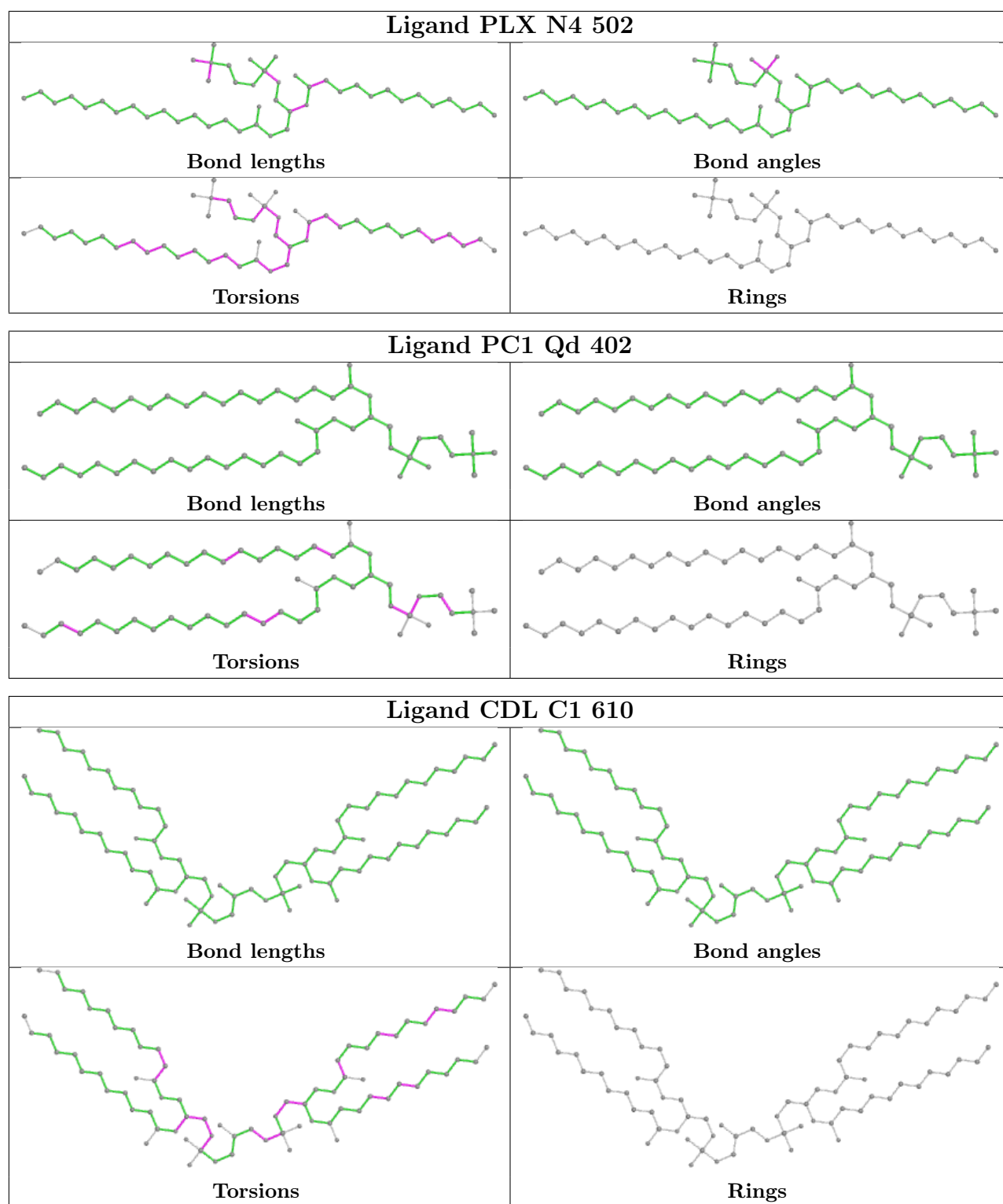


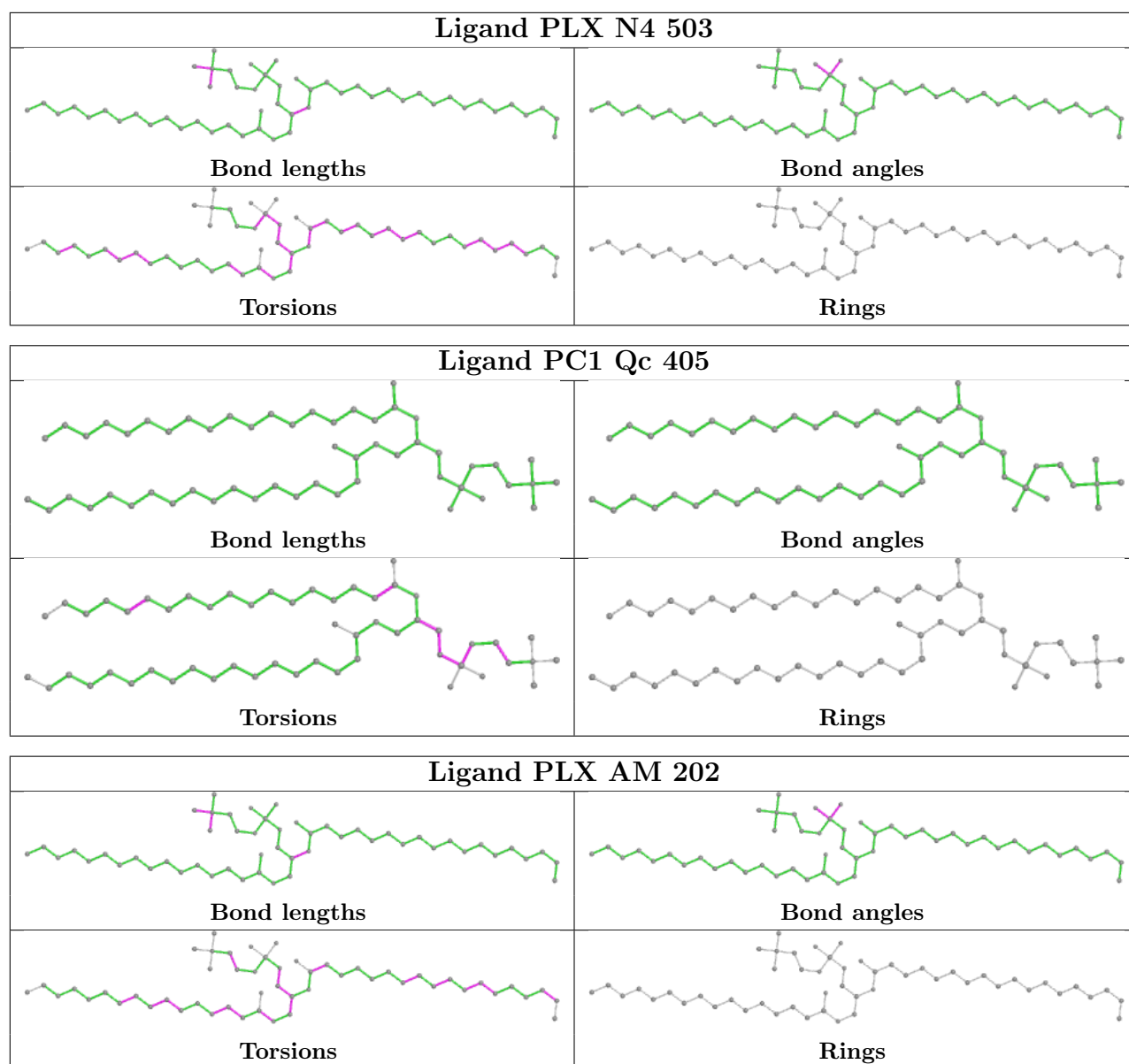


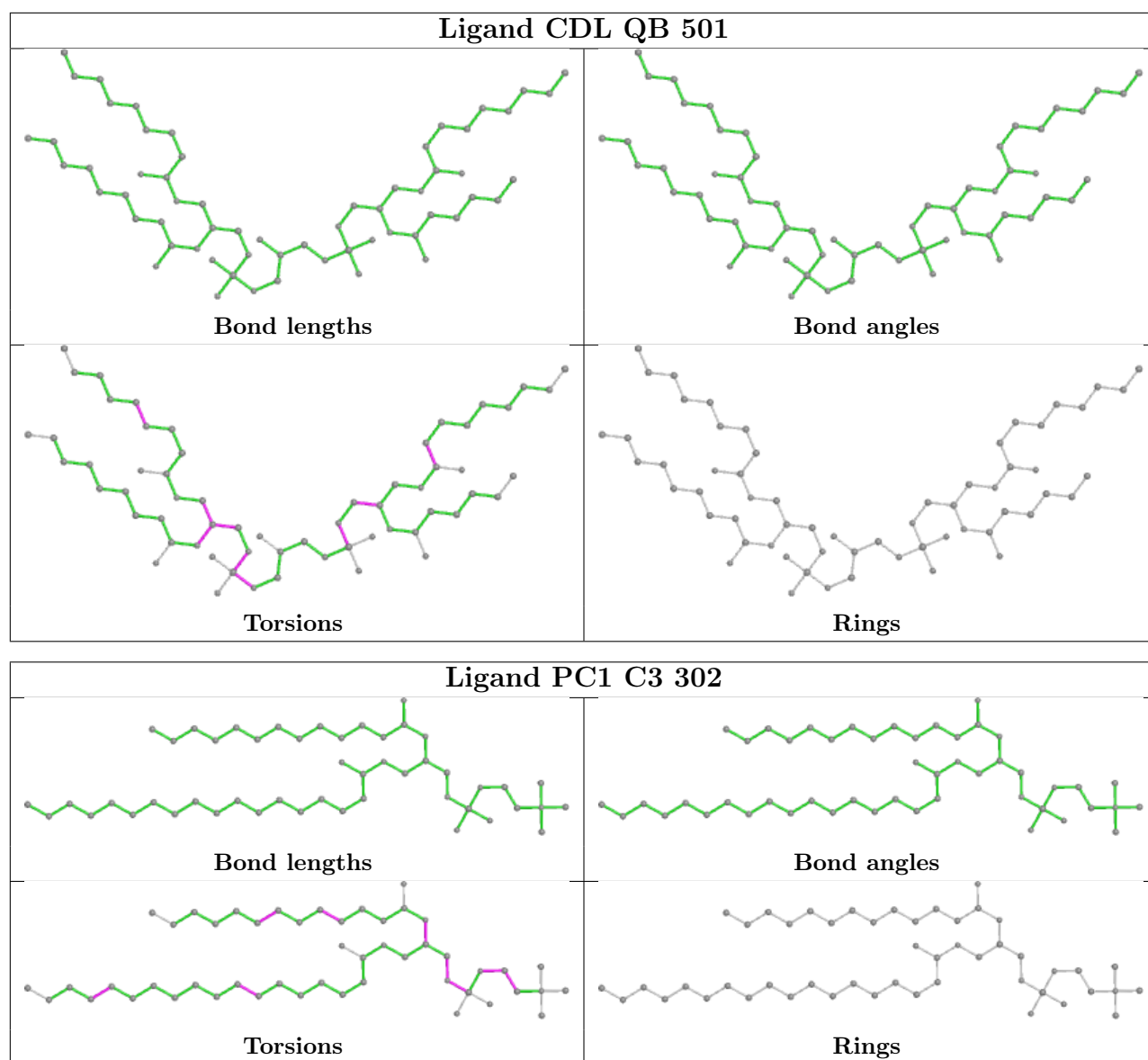


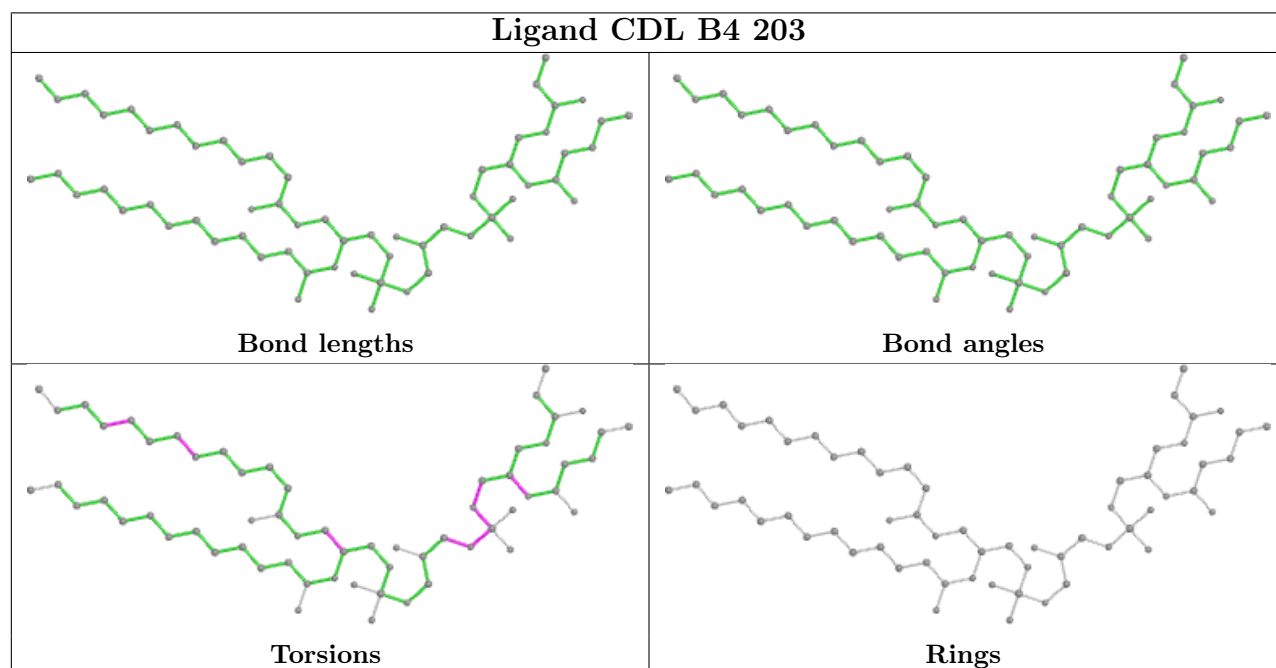
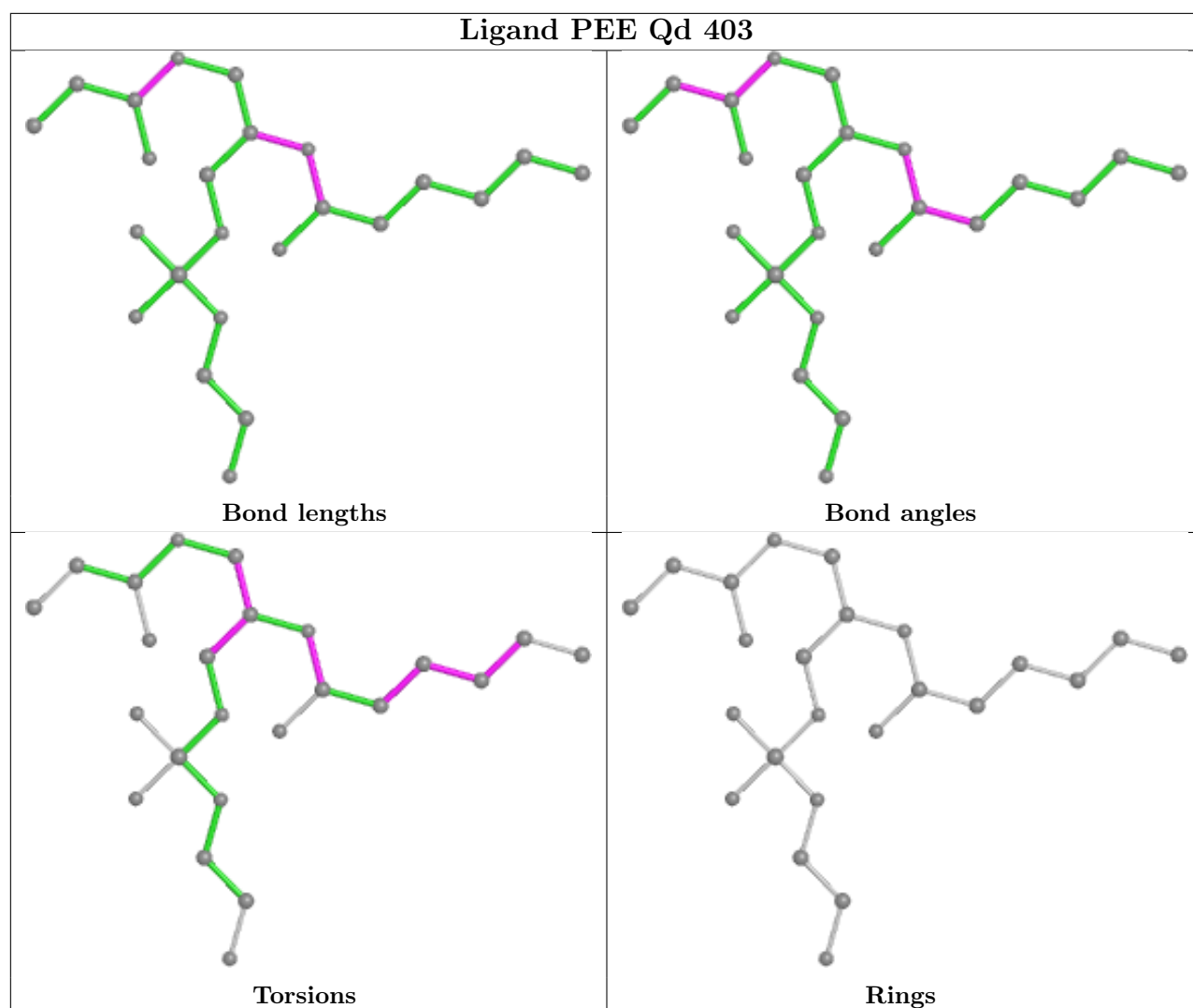


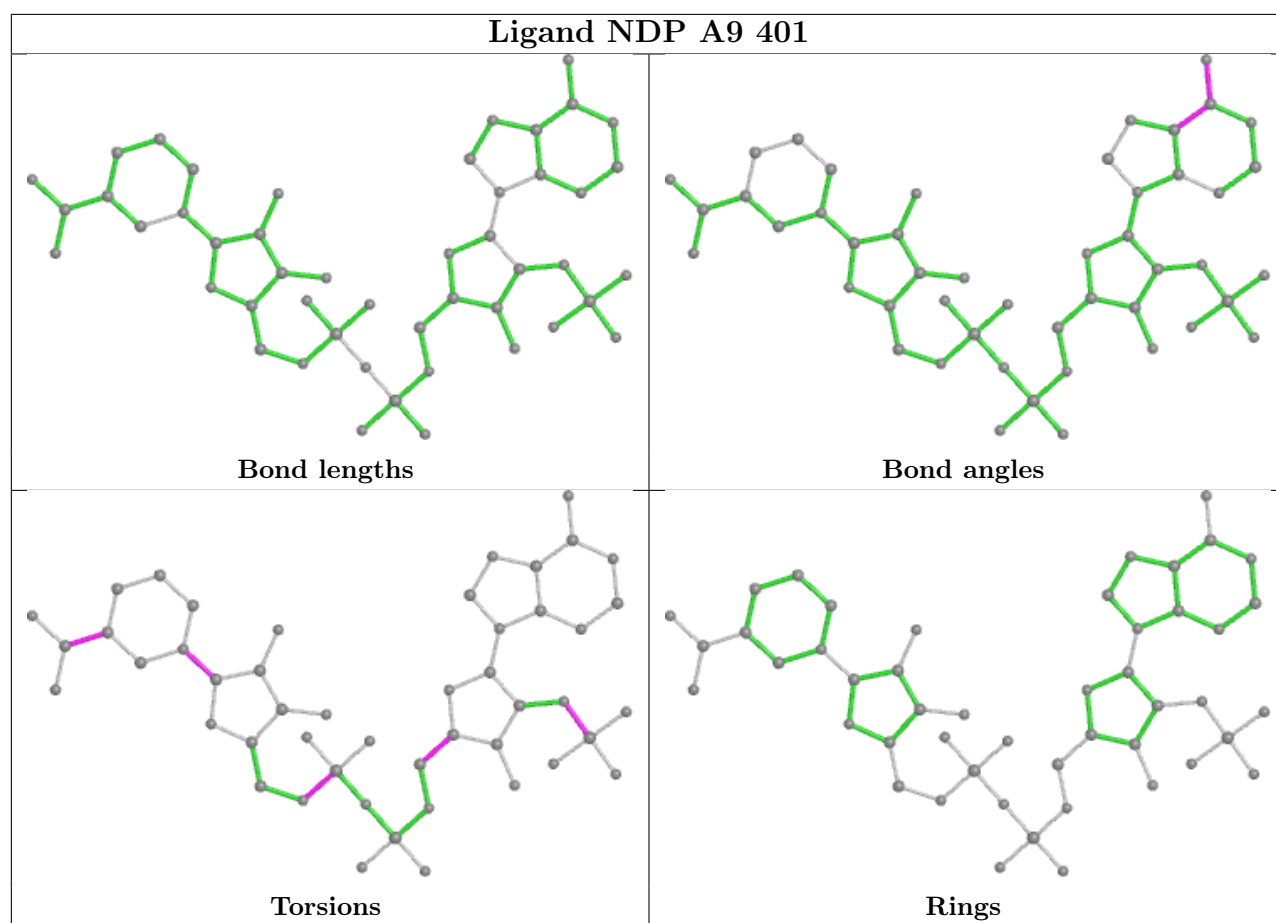




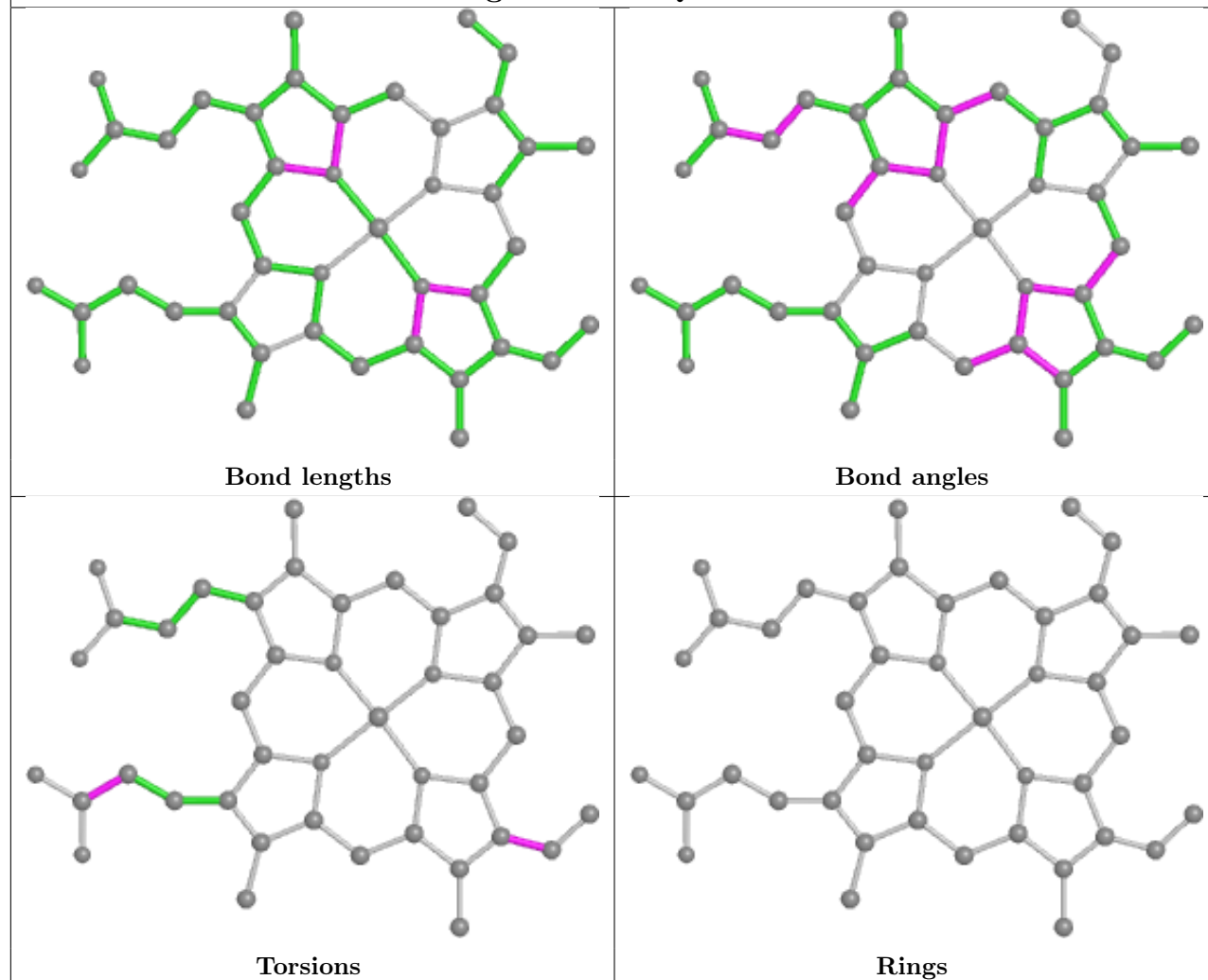




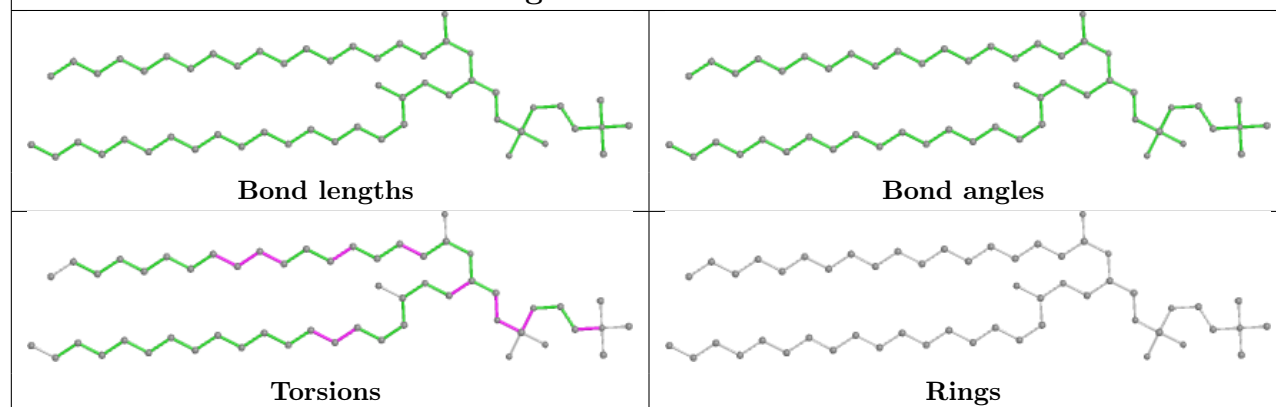


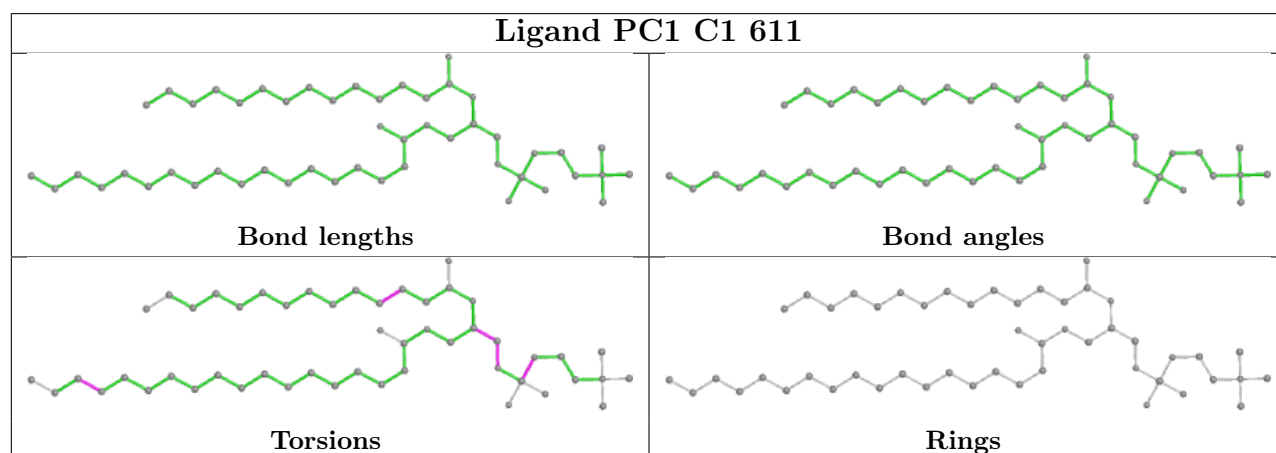
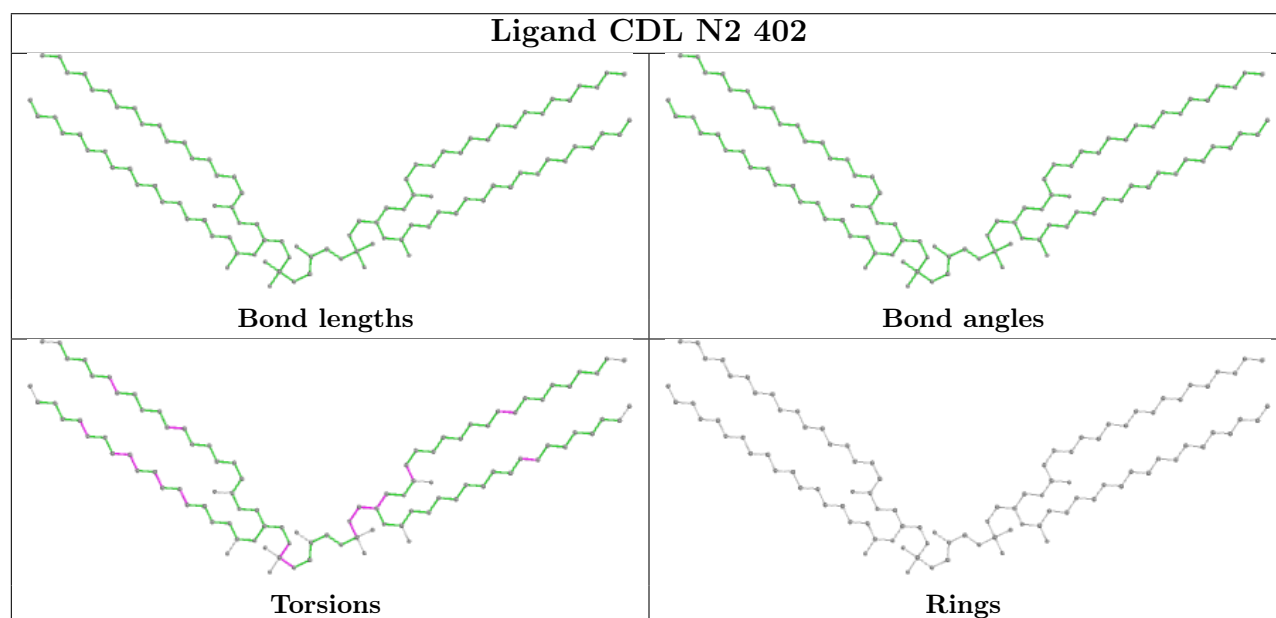
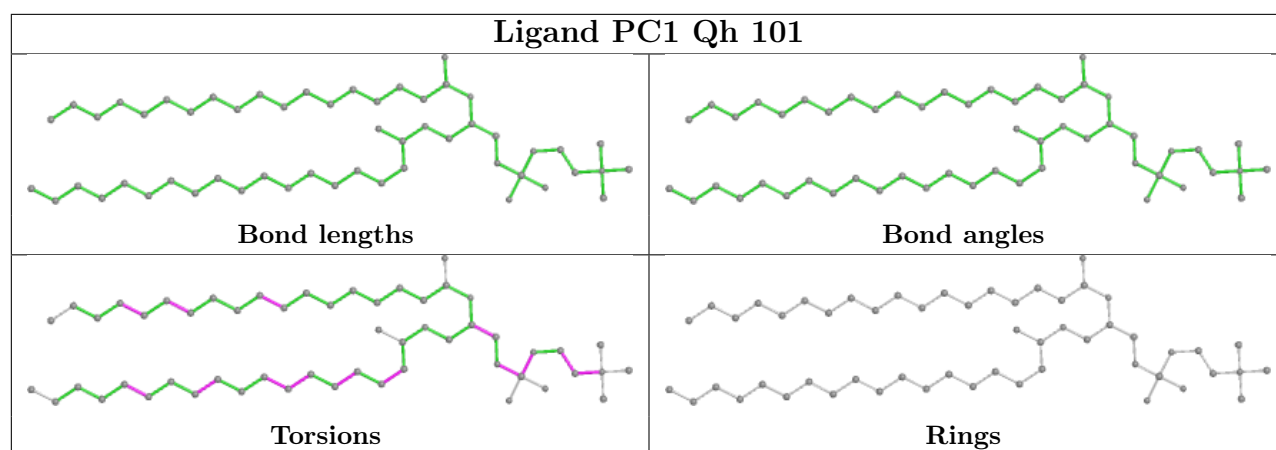


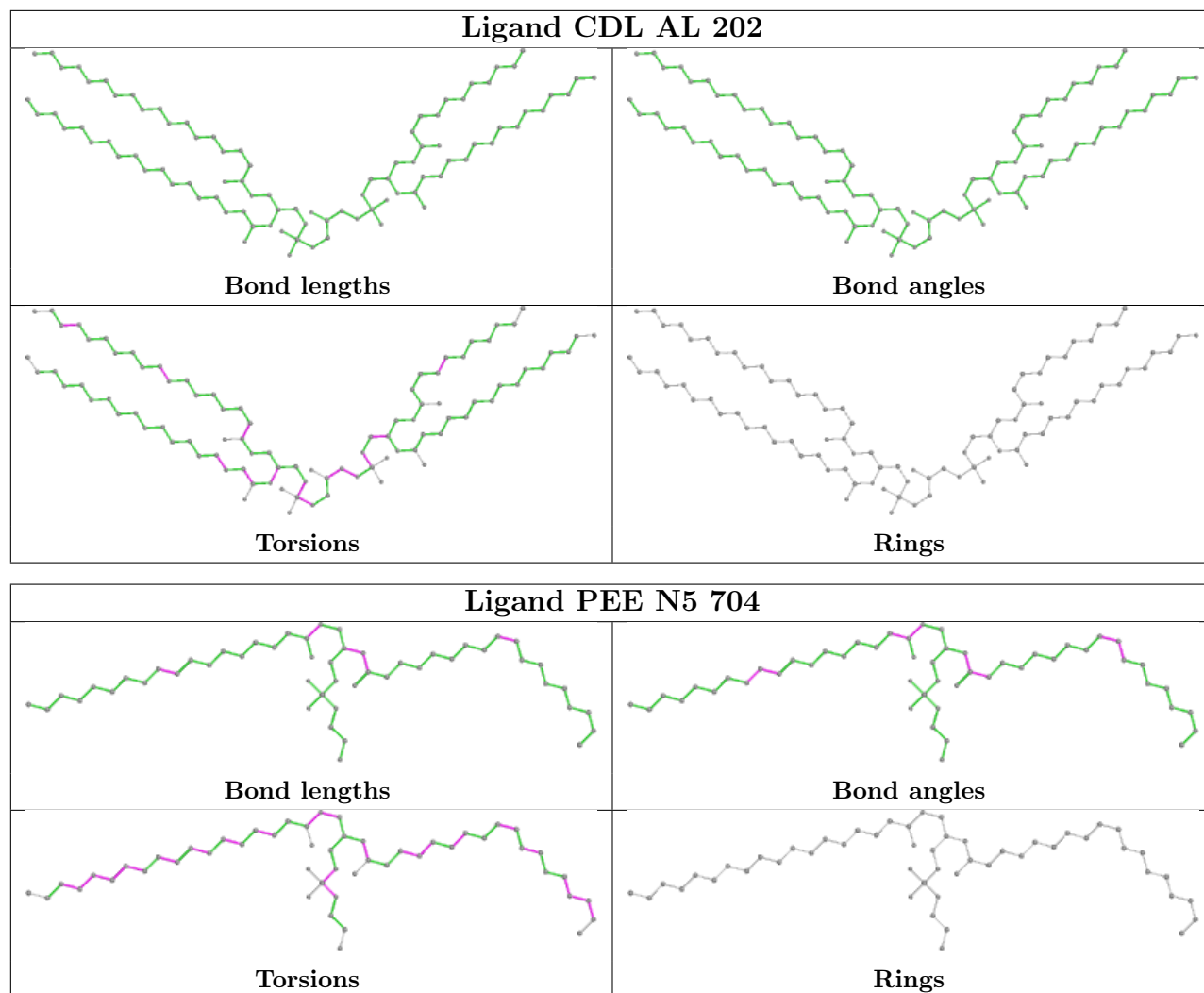
## Ligand HEM QC 402

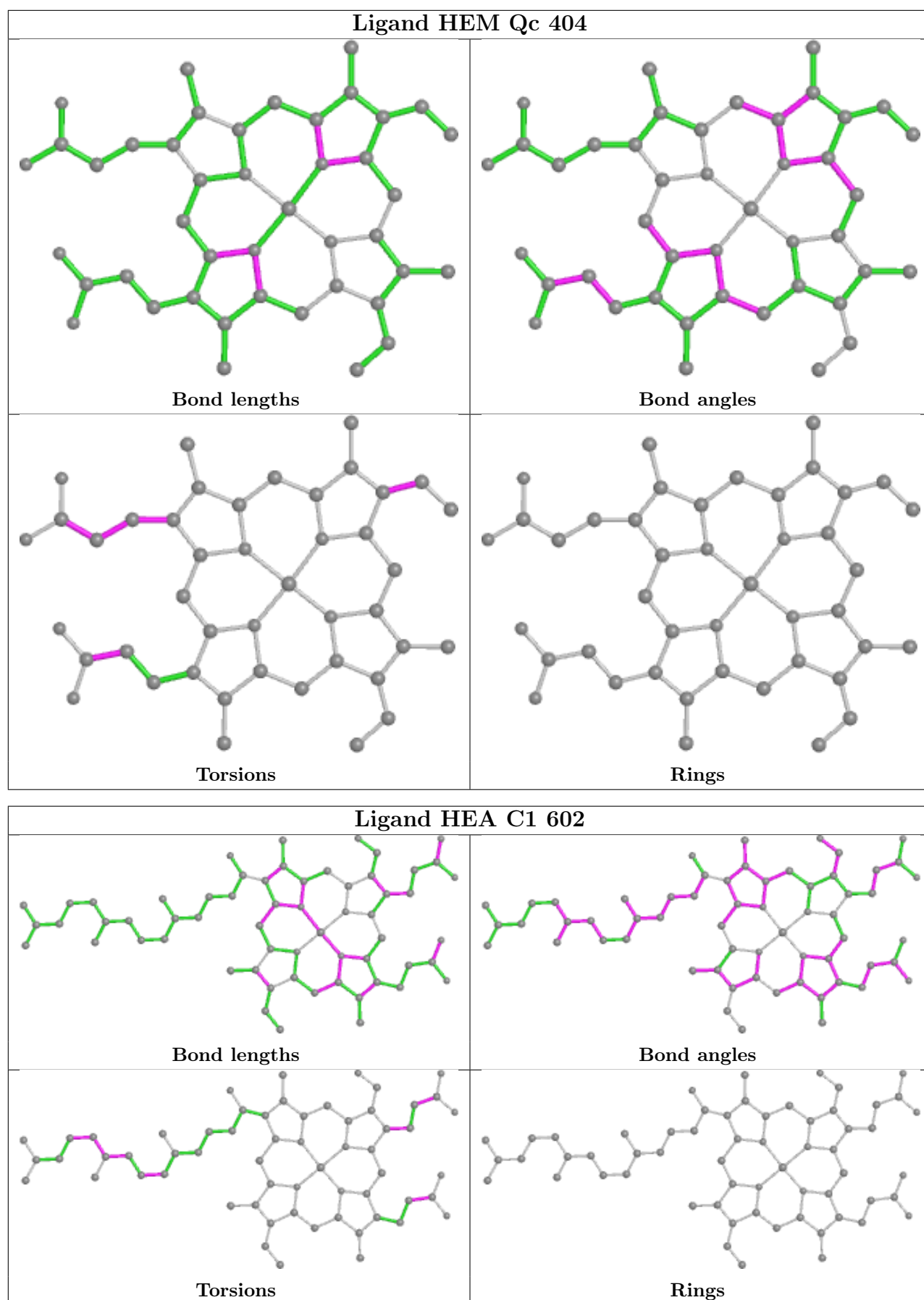


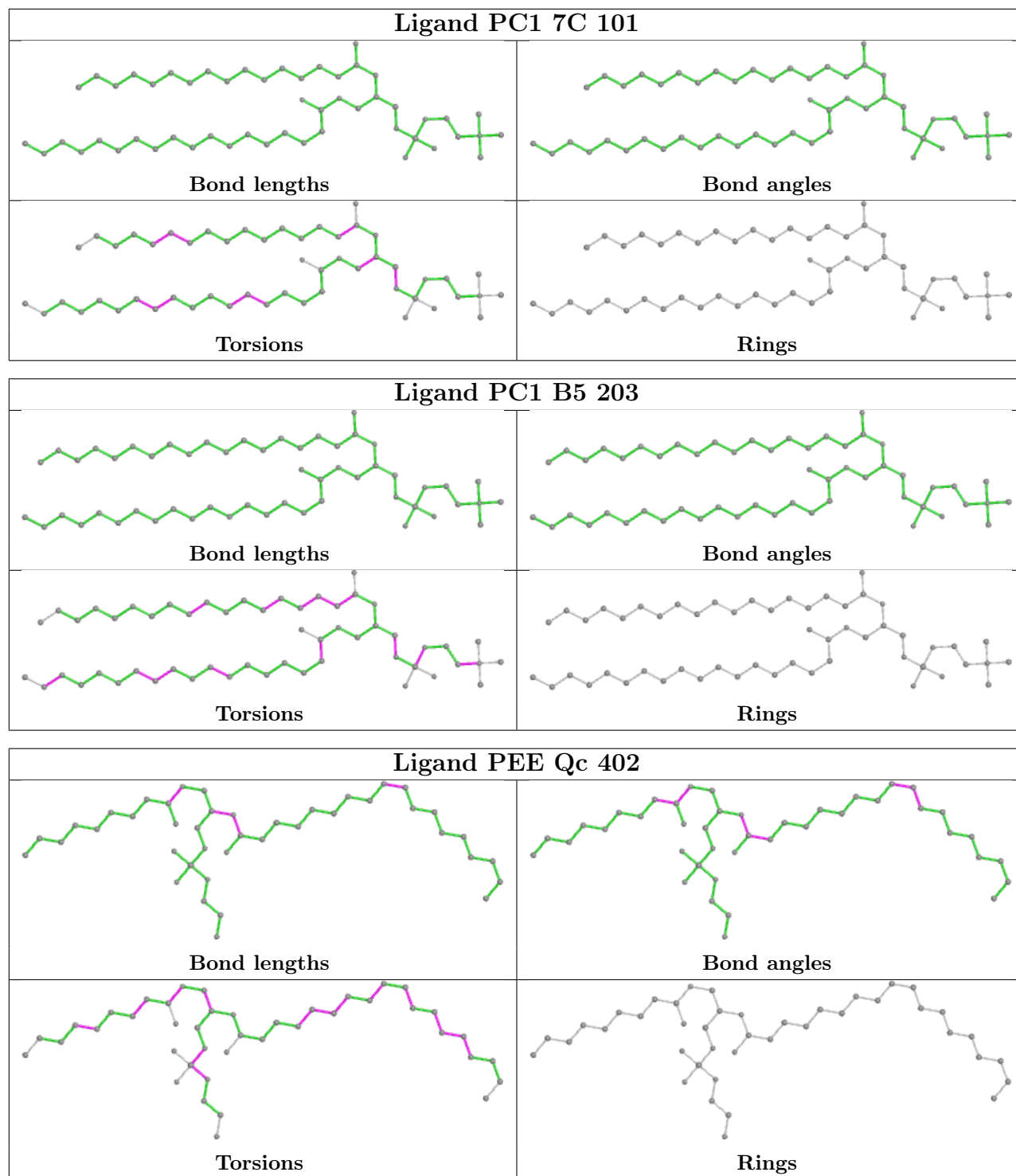
## Ligand PC1 N1 401

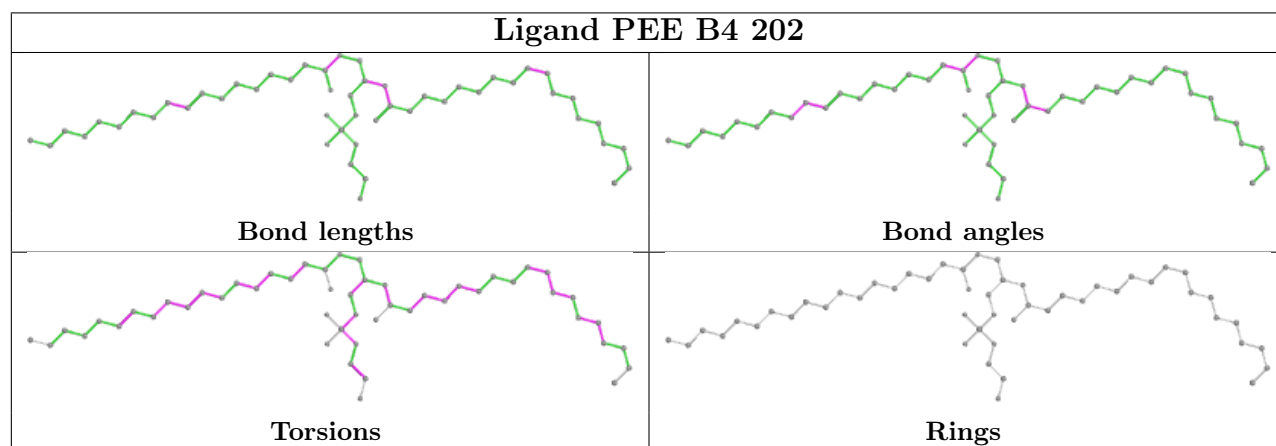
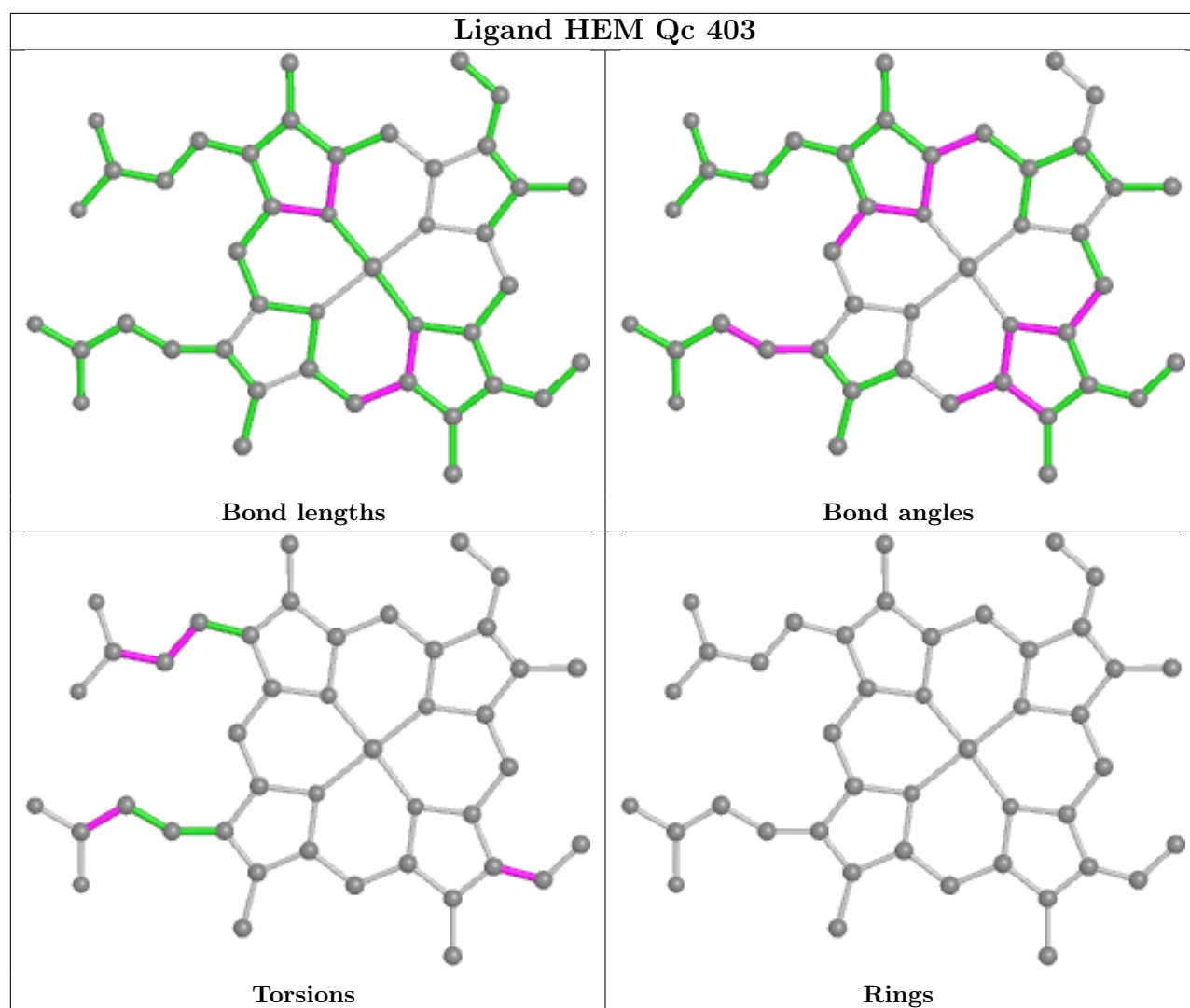


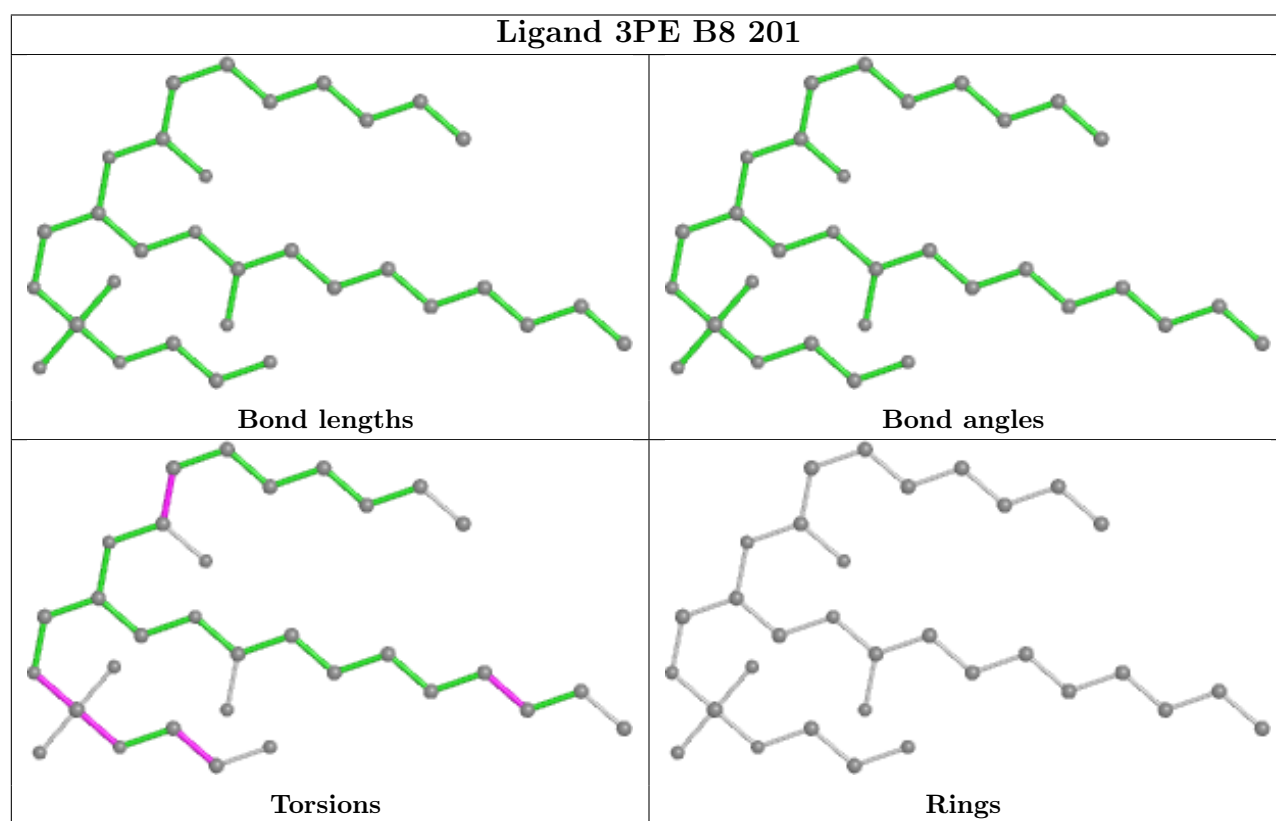
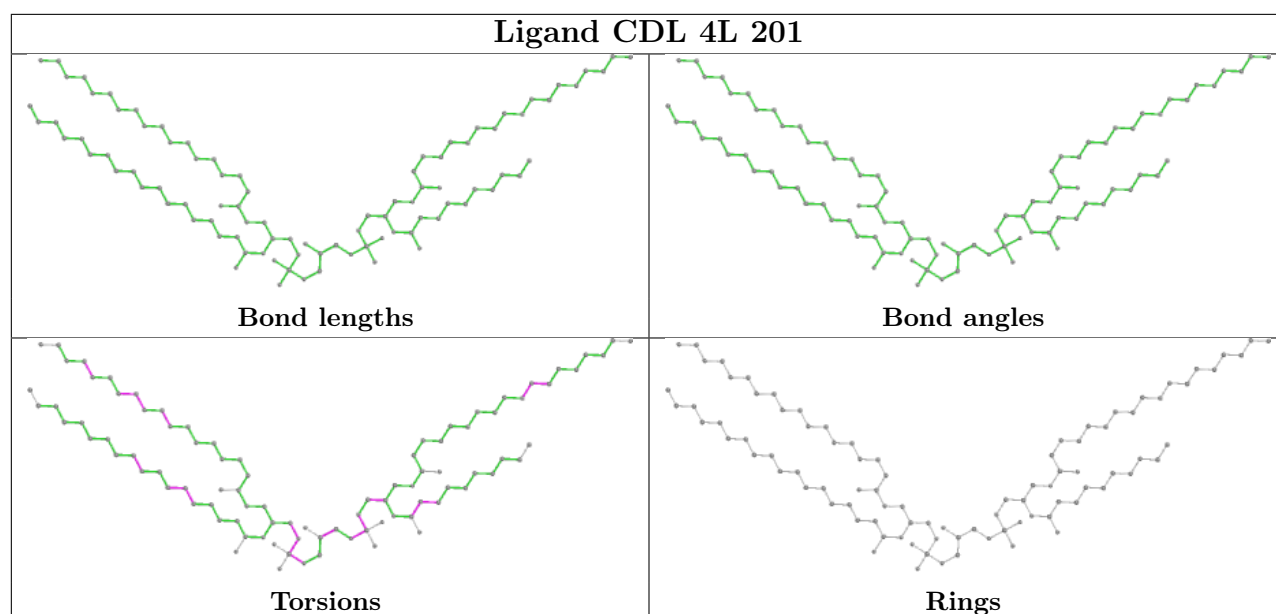


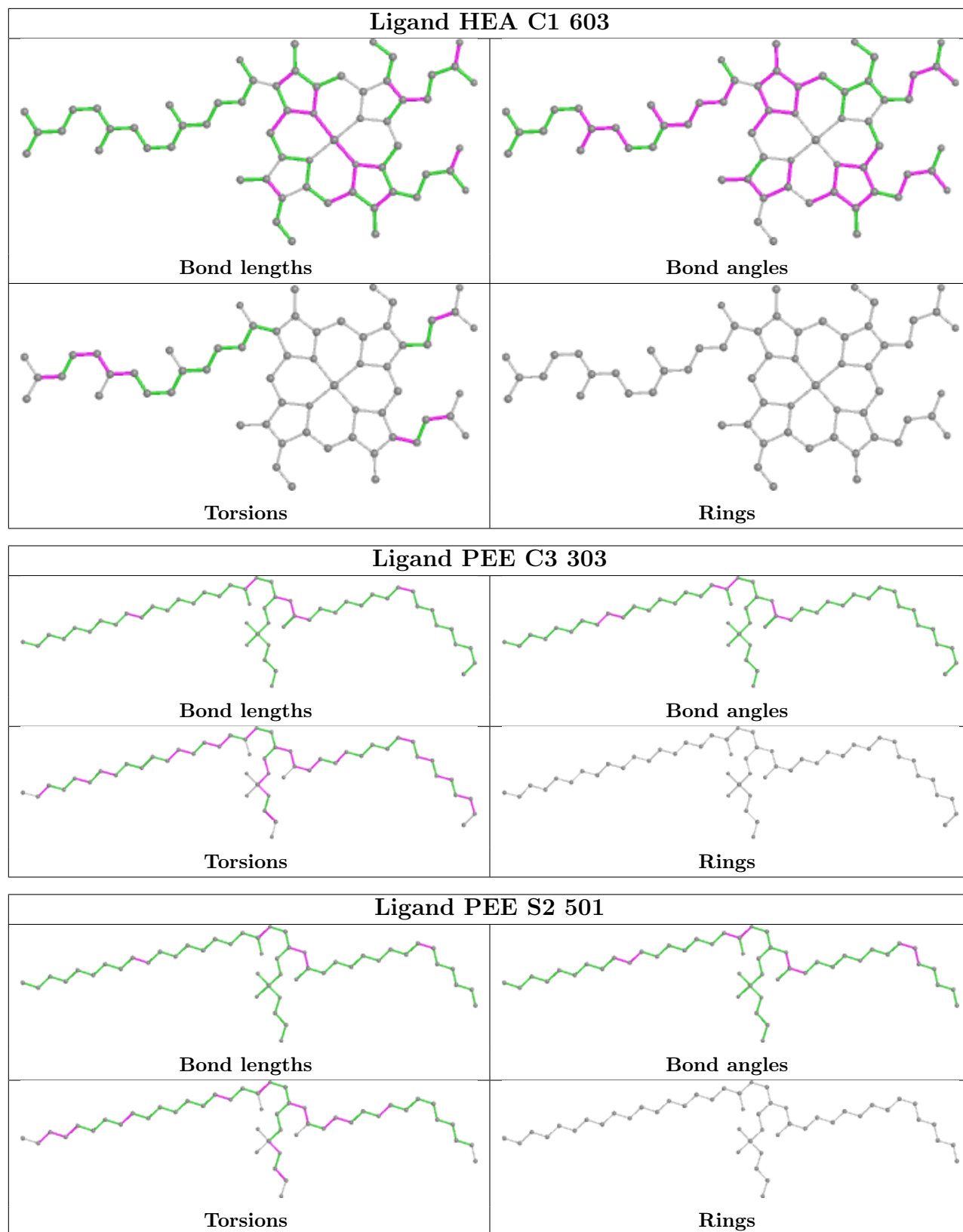


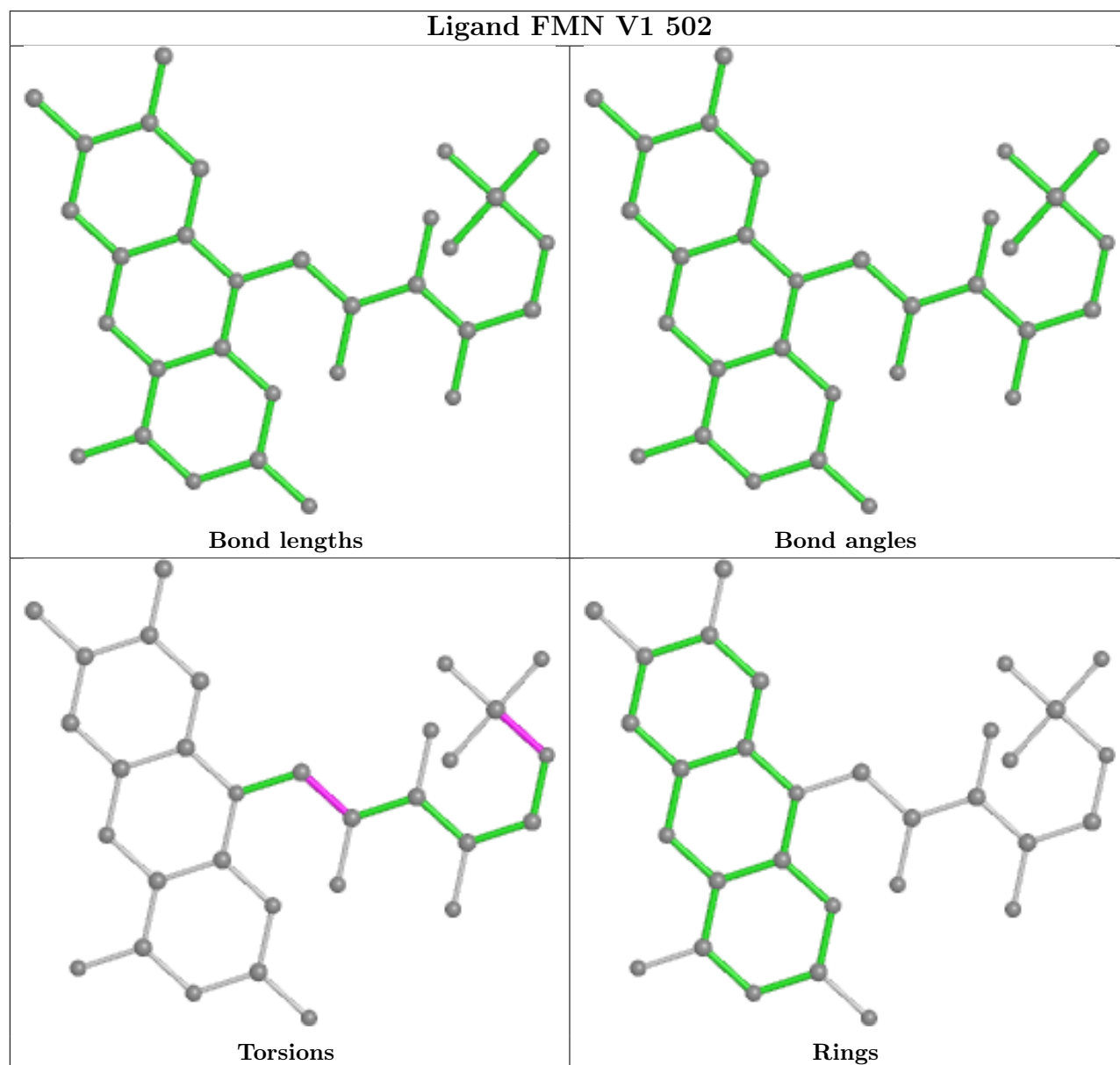
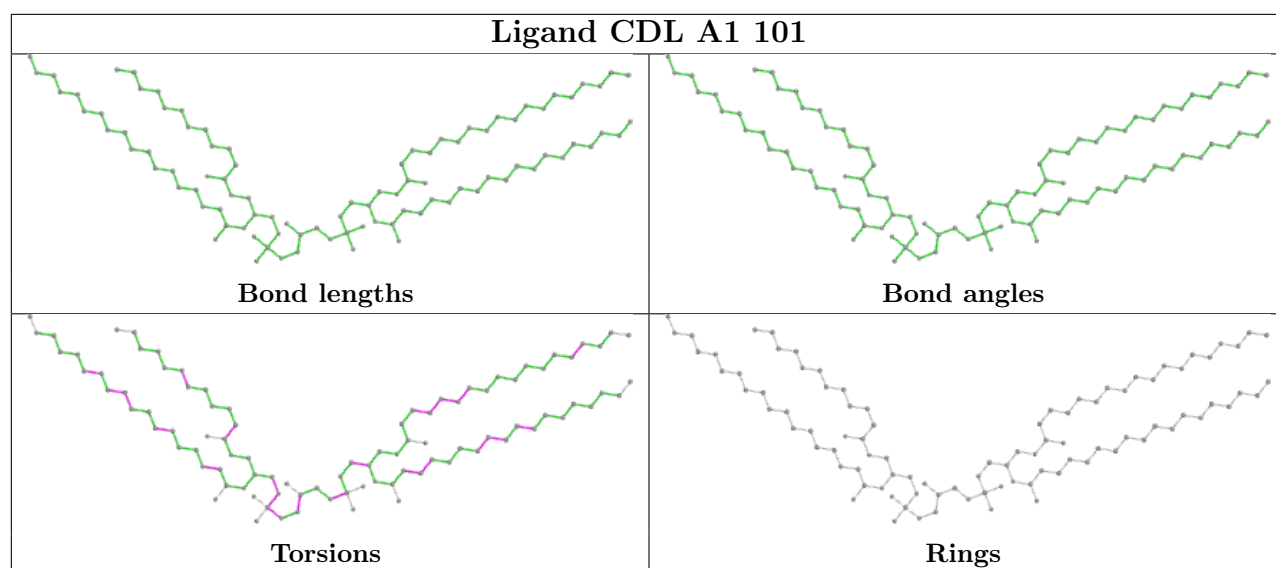


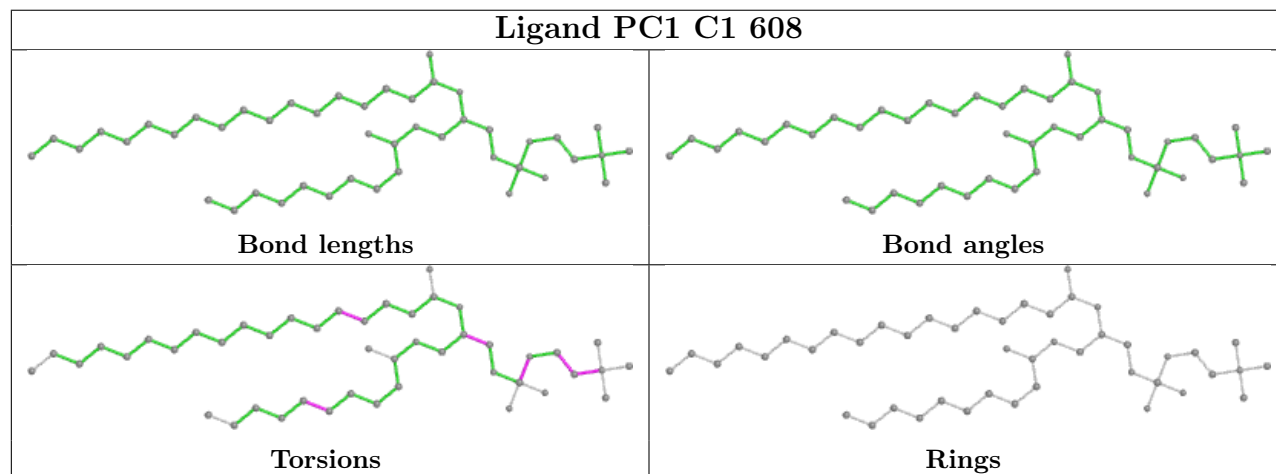
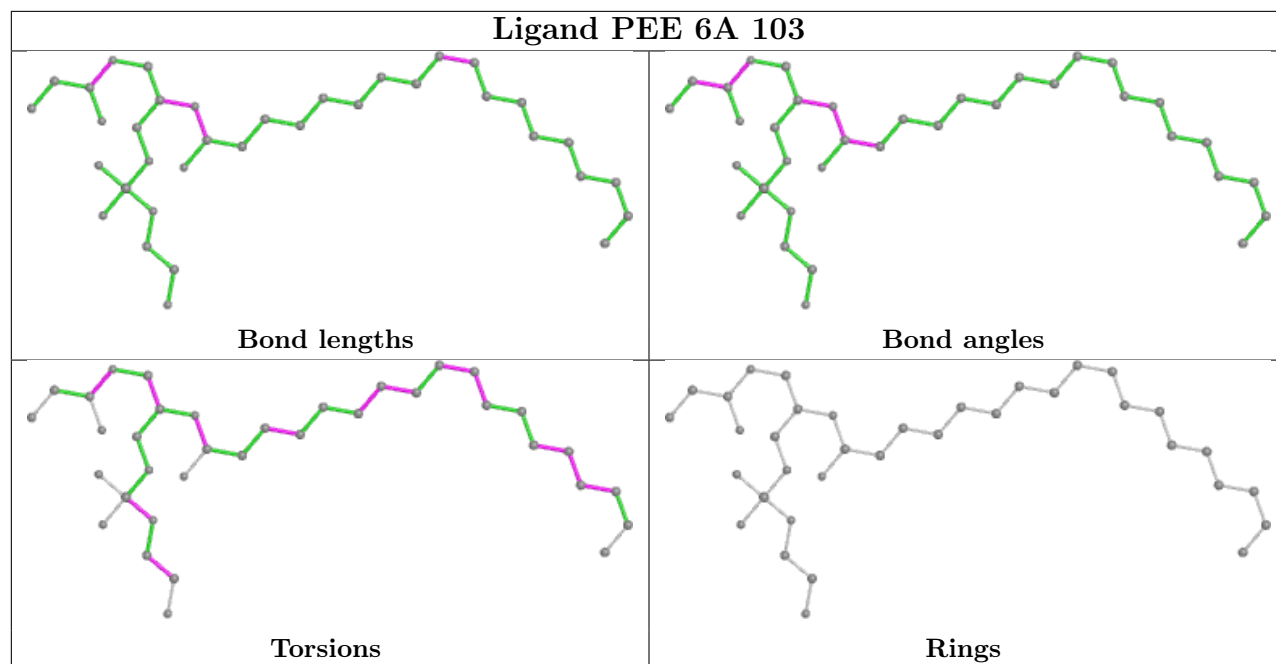


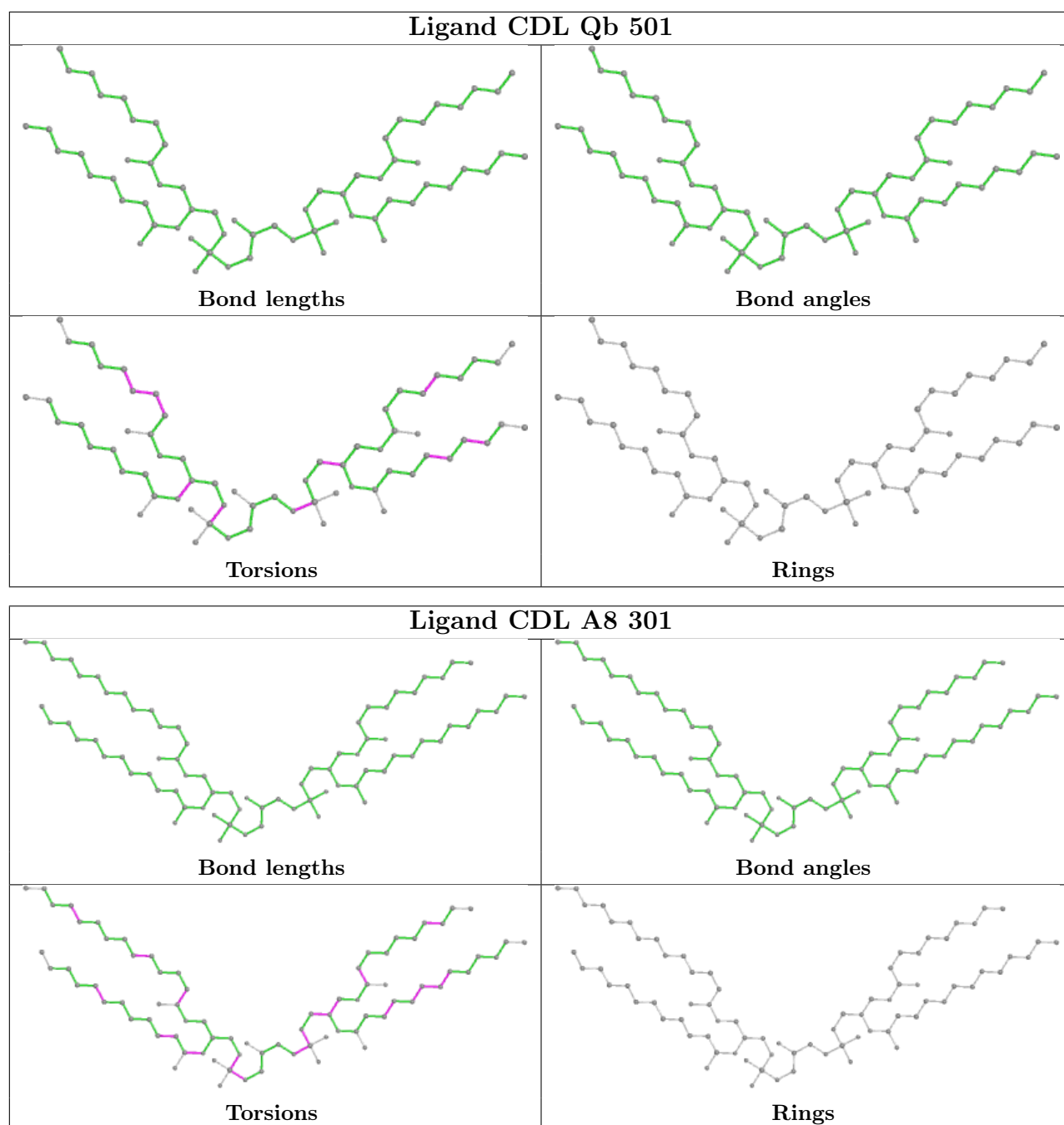


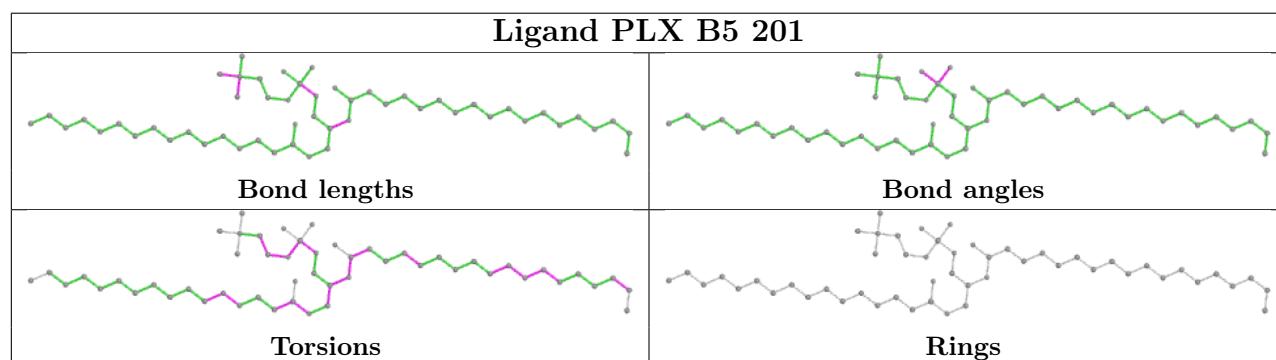
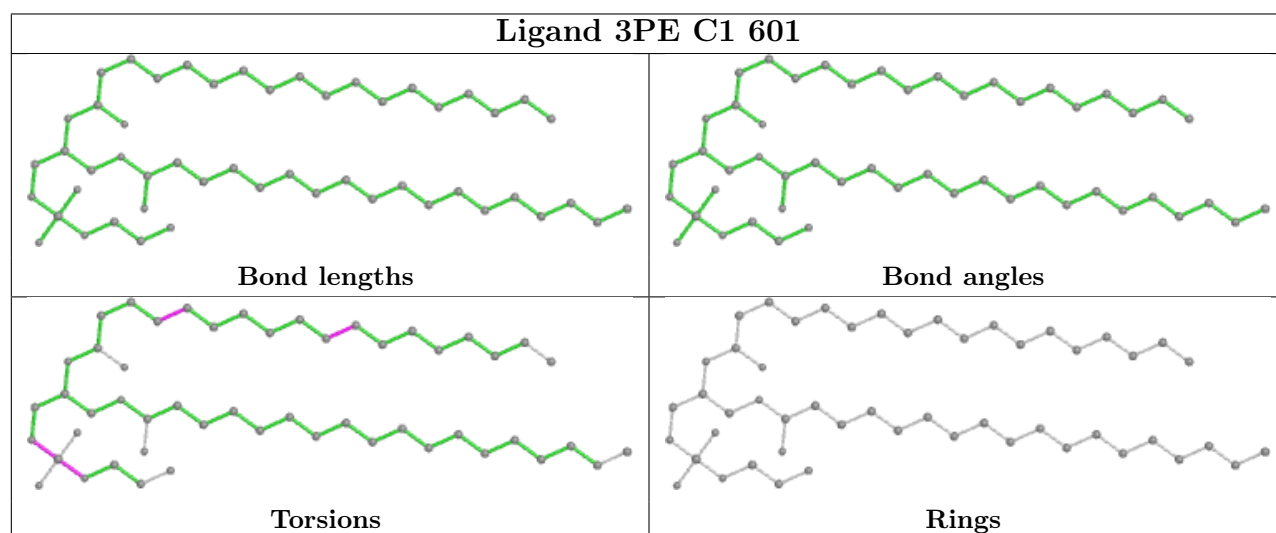
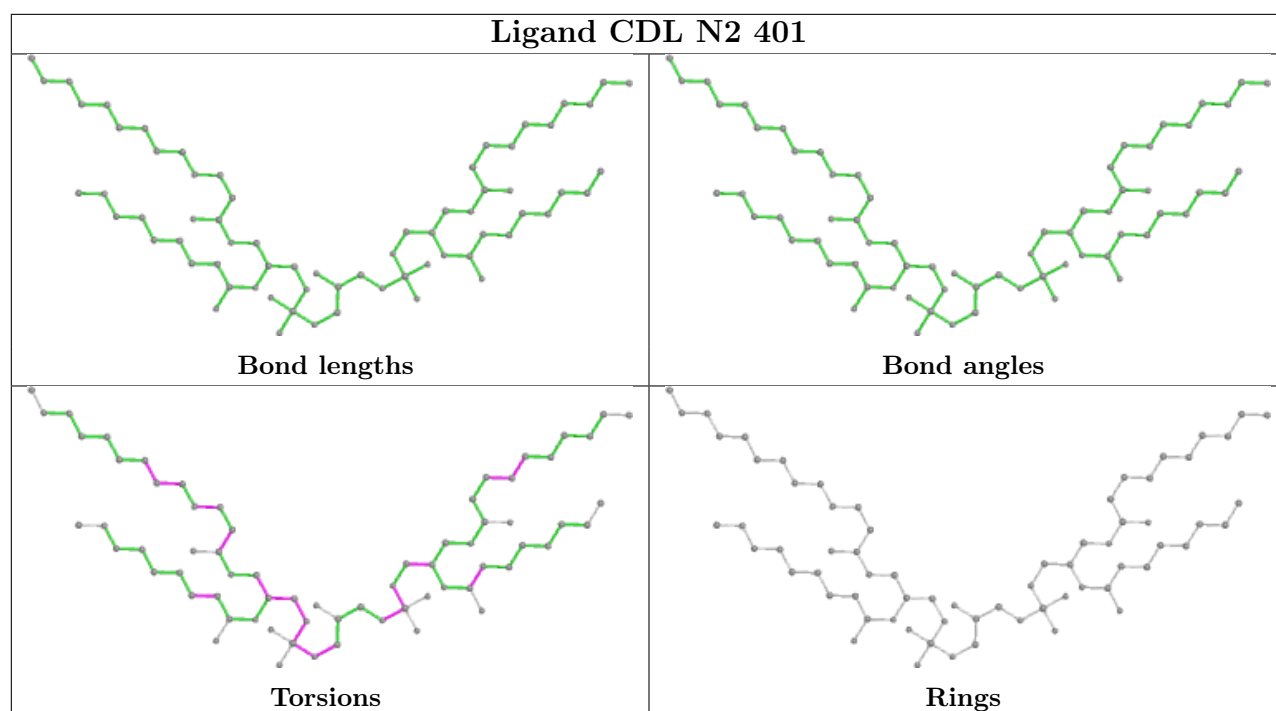


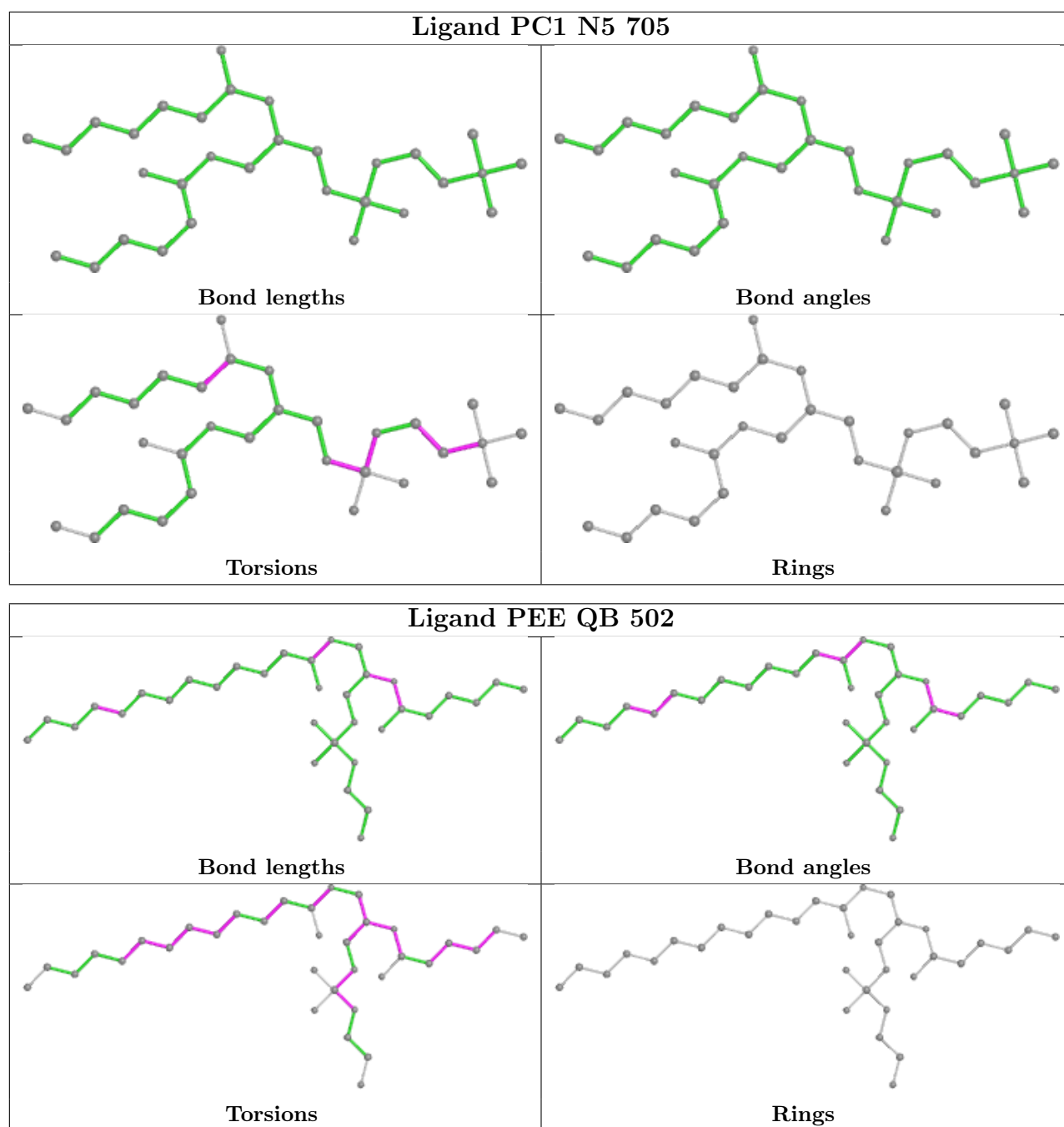


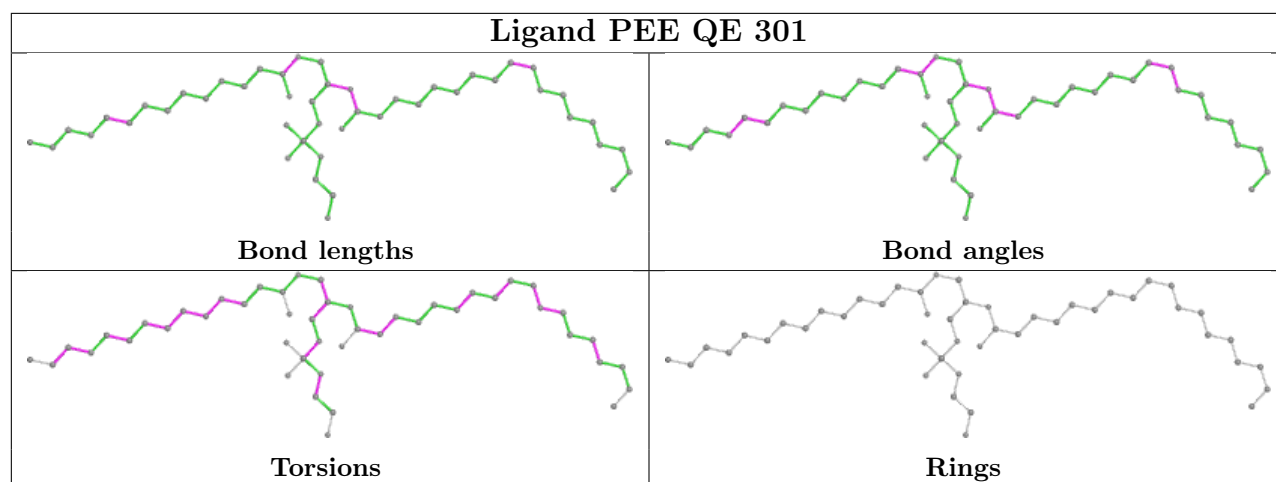
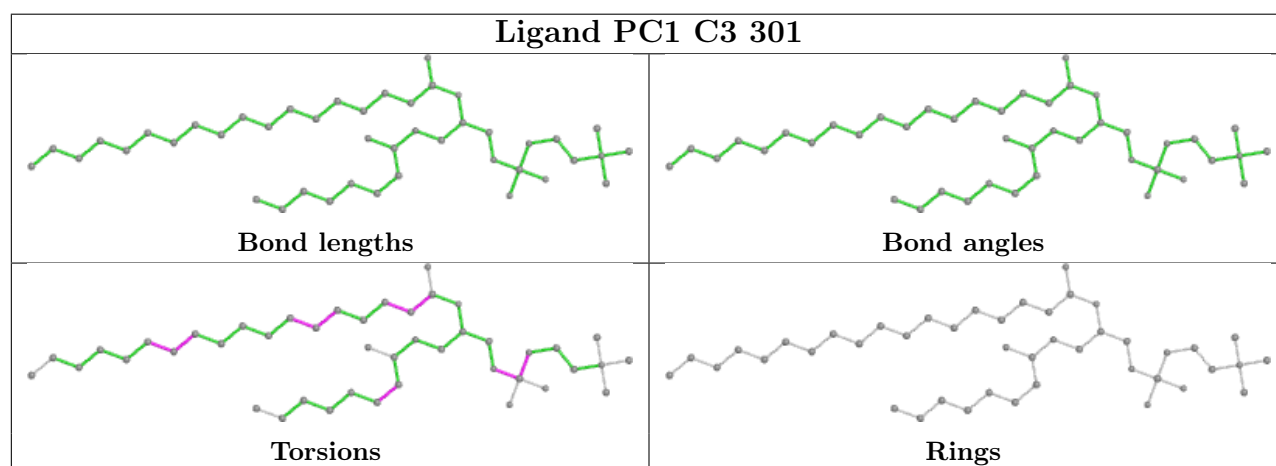
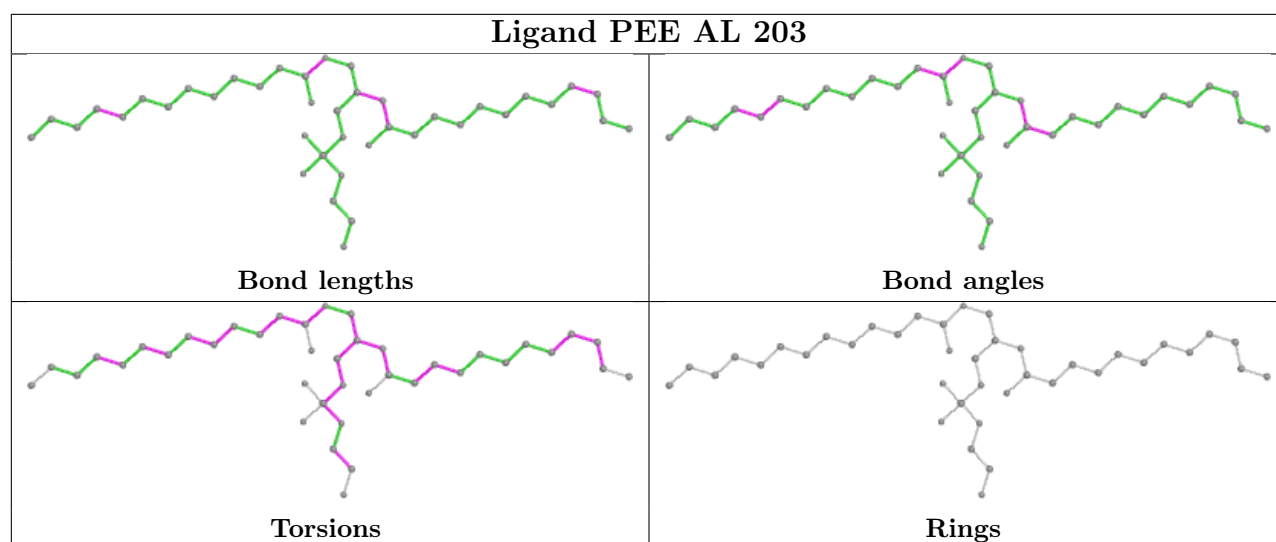


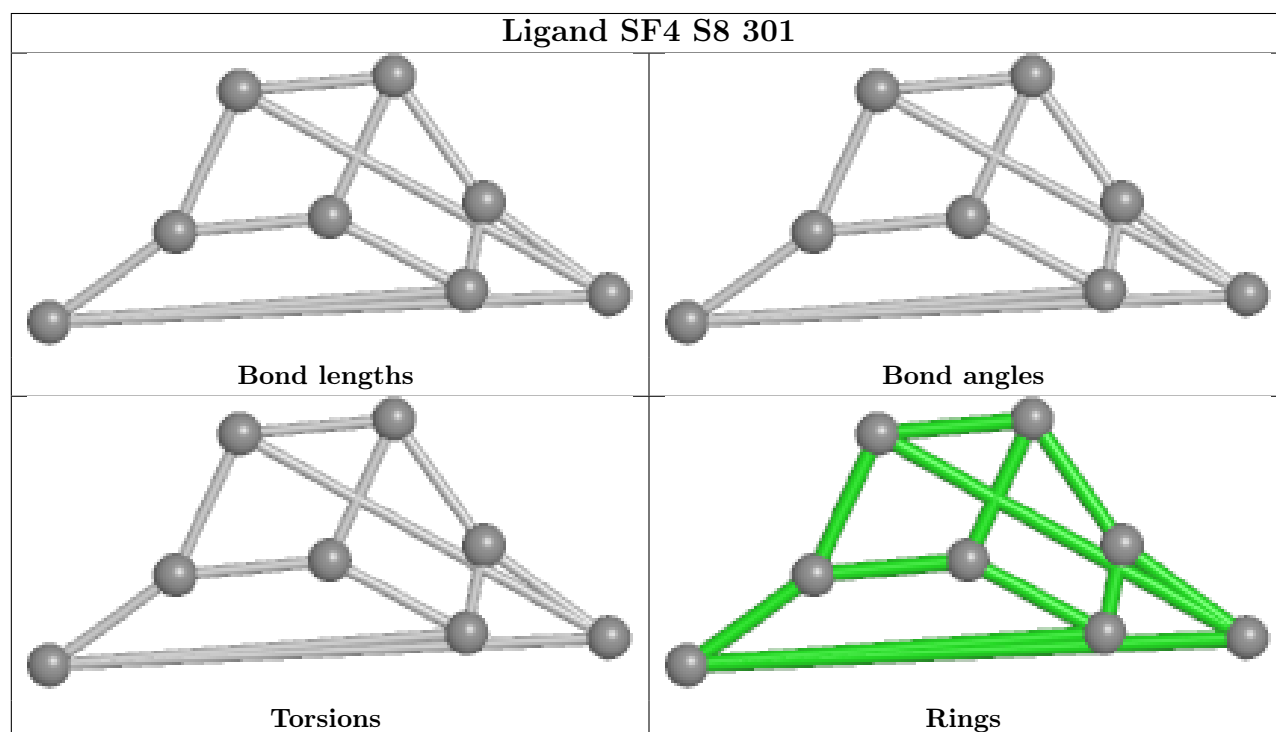
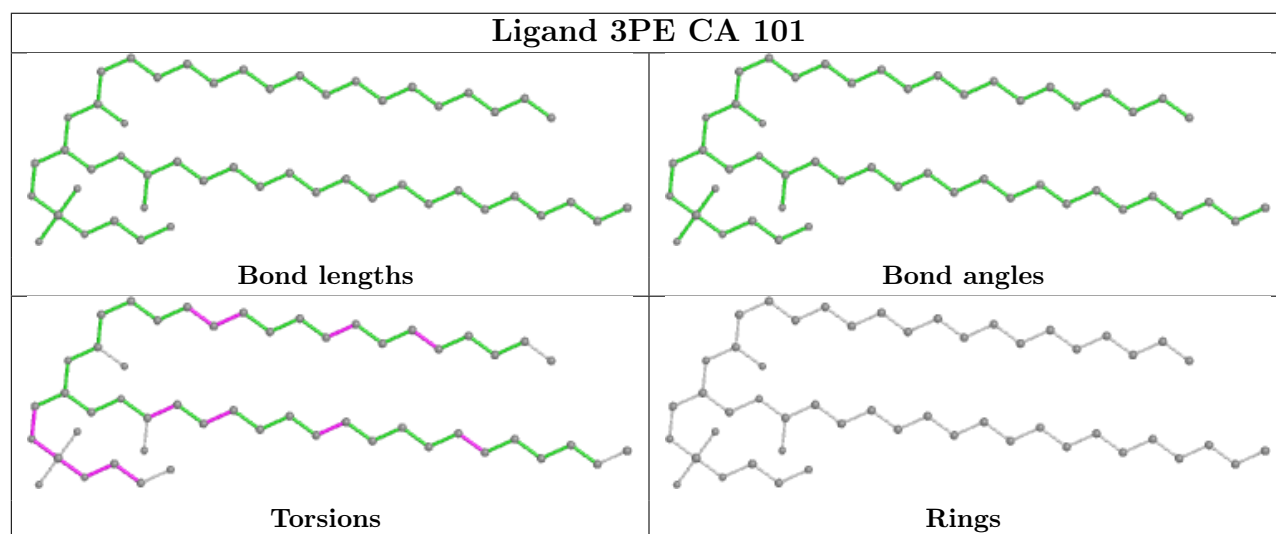
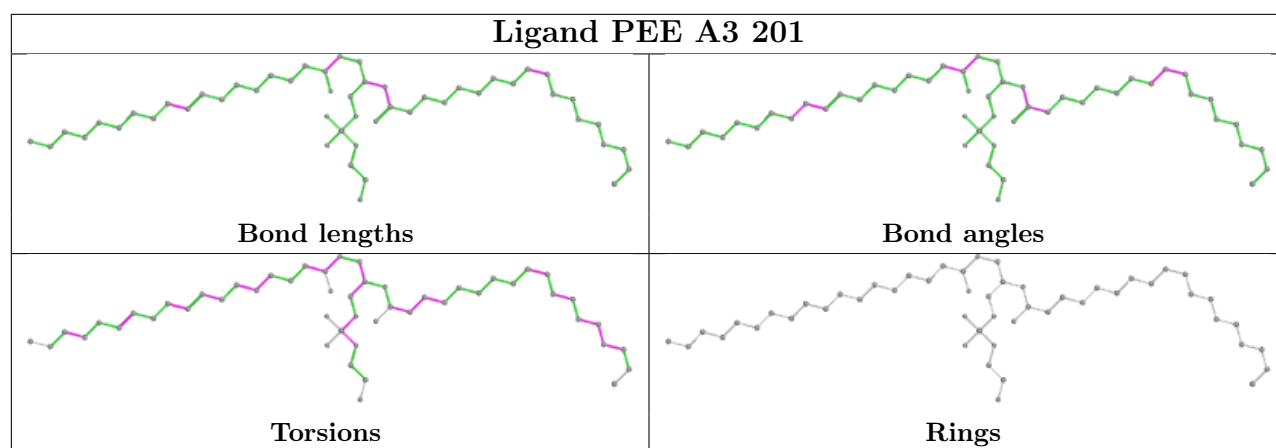




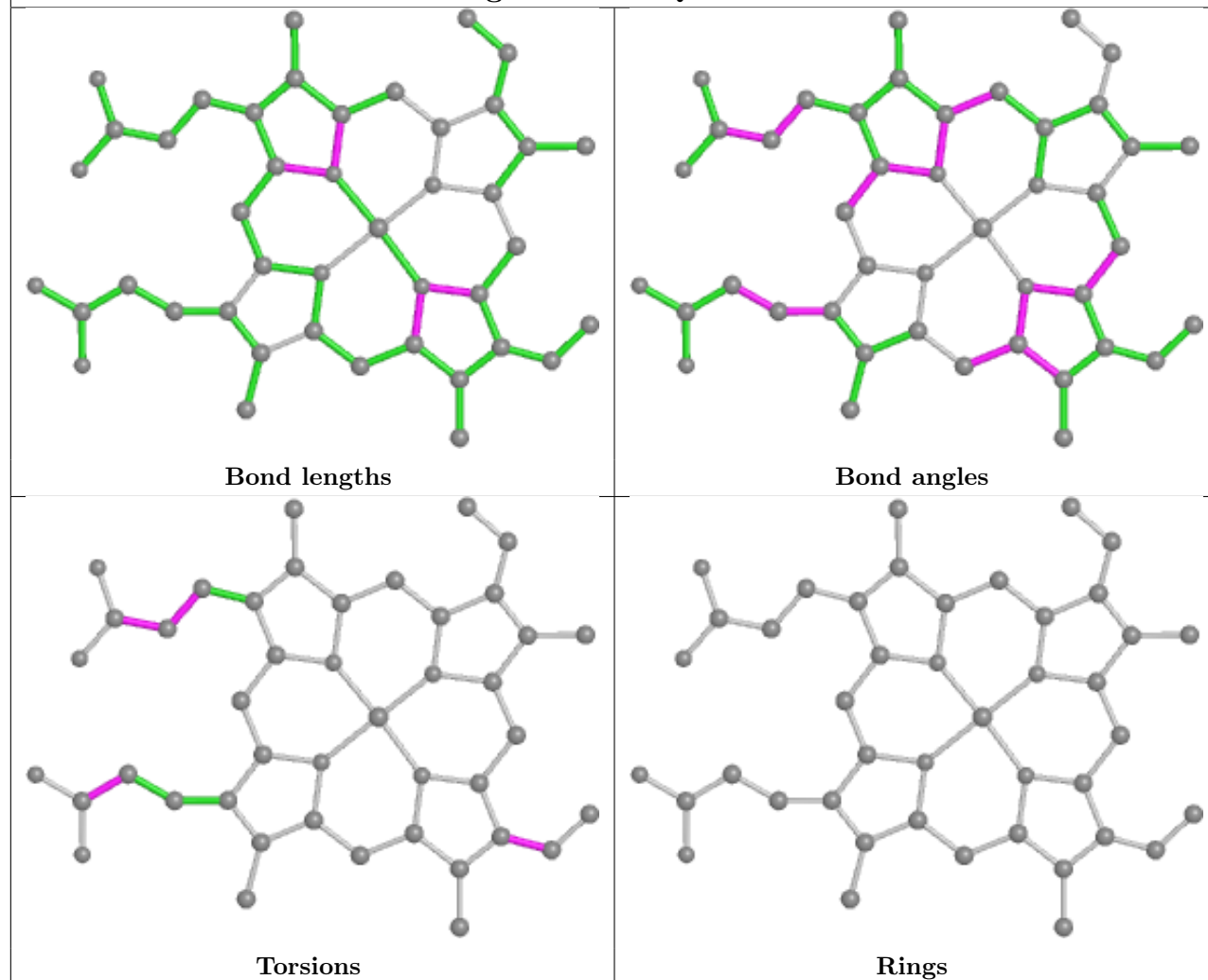




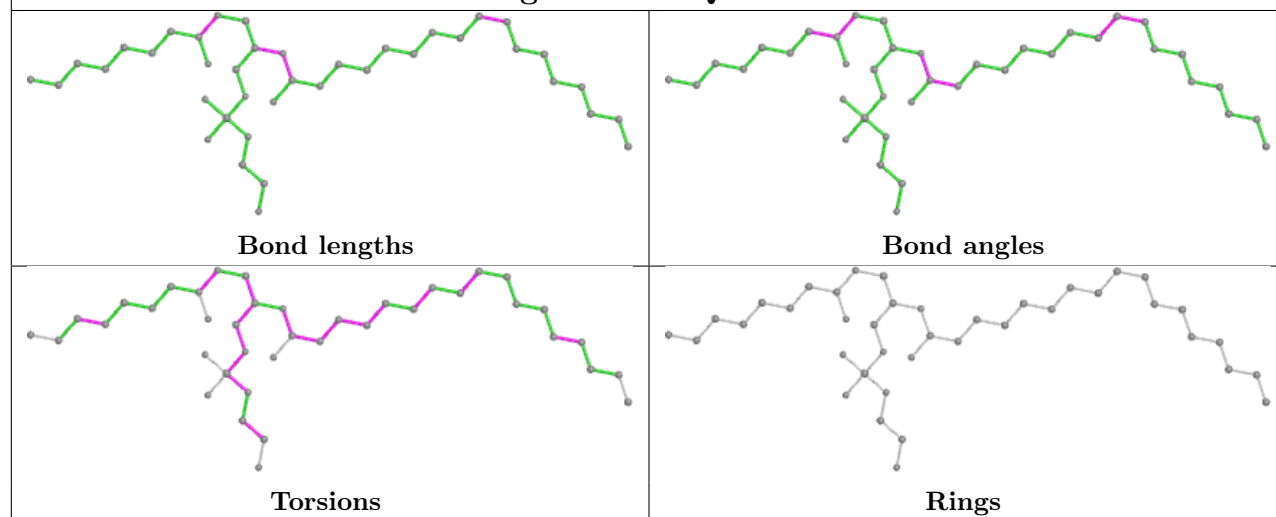


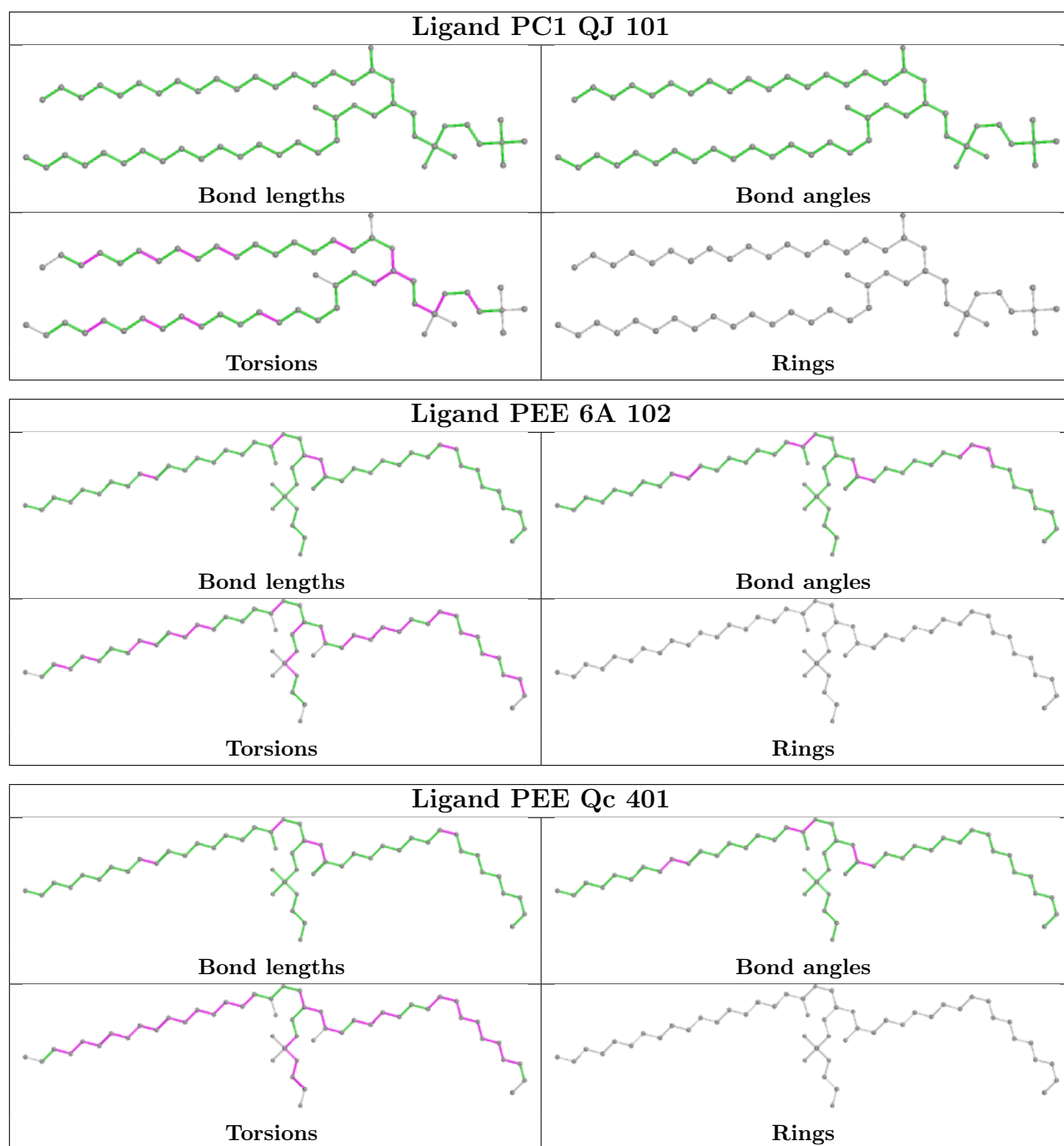


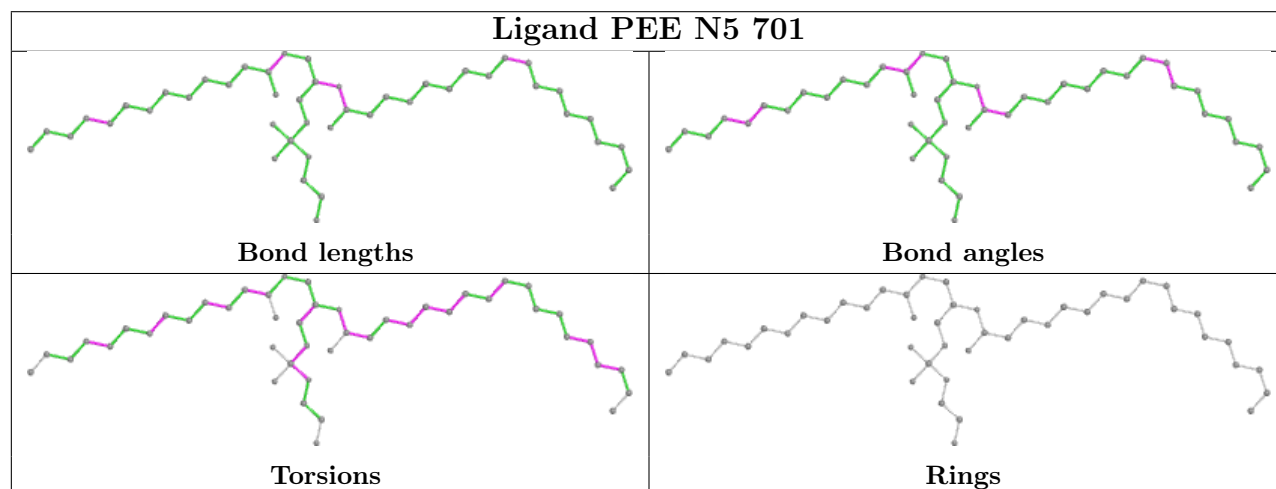
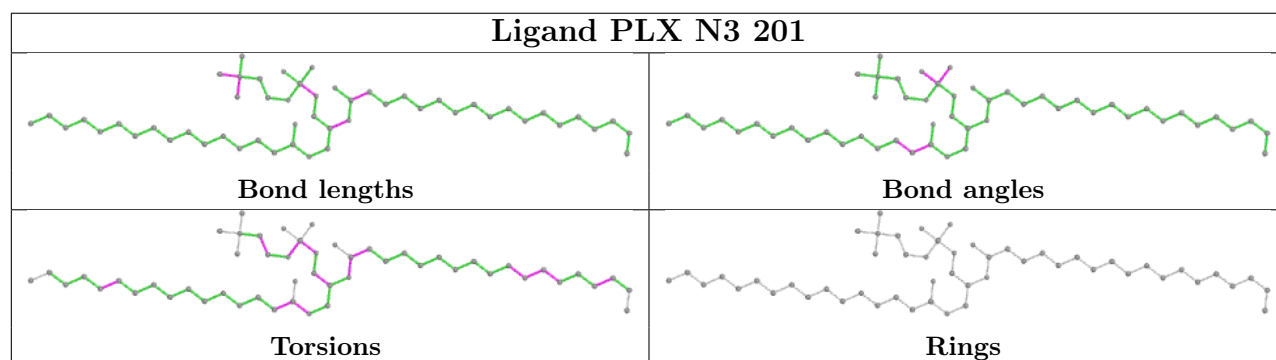
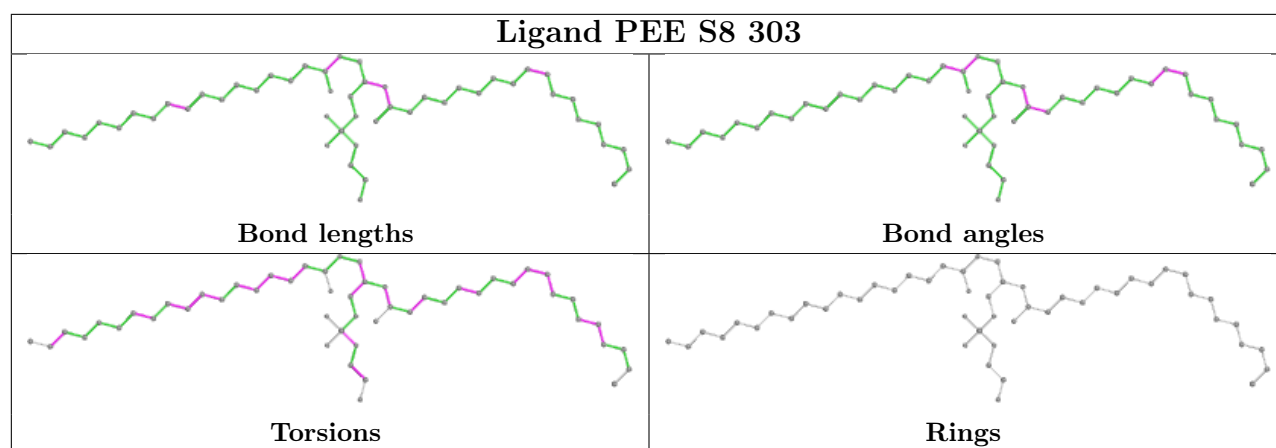
## Ligand HEM QC 401



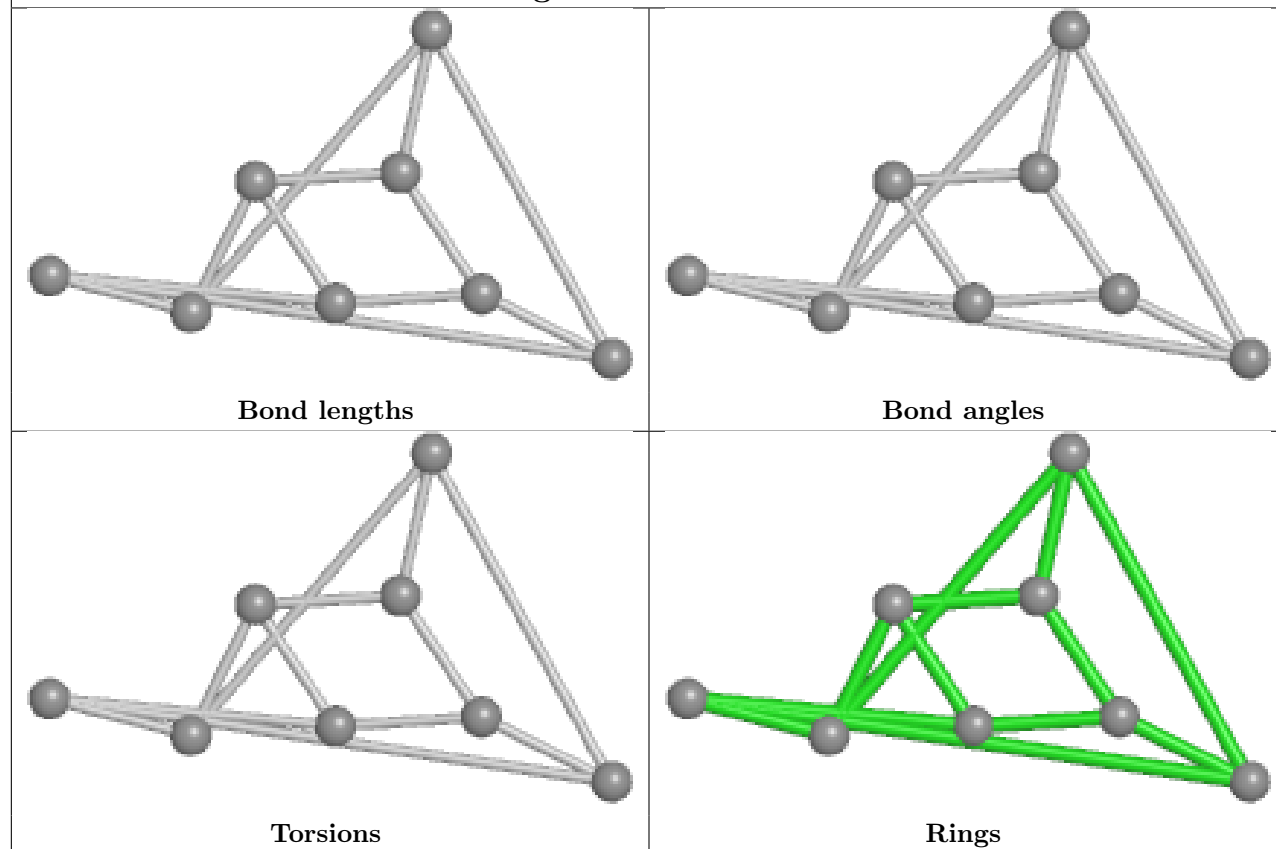
## Ligand PEE QC 403



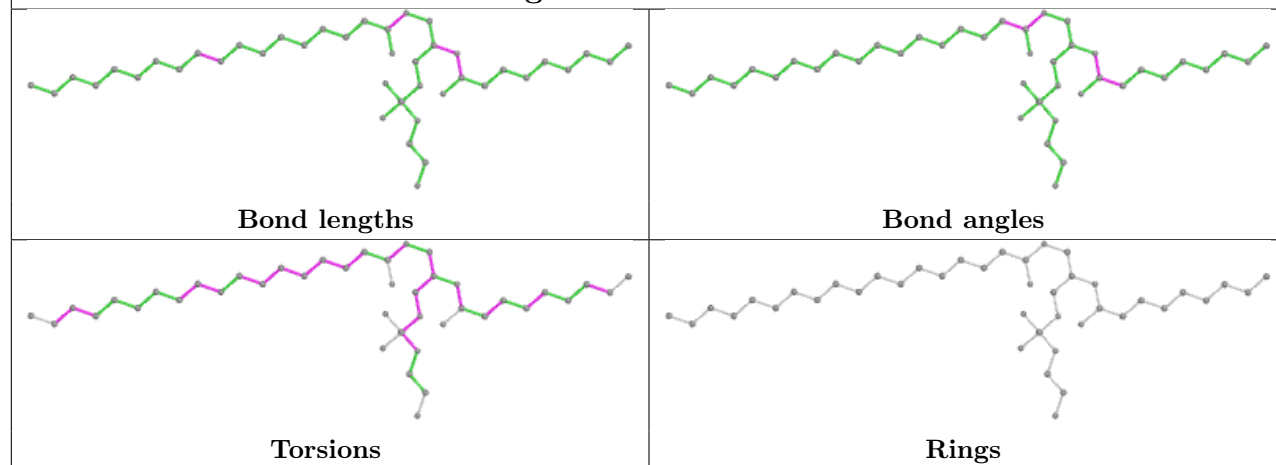


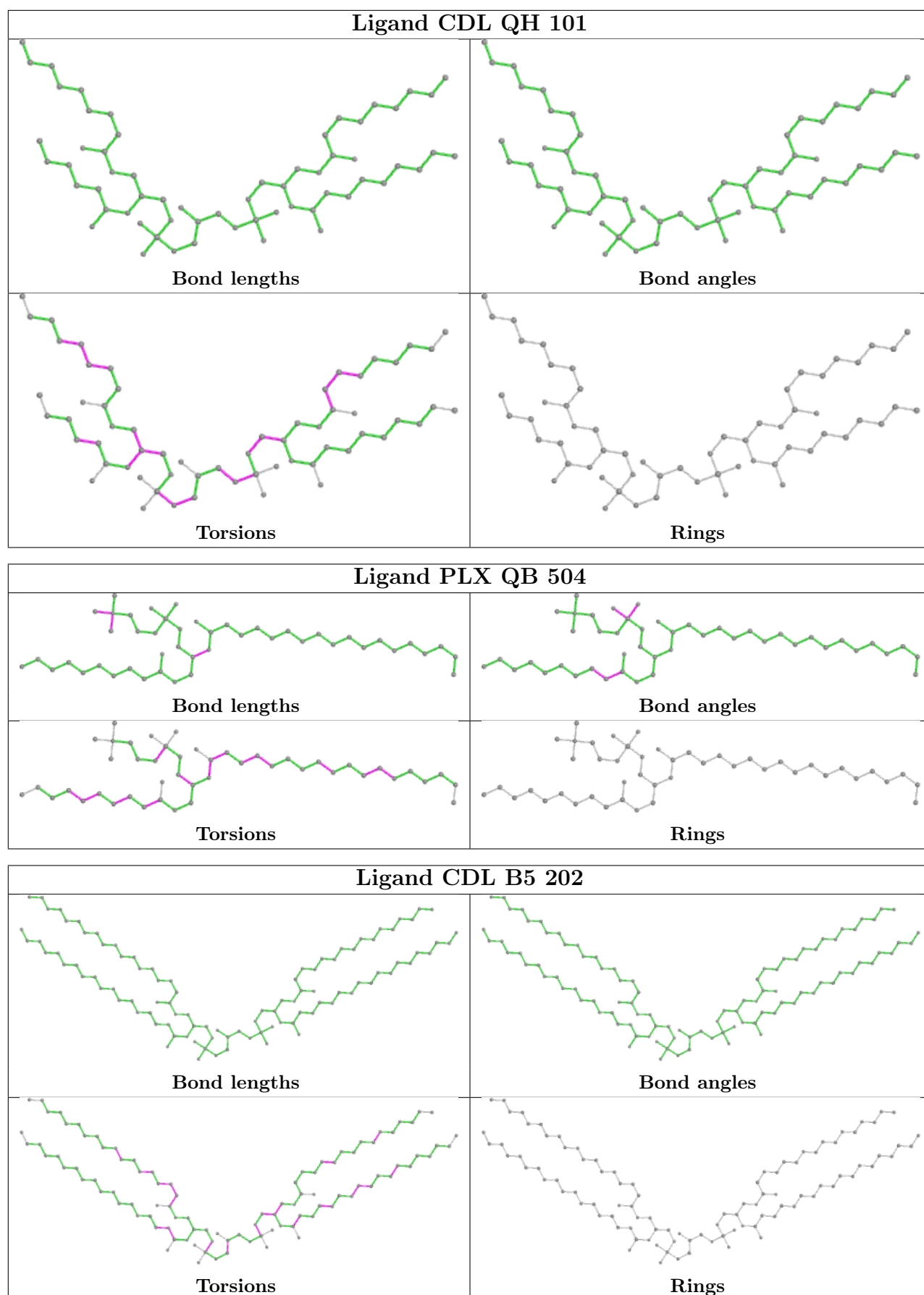


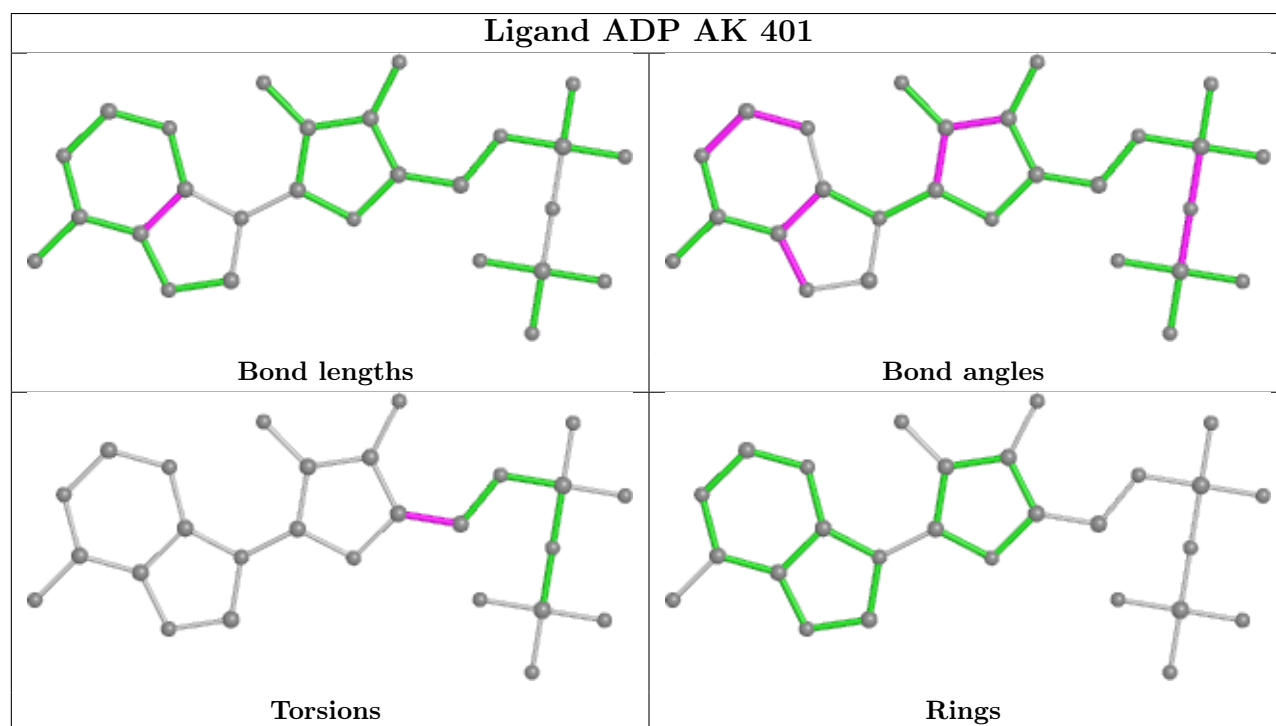
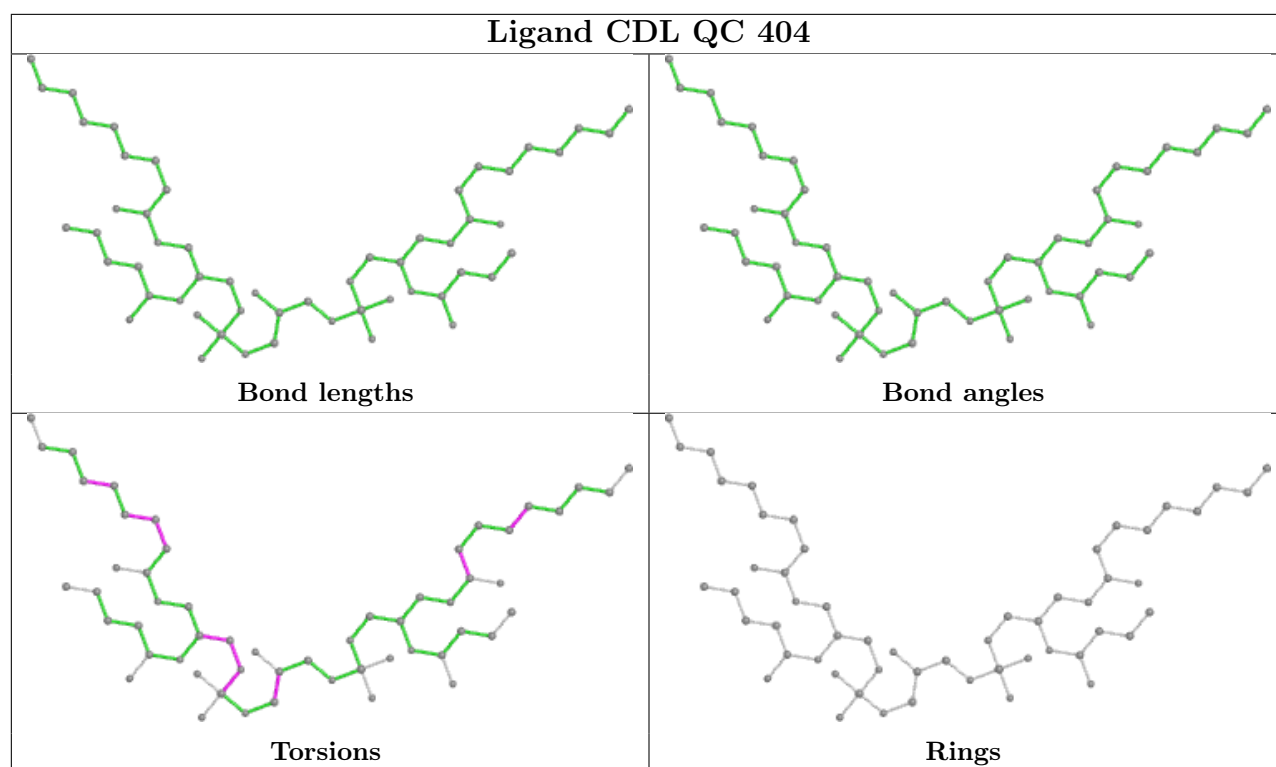
## Ligand SF4 S1 801

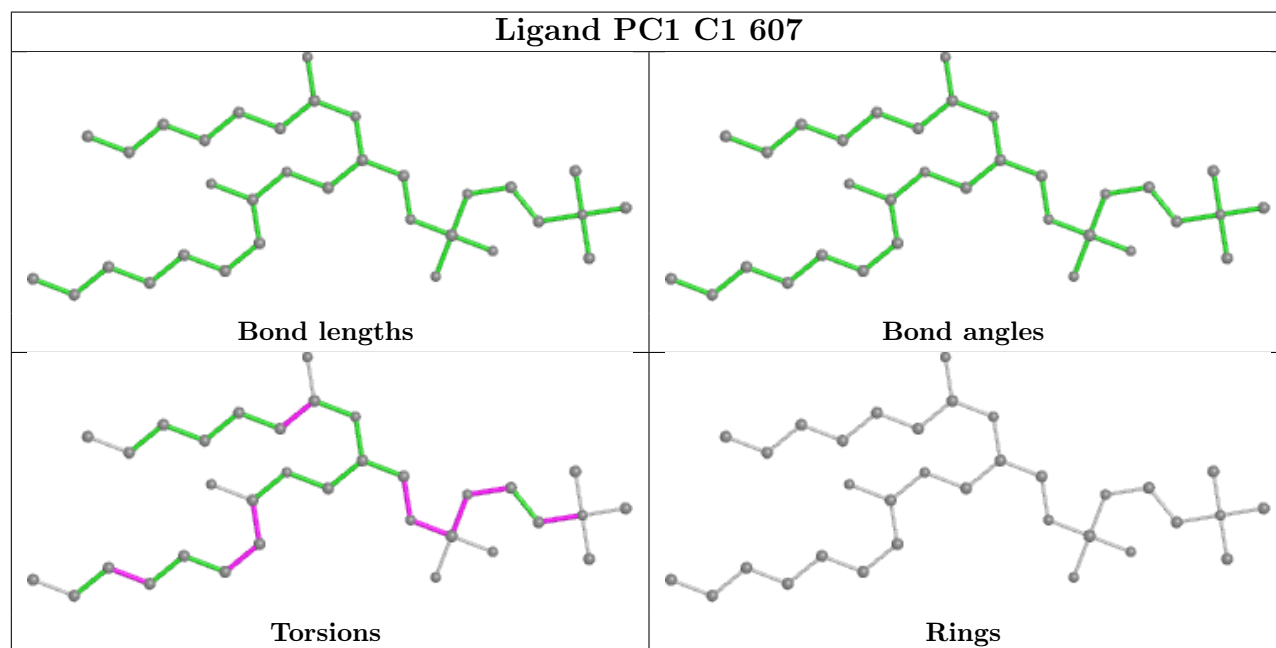
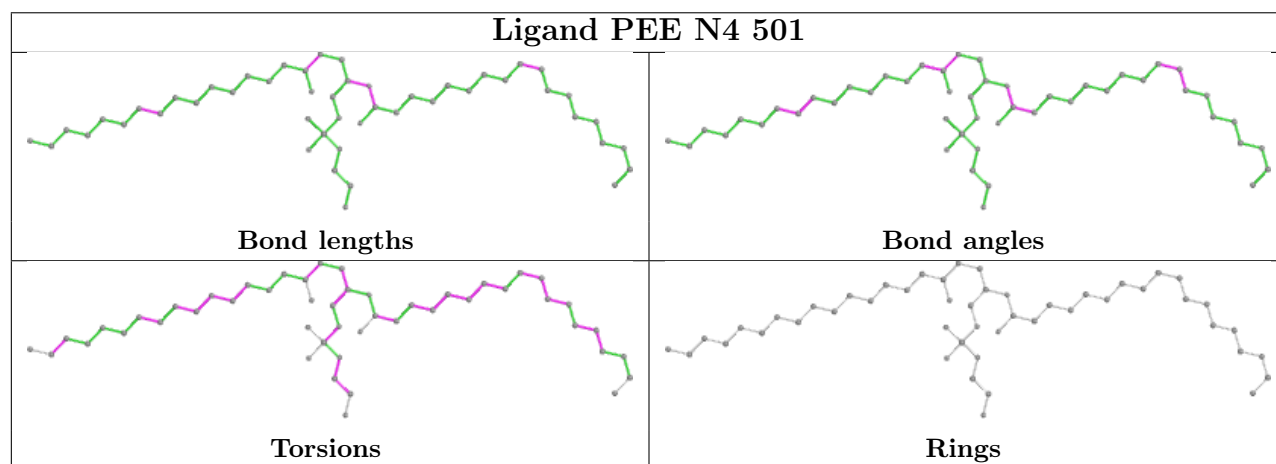
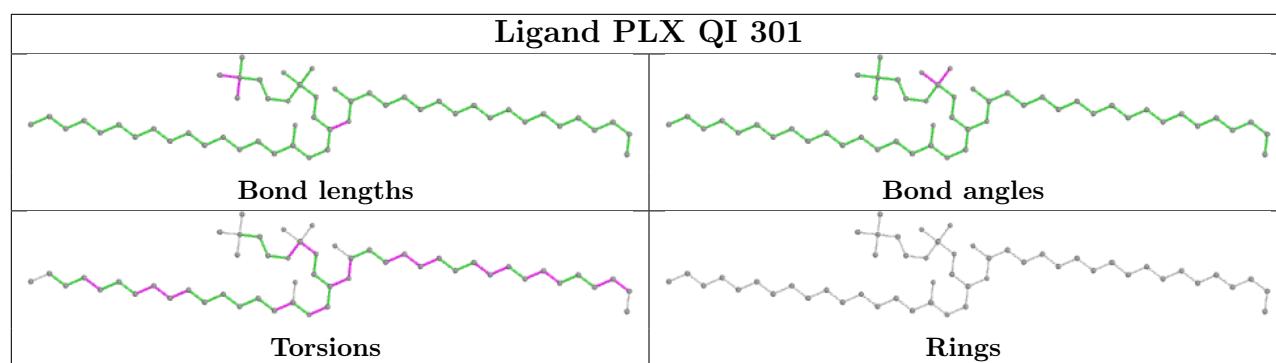


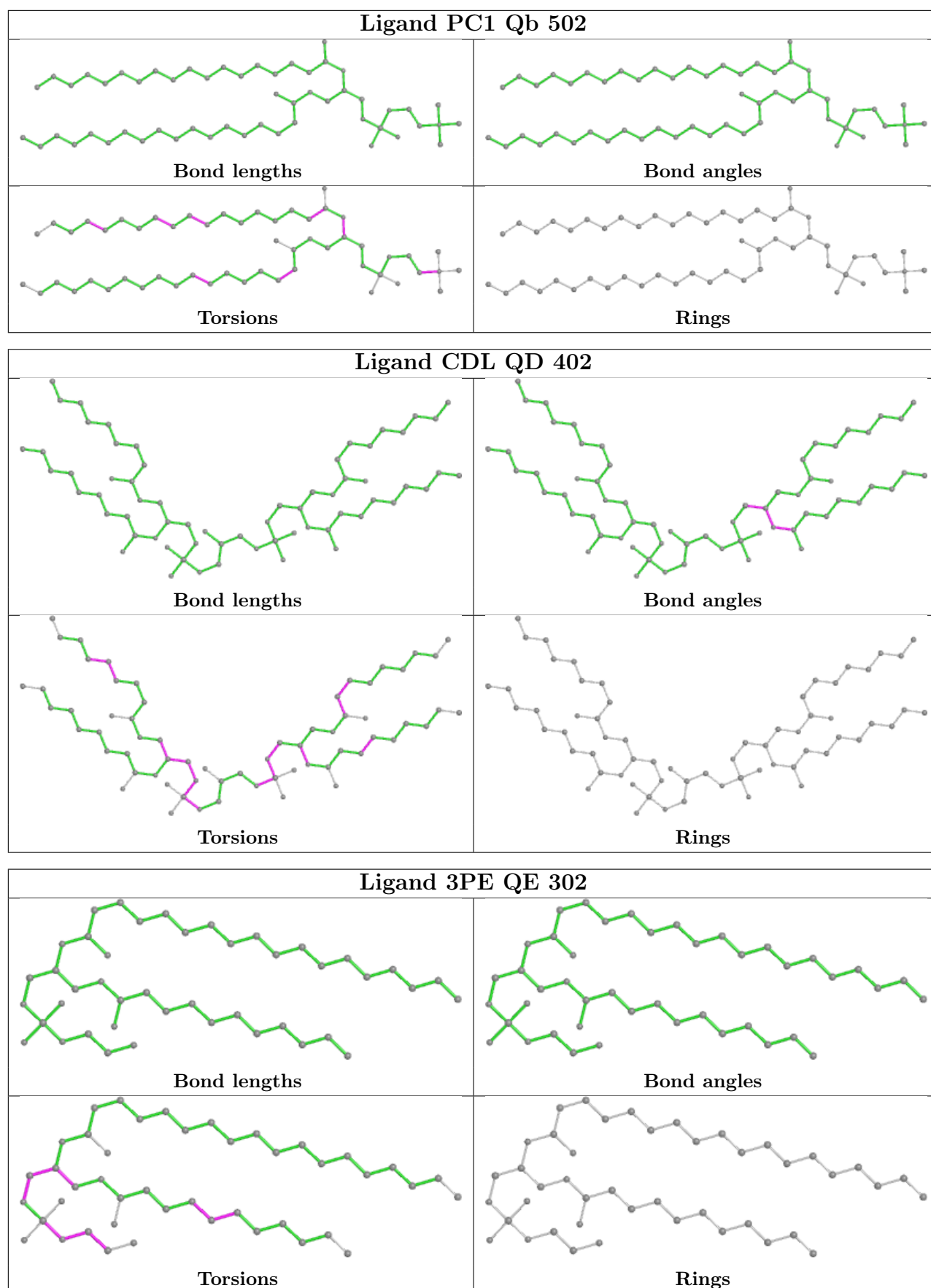
## Ligand PEE 8B 201

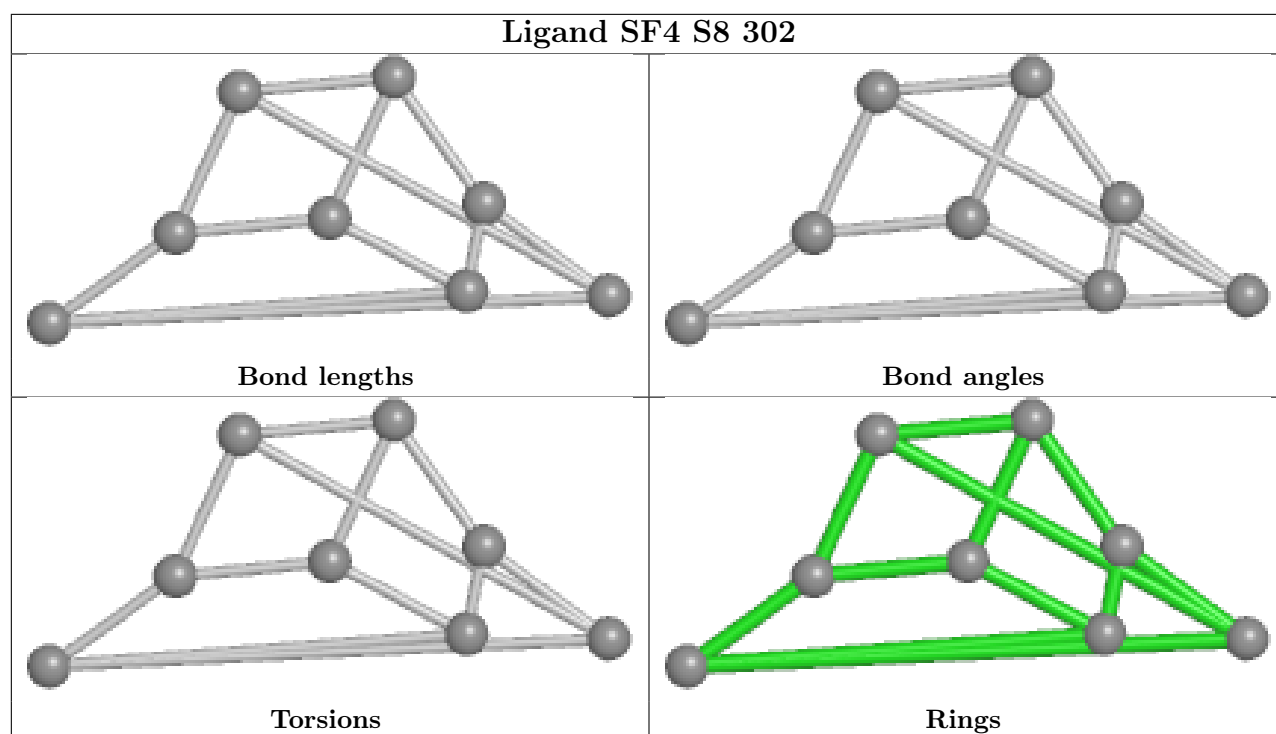












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

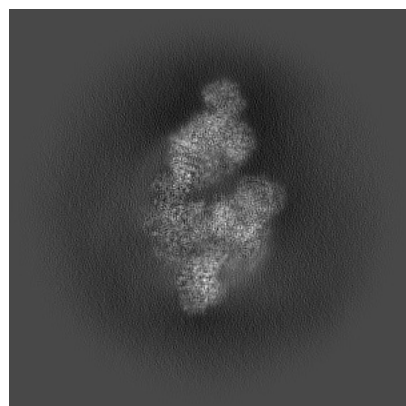
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60329. These allow visual inspection of the internal detail of the map and identification of artifacts.

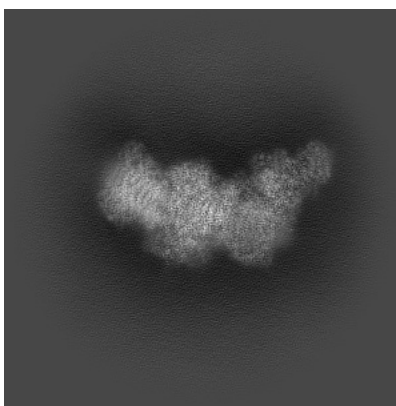
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

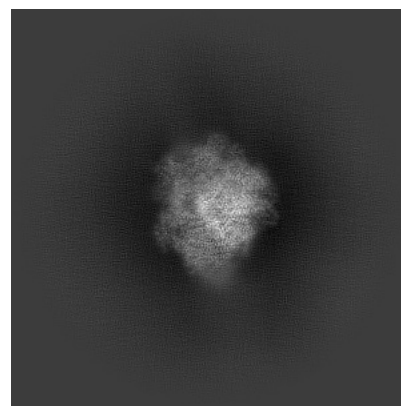
#### 6.1.1 Primary map



X

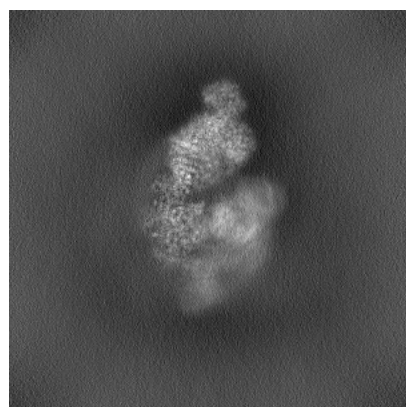


Y

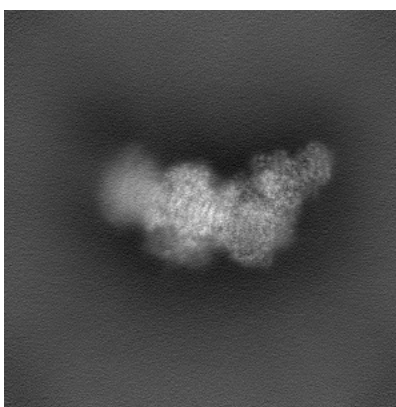


Z

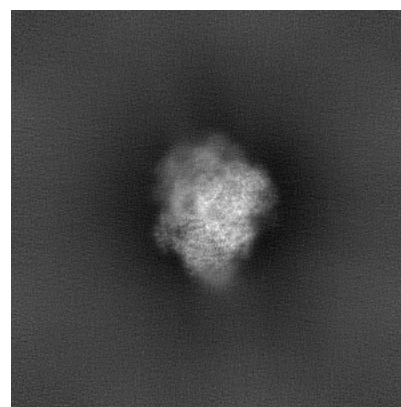
#### 6.1.2 Raw map



X



Y

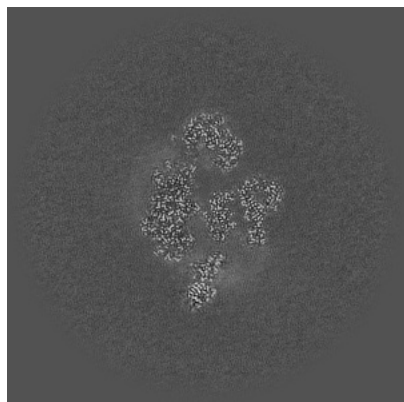


Z

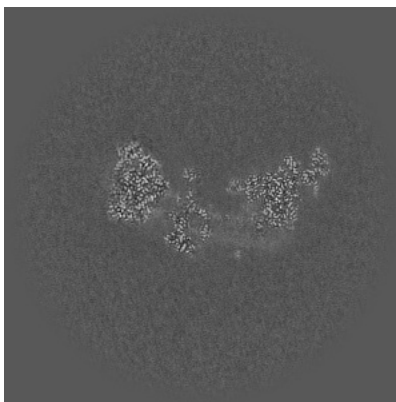
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

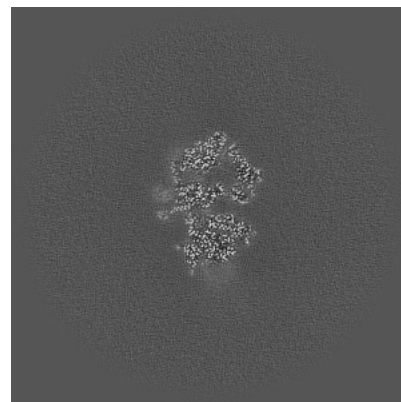
### 6.2.1 Primary map



X Index: 240

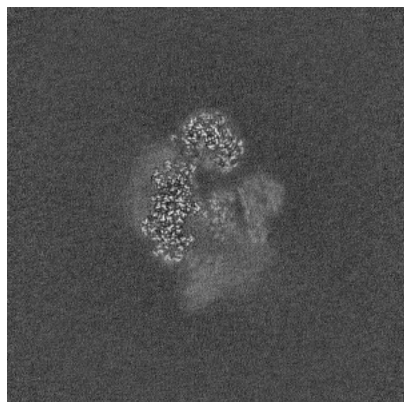


Y Index: 240

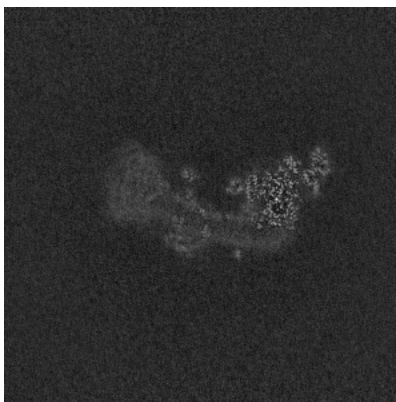


Z Index: 240

### 6.2.2 Raw map



X Index: 240



Y Index: 240

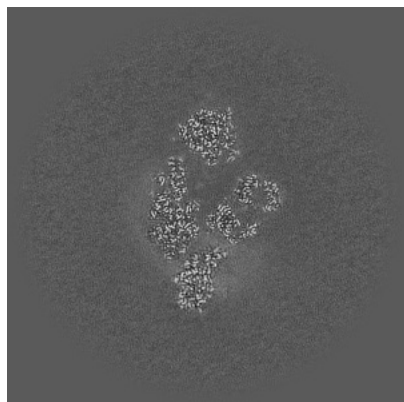


Z Index: 240

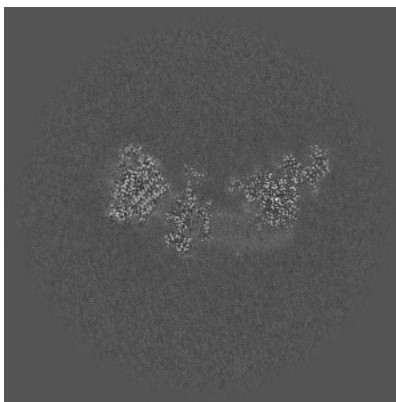
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

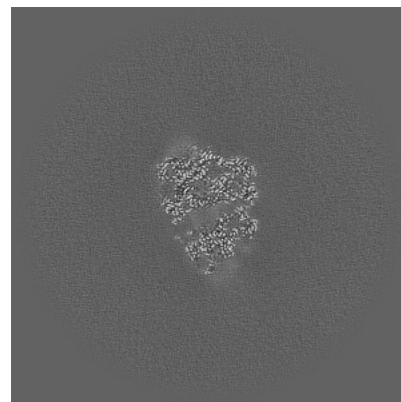
### 6.3.1 Primary map



X Index: 252

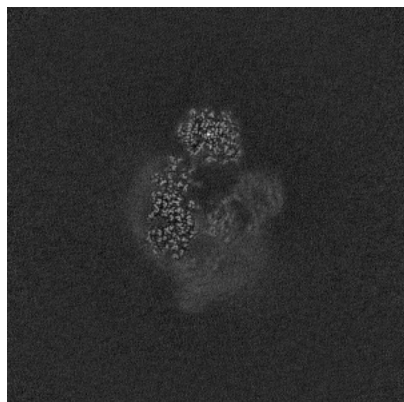


Y Index: 242

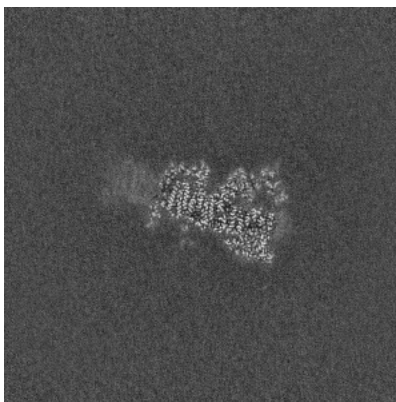


Z Index: 217

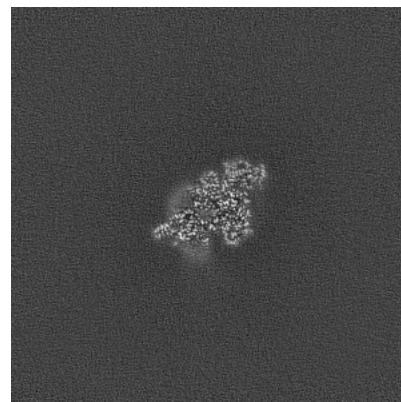
### 6.3.2 Raw map



X Index: 248



Y Index: 206

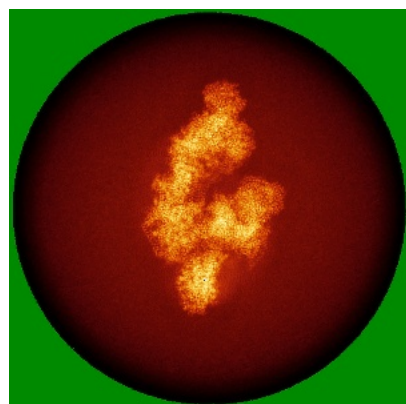


Z Index: 317

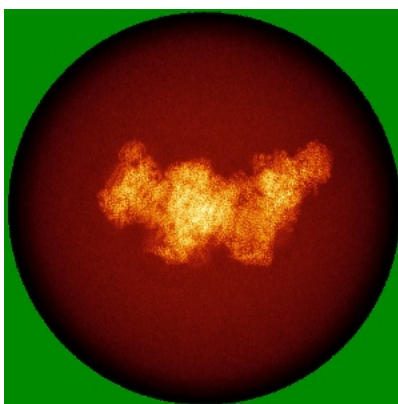
The images above show the largest variance slices of the map in three orthogonal directions.

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

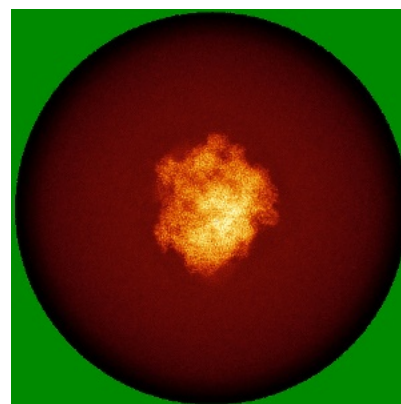
### 6.4.1 Primary map



X

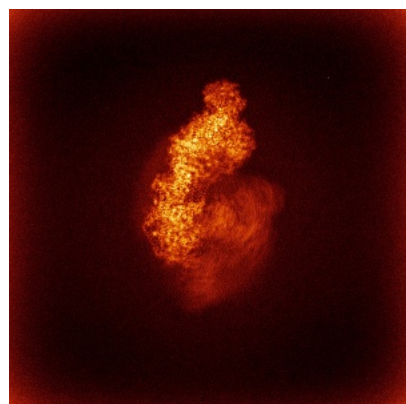


Y

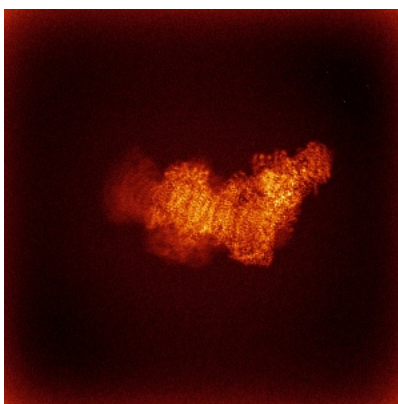


Z

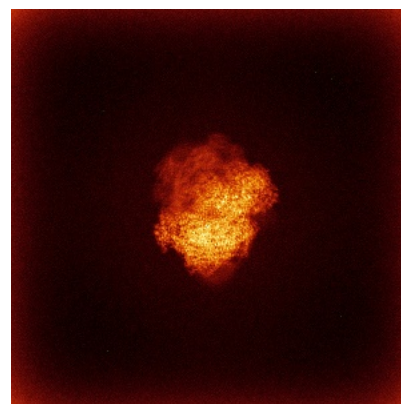
### 6.4.2 Raw map



X



Y

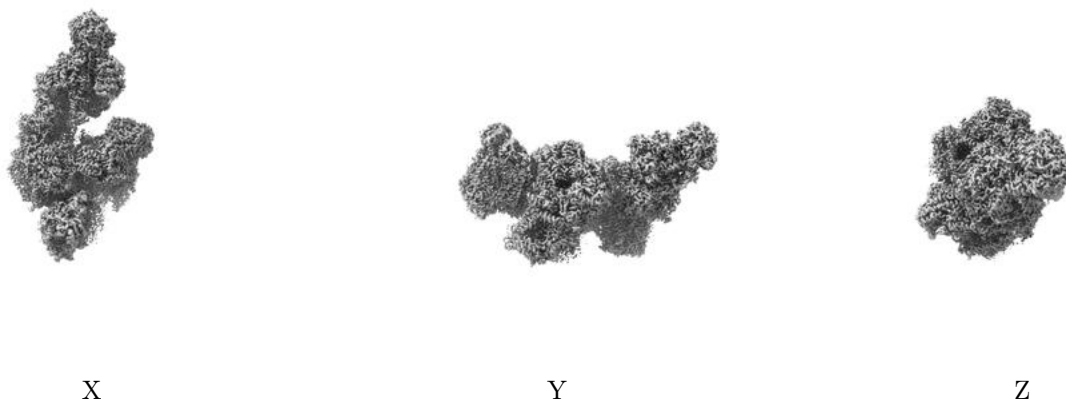


Z

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.

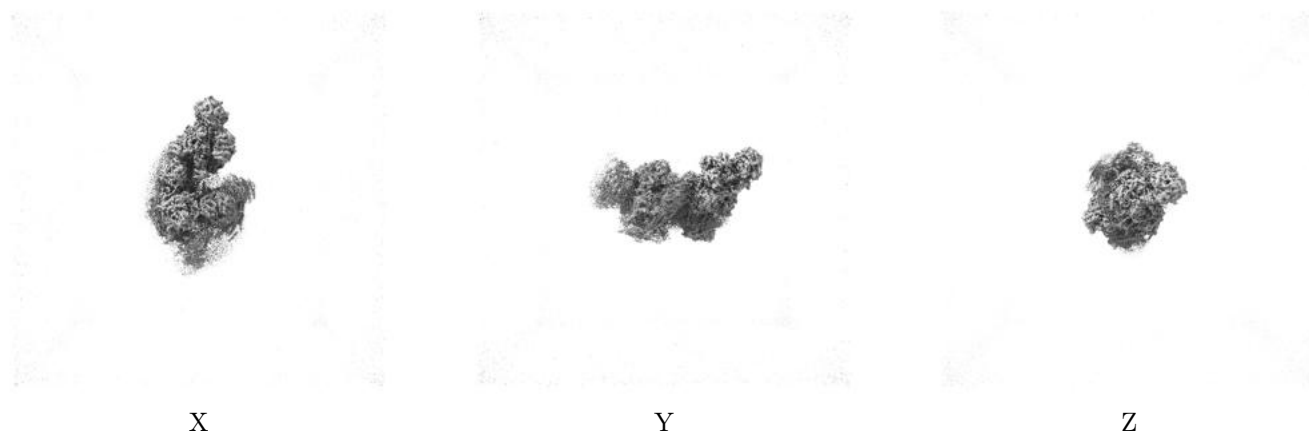
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.0. 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



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.

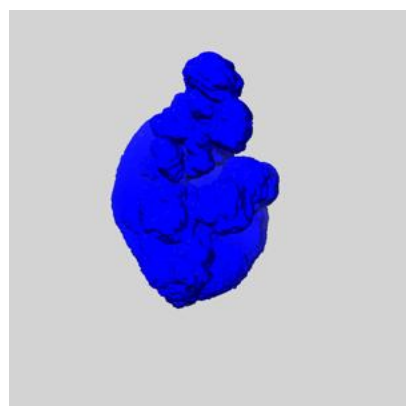
## 6.6 Mask visualisation [i](#)

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

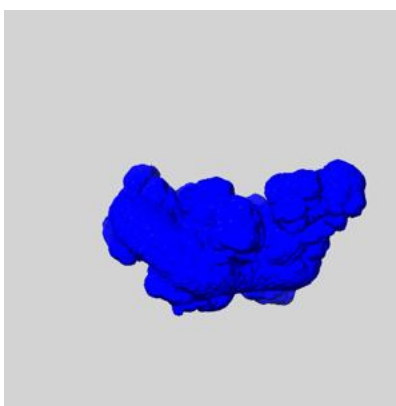
A mask typically either:

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

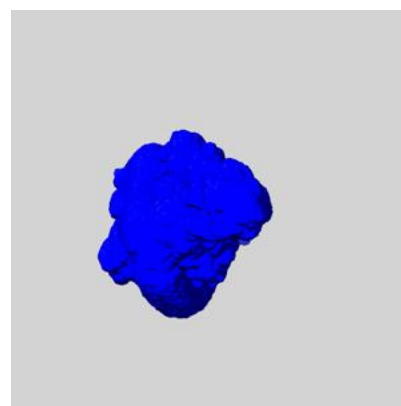
### 6.6.1 emd\_60329\_msk\_1.map [i](#)



X



Y

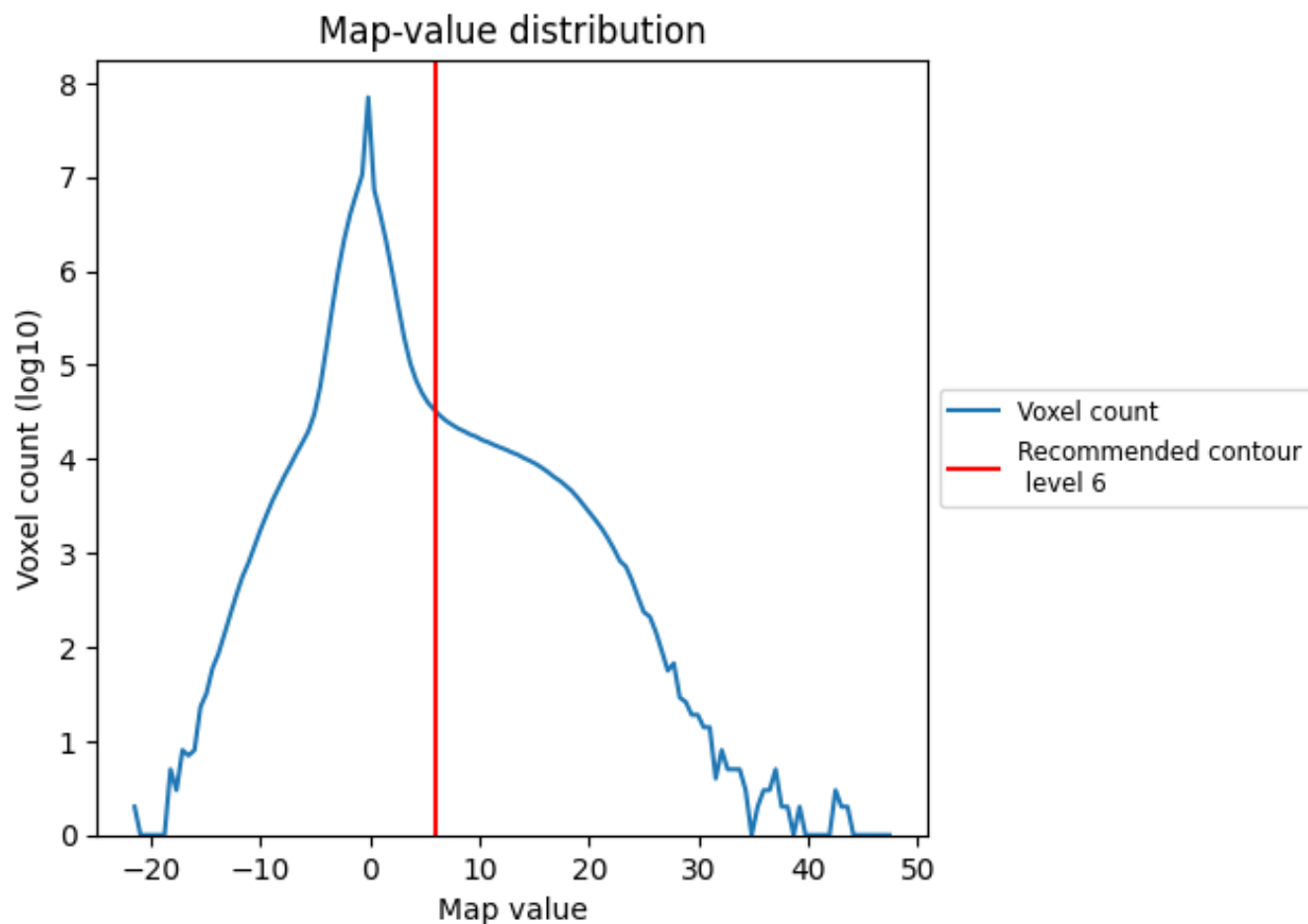


Z

## 7 Map analysis [i](#)

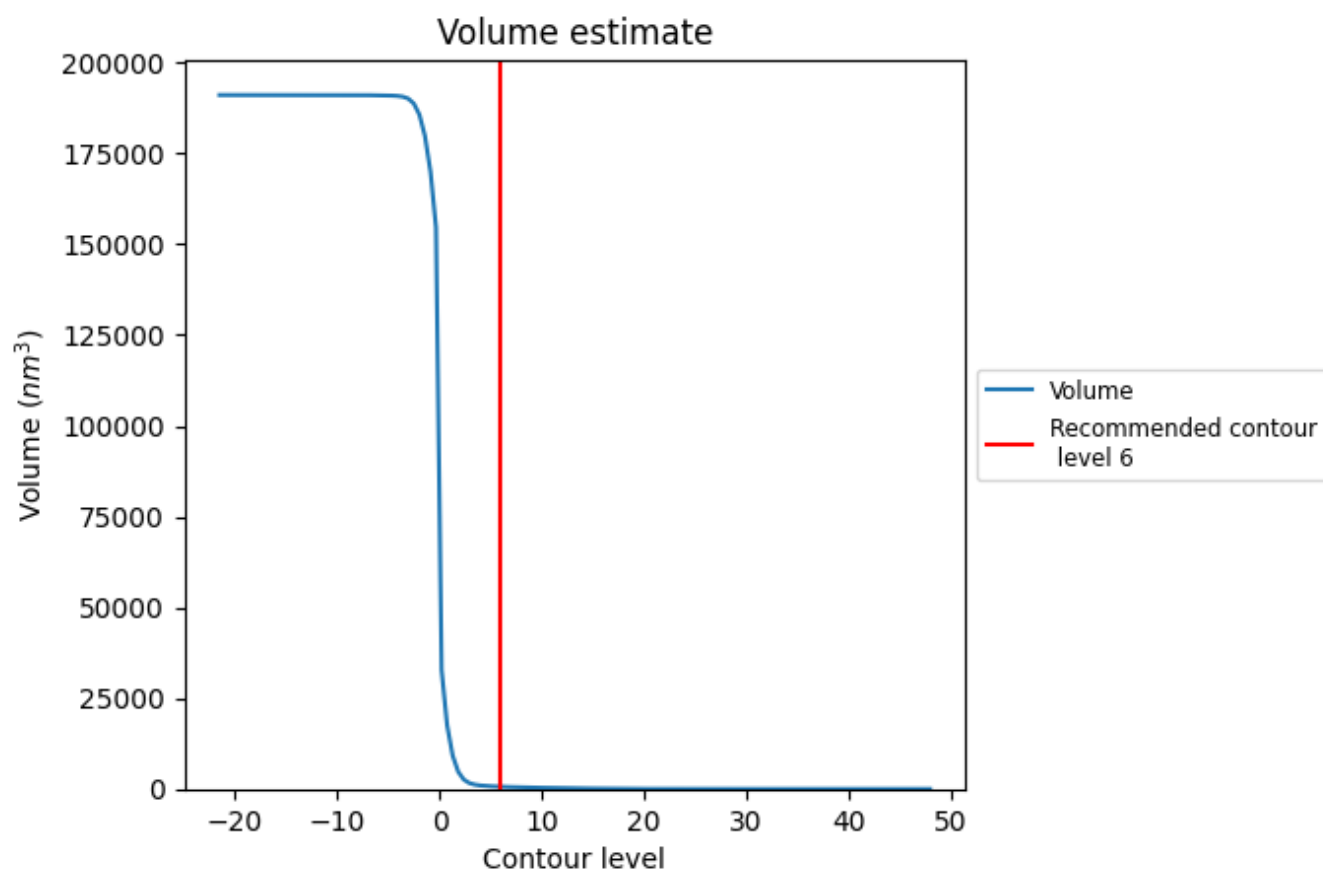
This section contains the results of statistical analysis of the map.

### 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.

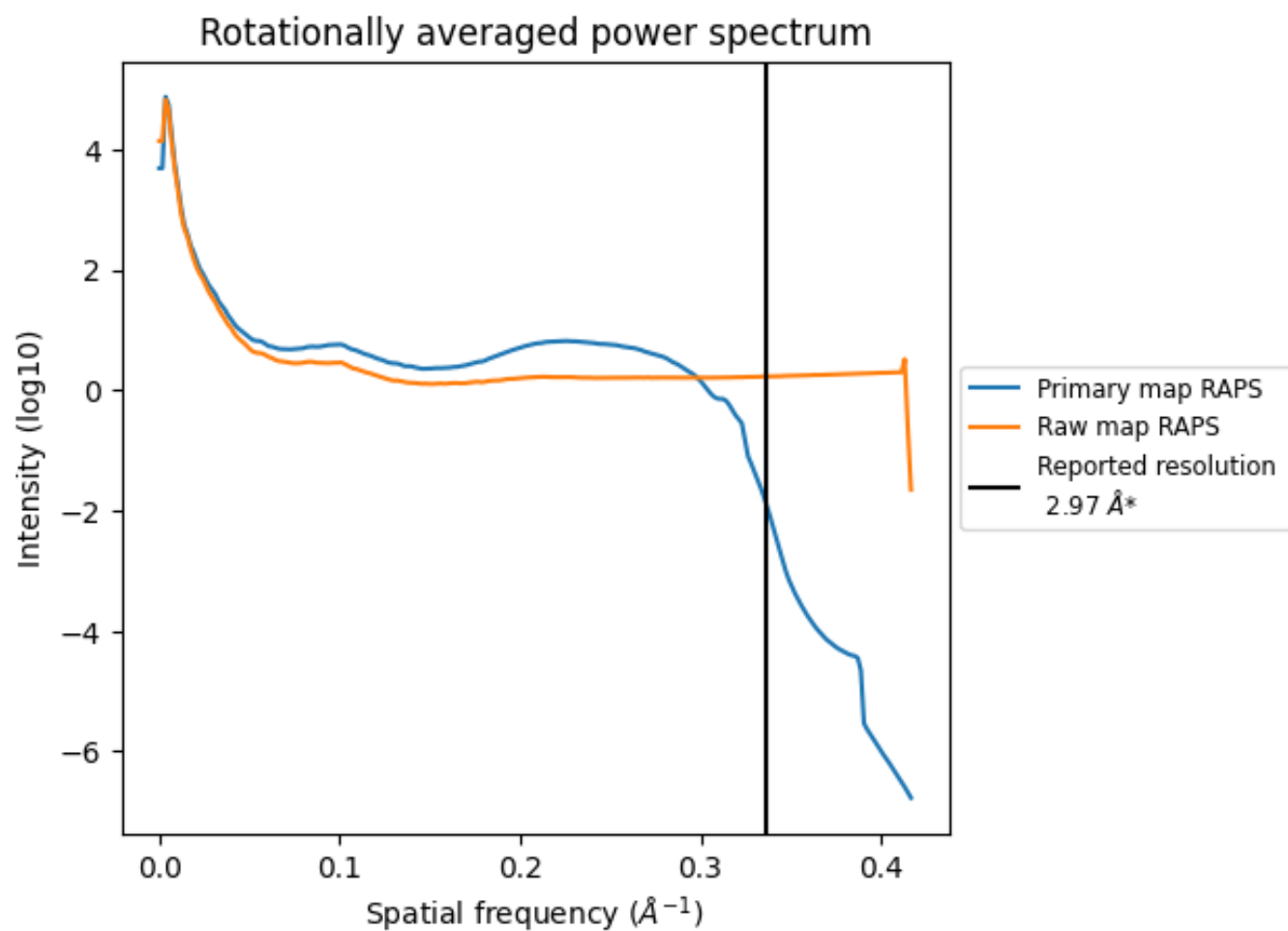
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 620  $\text{nm}^3$ ; this corresponds to an approximate mass of 560 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 ⓘ

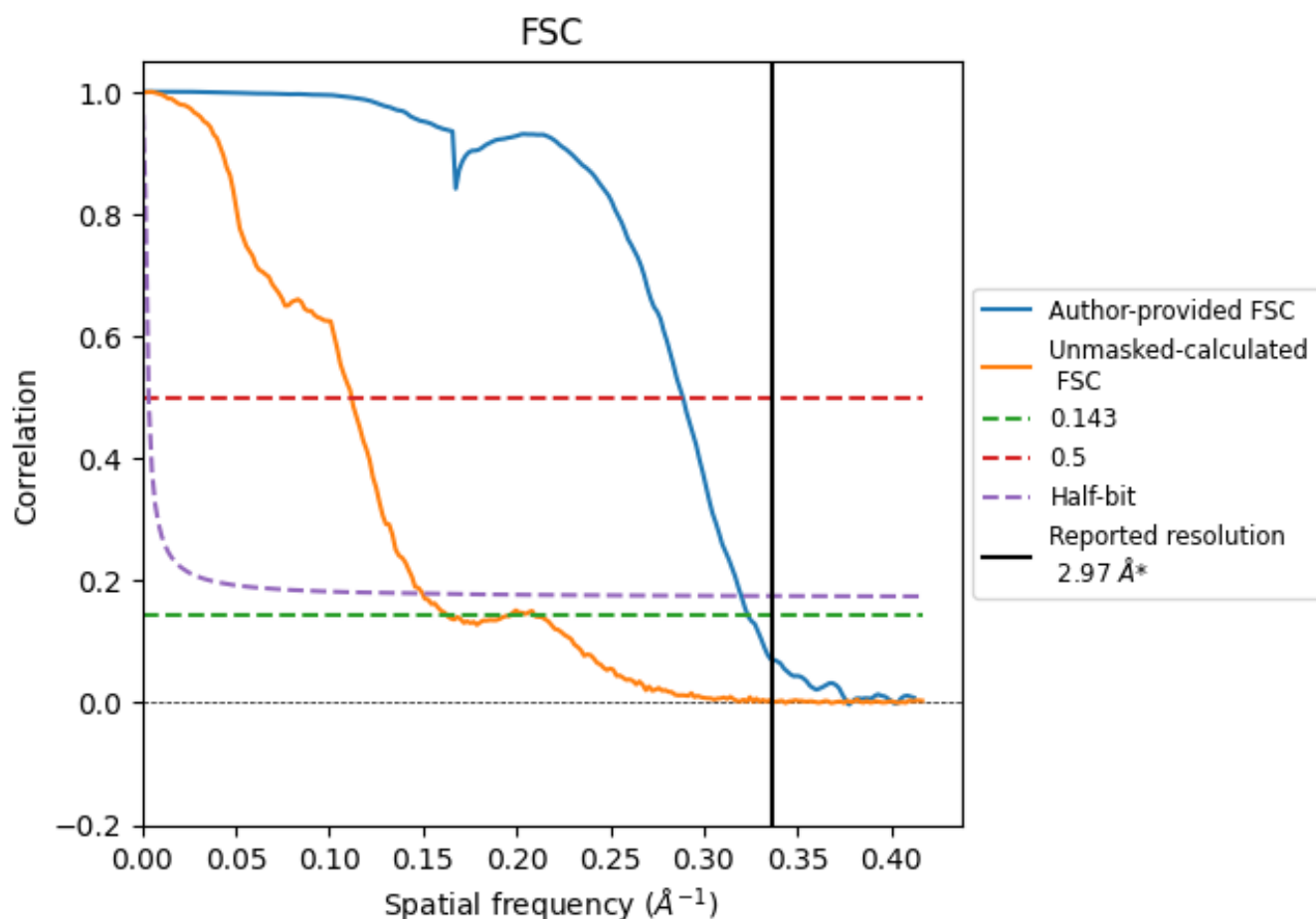


\*Reported resolution corresponds to spatial frequency of 0.337  $\text{\AA}^{-1}$

## 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 0.337  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

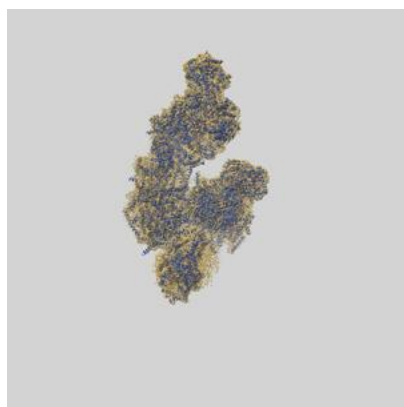
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	3.09	3.46	3.12
Unmasked-calculated*	6.14	8.94	6.68

\*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 6.14 differs from the reported value 2.97 by more than 10 %

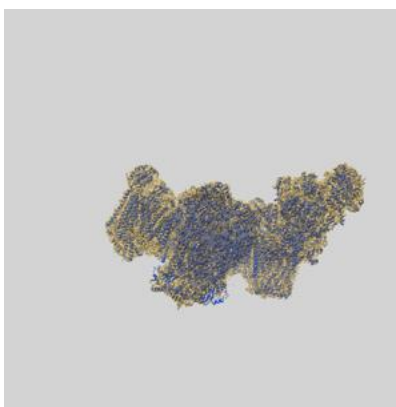
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60329 and PDB model 8ZP8. Per-residue inclusion information can be found in section [3](#) on page [30](#).

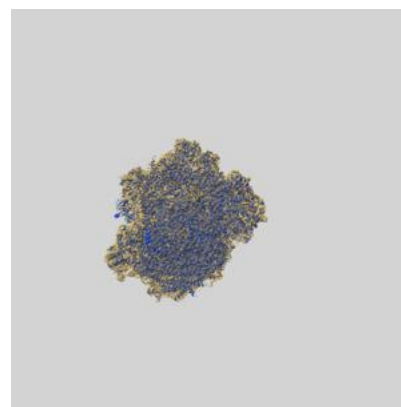
### 9.1 Map-model overlay [i](#)



X



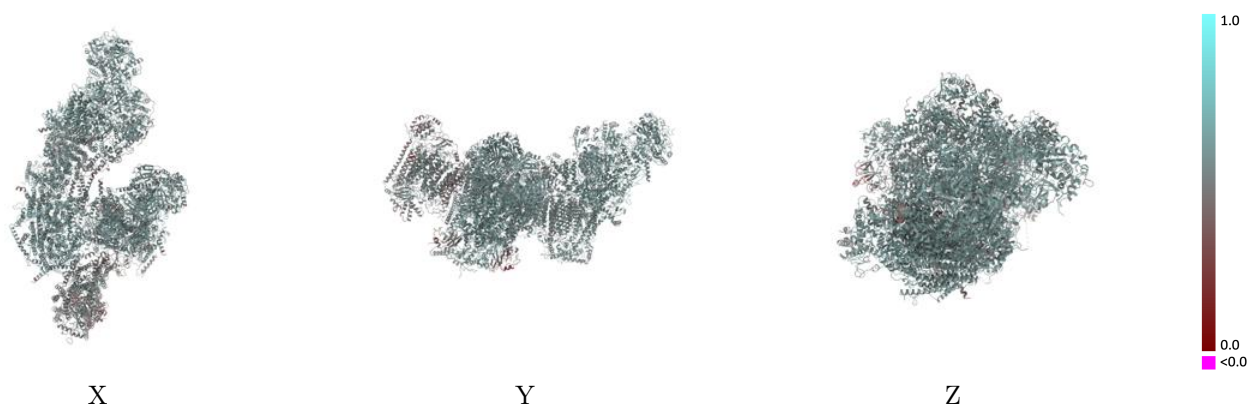
Y



Z

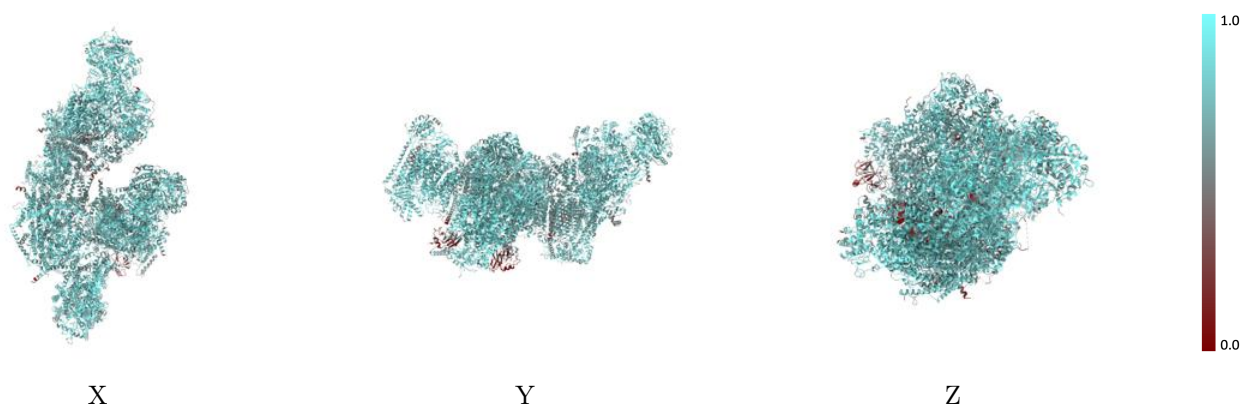
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



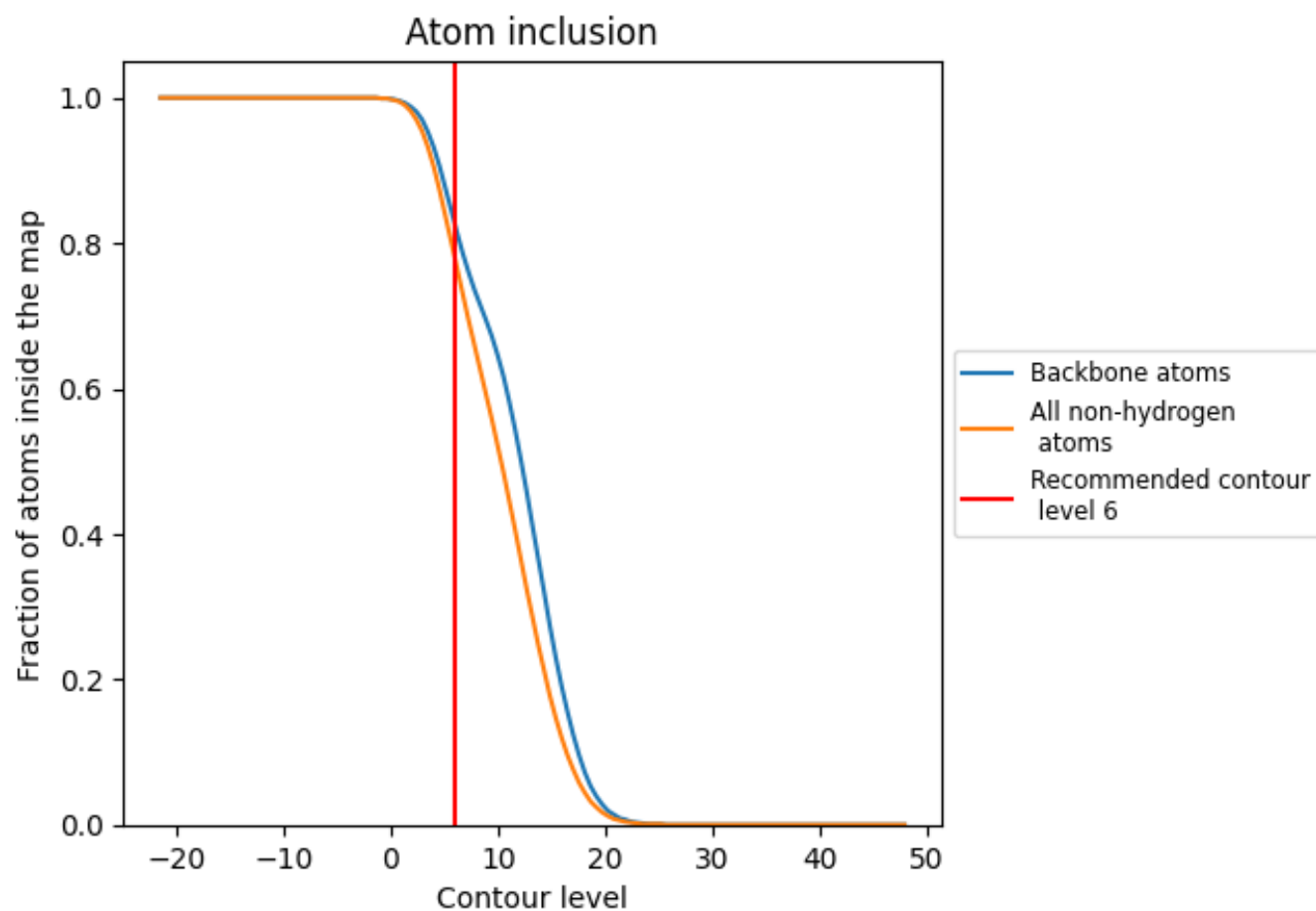
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7800	 0.5560
4L	 0.7630	 0.5730
5A	 0.7340	 0.4440
5B	 0.7710	 0.4480
6A	 0.7530	 0.4640
6B	 0.8310	 0.4680
6C	 0.7150	 0.4600
7A	 0.7400	 0.4690
7B	 0.6710	 0.4820
7C	 0.8280	 0.5000
8B	 0.7910	 0.5020
A1	 0.7330	 0.5610
A2	 0.7170	 0.5510
A3	 0.7810	 0.5650
A5	 0.7590	 0.5610
A6	 0.7540	 0.5650
A7	 0.6940	 0.5620
A8	 0.8060	 0.5690
A9	 0.7610	 0.5610
AB	 0.5630	 0.4900
AC	 0.7940	 0.5810
AK	 0.7530	 0.5440
AL	 0.6600	 0.5510
AM	 0.6660	 0.5550
AN	 0.8130	 0.5670
B1	 0.6940	 0.5520
B2	 0.7730	 0.5750
B3	 0.7280	 0.5510
B4	 0.7100	 0.5760
B5	 0.8200	 0.5920
B6	 0.7230	 0.5550
B7	 0.7230	 0.5670
B8	 0.7960	 0.5840
B9	 0.8250	 0.5870
BK	 0.7740	 0.5750









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Chain	Atom inclusion	Q-score
BL	 0.7890	 0.5740
C1	 0.8580	 0.5230
C2	 0.7970	 0.5000
C3	 0.8360	 0.4970
C4	 0.7730	 0.4690
CA	 0.7300	 0.5600
CB	 0.8320	 0.5810
N1	 0.7940	 0.5660
N2	 0.8340	 0.5810
N3	 0.6970	 0.5550
N4	 0.8460	 0.5890
N5	 0.8270	 0.5880
N6	 0.6690	 0.5170
QA	 0.7980	 0.5610
QB	 0.7930	 0.5660
QC	 0.8440	 0.5760
QD	 0.8150	 0.5700
QE	 0.4380	 0.4700
QF	 0.6430	 0.5010
QG	 0.7910	 0.5610
QH	 0.7390	 0.5530
QI	 0.7510	 0.5580
QJ	 0.6390	 0.5230
QK	 0.5660	 0.5290
Qa	 0.7680	 0.5620
Qb	 0.7930	 0.5680
Qc	 0.8230	 0.5730
Qd	 0.8100	 0.5720
Qe	 0.3750	 0.4230
Qf	 0.6360	 0.5190
Qg	 0.7920	 0.5650
Qh	 0.7590	 0.5640
Qi	 0.8090	 0.5720
Qj	 0.7770	 0.5460
S1	 0.8170	 0.5720
S2	 0.8350	 0.5810
S3	 0.8720	 0.5980
S4	 0.8050	 0.5840
S5	 0.7710	 0.5660
S6	 0.7700	 0.5740
S7	 0.8500	 0.5820
S8	 0.8970	 0.5910

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Chain	Atom inclusion	Q-score
V1	 0.8000	 0.5630
V2	 0.7540	 0.5580
V3	 0.7440	 0.5670