



Full wwPDB EM Validation Report ⓘ

Nov 11, 2025 – 08:30 PM JST

PDB ID : 8ZOU / pdb_00008zou
EMDB ID : EMD-60319
Title : Respirasome open state 2 in presence of metformin (SC-MetO2)
Authors : Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.
Deposited on : 2024-05-29
Resolution : 3.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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) : 2.46

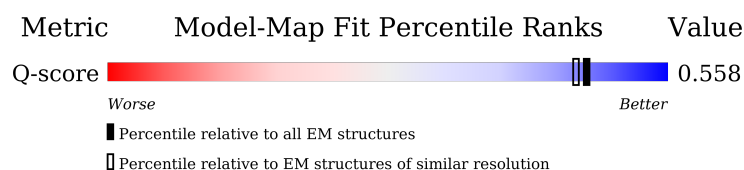
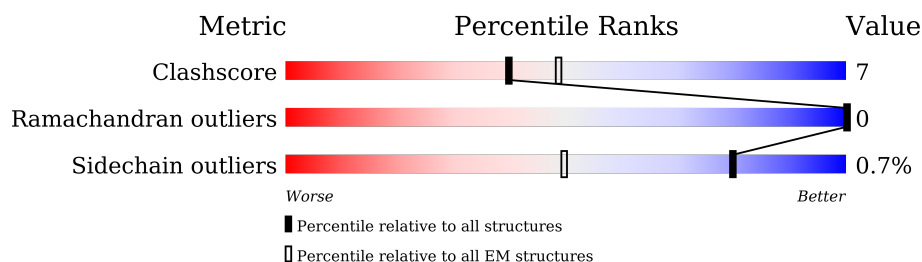
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.01 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	13882 (2.51 - 3.51)

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

Mol	Chain	Length	Quality of chain
1	4L	98	<div> <div>5%</div> <div>85%</div> <div>15%</div> </div>
2	5A	102	<div> <div>5%</div> <div>93%</div> <div>7%</div> </div>
3	5B	95	<div> <div>5%</div> <div>79%</div> <div>21%</div> </div>
4	6A	75	<div> <div>7%</div> <div>83%</div> <div>17%</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	102	
35	C1	514	
36	C2	228	
37	C3	261	
38	C4	138	
39	CA	49	
40	CB	121	
41	N1	318	
42	N2	347	
43	N3	114	
44	N4	459	
45	N5	603	
46	N6	174	
47	QA	419	
47	Qa	419	
48	QB	446	
48	Qb	446	
49	QC	379	
49	Qc	379	
50	QD	241	

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Mol	Chain	Length	Quality of chain
50	Qd	241	
51	QE	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	63	
55	Qi	63	
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	-
84	SF4	S8	302	-	-	X	-

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 118456 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A9	335	Total	C	N	O	S	0	0
			2684	1737	470	468	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
			1172	754	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	104	Total	C	N	O	S	0	0
			890	583	157	149	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	308	Total	C	N	O	S	0	0
			2436	1634	374	407	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	97	Total	C	N	O	S	0	0
			779	531	113	130	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	164	Total	C	N	O	S	0	0
			1243	835	178	219	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
			3143	1969	557	609	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 c domain-containing protein.

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	689	Total	C	N	O	S	0	0
			5290	3317	922	1012	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
58	S2	425	Total	C	N	O	S	0	0
			3423	2190	589	620	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
			3312	2090	591	611	20		

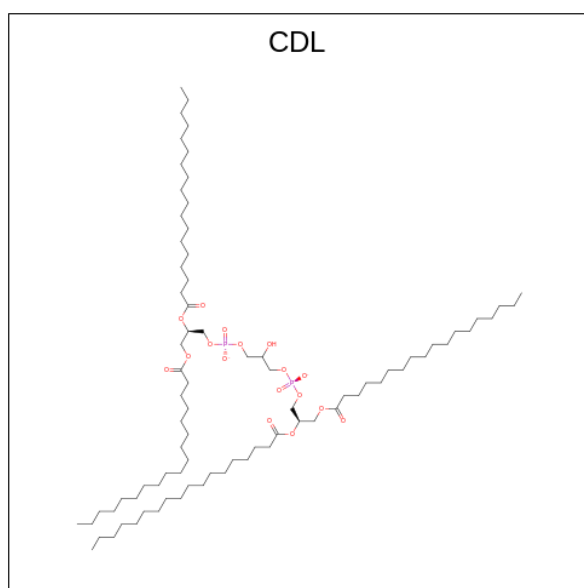
- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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	A7	1	Total	C	O	P	0
			94	75	17	2	
68	A8	1	Total	C	O	P	0
			83	64	17	2	
68	AL	1	Total	C	O	P	0
			94	75	17	2	
68	AL	1	Total	C	O	P	0
			82	63	17	2	
68	AL	1	Total	C	O	P	0
			80	61	17	2	
68	AN	1	Total	C	O	P	0
			81	62	17	2	
68	AN	1	Total	C	O	P	0
			66	47	17	2	
68	B4	1	Total	C	O	P	0
			62	43	17	2	
68	B5	1	Total	C	O	P	0
			96	77	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	N4	1	Total	C	O	P	0
			100	81	17	2	
68	N5	1	Total	C	O	P	0
			89	70	17	2	
68	N5	1	Total	C	O	P	0
			100	81	17	2	
68	QB	1	Total	C	O	P	0
			64	45	17	2	
68	QC	1	Total	C	O	P	0
			90	71	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	Qb	1	Total	C	O	P	0
			64	45	17	2	
68	Qc	1	Total	C	O	P	0
			61	42	17	2	
68	Qc	1	Total	C	O	P	0
			64	45	17	2	

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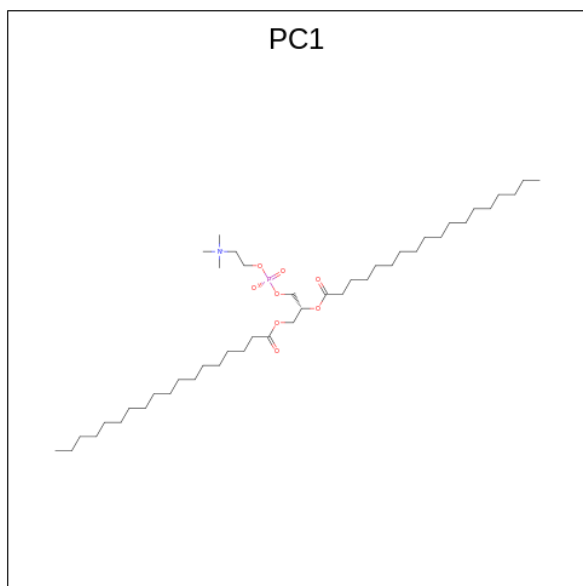
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Mol	Chain	Residues	Atoms				AltConf
68	Qh	1	Total	C	O	P	0
			100	81	17	2	
68	Qj	1	Total	C	O	P	0
			96	77	17	2	

- 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: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
70	6A	1	Total	C	N	O	P	0
			45	35	1	8	1	
70	7A	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	7C	1	Total	C	N	O	P	0
			42	32	1	8	1	
70	B5	1	Total	C	N	O	P	0
			54	44	1	8	1	

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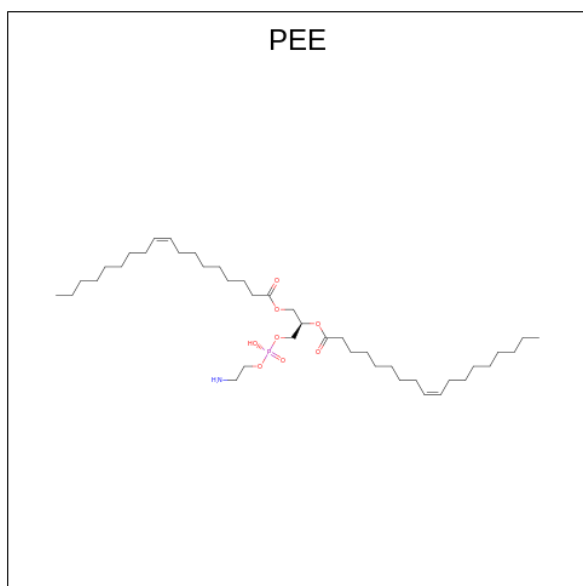
Mol	Chain	Residues	Atoms					AltConf
70	B7	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	B8	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	C1	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	C1	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	C1	1	Total	C	N	O	P	0
			50	40	1	8	1	
70	C3	1	Total	C	N	O	P	0
			49	39	1	8	1	
70	C3	1	Total	C	N	O	P	0
			51	41	1	8	1	
70	C4	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	N4	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	N6	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	QB	1	Total	C	N	O	P	0
			51	41	1	8	1	
70	QB	1	Total	C	N	O	P	0
			32	22	1	8	1	
70	QI	1	Total	C	N	O	P	0
			54	44	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
			38	28	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
			42	32	1	8	1	
70	Qc	1	Total	C	N	O	P	0
			48	38	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
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	
70	S8	1	Total	C	N	O	P	0
			45	35	1	8	1	

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



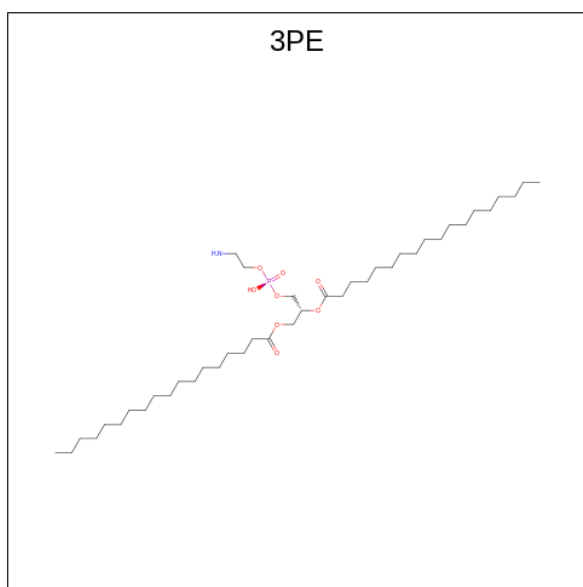
Mol	Chain	Residues	Atoms					AltConf
71	6A	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	6A	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	8B	1	Total	C	N	O	P	0
			42	32	1	8	1	
71	A3	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	A7	1	Total	C	N	O	P	0
			28	18	1	8	1	
71	AL	1	Total	C	N	O	P	0
			36	26	1	8	1	
71	AL	1	Total	C	N	O	P	0
			40	30	1	8	1	

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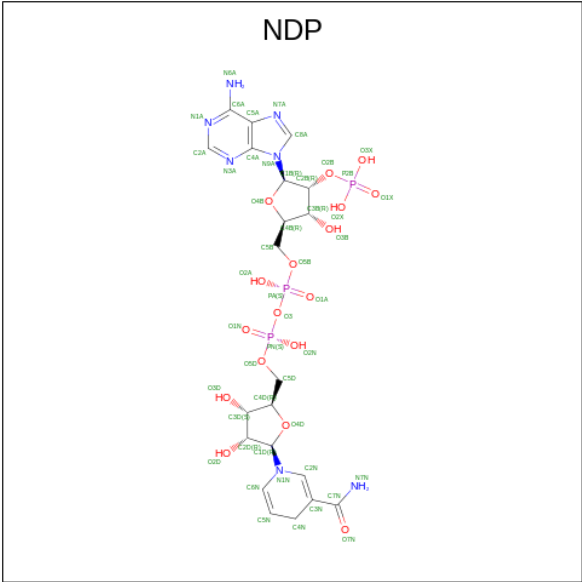
Mol	Chain	Residues	Atoms					AltConf
71	AN	1	Total 51	C 41	N 1	O 8	P 1	0
71	BL	1	Total 51	C 41	N 1	O 8	P 1	0
71	C1	1	Total 33	C 23	N 1	O 8	P 1	0
71	C3	1	Total 51	C 41	N 1	O 8	P 1	0
71	C3	1	Total 51	C 41	N 1	O 8	P 1	0
71	CB	1	Total 37	C 27	N 1	O 8	P 1	0
71	N5	1	Total 46	C 36	N 1	O 8	P 1	0
71	N5	1	Total 51	C 41	N 1	O 8	P 1	0
71	N5	1	Total 44	C 34	N 1	O 8	P 1	0
71	QC	1	Total 40	C 30	N 1	O 8	P 1	0
71	QC	1	Total 35	C 25	N 1	O 8	P 1	0
71	QC	1	Total 43	C 33	N 1	O 8	P 1	0
71	QE	1	Total 47	C 37	N 1	O 8	P 1	0
71	QH	1	Total 51	C 41	N 1	O 8	P 1	0
71	Qb	1	Total 51	C 41	N 1	O 8	P 1	0
71	Qc	1	Total 42	C 32	N 1	O 8	P 1	0
71	Qc	1	Total 48	C 38	N 1	O 8	P 1	0
71	Qe	1	Total 50	C 40	N 1	O 8	P 1	0
71	Qh	1	Total 51	C 41	N 1	O 8	P 1	0
71	S8	1	Total 51	C 41	N 1	O 8	P 1	0

- Molecule 72 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



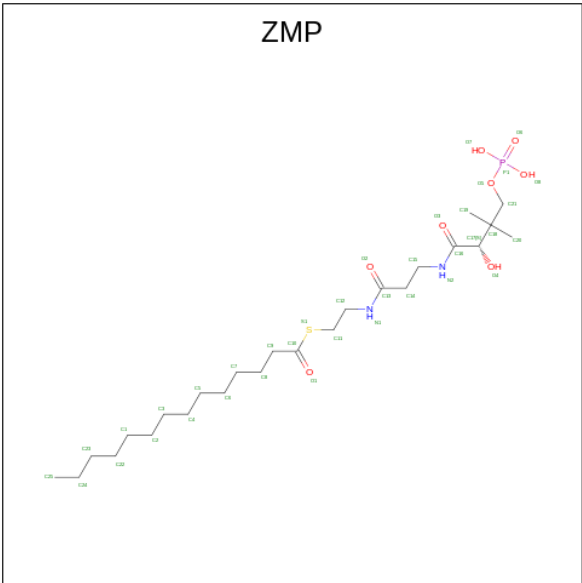
Mol	Chain	Residues	Atoms					AltConf
72	7B	1	Total	C	N	O	P	0
			51	41	1	8	1	
72	C1	1	Total	C	N	O	P	0
			51	41	1	8	1	
72	CA	1	Total	C	N	O	P	0
			51	41	1	8	1	
72	CB	1	Total	C	N	O	P	0
			46	36	1	8	1	
72	Qc	1	Total	C	N	O	P	0
			44	34	1	8	1	
72	Qc	1	Total	C	N	O	P	0
			48	38	1	8	1	

- Molecule 73 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



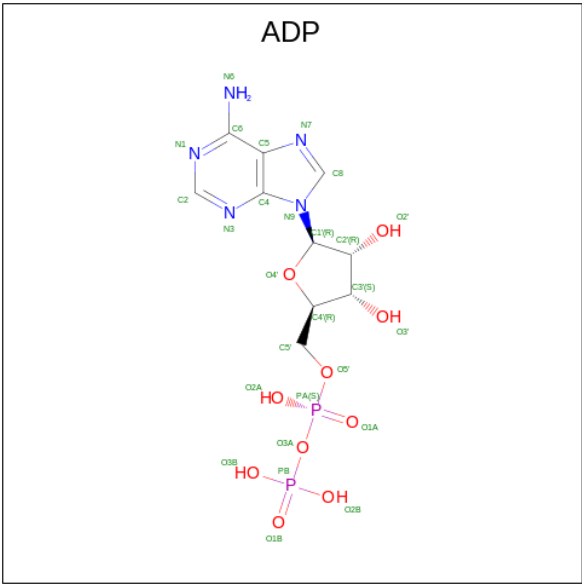
Mol	Chain	Residues	Atoms					AltConf
73	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 74 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



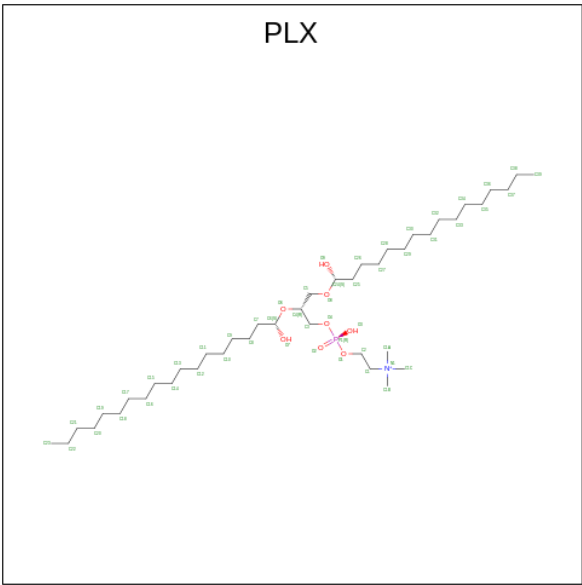
Mol	Chain	Residues	Atoms						AltConf
74	AB	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	
74	AC	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 75 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



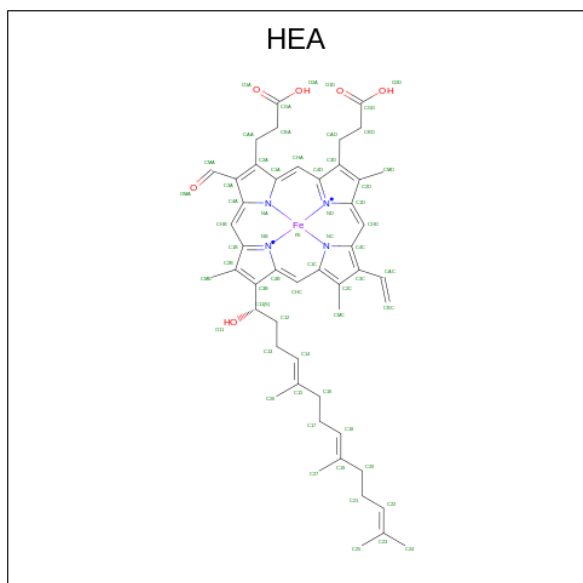
Mol	Chain	Residues	Atoms					AltConf
75	AK	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 76 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P).



Mol	Chain	Residues	Atoms					AltConf
76	AL	1	Total	C	N	O	P	0
			47	37	1	8	1	
76	AM	1	Total	C	N	O	P	0
			52	42	1	8	1	
76	B1	1	Total	C	N	O	P	0
			52	42	1	8	1	
76	BL	1	Total	C	N	O	P	0
			52	42	1	8	1	
76	C2	1	Total	C	N	O	P	0
			39	29	1	8	1	
76	CB	1	Total	C	N	O	P	0
			52	42	1	8	1	
76	N3	1	Total	C	N	O	P	0
			52	42	1	8	1	
76	QE	1	Total	C	N	O	P	0
			46	36	1	8	1	
76	QI	1	Total	C	N	O	P	0
			52	42	1	8	1	
76	S7	1	Total	C	N	O	P	0
			52	42	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	

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

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

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

- # HEM

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

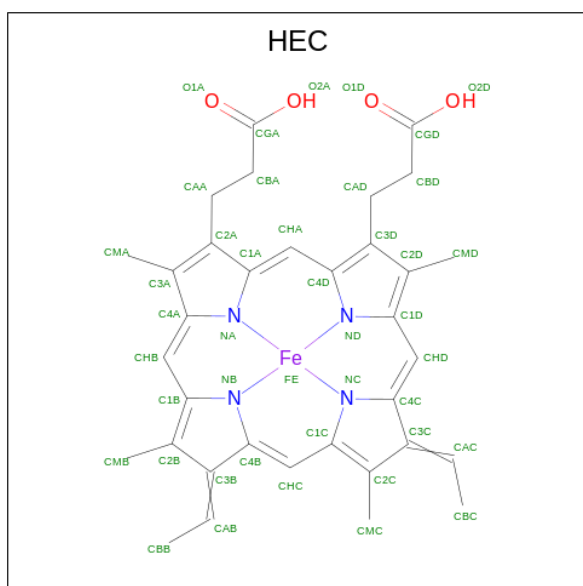


WORLD WIDE
PDB
PROTEIN DATA BANK

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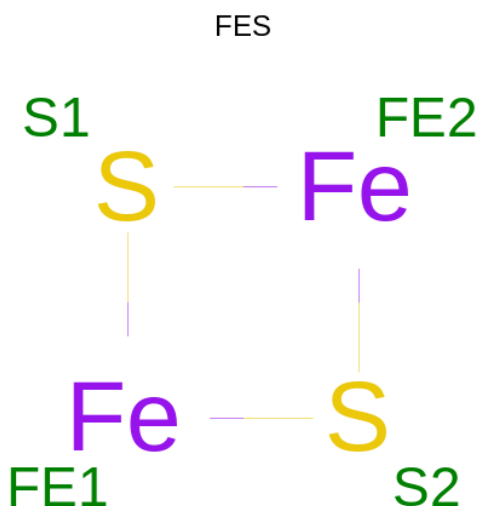
Mol	Chain	Residues	Atoms					AltConf
80	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
80	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
80	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 81 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



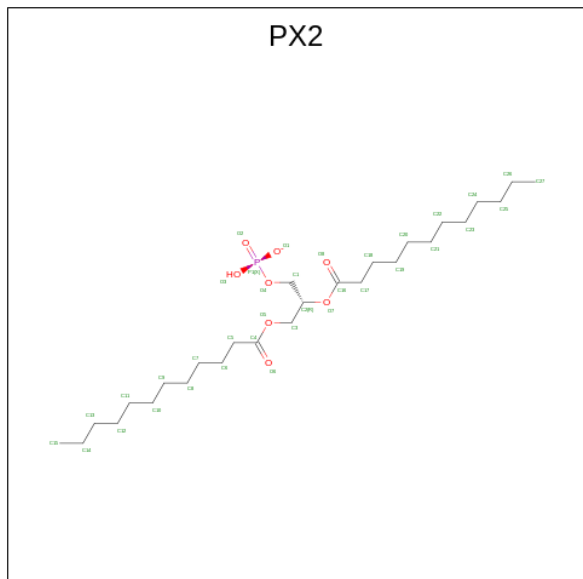
Mol	Chain	Residues	Atoms					AltConf
81	QD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
81	Qd	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 82 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



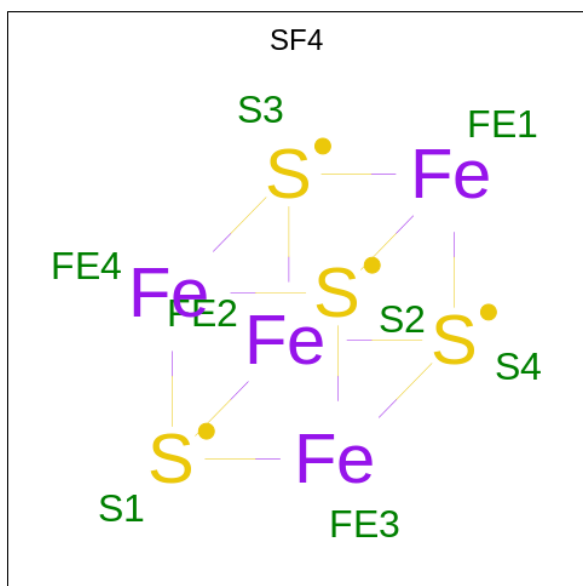
Mol	Chain	Residues	Atoms			AltConf
82	QE	1	Total 4	Fe 2	S 2	0
82	Qe	1	Total 4	Fe 2	S 2	0
82	S1	1	Total 4	Fe 2	S 2	0
82	V2	1	Total 4	Fe 2	S 2	0

- Molecule 83 is 1,2-DILAULOYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: $C_{27}H_{52}O_8P$).



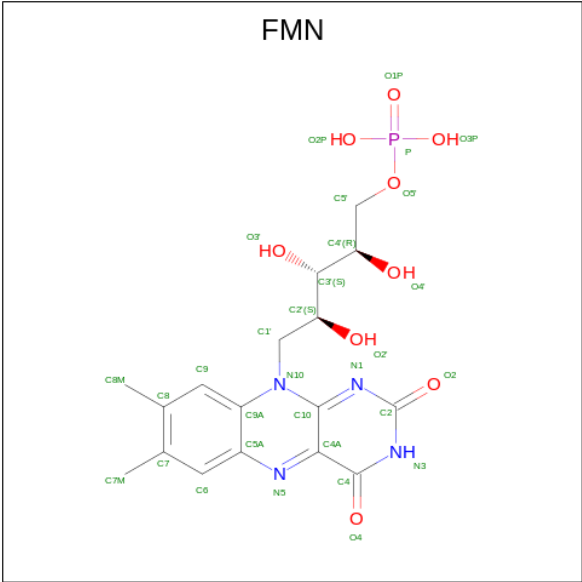
Mol	Chain	Residues	Atoms				AltConf
83	QH	1	Total	C	O	P	0
			36	27	8	1	

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



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

- Molecule 85 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).




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

3 Residue-property plots [i](#)

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

- Molecule 1: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L:  85% 15%




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

Chain 5A:  5% 93% 7%




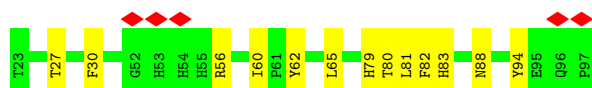
- Molecule 3: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 5B:  5% 79% 21%




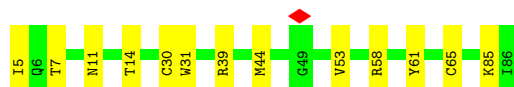
- Molecule 4: Cytochrome c oxidase subunit

Chain 6A:  7% 83% 17%

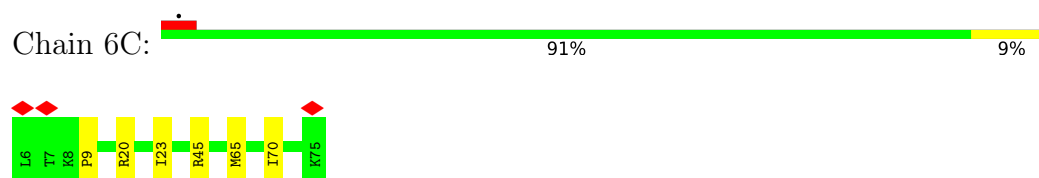


- Molecule 5: Cytochrome c oxidase subunit

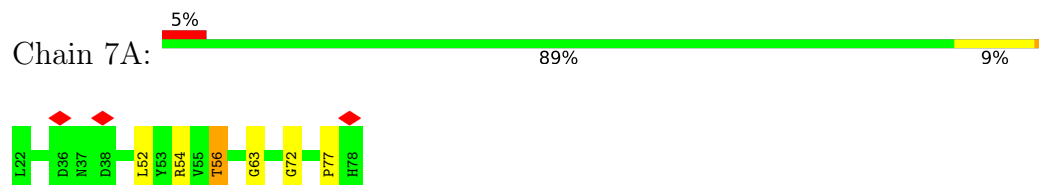
Chain 6B:  84% 16%



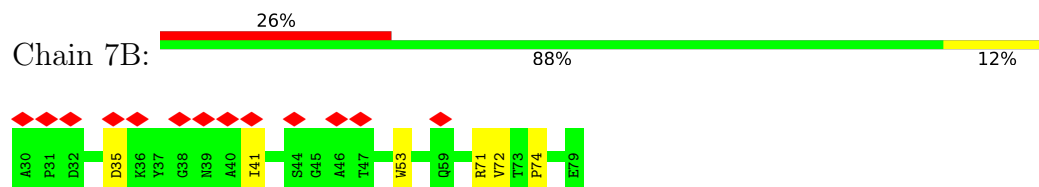
- Molecule 6: Cytochrome c oxidase subunit 6C



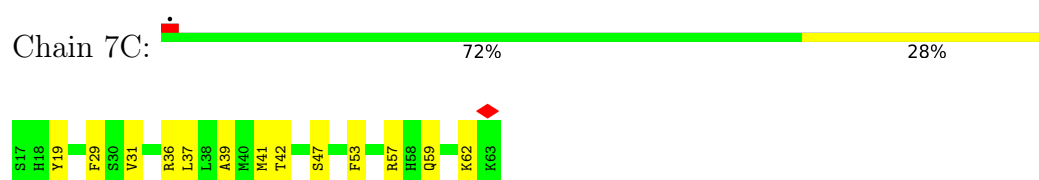
- Molecule 7: Cytochrome c oxidase subunit 7A1, mitochondrial



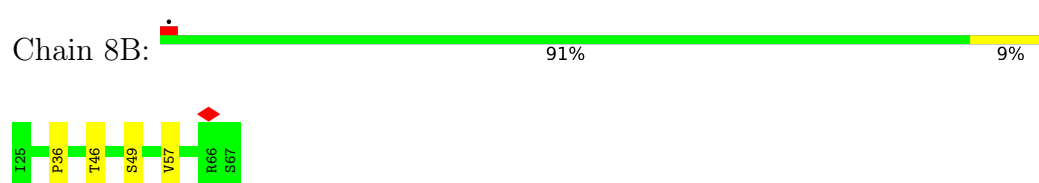
- Molecule 8: Cytochrome c oxidase subunit 7B, mitochondrial



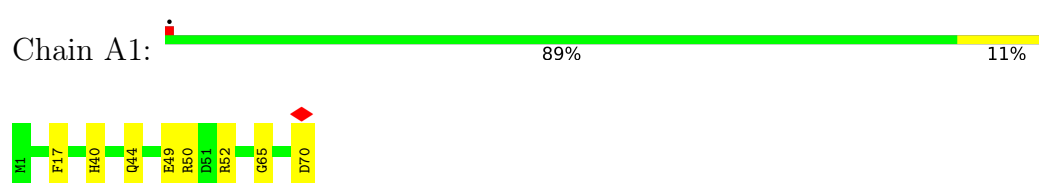
- Molecule 9: Cytochrome c oxidase subunit 7C, mitochondrial



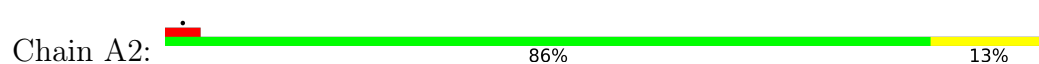
- Molecule 10: Cytochrome c oxidase subunit 8



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

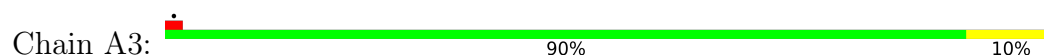


- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2





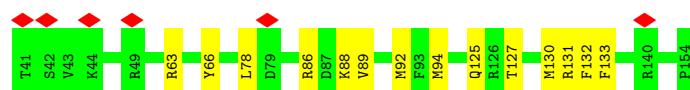
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



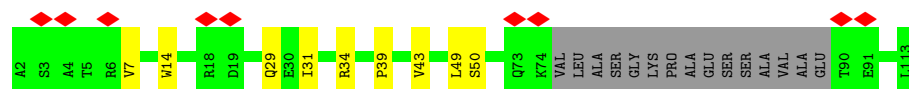
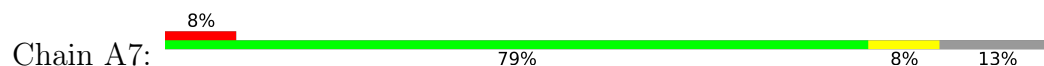
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



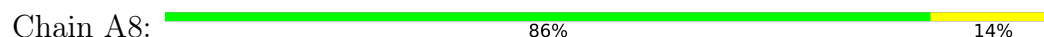
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



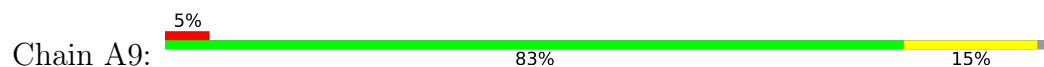
- Molecule 16: Complex I-B14.5a

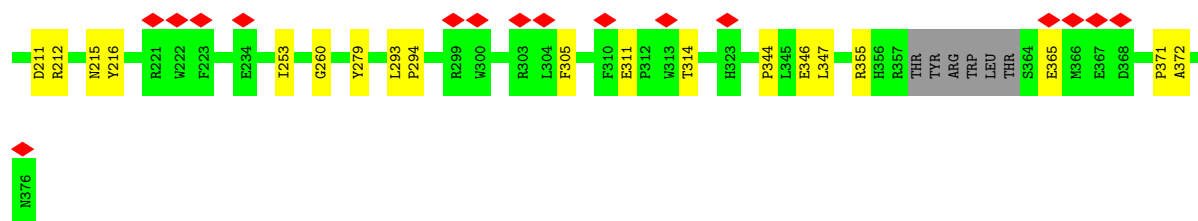


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

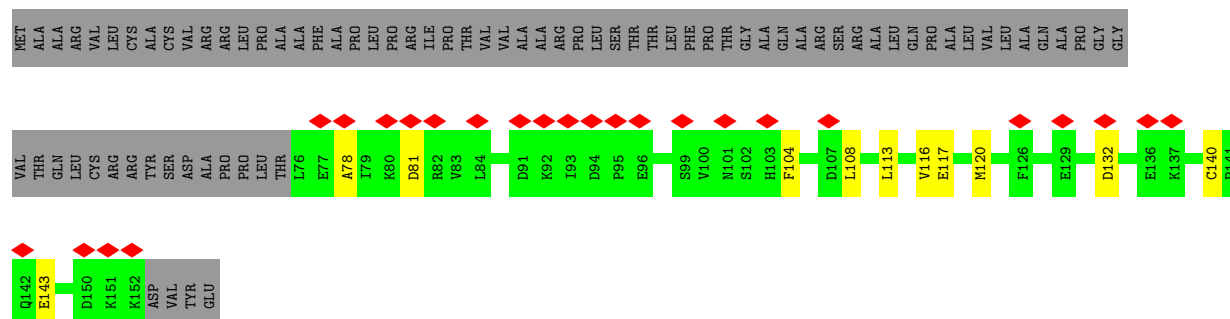
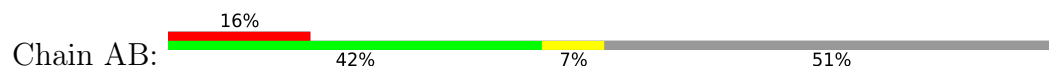


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

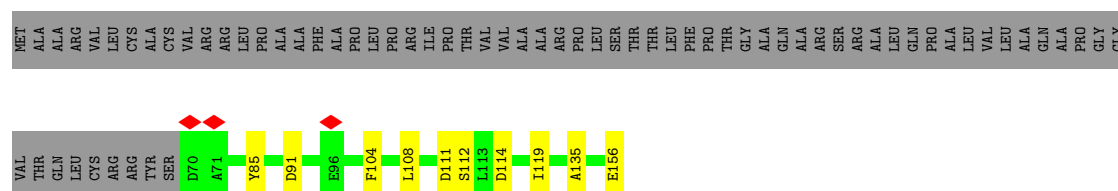




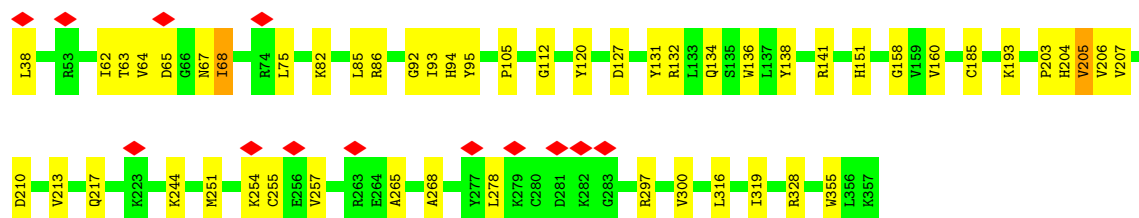
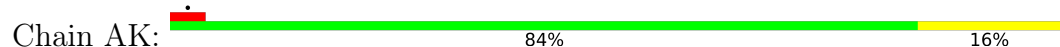
- Molecule 19: Acyl carrier protein



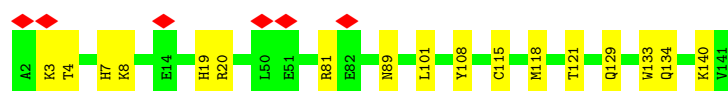
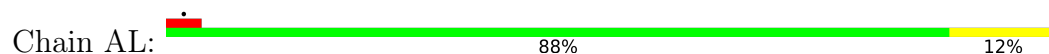
- Molecule 19: Acyl carrier protein



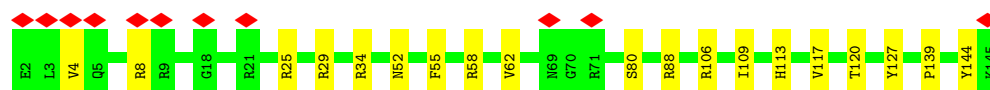
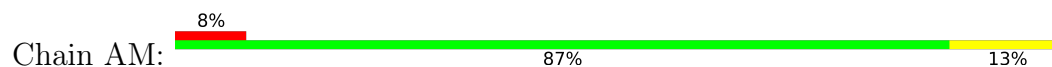
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



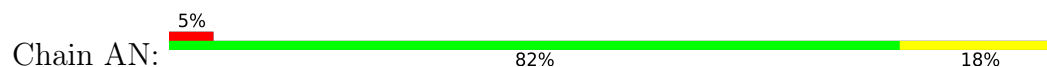
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



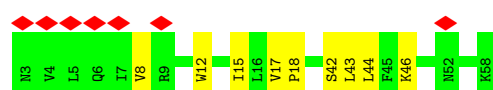
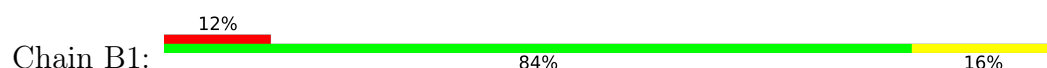
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



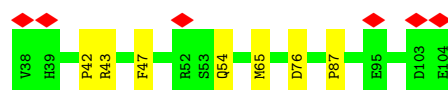
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



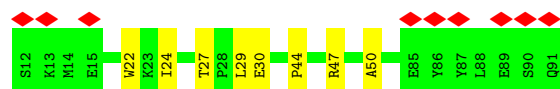
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



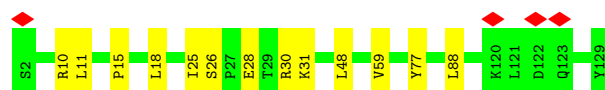
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



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



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

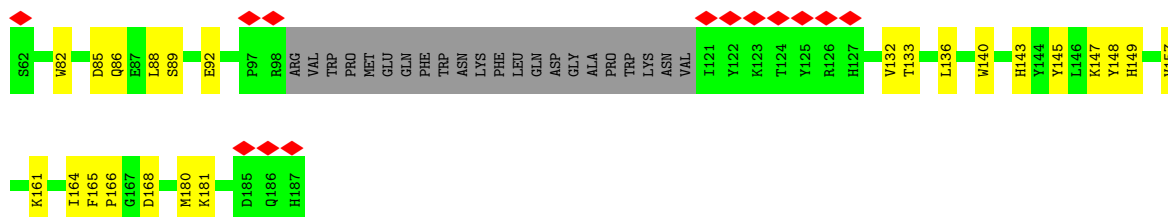


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

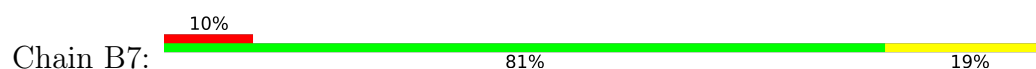




- Molecule 29: Complex I-B17



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



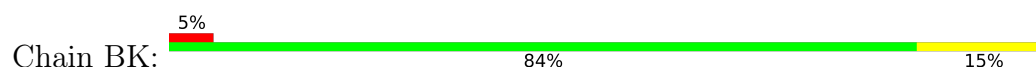
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



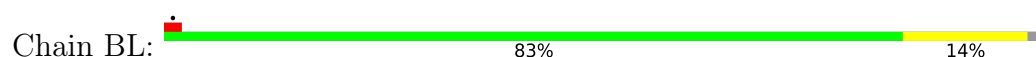
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



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

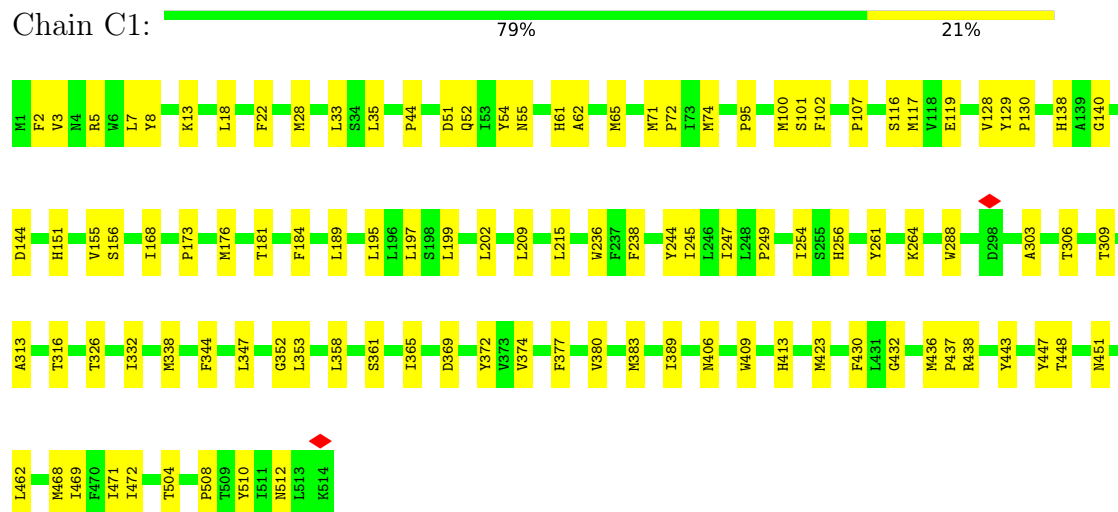


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

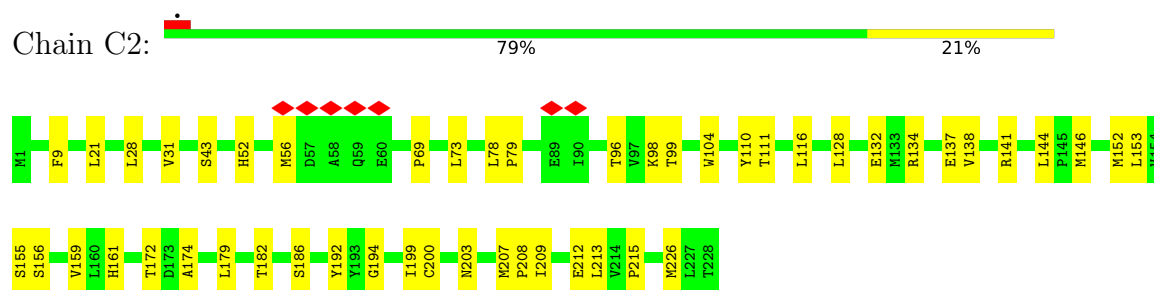




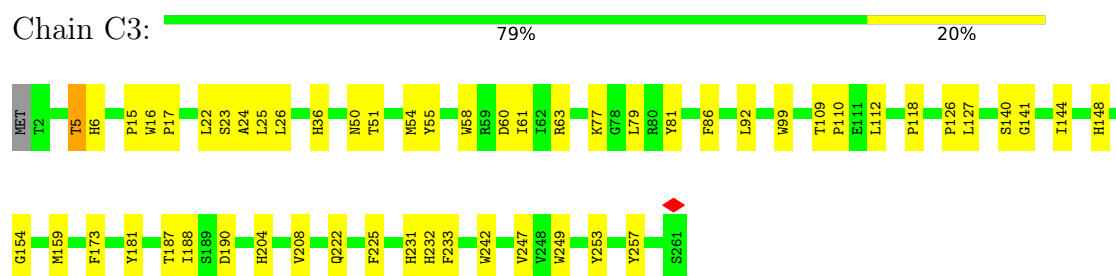
• Molecule 35: Cytochrome c oxidase subunit 1



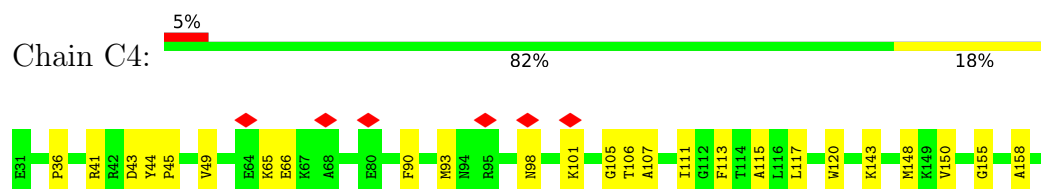
• Molecule 36: Cytochrome c oxidase subunit 2



• Molecule 37: Cytochrome c oxidase subunit 3

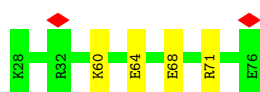


• Molecule 38: Cytochrome c oxidase subunit 4



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

Chain CA:  92% 8%




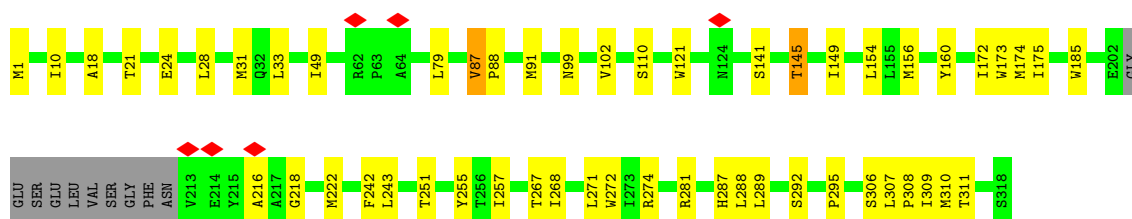
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain CB:  91% 9%




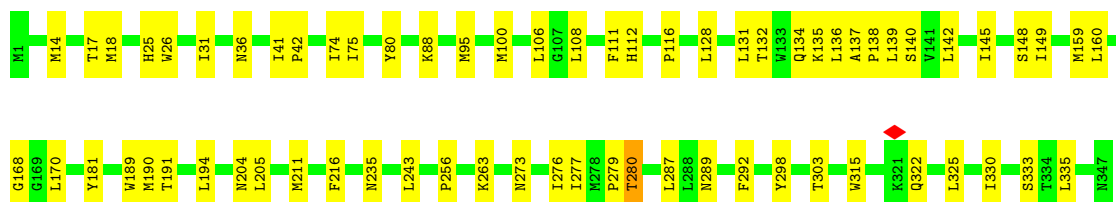
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain N1:  80% 16% ..




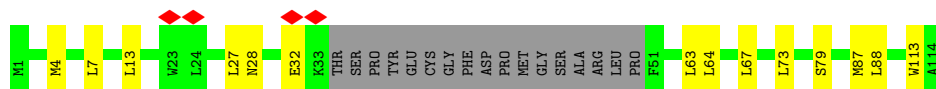
- Molecule 42: NADH-ubiquinone oxidoreductase chain 2

Chain N2:  81% 19%




- Molecule 43: NADH-ubiquinone oxidoreductase chain 3

Chain N3:  73% 12% 15%

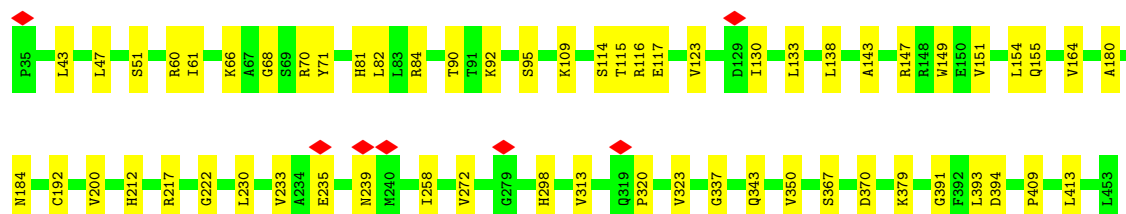


- Molecule 44: NADH-ubiquinone oxidoreductase chain 4

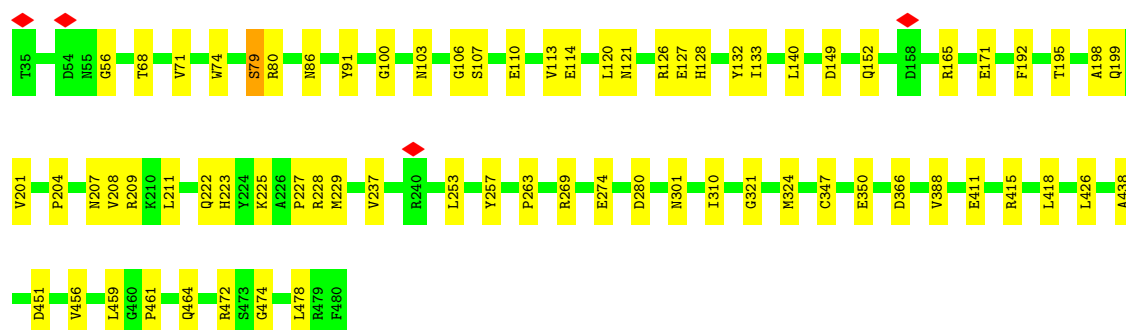
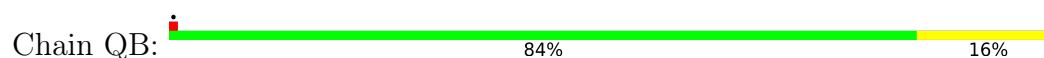
Chain N4:  78% 22%



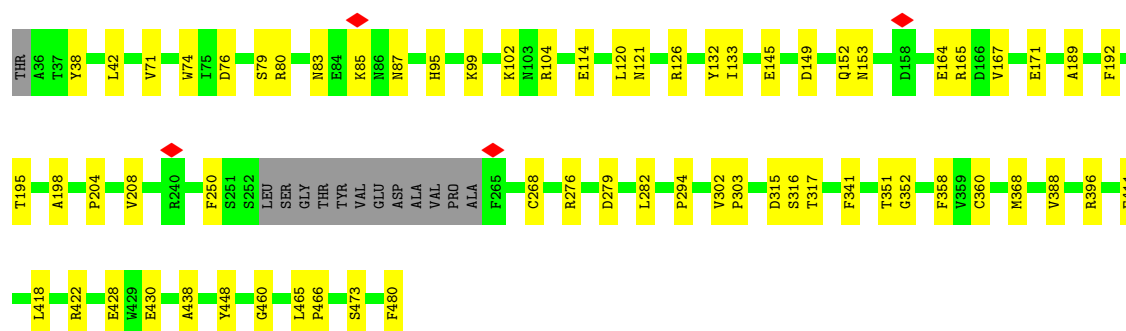
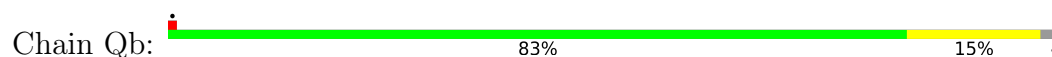
- Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial



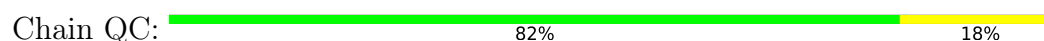
- Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial



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

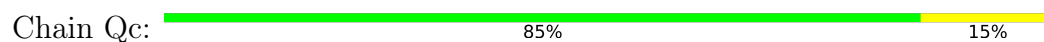


- Molecule 49: Cytochrome b

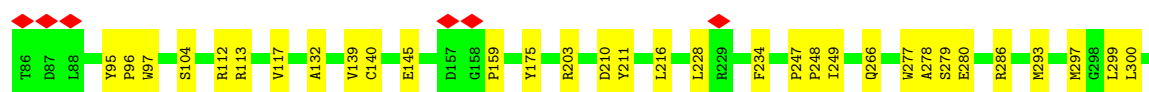




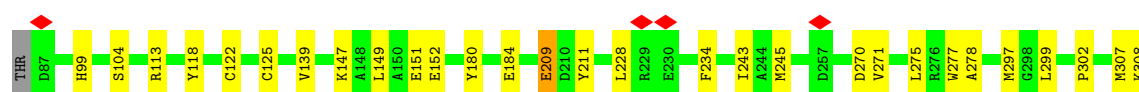
• Molecule 49: Cytochrome b



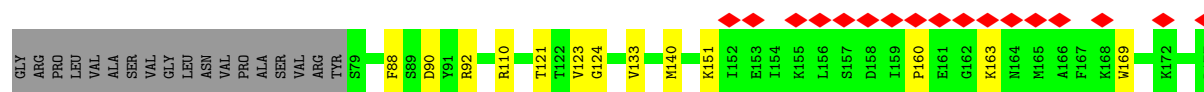
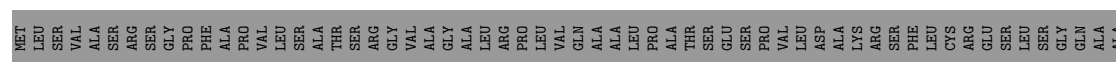
• Molecule 50: Cytochrome c domain-containing protein

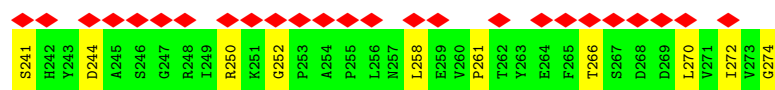


• Molecule 50: Cytochrome c domain-containing protein

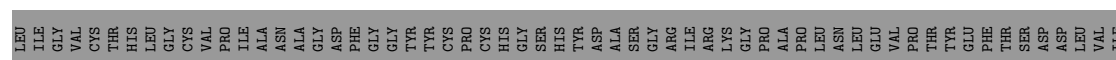
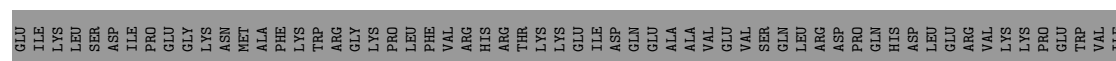
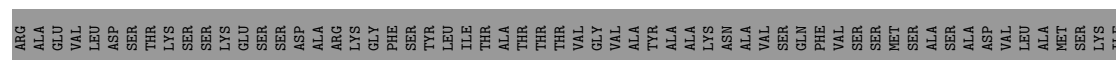
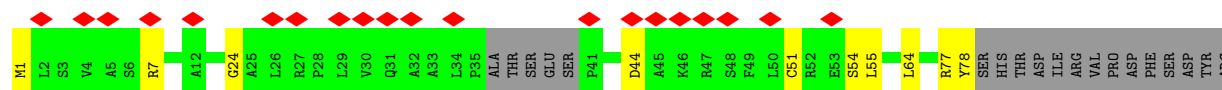


• Molecule 51: Cytochrome b-c1 complex subunit Rieske, mitochondrial

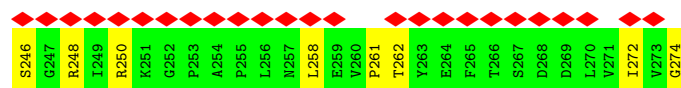
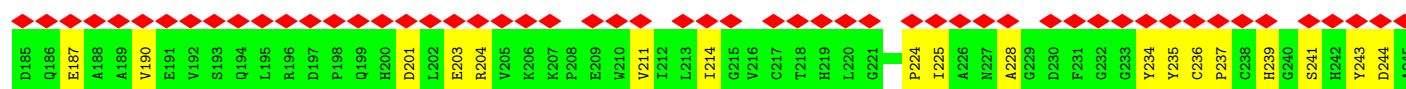
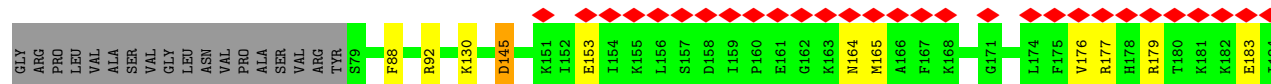
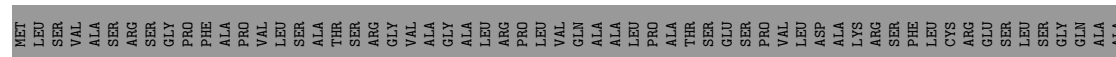




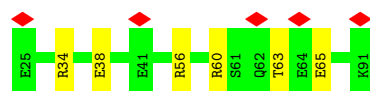
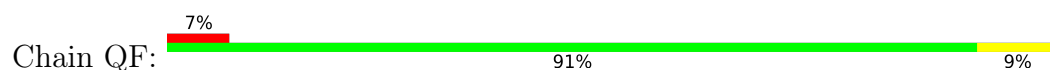
- Molecule 51: Cytochrome b-c1 complex subunit Rieske, mitochondrial



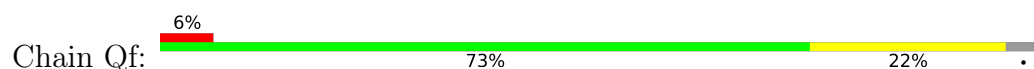
- Molecule 51: Cytochrome b-c1 complex subunit Rieske, mitochondrial

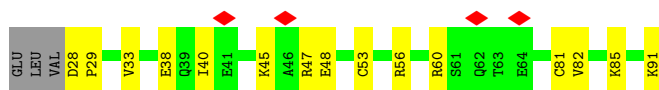


- Molecule 52: Cytochrome b-c1 complex subunit 6



- Molecule 52: Cytochrome b-c1 complex subunit 6

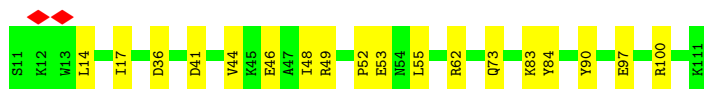
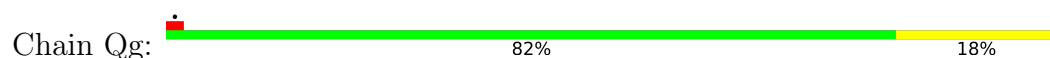




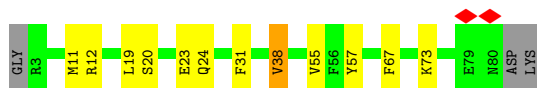
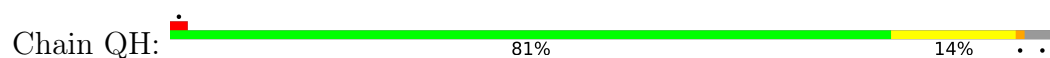
- Molecule 53: Cytochrome b-c1 complex subunit 7



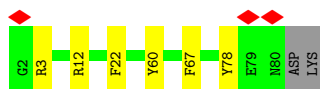
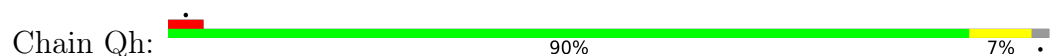
- Molecule 53: Cytochrome b-c1 complex subunit 7



- Molecule 54: Cytochrome b-c1 complex subunit 8



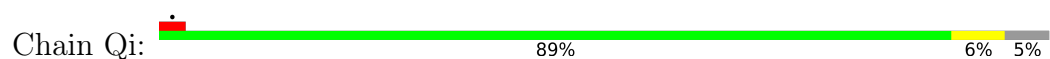
- Molecule 54: Cytochrome b-c1 complex subunit 8



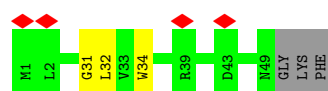
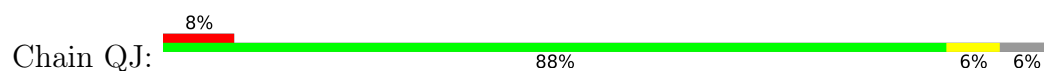
- Molecule 55: Complex III subunit 9



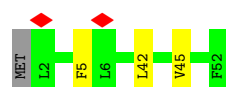
- Molecule 55: Complex III subunit 9



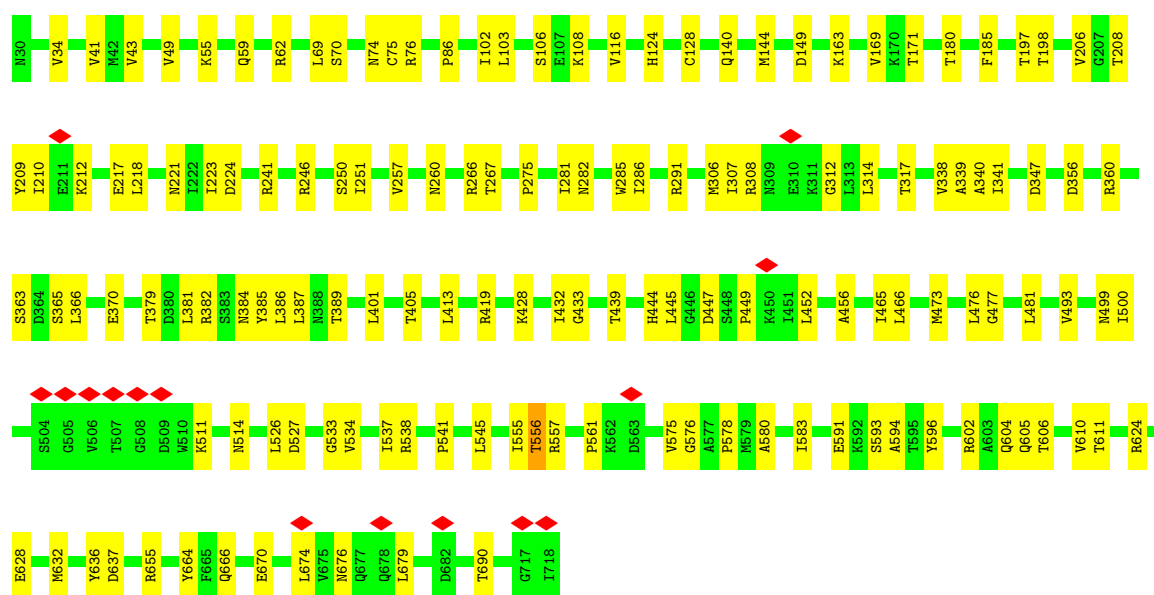
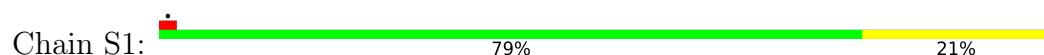
- Molecule 56: Cytochrome b-c1 complex subunit 10



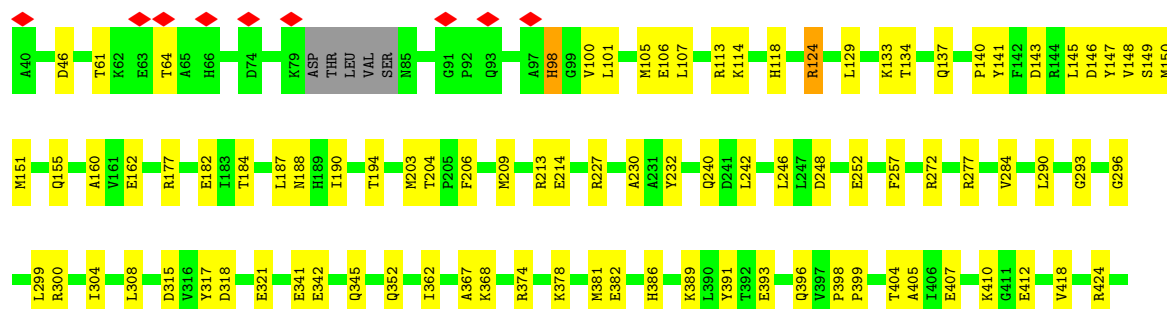
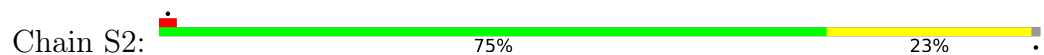
- Molecule 56: Cytochrome b-c1 complex subunit 10

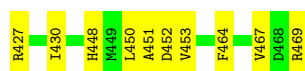


- Molecule 57: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



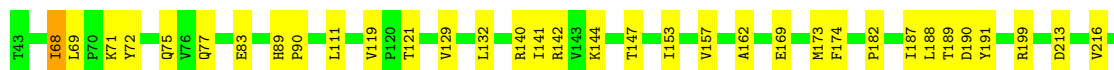
- Molecule 58: Complex I-49kD





• Molecule 59: Complex I-30kD

Chain S3: 82% 17%



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

Chain S4: 6% 86% 14%



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

Chain S5: 5% 89% 11%



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

Chain S6: 6% 88% 12%



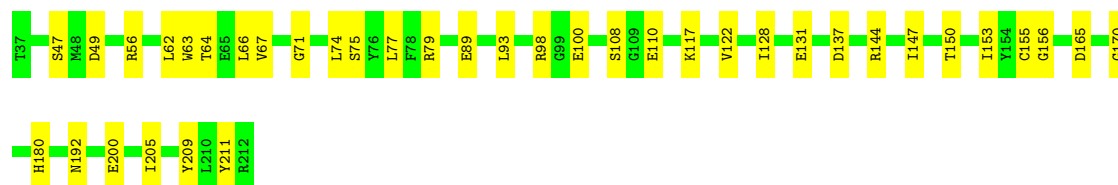
• Molecule 63: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain S7: 78% 21%

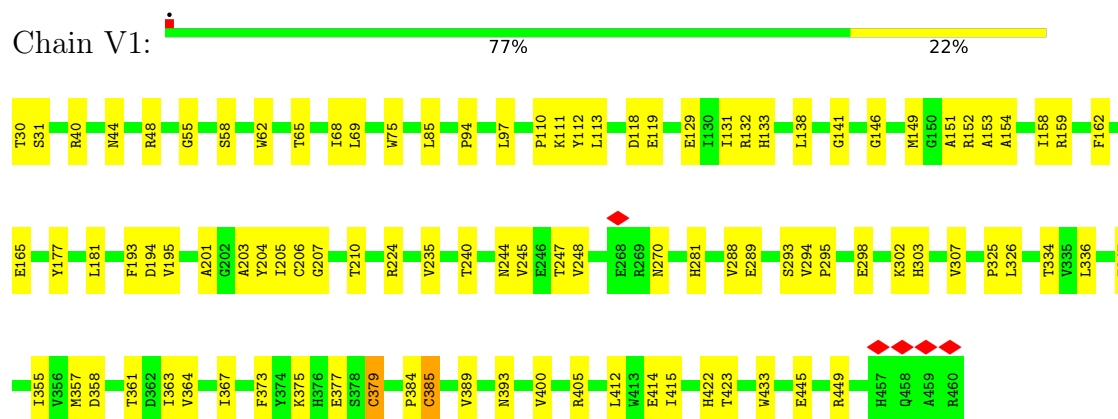


• Molecule 64: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

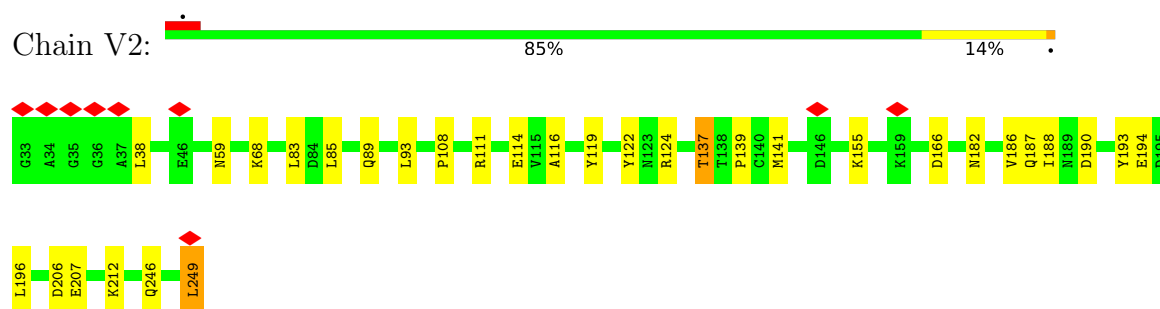
Chain S8: 78% 22%



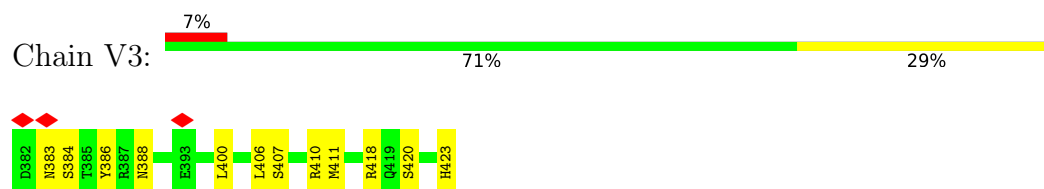
- Molecule 65: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



- 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, C1	Depositor
Number of particles used	250490	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	47.821	Depositor
Minimum map value	-24.261	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	1.078	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: NDP, HEC, ZN, PEE, ADP, PX2, 2MR, CDL, ZMP, 3PE, MG, PLX, PC1, FMN, CU, FES, HEA, SF4, HEM

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	0.16	0/759	0.26	0/1029
2	5A	0.11	0/843	0.23	0/1145
3	5B	0.14	0/739	0.30	0/1002
4	6A	0.12	0/648	0.27	0/888
5	6B	0.13	0/704	0.23	0/951
6	6C	0.12	0/587	0.22	0/781
7	7A	0.12	0/457	0.25	0/620
8	7B	0.11	0/405	0.24	0/555
9	7C	0.14	0/400	0.23	0/536
10	8B	0.14	0/349	0.26	0/477
11	A1	0.14	0/577	0.28	0/777
12	A2	0.10	0/697	0.25	0/938
13	A3	0.12	0/664	0.25	0/912
14	A5	0.13	0/929	0.21	0/1258
15	A6	0.13	0/991	0.26	0/1335
16	A7	0.12	0/798	0.23	0/1079
17	A8	0.13	0/1436	0.23	0/1938
18	A9	0.12	0/2757	0.25	0/3734
19	AB	0.08	0/633	0.21	0/851
19	AC	0.13	0/714	0.23	0/965
20	AK	0.15	0/2650	0.36	2/3588 (0.1%)
21	AL	0.13	0/1042	0.21	0/1411
22	AM	0.12	0/1245	0.23	0/1694
23	AN	0.14	0/1203	0.26	0/1622
24	B1	0.14	0/491	0.28	0/663
25	B2	0.13	0/610	0.26	0/836
26	B3	0.13	0/660	0.25	0/892
27	B4	0.14	0/1092	0.25	0/1481
28	B5	0.16	0/1184	0.27	0/1603
29	B6	0.15	0/918	0.31	0/1248
30	B7	0.12	0/1092	0.23	0/1459

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	B8	0.13	0/1371	0.25	0/1875
32	B9	0.14	0/1590	0.27	0/2155
33	BK	0.15	0/1489	0.24	0/2008
34	BL	0.15	0/851	0.29	0/1155
35	C1	0.19	0/4164	0.31	0/5689
36	C2	0.16	0/1880	0.27	0/2564
37	C3	0.16	0/2186	0.26	0/2991
38	C4	0.13	0/1187	0.23	0/1606
39	CA	0.12	0/430	0.22	0/581
40	CB	0.15	0/1031	0.25	0/1394
41	N1	0.17	0/2507	0.32	0/3428
42	N2	0.19	0/2773	0.33	0/3768
43	N3	0.15	0/797	0.26	0/1087
44	N4	0.19	0/3723	0.32	0/5078
45	N5	0.17	0/4914	0.34	0/6683
46	N6	0.15	0/1273	0.31	0/1722
47	QA	0.15	0/3196	0.27	0/4328
47	Qa	0.14	0/3200	0.26	0/4333
48	QB	0.15	0/3531	0.29	0/4793
48	Qb	0.14	0/3436	0.27	0/4659
49	QC	0.17	0/3123	0.30	0/4269
49	Qc	0.17	0/3123	0.30	0/4269
50	QD	0.14	0/1979	0.25	0/2684
50	Qd	0.14	0/1962	0.26	0/2663
51	QE	0.12	0/1550	0.25	0/2098
51	QK	0.11	0/528	0.26	0/716
51	Qe	0.12	0/1550	0.27	0/2098
52	QF	0.11	0/558	0.22	0/747
52	Qf	0.13	0/534	0.24	0/714
53	QG	0.14	0/913	0.24	0/1223
53	Qg	0.14	0/913	0.25	0/1223
54	QH	0.14	0/684	0.29	0/926
54	Qh	0.14	0/688	0.27	0/931
55	QI	0.11	0/520	0.18	0/701
55	Qi	0.15	0/506	0.24	0/683
56	QJ	0.10	0/420	0.24	0/576
56	Qj	0.14	0/437	0.28	0/598
57	S1	0.15	0/5378	0.29	0/7287
58	S2	0.18	0/3501	0.30	0/4743
59	S3	0.15	0/1789	0.27	0/2436
60	S4	0.15	0/1030	0.28	0/1391
61	S5	0.13	0/889	0.23	0/1190
62	S6	0.13	0/755	0.26	0/1018

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
63	S7	0.17	0/1279	0.28	0/1730
64	S8	0.17	0/1443	0.26	0/1952
65	V1	0.14	0/3387	0.29	0/4578
66	V2	0.12	0/1711	0.28	0/2328
67	V3	0.10	0/365	0.25	0/493
All	All	0.15	0/115318	0.28	2/156430 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AK	204	HIS	CA-C-N	-6.18	114.45	123.10
20	AK	204	HIS	C-N-CA	-6.18	114.45	123.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4L	748	0	799	13	0
2	5A	825	0	823	5	0
3	5B	724	0	705	12	0
4	6A	620	0	589	13	0
5	6B	684	0	649	9	0
6	6C	574	0	590	4	0
7	7A	447	0	443	5	0
8	7B	392	0	372	7	0
9	7C	387	0	385	13	0
10	8B	338	0	342	4	0
11	A1	562	0	557	6	0
12	A2	686	0	699	8	0
13	A3	643	0	642	6	0
14	A5	910	0	950	5	0
15	A6	967	0	972	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A7	780	0	808	7	0
17	A8	1398	0	1372	20	0
18	A9	2684	0	2704	31	0
19	AB	624	0	625	8	0
19	AC	702	0	694	8	0
20	AK	2590	0	2553	31	0
21	AL	1021	0	1025	13	0
22	AM	1204	0	1162	12	0
23	AN	1172	0	1162	23	0
24	B1	479	0	486	6	0
25	B2	584	0	529	6	0
26	B3	641	0	620	6	0
27	B4	1062	0	1072	9	0
28	B5	1151	0	1164	13	0
29	B6	890	0	910	23	0
30	B7	1068	0	1043	19	0
31	B8	1315	0	1208	14	0
32	B9	1534	0	1470	17	0
33	BK	1456	0	1426	22	0
34	BL	828	0	788	10	0
35	C1	4024	0	4005	80	0
36	C2	1833	0	1843	31	0
37	C3	2103	0	2034	48	0
38	C4	1153	0	1130	21	0
39	CA	417	0	422	2	0
40	CB	1000	0	994	11	0
41	N1	2436	0	2543	39	0
42	N2	2710	0	2874	54	0
43	N3	779	0	829	12	0
44	N4	3631	0	3839	70	0
45	N5	4785	0	4933	95	0
46	N6	1243	0	1248	26	0
47	QA	3143	0	3125	42	0
47	Qa	3147	0	3129	38	0
48	QB	3459	0	3350	46	0
48	Qb	3367	0	3262	38	0
49	QC	3025	0	3090	55	0
49	Qc	3025	0	3090	51	0
50	QD	1921	0	1867	23	0
50	Qd	1904	0	1849	24	0
51	QE	1517	0	1500	33	0
51	QK	520	0	554	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	Qe	1517	0	1500	24	0
52	QF	552	0	536	4	0
52	Qf	528	0	510	9	0
53	QG	893	0	888	5	0
53	Qg	893	0	888	11	0
54	QH	662	0	660	12	0
54	Qh	666	0	663	6	0
55	QI	507	0	509	3	0
55	Qi	493	0	491	4	0
56	QJ	405	0	405	3	0
56	Qj	421	0	418	2	0
57	S1	5290	0	5321	91	0
58	S2	3423	0	3359	71	0
59	S3	1738	0	1693	25	0
60	S4	1007	0	1008	11	0
61	S5	867	0	871	16	0
62	S6	741	0	701	10	0
63	S7	1248	0	1254	24	0
64	S8	1412	0	1363	32	0
65	V1	3312	0	3266	58	0
66	V2	1671	0	1673	19	0
67	V3	355	0	329	9	0
68	4L	92	0	137	3	0
68	A7	94	0	141	5	0
68	A8	83	0	113	7	0
68	AL	256	0	359	14	0
68	AN	147	0	188	10	0
68	B4	62	0	68	3	0
68	B5	96	0	145	7	0
68	C1	77	0	98	5	0
68	N2	68	0	80	1	0
68	N4	100	0	156	10	0
68	N5	189	0	284	12	0
68	QB	64	0	72	10	0
68	QC	145	0	187	4	0
68	QD	64	0	72	2	0
68	Qb	64	0	72	4	0
68	Qc	125	0	138	8	0
68	Qh	100	0	156	2	0
68	Qj	96	0	145	4	0
69	5B	1	0	0	0	0
69	S6	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	6A	45	0	64	13	0
70	7A	54	0	88	2	0
70	7C	42	0	58	6	0
70	B5	54	0	88	0	0
70	B7	54	0	88	1	0
70	B8	54	0	88	1	0
70	C1	144	0	219	16	0
70	C3	100	0	154	7	0
70	C4	54	0	88	1	0
70	N1	54	0	88	7	0
70	N3	54	0	88	3	0
70	N4	54	0	88	11	0
70	N5	31	0	36	2	0
70	N6	54	0	88	8	0
70	QB	83	0	117	16	0
70	QI	54	0	88	3	0
70	QJ	54	0	88	4	0
70	Qb	38	0	50	5	0
70	Qc	198	0	310	13	0
70	Qd	54	0	88	3	0
70	Qh	54	0	88	5	0
70	S8	45	0	67	10	0
71	6A	102	0	164	6	0
71	8B	42	0	61	3	0
71	A3	51	0	82	4	0
71	A7	28	0	30	1	0
71	AL	76	0	103	0	0
71	AN	51	0	82	5	0
71	BL	51	0	82	1	0
71	C1	33	0	40	3	0
71	C3	102	0	164	7	0
71	CB	37	0	51	3	0
71	N5	141	0	213	16	0
71	QC	118	0	161	12	0
71	QE	47	0	71	4	0
71	QH	51	0	82	4	0
71	Qb	51	0	82	1	0
71	Qc	90	0	134	6	0
71	Qe	50	0	77	3	0
71	Qh	51	0	82	3	0
71	S8	51	0	82	1	0
72	7B	51	0	82	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	C1	51	0	82	4	0
72	CA	51	0	82	4	0
72	CB	46	0	69	0	0
72	Qc	92	0	138	3	0
73	A9	48	0	26	2	0
74	AB	36	0	47	2	0
74	AC	36	0	47	5	0
75	AK	27	0	12	3	0
76	AL	47	0	75	4	0
76	AM	52	0	88	3	0
76	B1	52	0	88	1	0
76	BL	52	0	88	6	0
76	C2	39	0	56	4	0
76	CB	52	0	88	4	0
76	N3	52	0	88	3	0
76	QE	46	0	73	3	0
76	QI	52	0	88	5	0
76	S7	52	0	88	9	0
77	C1	120	0	108	19	0
78	C1	1	0	0	0	0
78	C2	2	0	0	0	0
79	C1	1	0	0	0	0
79	S1	1	0	0	0	0
80	QC	86	0	60	8	0
80	Qc	86	0	60	10	0
81	QD	43	0	30	1	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	QH	36	0	52	1	0
84	S1	16	0	0	1	0
84	S7	8	0	0	0	0
84	S8	16	0	0	2	0
84	V1	8	0	0	0	0
85	V1	31	0	19	2	0
All	All	118456	0	120593	1656	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 (1656) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BK:140:GLN:O	33:BK:144:SER:HB2	1.66	0.95
49:Qc:98:VAL:HG22	80:Qc:405:HEM:HBC2	1.61	0.82
49:QC:97:HIS:HE1	80:QC:402:HEM:ND	1.81	0.79
29:B6:88:LEU:HD22	29:B6:92:GLU:HG2	1.65	0.79
49:QC:237:LEU:HB2	50:QD:297:MET:HE2	1.66	0.78
21:AL:140:LYS:H	42:N2:273:ASN:HD22	1.32	0.78
65:V1:205:ILE:HG12	65:V1:379:CYS:HB3	1.65	0.78
18:A9:198:ALA:O	18:A9:260:GLY:HA2	1.86	0.76
42:N2:88:LYS:HG3	42:N2:148:SER:HB3	1.68	0.75
68:A7:201:CDL:H521	68:A7:201:CDL:H112	1.68	0.75
36:C2:132:GLU:HB3	36:C2:137:GLU:HG3	1.67	0.74
68:QB:501:CDL:HB62	70:QB:502:PC1:H221	1.69	0.74
65:V1:235:VAL:HG12	65:V1:240:THR:HG21	1.69	0.74
65:V1:110:PRO:HB3	65:V1:152:ARG:HD3	1.69	0.74
7:7A:77:PRO:HG3	9:7C:62:LYS:HG3	1.70	0.74
63:S7:188:LYS:HB2	63:S7:191:ARG:HB2	1.68	0.74
18:A9:129:LEU:HD23	18:A9:167:ILE:HG13	1.69	0.73
70:QJ:101:PC1:H321	71:Qe:302:PEE:H16	1.70	0.73
6:6C:45:ARG:NH2	76:C2:301:PLX:O2	2.22	0.72
33:BK:107:GLN:HE22	45:N5:194:ASN:HD22	1.36	0.72
35:C1:406:ASN:HD22	35:C1:409:TRP:HD1	1.37	0.72
57:S1:338:VAL:O	57:S1:365:SER:HB2	1.89	0.72
70:C1:610:PC1:H3A1	37:C3:24:ALA:HB2	1.71	0.71
57:S1:282:ASN:ND2	57:S1:285:TRP:O	2.23	0.71
71:AN:202:PEE:H37	70:N1:401:PC1:H2F2	1.73	0.70
72:CA:101:3PE:H2G2	72:CA:101:3PE:H2B1	1.72	0.70
47:QA:178:HIS:NE2	47:QA:330:TYR:OH	2.24	0.70
48:QB:204:PRO:HG2	48:QB:207:ASN:HB2	1.72	0.70
20:AK:65:ASP:HB3	20:AK:206:VAL:HG13	1.74	0.70
56:QJ:32:LEU:HD21	70:QJ:101:PC1:H262	1.73	0.70
64:S8:64:THR:HG21	70:S8:304:PC1:H121	1.71	0.70
47:Qa:155:GLN:NE2	47:Qa:200:VAL:O	2.25	0.70
70:Qh:103:PC1:H2E1	70:Qh:103:PC1:H3F1	1.74	0.69
57:S1:124:HIS:HD2	58:S2:381:MET:HE2	1.55	0.69
22:AM:34:ARG:NH2	64:S8:89:GLU:OE2	2.25	0.69
68:B5:201:CDL:H661	45:N5:12:LEU:HB3	1.74	0.69
17:A8:107:HIS:HB3	17:A8:197:PRO:HD2	1.75	0.69
49:QC:138:MET:HB2	49:QC:255:ASN:HD22	1.57	0.69
57:S1:433:GLY:HA2	57:S1:447:ASP:HA	1.75	0.69
60:S4:62:THR:HG23	60:S4:72:ILE:HD13	1.75	0.69
48:QB:195:THR:HG21	48:QB:269:ARG:H	1.58	0.68
48:Qb:388:VAL:HG21	48:Qb:438:ALA:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A2:24:CYS:N	12:A2:58:CYS:SG	2.66	0.68
45:N5:530:PRO:O	45:N5:534:HIS:HB2	1.94	0.68
71:6A:102:PEE:H17	71:6A:103:PEE:H50	1.76	0.68
48:QB:100:GLY:HA2	48:QB:106:GLY:H	1.56	0.68
35:C1:51:ASP:O	35:C1:55:ASN:ND2	2.27	0.68
37:C3:86:PHE:HZ	70:C3:301:PC1:H3C1	1.58	0.67
16:A7:14:TRP:HB2	71:A7:202:PEE:H10	1.77	0.67
51:QK:1:MET:O	51:QK:7:ARG:NH1	2.27	0.67
51:QE:110:ARG:NH1	54:Qh:22:PHE:O	2.27	0.67
70:QI:101:PC1:H3B2	70:QI:101:PC1:H2F2	1.76	0.67
57:S1:433:GLY:O	57:S1:444:HIS:NE2	2.22	0.67
68:B5:201:CDL:H192	68:B5:201:CDL:H791	1.76	0.67
36:C2:161:HIS:CE1	36:C2:200:CYS:SG	2.87	0.67
12:A2:59:SER:HB2	57:S1:655:ARG:HD3	1.76	0.66
53:Qg:36:ASP:OD1	53:Qg:90:TYR:OH	2.11	0.66
58:S2:374:ARG:NH2	64:S8:165:ASP:OD1	2.28	0.66
58:S2:290:LEU:O	58:S2:293:GLY:N	2.28	0.66
44:N4:114:GLU:HG2	44:N4:116:ILE:HG22	1.77	0.66
47:Qa:82:LEU:HD11	47:Qa:154:LEU:HB3	1.78	0.66
47:Qa:155:GLN:HE22	47:Qa:200:VAL:HB	1.60	0.66
49:Qc:237:LEU:HD13	50:Qd:297:MET:HG2	1.77	0.66
57:S1:224:ASP:OD2	57:S1:291:ARG:NH2	2.27	0.66
65:V1:112:TYR:HB2	65:V1:240:THR:HG22	1.78	0.66
20:AK:94:HIS:HB3	20:AK:105:PRO:HB3	1.78	0.66
49:QC:98:VAL:HG22	80:QC:402:HEM:HBC2	1.76	0.66
20:AK:92:GLY:H	20:AK:95:TYR:HB3	1.61	0.66
57:S1:208:THR:HG21	57:S1:212:LYS:HB3	1.78	0.66
3:5B:41:GLU:HG2	3:5B:56:ARG:HH22	1.61	0.65
12:A2:46:LYS:HE2	57:S1:674:LEU:HD21	1.78	0.65
68:N5:702:CDL:HA4	68:N5:702:CDL:H541	1.79	0.65
26:B3:27:THR:HG22	26:B3:29:LEU:H	1.60	0.65
63:S7:63:TRP:HA	63:S7:92:VAL:HG22	1.78	0.65
47:QA:399:GLN:HA	47:QA:402:VAL:HG22	1.77	0.65
49:QC:97:HIS:HE1	80:QC:402:HEM:C1D	2.14	0.65
49:QC:246:SER:HB2	49:QC:249:LEU:HB2	1.78	0.65
65:V1:40:ARG:NH1	65:V1:289:GLU:O	2.29	0.65
70:6A:101:PC1:H112	37:C3:187:THR:HA	1.79	0.65
68:A7:201:CDL:H771	68:A7:201:CDL:H602	1.77	0.65
76:C2:301:PLX:H6	76:C2:301:PLX:H251	1.79	0.65
70:QB:502:PC1:H2B2	70:QB:503:PC1:H392	1.79	0.65
9:7C:59:GLN:NE2	35:C1:116:SER:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:N2:108:LEU:HD11	42:N2:191:THR:HG21	1.78	0.64
29:B6:132:VAL:O	29:B6:136:LEU:HB3	1.97	0.64
50:QD:266:GLN:HE22	52:Qf:91:LYS:H	1.45	0.64
70:C1:610:PC1:H2A1	70:C3:301:PC1:H3B2	1.80	0.64
41:N1:156:MET:HB3	41:N1:174:MET:HE1	1.80	0.64
68:Qc:411:CDL:H712	68:Qc:411:CDL:H311	1.79	0.64
57:S1:163:LYS:O	57:S1:171:THR:OG1	2.16	0.64
68:AL:202:CDL:H242	70:N5:705:PC1:H232	1.80	0.64
36:C2:104:TRP:CG	36:C2:203:ASN:HB2	2.32	0.64
38:C4:155:GLY:H	38:C4:158:ALA:HB3	1.63	0.64
19:AC:156:GLU:OE1	28:B5:52:LYS:NZ	2.30	0.64
68:AN:203:CDL:H141	70:S8:304:PC1:H2E1	1.80	0.64
29:B6:85:ASP:OD2	32:B9:167:TRP:NE1	2.29	0.64
47:Qa:90:THR:HG23	47:Qa:95:SER:HA	1.78	0.64
49:Qc:311:LYS:NZ	49:Qc:379:TRP:OXT	2.31	0.64
45:N5:3:PRO:HB2	45:N5:53:MET:HE1	1.80	0.64
49:Qc:356:ILE:HD11	70:Qc:407:PC1:H2A2	1.79	0.64
5:6B:39:ARG:NH1	5:6B:85:LYS:O	2.29	0.64
70:6A:101:PC1:H241	35:C1:215:LEU:HD21	1.79	0.63
66:V2:187:GLN:HE21	66:V2:190:ASP:HA	1.64	0.63
70:S8:304:PC1:H2E2	70:S8:304:PC1:H381	1.79	0.63
15:A6:78:LEU:HD22	15:A6:130:MET:HE3	1.79	0.63
20:AK:93:ILE:HA	20:AK:136:TRP:HE1	1.63	0.63
51:Qe:204:ARG:NH2	51:Qe:258:LEU:O	2.30	0.63
68:AL:204:CDL:H322	27:B4:88:LEU:HD11	1.80	0.63
35:C1:406:ASN:HD22	35:C1:409:TRP:CD1	2.17	0.63
35:C1:443:TYR:O	36:C2:134:ARG:NH2	2.32	0.63
51:Qe:244:ASP:OD2	51:Qe:250:ARG:NH2	2.31	0.63
63:S7:55:ASN:ND2	63:S7:187:GLU:O	2.29	0.63
65:V1:111:LYS:HB2	65:V1:151:ALA:HA	1.79	0.63
45:N5:362:LEU:HA	45:N5:365:ALA:HB3	1.80	0.63
57:S1:149:ASP:HB2	58:S2:367:ALA:HB3	1.81	0.63
19:AB:116:VAL:HG12	19:AB:120:MET:HE2	1.80	0.63
55:Ql:48:ASN:HD21	50:Qd:104:SER:HA	1.63	0.63
51:QK:24:GLY:HA3	47:Qa:109:LYS:HE3	1.81	0.63
51:Qe:145:ASP:N	51:Qe:145:ASP:OD1	2.31	0.63
35:C1:447:TYR:O	35:C1:451:ASN:ND2	2.28	0.62
66:V2:59:ASN:ND2	66:V2:89:GLN:OE1	2.32	0.62
36:C2:146:MET:HE2	36:C2:215:PRO:HG3	1.81	0.62
37:C3:77:LYS:NZ	37:C3:81:TYR:OH	2.32	0.62
47:QA:90:THR:HG23	47:QA:95:SER:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Qa:81:HIS:HD2	47:Qa:192:CYS:H	1.47	0.62
58:S2:106:GLU:HB2	58:S2:114:LYS:HB3	1.81	0.62
66:V2:182:ASN:HB3	66:V2:194:GLU:HB3	1.82	0.62
36:C2:52:HIS:HD2	36:C2:56:MET:HE2	1.63	0.62
4:6A:83:HIS:HA	70:6A:101:PC1:H132	1.81	0.62
18:A9:43:HIS:O	18:A9:50:SER:OG	2.16	0.62
42:N2:289:ASN:HA	42:N2:292:PHE:CE2	2.35	0.62
68:Qj:101:CDL:HA61	68:Qj:101:CDL:HA21	1.80	0.62
8:7B:53:TRP:HE1	38:C4:111:ILE:HG22	1.65	0.62
20:AK:62:ILE:O	20:AK:160:VAL:HA	2.00	0.62
8:7B:71:ARG:HG3	8:7B:72:VAL:HG23	1.82	0.62
46:N6:111:GLU:HG3	46:N6:120:ASN:HA	1.82	0.62
44:N4:391:ILE:HG23	44:N4:394:ILE:HD12	1.82	0.61
47:Qa:235:GLU:OE1	47:Qa:239:ASN:ND2	2.32	0.61
57:S1:593:SER:HA	57:S1:606:THR:O	2.00	0.61
58:S2:300:ARG:NH2	58:S2:407:GLU:OE2	2.33	0.61
31:B8:83:GLN:HA	31:B8:86:ARG:HG3	1.81	0.61
44:N4:122:PHE:HE2	44:N4:206:LYS:HG3	1.64	0.61
50:Qd:211:TYR:OH	81:Qd:401:HEC:O1A	2.15	0.61
20:AK:120:TYR:OH	75:AK:401:ADP:O2'	2.11	0.61
49:Qc:27:ILE:HD12	71:Qc:408:PEE:H34	1.82	0.61
66:V2:68:LYS:NZ	67:V3:407:SER:OG	2.32	0.61
76:AM:201:PLX:H71	76:S7:302:PLX:H72	1.81	0.61
30:B7:92:HIS:ND1	45:N5:481:THR:OG1	2.29	0.61
47:QA:155:GLN:HE21	47:QA:198:GLY:H	1.48	0.61
57:S1:387:LEU:HD12	57:S1:514:ASN:HB3	1.82	0.61
68:AN:203:CDL:HB32	68:AN:203:CDL:HA31	1.83	0.61
76:BL:202:PLX:H272	44:N4:446:LEU:HB3	1.82	0.61
58:S2:321:GLU:O	58:S2:352:GLN:NE2	2.31	0.61
71:A3:201:PEE:H29	41:N1:295:PRO:HB3	1.82	0.61
50:QD:228:LEU:HD11	50:QD:234:PHE:HB2	1.82	0.61
47:Qa:84:ARG:NH1	47:Qa:114:SER:OG	2.30	0.61
47:Qa:66:LYS:O	47:Qa:217:ARG:NH2	2.31	0.61
70:Qc:410:PC1:H371	70:Qc:410:PC1:H331	1.83	0.61
51:Qe:234:TYR:HB2	51:Qe:243:TYR:HB2	1.83	0.61
53:Qg:53:GLU:OE2	54:Qh:12:ARG:NH1	2.34	0.61
44:N4:371:PRO:HD2	68:N5:702:CDL:H391	1.83	0.61
68:AL:202:CDL:H461	68:AL:202:CDL:H201	1.82	0.60
23:AN:51:MET:HE2	41:N1:311:THR:HB	1.83	0.60
35:C1:173:PRO:HD2	35:C1:176:MET:HE2	1.82	0.60
37:C3:126:PRO:HG2	37:C3:127:LEU:HD12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Qd:147:LYS:NZ	50:Qd:151:GLU:OE2	2.34	0.60
1:4L:56:ALA:HA	61:S5:18:MET:HE3	1.83	0.60
13:A3:117:LEU:HD23	41:N1:310:MET:HE1	1.84	0.60
37:C3:16:TRP:NE1	37:C3:60:ASP:OD2	2.34	0.60
47:Qa:51:SER:HB3	47:Qa:230:LEU:HD12	1.83	0.60
42:N2:42:PRO:HG2	46:N6:167:VAL:HG22	1.83	0.60
28:B5:152:LYS:HD3	40:CB:96:VAL:HG21	1.84	0.60
68:QB:501:CDL:H712	70:QB:502:PC1:H342	1.84	0.60
57:S1:210:ILE:HD11	57:S1:212:LYS:HE2	1.84	0.60
12:A2:18:GLU:HG2	12:A2:68:ARG:HB3	1.83	0.60
23:AN:85:GLN:OE1	61:S5:105:ARG:NH1	2.33	0.60
68:AN:201:CDL:H511	68:AN:201:CDL:H751	1.82	0.60
45:N5:100:ILE:HG21	45:N5:246:LEU:HB2	1.84	0.60
64:S8:71:GLY:HA3	70:S8:304:PC1:H241	1.83	0.60
66:V2:108:PRO:HB2	66:V2:111:ARG:HG2	1.84	0.60
44:N4:445:LEU:HB3	68:N5:702:CDL:H452	1.84	0.59
57:S1:246:ARG:HH22	60:S4:123:ASN:HD21	1.50	0.59
17:A8:174:PHE:HB3	17:A8:178:ARG:HH12	1.67	0.59
15:A6:66:TYR:O	15:A6:86:ARG:NH1	2.35	0.59
57:S1:275:PRO:HG3	57:S1:286:ILE:HG12	1.83	0.59
58:S2:106:GLU:HG3	58:S2:114:LYS:HE2	1.84	0.59
18:A9:135:GLU:HG3	18:A9:140:ASP:HA	1.84	0.59
28:B5:139:ILE:HG23	44:N4:54:LEU:HD23	1.84	0.59
30:B7:29:TYR:O	30:B7:104:ARG:NH2	2.35	0.59
35:C1:22:PHE:HD1	70:C1:608:PC1:H11	1.67	0.59
44:N4:195:MET:HB2	70:N4:502:PC1:H222	1.84	0.59
48:QB:301:ASN:ND2	48:QB:347:CYS:SG	2.75	0.59
57:S1:308:ARG:NH1	57:S1:312:GLY:O	2.35	0.59
65:V1:94:PRO:HB2	65:V1:97:LEU:HB2	1.84	0.59
68:A8:301:CDL:H381	42:N2:256:PRO:HB2	1.83	0.59
48:QB:152:GLN:HE21	48:QB:253:LEU:HB2	1.68	0.59
19:AC:114:ASP:OD1	32:B9:87:ARG:NH2	2.36	0.59
19:AC:91:ASP:OD1	26:B3:47:ARG:NH2	2.34	0.59
35:C1:508:PRO:HG3	37:C3:6:HIS:HB3	1.85	0.59
40:CB:13:LEU:HD21	61:S5:4:PHE:HB3	1.83	0.59
49:QC:71:ARG:NH2	50:QD:278:ALA:O	2.32	0.59
62:S6:74:GLN:HG3	64:S8:108:SER:HB2	1.84	0.59
34:BL:95:PHE:O	34:BL:99:LEU:HB2	2.03	0.59
49:Qc:8:HIS:HB3	49:Qc:11:MET:HB2	1.84	0.59
20:AK:64:VAL:HG13	20:AK:207:VAL:HB	1.85	0.59
68:Qc:411:CDL:H751	68:Qc:411:CDL:H352	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:N4:501:CDL:OB9	68:N4:501:CDL:O1	2.19	0.58
70:N3:202:PC1:H3C1	76:S7:302:PLX:H391	1.84	0.58
65:V1:118:ASP:HB3	65:V1:207:GLY:HA2	1.85	0.58
70:6A:101:PC1:H32	37:C3:188:ILE:HD12	1.86	0.58
33:BK:114:GLN:HG3	45:N5:203:MET:HG2	1.85	0.58
35:C1:74:MET:HE3	35:C1:389:ILE:HG13	1.85	0.58
43:N3:73:LEU:HD13	46:N6:55:MET:HE1	1.86	0.58
48:Qb:83:ASN:HD22	48:Qb:85:LYS:H	1.51	0.58
21:AL:133:TRP:CE2	70:N4:502:PC1:H31	2.39	0.58
45:N5:419:THR:HA	45:N5:422:TYR:CE2	2.39	0.58
58:S2:308:LEU:HB2	58:S2:407:GLU:HB2	1.85	0.58
59:S3:83:GLU:OE1	59:S3:142:ARG:NH2	2.33	0.58
65:V1:113:LEU:HD13	65:V1:149:MET:HE1	1.85	0.58
18:A9:293:LEU:HD12	18:A9:294:PRO:HD2	1.85	0.58
42:N2:235:ASN:O	42:N2:315:TRP:NE1	2.36	0.58
45:N5:295:GLN:O	45:N5:425:ARG:NH1	2.37	0.58
18:A9:61:ALA:HB3	18:A9:82:VAL:HG13	1.85	0.58
71:AN:202:PEE:H60	41:N1:310:MET:HE2	1.85	0.58
35:C1:347:LEU:HD13	35:C1:383:MET:HE2	1.85	0.58
77:C1:602:HEA:HMA	77:C1:602:HEA:HBA2	1.85	0.58
44:N4:133:ILE:HD11	44:N4:231:LEU:HD11	1.86	0.58
44:N4:369:LEU:HD21	45:N5:149:ILE:HD13	1.86	0.58
51:QE:204:ARG:NH2	51:QE:258:LEU:O	2.32	0.58
34:BL:89:VAL:HG21	44:N4:25:ILE:HG23	1.84	0.58
36:C2:104:TRP:HA	36:C2:207:MET:HG2	1.84	0.58
41:N1:99:ASN:N	70:N6:201:PC1:O12	2.37	0.58
47:QA:148:ARG:NH2	53:QG:50:ARG:O	2.37	0.58
47:Qa:81:HIS:CD2	47:Qa:192:CYS:H	2.21	0.58
57:S1:251:ILE:HD13	57:S1:604:GLN:HB2	1.86	0.58
65:V1:119:GLU:O	65:V1:159:ARG:NH1	2.36	0.57
17:A8:196:ARG:NH2	23:AN:63:GLU:OE2	2.38	0.57
49:QC:233:LEU:HG	50:QD:297:MET:HE1	1.86	0.57
57:S1:250:SER:HB2	57:S1:606:THR:HG23	1.85	0.57
76:BL:202:PLX:H1C2	71:N5:701:PEE:H3	1.86	0.57
77:C1:602:HEA:HBA2	77:C1:602:HEA:CMA	2.34	0.57
42:N2:100:MET:HE1	45:N5:595:ILE:HG23	1.86	0.57
44:N4:392:THR:O	44:N4:396:MET:HG2	2.05	0.57
57:S1:198:THR:HG21	57:S1:209:TYR:HB2	1.86	0.57
14:A5:49:GLU:O	14:A5:53:ASN:ND2	2.36	0.57
49:QC:214:ASP:OD1	54:Qh:3:ARG:NH2	2.37	0.57
52:QF:34:ARG:O	52:QF:38:GLU:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6B:30:CYS:HB2	5:6B:65:CYS:SG	2.45	0.57
17:A8:146:ASP:OD1	17:A8:149:ARG:NH2	2.37	0.57
41:N1:24:GLU:OE2	41:N1:274:ARG:NH1	2.36	0.57
50:Qd:228:LEU:HD11	50:Qd:234:PHE:HB2	1.86	0.57
2:5A:104:PHE:N	38:C4:66:GLU:OE2	2.33	0.57
42:N2:298:TYR:O	42:N2:303:THR:OG1	2.20	0.57
48:QB:103:ASN:ND2	48:QB:149:ASP:OD1	2.37	0.57
68:QD:402:CDL:H312	68:QD:402:CDL:H731	1.87	0.57
68:B5:201:CDL:H271	76:BL:202:PLX:H181	1.86	0.57
37:C3:55:TYR:HA	71:C3:302:PEE:H61	1.87	0.57
44:N4:403:THR:HA	44:N4:406:TYR:CE2	2.40	0.57
57:S1:666:GLN:NE2	57:S1:670:GLU:OE2	2.38	0.57
48:QB:478:LEU:HG	70:QB:503:PC1:H152	1.87	0.57
49:Qc:114:ASN:ND2	70:Qc:410:PC1:O12	2.38	0.57
22:AM:88:ARG:HD3	64:S8:200:GLU:HG3	1.86	0.57
25:B2:43:ARG:NH1	25:B2:47:PHE:O	2.38	0.57
50:Qd:125:CYS:SG	81:Qd:401:HEC:HAC	2.44	0.57
64:S8:205:ILE:O	64:S8:209:TYR:HB3	2.04	0.57
45:N5:249:SER:HA	45:N5:306:THR:HG21	1.85	0.57
49:Qc:220:PHE:HE1	71:Qc:408:PEE:H31	1.69	0.57
35:C1:409:TRP:HB3	35:C1:471:ILE:HG12	1.87	0.56
57:S1:338:VAL:HB	57:S1:363:SER:HB2	1.87	0.56
18:A9:211:ASP:O	18:A9:215:ASN:ND2	2.38	0.56
44:N4:373:ILE:HD11	44:N4:444:LEU:HD23	1.86	0.56
48:QB:280:ASP:HA	48:QB:461:PRO:HB3	1.86	0.56
48:QB:411:GLU:OE2	48:QB:415:ARG:NH2	2.38	0.56
66:V2:111:ARG:NH1	66:V2:114:GLU:OE2	2.39	0.56
11:A1:70:ASP:O	17:A8:152:LYS:NZ	2.37	0.56
20:AK:141:ARG:NH2	75:AK:401:ADP:N7	2.53	0.56
37:C3:140:SER:HB2	37:C3:242:TRP:HE1	1.70	0.56
47:QA:151:VAL:O	47:QA:155:GLN:HG2	2.05	0.56
55:QI:19:SER:OG	48:Qb:480:PHE:O	2.23	0.56
64:S8:47:SER:O	64:S8:56:ARG:NH2	2.39	0.56
64:S8:64:THR:HG23	70:S8:304:PC1:H32	1.86	0.56
65:V1:138:LEU:HD13	65:V1:245:VAL:HG13	1.88	0.56
14:A5:99:PRO:HA	59:S3:71:LYS:HE2	1.87	0.56
49:QC:8:HIS:HB3	49:QC:11:MET:HB2	1.88	0.56
64:S8:63:TRP:HB3	64:S8:66:LEU:HD12	1.87	0.56
10:8B:46:THR:O	10:8B:49:SER:OG	2.22	0.56
68:B5:201:CDL:HB22	71:N5:701:PEE:H50	1.87	0.56
29:B6:85:ASP:O	32:B9:163:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Qe:204:ARG:NE	51:Qe:246:SER:O	2.35	0.56
57:S1:405:THR:HB	57:S1:477:GLY:HA3	1.87	0.56
58:S2:155:GLN:NE2	58:S2:315:ASP:OD2	2.33	0.56
1:4L:73:LEU:HD21	42:N2:41:ILE:HG13	1.87	0.56
72:7B:101:3PE:H2D1	35:C1:423:MET:HA	1.87	0.56
74:AC:201:ZMP:H5A	32:B9:109:ALA:HB1	1.87	0.56
36:C2:116:LEU:HD21	36:C2:226:MET:HG2	1.88	0.56
41:N1:281:ARG:NH1	58:S2:452:ASP:OD1	2.39	0.56
17:A8:115:LYS:NZ	17:A8:119:GLU:OE2	2.36	0.56
17:A8:219:TYR:OH	28:B5:189:ASN:ND2	2.38	0.56
44:N4:196:TRP:CD1	44:N4:250:LEU:HB3	2.41	0.56
57:S1:389:THR:HG21	57:S1:473:MET:HE2	1.86	0.56
49:Qc:300:ILE:HD11	49:Qc:363:LEU:HD21	1.87	0.56
5:6B:7:THR:O	5:6B:11:ASN:ND2	2.39	0.56
49:QC:126:THR:HG21	80:QC:401:HEM:HBB2	1.88	0.56
9:7C:42:THR:OG1	10:8B:49:SER:HB3	2.05	0.55
35:C1:107:PRO:HB3	37:C3:25:LEU:HB2	1.88	0.55
49:QC:190:THR:HG23	70:Qc:409:PC1:H2E2	1.88	0.55
48:Qb:315:ASP:OD1	48:Qb:316:SER:N	2.39	0.55
58:S2:242:LEU:HD22	58:S2:246:LEU:HD23	1.88	0.55
33:BK:2:PRO:O	33:BK:7:LYS:NZ	2.39	0.55
71:QH:102:PEE:H36	49:Qc:332:LEU:HD13	1.88	0.55
47:Qa:272:VAL:HA	47:Qa:337:GLY:HA3	1.89	0.55
48:Qb:87:ASN:HD22	48:Qb:204:PRO:HD3	1.70	0.55
18:A9:205:ASP:N	18:A9:205:ASP:OD1	2.39	0.55
35:C1:62:ALA:HB2	77:C1:602:HEA:HBD1	1.87	0.55
48:Qb:121:ASN:ND2	48:Qb:132:TYR:OH	2.39	0.55
70:Qb:501:PC1:H132	68:Qb:502:CDL:HA31	1.87	0.55
71:6A:102:PEE:H50	71:6A:102:PEE:H62	1.88	0.55
48:Qb:422:ARG:NH2	48:Qb:428:GLU:OE1	2.37	0.55
57:S1:466:LEU:HD13	57:S1:500:ILE:HD11	1.87	0.55
70:QB:502:PC1:H262	49:QC:11:MET:HE3	1.89	0.55
59:S3:174:PHE:O	59:S3:199:ARG:NE	2.38	0.55
22:AM:106:ARG:HB2	22:AM:109:ILE:HG13	1.88	0.55
41:N1:141:SER:HB2	41:N1:289:LEU:HD22	1.89	0.55
43:N3:4:MET:HG2	70:N6:201:PC1:H351	1.89	0.55
44:N4:266:MET:HB3	44:N4:395:LEU:HD13	1.88	0.55
47:Qa:151:VAL:O	47:Qa:155:GLN:HG2	2.06	0.55
51:Qe:190:VAL:HG21	51:Qe:250:ARG:HH22	1.69	0.55
60:S4:109:ASN:ND2	60:S4:111:LEU:O	2.40	0.55
23:AN:98:MET:HE3	23:AN:101:VAL:HG21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:CA:101:3PE:H381	42:N2:325:LEU:H	1.72	0.55
49:Qc:24:PRO:HB2	49:Qc:27:ILE:HG23	1.88	0.55
60:S4:84:ARG:NH1	60:S4:88:GLN:O	2.39	0.55
64:S8:100:GLU:O	64:S8:170:GLY:N	2.39	0.55
33:BK:142:ARG:NH1	33:BK:143:TYR:OH	2.40	0.55
51:QE:209:GLU:HG3	51:QE:210:TRP:CD1	2.42	0.55
58:S2:412:GLU:OE2	59:S3:140:ARG:NH2	2.40	0.55
49:QC:278:TYR:HD1	71:QC:405:PEE:H60	1.72	0.55
58:S2:393:GLU:OE2	58:S2:396:GLN:NE2	2.40	0.55
29:B6:147:LYS:NZ	33:BK:42:ASP:OD1	2.40	0.54
42:N2:36:ASN:OD1	42:N2:134:GLN:NE2	2.35	0.54
58:S2:187:LEU:HD23	58:S2:213:ARG:HG2	1.89	0.54
37:C3:148:HIS:HE1	37:C3:232:HIS:HE1	1.55	0.54
45:N5:15:LEU:HD11	45:N5:94:LEU:HD21	1.89	0.54
45:N5:253:VAL:HG23	45:N5:310:LEU:HD21	1.89	0.54
49:Qc:155:TYR:HB3	70:Qc:412:PC1:H382	1.89	0.54
65:V1:119:GLU:HA	85:V1:502:FMN:HM71	1.89	0.54
11:A1:49:GLU:OE1	11:A1:52:ARG:NH2	2.40	0.54
33:BK:115:GLN:HG2	45:N5:62:ILE:HG12	1.90	0.54
62:S6:61:GLU:OE2	64:S8:192:ASN:ND2	2.41	0.54
41:N1:160:TYR:OH	43:N3:73:LEU:O	2.25	0.54
52:Qf:85:LYS:HB2	52:Qf:85:LYS:HZ2	1.72	0.54
63:S7:69:LEU:HB2	63:S7:107:GLY:HA3	1.89	0.54
17:A8:239:LYS:HD3	28:B5:149:LEU:HD11	1.89	0.54
35:C1:51:ASP:OD1	35:C1:55:ASN:ND2	2.39	0.54
41:N1:149:ILE:HG21	41:N1:185:TRP:HB2	1.89	0.54
44:N4:73:LEU:HA	44:N4:76:MET:HE2	1.88	0.54
49:QC:207:ASN:OD1	49:QC:209:THR:OG1	2.20	0.54
50:QD:280:GLU:OE2	50:QD:286:ARG:NH1	2.39	0.54
47:Qa:70:ARG:HD2	47:Qa:117:GLU:HG2	1.89	0.54
58:S2:129:LEU:O	58:S2:133:LYS:HG2	2.08	0.54
31:B8:108:ASP:HB3	31:B8:111:MET:HG2	1.89	0.54
31:B8:173:ASP:OD2	31:B8:176:LYS:NZ	2.38	0.54
51:QE:90:ASP:OD1	51:QE:90:ASP:N	2.41	0.54
57:S1:307:ILE:HG23	57:S1:317:THR:HG21	1.89	0.54
29:B6:145:TYR:HE1	71:N5:701:PEE:H48	1.71	0.54
44:N4:1:MET:HE2	44:N4:111:THR:HG21	1.90	0.54
53:QG:43:ASP:OD2	53:QG:102:ARG:NH1	2.41	0.54
71:QH:102:PEE:H11	71:QH:102:PEE:H48	1.89	0.54
2:5A:124:ILE:HG12	6:6C:9:PRO:HG2	1.89	0.54
70:6A:101:PC1:H133	37:C3:187:THR:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A3:151:VAL:O	17:A8:207:LYS:NZ	2.29	0.54
13:A3:160:GLY:HA3	17:A8:204:LYS:HD2	1.89	0.54
36:C2:155:SER:HB2	36:C2:179:LEU:HD23	1.89	0.54
65:V1:162:PHE:HB3	65:V1:165:GLU:HB2	1.89	0.54
23:AN:99:LYS:NZ	23:AN:100:ASP:OD1	2.41	0.54
42:N2:112:HIS:O	42:N2:116:PRO:HD2	2.08	0.54
70:N6:201:PC1:H11	70:N6:201:PC1:H132	1.90	0.54
21:AL:129:GLN:HG2	68:AL:202:CDL:HB62	1.89	0.54
76:B1:101:PLX:H282	76:B1:101:PLX:H92	1.90	0.54
35:C1:197:LEU:HA	37:C3:92:LEU:HD13	1.90	0.54
57:S1:251:ILE:HD11	57:S1:596:TYR:HB2	1.90	0.54
70:7A:101:PC1:H221	70:C1:608:PC1:H2E1	1.90	0.53
25:B2:54:GLN:NE2	45:N5:367:PRO:HD2	2.23	0.53
27:B4:59:VAL:HG22	44:N4:423:ILE:HG12	1.90	0.53
30:B7:29:TYR:OH	30:B7:111:ARG:NH2	2.41	0.53
41:N1:173:TRP:HB3	41:N1:175:ILE:HG22	1.90	0.53
57:S1:449:PRO:HB2	57:S1:679:LEU:HD13	1.90	0.53
41:N1:174:MET:HB2	41:N1:242:PHE:HA	1.91	0.53
57:S1:419:ARG:NH1	57:S1:439:THR:O	2.41	0.53
45:N5:562:LEU:HB3	45:N5:563:PRO:HD3	1.89	0.53
18:A9:188:GLU:HG3	18:A9:200:ILE:HD13	1.89	0.53
68:N5:703:CDL:H321	68:N5:703:CDL:H751	1.90	0.53
51:QE:123:VAL:HG13	55:Qi:29:ALA:HA	1.91	0.53
58:S2:134:THR:HA	58:S2:424:ARG:HG2	1.91	0.53
72:7B:101:3PE:H292	35:C1:430:PHE:HE2	1.71	0.53
48:QB:165:ARG:HD3	48:QB:209:ARG:HA	1.90	0.53
48:Qb:396:ARG:NE	48:Qb:430:GLU:OE2	2.41	0.53
58:S2:194:THR:HB	58:S2:206:PHE:HA	1.90	0.53
1:4L:98:CYS:HB3	45:N5:580:GLN:HB2	1.90	0.53
6:6C:65:MET:HB3	6:6C:70:ILE:HD11	1.91	0.53
35:C1:35:LEU:HD21	35:C1:462:LEU:HD22	1.90	0.53
46:N6:34:ILE:HG22	70:N6:201:PC1:H3G2	1.89	0.53
57:S1:389:THR:OG1	57:S1:511:LYS:O	2.27	0.53
62:S6:67:ALA:HB1	64:S8:110:GLU:HA	1.90	0.53
65:V1:364:VAL:HG12	65:V1:400:VAL:HG12	1.90	0.53
66:V2:38:LEU:O	66:V2:124:ARG:NH2	2.28	0.53
14:A5:44:TYR:O	14:A5:48:THR:HG22	2.09	0.53
19:AC:104:PHE:HD1	19:AC:108:LEU:HD12	1.73	0.53
47:QA:116:ARG:NH1	47:QA:188:ASN:O	2.42	0.53
51:QE:140:MET:HE3	49:Qc:177:ARG:HE	1.74	0.53
49:Qc:126:THR:HG21	80:Qc:404:HEM:HBB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:S1:251:ILE:HG21	57:S1:604:GLN:HB3	1.91	0.53
57:S1:266:ARG:HD2	57:S1:267:THR:HG23	1.91	0.53
36:C2:28:LEU:HA	36:C2:31:VAL:HG22	1.90	0.53
37:C3:112:LEU:HD13	37:C3:118:PRO:HG3	1.90	0.53
48:QB:474:GLY:HA2	70:QB:503:PC1:H142	1.89	0.53
51:QE:266:THR:OG1	51:QE:270:LEU:O	2.23	0.53
51:Qe:179:ARG:NH1	51:Qe:246:SER:OG	2.42	0.53
45:N5:6:SER:O	45:N5:10:THR:OG1	2.19	0.53
3:5B:105:VAL:HA	3:5B:111:GLN:HG3	1.91	0.53
8:7B:41:ILE:HG22	38:C4:105:GLY:HA3	1.91	0.53
49:QC:267:HIS:HD2	49:QC:269:LYS:HG2	1.73	0.53
50:Qd:243:ILE:HG12	50:Qd:245:MET:H	1.73	0.53
58:S2:61:THR:N	58:S2:64:THR:OG1	2.41	0.53
18:A9:85:ARG:HH12	63:S7:196:ARG:HA	1.74	0.52
45:N5:65:ASN:HD21	45:N5:78:LEU:HD23	1.74	0.52
49:Qc:227:LYS:HG2	50:Qd:308:LYS:HE2	1.91	0.52
18:A9:279:TYR:HB2	18:A9:372:ALA:HB2	1.91	0.52
18:A9:305:PHE:HD2	18:A9:314:THR:HG22	1.73	0.52
35:C1:468:MET:HE1	77:C1:602:HEA:H211	1.90	0.52
37:C3:253:TYR:HA	37:C3:257:TYR:HD1	1.75	0.52
38:C4:90:PHE:HA	38:C4:93:MET:HG2	1.90	0.52
47:QA:77:LEU:O	47:QA:196:ARG:NH1	2.33	0.52
48:Qb:276:ARG:NH2	48:Qb:466:PRO:O	2.42	0.52
53:Qg:14:LEU:HD12	53:Qg:17:ILE:HD11	1.91	0.52
68:A8:301:CDL:H201	68:A8:301:CDL:H781	1.91	0.52
32:B9:119:PRO:HB3	45:N5:525:MET:HE2	1.92	0.52
35:C1:372:TYR:N	35:C1:432:GLY:HA3	2.24	0.52
43:N3:64:LEU:HD13	46:N6:165:VAL:HG22	1.91	0.52
51:Qe:214:ILE:HG13	51:Qe:261:PRO:HD3	1.90	0.52
29:B6:181:LYS:HG3	30:B7:40:VAL:HG13	1.90	0.52
48:QB:152:GLN:HG2	48:QB:253:LEU:HD13	1.91	0.52
30:B7:56:ARG:NH2	33:BK:120:SER:OG	2.36	0.52
33:BK:33:LEU:HD13	45:N5:49:VAL:HG13	1.92	0.52
47:Qa:379:LYS:HG2	47:Qa:413:LEU:HD22	1.91	0.52
57:S1:341:ILE:HG13	57:S1:545:LEU:HD11	1.92	0.52
65:V1:203:ALA:HB3	65:V1:206:CYS:HB2	1.91	0.52
16:A7:29:GLN:HE21	22:AM:52:ASN:HB3	1.74	0.52
70:QJ:101:PC1:H261	70:QJ:101:PC1:H2A1	1.91	0.52
57:S1:456:ALA:O	57:S1:499:ASN:ND2	2.43	0.52
60:S4:111:LEU:HG	60:S4:112:MET:HG2	1.91	0.52
58:S2:214:GLU:OE2	58:S2:227:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B5:92:PHE:O	33:BK:59:ASN:ND2	2.42	0.52
40:CB:13:LEU:HD11	61:S5:6:VAL:HG12	1.92	0.52
54:QH:38:VAL:HG22	68:Qc:402:CDL:H112	1.92	0.52
70:7C:101:PC1:H352	70:C1:608:PC1:H132	1.92	0.52
41:N1:24:GLU:HA	41:N1:271:LEU:HD13	1.92	0.52
44:N4:267:TRP:O	44:N4:271:MET:HG2	2.10	0.52
57:S1:306:MET:HE2	57:S1:314:LEU:HB3	1.92	0.52
68:C1:607:CDL:H761	68:C1:607:CDL:H721	1.92	0.51
49:Qc:71:ARG:NH2	50:Qd:278:ALA:O	2.38	0.51
68:4L:101:CDL:H191	45:N5:593:ILE:HG12	1.93	0.51
30:B7:103:GLU:O	30:B7:107:ARG:HG2	2.10	0.51
45:N5:559:GLU:O	45:N5:564:LYS:HB2	2.11	0.51
50:QD:216:LEU:HB3	50:QD:249:ILE:HD11	1.92	0.51
47:Qa:68:GLY:H	47:Qa:71:TYR:HD2	1.58	0.51
51:Qe:153:GLU:HG2	51:Qe:272:ILE:HG12	1.92	0.51
57:S1:49:VAL:HG13	57:S1:102:ILE:HD13	1.92	0.51
8:7B:53:TRP:CE2	38:C4:115:ALA:HB2	2.45	0.51
20:AK:205:VAL:HG12	20:AK:207:VAL:HG22	1.92	0.51
44:N4:194:PHE:HD1	70:N4:502:PC1:H2B1	1.76	0.51
47:QA:153:ALA:O	47:QA:156:SER:OG	2.21	0.51
48:QB:56:GLY:HA3	48:QB:227:PRO:HB3	1.91	0.51
48:QB:451:ASP:OD1	48:QB:472:ARG:NH2	2.33	0.51
52:Qf:33:VAL:HG12	52:Qf:82:VAL:HG22	1.92	0.51
65:V1:113:LEU:O	65:V1:154:ALA:HA	2.10	0.51
30:B7:107:ARG:HA	30:B7:110:GLN:HG2	1.93	0.51
45:N5:421:ALA:O	45:N5:424:THR:OG1	2.26	0.51
48:QB:120:LEU:HD13	48:QB:133:ILE:HG12	1.92	0.51
57:S1:624:ARG:NH1	57:S1:628:GLU:OE1	2.28	0.51
65:V1:55:GLY:O	65:V1:58:SER:OG	2.24	0.51
66:V2:93:LEU:HD12	66:V2:122:TYR:HB3	1.91	0.51
70:7C:101:PC1:H2B2	35:C1:472:ILE:HG21	1.93	0.51
70:7C:101:PC1:H332	68:C1:607:CDL:H142	1.92	0.51
42:N2:131:LEU:O	42:N2:135:LYS:HG2	2.11	0.51
57:S1:347:ASP:OD1	57:S1:347:ASP:N	2.36	0.51
64:S8:131:GLU:HB2	64:S8:144:ARG:HB3	1.93	0.51
68:A7:201:CDL:H611	68:A7:201:CDL:H792	1.92	0.51
17:A8:160:THR:HA	17:A8:163:TRP:CD1	2.45	0.51
19:AB:140:CYS:HB2	19:AB:143:GLU:HG3	1.92	0.51
30:B7:15:LYS:HG2	30:B7:113:LYS:HG3	1.93	0.51
36:C2:9:PHE:HB2	36:C2:21:LEU:HD21	1.93	0.51
42:N2:26:TRP:HB3	42:N2:74:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:N3:79:SER:HA	43:N3:87:MET:HE2	1.92	0.51
68:QB:501:CDL:H561	70:QB:502:PC1:H3F1	1.91	0.51
47:Qa:320:PRO:HG2	47:Qa:343:GLN:HE21	1.75	0.51
19:AC:91:ASP:HB2	26:B3:44:PRO:HB3	1.93	0.51
68:AN:203:CDL:H452	70:S8:304:PC1:H382	1.92	0.51
25:B2:87:PRO:HD2	30:B7:99:MET:HE1	1.93	0.51
27:B4:26:SER:OG	27:B4:28:GLU:OE1	2.27	0.51
33:BK:73:ASP:OD1	33:BK:73:ASP:N	2.41	0.51
34:BL:150:PRO:HG3	40:CB:115:LEU:HD22	1.93	0.51
35:C1:144:ASP:OD2	37:C3:36:HIS:NE2	2.34	0.51
46:N6:60:TYR:HD2	46:N6:61:LEU:HD12	1.74	0.51
47:QA:364:GLY:HA2	47:QA:425:ILE:HD13	1.93	0.51
48:QB:192:PHE:O	48:QB:198:ALA:HB2	2.11	0.51
50:QD:211:TYR:OH	81:QD:401:HEC:O2A	2.19	0.51
57:S1:43:VAL:HG12	57:S1:55:LYS:HD2	1.92	0.51
63:S7:62:LEU:O	63:S7:91:VAL:HA	2.10	0.51
64:S8:153:ILE:HG12	84:S8:302:SF4:S1	2.51	0.51
65:V1:118:ASP:HA	65:V1:159:ARG:HB3	1.93	0.51
8:7B:53:TRP:NE1	38:C4:111:ILE:HG22	2.26	0.51
9:7C:41:MET:HG2	70:7C:101:PC1:H272	1.92	0.51
14:A5:48:THR:HA	14:A5:51:ILE:HG12	1.92	0.51
44:N4:318:ALA:HB2	44:N4:373:ILE:HG13	1.93	0.51
71:QH:102:PEE:H33	49:Qc:332:LEU:HB3	1.92	0.51
48:Qb:152:GLN:NE2	48:Qb:250:PHE:HA	2.25	0.51
50:Qd:99:HIS:HE2	50:Qd:209:GLU:CD	2.18	0.51
65:V1:112:TYR:CD1	65:V1:153:ALA:HB3	2.46	0.51
20:AK:206:VAL:HB	20:AK:257:VAL:HG13	1.92	0.51
20:AK:210:ASP:OD1	20:AK:244:LYS:NZ	2.36	0.51
23:AN:30:LEU:HD11	68:AN:203:CDL:H321	1.93	0.51
30:B7:22:MET:HE1	30:B7:102:PHE:CD2	2.46	0.51
59:S3:111:LEU:HD23	59:S3:162:ALA:HB3	1.93	0.51
16:A7:39:PRO:HG3	64:S8:211:TYR:CZ	2.46	0.51
42:N2:128:LEU:HD12	42:N2:216:PHE:HB3	1.92	0.51
44:N4:375:LEU:HD11	45:N5:141:PHE:HE2	1.76	0.51
46:N6:17:PHE:HA	46:N6:20:PHE:CE2	2.46	0.51
50:QD:112:ARG:NH2	50:QD:145:GLU:OE1	2.44	0.51
51:Qe:211:VAL:HG11	51:Qe:246:SER:HA	1.93	0.51
1:4L:37:MET:HG3	1:4L:67:ALA:CB	2.41	0.50
7:7A:72:GLY:HA3	70:7A:101:PC1:H321	1.93	0.50
35:C1:130:PRO:HG3	35:C1:209:LEU:HD13	1.92	0.50
38:C4:148:MET:HG3	38:C4:150:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:QE:301:PLX:H233	71:QE:302:PEE:H28	1.94	0.50
57:S1:624:ARG:NH2	57:S1:637:ASP:OD1	2.40	0.50
4:6A:82:PHE:O	70:6A:101:PC1:H143	2.11	0.50
15:A6:63:ARG:NH2	19:AB:132:ASP:OD2	2.45	0.50
18:A9:163:LYS:NZ	18:A9:253:ILE:O	2.33	0.50
35:C1:316:THR:HG21	77:C1:603:HEA:C14	2.40	0.50
35:C1:374:VAL:HA	35:C1:377:PHE:CE2	2.46	0.50
42:N2:139:LEU:HD13	42:N2:190:MET:HE1	1.94	0.50
58:S2:160:ALA:HA	58:S2:404:THR:HG21	1.93	0.50
64:S8:150:THR:HG21	64:S8:180:HIS:CD2	2.46	0.50
18:A9:346:GLU:HG2	18:A9:371:PRO:HB3	1.93	0.50
36:C2:161:HIS:HB2	36:C2:174:ALA:HB3	1.93	0.50
45:N5:293:ILE:HD12	68:N5:703:CDL:H521	1.94	0.50
51:QE:241:SER:OG	82:QE:303:FES:S1	2.61	0.50
51:Qe:183:GLU:O	51:Qe:187:GLU:HG2	2.11	0.50
23:AN:16:TYR:OH	58:S2:248:ASP:OD1	2.27	0.50
45:N5:7:LEU:HD22	45:N5:46:LEU:HD11	1.94	0.50
45:N5:290:LEU:O	45:N5:523:SER:OG	2.29	0.50
50:QD:97:TRP:NE1	50:QD:210:ASP:OD1	2.39	0.50
49:Qc:97:HIS:HD2	80:Qc:405:HEM:C1C	2.29	0.50
70:Qh:103:PC1:H31	70:Qh:103:PC1:H111	1.92	0.50
66:V2:246:GLN:HB3	66:V2:249:LEU:HB3	1.93	0.50
13:A3:111:GLY:HA3	71:A3:201:PEE:H39	1.94	0.50
68:C1:607:CDL:H582	37:C3:22:LEU:HD21	1.93	0.50
41:N1:31:MET:HG2	64:S8:77:LEU:HB2	1.94	0.50
44:N4:408:LEU:HD12	45:N5:172:ILE:HG21	1.92	0.50
58:S2:140:PRO:HB2	63:S7:142:TYR:CE2	2.46	0.50
4:6A:81:LEU:HD22	70:6A:101:PC1:H221	1.94	0.50
21:AL:134:GLN:HB3	68:AL:202:CDL:HA22	1.93	0.50
33:BK:74:ILE:HG23	33:BK:156:LEU:HD22	1.94	0.50
76:CB:201:PLX:H92	71:CB:203:PEE:H28	1.93	0.50
42:N2:170:LEU:HD23	45:N5:574:SER:HB3	1.93	0.50
44:N4:233:ALA:HA	44:N4:320:GLY:HA2	1.92	0.50
44:N4:361:VAL:HG13	68:N5:702:CDL:H351	1.93	0.50
47:QA:313:VAL:HG11	47:QA:350:VAL:HG13	1.94	0.50
51:Qe:88:PHE:O	51:Qe:92:ARG:HG3	2.12	0.50
15:A6:88:LYS:NZ	15:A6:132:PHE:O	2.38	0.50
48:QB:388:VAL:HG21	48:QB:438:ALA:HA	1.92	0.50
3:5B:33:SER:OG	3:5B:34:GLY:N	2.45	0.50
45:N5:400:ASN:HB3	45:N5:486:MET:HE3	1.93	0.50
47:Qa:61:ILE:HG12	47:Qa:130:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:Qg:44:VAL:O	53:Qg:48:ILE:HG12	2.11	0.50
57:S1:69:LEU:O	60:S4:158:LYS:NZ	2.30	0.50
58:S2:277:ARG:NH2	58:S2:451:ALA:HB1	2.27	0.50
4:6A:27:THR:HA	4:6A:30:PHE:CE2	2.47	0.50
68:B5:201:CDL:H362	29:B6:140:TRP:HB3	1.93	0.50
36:C2:43:SER:HB3	70:C4:201:PC1:H3C2	1.93	0.50
37:C3:247:VAL:HG11	70:C3:304:PC1:H3C2	1.93	0.50
44:N4:176:PHE:HA	44:N4:179:ILE:HG12	1.93	0.50
45:N5:526:LEU:HD12	45:N5:530:PRO:HG3	1.93	0.50
48:QB:165:ARG:NH1	48:QB:208:VAL:O	2.45	0.50
49:QC:112:THR:HG22	49:QC:196:HIS:CE1	2.46	0.50
59:S3:232:LYS:HB2	60:S4:123:ASN:HD22	1.76	0.50
20:AK:82:LYS:HZ2	20:AK:268:ALA:HB3	1.77	0.49
44:N4:211:GLY:H	44:N4:213:HIS:HD2	1.59	0.49
68:QB:501:CDL:H161	70:QB:502:PC1:H241	1.94	0.49
49:QC:113:TRP:NE1	49:QC:301:LEU:O	2.27	0.49
54:QH:12:ARG:NH1	48:Qb:279:ASP:OD1	2.42	0.49
47:Qa:71:TYR:HB3	47:Qa:212:HIS:CE1	2.47	0.49
47:Qa:409:PRO:O	47:Qa:413:LEU:HG	2.12	0.49
48:Qb:76:ASP:HB2	48:Qb:418:LEU:HD22	1.93	0.49
65:V1:44:ASN:ND2	65:V1:44:ASN:O	2.45	0.49
65:V1:295:PRO:HG2	65:V1:298:GLU:HB2	1.93	0.49
24:B1:44:LEU:HD11	33:BK:68:PHE:HD1	1.77	0.49
29:B6:149:HIS:CD2	71:N5:701:PEE:H49	2.47	0.49
47:QA:61:ILE:HG12	47:QA:130:ILE:HD11	1.94	0.49
48:Qb:104:ARG:NH1	48:Qb:149:ASP:OD2	2.45	0.49
58:S2:391:TYR:HD1	64:S8:122:VAL:HG21	1.76	0.49
59:S3:89:HIS:CG	59:S3:90:PRO:HD2	2.47	0.49
9:7C:53:PHE:HB3	10:8B:57:VAL:HG11	1.95	0.49
18:A9:355:ARG:NH1	43:N3:32:GLU:OE2	2.44	0.49
20:AK:213:VAL:HG12	20:AK:217:GLN:HE21	1.76	0.49
23:AN:95:ALA:HA	23:AN:106:VAL:HG11	1.94	0.49
44:N4:416:ARG:HG2	45:N5:159:HIS:HB3	1.93	0.49
47:QA:233:VAL:HG22	47:QA:236:ARG:HH12	1.78	0.49
49:QC:5:ARG:HA	49:QC:11:MET:HE2	1.94	0.49
49:QC:197:LEU:HD11	80:QC:402:HEM:HMA3	1.94	0.49
51:QE:186:GLN:O	51:QE:190:VAL:HG23	2.13	0.49
47:Qa:123:VAL:HB	47:Qa:133:LEU:HD23	1.94	0.49
4:6A:88:ASN:ND2	70:6A:101:PC1:H151	2.27	0.49
15:A6:63:ARG:HG2	19:AB:120:MET:SD	2.52	0.49
35:C1:236:TRP:O	35:C1:288:TRP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:C3:231:HIS:HB3	70:C3:301:PC1:H133	1.93	0.49
72:CA:101:3PE:H231	40:CB:65:LEU:HD23	1.93	0.49
45:N5:327:LEU:O	45:N5:331:MET:HG2	2.12	0.49
45:N5:504:LEU:HD12	68:N5:703:CDL:H511	1.94	0.49
68:QB:501:CDL:H162	68:QB:501:CDL:HB61	1.95	0.49
57:S1:128:CYS:SG	57:S1:140:GLN:NE2	2.85	0.49
5:6B:14:THR:OG1	36:C2:96:THR:OG1	2.29	0.49
16:A7:34:ARG:NH2	64:S8:93:LEU:O	2.45	0.49
37:C3:204:HIS:NE2	37:C3:249:TRP:HB2	2.28	0.49
45:N5:368:PHE:CZ	45:N5:455:LYS:HG3	2.47	0.49
70:Qh:103:PC1:H2C2	70:Qh:103:PC1:H3H2	1.95	0.49
65:V1:293:SER:HB3	65:V1:336:LEU:HD23	1.95	0.49
45:N5:176:ARG:HD3	45:N5:179:ASP:HB2	1.95	0.49
49:Qc:100:ARG:NH2	80:Qc:405:HEM:O1A	2.44	0.49
52:Qf:38:GLU:OE1	52:Qf:47:ARG:NH2	2.45	0.49
57:S1:591:GLU:HG2	57:S1:610:VAL:HG23	1.95	0.49
58:S2:382:GLU:O	58:S2:386:HIS:ND1	2.42	0.49
14:A5:101:GLU:HB2	59:S3:71:LYS:HD3	1.94	0.49
15:A6:92:MET:HB2	74:AB:201:ZMP:H4A	1.95	0.49
70:C1:610:PC1:H351	37:C3:54:MET:HG2	1.95	0.49
44:N4:197:LEU:HB3	70:N4:502:PC1:H2C2	1.94	0.49
45:N5:368:PHE:HZ	45:N5:455:LYS:HG3	1.77	0.49
48:QB:310:ILE:HD11	48:QB:388:VAL:HA	1.95	0.49
76:QI:102:PLX:H341	56:QJ:31:GLY:HA3	1.94	0.49
45:N5:190:LEU:HB2	45:N5:196:TRP:NE1	2.28	0.49
49:Qc:119:LEU:HD22	80:Qc:405:HEM:HBB2	1.93	0.49
57:S1:180:THR:N	84:S1:802:SF4:S4	2.85	0.49
57:S1:306:MET:HB2	57:S1:583:ILE:HB	1.95	0.49
68:4L:101:CDL:H822	45:N5:596:MET:HE2	1.95	0.49
22:AM:55:PHE:CZ	22:AM:58:ARG:HG3	2.48	0.49
32:B9:143:GLU:O	32:B9:164:ARG:NH2	2.46	0.49
34:BL:106:VAL:HG13	44:N4:453:MET:HE3	1.94	0.49
35:C1:468:MET:SD	77:C1:602:HEA:H242	2.53	0.49
47:QA:82:LEU:HD23	47:QA:205:LEU:HD11	1.93	0.49
48:QB:192:PHE:HB3	48:QB:195:THR:OG1	2.12	0.49
49:QC:141:TRP:CD1	49:QC:265:PRO:HD3	2.48	0.49
49:Qc:29:SER:OG	68:Qc:411:CDL:OA7	2.24	0.49
57:S1:389:THR:N	57:S1:514:ASN:OD1	2.42	0.49
62:S6:36:GLU:OE2	62:S6:60:LYS:NZ	2.42	0.49
65:V1:30:THR:OG1	65:V1:31:SER:N	2.45	0.49
12:A2:21:ILE:HD11	12:A2:91:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AN:68:ARG:O	23:AN:72:MET:HG3	2.13	0.49
30:B7:12:ASP:OD1	30:B7:14:SER:OG	2.25	0.49
36:C2:144:LEU:HB2	36:C2:213:LEU:HD23	1.95	0.49
42:N2:135:LYS:O	42:N2:139:LEU:HD12	2.12	0.49
45:N5:566:THR:O	45:N5:570:GLN:HG2	2.12	0.49
53:QG:72:ARG:NH1	53:QG:74:GLN:OE1	2.44	0.49
80:Qc:405:HEM:HBA2	71:Qc:408:PEE:H25	1.94	0.49
58:S2:300:ARG:NH1	58:S2:342:GLU:OE2	2.45	0.49
35:C1:3:VAL:HG13	35:C1:7:LEU:HD12	1.95	0.48
36:C2:110:TYR:HB2	36:C2:116:LEU:HB3	1.94	0.48
42:N2:42:PRO:HG3	46:N6:167:VAL:HG13	1.95	0.48
44:N4:76:MET:SD	44:N4:230:VAL:HB	2.52	0.48
44:N4:216:LEU:HB3	44:N4:217:PRO:HD3	1.95	0.48
57:S1:541:PRO:HB3	57:S1:561:PRO:HD3	1.95	0.48
59:S3:129:VAL:HG22	59:S3:144:LYS:HD2	1.95	0.48
59:S3:157:VAL:HG21	59:S3:182:PRO:HD3	1.94	0.48
1:4L:68:ALA:HB2	46:N6:64:MET:HE2	1.94	0.48
18:A9:173:ASP:HB3	18:A9:176:SER:HB2	1.95	0.48
19:AB:117:GLU:HA	19:AB:120:MET:HE3	1.95	0.48
20:AK:134:GLN:HE22	75:AK:401:ADP:HN62	1.60	0.48
32:B9:77:ASP:OD1	32:B9:77:ASP:N	2.46	0.48
77:C1:602:HEA:HBD2	77:C1:602:HEA:HHA	1.94	0.48
37:C3:253:TYR:HA	37:C3:257:TYR:CD1	2.48	0.48
45:N5:103:PHE:HB2	45:N5:341:MET:HE3	1.95	0.48
45:N5:248:HIS:O	45:N5:253:VAL:HG22	2.12	0.48
49:QC:344:GLU:HG3	54:Qh:67:PHE:HE1	1.79	0.48
51:QE:239:HIS:HB2	82:QE:303:FES:S1	2.53	0.48
76:QI:102:PLX:H191	70:Qd:402:PC1:H3C1	1.95	0.48
49:Qc:234:PHE:CE2	68:Qc:411:CDL:H321	2.49	0.48
72:Qc:401:3PE:O32	70:Qc:412:PC1:H241	2.13	0.48
57:S1:432:ILE:HG12	57:S1:445:LEU:HB2	1.94	0.48
57:S1:534:VAL:HG22	57:S1:537:ILE:HB	1.94	0.48
59:S3:147:THR:HB	59:S3:153:ILE:HD11	1.95	0.48
65:V1:210:THR:HB	65:V1:224:ARG:H	1.77	0.48
18:A9:206:ILE:HG13	73:A9:401:NDP:H42N	1.95	0.48
68:AN:203:CDL:HA4	70:S8:304:PC1:O22	2.13	0.48
49:QC:101:GLY:HA2	49:QC:106:SER:HB2	1.95	0.48
51:QE:133:VAL:HG12	72:Qc:401:3PE:H262	1.93	0.48
48:Qb:152:GLN:HE22	48:Qb:250:PHE:HA	1.79	0.48
18:A9:132:ARG:NH2	73:A9:401:NDP:O1A	2.46	0.48
34:BL:77:ASP:OD1	34:BL:78:LYS:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C1:352:GLY:HA3	77:C1:603:HEA:H162	1.95	0.48
41:N1:18:ALA:O	41:N1:21:THR:OG1	2.23	0.48
41:N1:309:ILE:HD12	43:N3:88:LEU:HD13	1.96	0.48
5:6B:14:THR:HG1	36:C2:96:THR:HG1	1.60	0.48
7:7A:52:LEU:O	7:7A:56:THR:OG1	2.29	0.48
29:B6:89:SER:HB2	29:B6:92:GLU:HB2	1.96	0.48
29:B6:143:HIS:CD2	33:BK:45:VAL:HG21	2.48	0.48
30:B7:43:GLN:NE2	31:B8:169:GLU:OE2	2.42	0.48
30:B7:103:GLU:OE2	30:B7:106:ARG:NH2	2.45	0.48
35:C1:195:LEU:HD23	35:C1:245:ILE:HD13	1.95	0.48
41:N1:243:LEU:HD13	70:N1:401:PC1:H372	1.96	0.48
42:N2:142:LEU:HB3	42:N2:194:LEU:HD21	1.96	0.48
65:V1:412:LEU:HD12	65:V1:415:ILE:HD11	1.95	0.48
2:5A:68:ASP:HA	2:5A:101:LEU:HD21	1.96	0.48
29:B6:147:LYS:HE3	29:B6:148:TYR:CZ	2.49	0.48
44:N4:211:GLY:H	44:N4:213:HIS:CD2	2.32	0.48
44:N4:412:ILE:HG12	44:N4:416:ARG:HD2	1.94	0.48
46:N6:45:LEU:HD23	46:N6:50:SER:HA	1.96	0.48
46:N6:57:PHE:CZ	70:N6:201:PC1:H282	2.49	0.48
47:QA:155:GLN:NE2	47:QA:198:GLY:H	2.11	0.48
57:S1:185:PHE:CZ	57:S1:221:ASN:HB2	2.49	0.48
57:S1:217:GLU:HG2	57:S1:218:LEU:HG	1.94	0.48
65:V1:112:TYR:O	65:V1:240:THR:HA	2.14	0.48
65:V1:204:TYR:HB3	65:V1:377:GLU:HB3	1.95	0.48
65:V1:288:VAL:HG21	65:V1:303:HIS:CD2	2.49	0.48
4:6A:56:ARG:HH21	4:6A:94:TYR:HB3	1.78	0.48
27:B4:15:PRO:HG2	27:B4:18:LEU:HB2	1.95	0.48
35:C1:95:PRO:HD2	70:C1:610:PC1:H111	1.95	0.48
35:C1:101:SER:O	35:C1:156:SER:OG	2.23	0.48
77:C1:602:HEA:H212	77:C1:602:HEA:H271	1.48	0.48
45:N5:230:HIS:H	45:N5:230:HIS:CD2	2.30	0.48
45:N5:536:LEU:HB3	45:N5:537:PRO:HD3	1.96	0.48
47:QA:177:LEU:HD11	47:QA:272:VAL:HG22	1.96	0.48
48:Qb:189:ALA:HA	48:Qb:198:ALA:HB1	1.96	0.48
50:Qd:118:TYR:HA	50:Qd:122:CYS:SG	2.54	0.48
58:S2:430:ILE:HB	58:S2:469:ARG:HD2	1.96	0.48
65:V1:326:LEU:HD22	65:V1:363:ILE:HD11	1.94	0.48
17:A8:115:LYS:HB3	17:A8:116:PRO:HD3	1.96	0.48
35:C1:264:LYS:NZ	35:C1:326:THR:O	2.41	0.48
35:C1:313:ALA:HA	77:C1:603:HEA:H262	1.95	0.48
68:QB:501:CDL:H551	70:QB:502:PC1:H3A2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:QI:50:GLY:H	55:QI:55:HIS:CD2	2.32	0.48
51:QK:51:CYS:HG	51:QK:54:SER:HG	1.59	0.48
58:S2:145:LEU:HD11	58:S2:430:ILE:HD13	1.95	0.48
12:A2:89:ARG:O	12:A2:93:ASN:ND2	2.29	0.48
28:B5:176:LYS:H	61:S5:45:HIS:CD2	2.32	0.48
32:B9:64:ARG:NH2	32:B9:110:GLU:OE1	2.47	0.48
45:N5:49:VAL:HB	45:N5:50:PRO:HD3	1.95	0.48
51:QE:179:ARG:NH2	51:QE:208:PRO:O	2.32	0.48
9:7C:62:LYS:NZ	35:C1:117:MET:O	2.45	0.48
26:B3:47:ARG:HA	26:B3:50:ALA:HB3	1.95	0.48
36:C2:152:MET:HB2	36:C2:182:THR:HG22	1.95	0.48
42:N2:132:THR:HG21	68:N2:401:CDL:H362	1.96	0.48
58:S2:190:ILE:HG23	58:S2:209:MET:HB3	1.96	0.48
66:V2:85:LEU:HD13	67:V3:400:LEU:HD22	1.96	0.48
31:B8:62:TYR:OH	31:B8:74:ASP:O	2.24	0.47
76:BL:202:PLX:H112	71:N5:701:PEE:H27	1.94	0.47
71:CB:203:PEE:H39	42:N2:136:LEU:HD11	1.94	0.47
44:N4:201:MET:HE1	44:N4:212:LEU:HD11	1.96	0.47
76:QI:102:PLX:H212	70:Qd:402:PC1:H291	1.96	0.47
65:V1:385:CYS:O	65:V1:389:VAL:HB	2.14	0.47
5:6B:5:ILE:HG13	5:6B:7:THR:H	1.79	0.47
20:AK:75:LEU:HD22	20:AK:265:ALA:HB1	1.96	0.47
35:C1:13:LYS:NZ	35:C1:504:THR:OG1	2.47	0.47
45:N5:375:ILE:HD12	45:N5:458:LEU:HD11	1.95	0.47
48:QB:86:ASN:HA	48:QB:211:LEU:HD21	1.96	0.47
68:QC:407:CDL:HA61	68:QC:407:CDL:CB5	2.44	0.47
59:S3:132:LEU:HB2	59:S3:141:ILE:HG22	1.95	0.47
65:V1:85:LEU:HD21	65:V1:247:THR:HG23	1.96	0.47
18:A9:87:GLU:HG3	18:A9:89:TYR:H	1.78	0.47
28:B5:147:ALA:HB2	44:N4:173:SER:HB2	1.95	0.47
29:B6:165:PHE:O	29:B6:168:ASP:HB2	2.15	0.47
35:C1:168:ILE:HG21	35:C1:189:LEU:HB2	1.97	0.47
36:C2:161:HIS:HE1	36:C2:200:CYS:SG	2.34	0.47
38:C4:41:ARG:NH1	38:C4:43:ASP:OD2	2.47	0.47
48:QB:366:ASP:HB2	48:QB:464:GLN:HG2	1.94	0.47
71:QC:403:PEE:H28	68:QC:407:CDL:H772	1.96	0.47
65:V1:357:MET:HB3	65:V1:361:THR:HG21	1.97	0.47
39:CA:60:LYS:O	39:CA:64:GLU:HG2	2.15	0.47
50:QD:159:PRO:HB2	50:Qd:184:GLU:HG3	1.96	0.47
48:Qb:74:TRP:CZ2	48:Qb:411:GLU:HA	2.49	0.47
48:Qb:192:PHE:O	48:Qb:195:THR:OG1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Qd:322:TYR:CZ	50:Qd:324:PRO:HG3	2.49	0.47
57:S1:260:ASN:OD1	57:S1:604:GLN:NE2	2.47	0.47
58:S2:230:ALA:O	64:S8:98:ARG:NH2	2.48	0.47
66:V2:155:LYS:NZ	66:V2:206:ASP:OD1	2.42	0.47
3:5B:89:VAL:HG22	35:C1:510:TYR:HB3	1.95	0.47
19:AC:111:ASP:N	19:AC:111:ASP:OD1	2.47	0.47
20:AK:131:TYR:CD1	20:AK:185:CYS:HB3	2.49	0.47
31:B8:161:TYR:HB3	31:B8:166:LEU:HG	1.96	0.47
32:B9:144:TRP:HA	32:B9:147:ASP:OD2	2.15	0.47
33:BK:60:ARG:NH1	33:BK:62:TYR:OH	2.47	0.47
35:C1:28:MET:HE3	35:C1:469:ILE:HD11	1.96	0.47
41:N1:33:LEU:O	63:S7:82:PRO:HB3	2.15	0.47
42:N2:111:PHE:HA	45:N5:591:PHE:CE1	2.49	0.47
45:N5:292:ALA:HB2	45:N5:304:PHE:HB3	1.97	0.47
47:Qa:92:LYS:HD3	47:Qa:143:ALA:HB1	1.96	0.47
49:Qc:112:THR:HG22	49:Qc:196:HIS:CE1	2.49	0.47
59:S3:68:ILE:HG22	59:S3:69:LEU:HG	1.96	0.47
64:S8:153:ILE:HG13	64:S8:155:CYS:HB3	1.95	0.47
36:C2:192:TYR:CE1	36:C2:213:LEU:HD12	2.50	0.47
47:QA:193:PRO:HG2	47:QA:196:ARG:HG3	1.96	0.47
71:QC:403:PEE:H30	71:QC:403:PEE:H36	1.68	0.47
70:Qb:501:PC1:H291	49:Qc:229:ILE:HD11	1.97	0.47
53:Qg:36:ASP:OD2	53:Qg:62:ARG:NH1	2.48	0.47
57:S1:74:ASN:OD1	57:S1:75:CYS:N	2.47	0.47
3:5B:37:VAL:HB	37:C3:154:GLY:HA2	1.97	0.47
3:5B:41:GLU:HG2	3:5B:56:ARG:NH2	2.29	0.47
3:5B:63:ASN:ND2	37:C3:5:THR:O	2.48	0.47
4:6A:88:ASN:HD21	70:6A:101:PC1:H151	1.80	0.47
70:6A:101:PC1:H152	37:C3:187:THR:HA	1.97	0.47
12:A2:65:LEU:HD11	12:A2:91:LEU:HG	1.96	0.47
17:A8:124:ARG:NE	23:AN:80:ASP:OD2	2.44	0.47
17:A8:141:ASN:HD21	23:AN:81:ARG:HH21	1.62	0.47
19:AB:104:PHE:HA	19:AB:108:LEU:HD12	1.95	0.47
74:AC:201:ZMP:H8A	32:B9:109:ALA:HB2	1.95	0.47
35:C1:352:GLY:HA3	77:C1:603:HEA:C14	2.45	0.47
71:C1:609:PEE:H19	71:C1:609:PEE:H14	1.36	0.47
48:QB:74:TRP:HB3	48:QB:418:LEU:HD11	1.97	0.47
49:QC:165:TRP:O	49:QC:174:THR:OG1	2.27	0.47
50:QD:112:ARG:HB2	50:QD:140:CYS:HB2	1.96	0.47
63:S7:65:MET:HE1	63:S7:120:VAL:HG21	1.95	0.47
64:S8:128:ILE:HG12	64:S8:147:ILE:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:V1:201:ALA:HB3	66:V2:119:TYR:CD1	2.50	0.47
65:V1:355:ILE:HD13	66:V2:139:PRO:HG3	1.95	0.47
9:7C:36:ARG:NH2	70:7C:101:PC1:O14	2.32	0.47
9:7C:57:ARG:HH21	70:C1:608:PC1:H2I1	1.79	0.47
35:C1:8:TYR:CZ	37:C3:15:PRO:HB3	2.50	0.47
45:N5:241:THR:HG21	45:N5:344:GLY:HA3	1.96	0.47
48:QB:79:SER:OG	48:QB:201:VAL:HA	2.15	0.47
48:QB:321:GLY:HA2	48:QB:324:MET:HE2	1.96	0.47
48:Qb:102:LYS:HG2	48:Qb:153:ASN:HB3	1.97	0.47
57:S1:575:VAL:C	57:S1:578:PRO:HD2	2.40	0.47
58:S2:464:PHE:HA	58:S2:467:VAL:HB	1.96	0.47
17:A8:160:THR:HA	17:A8:163:TRP:NE1	2.30	0.47
46:N6:124:ASP:OD1	46:N6:124:ASP:N	2.48	0.47
49:QC:236:MET:HG2	71:QE:302:PEE:H61	1.96	0.47
51:QE:202:LEU:HD11	51:QE:208:PRO:HB3	1.96	0.47
57:S1:338:VAL:HB	57:S1:363:SER:CB	2.44	0.47
66:V2:207:GLU:HG3	66:V2:212:LYS:HD2	1.96	0.47
18:A9:85:ARG:HH22	63:S7:196:ARG:HG3	1.79	0.47
41:N1:87:VAL:HG22	41:N1:88:PRO:HD3	1.97	0.47
50:Qd:139:VAL:HG21	50:Qd:277:TRP:CZ2	2.50	0.47
51:Qe:241:SER:OG	82:Qe:301:FES:S2	2.57	0.47
56:Qj:5:PHE:HB3	68:Qj:101:CDL:H131	1.97	0.47
58:S2:98:HIS:HB3	58:S2:101:LEU:HD23	1.97	0.47
5:6B:44:MET:HE3	5:6B:53:VAL:HG11	1.97	0.46
71:8B:101:PEE:H26	38:C4:117:LEU:HD22	1.96	0.46
68:N4:501:CDL:H472	68:N4:501:CDL:H412	1.96	0.46
50:Qd:125:CYS:SG	50:Qd:180:TYR:OH	2.70	0.46
68:C1:607:CDL:H402	68:C1:607:CDL:H331	1.96	0.46
70:C1:610:PC1:H2B1	70:C1:610:PC1:H362	1.96	0.46
37:C3:58:TRP:CG	70:C3:301:PC1:H252	2.50	0.46
76:QE:301:PLX:H22	76:QE:301:PLX:H1A3	1.61	0.46
57:S1:347:ASP:HB3	57:S1:594:ALA:HB1	1.96	0.46
58:S2:188:ASN:OD1	58:S2:410:LYS:NZ	2.47	0.46
63:S7:66:THR:HG21	63:S7:76:MET:HE2	1.96	0.46
65:V1:62:TRP:CD2	65:V1:181:LEU:HD13	2.50	0.46
65:V1:325:PRO:HG3	65:V1:433:TRP:HB3	1.97	0.46
76:AM:201:PLX:H382	41:N1:49:ILE:HG12	1.97	0.46
34:BL:90:VAL:HG22	44:N4:28:THR:HG21	1.97	0.46
37:C3:159:MET:HE2	37:C3:222:GLN:HE21	1.79	0.46
48:QB:107:SER:HA	48:QB:110:GLU:HG2	1.96	0.46
49:QC:137:GLN:NE2	49:QC:263:ASN:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:QK:64:LEU:HA	51:QK:77:ARG:O	2.16	0.46
57:S1:59:GLN:HE22	60:S4:90:GLY:HA2	1.80	0.46
57:S1:197:THR:HG22	57:S1:206:VAL:HG22	1.97	0.46
58:S2:296:GLY:HA2	58:S2:300:ARG:HH21	1.80	0.46
59:S3:119:VAL:HG12	59:S3:121:THR:HG22	1.97	0.46
70:S8:304:PC1:H281	70:S8:304:PC1:H2C2	1.97	0.46
15:A6:88:LYS:HD2	15:A6:88:LYS:HA	1.71	0.46
35:C1:184:PHE:H	35:C1:256:HIS:CE1	2.34	0.46
35:C1:303:ALA:O	35:C1:306:THR:OG1	2.29	0.46
42:N2:190:MET:HG2	42:N2:204:ASN:HB3	1.97	0.46
68:Qb:502:CDL:H722	68:Qb:502:CDL:H121	1.97	0.46
68:Qh:102:CDL:H142	68:Qh:102:CDL:HA62	1.97	0.46
57:S1:281:ILE:HD11	57:S1:602:ARG:NE	2.31	0.46
58:S2:162:GLU:OE2	58:S2:177:ARG:NH2	2.35	0.46
20:AK:138:TYR:OH	20:AK:193:LYS:HA	2.16	0.46
71:QC:405:PEE:H16	71:QC:405:PEE:H22	1.68	0.46
49:Qc:114:ASN:HB3	70:Qc:410:PC1:H231	1.98	0.46
50:Qd:209:GLU:H	50:Qd:209:GLU:HG2	1.51	0.46
71:Qe:302:PEE:H13	71:Qe:302:PEE:H20	1.79	0.46
3:5B:43:GLN:NE2	37:C3:225:PHE:O	2.33	0.46
29:B6:157:VAL:HG22	45:N5:63:ILE:HG23	1.97	0.46
35:C1:254:ILE:HG13	35:C1:344:PHE:CD2	2.50	0.46
39:CA:68:GLU:OE2	39:CA:71:ARG:NH2	2.49	0.46
76:N3:201:PLX:H1C2	76:N3:201:PLX:H22	1.73	0.46
76:N3:201:PLX:H221	76:N3:201:PLX:H191	1.60	0.46
45:N5:399:VAL:HG12	45:N5:409:LEU:HD13	1.98	0.46
50:QD:300:LEU:HD21	51:QE:124:GLY:HA3	1.97	0.46
71:Qh:101:PEE:H36	71:Qh:101:PEE:H41	1.79	0.46
57:S1:538:ARG:HG2	57:S1:555:ILE:HD11	1.98	0.46
85:V1:502:FMN:H9	85:V1:502:FMN:H4'	1.98	0.46
25:B2:65:MET:SD	45:N5:375:ILE:HG12	2.56	0.46
35:C1:155:VAL:HG11	70:C1:610:PC1:H3B1	1.98	0.46
68:QB:501:CDL:HB21	70:QB:503:PC1:H131	1.98	0.46
49:QC:102:LEU:HD12	71:QC:403:PEE:H41	1.97	0.46
83:QH:101:PX2:H14	50:Qd:302:PRO:HB2	1.98	0.46
48:Qb:165:ARG:NH1	48:Qb:208:VAL:O	2.48	0.46
52:Qf:28:ASP:HB3	52:Qf:29:PRO:HD3	1.98	0.46
9:7C:31:VAL:HG13	9:7C:37:LEU:HD22	1.97	0.46
18:A9:65:LEU:HG	18:A9:129:LEU:HD22	1.98	0.46
71:C1:609:PEE:H27	71:C1:609:PEE:H21	1.49	0.46
40:CB:51:ARG:CZ	42:N2:322:GLN:HG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:N2:243:LEU:HD23	68:N4:501:CDL:H351	1.97	0.46
44:N4:12:LEU:HB2	44:N4:13:PRO:HD3	1.97	0.46
44:N4:94:LEU:HD11	68:N4:501:CDL:H312	1.97	0.46
44:N4:370:PRO:HB2	45:N5:142:ILE:HA	1.98	0.46
49:QC:274:PHE:HB3	71:QC:405:PEE:H56	1.98	0.46
51:QE:140:MET:O	49:Qc:177:ARG:NH2	2.48	0.46
70:QI:101:PC1:H2I3	50:Qd:299:LEU:HD21	1.98	0.46
48:Qb:302:VAL:HB	48:Qb:303:PRO:HD3	1.96	0.46
58:S2:190:ILE:HD11	58:S2:257:PHE:CZ	2.50	0.46
71:6A:102:PEE:H23	71:6A:102:PEE:H18	1.74	0.46
68:B5:201:CDL:H512	71:N5:701:PEE:H14	1.98	0.46
76:BL:202:PLX:H1C2	76:BL:202:PLX:H22	1.70	0.46
36:C2:78:LEU:HB2	36:C2:79:PRO:HD3	1.98	0.46
42:N2:106:LEU:O	42:N2:135:LYS:HE3	2.15	0.46
45:N5:79:SER:O	45:N5:139:GLN:NE2	2.46	0.46
45:N5:289:ALA:O	45:N5:293:ILE:HG23	2.16	0.46
54:QH:38:VAL:HG23	68:Qc:411:CDL:HB31	1.96	0.46
54:QH:55:VAL:HG11	72:Qc:406:3PE:H3H1	1.97	0.46
47:Qa:164:VAL:HG21	48:Qb:317:THR:HG21	1.98	0.46
48:Qb:282:LEU:HD12	48:Qb:460:GLY:HA2	1.98	0.46
48:Qb:465:LEU:HD12	48:Qb:466:PRO:HD2	1.98	0.46
49:Qc:42:ILE:HG12	71:Qc:408:PEE:H57	1.98	0.46
51:Qe:165:MET:HB3	51:Qe:176:VAL:HG23	1.98	0.46
51:Qe:228:ALA:HB3	51:Qe:235:TYR:HB3	1.98	0.46
57:S1:34:VAL:HG23	57:S1:41:VAL:HG13	1.98	0.46
57:S1:241:ARG:HG2	64:S8:117:LYS:HD2	1.98	0.46
57:S1:257:VAL:HG11	57:S1:413:LEU:HB2	1.98	0.46
64:S8:75:SER:O	64:S8:79:ARG:HG3	2.16	0.46
17:A8:111:ALA:HB2	17:A8:197:PRO:HG3	1.98	0.46
68:AL:201:CDL:H341	68:AL:201:CDL:H162	1.98	0.46
32:B9:52:LEU:O	32:B9:57:LYS:NZ	2.49	0.46
36:C2:161:HIS:ND1	36:C2:207:MET:HE1	2.31	0.46
38:C4:41:ARG:HB2	38:C4:44:TYR:HB3	1.97	0.46
42:N2:168:GLY:HA3	42:N2:181:TYR:CE1	2.50	0.46
44:N4:282:LEU:HD13	44:N4:342:MET:HG3	1.98	0.46
51:QE:178:HIS:ND1	51:QE:209:GLU:O	2.48	0.46
50:Qd:113:ARG:NH1	50:Qd:270:ASP:OD1	2.49	0.46
62:S6:116:LEU:HD23	62:S6:116:LEU:HA	1.85	0.46
29:B6:132:VAL:O	29:B6:136:LEU:CB	2.64	0.45
35:C1:129:TYR:OH	35:C1:236:TRP:NE1	2.42	0.45
35:C1:261:TYR:HB2	35:C1:338:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:C2:186:SER:OG	36:C2:213:LEU:HD13	2.17	0.45
47:QA:125:CYS:HB3	47:QA:133:LEU:HD22	1.98	0.45
48:QB:126:ARG:NH1	48:QB:199:GLN:O	2.48	0.45
49:QC:30:TRP:HB3	49:QC:100:ARG:HG3	1.97	0.45
51:QE:88:PHE:O	51:QE:92:ARG:HG3	2.16	0.45
49:Qc:33:PHE:HA	49:Qc:36:LEU:HB2	1.98	0.45
52:Qf:53:CYS:SG	52:Qf:56:ARG:NH2	2.89	0.45
28:B5:74:TYR:O	34:BL:96:SER:OG	2.23	0.45
76:C2:301:PLX:H252	76:C2:301:PLX:H282	1.68	0.45
41:N1:102:VAL:HG21	41:N1:154:LEU:HD11	1.98	0.45
45:N5:298:ILE:O	45:N5:302:VAL:HG23	2.16	0.45
47:QA:70:ARG:HG3	47:QA:185:ALA:HB1	1.98	0.45
48:QB:121:ASN:ND2	48:QB:132:TYR:OH	2.45	0.45
51:QE:178:HIS:CE1	51:QE:209:GLU:HB2	2.51	0.45
49:Qc:97:HIS:CE1	49:Qc:100:ARG:HH22	2.35	0.45
51:Qe:164:ASN:HB2	51:Qe:177:ARG:CZ	2.46	0.45
57:S1:144:MET:HG3	58:S2:389:LYS:HG3	1.98	0.45
65:V1:65:THR:O	65:V1:69:LEU:HG	2.17	0.45
15:A6:89:VAL:HG22	74:AB:201:ZMP:H1	1.97	0.45
21:AL:19:HIS:CD2	21:AL:20:ARG:HG3	2.51	0.45
76:AL:205:PLX:H251	76:AL:205:PLX:H282	1.76	0.45
22:AM:144:TYR:HD1	22:AM:144:TYR:H	1.63	0.45
44:N4:119:TYR:CZ	44:N4:161:LEU:HB2	2.51	0.45
47:QA:49:ILE:HD13	47:QA:220:LEU:HB3	1.98	0.45
48:QB:478:LEU:HD11	70:QB:503:PC1:H11	1.98	0.45
70:QI:101:PC1:H3C1	70:QI:101:PC1:H3F2	1.81	0.45
57:S1:385:TYR:OH	57:S1:527:ASP:OD1	2.29	0.45
58:S2:190:ILE:HD11	58:S2:257:PHE:HZ	1.81	0.45
65:V1:146:GLY:HA3	65:V1:193:PHE:CE1	2.52	0.45
35:C1:184:PHE:H	35:C1:256:HIS:HE1	1.64	0.45
44:N4:400:MET:HE1	45:N5:183:VAL:HG21	1.97	0.45
48:QB:478:LEU:C	55:Qi:18:THR:HG21	2.41	0.45
57:S1:340:ALA:HB3	57:S1:366:LEU:HD23	1.98	0.45
65:V1:195:VAL:O	67:V3:410:ARG:NH1	2.37	0.45
5:6B:31:TRP:CD2	37:C3:110:PRO:HB3	2.51	0.45
23:AN:82:ARG:HA	61:S5:105:ARG:HD3	1.98	0.45
50:QD:299:LEU:HD11	68:Qh:102:CDL:H671	1.98	0.45
51:QE:207:LYS:HE3	51:QE:210:TRP:CD1	2.52	0.45
51:QE:223:VAL:HG23	49:Qc:264:THR:HG23	1.98	0.45
57:S1:86:PRO:O	57:S1:108:LYS:NZ	2.50	0.45
58:S2:145:LEU:HD13	58:S2:430:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:S2:448:HIS:HB3	58:S2:452:ASP:HB2	1.99	0.45
65:V1:384:PRO:HB2	65:V1:423:THR:HG22	1.99	0.45
67:V3:386:TYR:CZ	67:V3:388:ASN:HB3	2.51	0.45
1:4L:4:VAL:O	1:4L:8:ILE:HG12	2.17	0.45
15:A6:94:MET:HE2	19:AB:113:LEU:HD12	1.99	0.45
16:A7:14:TRP:O	23:AN:28:ARG:NH2	2.50	0.45
20:AK:297:ARG:HA	20:AK:300:VAL:HG22	1.99	0.45
21:AL:133:TRP:CD1	70:N4:502:PC1:H112	2.52	0.45
29:B6:145:TYR:CE1	71:N5:701:PEE:H48	2.50	0.45
29:B6:161:LYS:HG3	30:B7:50:GLN:NE2	2.32	0.45
41:N1:216:ALA:C	41:N1:218:GLY:H	2.25	0.45
46:N6:33:LEU:HG	46:N6:65:LEU:HD21	1.98	0.45
50:QD:203:ARG:HB2	50:QD:279:SER:HB2	1.99	0.45
48:Qb:294:PRO:HG3	48:Qb:448:TYR:CZ	2.52	0.45
48:Qb:341:PHE:HB2	48:Qb:358:PHE:HB3	1.98	0.45
57:S1:169:VAL:HG22	57:S1:223:ILE:HD11	1.99	0.45
58:S2:147:TYR:CB	63:S7:71:CYS:HB3	2.46	0.45
59:S3:173:MET:HE1	59:S3:189:THR:HG23	1.99	0.45
65:V1:48:ARG:HH21	67:V3:384:SER:HA	1.81	0.45
1:4L:38:LEU:O	1:4L:42:ILE:HG12	2.17	0.45
2:5A:86:PRO:HB2	2:5A:91:ILE:HD11	1.98	0.45
20:AK:112:GLY:HA2	20:AK:136:TRP:CD2	2.51	0.45
68:AN:203:CDL:H392	64:S8:62:LEU:HD23	1.99	0.45
32:B9:87:ARG:NH1	32:B9:91:ASP:OD2	2.49	0.45
46:N6:124:ASP:O	46:N6:127:ILE:HG12	2.17	0.45
68:QC:406:CDL:HA61	68:QC:406:CDL:HA22	1.99	0.45
57:S1:576:GLY:O	57:S1:580:ALA:HB2	2.16	0.45
65:V1:326:LEU:HD23	65:V1:367:ILE:HD11	1.98	0.45
66:V2:166:ASP:OD1	66:V2:166:ASP:N	2.44	0.45
3:5B:69:ALA:HB2	35:C1:512:ASN:HB3	1.99	0.45
20:AK:127:ASP:O	20:AK:132:ARG:NH1	2.48	0.45
70:C1:608:PC1:H352	70:C1:608:PC1:H252	1.98	0.45
44:N4:79:ALA:O	44:N4:82:SER:HB3	2.17	0.45
47:QA:70:ARG:NH2	47:QA:332:ASP:OD2	2.50	0.45
47:QA:134:MET:HE2	47:QA:233:VAL:HG21	1.99	0.45
48:QB:222:GLN:HE21	48:QB:263:PRO:HG3	1.81	0.45
51:QE:244:ASP:OD2	51:QE:250:ARG:NH2	2.50	0.45
70:Qc:407:PC1:H3G2	70:Qc:407:PC1:H3B1	1.98	0.45
59:S3:71:LYS:HE3	59:S3:72:TYR:CZ	2.52	0.45
21:AL:118:MET:HA	21:AL:121:THR:HG22	1.99	0.45
23:AN:93:GLU:HG3	61:S5:98:HIS:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B4:10:ARG:HG3	27:B4:11:LEU:HG	1.98	0.45
29:B6:161:LYS:HG2	33:BK:116:ARG:O	2.17	0.45
29:B6:166:PRO:HG2	29:B6:180:MET:HG3	1.99	0.45
33:BK:107:GLN:HE22	45:N5:194:ASN:ND2	2.10	0.45
45:N5:534:HIS:ND1	71:N5:704:PEE:O1P	2.37	0.45
46:N6:103:MET:HE1	46:N6:115:ILE:HG13	1.98	0.45
48:QB:229:MET:SD	48:QB:253:LEU:HD21	2.57	0.45
49:QC:42:ILE:HG12	70:Qc:409:PC1:H2D2	1.99	0.45
71:Qb:503:PEE:H66	71:Qb:503:PEE:H72	1.59	0.45
57:S1:62:ARG:HB2	82:S1:803:FES:S1	2.57	0.45
58:S2:146:ASP:OD2	58:S2:149:SER:OG	2.35	0.45
58:S2:374:ARG:O	58:S2:378:LYS:HG2	2.16	0.45
65:V1:141:GLY:HA3	65:V1:248:VAL:O	2.17	0.45
65:V1:375:LYS:HD2	65:V1:393:ASN:ND2	2.32	0.45
1:4L:62:ILE:HG21	42:N2:31:ILE:HD11	1.99	0.45
16:A7:49:LEU:HD11	65:V1:405:ARG:HH22	1.81	0.45
68:B5:201:CDL:H511	71:N5:701:PEE:H51	1.99	0.45
76:C2:301:PLX:H21	76:C2:301:PLX:H1C2	1.59	0.45
71:C3:302:PEE:H19	71:C3:302:PEE:H25	1.77	0.45
41:N1:10:ILE:HG21	43:N3:13:LEU:HD23	1.99	0.45
41:N1:79:LEU:HD22	41:N1:222:MET:HG3	1.98	0.45
70:N1:401:PC1:H382	70:S8:304:PC1:H2H2	1.98	0.45
44:N4:106:LEU:HD13	44:N4:234:VAL:HG11	1.98	0.45
71:N5:704:PEE:H72	71:N5:704:PEE:H67	1.78	0.45
47:QA:235:GLU:O	47:QA:239:ASN:ND2	2.49	0.45
51:QE:222:CYS:HA	49:Qc:264:THR:HG21	1.98	0.45
47:Qa:367:SER:OG	47:Qa:370:ASP:OD2	2.23	0.45
9:7C:47:SER:HB2	70:C1:608:PC1:H342	1.99	0.44
71:A3:201:PEE:H73	71:A3:201:PEE:H78	1.75	0.44
76:AL:205:PLX:H72	68:B4:201:CDL:HA61	1.99	0.44
37:C3:51:THR:HB	71:C3:302:PEE:H73	1.99	0.44
68:N4:501:CDL:H822	68:N4:501:CDL:H422	1.99	0.44
45:N5:14:ILE:HD11	45:N5:43:ALA:HA	1.98	0.44
45:N5:162:THR:O	45:N5:166:THR:HG23	2.17	0.44
48:QB:91:TYR:OH	48:QB:171:GLU:OE1	2.23	0.44
57:S1:381:LEU:HD13	57:S1:664:TYR:HB3	1.98	0.44
58:S2:106:GLU:O	58:S2:113:ARG:HB2	2.16	0.44
1:4L:14:ILE:HG12	68:4L:101:CDL:H771	1.99	0.44
7:7A:54:ARG:HG2	45:N5:503:GLU:HG3	1.99	0.44
9:7C:29:PHE:CD2	70:7C:101:PC1:H251	2.52	0.44
32:B9:69:LEU:HD21	32:B9:82:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C1:353:LEU:HD21	77:C1:603:HEA:H22	1.99	0.44
45:N5:97:THR:HG21	45:N5:125:LEU:HD22	1.98	0.44
48:QB:127:GLU:O	48:QB:128:HIS:ND1	2.51	0.44
48:QB:426:LEU:HD12	48:QB:426:LEU:HA	1.84	0.44
51:Qe:201:ASP:C	51:Qe:203:GLU:H	2.25	0.44
58:S2:101:LEU:HD13	58:S2:464:PHE:HZ	1.81	0.44
63:S7:131:VAL:HG22	63:S7:161:ILE:HB	1.99	0.44
13:A3:135:PRO:HB2	23:AN:69:ILE:HD11	1.99	0.44
74:AC:201:ZMP:H14	32:B9:102:ALA:HB1	1.99	0.44
68:AL:202:CDL:H442	42:N2:159:MET:HG2	1.99	0.44
37:C3:63:ARG:NH2	71:C3:302:PEE:O2P	2.51	0.44
71:C3:303:PEE:H57	71:C3:303:PEE:H62	1.84	0.44
42:N2:276:ILE:HG13	70:N4:502:PC1:H11	1.99	0.44
47:QA:259:ARG:HB3	47:QA:444:LEU:HD13	1.99	0.44
48:QB:100:GLY:HA2	48:QB:106:GLY:N	2.30	0.44
48:QB:110:GLU:HA	48:QB:113:VAL:HG22	1.98	0.44
71:QC:405:PEE:H26	71:QC:405:PEE:H31	1.54	0.44
50:Qd:149:LEU:O	50:Qd:152:GLU:HG2	2.17	0.44
18:A9:212:ARG:O	18:A9:216:TYR:N	2.40	0.44
68:AL:201:CDL:H621	42:N2:160:LEU:HD11	1.98	0.44
29:B6:148:TYR:CE1	33:BK:49:ARG:HG2	2.53	0.44
71:CB:203:PEE:H38	71:CB:203:PEE:H32	1.60	0.44
42:N2:243:LEU:HD22	42:N2:330:ILE:HG21	2.00	0.44
48:QB:223:HIS:HA	48:QB:228:ARG:NH2	2.33	0.44
50:QD:293:MET:HE2	50:QD:293:MET:HB3	1.89	0.44
70:Qh:103:PC1:H272	70:Qh:103:PC1:H382	1.99	0.44
58:S2:137:GLN:O	63:S7:142:TYR:OH	2.34	0.44
71:8B:101:PEE:H25	38:C4:120:TRP:CE3	2.52	0.44
11:A1:50:ARG:NH2	17:A8:95:VAL:O	2.50	0.44
19:AB:78:ALA:HA	19:AB:81:ASP:OD2	2.18	0.44
37:C3:141:GLY:O	37:C3:144:ILE:HG22	2.18	0.44
41:N1:110:SER:HB2	46:N6:62:GLY:HA3	2.00	0.44
43:N3:28:ASN:HD21	70:N3:202:PC1:H232	1.82	0.44
44:N4:16:TRP:CE2	68:N4:501:CDL:H272	2.52	0.44
44:N4:372:SER:HB3	68:N5:702:CDL:H381	1.98	0.44
76:QI:102:PLX:H71	50:Qd:307:MET:HE1	1.98	0.44
65:V1:129:GLU:OE2	65:V1:132:ARG:NH2	2.50	0.44
3:5B:45:THR:OG1	3:5B:46:GLY:N	2.51	0.44
4:6A:79:HIS:HD2	4:6A:83:HIS:CD2	2.36	0.44
19:AC:119:ILE:HG21	19:AC:135:ALA:HB1	1.99	0.44
34:BL:130:GLU:HB3	34:BL:136:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C1:176:MET:HE3	35:C1:181:THR:HG22	1.98	0.44
36:C2:128:LEU:HD11	36:C2:134:ARG:HA	1.98	0.44
71:C3:302:PEE:H81	71:C3:302:PEE:H75	1.83	0.44
47:QA:222:GLY:HA3	47:QA:230:LEU:HD11	1.98	0.44
49:QC:233:LEU:HD13	76:QE:301:PLX:H152	1.99	0.44
51:QE:151:LYS:HE2	51:QE:272:ILE:HD11	1.99	0.44
70:Qd:402:PC1:H262	70:Qd:402:PC1:H232	1.82	0.44
51:Qe:187:GLU:OE1	51:Qe:248:ARG:NH2	2.49	0.44
57:S1:401:LEU:HD11	57:S1:432:ILE:HG13	1.99	0.44
15:A6:88:LYS:NZ	15:A6:133:PHE:HA	2.33	0.44
17:A8:202:LEU:HD13	23:AN:70:ALA:HB2	1.99	0.44
74:AC:201:ZMP:H25B	74:AC:201:ZMP:H22A	1.67	0.44
33:BK:99:ASP:OD2	33:BK:142:ARG:NH1	2.50	0.44
34:BL:137:MET:HE3	34:BL:137:MET:HB2	1.86	0.44
37:C3:58:TRP:CD2	70:C3:301:PC1:H252	2.52	0.44
45:N5:233:LEU:HB3	45:N5:234:PRO:HD3	1.99	0.44
49:Qc:200:LEU:CD2	80:Qc:405:HEM:HAA1	2.47	0.44
52:Qf:45:LYS:O	52:Qf:48:GLU:HG2	2.18	0.44
57:S1:382:ARG:CZ	57:S1:386:LEU:HD11	2.48	0.44
63:S7:140:GLY:HA3	63:S7:144:HIS:HA	2.00	0.44
18:A9:64:PHE:O	18:A9:67:ARG:HG2	2.17	0.44
70:N4:502:PC1:H132	70:N4:502:PC1:H111	1.84	0.44
49:QC:8:HIS:O	49:QC:12:LYS:N	2.43	0.44
49:QC:150:LEU:HD11	71:QC:405:PEE:H15	1.99	0.44
68:QD:402:CDL:HB21	53:Qg:73:GLN:HB2	1.98	0.44
71:Qh:101:PEE:H13	71:Qh:101:PEE:H19	1.59	0.44
68:A8:301:CDL:H112	40:CB:32:ARG:HG2	1.99	0.44
22:AM:127:TYR:OH	62:S6:61:GLU:O	2.27	0.44
23:AN:87:LEU:HD11	23:AN:119:PRO:HG3	1.99	0.44
35:C1:436:MET:HE3	35:C1:443:TYR:HB3	1.98	0.44
42:N2:95:MET:HE2	42:N2:149:ILE:HA	1.99	0.44
68:N5:703:CDL:H221	68:N5:703:CDL:H192	1.80	0.44
70:QB:503:PC1:O22	49:QC:221:HIS:HE1	2.00	0.44
49:QC:185:LEU:HD23	49:QC:188:ILE:HD12	1.98	0.44
51:QE:207:LYS:HE3	51:QE:210:TRP:HD1	1.83	0.44
47:Qa:66:LYS:HB2	47:Qa:217:ARG:HB3	2.00	0.44
49:Qc:197:LEU:HD11	80:Qc:405:HEM:HMA2	1.98	0.44
49:Qc:233:LEU:HD23	49:Qc:233:LEU:HA	1.80	0.44
18:A9:212:ARG:NH1	18:A9:311:GLU:OE2	2.51	0.43
27:B4:48:LEU:HB3	32:B9:208:LEU:HD13	1.99	0.43
35:C1:377:PHE:HA	35:C1:380:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:N5:67:HIS:NE2	45:N5:70:THR:OG1	2.51	0.43
47:QA:92:LYS:HD2	47:QA:143:ALA:HB1	1.99	0.43
47:QA:138:LEU:O	47:QA:142:ALA:HB3	2.18	0.43
48:QB:80:ARG:NH2	48:QB:350:GLU:OE1	2.51	0.43
68:QB:501:CDL:H762	70:QB:502:PC1:H3A1	1.99	0.43
54:QH:19:LEU:HD23	54:QH:24:GLN:HB3	1.99	0.43
47:Qa:180:ALA:HB2	47:Qa:258:ILE:HG13	2.00	0.43
47:Qa:313:VAL:HG11	47:Qa:350:VAL:HG13	2.00	0.43
71:6A:103:PEE:H49	71:6A:103:PEE:H55	1.89	0.43
18:A9:344:PRO:HG2	18:A9:347:LEU:HD13	2.00	0.43
33:BK:78:GLU:HA	40:CB:110:THR:HA	2.00	0.43
41:N1:272:TRP:CZ2	64:S8:74:LEU:HB2	2.53	0.43
46:N6:109:LYS:HA	46:N6:109:LYS:HD3	1.84	0.43
51:QE:169:TRP:HZ2	51:QE:274:GLY:HA2	1.82	0.43
76:QI:102:PLX:H1A3	76:QI:102:PLX:H22	1.73	0.43
48:Qb:99:LYS:HA	48:Qb:99:LYS:HD3	1.91	0.43
49:Qc:128:PHE:O	49:Qc:132:VAL:HG23	2.19	0.43
49:Qc:131:TYR:O	49:Qc:134:PRO:HD2	2.18	0.43
51:Qe:239:HIS:HB2	82:Qe:301:FES:S2	2.58	0.43
52:Qf:40:ILE:HD13	52:Qf:81:CYS:SG	2.58	0.43
59:S3:173:MET:HE3	59:S3:188:LEU:HB2	2.00	0.43
37:C3:58:TRP:HD1	37:C3:61:ILE:HD12	1.83	0.43
44:N4:127:VAL:HG11	68:N4:501:CDL:H471	2.00	0.43
49:Qc:181:PHE:HA	49:Qc:184:ILE:HG22	2.00	0.43
57:S1:370:GLU:O	57:S1:533:GLY:N	2.46	0.43
57:S1:556:THR:OG1	57:S1:557:ARG:N	2.51	0.43
58:S2:118:HIS:ND1	59:S3:191:TYR:OH	2.50	0.43
58:S2:133:LYS:HG3	58:S2:141:TYR:HE2	1.83	0.43
9:7C:39:ALA:O	9:7C:42:THR:HG22	2.18	0.43
19:AC:85:TYR:OH	26:B3:22:TRP:NE1	2.36	0.43
76:AL:205:PLX:H142	68:B4:201:CDL:H342	2.00	0.43
30:B7:95:TYR:CZ	31:B8:156:VAL:HG11	2.54	0.43
35:C1:65:MET:HB3	77:C1:602:HEA:CAC	2.48	0.43
35:C1:244:TYR:HA	35:C1:247:ILE:HG22	1.99	0.43
72:C1:601:3PE:H2G1	38:C4:113:PHE:HB2	2.00	0.43
36:C2:194:GLY:N	36:C2:209:ILE:O	2.49	0.43
41:N1:121:TRP:CE2	46:N6:27:ILE:HG13	2.53	0.43
48:QB:74:TRP:CZ2	48:QB:411:GLU:HA	2.54	0.43
49:QC:121:PHE:HD1	71:QC:405:PEE:H30	1.83	0.43
48:Qb:360:CYS:SG	48:Qb:368:MET:HG3	2.58	0.43
70:Qb:501:PC1:H32	68:Qb:502:CDL:H131	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:Qb:501:PC1:H2B2	68:Qb:502:CDL:H351	2.01	0.43
49:Qc:299:LEU:HD23	70:Qc:407:PC1:H133	1.99	0.43
57:S1:339:ALA:HA	57:S1:365:SER:HB2	2.01	0.43
61:S5:15:ASP:OD1	61:S5:15:ASP:N	2.50	0.43
63:S7:75:GLU:HG3	63:S7:167:PRO:HB2	1.99	0.43
3:5B:80:VAL:N	3:5B:121:LYS:O	2.48	0.43
68:A8:301:CDL:H202	68:A8:301:CDL:H541	2.00	0.43
18:A9:174:ILE:HG23	18:A9:175:LYS:HG3	2.01	0.43
21:AL:81:ARG:NH1	21:AL:89:ASN:OD1	2.50	0.43
71:AN:202:PEE:H12	71:AN:202:PEE:H2	2.01	0.43
72:C1:601:3PE:H3B2	72:C1:601:3PE:H2E2	2.00	0.43
42:N2:287:LEU:HB2	71:N5:706:PEE:H62	2.00	0.43
45:N5:10:THR:O	45:N5:14:ILE:HG23	2.18	0.43
53:Qg:41:ASP:OD1	53:Qg:41:ASP:N	2.51	0.43
64:S8:49:ASP:OD1	64:S8:49:ASP:N	2.52	0.43
66:V2:188:ILE:HB	66:V2:193:TYR:HE2	1.83	0.43
67:V3:383:ASN:O	67:V3:383:ASN:ND2	2.52	0.43
13:A3:126:TYR:HE1	13:A3:129:ARG:HH21	1.67	0.43
18:A9:64:PHE:HZ	18:A9:208:GLY:HA3	1.83	0.43
23:AN:28:ARG:NH1	68:AN:203:CDL:OA4	2.51	0.43
29:B6:82:TRP:O	29:B6:86:GLN:HG2	2.19	0.43
38:C4:36:PRO:HB2	38:C4:49:VAL:HG13	2.00	0.43
72:CA:101:3PE:H3H2	72:CA:101:3PE:H291	2.00	0.43
40:CB:35:TYR:OH	42:N2:335:LEU:O	2.34	0.43
68:N4:501:CDL:H273	68:N4:501:CDL:H712	2.01	0.43
45:N5:341:MET:SD	45:N5:457:LEU:HD12	2.58	0.43
71:N5:704:PEE:H76	71:N5:704:PEE:H71	1.78	0.43
53:Qg:97:GLU:OE1	53:Qg:100:ARG:NH1	2.51	0.43
58:S2:118:HIS:HD1	59:S3:191:TYR:HH	1.65	0.43
76:S7:302:PLX:H152	76:S7:302:PLX:H182	1.75	0.43
2:5A:77:ASN:HD22	38:C4:45:PRO:HD2	1.84	0.43
20:AK:63:THR:CG2	20:AK:203:PRO:HB3	2.49	0.43
76:AL:205:PLX:H352	76:AL:205:PLX:H381	1.77	0.43
42:N2:137:ALA:HB3	42:N2:138:PRO:HD3	2.01	0.43
47:QA:35:PRO:HB2	47:QA:36:GLN:H	1.60	0.43
49:QC:131:TYR:O	49:QC:134:PRO:HD2	2.18	0.43
50:QD:113:ARG:O	50:QD:117:VAL:HG23	2.19	0.43
58:S2:194:THR:HG21	58:S2:209:MET:HB2	2.00	0.43
58:S2:469:ARG:NH2	59:S3:169:GLU:OE2	2.51	0.43
68:A8:301:CDL:H182	68:A8:301:CDL:H522	2.00	0.43
74:AC:201:ZMP:H6	32:B9:90:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AN:49:SER:HB2	41:N1:172:ILE:HD13	2.01	0.43
23:AN:94:GLU:OE2	61:S5:75:ARG:NH2	2.52	0.43
25:B2:76:ASP:O	45:N5:385:TYR:OH	2.23	0.43
76:BL:202:PLX:H312	76:BL:202:PLX:H281	1.74	0.43
35:C1:413:HIS:CE1	35:C1:468:MET:HB2	2.54	0.43
44:N4:200:ILE:O	44:N4:204:MET:HG2	2.19	0.43
44:N4:203:PHE:CE1	44:N4:242:GLY:HA3	2.54	0.43
44:N4:210:TYR:CG	44:N4:268:GLY:HA3	2.53	0.43
47:QA:272:VAL:HA	47:QA:337:GLY:HA3	2.00	0.43
54:QH:67:PHE:HE1	49:Qc:344:GLU:HG3	1.84	0.43
56:QJ:34:TRP:CE2	51:Qe:130:LYS:HD2	2.53	0.43
49:Qc:234:PHE:HE2	68:Qc:411:CDL:H321	1.83	0.43
57:S1:594:ALA:O	57:S1:605:GLN:HA	2.18	0.43
65:V1:68:ILE:HG23	65:V1:75:TRP:HZ3	1.84	0.43
65:V1:281:HIS:ND1	65:V1:358:ASP:OD1	2.52	0.43
66:V2:83:LEU:HD21	66:V2:116:ALA:HB2	2.00	0.43
67:V3:420:SER:HB3	67:V3:423:HIS:ND1	2.33	0.43
71:8B:101:PEE:H77	71:8B:101:PEE:H71	1.69	0.43
20:AK:64:VAL:HA	20:AK:205:VAL:O	2.19	0.43
24:B1:17:VAL:HG13	44:N4:7:PRO:HB3	2.01	0.43
70:C1:610:PC1:H332	70:C1:610:PC1:H361	1.81	0.43
38:C4:65:LYS:HE2	38:C4:65:LYS:HB3	1.86	0.43
42:N2:189:TRP:CH2	42:N2:263:LYS:HG3	2.54	0.43
44:N4:221:VAL:HA	44:N4:283:LYS:HD3	2.01	0.43
44:N4:296:LEU:HD21	44:N4:378:GLU:HG3	2.01	0.43
70:N6:201:PC1:O12	70:N6:201:PC1:H121	2.19	0.43
52:QF:65:GLU:HG3	54:QH:73:LYS:NZ	2.34	0.43
51:Qe:262:THR:HB	51:Qe:274:GLY:O	2.18	0.43
52:Qf:60:ARG:NH1	54:Qh:78:TYR:O	2.49	0.43
57:S1:356:ASP:O	57:S1:360:ARG:HG2	2.19	0.43
58:S2:46:ASP:OD1	58:S2:46:ASP:N	2.50	0.43
4:6A:88:ASN:CG	70:6A:101:PC1:H131	2.44	0.43
20:AK:316:LEU:HB2	20:AK:319:ILE:HG12	2.00	0.43
68:AL:204:CDL:H711	68:AL:204:CDL:H522	2.01	0.43
24:B1:42:SER:O	24:B1:46:LYS:HB2	2.19	0.43
71:BL:201:PEE:H23	71:BL:201:PEE:H18	1.70	0.43
42:N2:280:THR:HG23	44:N4:162:VAL:HG11	2.01	0.43
46:N6:17:PHE:HA	46:N6:20:PHE:CD2	2.54	0.43
71:QC:403:PEE:H30	71:QC:403:PEE:H23	1.59	0.43
59:S3:213:ASP:HB3	59:S3:216:VAL:HG22	2.00	0.43
44:N4:131:ILE:O	44:N4:135:ARG:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:N5:136:ASN:ND2	45:N5:139:GLN:H	2.17	0.42
47:QA:51:SER:OG	47:QA:230:LEU:HD12	2.19	0.42
50:QD:247:PRO:HA	50:QD:248:PRO:HD3	1.84	0.42
49:Qc:285:PRO:HD2	70:Qc:407:PC1:H391	2.01	0.42
54:Qh:60:TYR:CE1	70:Qh:103:PC1:H362	2.54	0.42
62:S6:79:VAL:O	62:S6:121:PRO:HD3	2.19	0.42
64:S8:67:VAL:HG12	70:S8:304:PC1:H231	2.01	0.42
4:6A:60:ILE:O	4:6A:62:TYR:N	2.45	0.42
15:A6:127:THR:O	15:A6:131:ARG:HG3	2.20	0.42
16:A7:50:SER:HG	65:V1:414:GLU:CD	2.26	0.42
35:C1:195:LEU:HD22	35:C1:199:LEU:HD11	2.01	0.42
42:N2:280:THR:HG21	70:N4:502:PC1:H272	2.00	0.42
46:N6:122:LEU:HG	46:N6:126:VAL:HG21	2.01	0.42
48:QB:459:LEU:HD12	48:QB:459:LEU:HA	1.88	0.42
58:S2:149:SER:HA	58:S2:184:THR:HG22	1.99	0.42
58:S2:418:VAL:HB	58:S2:427:ARG:HB3	2.01	0.42
62:S6:71:ILE:HD12	62:S6:71:ILE:HA	1.91	0.42
63:S7:96:SER:HB2	63:S7:99:GLN:HG2	2.01	0.42
63:S7:119:LYS:HE2	63:S7:119:LYS:HB3	1.83	0.42
65:V1:62:TRP:CE2	65:V1:181:LEU:HD13	2.53	0.42
65:V1:244:ASN:OD1	65:V1:245:VAL:N	2.52	0.42
10:8B:36:PRO:HB3	72:C1:601:3PE:H341	2.01	0.42
11:A1:40:HIS:N	11:A1:44:GLN:OE1	2.50	0.42
18:A9:109:ASN:HB3	18:A9:112:ASP:HB2	2.00	0.42
20:AK:63:THR:HG23	20:AK:203:PRO:HB3	2.00	0.42
20:AK:355:TRP:H	20:AK:355:TRP:CD1	2.38	0.42
42:N2:17:THR:HG23	42:N2:137:ALA:HB2	2.00	0.42
42:N2:140:SER:HB3	61:S5:2:PRO:HA	2.01	0.42
45:N5:213:LEU:HD23	45:N5:213:LEU:HA	1.74	0.42
49:QC:116:GLY:HA3	80:QC:402:HEM:C3C	2.54	0.42
49:QC:267:HIS:CD2	49:QC:269:LYS:HG2	2.54	0.42
52:QF:56:ARG:O	52:QF:60:ARG:HG3	2.19	0.42
50:Qd:122:CYS:SG	81:Qd:401:HEC:HAB	2.58	0.42
51:Qe:190:VAL:HG11	51:Qe:250:ARG:NH2	2.33	0.42
35:C1:44:PRO:HD3	35:C1:448:THR:HG23	2.00	0.42
42:N2:276:ILE:C	42:N2:279:PRO:HD2	2.44	0.42
49:QC:130:GLY:O	49:QC:134:PRO:HD3	2.19	0.42
49:Qc:182:HIS:HE1	80:Qc:404:HEM:C1B	2.38	0.42
58:S2:203:MET:O	58:S2:206:PHE:HB3	2.20	0.42
59:S3:187:ILE:HG23	59:S3:188:LEU:HG	2.00	0.42
11:A1:17:PHE:CE1	41:N1:257:ILE:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A9:198:ALA:O	18:A9:260:GLY:CA	2.64	0.42
24:B1:15:ILE:C	24:B1:18:PRO:HD2	2.44	0.42
29:B6:164:ILE:HB	30:B7:48:ASP:HB3	2.01	0.42
35:C1:436:MET:HA	35:C1:437:PRO:HD3	1.91	0.42
36:C2:156:SER:OG	36:C2:159:VAL:O	2.23	0.42
41:N1:287:HIS:CE1	43:N3:113:TRP:HD1	2.37	0.42
43:N3:63:LEU:O	43:N3:67:LEU:HG	2.19	0.42
44:N4:70:THR:HA	44:N4:103:GLN:HE21	1.83	0.42
45:N5:569:ILE:HG23	70:N5:705:PC1:H12	2.02	0.42
47:QA:147:ARG:HD3	47:QA:149:TRP:CZ2	2.55	0.42
68:QC:406:CDL:H632	49:Qc:188:ILE:HG23	2.01	0.42
48:Qb:120:LEU:HD13	48:Qb:133:ILE:HG12	2.01	0.42
48:Qb:167:VAL:O	48:Qb:171:GLU:HG2	2.20	0.42
57:S1:382:ARG:C	57:S1:384:ASN:H	2.27	0.42
65:V1:384:PRO:HG2	65:V1:422:HIS:O	2.19	0.42
4:6A:88:ASN:OD1	70:6A:101:PC1:H141	2.19	0.42
71:A3:201:PEE:H32	41:N1:295:PRO:HA	2.02	0.42
21:AL:101:LEU:HD21	68:AL:201:CDL:H332	2.00	0.42
26:B3:24:ILE:O	26:B3:30:GLU:HB3	2.20	0.42
27:B4:25:ILE:HG21	27:B4:30:ARG:CZ	2.49	0.42
28:B5:163:ARG:NH1	40:CB:102:ASP:OD2	2.27	0.42
30:B7:17:PRO:HB3	30:B7:105:GLU:HG2	2.02	0.42
35:C1:71:MET:HB2	35:C1:72:PRO:HD3	2.01	0.42
35:C1:202:LEU:HD22	35:C1:238:PHE:CE2	2.54	0.42
70:C1:610:PC1:H153	70:C1:610:PC1:H112	1.86	0.42
76:CB:201:PLX:H362	76:CB:201:PLX:H332	1.86	0.42
71:N5:701:PEE:H31	68:N5:702:CDL:H231	2.01	0.42
54:QH:20:SER:HB3	54:QH:23:GLU:HG2	2.02	0.42
57:S1:611:THR:HG21	60:S4:105:GLU:HA	2.01	0.42
67:V3:411:MET:HE2	67:V3:411:MET:HB3	1.94	0.42
72:7B:101:3PE:H242	72:7B:101:3PE:H361	2.01	0.42
9:7C:19:TYR:CE2	35:C1:5:ARG:HG3	2.54	0.42
20:AK:85:LEU:HD22	20:AK:158:GLY:HA3	2.01	0.42
20:AK:251:MET:SD	20:AK:254:LYS:HD2	2.60	0.42
35:C1:469:ILE:HD13	35:C1:469:ILE:HA	1.91	0.42
37:C3:231:HIS:CE1	70:C3:301:PC1:H152	2.54	0.42
41:N1:91:MET:HA	41:N1:255:TYR:HE1	1.85	0.42
70:N1:401:PC1:H391	70:N1:401:PC1:H3C2	1.81	0.42
45:N5:229:LEU:HG	71:N5:704:PEE:H38	2.01	0.42
47:QA:82:LEU:HD11	47:QA:154:LEU:HB3	2.02	0.42
49:QC:128:PHE:O	49:QC:132:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:QC:378:LYS:NZ	53:Qg:84:TYR:OH	2.50	0.42
71:QE:302:PEE:H47	71:QE:302:PEE:H39	1.87	0.42
47:Qa:70:ARG:NH1	47:Qa:117:GLU:OE2	2.44	0.42
47:Qa:147:ARG:HD3	47:Qa:149:TRP:CZ2	2.54	0.42
57:S1:452:LEU:HD21	57:S1:493:VAL:HG13	2.02	0.42
59:S3:190:ASP:OD1	59:S3:191:TYR:N	2.53	0.42
62:S6:54:ARG:O	62:S6:58:ARG:NH2	2.53	0.42
1:4L:1:MET:SD	42:N2:80:TYR:OH	2.76	0.42
31:B8:116:ARG:HG3	71:N5:704:PEE:H49	2.02	0.42
35:C1:119:GLU:HG3	35:C1:140:GLY:HA3	2.01	0.42
70:N3:202:PC1:H321	70:N3:202:PC1:H351	1.85	0.42
45:N5:356:ILE:HB	45:N5:429:PHE:HB3	2.02	0.42
51:QK:51:CYS:SG	51:QK:54:SER:OG	2.71	0.42
48:Qb:473:SER:HB3	70:Qb:501:PC1:H121	2.02	0.42
71:Qe:302:PEE:H66	71:Qe:302:PEE:H61	1.67	0.42
68:Qj:101:CDL:H341	68:Qj:101:CDL:H312	1.85	0.42
68:Qj:101:CDL:H361	68:Qj:101:CDL:H392	1.92	0.42
63:S7:62:LEU:HD23	63:S7:62:LEU:HA	1.88	0.42
66:V2:186:VAL:HG22	66:V2:196:LEU:HD11	2.02	0.42
71:6A:103:PEE:H67	71:6A:103:PEE:H73	1.80	0.42
8:7B:35:ASP:HA	38:C4:98:ASN:HD22	1.85	0.42
30:B7:99:MET:HG3	31:B8:156:VAL:HG12	2.02	0.42
35:C1:2:PHE:HE2	68:C1:607:CDL:H112	1.85	0.42
35:C1:309:THR:HG22	77:C1:603:HEA:HMB1	2.01	0.42
35:C1:361:SER:O	35:C1:365:ILE:HG12	2.19	0.42
72:C1:601:3PE:H2B1	38:C4:106:THR:HG23	2.01	0.42
38:C4:107:ALA:O	38:C4:111:ILE:HG13	2.20	0.42
51:Qe:225:ILE:HG12	51:Qe:237:PRO:HD3	2.01	0.42
57:S1:76:ARG:O	57:S1:116:VAL:HG21	2.19	0.42
57:S1:103:LEU:HB3	57:S1:106:SER:HB2	2.01	0.42
64:S8:74:LEU:HD12	64:S8:77:LEU:HD23	2.02	0.42
4:6A:80:THR:HG21	37:C3:187:THR:HB	2.02	0.42
6:6C:20:ARG:O	6:6C:23:ILE:HG22	2.20	0.42
8:7B:74:PRO:HB3	38:C4:143:LYS:HB2	2.02	0.42
21:AL:3:LYS:HE3	21:AL:7:HIS:NE2	2.35	0.42
68:AN:201:CDL:H392	68:AN:201:CDL:H442	2.02	0.42
71:AN:202:PEE:H26	71:AN:202:PEE:H31	1.68	0.42
70:B7:201:PC1:H391	70:B7:201:PC1:H352	2.02	0.42
42:N2:136:LEU:HD12	42:N2:205:LEU:HD21	2.02	0.42
45:N5:503:GLU:O	45:N5:507:THR:HG23	2.20	0.42
45:N5:572:LYS:HD3	45:N5:572:LYS:HA	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:QA:48:VAL:HG11	47:QA:400:ALA:HB1	2.02	0.42
47:QA:371:VAL:HG12	47:QA:375:LYS:HE3	2.00	0.42
53:QG:60:VAL:HG11	54:QH:11:MET:HG2	2.01	0.42
47:Qa:43:LEU:HD12	47:Qa:47:LEU:HD23	2.01	0.42
49:Qc:200:LEU:HD22	80:Qc:405:HEM:HAA1	2.01	0.42
63:S7:108:THR:HA	63:S7:136:CYS:HB3	2.02	0.42
71:6A:103:PEE:H15	71:6A:103:PEE:H21	1.69	0.41
17:A8:117:ASN:HB3	23:AN:73:PRO:HG2	2.02	0.41
20:AK:93:ILE:HG23	20:AK:136:TRP:NE1	2.35	0.41
77:C1:602:HEA:HMB1	77:C1:602:HEA:HHB	1.83	0.41
36:C2:98:LYS:HG2	36:C2:153:LEU:HB2	2.02	0.41
45:N5:7:LEU:O	45:N5:11:THR:HG23	2.20	0.41
45:N5:15:LEU:HD23	45:N5:15:LEU:HA	1.93	0.41
68:N5:703:CDL:H192	68:N5:703:CDL:H152	2.00	0.41
47:QA:348:GLY:HA2	47:QA:448:PRO:HD3	2.02	0.41
49:QC:132:VAL:HG11	49:QC:178:PHE:HD2	1.83	0.41
57:S1:476:LEU:HD21	57:S1:481:LEU:HD21	2.01	0.41
58:S2:124:2MR:O	63:S7:146:SER:OG	2.21	0.41
58:S2:405:ALA:HB1	58:S2:412:GLU:HG3	2.02	0.41
62:S6:46:ASP:OD1	62:S6:46:ASP:N	2.39	0.41
63:S7:186:ARG:HE	63:S7:186:ARG:HB2	1.72	0.41
76:S7:302:PLX:H261	76:S7:302:PLX:H292	1.92	0.41
67:V3:418:ARG:NH1	67:V3:423:HIS:O	2.53	0.41
68:A7:201:CDL:H732	68:A7:201:CDL:H761	1.93	0.41
27:B4:31:LYS:HE3	27:B4:31:LYS:HB2	1.91	0.41
70:N1:401:PC1:H251	70:N1:401:PC1:H281	1.82	0.41
43:N3:7:LEU:HD11	70:N6:201:PC1:H251	2.02	0.41
71:QC:404:PEE:H13	71:QC:404:PEE:H19	1.87	0.41
50:QD:95:TYR:HA	50:QD:96:PRO:HD3	1.92	0.41
71:Qc:403:PEE:H23	71:Qc:403:PEE:H29	1.82	0.41
57:S1:632:MET:H	57:S1:632:MET:HG2	1.72	0.41
58:S2:151:MET:HE2	58:S2:232:TYR:HB3	2.01	0.41
58:S2:248:ASP:O	58:S2:252:GLU:HG2	2.19	0.41
58:S2:341:GLU:O	58:S2:345:GLN:HG2	2.20	0.41
68:AL:204:CDL:H342	71:Qh:101:PEE:H65	2.01	0.41
76:AM:201:PLX:H262	76:S7:302:PLX:H122	2.02	0.41
35:C1:52:GLN:HE22	35:C1:138:HIS:HE1	1.67	0.41
35:C1:100:MET:N	37:C3:17:PRO:HB3	2.35	0.41
37:C3:79:LEU:HB3	37:C3:233:PHE:CE2	2.55	0.41
37:C3:204:HIS:CE1	37:C3:249:TRP:HB2	2.54	0.41
70:QB:502:PC1:H151	49:QC:1:MET:H2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:V1:302:LYS:HE3	65:V1:303:HIS:CE1	2.55	0.41
66:V2:137:THR:O	66:V2:141:MET:N	2.51	0.41
70:6A:101:PC1:H142	37:C3:181:TYR:O	2.20	0.41
35:C1:2:PHE:HZ	70:C1:608:PC1:H141	1.85	0.41
35:C1:74:MET:SD	35:C1:249:PRO:HG2	2.61	0.41
77:C1:603:HEA:HHA	77:C1:603:HEA:HAD2	1.93	0.41
36:C2:104:TRP:CD1	36:C2:203:ASN:HB2	2.55	0.41
37:C3:54:MET:HB3	37:C3:58:TRP:CZ3	2.55	0.41
44:N4:127:VAL:HB	44:N4:128:PRO:HD3	2.01	0.41
44:N4:346:ARG:O	44:N4:419:TYR:HA	2.21	0.41
45:N5:297:ASP:O	45:N5:301:ILE:HG13	2.21	0.41
49:Qc:11:MET:SD	70:Qc:410:PC1:H362	2.60	0.41
51:QE:196:ARG:NH2	51:QE:252:GLY:O	2.49	0.41
51:QE:214:ILE:HG13	51:QE:261:PRO:HD3	2.03	0.41
49:Qc:24:PRO:O	49:Qc:224:TYR:OH	2.17	0.41
49:Qc:141:TRP:CD1	49:Qc:265:PRO:HD3	2.55	0.41
70:Qc:412:PC1:H381	70:Qc:412:PC1:H352	1.94	0.41
58:S2:272:ARG:NH1	71:S8:303:PEE:H1	2.35	0.41
60:S4:75:ARG:HA	60:S4:75:ARG:HD2	1.83	0.41
63:S7:49:LYS:HE3	76:S7:302:PLX:H301	2.02	0.41
65:V1:373:PHE:CE1	65:V1:377:GLU:HG3	2.56	0.41
11:A1:65:GLY:HA2	17:A8:97:VAL:HG12	2.02	0.41
28:B5:53:ARG:NH2	29:B6:89:SER:O	2.53	0.41
35:C1:358:LEU:HB3	77:C1:603:HEA:HMA	2.03	0.41
44:N4:97:THR:HG21	68:N4:501:CDL:H232	2.02	0.41
44:N4:225:ILE:HD13	44:N4:331:ASN:HB2	2.03	0.41
46:N6:129:ASP:HB2	61:S5:32:ARG:NH1	2.35	0.41
47:Qa:313:VAL:HG21	47:Qa:323:VAL:HG11	2.02	0.41
48:Qb:104:ARG:NH2	48:Qb:145:GLU:OE2	2.53	0.41
53:Qg:46:GLU:HA	53:Qg:49:ARG:HG2	2.03	0.41
58:S2:143:ASP:OD1	58:S2:150:MET:HB3	2.19	0.41
58:S2:299:LEU:HD22	58:S2:304:ILE:HD12	2.02	0.41
58:S2:318:ASP:OD1	58:S2:318:ASP:N	2.47	0.41
18:A9:56:ALA:HA	18:A9:125:VAL:O	2.19	0.41
18:A9:106:MET:HE2	18:A9:118:LYS:HE3	2.03	0.41
31:B8:78:LEU:HD12	31:B8:106:HIS:HA	2.02	0.41
36:C2:141:ARG:HD2	36:C2:212:GLU:OE1	2.20	0.41
37:C3:23:SER:HB3	37:C3:50:ASN:HB2	2.03	0.41
37:C3:173:PHE:CE1	37:C3:208:VAL:HG21	2.56	0.41
41:N1:268:ILE:HG22	70:N1:401:PC1:H3I2	2.01	0.41
41:N1:306:SER:O	41:N1:310:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:N2:95:MET:HE1	42:N2:145:ILE:HD12	2.03	0.41
42:N2:211:MET:HG2	42:N2:333:SER:HB2	2.02	0.41
44:N4:242:GLY:O	44:N4:246:ILE:HG12	2.21	0.41
47:Qa:60:ARG:HD3	47:Qa:393:LEU:HD22	2.02	0.41
48:Qb:80:ARG:NH2	48:Qb:268:CYS:SG	2.93	0.41
56:Qj:42:LEU:HA	56:Qj:45:VAL:HG22	2.02	0.41
59:S3:75:GLN:NE2	59:S3:77:GLN:HE21	2.18	0.41
76:S7:302:PLX:H22	76:S7:302:PLX:H1A2	1.81	0.41
1:4L:40:LEU:HD22	42:N2:75:ILE:HD12	2.02	0.41
24:B1:8:VAL:O	24:B1:12:TRP:HB3	2.20	0.41
76:N3:201:PLX:H352	76:N3:201:PLX:H382	1.72	0.41
45:N5:504:LEU:O	45:N5:507:THR:OG1	2.38	0.41
49:QC:102:LEU:HD22	49:QC:304:MET:HE2	2.02	0.41
49:Qc:278:TYR:HE2	49:Qc:282:ARG:HH21	1.68	0.41
57:S1:476:LEU:HD22	57:S1:493:VAL:HG21	2.03	0.41
63:S7:56:TRP:NE1	76:S7:302:PLX:H82	2.36	0.41
65:V1:445:GLU:OE1	65:V1:449:ARG:NH2	2.54	0.41
5:6B:58:ARG:HA	5:6B:61:TYR:CE2	2.55	0.41
72:7B:101:3PE:H2F1	72:7B:101:3PE:H3G2	2.03	0.41
12:A2:85:ASP:OD1	12:A2:85:ASP:N	2.53	0.41
20:AK:328:ARG:HH21	34:BL:58:ASP:CG	2.29	0.41
21:AL:4:THR:HG22	21:AL:8:LYS:HE3	2.03	0.41
21:AL:108:TYR:CE1	68:AL:204:CDL:H111	2.56	0.41
30:B7:92:HIS:O	30:B7:96:VAL:HG13	2.21	0.41
35:C1:18:LEU:HB3	35:C1:102:PHE:CZ	2.56	0.41
76:CB:201:PLX:H1A2	61:S5:2:PRO:HD2	2.02	0.41
70:N4:502:PC1:H352	70:N4:502:PC1:H3C2	2.02	0.41
45:N5:341:MET:HE2	45:N5:454:ILE:HG12	2.03	0.41
68:N5:702:CDL:H361	68:N5:702:CDL:H401	2.01	0.41
49:QC:138:MET:HE1	49:QC:269:LYS:H	1.85	0.41
49:QC:186:PRO:HG2	80:QC:401:HEM:HMC3	2.02	0.41
50:QD:104:SER:HA	55:Qi:48:ASN:HD21	1.85	0.41
51:QE:160:PRO:HD2	51:QE:163:LYS:HG2	2.03	0.41
48:Qb:38:TYR:CZ	48:Qb:42:LEU:HD11	2.56	0.41
58:S2:107:LEU:HD22	58:S2:450:LEU:HD11	2.02	0.41
58:S2:398:PRO:HA	58:S2:399:PRO:HD3	1.96	0.41
65:V1:131:ILE:HD13	65:V1:158:ILE:HD13	2.03	0.41
15:A6:127:THR:HG23	59:S3:219:VAL:O	2.21	0.41
22:AM:25:ARG:O	22:AM:29:ARG:HG2	2.21	0.41
22:AM:139:PRO:HG3	57:S1:306:MET:HE1	2.02	0.41
68:AN:201:CDL:H181	68:AN:201:CDL:H141	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B1:43:LEU:O	33:BK:69:ARG:HD2	2.21	0.41
28:B5:67:PHE:CE2	44:N4:434:ASN:HB3	2.56	0.41
31:B8:83:GLN:O	31:B8:98:ARG:HD2	2.21	0.41
31:B8:149:ILE:HD12	70:B8:201:PC1:H221	2.03	0.41
32:B9:123:ILE:HD13	32:B9:129:GLY:HA3	2.03	0.41
35:C1:33:LEU:HB3	35:C1:61:HIS:HB2	2.03	0.41
35:C1:54:TYR:OH	77:C1:602:HEA:O1A	2.29	0.41
71:C1:609:PEE:H54	37:C3:99:TRP:CE2	2.56	0.41
36:C2:138:VAL:HG12	36:C2:208:PRO:HG2	2.02	0.41
41:N1:145:THR:OG1	41:N1:289:LEU:HD11	2.21	0.41
41:N1:267:THR:O	41:N1:271:LEU:HG	2.21	0.41
44:N4:74:PRO:O	44:N4:78:MET:HG3	2.21	0.41
44:N4:398:MET:HG2	71:N5:704:PEE:H78	2.03	0.41
45:N5:583:LEU:HD23	45:N5:583:LEU:HA	1.92	0.41
46:N6:106:TYR:HB3	46:N6:112:GLU:OE1	2.21	0.41
46:N6:135:PHE:HD1	46:N6:135:PHE:HA	1.78	0.41
47:QA:290:GLN:HB2	47:QA:336:PHE:HE1	1.85	0.41
47:QA:379:LYS:NZ	47:QA:417:ASP:OD1	2.42	0.41
47:QA:384:MET:HG2	48:QB:68:THR:HG21	2.01	0.41
48:QB:225:LYS:HD2	48:QB:257:TYR:CE2	2.56	0.41
68:QB:501:CDL:H511	70:QB:502:PC1:H361	2.01	0.41
49:QC:82:LEU:HD23	49:QC:82:LEU:HA	1.97	0.41
49:QC:156:ILE:HD12	70:QJ:101:PC1:H342	2.01	0.41
49:QC:300:ILE:HD11	49:QC:363:LEU:HD21	2.03	0.41
50:QD:139:VAL:HG11	50:QD:277:TRP:CE2	2.56	0.41
54:QH:57:TYR:CD1	71:QH:102:PEE:H50	2.56	0.41
47:Qa:184:ASN:OD1	47:Qa:184:ASN:N	2.54	0.41
47:Qa:222:GLY:HA3	47:Qa:230:LEU:HD11	2.03	0.41
48:Qb:79:SER:HB3	48:Qb:126:ARG:HA	2.02	0.41
49:Qc:190:THR:HG23	71:Qc:408:PEE:H55	2.02	0.41
49:Qc:310:SER:HA	49:Qc:374:ASN:HD21	1.86	0.41
55:Qi:54:LYS:HE2	55:Qi:54:LYS:HB3	1.84	0.41
57:S1:70:SER:HB2	60:S4:163:ASN:HD21	1.85	0.41
57:S1:379:THR:HG21	57:S1:526:LEU:HD22	2.03	0.41
57:S1:534:VAL:HG23	57:S1:537:ILE:HD12	2.03	0.41
65:V1:177:TYR:OH	65:V1:194:ASP:OD1	2.32	0.41
1:4L:37:MET:HE1	46:N6:64:MET:HE1	2.03	0.41
23:AN:93:GLU:OE1	61:S5:92:TYR:OH	2.35	0.41
71:AN:202:PEE:H71	71:AN:202:PEE:H76	1.87	0.41
25:B2:42:PRO:HB3	45:N5:442:LEU:HD23	2.03	0.41
33:BK:43:ARG:HB2	33:BK:44:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:C3:302:PEE:H66	71:C3:302:PEE:H72	1.74	0.41
42:N2:277:ILE:HG13	70:N4:502:PC1:H331	2.02	0.41
44:N4:118:PHE:O	44:N4:122:PHE:HB3	2.21	0.41
68:N4:501:CDL:H231	68:N4:501:CDL:H832	2.02	0.41
45:N5:96:VAL:O	45:N5:100:ILE:HG12	2.21	0.41
48:QB:274:GLU:HA	48:QB:456:VAL:O	2.20	0.41
49:QC:51:LEU:O	49:QC:55:TYR:HB2	2.21	0.41
71:QE:302:PEE:H23	71:QE:302:PEE:H30	1.77	0.41
54:QH:31:PHE:CD1	68:Qc:411:CDL:H521	2.55	0.41
48:Qb:418:LEU:HD23	48:Qb:418:LEU:HA	1.89	0.41
51:Qe:224:PRO:HA	51:Qe:236:CYS:HA	2.02	0.41
53:Qg:52:PRO:HD2	53:Qg:55:LEU:HD12	2.03	0.41
20:AK:67:ASN:CG	20:AK:68:ILE:H	2.30	0.40
20:AK:86:ARG:HH11	20:AK:151:HIS:CD2	2.39	0.40
21:AL:140:LYS:HE2	28:B5:158:ARG:HD2	2.03	0.40
35:C1:369:ASP:HA	35:C1:438:ARG:HD3	2.03	0.40
42:N2:25:HIS:HB2	61:S5:15:ASP:HB2	2.03	0.40
42:N2:276:ILE:HG21	70:N4:502:PC1:H242	2.03	0.40
44:N4:216:LEU:HD23	44:N4:287:ALA:HB1	2.02	0.40
45:N5:401:MET:HE3	45:N5:401:MET:HB3	1.96	0.40
45:N5:530:PRO:O	45:N5:534:HIS:CB	2.67	0.40
70:N6:201:PC1:H3B2	70:N6:201:PC1:H3E1	1.85	0.40
47:QA:266:LEU:HD13	51:QK:55:LEU:HD21	2.03	0.40
49:QC:133:LEU:HD23	49:QC:133:LEU:HA	1.75	0.40
51:QE:151:LYS:HB3	51:QE:272:ILE:HD11	2.02	0.40
47:Qa:298:HIS:HB2	48:Qb:114:GLU:HG2	2.02	0.40
50:Qd:271:VAL:O	50:Qd:275:LEU:HG	2.21	0.40
58:S2:105:MET:HE1	58:S2:453:VAL:HG21	2.03	0.40
58:S2:290:LEU:O	58:S2:293:GLY:CA	2.69	0.40
3:5B:44:ALA:O	3:5B:49:ARG:NH1	2.51	0.40
7:7A:63:GLY:C	37:C3:26:LEU:HD21	2.46	0.40
72:7B:101:3PE:H331	72:7B:101:3PE:H362	1.87	0.40
22:AM:80:SER:O	22:AM:113:HIS:HE1	2.05	0.40
31:B8:88:PRO:HB3	31:B8:98:ARG:NH2	2.35	0.40
31:B8:162:PRO:HB2	31:B8:163:TYR:CD2	2.56	0.40
35:C1:155:VAL:HG21	70:C1:610:PC1:H3D1	2.03	0.40
40:CB:27:LYS:O	40:CB:30:ASP:HB2	2.22	0.40
41:N1:307:LEU:HB3	41:N1:308:PRO:HD3	2.03	0.40
42:N2:14:MET:O	42:N2:18:MET:HG2	2.20	0.40
44:N4:357:THR:O	44:N4:361:VAL:HG23	2.22	0.40
45:N5:286:LEU:HD22	45:N5:411:MET:SD	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:N5:290:LEU:O	45:N5:293:ILE:HG12	2.22	0.40
45:N5:584:ILE:HG22	45:N5:587:TYR:OH	2.21	0.40
47:QA:231:LYS:HE2	47:QA:231:LYS:HB3	1.88	0.40
47:QA:306:THR:OG1	48:QB:114:GLU:OE1	2.28	0.40
51:QE:209:GLU:HG3	51:QE:210:TRP:HD1	1.85	0.40
49:Qc:8:HIS:CD2	49:Qc:10:LEU:H	2.39	0.40
58:S2:182:GLU:OE2	58:S2:317:TYR:OH	2.31	0.40
4:6A:65:LEU:HD22	37:C3:190:ASP:HB3	2.04	0.40
68:A7:201:CDL:H232	68:A7:201:CDL:H201	1.89	0.40
68:A8:301:CDL:H222	68:A8:301:CDL:H251	1.89	0.40
68:AL:202:CDL:H331	68:AL:202:CDL:H361	1.89	0.40
22:AM:117:VAL:O	22:AM:120:THR:OG1	2.37	0.40
23:AN:120:MET:HG3	61:S5:32:ARG:NH2	2.37	0.40
38:C4:98:ASN:HB3	38:C4:101:LYS:HD2	2.01	0.40
76:CB:201:PLX:H152	76:CB:201:PLX:H182	1.88	0.40
44:N4:145:ALA:HB1	44:N4:219:ALA:HA	2.03	0.40
45:N5:208:CYS:HA	45:N5:209:PRO:HD3	1.79	0.40
45:N5:285:THR:HA	45:N5:308:SER:HA	2.03	0.40
47:QA:121:TYR:HB3	47:QA:137:LEU:HD11	2.03	0.40
48:QB:140:LEU:HD22	48:QB:237:VAL:HG12	2.03	0.40
50:QD:303:LEU:HB3	51:QE:121:THR:OG1	2.22	0.40
51:QE:207:LYS:HG2	51:QE:209:GLU:HG2	2.03	0.40
52:QF:60:ARG:HD3	52:QF:63:THR:HG21	2.03	0.40
53:QG:44:VAL:O	53:QG:48:ILE:HG12	2.21	0.40
47:Qa:138:LEU:HD11	47:Qa:233:VAL:HB	2.03	0.40
47:Qa:391:GLY:HA2	47:Qa:394:ASP:OD2	2.21	0.40
48:Qb:351:THR:OG1	48:Qb:352:GLY:N	2.55	0.40
49:Qc:132:VAL:HG22	49:Qc:143:ALA:HB2	2.03	0.40
64:S8:137:ASP:OD1	64:S8:137:ASP:N	2.55	0.40
64:S8:156:GLY:N	84:S8:302:SF4:S4	2.80	0.40
65:V1:44:ASN:HD22	65:V1:133:HIS:HB3	1.86	0.40
1:4L:55:LEU:HD13	61:S5:17:TRP:HE3	1.87	0.40
27:B4:77:TYR:OH	45:N5:564:LYS:HG2	2.21	0.40
77:C1:602:HEA:H122	77:C1:602:HEA:HHC	2.03	0.40
36:C2:69:PRO:O	36:C2:73:LEU:HG	2.21	0.40
41:N1:288:LEU:O	41:N1:292:SER:HB2	2.21	0.40
70:N1:401:PC1:H3E2	70:N1:401:PC1:H3B1	1.92	0.40
45:N5:11:THR:HG22	45:N5:46:LEU:HB3	2.03	0.40
46:N6:165:VAL:O	46:N6:168:ILE:HG13	2.22	0.40
50:QD:132:ALA:HA	50:QD:175:TYR:HA	2.03	0.40
47:Qa:115:THR:OG1	47:Qa:116:ARG:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:S1:428:LYS:HE2	57:S1:465:ILE:HD13	2.04	0.40
76:S7:302:PLX:H211	76:S7:302:PLX:H181	1.94	0.40
68:A8:301:CDL:H381	42:N2:256:PRO:CB	2.48	0.40
68:AL:204:CDL:H872	68:B4:201:CDL:H521	2.04	0.40
22:AM:4:VAL:O	22:AM:8:ARG:HG2	2.21	0.40
35:C1:332:ILE:HG23	35:C1:338:MET:HE3	2.02	0.40
46:N6:123:GLY:O	46:N6:127:ILE:HG23	2.21	0.40
68:QB:501:CDL:H152	70:QB:502:PC1:H2A1	2.04	0.40
49:QC:119:LEU:HD22	80:QC:402:HEM:HBB2	2.04	0.40
49:QC:326:TRP:CH2	71:QC:403:PEE:H48	2.56	0.40
51:QE:220:LEU:HD12	51:QE:239:HIS:HE1	1.86	0.40
54:QH:20:SER:O	54:QH:24:GLN:HG2	2.22	0.40
48:Qb:99:LYS:NZ	48:Qb:164:GLU:OE2	2.50	0.40
50:Qd:311:LYS:HD3	50:Qd:311:LYS:HA	1.86	0.40
58:S2:368:LYS:HE3	58:S2:368:LYS:HB2	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4L	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
2	5A	100/102 (98%)	100 (100%)	0	0	100	100
3	5B	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
4	6A	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
5	6B	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
6	6C	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
7	7A	55/57 (96%)	55 (100%)	0	0	100	100
8	7B	48/50 (96%)	45 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	7C	45/47 (96%)	45 (100%)	0	0	100	100
10	8B	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
11	A1	68/70 (97%)	68 (100%)	0	0	100	100
12	A2	83/85 (98%)	79 (95%)	4 (5%)	0	100	100
13	A3	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
14	A5	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
15	A6	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
16	A7	93/112 (83%)	91 (98%)	2 (2%)	0	100	100
17	A8	169/171 (99%)	164 (97%)	5 (3%)	0	100	100
18	A9	331/341 (97%)	322 (97%)	9 (3%)	0	100	100
19	AB	75/156 (48%)	75 (100%)	0	0	100	100
19	AC	85/156 (54%)	85 (100%)	0	0	100	100
20	AK	318/320 (99%)	302 (95%)	16 (5%)	0	100	100
21	AL	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
22	AM	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
23	AN	140/142 (99%)	130 (93%)	10 (7%)	0	100	100
24	B1	54/56 (96%)	54 (100%)	0	0	100	100
25	B2	65/67 (97%)	65 (100%)	0	0	100	100
26	B3	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
27	B4	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
28	B5	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
29	B6	100/126 (79%)	97 (97%)	3 (3%)	0	100	100
30	B7	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
31	B8	154/156 (99%)	151 (98%)	3 (2%)	0	100	100
32	B9	176/178 (99%)	174 (99%)	2 (1%)	0	100	100
33	BK	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
34	BL	97/102 (95%)	90 (93%)	7 (7%)	0	100	100
35	C1	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
36	C2	226/228 (99%)	220 (97%)	6 (3%)	0	100	100
37	C3	258/261 (99%)	251 (97%)	7 (3%)	0	100	100
38	C4	136/138 (99%)	133 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	CA	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
40	CB	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
41	N1	304/318 (96%)	290 (95%)	14 (5%)	0	100	100
42	N2	345/347 (99%)	333 (96%)	12 (4%)	0	100	100
43	N3	93/114 (82%)	90 (97%)	3 (3%)	0	100	100
44	N4	457/459 (100%)	453 (99%)	4 (1%)	0	100	100
45	N5	601/603 (100%)	577 (96%)	24 (4%)	0	100	100
46	N6	160/174 (92%)	145 (91%)	15 (9%)	0	100	100
47	QA	417/419 (100%)	407 (98%)	10 (2%)	0	100	100
47	Qa	417/419 (100%)	413 (99%)	4 (1%)	0	100	100
48	QB	444/446 (100%)	432 (97%)	12 (3%)	0	100	100
48	Qb	429/446 (96%)	422 (98%)	7 (2%)	0	100	100
49	QC	377/379 (100%)	371 (98%)	6 (2%)	0	100	100
49	Qc	377/379 (100%)	371 (98%)	6 (2%)	0	100	100
50	QD	239/241 (99%)	231 (97%)	8 (3%)	0	100	100
50	Qd	237/241 (98%)	230 (97%)	7 (3%)	0	100	100
51	QE	194/274 (71%)	190 (98%)	4 (2%)	0	100	100
51	QK	69/274 (25%)	69 (100%)	0	0	100	100
51	Qe	194/274 (71%)	188 (97%)	6 (3%)	0	100	100
52	QF	65/67 (97%)	65 (100%)	0	0	100	100
52	Qf	62/67 (92%)	62 (100%)	0	0	100	100
53	QG	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
53	Qg	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
54	QH	76/81 (94%)	75 (99%)	1 (1%)	0	100	100
54	Qh	77/81 (95%)	76 (99%)	1 (1%)	0	100	100
55	QI	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
55	Qi	58/63 (92%)	58 (100%)	0	0	100	100
56	QJ	47/52 (90%)	47 (100%)	0	0	100	100
56	Qj	49/52 (94%)	47 (96%)	2 (4%)	0	100	100
57	S1	687/689 (100%)	663 (96%)	24 (4%)	0	100	100
58	S2	420/430 (98%)	396 (94%)	24 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	S3	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
60	S4	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
61	S5	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
62	S6	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
63	S7	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
64	S8	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
65	V1	429/431 (100%)	407 (95%)	22 (5%)	0	100	100
66	V2	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
67	V3	40/42 (95%)	37 (92%)	3 (8%)	0	100	100
All	All	13913/14717 (94%)	13526 (97%)	387 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4L	85/85 (100%)	85 (100%)	0	100	100
2	5A	89/89 (100%)	89 (100%)	0	100	100
3	5B	80/80 (100%)	77 (96%)	3 (4%)	28	61
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%)	47 (98%)	1 (2%)	48	76
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%)	75 (99%)	1 (1%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	A3	69/69 (100%)	68 (99%)	1 (1%)	62	83
14	A5	99/99 (100%)	99 (100%)	0	100	100
15	A6	107/107 (100%)	106 (99%)	1 (1%)	75	89
16	A7	87/97 (90%)	84 (97%)	3 (3%)	32	65
17	A8	153/153 (100%)	153 (100%)	0	100	100
18	A9	289/295 (98%)	287 (99%)	2 (1%)	81	91
19	AB	71/132 (54%)	71 (100%)	0	100	100
19	AC	80/132 (61%)	79 (99%)	1 (1%)	65	84
20	AK	283/283 (100%)	278 (98%)	5 (2%)	54	79
21	AL	101/101 (100%)	100 (99%)	1 (1%)	73	88
22	AM	130/130 (100%)	129 (99%)	1 (1%)	79	90
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	99/119 (83%)	98 (99%)	1 (1%)	73	88
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	91/94 (97%)	90 (99%)	1 (1%)	70	87
35	C1	425/425 (100%)	423 (100%)	2 (0%)	86	94
36	C2	212/212 (100%)	208 (98%)	4 (2%)	52	78
37	C3	224/225 (100%)	222 (99%)	2 (1%)	75	89
38	C4	123/123 (100%)	123 (100%)	0	100	100
39	CA	45/45 (100%)	45 (100%)	0	100	100
40	CB	108/108 (100%)	108 (100%)	0	100	100
41	N1	267/275 (97%)	262 (98%)	5 (2%)	52	78
42	N2	311/311 (100%)	310 (100%)	1 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	N3	85/99 (86%)	84 (99%)	1 (1%)	67	85
44	N4	410/410 (100%)	409 (100%)	1 (0%)	92	97
45	N5	537/537 (100%)	534 (99%)	3 (1%)	84	92
46	N6	130/140 (93%)	127 (98%)	3 (2%)	45	74
47	QA	329/330 (100%)	329 (100%)	0	100	100
47	Qa	330/330 (100%)	330 (100%)	0	100	100
48	QB	372/372 (100%)	370 (100%)	2 (0%)	86	94
48	Qb	362/372 (97%)	360 (99%)	2 (1%)	84	92
49	QC	332/332 (100%)	331 (100%)	1 (0%)	91	96
49	Qc	332/332 (100%)	330 (99%)	2 (1%)	84	92
50	QD	206/206 (100%)	206 (100%)	0	100	100
50	Qd	204/206 (99%)	203 (100%)	1 (0%)	86	94
51	QE	166/225 (74%)	165 (99%)	1 (1%)	84	92
51	QK	55/225 (24%)	53 (96%)	2 (4%)	30	62
51	Qe	166/225 (74%)	165 (99%)	1 (1%)	84	92
52	QF	64/64 (100%)	64 (100%)	0	100	100
52	Qf	61/64 (95%)	61 (100%)	0	100	100
53	QG	93/93 (100%)	93 (100%)	0	100	100
53	Qg	93/93 (100%)	92 (99%)	1 (1%)	70	87
54	QH	70/72 (97%)	69 (99%)	1 (1%)	62	83
54	Qh	70/72 (97%)	70 (100%)	0	100	100
55	QI	50/51 (98%)	50 (100%)	0	100	100
55	Qi	49/51 (96%)	49 (100%)	0	100	100
56	QJ	40/42 (95%)	40 (100%)	0	100	100
56	Qj	41/42 (98%)	41 (100%)	0	100	100
57	S1	579/579 (100%)	575 (99%)	4 (1%)	81	91
58	S2	365/370 (99%)	358 (98%)	7 (2%)	52	78
59	S3	190/190 (100%)	188 (99%)	2 (1%)	70	87
60	S4	112/112 (100%)	108 (96%)	4 (4%)	30	62
61	S5	93/93 (100%)	93 (100%)	0	100	100
62	S6	79/79 (100%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	S7	132/132 (100%)	130 (98%)	2 (2%)	60	82
64	S8	151/151 (100%)	151 (100%)	0	100	100
65	V1	343/344 (100%)	336 (98%)	7 (2%)	50	77
66	V2	183/183 (100%)	181 (99%)	2 (1%)	70	87
67	V3	41/41 (100%)	40 (98%)	1 (2%)	44	73
All	All	12138/12644 (96%)	12051 (99%)	87 (1%)	80	91

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	5B	94	GLU
3	5B	99	THR
3	5B	100	VAL
7	7A	56	THR
12	A2	85	ASP
13	A3	120	LEU
15	A6	125	GLN
16	A7	7	VAL
16	A7	31	ILE
16	A7	43	VAL
18	A9	129	LEU
18	A9	365	GLU
19	AC	112	SER
20	AK	38	LEU
20	AK	68	ILE
20	AK	205	VAL
20	AK	255	CYS
20	AK	278	LEU
21	AL	115	CYS
22	AM	62	VAL
29	B6	133	THR
34	BL	83	ASP
35	C1	128	VAL
35	C1	151	HIS
36	C2	99	THR
36	C2	111	THR
36	C2	172	THR
36	C2	199	ILE
37	C3	5	THR
37	C3	109	THR

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Mol	Chain	Res	Type
41	N1	1	MET
41	N1	28	LEU
41	N1	87	VAL
41	N1	145	THR
41	N1	251	THR
42	N2	280	THR
43	N3	27	LEU
44	N4	122	PHE
45	N5	286	LEU
45	N5	340	PHE
45	N5	387	THR
46	N6	57	PHE
46	N6	116	ILE
46	N6	135	PHE
48	QB	71	VAL
48	QB	79	SER
49	QC	281	LEU
51	QE	211	VAL
54	QH	38	VAL
51	QK	44	ASP
51	QK	78	TYR
48	Qb	71	VAL
48	Qb	95	HIS
49	Qc	68	HIS
49	Qc	100	ARG
50	Qd	209	GLU
51	Qe	145	ASP
53	Qg	83	LYS
57	S1	556	THR
57	S1	636	TYR
57	S1	676	ASN
57	S1	690	THR
58	S2	98	HIS
58	S2	100	VAL
58	S2	148	VAL
58	S2	204	THR
58	S2	240	GLN
58	S2	284	VAL
58	S2	362	ILE
59	S3	68	ILE
59	S3	225	GLU
60	S4	53	ILE

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Mol	Chain	Res	Type
60	S4	58	LYS
60	S4	77	VAL
60	S4	129	SER
63	S7	67	PHE
63	S7	71	CYS
65	V1	270	ASN
65	V1	294	VAL
65	V1	307	VAL
65	V1	334	THR
65	V1	347	THR
65	V1	379	CYS
65	V1	385	CYS
66	V2	137	THR
66	V2	249	LEU
67	V3	406	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (267) such sidechains are listed below:

Mol	Chain	Res	Type
1	4L	7	ASN
2	5A	77	ASN
3	5B	97	ASN
4	6A	50	HIS
4	6A	54	HIS
4	6A	64	HIS
4	6A	83	HIS
5	6B	11	ASN
5	6B	24	GLN
5	6B	25	ASN
5	6B	26	GLN
5	6B	33	ASN
7	7A	50	ASN
8	7B	34	HIS
8	7B	59	GLN
9	7C	18	HIS
9	7C	59	GLN
12	A2	86	GLN
13	A3	96	ASN
14	A5	71	GLN
14	A5	86	ASN
14	A5	111	GLN
15	A6	84	GLN

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Mol	Chain	Res	Type
16	A7	9	GLN
16	A7	29	GLN
16	A7	51	ASN
17	A8	107	HIS
17	A8	112	GLN
17	A8	141	ASN
17	A8	142	GLN
17	A8	176	HIS
17	A8	220	HIS
18	A9	37	HIS
18	A9	72	HIS
18	A9	138	ASN
18	A9	154	GLN
18	A9	215	ASN
18	A9	238	GLN
18	A9	295	HIS
19	AB	101	ASN
19	AC	142	GLN
20	AK	67	ASN
20	AK	134	GLN
20	AK	151	HIS
20	AK	178	GLN
20	AK	217	GLN
20	AK	221	GLN
21	AL	79	GLN
21	AL	129	GLN
22	AM	31	ASN
22	AM	113	HIS
23	AN	61	GLN
24	B1	3	ASN
24	B1	6	GLN
24	B1	14	HIS
25	B2	49	GLN
25	B2	57	GLN
26	B3	33	GLN
26	B3	91	GLN
27	B4	50	GLN
28	B5	132	ASN
28	B5	170	GLN
28	B5	189	ASN
29	B6	149	HIS
30	B7	110	GLN

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Mol	Chain	Res	Type
31	B8	94	HIS
31	B8	115	ASN
31	B8	127	ASN
31	B8	132	HIS
32	B9	104	GLN
32	B9	117	GLN
33	BK	107	GLN
33	BK	124	ASN
33	BK	161	GLN
35	C1	4	ASN
35	C1	12	HIS
35	C1	43	GLN
35	C1	80	ASN
35	C1	138	HIS
35	C1	151	HIS
35	C1	178	GLN
35	C1	233	HIS
35	C1	256	HIS
35	C1	328	HIS
35	C1	422	ASN
35	C1	491	ASN
36	C2	10	GLN
36	C2	52	HIS
36	C2	59	GLN
36	C2	181	GLN
36	C2	203	ASN
37	C3	6	HIS
37	C3	70	HIS
37	C3	125	ASN
37	C3	133	ASN
37	C3	148	HIS
37	C3	161	GLN
37	C3	204	HIS
37	C3	232	HIS
38	C4	141	GLN
38	C4	154	GLN
39	CA	62	HIS
39	CA	73	ASN
41	N1	138	GLN
41	N1	317	GLN
42	N2	49	ASN
42	N2	77	ASN

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Mol	Chain	Res	Type
42	N2	112	HIS
42	N2	144	GLN
42	N2	273	ASN
42	N2	322	GLN
42	N2	347	ASN
43	N3	28	ASN
44	N4	30	HIS
44	N4	51	ASN
44	N4	81	GLN
44	N4	168	GLN
44	N4	192	ASN
44	N4	213	HIS
44	N4	251	ASN
44	N4	279	GLN
45	N5	56	HIS
45	N5	135	ASN
45	N5	159	HIS
45	N5	175	ASN
45	N5	199	GLN
45	N5	205	ASN
45	N5	230	HIS
45	N5	470	ASN
45	N5	518	GLN
45	N5	524	ASN
45	N5	579	ASN
45	N5	580	GLN
47	QA	167	GLN
47	QA	168	ASN
47	QA	176	ASN
47	QA	184	ASN
47	QA	227	HIS
47	QA	284	ASN
47	QA	291	HIS
47	QA	357	GLN
47	QA	365	ASN
47	QA	415	GLN
47	QA	426	ASN
48	QB	49	GLN
48	QB	119	HIS
48	QB	152	GLN
48	QB	170	GLN
48	QB	173	GLN

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Mol	Chain	Res	Type
48	QB	188	HIS
48	QB	222	GLN
48	QB	223	HIS
48	QB	239	HIS
48	QB	298	ASN
48	QB	301	ASN
48	QB	357	HIS
48	QB	464	GLN
49	QC	54	HIS
49	QC	68	HIS
49	QC	97	HIS
49	QC	201	HIS
49	QC	255	ASN
49	QC	267	HIS
49	QC	308	HIS
49	QC	312	GLN
49	QC	322	GLN
50	QD	91	HIS
50	QD	206	HIS
50	QD	266	GLN
51	QE	135	GLN
51	QE	186	GLN
51	QE	199	GLN
51	QE	257	ASN
52	QF	88	ASN
53	QG	54	ASN
54	QH	80	ASN
55	QI	38	GLN
55	QI	46	HIS
55	QI	48	ASN
55	QI	55	HIS
51	QK	58	GLN
47	Qa	36	GLN
47	Qa	155	GLN
47	Qa	167	GLN
47	Qa	172	GLN
47	Qa	211	ASN
47	Qa	212	HIS
47	Qa	290	GLN
47	Qa	291	HIS
47	Qa	304	ASN
47	Qa	319	GLN

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Mol	Chain	Res	Type
47	Qa	343	GLN
47	Qa	376	ASN
47	Qa	408	GLN
48	Qb	43	GLN
48	Qb	83	ASN
48	Qb	87	ASN
48	Qb	95	HIS
48	Qb	160	GLN
48	Qb	170	GLN
48	Qb	188	HIS
48	Qb	223	HIS
48	Qb	239	HIS
48	Qb	249	HIS
48	Qb	313	HIS
48	Qb	357	HIS
48	Qb	469	ASN
49	Qc	8	HIS
49	Qc	54	HIS
50	Qd	116	GLN
50	Qd	190	ASN
50	Qd	206	HIS
50	Qd	310	HIS
51	Qe	186	GLN
51	Qe	194	GLN
51	Qe	199	GLN
52	Qf	36	GLN
52	Qf	55	GLN
53	Qg	23	ASN
54	Qh	13	HIS
54	Qh	65	GLN
55	Qi	38	GLN
55	Qi	48	ASN
57	S1	39	GLN
57	S1	59	GLN
57	S1	142	GLN
57	S1	282	ASN
57	S1	331	GLN
57	S1	336	ASN
57	S1	425	ASN
57	S1	453	GLN
57	S1	498	GLN
57	S1	604	GLN

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Mol	Chain	Res	Type
57	S1	652	ASN
57	S1	688	GLN
58	S2	52	GLN
58	S2	85	ASN
58	S2	98	HIS
58	S2	153	ASN
58	S2	239	HIS
58	S2	240	GLN
58	S2	271	ASN
59	S3	75	GLN
59	S3	82	ASN
59	S3	123	GLN
59	S3	196	HIS
60	S4	123	ASN
60	S4	163	ASN
61	S5	45	HIS
62	S6	74	GLN
62	S6	117	GLN
65	V1	44	ASN
65	V1	49	HIS
65	V1	303	HIS
65	V1	344	GLN
65	V1	381	GLN
65	V1	393	ASN
65	V1	452	GLN
66	V2	131	HIS
66	V2	133	GLN
66	V2	153	GLN
66	V2	182	ASN
66	V2	187	GLN
66	V2	246	GLN
67	V3	388	ASN
67	V3	392	HIS
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	2.43	2 (20%)	5,13,15	1.07	0

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	S2	124	2MR	CZ-NE	5.20	1.45	1.34
58	S2	124	2MR	CZ-NH2	5.00	1.44	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	S2	124	2MR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 127 ligands modelled in this entry, 7 are monoatomic - leaving 120 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
71	PEE	AN	202	-	50,50,50	1.33	5 (10%)	53,55,55	1.15	2 (3%)
70	PC1	N5	705	-	30,30,53	0.37	0	36,38,61	0.40	0
68	CDL	N5	703	-	99,99,99	0.31	0	105,111,111	0.28	0
84	SF4	S8	302	64	0,12,12	-	-	-		
68	CDL	AL	201	-	93,93,99	0.31	0	99,105,111	0.27	0
77	HEA	C1	602	35	57,67,67	2.00	16 (28%)	61,103,103	2.65	27 (44%)
71	PEE	A7	202	-	27,27,50	1.34	3 (11%)	30,32,55	1.15	2 (6%)
70	PC1	C3	301	-	48,48,53	0.31	0	54,56,61	0.34	0
76	PLX	N3	201	-	51,51,51	1.11	4 (7%)	55,59,59	0.86	1 (1%)
71	PEE	8B	101	-	41,41,50	1.29	5 (12%)	44,46,55	1.23	2 (4%)
74	ZMP	AB	201	19	29,35,36	0.66	1 (3%)	34,42,45	0.80	1 (2%)
76	PLX	CB	201	-	51,51,51	1.11	4 (7%)	55,59,59	0.83	1 (1%)
76	PLX	S7	302	-	51,51,51	1.10	3 (5%)	55,59,59	0.91	1 (1%)
70	PC1	Qb	501	-	37,37,53	0.35	0	43,45,61	0.33	0
82	FES	S1	803	57	0,4,4	-	-	-		
72	3PE	CB	202	-	45,45,50	0.31	0	48,50,55	0.33	0
71	PEE	QC	404	-	34,34,50	1.41	4 (11%)	36,39,55	1.23	3 (8%)
84	SF4	S8	301	64	0,12,12	-	-	-		
71	PEE	QH	102	-	50,50,50	1.32	5 (10%)	53,55,55	1.17	3 (5%)
82	FES	QE	303	51	0,4,4	-	-	-		
76	PLX	QE	301	-	45,45,51	1.17	5 (11%)	49,53,59	0.88	1 (2%)
72	3PE	7B	101	-	50,50,50	0.30	0	53,55,55	0.33	0
70	PC1	Qh	103	-	53,53,53	0.29	0	59,61,61	0.27	0
68	CDL	A7	201	-	93,93,99	0.31	0	99,105,111	0.31	0
68	CDL	AN	201	-	80,80,99	0.33	0	86,92,111	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	CDL	N4	501	-	99,99,99	0.30	0	105,111,111	0.28	0
72	3PE	Qc	401	-	43,43,50	0.32	0	46,48,55	0.32	0
70	PC1	N6	201	-	53,53,53	0.30	0	59,61,61	0.40	0
71	PEE	Qc	408	-	47,47,50	1.36	5 (10%)	50,52,55	1.16	4 (8%)
70	PC1	N1	401	-	53,53,53	0.29	0	59,61,61	0.30	0
71	PEE	N5	706	-	43,43,50	1.41	5 (11%)	46,48,55	1.19	3 (6%)
81	HEC	Qd	401	50	32,50,50	2.03	4 (12%)	24,82,82	2.31	14 (58%)
82	FES	V2	301	66	0,4,4	-	-	-	-	-
68	CDL	AN	203	-	65,65,99	0.36	0	71,77,111	0.38	0
84	SF4	V1	501	65	0,12,12	-	-	-	-	-
75	ADP	AK	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.42	4 (13%)
73	NDP	A9	401	-	45,52,52	0.53	0	53,80,80	0.53	1 (1%)
76	PLX	BL	202	-	51,51,51	1.11	6 (11%)	55,59,59	0.86	1 (1%)
83	PX2	QH	101	-	35,35,35	0.97	4 (11%)	39,40,40	1.03	2 (5%)
71	PEE	Qb	503	-	50,50,50	1.32	5 (10%)	53,55,55	1.10	2 (3%)
76	PLX	B1	101	-	51,51,51	1.11	4 (7%)	55,59,59	0.88	1 (1%)
68	CDL	AL	204	-	79,79,99	0.34	0	85,91,111	0.41	1 (1%)
70	PC1	7A	101	-	53,53,53	0.31	0	59,61,61	0.42	0
74	ZMP	AC	201	19	29,35,36	0.67	1 (3%)	34,42,45	0.75	0
68	CDL	C1	607	-	76,76,99	0.34	0	82,88,111	0.32	0
70	PC1	C4	201	-	53,53,53	0.30	0	59,61,61	0.36	0
84	SF4	S1	802	57	0,12,12	-	-	-	-	-
84	SF4	S1	801	57	0,12,12	-	-	-	-	-
71	PEE	N5	701	-	45,45,50	1.37	5 (11%)	48,50,55	1.19	2 (4%)
71	PEE	6A	103	-	50,50,50	1.32	5 (10%)	53,55,55	1.15	4 (7%)
82	FES	Qe	301	51	0,4,4	-	-	-	-	-
70	PC1	6A	101	-	44,44,53	0.32	0	50,52,61	0.32	0
70	PC1	C3	304	-	50,50,53	0.30	0	56,58,61	0.28	0
68	CDL	Qb	502	-	63,63,99	0.38	0	69,75,111	0.41	0
71	PEE	Qh	101	-	50,50,50	1.32	5 (10%)	53,55,55	1.16	3 (5%)
71	PEE	Qe	302	-	49,49,50	1.33	5 (10%)	52,54,55	1.20	3 (5%)
77	HEA	C1	603	35	57,67,67	2.02	16 (28%)	61,103,103	2.67	28 (45%)
68	CDL	QC	406	-	89,89,99	0.32	0	95,101,111	0.34	0
72	3PE	Qc	406	-	47,47,50	0.31	0	50,52,55	0.37	0
71	PEE	C3	302	-	50,50,50	1.32	5 (10%)	53,55,55	1.10	3 (5%)
72	3PE	C1	601	-	50,50,50	0.31	0	53,55,55	0.29	0
71	PEE	QC	403	-	39,39,50	1.31	4 (10%)	42,44,55	1.18	2 (4%)
80	HEM	QC	402	49	41,50,50	1.25	5 (12%)	45,82,82	1.69	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
70	PC1	C1	610	-	49,49,53	0.31	0	55,57,61	0.31	0
71	PEE	N5	704	-	50,50,50	1.31	5 (10%)	53,55,55	1.16	3 (5%)
68	CDL	QC	407	-	54,54,99	0.40	0	60,66,111	0.37	0
70	PC1	QJ	101	-	53,53,53	0.30	0	59,61,61	0.29	0
70	PC1	Qc	409	-	41,41,53	0.33	0	47,49,61	0.29	0
70	PC1	N3	202	-	53,53,53	0.29	0	59,61,61	0.35	0
68	CDL	Qj	101	-	95,95,99	0.31	0	101,107,111	0.36	0
76	PLX	AL	205	-	46,46,51	1.16	4 (8%)	50,54,59	0.88	1 (2%)
70	PC1	C1	608	-	47,47,53	0.31	0	53,55,61	0.30	0
70	PC1	N4	502	-	53,53,53	0.30	0	59,61,61	0.32	0
68	CDL	N2	401	-	67,67,99	0.35	0	73,79,111	0.32	0
68	CDL	B5	201	-	95,95,99	0.31	0	101,107,111	0.34	0
71	PEE	AL	203	-	35,35,50	1.36	4 (11%)	38,40,55	1.14	3 (7%)
80	HEM	Qc	405	49	41,50,50	1.24	3 (7%)	45,82,82	1.69	9 (20%)
71	PEE	Qc	403	-	41,41,50	1.28	4 (9%)	44,46,55	1.17	2 (4%)
71	PEE	6A	102	-	50,50,50	1.32	5 (10%)	53,55,55	1.14	3 (5%)
71	PEE	S8	303	-	50,50,50	1.31	5 (10%)	53,55,55	1.15	3 (5%)
70	PC1	Qd	402	-	53,53,53	0.29	0	59,61,61	0.30	0
80	HEM	Qc	404	49	41,50,50	1.22	4 (9%)	45,82,82	1.69	7 (15%)
68	CDL	A8	301	-	82,82,99	0.33	0	88,94,111	0.31	0
68	CDL	Qh	102	-	99,99,99	0.30	0	105,111,111	0.29	0
70	PC1	C1	606	-	45,45,53	0.31	0	51,53,61	0.36	0
70	PC1	B7	201	-	53,53,53	0.30	0	59,61,61	0.30	0
70	PC1	S8	304	-	44,44,53	0.33	0	50,52,61	0.34	0
68	CDL	N5	702	-	88,88,99	0.32	0	94,100,111	0.34	0
76	PLX	QI	102	-	51,51,51	1.11	4 (7%)	55,59,59	0.86	1 (1%)
70	PC1	Qc	412	-	53,53,53	0.30	0	59,61,61	0.41	0
76	PLX	AM	201	-	51,51,51	1.12	4 (7%)	55,59,59	0.85	1 (1%)
71	PEE	QE	302	-	46,46,50	1.37	5 (10%)	49,51,55	1.23	4 (8%)
70	PC1	Qc	410	-	47,47,53	0.31	0	53,55,61	0.32	0
80	HEM	QC	401	49	41,50,50	1.22	4 (9%)	45,82,82	1.68	7 (15%)
68	CDL	QD	402	-	63,63,99	0.37	0	69,75,111	0.30	0
70	PC1	QI	101	-	53,53,53	0.29	0	59,61,61	0.28	0
71	PEE	C3	303	-	50,50,50	1.33	6 (12%)	53,55,55	1.19	2 (3%)
71	PEE	AL	206	-	39,39,50	1.48	6 (15%)	41,44,55	1.22	2 (4%)
71	PEE	CB	203	-	36,36,50	1.37	5 (13%)	39,41,55	1.19	3 (7%)
85	FMN	V1	502	-	33,33,33	0.23	0	48,50,50	0.45	0
72	3PE	CA	101	-	50,50,50	0.31	0	53,55,55	0.40	0
68	CDL	B4	201	-	61,61,99	0.37	0	67,73,111	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
70	PC1	B5	202	-	53,53,53	0.29	0	59,61,61	0.28	0
68	CDL	Qc	411	-	63,63,99	0.37	0	69,75,111	0.36	0
70	PC1	QB	502	-	50,50,53	0.30	0	56,58,61	0.43	0
70	PC1	B8	201	-	53,53,53	0.30	0	59,61,61	0.26	0
68	CDL	QB	501	-	63,63,99	0.37	0	69,75,111	0.40	0
68	CDL	4L	101	-	91,91,99	0.31	0	97,103,111	0.29	0
70	PC1	Qc	407	-	53,53,53	0.29	0	59,61,61	0.29	0
71	PEE	QC	405	-	42,42,50	1.42	5 (11%)	45,47,55	1.21	3 (6%)
68	CDL	Qc	402	-	60,60,99	0.38	0	66,72,111	0.35	0
71	PEE	A3	201	-	50,50,50	1.32	5 (10%)	53,55,55	1.14	2 (3%)
68	CDL	AL	202	-	81,81,99	0.33	0	87,93,111	0.41	0
84	SF4	S7	301	63	0,12,12	-	-	-	-	-
70	PC1	7C	101	-	41,41,53	0.32	0	47,49,61	0.37	0
71	PEE	C1	609	-	32,32,50	1.39	4 (12%)	35,37,55	1.27	4 (11%)
70	PC1	QB	503	-	31,31,53	0.38	0	37,39,61	0.35	0
81	HEC	QD	401	50	32,50,50	2.04	4 (12%)	24,82,82	2.32	15 (62%)
71	PEE	BL	201	-	50,50,50	1.32	5 (10%)	53,55,55	1.18	2 (3%)
76	PLX	C2	301	-	38,38,51	1.22	3 (7%)	42,46,59	0.85	1 (2%)

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
71	PEE	AN	202	-	-	37/54/54/54	-
70	PC1	N5	705	-	-	11/34/34/57	-
68	CDL	N5	703	-	-	24/110/110/110	-
84	SF4	S8	302	64	-	-	0/6/5/5
68	CDL	AL	201	-	-	21/104/104/110	-
77	HEA	C1	602	35	-	14/32/76/76	-
71	PEE	A7	202	-	-	11/31/31/54	-
70	PC1	C3	301	-	-	15/52/52/57	-
76	PLX	N3	201	-	-	21/55/55/55	-
71	PEE	8B	101	-	-	23/45/45/54	-
74	ZMP	AB	201	19	-	12/40/42/43	-
76	PLX	CB	201	-	-	27/55/55/55	-
76	PLX	S7	302	-	-	21/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	PC1	Qb	501	-	-	11/41/41/57	-
82	FES	S1	803	57	-	-	0/1/1/1
72	3PE	CB	202	-	-	11/49/49/54	-
71	PEE	QC	404	-	-	22/38/38/54	-
84	SF4	S8	301	64	-	-	0/6/5/5
71	PEE	QH	102	-	-	27/54/54/54	-
82	FES	QE	303	51	-	-	0/1/1/1
76	PLX	QE	301	-	-	17/49/49/55	-
72	3PE	7B	101	-	-	15/54/54/54	-
70	PC1	Qh	103	-	-	13/57/57/57	-
68	CDL	A7	201	-	-	25/104/104/110	-
68	CDL	AN	201	-	-	27/91/91/110	-
68	CDL	N4	501	-	-	26/110/110/110	-
72	3PE	Qc	401	-	-	13/47/47/54	-
70	PC1	N6	201	-	-	22/57/57/57	-
71	PEE	Qc	408	-	-	24/51/51/54	-
70	PC1	N1	401	-	-	20/57/57/57	-
71	PEE	N5	706	-	-	20/47/47/54	-
81	HEC	Qd	401	50	-	2/10/54/54	-
82	FES	V2	301	66	-	-	0/1/1/1
68	CDL	AN	203	-	-	26/76/76/110	-
84	SF4	V1	501	65	-	-	0/6/5/5
75	ADP	AK	401	-	-	3/12/32/32	0/3/3/3
73	NDP	A9	401	-	-	5/30/77/77	0/5/5/5
76	PLX	BL	202	-	-	25/55/55/55	-
83	PX2	QH	101	-	-	25/37/37/37	-
71	PEE	Qb	503	-	-	30/54/54/54	-
76	PLX	B1	101	-	-	16/55/55/55	-
68	CDL	AL	204	-	-	24/90/90/110	-
70	PC1	7A	101	-	-	22/57/57/57	-
74	ZMP	AC	201	19	-	19/40/42/43	-
68	CDL	C1	607	-	-	19/87/87/110	-
70	PC1	C4	201	-	-	16/57/57/57	-
84	SF4	S1	802	57	-	-	0/6/5/5
84	SF4	S1	801	57	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	PEE	N5	701	-	-	18/49/49/54	-
71	PEE	6A	103	-	-	29/54/54/54	-
82	FES	Qe	301	51	-	-	0/1/1/1
70	PC1	6A	101	-	-	15/48/48/57	-
70	PC1	C3	304	-	-	12/54/54/57	-
68	CDL	Qb	502	-	-	9/74/74/110	-
71	PEE	Qh	101	-	-	35/54/54/54	-
71	PEE	Qe	302	-	-	30/53/53/54	-
77	HEA	C1	603	35	-	12/32/76/76	-
68	CDL	QC	406	-	-	29/100/100/110	-
72	3PE	Qc	406	-	-	14/51/51/54	-
71	PEE	C3	302	-	-	25/54/54/54	-
72	3PE	C1	601	-	-	11/54/54/54	-
71	PEE	QC	403	-	-	15/43/43/54	-
80	HEM	QC	402	49	-	4/12/54/54	-
70	PC1	C1	610	-	-	10/53/53/57	-
71	PEE	N5	704	-	-	28/54/54/54	-
68	CDL	QC	407	-	-	10/65/65/110	-
70	PC1	QJ	101	-	-	11/57/57/57	-
70	PC1	Qc	409	-	-	11/45/45/57	-
70	PC1	N3	202	-	-	13/57/57/57	-
68	CDL	Qj	101	-	-	29/106/106/110	-
76	PLX	AL	205	-	-	19/50/50/55	-
70	PC1	C1	608	-	-	14/51/51/57	-
70	PC1	N4	502	-	-	20/57/57/57	-
68	CDL	N2	401	-	-	16/78/78/110	-
68	CDL	B5	201	-	-	16/106/106/110	-
71	PEE	AL	203	-	-	25/39/39/54	-
80	HEM	Qc	405	49	-	9/12/54/54	-
71	PEE	Qc	403	-	-	21/45/45/54	-
71	PEE	6A	102	-	-	28/54/54/54	-
71	PEE	S8	303	-	-	22/54/54/54	-
70	PC1	Qd	402	-	-	12/57/57/57	-
80	HEM	Qc	404	49	-	7/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	CDL	A8	301	-	-	22/93/93/110	-
68	CDL	Qh	102	-	-	30/110/110/110	-
70	PC1	C1	606	-	-	16/49/49/57	-
70	PC1	B7	201	-	-	24/57/57/57	-
70	PC1	S8	304	-	-	8/48/48/57	-
68	CDL	N5	702	-	-	26/99/99/110	-
76	PLX	QI	102	-	-	21/55/55/55	-
70	PC1	Qc	412	-	-	13/57/57/57	-
76	PLX	AM	201	-	-	15/55/55/55	-
71	PEE	QE	302	-	-	20/50/50/54	-
70	PC1	Qc	410	-	-	14/51/51/57	-
80	HEM	QC	401	49	-	7/12/54/54	-
68	CDL	QD	402	-	-	19/74/74/110	-
70	PC1	QI	101	-	-	17/57/57/57	-
71	PEE	C3	303	-	-	24/54/54/54	-
71	PEE	AL	206	-	-	23/43/43/54	-
71	PEE	CB	203	-	-	26/40/40/54	-
85	FMN	V1	502	-	-	5/18/18/18	0/3/3/3
72	3PE	CA	101	-	-	11/54/54/54	-
68	CDL	B4	201	-	-	17/72/72/110	-
70	PC1	B5	202	-	-	17/57/57/57	-
68	CDL	Qc	411	-	-	16/74/74/110	-
70	PC1	QB	502	-	-	18/54/54/57	-
70	PC1	B8	201	-	-	17/57/57/57	-
68	CDL	QB	501	-	-	23/74/74/110	-
68	CDL	4L	101	-	-	20/102/102/110	-
70	PC1	Qc	407	-	-	21/57/57/57	-
71	PEE	QC	405	-	-	27/46/46/54	-
68	CDL	Qc	402	-	-	16/71/71/110	-
71	PEE	A3	201	-	-	26/54/54/54	-
68	CDL	AL	202	-	-	21/92/92/110	-
84	SF4	S7	301	63	-	-	0/6/5/5
70	PC1	7C	101	-	-	8/45/45/57	-
71	PEE	C1	609	-	-	24/36/36/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	PC1	QB	503	-	-	17/35/35/57	-
81	HEC	QD	401	50	-	4/10/54/54	-
71	PEE	BL	201	-	-	26/54/54/54	-
76	PLX	C2	301	-	-	16/42/42/55	-

All (234) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	Qd	401	HEC	C3C-C2C	-6.46	1.34	1.40
81	QD	401	HEC	C3C-C2C	-6.42	1.34	1.40
81	QD	401	HEC	C2B-C3B	-6.34	1.34	1.40
81	Qd	401	HEC	C2B-C3B	-6.25	1.34	1.40
77	C1	602	HEA	C3B-C2B	5.06	1.46	1.34
77	C1	603	HEA	C3B-C2B	4.98	1.45	1.34
77	C1	603	HEA	C4B-NB	-4.62	1.32	1.40
77	C1	602	HEA	CHC-C4B	4.52	1.46	1.35
77	C1	602	HEA	C3A-C2A	4.51	1.46	1.40
77	C1	603	HEA	CHC-C4B	4.50	1.46	1.35
77	C1	602	HEA	C3C-C2C	4.15	1.46	1.40
77	C1	603	HEA	C3D-C2D	4.11	1.45	1.36
71	QC	405	PEE	C18-C19	4.09	1.55	1.31
77	C1	603	HEA	C3C-C2C	4.07	1.46	1.40
71	AN	202	PEE	C18-C19	4.06	1.55	1.31
71	C3	302	PEE	C18-C19	4.06	1.55	1.31
71	6A	102	PEE	C18-C19	4.06	1.55	1.31
71	Qh	101	PEE	C18-C19	4.05	1.55	1.31
71	QE	302	PEE	C18-C19	4.05	1.55	1.31
71	CB	203	PEE	C18-C19	4.05	1.55	1.31
71	C3	303	PEE	C18-C19	4.05	1.55	1.31
77	C1	603	HEA	C3A-C2A	4.05	1.46	1.40
71	Qb	503	PEE	C18-C19	4.04	1.55	1.31
71	6A	103	PEE	C18-C19	4.04	1.55	1.31
71	QC	403	PEE	C18-C19	4.04	1.55	1.31
71	S8	303	PEE	C18-C19	4.04	1.55	1.31
71	Qc	408	PEE	C18-C19	4.04	1.55	1.31
71	Qe	302	PEE	C18-C19	4.04	1.55	1.31
71	AL	206	PEE	C18-C19	4.03	1.55	1.31
71	N5	706	PEE	C18-C19	4.03	1.55	1.31
71	N5	701	PEE	C18-C19	4.03	1.55	1.31
71	Qc	403	PEE	C18-C19	4.02	1.55	1.31
77	C1	602	HEA	CHD-C1D	4.02	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	A3	201	PEE	C18-C19	4.02	1.55	1.31
71	QC	404	PEE	C18-C19	4.02	1.55	1.31
71	QH	102	PEE	C18-C19	4.01	1.55	1.31
71	N5	704	PEE	C18-C19	4.01	1.55	1.31
77	C1	603	HEA	C1D-ND	-4.00	1.33	1.40
71	BL	201	PEE	C18-C19	4.00	1.54	1.31
71	QH	102	PEE	C39-C38	3.96	1.54	1.31
71	AL	206	PEE	C39-C38	3.96	1.54	1.31
71	BL	201	PEE	C39-C38	3.95	1.54	1.31
77	C1	602	HEA	C3D-C2D	3.95	1.45	1.36
71	Qh	101	PEE	C39-C38	3.95	1.54	1.31
71	Qb	503	PEE	C39-C38	3.95	1.54	1.31
71	N5	706	PEE	C39-C38	3.95	1.54	1.31
71	6A	103	PEE	C39-C38	3.94	1.54	1.31
71	C3	303	PEE	C39-C38	3.94	1.54	1.31
71	A3	201	PEE	C39-C38	3.94	1.54	1.31
71	AN	202	PEE	C39-C38	3.94	1.54	1.31
71	AL	203	PEE	C39-C38	3.93	1.54	1.31
71	Qc	408	PEE	C39-C38	3.93	1.54	1.31
71	8B	101	PEE	C39-C38	3.93	1.54	1.31
77	C1	602	HEA	C4B-NB	-3.92	1.33	1.40
71	6A	102	PEE	C39-C38	3.92	1.54	1.31
71	N5	701	PEE	C39-C38	3.92	1.54	1.31
71	C3	302	PEE	C39-C38	3.92	1.54	1.31
71	QE	302	PEE	C39-C38	3.92	1.54	1.31
71	S8	303	PEE	C39-C38	3.91	1.54	1.31
71	Qe	302	PEE	C39-C38	3.90	1.54	1.31
80	QC	402	HEM	C4D-ND	-3.90	1.33	1.40
77	C1	603	HEA	CHD-C1D	3.90	1.45	1.35
71	N5	704	PEE	C39-C38	3.89	1.54	1.31
71	QC	405	PEE	C39-C38	3.85	1.54	1.28
80	Qc	405	HEM	C4D-ND	-3.78	1.33	1.40
80	QC	401	HEM	C4D-ND	-3.67	1.34	1.40
80	Qc	404	HEM	C4D-ND	-3.65	1.34	1.40
77	C1	602	HEA	C1D-ND	-3.64	1.34	1.40
71	C1	609	PEE	C18-C19	3.41	1.55	1.29
81	QD	401	HEC	CBC-CAC	-3.37	1.36	1.49
81	Qd	401	HEC	CBC-CAC	-3.35	1.36	1.49
71	AN	202	PEE	O3-C30	3.26	1.42	1.33
71	Qb	503	PEE	O3-C30	3.26	1.42	1.33
71	A7	202	PEE	O3-C30	3.25	1.42	1.33
71	A3	201	PEE	O3-C30	3.25	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	AL	203	PEE	O3-C30	3.25	1.42	1.33
71	QH	102	PEE	O3-C30	3.24	1.42	1.33
80	QC	402	HEM	C1B-NB	-3.24	1.34	1.40
71	CB	203	PEE	O3-C30	3.24	1.42	1.33
80	Qc	405	HEM	C1B-NB	-3.24	1.34	1.40
71	6A	102	PEE	O3-C30	3.24	1.42	1.33
71	AL	206	PEE	O3-C30	3.24	1.42	1.33
71	Qc	408	PEE	O3-C30	3.23	1.42	1.33
71	QC	405	PEE	O3-C30	3.23	1.42	1.33
71	QC	403	PEE	O3-C30	3.23	1.42	1.33
71	C3	303	PEE	O3-C30	3.22	1.42	1.33
71	N5	706	PEE	O3-C30	3.22	1.42	1.33
71	8B	101	PEE	O3-C30	3.21	1.42	1.33
71	BL	201	PEE	O3-C30	3.21	1.42	1.33
71	Qe	302	PEE	O3-C30	3.21	1.42	1.33
71	Qc	403	PEE	O3-C30	3.21	1.42	1.33
71	N5	704	PEE	O3-C30	3.20	1.42	1.33
71	QC	404	PEE	O3-C30	3.19	1.42	1.33
71	6A	103	PEE	O3-C30	3.19	1.42	1.33
71	QE	302	PEE	O3-C30	3.18	1.42	1.33
71	Qh	101	PEE	O3-C30	3.18	1.42	1.33
71	S8	303	PEE	O3-C30	3.16	1.42	1.33
71	C3	302	PEE	O3-C30	3.16	1.42	1.33
71	C1	609	PEE	O3-C30	3.12	1.42	1.33
71	N5	701	PEE	O3-C30	3.11	1.42	1.33
76	CB	201	PLX	O6-C4	-3.06	1.40	1.44
80	Qc	404	HEM	C1B-NB	-3.05	1.35	1.40
80	QC	401	HEM	C1B-NB	-3.04	1.35	1.40
76	BL	202	PLX	O6-C4	-3.02	1.40	1.44
77	C1	602	HEA	C1B-NB	-2.98	1.32	1.38
76	S7	302	PLX	O6-C4	-2.97	1.40	1.44
76	QE	301	PLX	O6-C4	-2.96	1.40	1.44
76	AM	201	PLX	O6-C4	-2.96	1.40	1.44
76	B1	101	PLX	O6-C4	-2.95	1.40	1.44
71	C3	302	PEE	O2-C10	2.95	1.42	1.34
76	AL	205	PLX	O6-C4	-2.95	1.40	1.44
76	C2	301	PLX	O6-C4	-2.91	1.40	1.44
76	N3	201	PLX	O6-C4	-2.90	1.40	1.44
71	6A	103	PEE	O2-C10	2.80	1.42	1.34
71	CB	203	PEE	O2-C10	2.79	1.42	1.34
71	AL	206	PEE	O2-C10	2.78	1.42	1.34
77	C1	603	HEA	CAA-C2A	-2.78	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	Qb	503	PEE	O2-C10	2.77	1.42	1.34
77	C1	603	HEA	C1B-NB	-2.75	1.33	1.38
77	C1	603	HEA	FE-ND	2.74	2.10	1.96
71	8B	101	PEE	O2-C10	2.72	1.42	1.34
71	S8	303	PEE	O2-C10	2.72	1.42	1.34
71	C3	303	PEE	O2-C10	2.70	1.41	1.34
71	Qc	408	PEE	O2-C10	2.67	1.41	1.34
71	6A	102	PEE	O2-C10	2.67	1.41	1.34
71	AL	203	PEE	O2-C10	2.66	1.41	1.34
77	C1	602	HEA	FE-ND	2.64	2.09	1.96
71	AN	202	PEE	O2-C10	2.64	1.41	1.34
71	Qe	302	PEE	O2-C10	2.64	1.41	1.34
71	QC	404	PEE	O2-C10	2.64	1.41	1.34
71	N5	701	PEE	O2-C10	2.63	1.41	1.34
80	Qc	405	HEM	C1D-ND	-2.63	1.33	1.38
71	QE	302	PEE	O2-C10	2.62	1.41	1.34
71	N5	706	PEE	O2-C10	2.61	1.41	1.34
71	Qh	101	PEE	O2-C10	2.61	1.41	1.34
71	A3	201	PEE	O2-C10	2.60	1.41	1.34
71	N5	704	PEE	O2-C10	2.60	1.41	1.34
71	A7	202	PEE	O2-C10	2.60	1.41	1.34
71	C1	609	PEE	O2-C10	2.60	1.41	1.34
71	QC	405	PEE	O2-C10	2.58	1.41	1.34
71	BL	201	PEE	O2-C10	2.58	1.41	1.34
71	QH	102	PEE	O2-C10	2.58	1.41	1.34
71	Qc	403	PEE	O2-C2	-2.57	1.40	1.46
71	C1	609	PEE	O2-C2	-2.55	1.40	1.46
71	QC	403	PEE	O2-C2	-2.55	1.40	1.46
71	A3	201	PEE	O2-C2	-2.54	1.40	1.46
80	QC	402	HEM	C1D-ND	-2.54	1.33	1.38
71	QC	403	PEE	O2-C10	2.53	1.41	1.34
71	QC	404	PEE	O2-C2	-2.53	1.40	1.46
76	QI	102	PLX	O6-C4	-2.52	1.41	1.44
71	QC	405	PEE	O2-C2	-2.52	1.40	1.46
71	Qc	403	PEE	O2-C10	2.52	1.41	1.34
80	QC	401	HEM	C1D-ND	-2.51	1.33	1.38
71	N5	704	PEE	O2-C2	-2.51	1.40	1.46
71	N5	706	PEE	O2-C2	-2.51	1.40	1.46
71	Qh	101	PEE	O2-C2	-2.51	1.40	1.46
80	Qc	404	HEM	C1D-ND	-2.51	1.33	1.38
77	C1	602	HEA	CAA-C2A	-2.50	1.47	1.52
71	A7	202	PEE	O2-C2	-2.50	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	AC	201	ZMP	C9-C10	-2.49	1.48	1.50
71	BL	201	PEE	O2-C2	-2.49	1.40	1.46
71	QH	102	PEE	O2-C2	-2.48	1.40	1.46
71	Qe	302	PEE	O2-C2	-2.48	1.40	1.46
71	QE	302	PEE	O2-C2	-2.48	1.40	1.46
71	Qc	408	PEE	O2-C2	-2.48	1.40	1.46
77	C1	603	HEA	FE-NB	2.47	2.09	1.96
74	AB	201	ZMP	C9-C10	-2.47	1.48	1.50
71	6A	102	PEE	O2-C2	-2.47	1.40	1.46
77	C1	602	HEA	FE-NB	2.47	2.09	1.96
71	AL	203	PEE	O2-C2	-2.46	1.40	1.46
71	C3	303	PEE	O2-C2	-2.46	1.40	1.46
71	AN	202	PEE	O2-C2	-2.46	1.40	1.46
77	C1	603	HEA	O2A-CGA	-2.45	1.22	1.30
71	N5	701	PEE	O2-C2	-2.45	1.40	1.46
77	C1	603	HEA	O2D-CGD	-2.44	1.22	1.30
77	C1	602	HEA	C4D-ND	-2.40	1.33	1.38
77	C1	602	HEA	O2D-CGD	-2.40	1.22	1.30
77	C1	602	HEA	O2A-CGA	-2.39	1.22	1.30
75	AK	401	ADP	C5-C4	2.37	1.47	1.40
81	QD	401	HEC	CBB-CAB	-2.35	1.40	1.49
81	Qd	401	HEC	CBB-CAB	-2.33	1.40	1.49
83	QH	101	PX2	O5-C4	2.33	1.40	1.33
77	C1	602	HEA	C4B-C3B	2.32	1.48	1.44
77	C1	603	HEA	C4B-C3B	2.28	1.48	1.44
76	QE	301	PLX	C1B-N1	-2.25	1.43	1.50
83	QH	101	PX2	O7-C2	-2.25	1.41	1.46
71	S8	303	PEE	O2-C2	-2.25	1.41	1.46
76	QI	102	PLX	C1B-N1	-2.22	1.43	1.50
76	B1	101	PLX	C1B-N1	-2.22	1.43	1.50
76	AL	205	PLX	C1B-N1	-2.21	1.43	1.50
76	S7	302	PLX	C1B-N1	-2.21	1.43	1.50
71	Qb	503	PEE	O2-C2	-2.20	1.41	1.46
83	QH	101	PX2	O7-C16	2.18	1.40	1.34
71	6A	103	PEE	O2-C2	-2.17	1.41	1.46
76	QE	301	PLX	C1A-N1	-2.17	1.43	1.50
76	N3	201	PLX	C1B-N1	-2.16	1.43	1.50
76	BL	202	PLX	C1B-N1	-2.16	1.43	1.50
71	CB	203	PEE	O2-C2	-2.16	1.41	1.46
76	QI	102	PLX	C1A-N1	-2.16	1.43	1.50
76	C2	301	PLX	C1B-N1	-2.16	1.43	1.50
76	CB	201	PLX	C1B-N1	-2.15	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	BL	202	PLX	C1A-N1	-2.15	1.43	1.50
83	QH	101	PX2	O5-C3	-2.15	1.40	1.45
71	AL	206	PEE	O2-C2	-2.14	1.41	1.46
76	CB	201	PLX	C1A-N1	-2.13	1.43	1.50
71	8B	101	PEE	C11-C10	2.12	1.56	1.50
76	AM	201	PLX	C1B-N1	-2.11	1.43	1.50
80	QC	402	HEM	CHB-C1B	2.10	1.40	1.35
76	S7	302	PLX	C1A-N1	-2.09	1.43	1.50
76	AM	201	PLX	P1-O4	2.08	1.67	1.59
71	C3	302	PEE	O2-C2	-2.08	1.41	1.46
77	C1	603	HEA	C1C-CHC	2.07	1.46	1.41
80	Qc	404	HEM	CHB-C1B	2.06	1.40	1.35
76	AL	205	PLX	C1A-N1	-2.06	1.44	1.50
71	CB	203	PEE	C11-C10	2.06	1.56	1.50
76	B1	101	PLX	C1A-N1	-2.06	1.44	1.50
76	C2	301	PLX	C1A-N1	-2.04	1.44	1.50
76	N3	201	PLX	P1-O4	2.04	1.67	1.59
76	B1	101	PLX	P1-O4	2.04	1.67	1.59
80	QC	401	HEM	CHB-C1B	2.04	1.40	1.35
71	8B	101	PEE	O2-C2	-2.03	1.41	1.46
71	AL	206	PEE	C11-C10	2.03	1.56	1.50
76	QE	301	PLX	C7-C6	2.03	1.55	1.50
76	N3	201	PLX	C1A-N1	-2.03	1.44	1.50
71	C3	303	PEE	C11-C10	2.03	1.56	1.50
76	AM	201	PLX	C1A-N1	-2.03	1.44	1.50
76	AL	205	PLX	P1-O4	2.02	1.67	1.59
80	QC	402	HEM	C4B-NB	-2.02	1.34	1.38
76	CB	201	PLX	P1-O3	-2.02	1.45	1.55
76	BL	202	PLX	P1-O3	-2.01	1.45	1.55
76	BL	202	PLX	C7-C6	2.01	1.55	1.50
76	QE	301	PLX	P1-O4	2.00	1.67	1.59
76	BL	202	PLX	P1-O4	2.00	1.67	1.59
76	QI	102	PLX	P1-O4	2.00	1.67	1.59

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	C1	603	HEA	CAD-CBD-CGD	-8.35	95.62	113.60
77	C1	602	HEA	CAD-CBD-CGD	-7.94	96.52	113.60
77	C1	603	HEA	C3D-C4D-ND	5.43	115.61	110.36
77	C1	602	HEA	C3D-C4D-ND	5.27	115.46	110.36
77	C1	603	HEA	CHB-C1B-C2B	-5.20	116.86	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	C1	602	HEA	C13-C12-C11	-5.02	106.81	114.35
77	C1	602	HEA	C2B-C1B-NB	4.98	115.84	109.88
77	C1	603	HEA	CAA-CBA-CGA	-4.89	100.04	113.76
77	C1	602	HEA	CHB-C1B-C2B	-4.87	117.37	124.98
80	Qc	404	HEM	CHC-C4B-NB	4.77	129.62	124.43
80	QC	401	HEM	CHC-C4B-NB	4.76	129.60	124.43
77	C1	602	HEA	C2D-C1D-ND	4.74	115.46	109.84
77	C1	603	HEA	C2D-C1D-ND	4.73	115.44	109.84
77	C1	603	HEA	C2B-C1B-NB	4.69	115.50	109.88
80	QC	402	HEM	C4D-ND-C1D	4.68	109.91	105.07
71	8B	101	PEE	O2-C10-C11	4.55	121.31	111.50
77	C1	602	HEA	C1D-C2D-C3D	-4.55	102.18	106.96
77	C1	603	HEA	C13-C12-C11	-4.54	107.53	114.35
77	C1	603	HEA	C1D-C2D-C3D	-4.38	102.35	106.96
77	C1	603	HEA	C3B-C4B-NB	4.34	114.98	109.84
71	C3	303	PEE	O2-C10-C11	4.33	120.84	111.50
71	QE	302	PEE	O2-C10-C11	4.33	120.83	111.50
71	AL	206	PEE	O2-C10-C11	4.31	120.79	111.50
77	C1	603	HEA	C3C-C4C-NC	4.30	114.77	109.21
80	Qc	405	HEM	CHC-C4B-NB	4.27	129.07	124.43
71	Qe	302	PEE	O2-C10-C11	4.25	120.67	111.50
81	QD	401	HEC	CMD-C2D-C1D	-4.23	121.97	128.46
71	QC	404	PEE	O2-C10-C11	4.22	120.59	111.50
83	QH	101	PX2	O7-C16-C17	4.20	120.56	111.50
71	CB	203	PEE	O2-C10-C11	4.19	120.52	111.50
71	6A	103	PEE	O2-C10-C11	4.17	120.48	111.50
77	C1	602	HEA	C3C-C4C-NC	4.16	114.59	109.21
71	BL	201	PEE	O2-C10-C11	4.16	120.47	111.50
81	Qd	401	HEC	CMD-C2D-C1D	-4.14	122.11	128.46
71	QC	403	PEE	O2-C10-C11	4.04	120.22	111.50
71	C1	609	PEE	O2-C10-C11	4.04	120.20	111.50
77	C1	602	HEA	C3B-C4B-NB	4.04	114.62	109.84
77	C1	602	HEA	CAA-CBA-CGA	-4.03	102.46	113.76
71	QH	102	PEE	O2-C10-C11	4.03	120.19	111.50
71	N5	701	PEE	O2-C10-C11	4.00	120.12	111.50
80	Qc	405	HEM	C4D-ND-C1D	4.00	109.20	105.07
71	S8	303	PEE	O2-C10-C11	3.99	120.10	111.50
71	AN	202	PEE	O2-C10-C11	3.97	120.06	111.50
71	Qc	408	PEE	O2-C10-C11	3.92	119.96	111.50
71	N5	706	PEE	O2-C10-C11	3.92	119.95	111.50
71	Qc	403	PEE	O2-C10-C11	3.90	119.92	111.50
80	QC	401	HEM	CHB-C1B-NB	3.90	129.19	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
71	6A	102	PEE	O2-C10-C11	3.89	119.89	111.50
80	QC	402	HEM	C1B-NB-C4B	3.87	109.07	105.07
71	N5	704	PEE	O2-C10-C11	3.86	119.83	111.50
71	QC	405	PEE	O2-C10-C11	3.85	119.81	111.50
71	Qh	101	PEE	O2-C10-C11	3.85	119.80	111.50
80	QC	402	HEM	CHC-C4B-NB	3.83	128.59	124.43
71	A7	202	PEE	O2-C10-C11	3.81	119.72	111.50
71	A3	201	PEE	O2-C10-C11	3.80	119.70	111.50
80	Qc	404	HEM	CHB-C1B-NB	3.77	129.04	124.38
77	C1	603	HEA	C4B-C3B-C2B	-3.67	101.14	107.41
71	Qb	503	PEE	O2-C10-C11	3.67	119.41	111.50
80	Qc	405	HEM	CHB-C1B-NB	3.66	128.90	124.38
77	C1	602	HEA	C4B-C3B-C2B	-3.64	101.19	107.41
81	Qd	401	HEC	CMB-C2B-C3B	3.55	129.99	125.82
81	Qd	401	HEC	CMB-C2B-C1B	-3.51	123.08	128.46
77	C1	602	HEA	CMC-C2C-C3C	3.48	131.18	124.68
75	AK	401	ADP	PA-O3A-PB	-3.45	120.99	132.83
81	QD	401	HEC	CMB-C2B-C3B	3.44	129.87	125.82
81	QD	401	HEC	CMB-C2B-C1B	-3.42	123.21	128.46
80	QC	402	HEM	CHB-C1B-NB	3.39	128.57	124.38
71	AL	203	PEE	O2-C10-C11	3.37	120.19	110.80
81	Qd	401	HEC	CMC-C2C-C3C	3.36	129.77	125.82
80	Qc	404	HEM	C4D-ND-C1D	3.34	108.52	105.07
80	QC	401	HEM	C4D-ND-C1D	3.32	108.50	105.07
81	QD	401	HEC	CMC-C2C-C3C	3.30	129.70	125.82
75	AK	401	ADP	N3-C2-N1	-3.26	123.58	128.68
77	C1	602	HEA	CHA-C4D-C3D	-3.22	120.11	124.84
71	C3	302	PEE	O2-C10-C11	3.21	118.42	111.50
77	C1	603	HEA	CMC-C2C-C3C	3.21	130.68	124.68
80	Qc	405	HEM	C1B-NB-C4B	3.18	108.36	105.07
80	QC	401	HEM	C1B-NB-C4B	3.16	108.33	105.07
77	C1	603	HEA	CHA-C4D-C3D	-3.15	120.20	124.84
80	Qc	404	HEM	C1B-NB-C4B	3.15	108.32	105.07
77	C1	602	HEA	C27-C19-C20	3.05	120.40	115.27
81	QD	401	HEC	CBD-CAD-C3D	2.95	117.66	112.62
81	QD	401	HEC	C4C-C3C-C2C	2.95	109.54	106.35
77	C1	603	HEA	CHB-C1B-NB	2.95	127.63	124.43
77	C1	602	HEA	C13-C14-C15	-2.94	120.59	127.66
77	C1	603	HEA	C27-C19-C20	2.91	120.16	115.27
81	Qd	401	HEC	C4C-C3C-C2C	2.87	109.45	106.35
80	QC	401	HEM	CHA-C4D-ND	2.84	127.89	124.38
80	Qc	404	HEM	CHA-C4D-ND	2.81	127.86	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	Qd	401	HEC	O1D-CGD-CBD	-2.79	114.13	123.08
71	AL	206	PEE	O3-C30-C31	2.77	120.61	111.91
71	QE	302	PEE	O3-C30-C31	2.76	120.58	111.91
71	Qc	403	PEE	O3-C30-C31	2.76	120.58	111.91
81	Qd	401	HEC	CMC-C2C-C1C	-2.75	124.23	128.46
81	QD	401	HEC	O1D-CGD-CBD	-2.75	114.24	123.08
77	C1	602	HEA	C17-C18-C19	-2.74	121.06	127.66
71	N5	704	PEE	O3-C30-C31	2.74	120.50	111.91
71	S8	303	PEE	O3-C30-C31	2.71	120.42	111.91
71	C3	303	PEE	O3-C30-C31	2.69	120.36	111.91
71	C1	609	PEE	C17-C18-C19	-2.69	109.66	131.07
77	C1	602	HEA	CMB-C2B-C1B	-2.69	120.94	125.04
71	N5	701	PEE	O3-C30-C31	2.69	120.34	111.91
71	QH	102	PEE	O3-C30-C31	2.67	120.30	111.91
77	C1	603	HEA	C13-C14-C15	-2.66	121.25	127.66
80	QC	401	HEM	CHD-C1D-ND	2.66	127.32	124.43
83	QH	101	PX2	O5-C4-C5	2.65	120.22	111.91
71	N5	706	PEE	O3-C30-C31	2.65	120.21	111.91
77	C1	602	HEA	C26-C15-C16	2.64	119.71	115.27
71	CB	203	PEE	O3-C30-C31	2.64	120.18	111.91
71	QC	403	PEE	O3-C30-C31	2.62	120.13	111.91
75	AK	401	ADP	C4-C5-N7	-2.62	106.67	109.40
81	Qd	401	HEC	CMA-C3A-C2A	2.61	129.87	124.94
71	QC	405	PEE	O3-C30-C31	2.60	120.07	111.91
77	C1	603	HEA	C17-C18-C19	-2.60	121.40	127.66
80	Qc	404	HEM	CHD-C1D-ND	2.58	127.23	124.43
80	Qc	405	HEM	CHA-C4D-ND	2.58	127.56	124.38
80	Qc	405	HEM	CHD-C1D-ND	2.57	127.23	124.43
71	AN	202	PEE	O3-C30-C31	2.57	119.97	111.91
71	C1	609	PEE	O3-C30-C31	2.57	119.96	111.91
71	A7	202	PEE	O3-C30-C31	2.56	119.94	111.91
71	8B	101	PEE	O3-C30-C31	2.55	119.92	111.91
75	AK	401	ADP	C3'-C2'-C1'	2.55	104.81	100.98
71	C3	302	PEE	O3-C30-C31	2.54	119.87	111.91
71	Qe	302	PEE	O3-C30-C31	2.54	119.87	111.91
71	QC	404	PEE	O3-C30-C31	2.54	119.87	111.91
71	QC	405	PEE	C37-C38-C39	-2.54	109.59	126.84
81	Qd	401	HEC	CBD-CAD-C3D	2.53	116.94	112.62
71	A3	201	PEE	O3-C30-C31	2.53	119.86	111.91
81	QD	401	HEC	CMC-C2C-C1C	-2.52	124.59	128.46
71	Qh	101	PEE	O3-C30-C31	2.50	119.75	111.91
80	QC	402	HEM	CHA-C4D-ND	2.50	127.47	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
71	AL	203	PEE	O3-C30-C31	2.49	119.73	111.91
71	6A	102	PEE	O3-C30-C31	2.48	119.68	111.91
81	QD	401	HEC	CMD-C2D-C3D	2.47	129.60	124.94
71	Qb	503	PEE	O3-C30-C31	2.46	119.63	111.91
77	C1	602	HEA	CBA-CAA-C2A	-2.42	108.52	112.60
71	BL	201	PEE	O3-C30-C31	2.41	119.48	111.91
77	C1	603	HEA	C4D-C3D-C2D	-2.40	103.39	106.90
77	C1	602	HEA	CMB-C2B-C3B	2.40	134.91	130.34
74	AB	201	ZMP	C15-C14-C13	-2.39	108.38	112.36
81	QD	401	HEC	O1A-CGA-CBA	-2.35	115.53	123.08
71	6A	103	PEE	O3-C30-C31	2.34	119.24	111.91
81	Qd	401	HEC	CMD-C2D-C3D	2.33	129.34	124.94
71	Qc	408	PEE	O3-C30-C31	2.32	119.19	111.91
68	AL	204	CDL	OA8-CA6-CA4	2.32	115.19	108.43
77	C1	603	HEA	O1D-CGD-CBD	-2.32	115.64	123.08
80	Qc	405	HEM	CAD-CBD-CGD	-2.30	108.66	113.60
77	C1	603	HEA	OMA-CMA-C3A	-2.29	119.92	124.91
80	QC	401	HEM	CHB-C1B-C2B	-2.28	120.41	126.72
76	B1	101	PLX	O3-P1-O2	-2.28	100.97	112.24
73	A9	401	NDP	C5A-C6A-N6A	2.27	123.81	120.35
77	C1	603	HEA	C1B-C2B-C3B	-2.27	104.08	106.80
76	QI	102	PLX	O3-P1-O2	-2.27	101.03	112.24
76	N3	201	PLX	O3-P1-O2	-2.26	101.08	112.24
77	C1	602	HEA	CHC-C4B-NB	-2.26	121.59	124.38
77	C1	603	HEA	CMB-C2B-C1B	-2.25	121.61	125.04
76	AM	201	PLX	O3-P1-O2	-2.25	101.12	112.24
76	QE	301	PLX	O3-P1-O2	-2.25	101.13	112.24
81	Qd	401	HEC	C1D-C2D-C3D	2.24	108.56	107.00
77	C1	602	HEA	C4D-C3D-C2D	-2.24	103.64	106.90
76	BL	202	PLX	O3-P1-O2	-2.24	101.18	112.24
76	AL	205	PLX	O3-P1-O2	-2.23	101.21	112.24
80	Qc	405	HEM	CHB-C1B-C2B	-2.22	120.58	126.72
76	C2	301	PLX	O3-P1-O2	-2.22	101.27	112.24
77	C1	602	HEA	C1B-C2B-C3B	-2.22	104.15	106.80
81	QD	401	HEC	CMA-C3A-C2A	2.21	129.11	124.94
76	CB	201	PLX	O3-P1-O2	-2.21	101.33	112.24
80	Qc	404	HEM	CHB-C1B-C2B	-2.19	120.66	126.72
77	C1	602	HEA	OMA-CMA-C3A	-2.19	120.14	124.91
76	S7	302	PLX	O3-P1-O2	-2.19	101.44	112.24
81	QD	401	HEC	O2A-CGA-O1A	2.18	128.74	123.30
81	QD	401	HEC	CBA-CAA-C2A	2.17	116.26	112.60
77	C1	602	HEA	CHB-C1B-NB	2.17	126.78	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	QD	401	HEC	C2B-C3B-C4B	2.17	108.69	106.35
81	Qd	401	HEC	O1A-CGA-CBA	-2.16	116.14	123.08
77	C1	602	HEA	C27-C19-C18	-2.14	118.18	123.68
77	C1	603	HEA	CAD-C3D-C2D	2.12	131.83	127.88
77	C1	603	HEA	C26-C15-C16	2.12	118.84	115.27
81	Qd	401	HEC	O2A-CGA-O1A	2.11	128.57	123.30
77	C1	603	HEA	C4D-CHA-C1A	2.11	125.34	122.56
80	QC	402	HEM	CAD-CBD-CGD	-2.10	109.08	113.60
71	S8	303	PEE	C37-C38-C39	-2.09	108.71	124.73
77	C1	603	HEA	CMB-C2B-C3B	2.08	134.31	130.34
71	Qc	408	PEE	C20-C19-C18	-2.07	108.86	124.73
71	Qe	302	PEE	C17-C18-C19	-2.06	108.91	124.73
81	QD	401	HEC	C1D-C2D-C3D	2.06	108.43	107.00
71	Qc	408	PEE	C17-C18-C19	-2.05	108.99	124.73
71	6A	102	PEE	C40-C39-C38	-2.05	109.00	124.73
71	N5	706	PEE	C37-C38-C39	-2.04	109.06	124.73
80	QC	402	HEM	C3C-C4C-NC	-2.04	107.09	110.94
71	6A	103	PEE	C20-C19-C18	-2.04	109.09	124.73
77	C1	602	HEA	CMD-C2D-C1D	2.04	128.14	125.04
71	QE	302	PEE	C40-C39-C38	-2.04	109.10	124.73
80	Qc	405	HEM	CMC-C2C-C3C	2.04	128.49	124.68
80	QC	402	HEM	CHD-C1D-ND	2.04	126.64	124.43
71	Qh	101	PEE	C17-C18-C19	-2.03	109.16	124.73
71	QH	102	PEE	C20-C19-C18	-2.02	109.21	124.73
71	6A	103	PEE	C37-C38-C39	-2.02	109.24	124.73
77	C1	603	HEA	CHC-C4B-NB	-2.01	121.89	124.38
71	AL	203	PEE	C37-C38-C39	-2.01	109.29	124.73
71	N5	704	PEE	C37-C38-C39	-2.01	109.30	124.73
81	Qd	401	HEC	C2B-C3B-C4B	2.01	108.52	106.35
71	C1	609	PEE	C20-C19-C18	-2.01	109.80	126.37
71	QE	302	PEE	C20-C19-C18	-2.01	109.33	124.73
71	QC	404	PEE	C17-C18-C19	-2.01	109.34	124.73
71	C3	302	PEE	C40-C39-C38	-2.00	109.36	124.73
71	CB	203	PEE	C20-C19-C18	-2.00	109.36	124.73
77	C1	603	HEA	O1A-CGA-CBA	-2.00	116.65	123.08

There are no chirality outliers.

All (2016) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
68	4L	101	CDL	CA2-OA2-PA1-OA3
68	4L	101	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
68	4L	101	CDL	CA2-OA2-PA1-OA5
68	4L	101	CDL	CB3-OB5-PB2-OB3
68	A7	201	CDL	CA2-OA2-PA1-OA3
68	A7	201	CDL	CA2-OA2-PA1-OA4
68	A7	201	CDL	CA2-OA2-PA1-OA5
68	A7	201	CDL	CA3-OA5-PA1-OA3
68	A7	201	CDL	CB2-OB2-PB2-OB3
68	A7	201	CDL	CB3-OB5-PB2-OB2
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-OA4
68	AL	201	CDL	CA2-OA2-PA1-OA3
68	AL	201	CDL	CA2-OA2-PA1-OA4
68	AL	201	CDL	CA2-OA2-PA1-OA5
68	AL	201	CDL	CA3-OA5-PA1-OA2
68	AL	201	CDL	CA3-OA5-PA1-OA3
68	AL	201	CDL	CA3-OA5-PA1-OA4
68	AL	201	CDL	C1-CB2-OB2-PB2
68	AL	201	CDL	CB3-OB5-PB2-OB2
68	AL	201	CDL	CB3-OB5-PB2-OB3
68	AL	201	CDL	CB3-OB5-PB2-OB4
68	AL	202	CDL	CA3-OA5-PA1-OA3
68	AL	202	CDL	CA3-OA5-PA1-OA4
68	AL	204	CDL	CA2-OA2-PA1-OA3
68	AL	204	CDL	CA2-OA2-PA1-OA4
68	AL	204	CDL	CA2-OA2-PA1-OA5
68	AL	204	CDL	CB2-OB2-PB2-OB3
68	AL	204	CDL	CB2-OB2-PB2-OB4
68	AL	204	CDL	CB2-OB2-PB2-OB5
68	AL	204	CDL	OB5-CB3-CB4-OB6
68	AN	201	CDL	CA2-C1-CB2-OB2
68	AN	201	CDL	CA3-OA5-PA1-OA3
68	AN	201	CDL	CB3-OB5-PB2-OB4
68	AN	203	CDL	CA2-OA2-PA1-OA3
68	AN	203	CDL	CA3-OA5-PA1-OA2
68	AN	203	CDL	CA3-OA5-PA1-OA3
68	AN	203	CDL	CA3-OA5-PA1-OA4
68	AN	203	CDL	CB2-OB2-PB2-OB4
68	AN	203	CDL	CB4-CB3-OB5-PB2
68	B4	201	CDL	CA2-OA2-PA1-OA3
68	B4	201	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
68	B5	201	CDL	CA2-OA2-PA1-OA3
68	C1	607	CDL	CB2-OB2-PB2-OB3
68	C1	607	CDL	CB2-OB2-PB2-OB4
68	C1	607	CDL	CB3-OB5-PB2-OB3
68	N2	401	CDL	CA2-OA2-PA1-OA3
68	N2	401	CDL	CA2-OA2-PA1-OA4
68	N2	401	CDL	CB2-OB2-PB2-OB4
68	N4	501	CDL	CA2-OA2-PA1-OA3
68	N4	501	CDL	CA3-OA5-PA1-OA3
68	N4	501	CDL	CA3-OA5-PA1-OA4
68	N4	501	CDL	CB3-OB5-PB2-OB2
68	N5	702	CDL	O1-C1-CB2-OB2
68	N5	702	CDL	CA2-OA2-PA1-OA3
68	N5	702	CDL	CA2-OA2-PA1-OA4
68	N5	702	CDL	CA2-OA2-PA1-OA5
68	N5	702	CDL	CA3-OA5-PA1-OA3
68	N5	702	CDL	CB3-OB5-PB2-OB3
68	N5	703	CDL	CB2-OB2-PB2-OB3
68	N5	703	CDL	CB2-OB2-PB2-OB4
68	N5	703	CDL	CB3-OB5-PB2-OB3
68	QB	501	CDL	CA2-OA2-PA1-OA3
68	QB	501	CDL	CA2-OA2-PA1-OA4
68	QB	501	CDL	CA2-OA2-PA1-OA5
68	QB	501	CDL	CA3-OA5-PA1-OA2
68	QB	501	CDL	CA3-OA5-PA1-OA3
68	QB	501	CDL	CA3-OA5-PA1-OA4
68	QB	501	CDL	CB3-OB5-PB2-OB3
68	QC	406	CDL	CB2-OB2-PB2-OB3
68	QC	406	CDL	CB3-OB5-PB2-OB3
68	QC	406	CDL	CB3-OB5-PB2-OB4
68	QC	407	CDL	CA2-OA2-PA1-OA4
68	QD	402	CDL	CA2-OA2-PA1-OA3
68	QD	402	CDL	CA3-OA5-PA1-OA3
68	QD	402	CDL	CB3-OB5-PB2-OB2
68	QD	402	CDL	CB3-OB5-PB2-OB3
68	QD	402	CDL	CB3-OB5-PB2-OB4
68	Qb	502	CDL	CA3-OA5-PA1-OA4
68	Qc	402	CDL	CA2-OA2-PA1-OA3
68	Qc	402	CDL	CA2-OA2-PA1-OA4
68	Qc	402	CDL	CA2-OA2-PA1-OA5
68	Qc	402	CDL	CB2-OB2-PB2-OB3
68	Qc	402	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
68	Qc	402	CDL	CB2-OB2-PB2-OB5
68	Qc	402	CDL	CB3-OB5-PB2-OB4
68	Qc	411	CDL	CA3-OA5-PA1-OA3
68	Qc	411	CDL	CB2-OB2-PB2-OB3
68	Qh	102	CDL	CA3-OA5-PA1-OA2
68	Qh	102	CDL	CA3-OA5-PA1-OA3
68	Qh	102	CDL	CA3-OA5-PA1-OA4
68	Qh	102	CDL	CB2-OB2-PB2-OB3
68	Qj	101	CDL	CA3-OA5-PA1-OA2
68	Qj	101	CDL	CA3-OA5-PA1-OA3
68	Qj	101	CDL	CA3-OA5-PA1-OA4
68	Qj	101	CDL	CB2-OB2-PB2-OB3
68	Qj	101	CDL	CB3-OB5-PB2-OB4
70	6A	101	PC1	C11-O13-P-O14
70	6A	101	PC1	C1-O11-P-O13
70	7A	101	PC1	C11-O13-P-O12
70	7A	101	PC1	C11-O13-P-O14
70	7A	101	PC1	C1-O11-P-O12
70	7A	101	PC1	C2-C1-O11-P
70	B5	202	PC1	C11-O13-P-O12
70	B5	202	PC1	C11-O13-P-O14
70	B7	201	PC1	C11-O13-P-O12
70	B7	201	PC1	C11-O13-P-O14
70	B7	201	PC1	C11-O13-P-O11
70	B7	201	PC1	C1-O11-P-O14
70	B8	201	PC1	C11-O13-P-O14
70	C1	606	PC1	C11-O13-P-O14
70	C1	606	PC1	C1-O11-P-O14
70	C1	606	PC1	C1-O11-P-O13
70	C1	608	PC1	C11-O13-P-O12
70	C1	608	PC1	C11-O13-P-O14
70	C1	610	PC1	C11-O13-P-O12
70	C1	610	PC1	C11-O13-P-O14
70	C1	610	PC1	C11-O13-P-O11
70	C3	301	PC1	C11-O13-P-O14
70	C3	301	PC1	C1-O11-P-O13
70	C3	304	PC1	C1-O11-P-O14
70	C4	201	PC1	C11-O13-P-O12
70	N1	401	PC1	C1-O11-P-O12
70	N1	401	PC1	O13-C11-C12-N
70	N3	202	PC1	C1-O11-P-O12
70	N3	202	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
70	N4	502	PC1	C11-O13-P-O12
70	N4	502	PC1	C11-O13-P-O14
70	N4	502	PC1	C1-O11-P-O12
70	N5	705	PC1	C1-O11-P-O12
70	N5	705	PC1	C1-O11-P-O14
70	N5	705	PC1	O13-C11-C12-N
70	N6	201	PC1	C12-C11-O13-P
70	N6	201	PC1	O13-C11-C12-N
70	QB	502	PC1	C11-O13-P-O14
70	QB	502	PC1	C1-O11-P-O14
70	QB	503	PC1	C11-O13-P-O12
70	QB	503	PC1	C11-O13-P-O14
70	QB	503	PC1	C1-O11-P-O14
70	QB	503	PC1	O13-C11-C12-N
70	QI	101	PC1	C11-O13-P-O12
70	QI	101	PC1	C11-O13-P-O14
70	QI	101	PC1	C11-O13-P-O11
70	QJ	101	PC1	C1-O11-P-O14
70	Qb	501	PC1	C11-O13-P-O14
70	Qc	407	PC1	C11-O13-P-O12
70	Qc	407	PC1	C11-O13-P-O14
70	Qc	407	PC1	C1-O11-P-O12
70	Qc	409	PC1	C11-O13-P-O12
70	Qc	410	PC1	C11-O13-P-O14
70	Qh	103	PC1	C1-O11-P-O12
70	Qh	103	PC1	C1-O11-P-O14
70	Qh	103	PC1	C1-O11-P-O13
70	S8	304	PC1	C11-O13-P-O12
71	6A	102	PEE	C1-O3P-P-O4P
71	6A	102	PEE	C4-O4P-P-O3P
71	6A	102	PEE	C4-O4P-P-O2P
71	6A	102	PEE	C4-O4P-P-O1P
71	6A	103	PEE	C11-C10-O2-C2
71	6A	103	PEE	C4-O4P-P-O2P
71	6A	103	PEE	O4P-C4-C5-N
71	8B	101	PEE	C11-C10-O2-C2
71	8B	101	PEE	C1-O3P-P-O1P
71	8B	101	PEE	C1-O3P-P-O4P
71	8B	101	PEE	C37-C38-C39-C40
71	A3	201	PEE	C17-C18-C19-C20
71	A3	201	PEE	C4-O4P-P-O2P
71	A3	201	PEE	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
71	A7	202	PEE	C2-C1-O3P-P
71	A7	202	PEE	C1-O3P-P-O2P
71	A7	202	PEE	O4P-C4-C5-N
71	AL	203	PEE	C1-O3P-P-O2P
71	AL	203	PEE	C1-O3P-P-O1P
71	AL	203	PEE	C4-O4P-P-O2P
71	AL	203	PEE	C4-O4P-P-O1P
71	AL	203	PEE	O4P-C4-C5-N
71	AL	203	PEE	C37-C38-C39-C40
71	AL	206	PEE	C18-C19-C20-C21
71	AL	206	PEE	C17-C18-C19-C20
71	AL	206	PEE	C11-C10-O2-C2
71	AL	206	PEE	C1-O3P-P-O2P
71	AL	206	PEE	C1-O3P-P-O1P
71	AL	206	PEE	C1-O3P-P-O4P
71	AN	202	PEE	C4-O4P-P-O2P
71	AN	202	PEE	O4P-C4-C5-N
71	BL	201	PEE	C17-C18-C19-C20
71	C1	609	PEE	C5-C4-O4P-P
71	C1	609	PEE	O4P-C4-C5-N
71	C3	302	PEE	O4P-C4-C5-N
71	C3	303	PEE	C17-C18-C19-C20
71	C3	303	PEE	C11-C10-O2-C2
71	C3	303	PEE	O4-C10-O2-C2
71	C3	303	PEE	C1-O3P-P-O2P
71	C3	303	PEE	C1-O3P-P-O4P
71	C3	303	PEE	C4-O4P-P-O1P
71	CB	203	PEE	C17-C18-C19-C20
71	CB	203	PEE	C11-C10-O2-C2
71	CB	203	PEE	C1-O3P-P-O2P
71	CB	203	PEE	C1-O3P-P-O1P
71	CB	203	PEE	C4-O4P-P-O3P
71	CB	203	PEE	C4-O4P-P-O2P
71	CB	203	PEE	C4-O4P-P-O1P
71	CB	203	PEE	O4P-C4-C5-N
71	N5	701	PEE	O4P-C4-C5-N
71	N5	704	PEE	C11-C10-O2-C2
71	N5	704	PEE	C1-O3P-P-O2P
71	N5	704	PEE	C1-O3P-P-O1P
71	N5	704	PEE	O4P-C4-C5-N
71	N5	706	PEE	O2-C2-C3-O3
71	N5	706	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
71	QC	403	PEE	O2-C2-C3-O3
71	QC	403	PEE	C4-O4P-P-O1P
71	QC	403	PEE	O4P-C4-C5-N
71	QC	404	PEE	O4P-C4-C5-N
71	QC	404	PEE	C31-C30-O3-C3
71	QC	405	PEE	C11-C10-O2-C2
71	QC	405	PEE	O4-C10-O2-C2
71	QC	405	PEE	C1-O3P-P-O2P
71	QC	405	PEE	C1-O3P-P-O1P
71	QC	405	PEE	C4-O4P-P-O2P
71	QC	405	PEE	C4-O4P-P-O1P
71	QH	102	PEE	C1-O3P-P-O2P
71	QH	102	PEE	C1-O3P-P-O1P
71	QH	102	PEE	O4P-C4-C5-N
71	Qb	503	PEE	C1-O3P-P-O2P
71	Qb	503	PEE	C1-O3P-P-O1P
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	Qb	503	PEE	O4P-C4-C5-N
71	Qc	403	PEE	C17-C18-C19-C20
71	Qc	408	PEE	C1-O3P-P-O1P
71	Qc	408	PEE	C1-O3P-P-O4P
71	Qc	408	PEE	C4-O4P-P-O3P
71	Qc	408	PEE	C4-O4P-P-O2P
71	Qc	408	PEE	C4-O4P-P-O1P
71	Qe	302	PEE	C11-C10-O2-C2
71	Qe	302	PEE	O4-C10-O2-C2
71	Qe	302	PEE	O3P-C1-C2-O2
71	Qe	302	PEE	C1-O3P-P-O2P
71	Qe	302	PEE	C1-O3P-P-O1P
71	Qe	302	PEE	O4P-C4-C5-N
71	Qh	101	PEE	C11-C10-O2-C2
71	Qh	101	PEE	O4P-C4-C5-N
71	S8	303	PEE	O4P-C4-C5-N
72	7B	101	3PE	O13-C11-C12-N
72	C1	601	3PE	C11-O13-P-O12
72	C1	601	3PE	O13-C11-C12-N
72	C1	601	3PE	O11-C1-C2-O21
72	CA	101	3PE	C1-O11-P-O14
72	CA	101	3PE	O13-C11-C12-N
72	CB	202	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
72	CB	202	3PE	O13-C11-C12-N
72	CB	202	3PE	O21-C2-C3-O31
72	Qc	401	3PE	C11-O13-P-O14
72	Qc	401	3PE	O13-C11-C12-N
72	Qc	406	3PE	C1-O11-P-O12
72	Qc	406	3PE	O13-C11-C12-N
74	AC	201	ZMP	C19-C18-C21-O5
74	AC	201	ZMP	C17-C18-C21-O5
74	AC	201	ZMP	S1-C11-C12-N1
74	AC	201	ZMP	O1-C10-S1-C11
74	AC	201	ZMP	C9-C10-S1-C11
74	AC	201	ZMP	C7-C8-C9-C10
75	AK	401	ADP	C5'-O5'-PA-O3A
76	AL	205	PLX	C3-O4-P1-O2
76	AL	205	PLX	C3-O4-P1-O3
76	AL	205	PLX	C2-O1-P1-O4
76	AL	205	PLX	C2-O1-P1-O2
76	AL	205	PLX	C2-O1-P1-O3
76	AL	205	PLX	N1-C1-C2-O1
76	AL	205	PLX	C25-C24-O8-C5
76	AL	205	PLX	O9-C24-C25-C26
76	AM	201	PLX	C25-C24-O8-C5
76	B1	101	PLX	O7-C6-O6-C4
76	B1	101	PLX	C2-O1-P1-O2
76	B1	101	PLX	C2-O1-P1-O3
76	B1	101	PLX	C25-C24-O8-C5
76	BL	202	PLX	O7-C6-C7-C8
76	BL	202	PLX	O7-C6-O6-C4
76	BL	202	PLX	N1-C1-C2-O1
76	C2	301	PLX	O7-C6-O6-C4
76	C2	301	PLX	C3-O4-P1-O2
76	C2	301	PLX	C3-O4-P1-O3
76	C2	301	PLX	C2-O1-P1-O2
76	C2	301	PLX	C2-O1-P1-O3
76	C2	301	PLX	O9-C24-O8-C5
76	C2	301	PLX	O9-C24-C25-C26
76	CB	201	PLX	O7-C6-O6-C4
76	CB	201	PLX	O4-C3-C4-O6
76	N3	201	PLX	N1-C1-C2-O1
76	N3	201	PLX	O9-C24-O8-C5
76	QE	301	PLX	O7-C6-C7-C8
76	QE	301	PLX	O7-C6-O6-C4

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Mol	Chain	Res	Type	Atoms
76	QE	301	PLX	O4-C3-C4-O6
76	QE	301	PLX	O9-C24-C25-C26
76	QI	102	PLX	C3-C4-O6-C6
76	QI	102	PLX	C2-O1-P1-O2
76	S7	302	PLX	O6-C6-C7-C8
76	S7	302	PLX	O4-C3-C4-O6
76	S7	302	PLX	C3-O4-P1-O3
77	C1	602	HEA	C1A-C2A-CAA-CBA
77	C1	602	HEA	C3A-C2A-CAA-CBA
77	C1	602	HEA	C17-C18-C19-C20
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	C17-C18-C19-C20
80	QC	401	HEM	C2B-C3B-CAB-CBB
80	QC	401	HEM	C4B-C3B-CAB-CBB
80	QC	402	HEM	C2B-C3B-CAB-CBB
80	QC	402	HEM	C4B-C3B-CAB-CBB
80	Qc	404	HEM	C2B-C3B-CAB-CBB
80	Qc	404	HEM	C4B-C3B-CAB-CBB
80	Qc	405	HEM	C1A-C2A-CAA-CBA
80	Qc	405	HEM	C3A-C2A-CAA-CBA
80	Qc	405	HEM	C2B-C3B-CAB-CBB
80	Qc	405	HEM	C4B-C3B-CAB-CBB
83	QH	101	PX2	C1-O4-P1-O1
83	QH	101	PX2	C1-O4-P1-O2
83	QH	101	PX2	C1-O4-P1-O3
83	QH	101	PX2	C1-C2-O7-C16
83	QH	101	PX2	C17-C16-O7-C2
85	V1	502	FMN	N10-C1'-C2'-O2'
85	V1	502	FMN	C5'-O5'-P-O1P
85	V1	502	FMN	C5'-O5'-P-O2P
85	V1	502	FMN	C5'-O5'-P-O3P
71	6A	102	PEE	O5-C30-O3-C3
71	6A	103	PEE	O5-C30-O3-C3
71	QC	404	PEE	O5-C30-O3-C3
71	QH	102	PEE	O5-C30-O3-C3
71	Qb	503	PEE	O5-C30-O3-C3
71	Qc	403	PEE	O5-C30-O3-C3
71	6A	102	PEE	C31-C30-O3-C3
71	6A	103	PEE	C31-C30-O3-C3
71	Qb	503	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
71	AL	203	PEE	O5-C30-O3-C3
71	AL	206	PEE	O5-C30-O3-C3
71	C1	609	PEE	O5-C30-O3-C3
71	CB	203	PEE	O5-C30-O3-C3
71	6A	103	PEE	O4-C10-O2-C2
71	AL	206	PEE	O4-C10-O2-C2
71	CB	203	PEE	O4-C10-O2-C2
71	N5	704	PEE	O4-C10-O2-C2
71	Qh	101	PEE	O4-C10-O2-C2
83	QH	101	PX2	O8-C16-O7-C2
71	AL	203	PEE	C31-C30-O3-C3
71	AL	206	PEE	C31-C30-O3-C3
71	C1	609	PEE	C31-C30-O3-C3
71	N5	706	PEE	C31-C30-O3-C3
71	QH	102	PEE	C31-C30-O3-C3
71	Qc	403	PEE	C31-C30-O3-C3
77	C1	603	HEA	C2D-C3D-CAD-CBD
71	CB	203	PEE	C31-C30-O3-C3
74	AC	201	ZMP	C14-C15-N2-C16
71	6A	102	PEE	C17-C18-C19-C20
71	C3	302	PEE	C17-C18-C19-C20
71	C3	303	PEE	C37-C38-C39-C40
71	N5	706	PEE	C37-C38-C39-C40
71	QH	102	PEE	C17-C18-C19-C20
71	QH	102	PEE	C37-C38-C39-C40
71	Qb	503	PEE	C17-C18-C19-C20
71	Qc	408	PEE	C17-C18-C19-C20
77	C1	603	HEA	C4D-C3D-CAD-CBD
77	C1	603	HEA	C17-C18-C19-C27
71	8B	101	PEE	O4-C10-O2-C2
68	AN	201	CDL	O1-C1-CB2-OB2
68	B5	201	CDL	O1-C1-CB2-OB2
71	QC	405	PEE	C31-C30-O3-C3
71	N5	706	PEE	O5-C30-O3-C3
83	QH	101	PX2	O6-C4-O5-C3
71	S8	303	PEE	C11-C10-O2-C2
83	QH	101	PX2	C5-C4-O5-C3
71	C1	609	PEE	C11-C12-C13-C14
70	C3	301	PC1	C2-C1-O11-P
71	QC	405	PEE	O5-C30-O3-C3
77	C1	602	HEA	C15-C16-C17-C18
77	C1	603	HEA	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
71	8B	101	PEE	C31-C30-O3-C3
71	QH	102	PEE	C11-C10-O2-C2
71	Qb	503	PEE	C11-C10-O2-C2
71	Qc	403	PEE	C11-C12-C13-C14
71	S8	303	PEE	O4-C10-O2-C2
70	B8	201	PC1	C11-C12-N-C14
70	N3	202	PC1	C11-C12-N-C13
70	Qc	407	PC1	C11-C12-N-C14
70	Qc	412	PC1	C11-C12-N-C15
70	Qd	402	PC1	C11-C12-N-C15
71	A3	201	PEE	C10-C11-C12-C13
71	6A	102	PEE	C11-C12-C13-C14
83	QH	101	PX2	C18-C19-C20-C21
71	CB	203	PEE	O3P-C1-C2-O2
68	N5	702	CDL	O1-C1-CA2-OA2
71	AL	203	PEE	C30-C31-C32-C33
68	AL	201	CDL	OA6-CA4-CA6-OA8
70	QB	503	PC1	O21-C2-C3-O31
77	C1	603	HEA	C18-C19-C20-C21
76	CB	201	PLX	C12-C13-C14-C15
68	AL	204	CDL	CA5-C11-C12-C13
70	B5	202	PC1	C21-C22-C23-C24
70	QI	101	PC1	C21-C22-C23-C24
80	Qc	405	HEM	C2A-CAA-CBA-CGA
68	AL	201	CDL	CB5-C51-C52-C53
68	Qj	101	CDL	CB7-C71-C72-C73
70	Qc	407	PC1	C21-C22-C23-C24
71	N5	701	PEE	C10-C11-C12-C13
71	Qe	302	PEE	C30-C31-C32-C33
71	AN	202	PEE	C37-C38-C39-C40
71	N5	701	PEE	C37-C38-C39-C40
71	S8	303	PEE	C17-C18-C19-C20
68	QC	406	CDL	CA5-C11-C12-C13
68	Qc	402	CDL	CA7-C31-C32-C33
68	Qj	101	CDL	CA7-C31-C32-C33
71	8B	101	PEE	C10-C11-C12-C13
71	N5	706	PEE	C10-C11-C12-C13
71	QE	302	PEE	C10-C11-C12-C13
71	QH	102	PEE	C30-C31-C32-C33
71	Qb	503	PEE	C10-C11-C12-C13
83	QH	101	PX2	C16-C17-C18-C19
71	8B	101	PEE	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
71	Qe	302	PEE	C31-C30-O3-C3
71	Qb	503	PEE	O4-C10-O2-C2
70	N3	202	PC1	C11-C12-N-C15
68	Qc	402	CDL	CB7-C71-C72-C73
70	B7	201	PC1	C31-C32-C33-C34
71	AL	206	PEE	C30-C31-C32-C33
71	QC	405	PEE	C12-C13-C14-C15
71	A7	202	PEE	C30-C31-C32-C33
68	4L	101	CDL	O1-C1-CB2-OB2
71	8B	101	PEE	O5-C30-O3-C3
71	C3	302	PEE	C30-C31-C32-C33
71	Qe	302	PEE	C17-C18-C19-C20
70	QB	502	PC1	C3A-C3B-C3C-C3D
71	Qh	101	PEE	C11-C12-C13-C14
71	QC	404	PEE	C11-C10-O2-C2
71	6A	103	PEE	C33-C34-C35-C36
71	C3	302	PEE	C12-C13-C14-C15
71	QE	302	PEE	C33-C34-C35-C36
76	CB	201	PLX	C15-C16-C17-C18
68	4L	101	CDL	CB3-OB5-PB2-OB2
68	A8	301	CDL	CB2-OB2-PB2-OB5
68	AL	201	CDL	CB2-OB2-PB2-OB5
68	AL	202	CDL	CA3-OA5-PA1-OA2
68	AL	204	CDL	CA3-OA5-PA1-OA2
68	AN	201	CDL	CB3-OB5-PB2-OB2
68	AN	203	CDL	CA2-OA2-PA1-OA5
68	AN	203	CDL	CB3-OB5-PB2-OB2
68	B4	201	CDL	CA2-OA2-PA1-OA5
68	B5	201	CDL	CB3-OB5-PB2-OB2
68	C1	607	CDL	CB2-OB2-PB2-OB5
68	C1	607	CDL	CB3-OB5-PB2-OB2
68	N2	401	CDL	CA2-OA2-PA1-OA5
68	N2	401	CDL	CB2-OB2-PB2-OB5
68	N4	501	CDL	CA3-OA5-PA1-OA2
68	N5	702	CDL	CA3-OA5-PA1-OA2
68	N5	702	CDL	CB2-OB2-PB2-OB5
68	N5	703	CDL	CA2-OA2-PA1-OA5
68	N5	703	CDL	CB2-OB2-PB2-OB5
68	N5	703	CDL	CB3-OB5-PB2-OB2
68	QB	501	CDL	CB3-OB5-PB2-OB2
68	QC	406	CDL	CA2-OA2-PA1-OA5
68	QC	406	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
68	QC	406	CDL	CB2-OB2-PB2-OB5
68	QC	406	CDL	CB3-OB5-PB2-OB2
68	QD	402	CDL	CA2-OA2-PA1-OA5
68	QD	402	CDL	CA3-OA5-PA1-OA2
68	Qc	411	CDL	CB2-OB2-PB2-OB5
68	Qj	101	CDL	CB3-OB5-PB2-OB2
70	7A	101	PC1	C11-O13-P-O11
70	7A	101	PC1	C1-O11-P-O13
70	B5	202	PC1	C11-O13-P-O11
70	B8	201	PC1	C11-O13-P-O11
70	C1	606	PC1	C11-O13-P-O11
70	C1	608	PC1	C11-O13-P-O11
70	C3	304	PC1	C1-O11-P-O13
70	C4	201	PC1	C11-O13-P-O11
70	N1	401	PC1	C11-O13-P-O11
70	N1	401	PC1	C1-O11-P-O13
70	N3	202	PC1	C1-O11-P-O13
70	N4	502	PC1	C11-O13-P-O11
70	N5	705	PC1	C11-O13-P-O11
70	N5	705	PC1	C1-O11-P-O13
70	N6	201	PC1	C1-O11-P-O13
70	QB	502	PC1	C11-O13-P-O11
70	QB	502	PC1	C1-O11-P-O13
70	QB	503	PC1	C11-O13-P-O11
70	Qc	407	PC1	C11-O13-P-O11
70	Qc	409	PC1	C1-O11-P-O13
70	Qd	402	PC1	C11-O13-P-O11
70	Qh	103	PC1	C11-O13-P-O11
70	S8	304	PC1	C11-O13-P-O11
71	6A	103	PEE	C4-O4P-P-O3P
71	A3	201	PEE	C1-O3P-P-O4P
71	A3	201	PEE	C4-O4P-P-O3P
71	A7	202	PEE	C1-O3P-P-O4P
71	AL	203	PEE	C1-O3P-P-O4P
71	AL	203	PEE	C4-O4P-P-O3P
71	AN	202	PEE	C1-O3P-P-O4P
71	BL	201	PEE	C1-O3P-P-O4P
71	BL	201	PEE	C4-O4P-P-O3P
71	C1	609	PEE	C4-O4P-P-O3P
71	C3	302	PEE	C4-O4P-P-O3P
71	C3	303	PEE	C4-O4P-P-O3P
71	CB	203	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
71	N5	704	PEE	C1-O3P-P-O4P
71	N5	706	PEE	C1-O3P-P-O4P
71	QC	405	PEE	C1-O3P-P-O4P
71	QC	405	PEE	C4-O4P-P-O3P
71	QE	302	PEE	C1-O3P-P-O4P
71	QH	102	PEE	C1-O3P-P-O4P
71	Qb	503	PEE	C1-O3P-P-O4P
71	Qe	302	PEE	C1-O3P-P-O4P
71	Qe	302	PEE	C4-O4P-P-O3P
71	Qh	101	PEE	C1-O3P-P-O4P
71	Qh	101	PEE	C4-O4P-P-O3P
72	7B	101	3PE	C1-O11-P-O13
72	C1	601	3PE	C11-O13-P-O11
72	CA	101	3PE	C1-O11-P-O13
72	CB	202	3PE	C11-O13-P-O11
76	AL	205	PLX	C3-O4-P1-O1
76	B1	101	PLX	C2-O1-P1-O4
76	C2	301	PLX	C3-O4-P1-O1
76	C2	301	PLX	C2-O1-P1-O4
76	S7	302	PLX	C3-O4-P1-O1
68	AN	201	CDL	CB7-C71-C72-C73
77	C1	602	HEA	C21-C22-C23-C24
71	Qe	302	PEE	O5-C30-O3-C3
71	Qc	403	PEE	C10-C11-C12-C13
68	4L	101	CDL	CA2-C1-CB2-OB2
68	N5	702	CDL	CA2-C1-CB2-OB2
71	QC	404	PEE	O4-C10-O2-C2
71	QH	102	PEE	O4-C10-O2-C2
68	A8	301	CDL	C33-C34-C35-C36
71	Qc	408	PEE	C20-C21-C22-C23
70	B7	201	PC1	C11-C12-N-C13
70	B7	201	PC1	C11-C12-N-C15
70	B8	201	PC1	C11-C12-N-C13
70	N6	201	PC1	C11-C12-N-C13
70	N6	201	PC1	C11-C12-N-C14
70	N6	201	PC1	C11-C12-N-C15
70	Qc	407	PC1	C11-C12-N-C13
70	Qc	412	PC1	C11-C12-N-C13
70	Qd	402	PC1	C11-C12-N-C14
76	AM	201	PLX	O6-C6-C7-C8
76	C2	301	PLX	O8-C24-C25-C26
76	N3	201	PLX	O8-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
71	6A	103	PEE	C39-C40-C41-C42
71	AL	203	PEE	C39-C40-C41-C42
71	C3	302	PEE	C35-C36-C37-C38
68	AN	203	CDL	CB5-C51-C52-C53
71	C1	609	PEE	C30-C31-C32-C33
68	AL	204	CDL	C76-C77-C78-C79
71	AN	202	PEE	C33-C34-C35-C36
68	A7	201	CDL	C79-C80-C81-C82
71	A3	201	PEE	C20-C21-C22-C23
71	AL	203	PEE	C43-C44-C45-C46
71	AN	202	PEE	C13-C14-C15-C16
71	C1	609	PEE	C13-C14-C15-C16
71	CB	203	PEE	C11-C12-C13-C14
71	Qe	302	PEE	C20-C21-C22-C23
71	Qe	302	PEE	C13-C14-C15-C16
71	Qh	101	PEE	C43-C44-C45-C46
74	AC	201	ZMP	C1-C2-C3-C4
76	S7	302	PLX	C11-C12-C13-C14
74	AC	201	ZMP	C20-C18-C21-O5
71	Qc	403	PEE	C22-C23-C24-C25
71	Qh	101	PEE	C40-C41-C42-C43
76	AM	201	PLX	C12-C13-C14-C15
76	N3	201	PLX	C33-C34-C35-C36
68	AL	202	CDL	C43-C44-C45-C46
70	N1	401	PC1	C27-C28-C29-C2A
71	A3	201	PEE	C32-C33-C34-C35
71	QC	404	PEE	C12-C13-C14-C15
76	QI	102	PLX	C26-C27-C28-C29
83	QH	101	PX2	C23-C24-C25-C26
70	6A	101	PC1	C23-C24-C25-C26
71	6A	103	PEE	C11-C12-C13-C14
76	BL	202	PLX	C18-C19-C20-C21
76	QI	102	PLX	C30-C31-C32-C33
68	QB	501	CDL	O1-C1-CB2-OB2
68	A7	201	CDL	C17-C18-C19-C20
71	AL	206	PEE	C33-C34-C35-C36
68	AL	204	CDL	CB7-C71-C72-C73
68	AN	201	CDL	OB6-CB4-CB6-OB8
68	N4	501	CDL	C54-C55-C56-C57
70	QJ	101	PC1	C2D-C2E-C2F-C2G
71	8B	101	PEE	C34-C35-C36-C37
71	Qc	403	PEE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
71	Qh	101	PEE	C42-C43-C44-C45
76	QE	301	PLX	C9-C10-C11-C12
76	S7	302	PLX	C14-C15-C16-C17
83	QH	101	PX2	C22-C23-C24-C25
68	N5	702	CDL	CB5-C51-C52-C53
70	B7	201	PC1	C32-C33-C34-C35
71	6A	102	PEE	C33-C34-C35-C36
71	N5	704	PEE	C14-C15-C16-C17
71	QC	403	PEE	C14-C15-C16-C17
71	QH	102	PEE	C20-C21-C22-C23
71	Qe	302	PEE	C42-C43-C44-C45
71	S8	303	PEE	C41-C42-C43-C44
72	C1	601	3PE	C27-C28-C29-C2A
74	AB	201	ZMP	C2-C3-C4-C5
76	N3	201	PLX	C13-C14-C15-C16
68	AN	203	CDL	C31-C32-C33-C34
70	N6	201	PC1	C2A-C2B-C2C-C2D
70	QI	101	PC1	C35-C36-C37-C38
71	Qc	408	PEE	C31-C32-C33-C34
76	BL	202	PLX	C14-C15-C16-C17
83	QH	101	PX2	C20-C21-C22-C23
68	B5	201	CDL	C23-C24-C25-C26
71	6A	103	PEE	C21-C22-C23-C24
71	AN	202	PEE	C31-C32-C33-C34
71	BL	201	PEE	C40-C41-C42-C43
71	C3	302	PEE	C21-C22-C23-C24
71	QE	302	PEE	C32-C33-C34-C35
71	Qe	302	PEE	C12-C13-C14-C15
76	QI	102	PLX	C34-C35-C36-C37
71	N5	704	PEE	C35-C36-C37-C38
71	Qe	302	PEE	C19-C20-C21-C22
70	B8	201	PC1	C29-C2A-C2B-C2C
70	N1	401	PC1	C26-C27-C28-C29
70	N6	201	PC1	C23-C24-C25-C26
70	QB	503	PC1	C32-C33-C34-C35
70	QI	101	PC1	C38-C39-C3A-C3B
71	6A	102	PEE	C22-C23-C24-C25
71	6A	102	PEE	C43-C44-C45-C46
71	AN	202	PEE	C20-C21-C22-C23
71	C3	303	PEE	C12-C13-C14-C15
71	N5	701	PEE	C21-C22-C23-C24
71	QC	403	PEE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
71	QC	403	PEE	C12-C13-C14-C15
71	QH	102	PEE	C11-C12-C13-C14
71	S8	303	PEE	C21-C22-C23-C24
76	CB	201	PLX	C11-C12-C13-C14
76	N3	201	PLX	C17-C18-C19-C20
70	B7	201	PC1	C11-C12-N-C14
70	B8	201	PC1	C11-C12-N-C15
70	N3	202	PC1	C11-C12-N-C14
70	Qc	407	PC1	C11-C12-N-C15
68	A7	201	CDL	C11-C12-C13-C14
68	A7	201	CDL	C80-C81-C82-C83
68	AN	201	CDL	C41-C42-C43-C44
70	B7	201	PC1	C2D-C2E-C2F-C2G
70	Qc	410	PC1	C28-C29-C2A-C2B
71	8B	101	PEE	C43-C44-C45-C46
71	AL	206	PEE	C32-C33-C34-C35
71	QC	404	PEE	C11-C12-C13-C14
74	AC	201	ZMP	C2-C3-C4-C5
76	N3	201	PLX	C9-C10-C11-C12
76	QI	102	PLX	C11-C10-C9-C8
68	QB	501	CDL	C12-C13-C14-C15
71	8B	101	PEE	C41-C42-C43-C44
71	A3	201	PEE	C11-C12-C13-C14
71	AN	202	PEE	C11-C12-C13-C14
71	N5	701	PEE	C11-C12-C13-C14
71	Qb	503	PEE	C22-C23-C24-C25
76	AM	201	PLX	C29-C30-C31-C32
71	8B	101	PEE	C12-C13-C14-C15
71	N5	706	PEE	C31-C32-C33-C34
76	N3	201	PLX	C11-C10-C9-C8
71	Qh	101	PEE	C32-C33-C34-C35
71	S8	303	PEE	C42-C43-C44-C45
68	A7	201	CDL	C74-C75-C76-C77
71	AL	206	PEE	C14-C15-C16-C17
71	Qh	101	PEE	C12-C13-C14-C15
74	AB	201	ZMP	C6-C7-C8-C9
76	QE	301	PLX	C7-C8-C9-C10
68	A8	301	CDL	C18-C19-C20-C21
68	N5	702	CDL	C56-C57-C58-C59
70	C4	201	PC1	C2E-C2F-C2G-C2H
71	N5	706	PEE	C11-C12-C13-C14
71	QH	102	PEE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
76	AM	201	PLX	C30-C31-C32-C33
76	N3	201	PLX	C14-C15-C16-C17
83	QH	101	PX2	C5-C6-C7-C8
83	QH	101	PX2	C21-C22-C23-C24
71	6A	103	PEE	C1-C2-C3-O3
71	AL	206	PEE	C37-C38-C39-C40
71	Qh	101	PEE	C37-C38-C39-C40
68	AL	204	CDL	C31-C32-C33-C34
70	Qc	412	PC1	C33-C34-C35-C36
71	8B	101	PEE	C11-C12-C13-C14
71	N5	706	PEE	C14-C15-C16-C17
71	Qb	503	PEE	C14-C15-C16-C17
72	C1	601	3PE	C2D-C2E-C2F-C2G
72	Qc	406	3PE	C23-C24-C25-C26
68	A7	201	CDL	CA5-C11-C12-C13
68	B4	201	CDL	C12-C13-C14-C15
71	C1	609	PEE	C11-C10-O2-C2
68	4L	101	CDL	C38-C39-C40-C41
71	N5	701	PEE	C23-C24-C25-C26
76	B1	101	PLX	O9-C24-C25-C26
76	QI	102	PLX	O7-C6-C7-C8
76	QI	102	PLX	O9-C24-C25-C26
76	S7	302	PLX	O7-C6-C7-C8
70	C4	201	PC1	C36-C37-C38-C39
71	C3	302	PEE	C22-C23-C24-C25
71	N5	701	PEE	C31-C32-C33-C34
71	N5	706	PEE	C12-C13-C14-C15
71	QH	102	PEE	C33-C34-C35-C36
71	CB	203	PEE	C30-C31-C32-C33
71	AN	202	PEE	C15-C16-C17-C18
71	C3	302	PEE	C19-C20-C21-C22
68	Qh	102	CDL	C37-C38-C39-C40
68	N5	703	CDL	O1-C1-CB2-OB2
74	AC	201	ZMP	C3-C4-C5-C6
71	QC	403	PEE	C16-C17-C18-C19
68	N4	501	CDL	C71-C72-C73-C74
71	C3	303	PEE	C14-C15-C16-C17
71	QH	102	PEE	C21-C22-C23-C24
83	QH	101	PX2	C11-C10-C9-C8
68	B5	201	CDL	CA2-C1-CB2-OB2
71	C3	302	PEE	C33-C34-C35-C36
71	QC	404	PEE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
74	AB	201	ZMP	C22-C1-C2-C3
71	C1	609	PEE	O4-C10-O2-C2
77	C1	602	HEA	C21-C22-C23-C25
70	C3	301	PC1	C36-C37-C38-C39
70	N3	202	PC1	C33-C34-C35-C36
71	6A	103	PEE	C14-C15-C16-C17
68	AN	201	CDL	C1-CB2-OB2-PB2
68	N4	501	CDL	C35-C36-C37-C38
70	N4	502	PC1	C29-C2A-C2B-C2C
70	N6	201	PC1	C35-C36-C37-C38
71	S8	303	PEE	C12-C13-C14-C15
70	Qc	410	PC1	C11-C12-N-C14
70	Qd	402	PC1	C11-C12-N-C13
70	Qh	103	PC1	C11-C12-N-C14
70	Qc	412	PC1	C21-C22-C23-C24
71	Qb	503	PEE	C30-C31-C32-C33
71	Qh	101	PEE	C30-C31-C32-C33
71	QC	404	PEE	C31-C32-C33-C34
76	CB	201	PLX	C7-C8-C9-C10
70	B5	202	PC1	C3B-C3C-C3D-C3E
70	N4	502	PC1	C37-C38-C39-C3A
76	CB	201	PLX	C27-C28-C29-C30
68	QB	501	CDL	CA7-C31-C32-C33
71	A3	201	PEE	C30-C31-C32-C33
71	CB	203	PEE	C10-C11-C12-C13
71	AN	202	PEE	C12-C13-C14-C15
70	N1	401	PC1	C2B-C2C-C2D-C2E
71	C3	302	PEE	C37-C38-C39-C40
71	QC	404	PEE	C17-C18-C19-C20
71	BL	201	PEE	C22-C23-C24-C25
74	AC	201	ZMP	C22-C23-C24-C25
71	AL	203	PEE	C35-C36-C37-C38
71	AN	202	PEE	C39-C40-C41-C42
71	N5	706	PEE	C35-C36-C37-C38
71	QE	302	PEE	C35-C36-C37-C38
71	QE	302	PEE	C39-C40-C41-C42
71	Qh	101	PEE	C39-C40-C41-C42
70	C4	201	PC1	C39-C3A-C3B-C3C
70	Qd	402	PC1	C22-C23-C24-C25
71	AN	202	PEE	C32-C33-C34-C35
71	Qb	503	PEE	C13-C14-C15-C16
70	Qb	501	PC1	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
72	CA	101	3PE	C34-C35-C36-C37
68	QD	402	CDL	C51-C52-C53-C54
71	Qe	302	PEE	C11-C12-C13-C14
68	A7	201	CDL	CA7-C31-C32-C33
68	Qj	101	CDL	CA5-C11-C12-C13
70	N1	401	PC1	C21-C22-C23-C24
83	QH	101	PX2	C4-C5-C6-C7
68	AL	201	CDL	C19-C20-C21-C22
68	QC	406	CDL	C71-C72-C73-C74
70	C1	608	PC1	C27-C28-C29-C2A
71	8B	101	PEE	C33-C34-C35-C36
72	Qc	401	3PE	C23-C24-C25-C26
76	BL	202	PLX	C13-C14-C15-C16
76	BL	202	PLX	C27-C28-C29-C30
70	7C	101	PC1	C29-C2A-C2B-C2C
71	A3	201	PEE	C22-C23-C24-C25
71	C3	303	PEE	C32-C33-C34-C35
68	B5	201	CDL	C77-C78-C79-C80
68	Qh	102	CDL	C71-C72-C73-C74
70	N4	502	PC1	C3B-C3C-C3D-C3E
70	QB	503	PC1	C35-C36-C37-C38
71	C3	302	PEE	C11-C12-C13-C14
70	Qd	402	PC1	C21-C22-C23-C24
71	AN	202	PEE	C10-C11-C12-C13
70	N1	401	PC1	O11-C1-C2-O21
71	6A	102	PEE	O3P-C1-C2-O2
68	Qh	102	CDL	C23-C24-C25-C26
68	Qj	101	CDL	C20-C21-C22-C23
71	6A	103	PEE	C22-C23-C24-C25
76	BL	202	PLX	C30-C31-C32-C33
71	N5	701	PEE	C38-C39-C40-C41
70	B5	202	PC1	C26-C27-C28-C29
71	8B	101	PEE	C40-C41-C42-C43
71	6A	102	PEE	C10-C11-C12-C13
70	N6	201	PC1	C33-C34-C35-C36
68	QD	402	CDL	OB6-CB4-CB6-OB8
70	6A	101	PC1	O21-C2-C3-O31
70	C3	304	PC1	O21-C2-C3-O31
71	A3	201	PEE	O2-C2-C3-O3
71	Qh	101	PEE	O2-C2-C3-O3
76	S7	302	PLX	O6-C4-C5-O8
70	C4	201	PC1	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
70	Qc	412	PC1	C11-C12-N-C14
68	Qh	102	CDL	C32-C33-C34-C35
71	BL	201	PEE	C33-C34-C35-C36
71	QC	405	PEE	C35-C36-C37-C38
71	Qb	503	PEE	C39-C40-C41-C42
71	Qh	101	PEE	C15-C16-C17-C18
68	Qc	411	CDL	C51-C52-C53-C54
70	N1	401	PC1	C3D-C3E-C3F-C3G
70	Qc	407	PC1	C2D-C2E-C2F-C2G
70	7A	101	PC1	C3B-C3C-C3D-C3E
71	AN	202	PEE	C43-C44-C45-C46
71	Qe	302	PEE	C37-C38-C39-C40
70	B5	202	PC1	C37-C38-C39-C3A
71	A3	201	PEE	C33-C34-C35-C36
71	C1	609	PEE	C33-C34-C35-C36
76	N3	201	PLX	C16-C17-C18-C19
68	N5	702	CDL	C20-C21-C22-C23
70	B8	201	PC1	C32-C33-C34-C35
76	QI	102	PLX	C25-C26-C27-C28
71	Qc	403	PEE	C11-C10-O2-C2
76	S7	302	PLX	C11-C10-C9-C8
71	Qh	101	PEE	C18-C19-C20-C21
68	AL	204	CDL	CA4-CA6-OA8-CA7
68	4L	101	CDL	CA3-OA5-PA1-OA2
68	AN	203	CDL	CB2-OB2-PB2-OB5
68	B5	201	CDL	CA2-OA2-PA1-OA5
68	QB	501	CDL	CB2-OB2-PB2-OB5
68	QC	407	CDL	CA2-OA2-PA1-OA5
68	Qb	502	CDL	CA3-OA5-PA1-OA2
68	Qc	402	CDL	CB3-OB5-PB2-OB2
70	Qc	407	PC1	C1-O11-P-O13
71	AN	202	PEE	C4-O4P-P-O3P
71	QH	102	PEE	C4-O4P-P-O3P
76	QI	102	PLX	C2-O1-P1-O4
71	Qe	302	PEE	C40-C41-C42-C43
68	AL	202	CDL	CA5-C11-C12-C13
68	QC	406	CDL	CA7-C31-C32-C33
68	N2	401	CDL	C1-CA2-OA2-PA1
71	6A	103	PEE	C2-C1-O3P-P
68	AL	202	CDL	C51-C52-C53-C54
71	A3	201	PEE	C13-C14-C15-C16
71	BL	201	PEE	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
68	AN	203	CDL	OB5-CB3-CB4-CB6
68	N2	401	CDL	OB5-CB3-CB4-CB6
68	Qh	102	CDL	OA5-CA3-CA4-CA6
70	Qc	407	PC1	O11-C1-C2-C3
71	A3	201	PEE	O3P-C1-C2-C3
71	C1	609	PEE	O3P-C1-C2-C3
71	Qe	302	PEE	O3P-C1-C2-C3
76	C2	301	PLX	O4-C3-C4-C5
76	CB	201	PLX	O4-C3-C4-C5
76	QE	301	PLX	O4-C3-C4-C5
76	QI	102	PLX	O4-C3-C4-C5
83	QH	101	PX2	O4-C1-C2-C3
71	N5	704	PEE	C12-C13-C14-C15
71	QC	403	PEE	C33-C34-C35-C36
71	BL	201	PEE	C34-C35-C36-C37
72	Qc	401	3PE	C22-C23-C24-C25
70	7A	101	PC1	C3C-C3D-C3E-C3F
70	Qc	407	PC1	C35-C36-C37-C38
71	C1	609	PEE	C12-C13-C14-C15
71	QH	102	PEE	C12-C13-C14-C15
71	Qc	408	PEE	C35-C36-C37-C38
71	Qh	101	PEE	C35-C36-C37-C38
68	4L	101	CDL	C15-C16-C17-C18
68	AL	201	CDL	C55-C56-C57-C58
68	N2	401	CDL	C36-C37-C38-C39
68	A8	301	CDL	C22-C23-C24-C25
76	QE	301	PLX	C17-C18-C19-C20
68	N2	401	CDL	C37-C38-C39-C40
71	Qc	403	PEE	C31-C32-C33-C34
70	QI	101	PC1	C37-C38-C39-C3A
71	A3	201	PEE	C42-C43-C44-C45
68	AN	203	CDL	CB3-CB4-CB6-OB8
68	B4	201	CDL	CA3-CA4-CA6-OA8
68	Qc	411	CDL	CA3-CA4-CA6-OA8
70	QB	503	PC1	C1-C2-C3-O31
71	C3	303	PEE	C1-C2-C3-O3
71	N5	706	PEE	C1-C2-C3-O3
71	Qc	403	PEE	C1-C2-C3-O3
76	AM	201	PLX	C3-C4-C5-O8
76	B1	101	PLX	C3-C4-C5-O8
71	N5	706	PEE	C17-C18-C19-C20
71	QE	302	PEE	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
71	C3	303	PEE	C11-C12-C13-C14
68	N5	702	CDL	C31-C32-C33-C34
70	7A	101	PC1	C26-C27-C28-C29
70	Qc	407	PC1	C3B-C3C-C3D-C3E
76	BL	202	PLX	C29-C30-C31-C32
71	Qh	101	PEE	C41-C42-C43-C44
76	AL	205	PLX	C32-C33-C34-C35
76	QI	102	PLX	C27-C28-C29-C30
68	Qh	102	CDL	CB7-C71-C72-C73
70	Qh	103	PC1	C31-C32-C33-C34
71	C1	609	PEE	C10-C11-C12-C13
71	Qc	403	PEE	O4-C10-O2-C2
74	AB	201	ZMP	O3-C16-C17-O4
77	C1	602	HEA	C19-C20-C21-C22
71	BL	201	PEE	C24-C25-C26-C27
71	BL	201	PEE	C38-C39-C40-C41
71	8B	101	PEE	C2-C3-O3-C30
71	AN	202	PEE	C44-C45-C46-C47
71	6A	102	PEE	C39-C40-C41-C42
71	AN	202	PEE	C35-C36-C37-C38
71	C3	302	PEE	C15-C16-C17-C18
71	C3	303	PEE	C19-C20-C21-C22
71	QC	405	PEE	C15-C16-C17-C18
71	QH	102	PEE	C35-C36-C37-C38
70	N3	202	PC1	C34-C35-C36-C37
68	QC	406	CDL	C84-C85-C86-C87
70	B5	202	PC1	C38-C39-C3A-C3B
83	QH	101	PX2	C12-C13-C14-C15
68	QC	406	CDL	CB5-C51-C52-C53
71	Qc	408	PEE	C21-C22-C23-C24
83	QH	101	PX2	C9-C10-C11-C12
70	B8	201	PC1	C37-C38-C39-C3A
70	N4	502	PC1	C2B-C2C-C2D-C2E
71	AL	206	PEE	C1-C2-O2-C10
71	Qb	503	PEE	C3-C2-O2-C10
71	S8	303	PEE	C3-C2-O2-C10
71	QH	102	PEE	C44-C45-C46-C47
71	Qc	403	PEE	C21-C22-C23-C24
68	Qb	502	CDL	C73-C74-C75-C76
70	B5	202	PC1	C23-C24-C25-C26
71	Qc	408	PEE	C41-C42-C43-C44
76	CB	201	PLX	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
71	Qc	403	PEE	C16-C17-C18-C19
68	N4	501	CDL	C80-C81-C82-C83
71	AL	203	PEE	C40-C41-C42-C43
71	QC	405	PEE	C33-C34-C35-C36
71	Qc	403	PEE	C35-C36-C37-C38
74	AB	201	ZMP	C3-C4-C5-C6
76	AL	205	PLX	C11-C10-C9-C8
68	C1	607	CDL	OB5-CB3-CB4-OB6
70	N6	201	PC1	O11-C1-C2-O21
71	QC	403	PEE	O3P-C1-C2-O2
71	QC	405	PEE	O3P-C1-C2-O2
71	AN	202	PEE	C17-C18-C19-C20
71	QC	405	PEE	C17-C18-C19-C20
70	QB	503	PC1	C11-C12-N-C15
70	Qc	410	PC1	C11-C12-N-C15
68	C1	607	CDL	C73-C74-C75-C76
68	QC	406	CDL	C58-C59-C60-C61
70	QB	502	PC1	C3E-C3F-C3G-C3H
71	BL	201	PEE	C23-C24-C25-C26
71	Qb	503	PEE	C21-C22-C23-C24
80	Qc	404	HEM	C3D-CAD-CBD-CGD
70	Qc	407	PC1	C3D-C3E-C3F-C3G
76	N3	201	PLX	C26-C27-C28-C29
70	6A	101	PC1	C35-C36-C37-C38
70	N6	201	PC1	C36-C37-C38-C39
71	A7	202	PEE	C33-C34-C35-C36
68	QB	501	CDL	OB6-CB4-CB6-OB8
71	C3	303	PEE	O2-C2-C3-O3
71	N5	704	PEE	O2-C2-C3-O3
68	N4	501	CDL	C82-C83-C84-C85
68	Qb	502	CDL	C75-C76-C77-C78
70	Qb	501	PC1	C23-C24-C25-C26
71	C3	303	PEE	C33-C34-C35-C36
71	Qb	503	PEE	C42-C43-C44-C45
71	N5	701	PEE	O3-C30-C31-C32
68	N5	703	CDL	C33-C34-C35-C36
71	CB	203	PEE	C20-C21-C22-C23
76	BL	202	PLX	C31-C32-C33-C34
72	C1	601	3PE	C3D-C3E-C3F-C3G
71	Qb	503	PEE	C40-C41-C42-C43
72	CA	101	3PE	C2D-C2E-C2F-C2G
71	C3	303	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
71	QC	404	PEE	C14-C15-C16-C17
71	6A	102	PEE	C35-C36-C37-C38
76	QE	301	PLX	C28-C29-C30-C31
76	QE	301	PLX	C11-C10-C9-C8
70	Qh	103	PC1	C11-C12-N-C15
70	7A	101	PC1	O11-C1-C2-C3
70	N1	401	PC1	O11-C1-C2-C3
70	QJ	101	PC1	O11-C1-C2-C3
70	S8	304	PC1	O11-C1-C2-C3
71	6A	102	PEE	O3P-C1-C2-C3
71	CB	203	PEE	O3P-C1-C2-C3
71	Qh	101	PEE	O3P-C1-C2-C3
72	C1	601	3PE	O11-C1-C2-C3
76	S7	302	PLX	O4-C3-C4-C5
71	QC	405	PEE	C23-C24-C25-C26
71	Qc	408	PEE	C11-C12-C13-C14
76	CB	201	PLX	C33-C34-C35-C36
71	6A	102	PEE	O4P-C4-C5-N
68	N4	501	CDL	C18-C19-C20-C21
68	Qb	502	CDL	C32-C33-C34-C35
71	S8	303	PEE	C33-C34-C35-C36
72	7B	101	3PE	C3F-C3G-C3H-C3I
68	A8	301	CDL	C16-C17-C18-C19
71	N5	706	PEE	C40-C41-C42-C43
74	AC	201	ZMP	C6-C7-C8-C9
70	C4	201	PC1	C31-C32-C33-C34
71	QC	403	PEE	C30-C31-C32-C33
71	A3	201	PEE	C21-C22-C23-C24
68	A8	301	CDL	O1-C1-CB2-OB2
68	N4	501	CDL	C21-C22-C23-C24
70	QB	503	PC1	C33-C34-C35-C36
71	QC	405	PEE	C32-C33-C34-C35
71	S8	303	PEE	C13-C14-C15-C16
68	4L	101	CDL	C13-C14-C15-C16
70	N4	502	PC1	C32-C33-C34-C35
76	C2	301	PLX	C7-C8-C9-C10
68	AL	201	CDL	C1-CA2-OA2-PA1
68	B4	201	CDL	CB4-CB3-OB5-PB2
68	QD	402	CDL	CA4-CA3-OA5-PA1
71	C1	609	PEE	C2-C1-O3P-P
71	Qe	302	PEE	C2-C1-O3P-P
71	6A	103	PEE	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
70	7A	101	PC1	C3A-C3B-C3C-C3D
72	Qc	406	3PE	C3D-C3E-C3F-C3G
76	AL	205	PLX	C15-C16-C17-C18
71	C3	303	PEE	C15-C16-C17-C18
68	N5	702	CDL	C17-C18-C19-C20
70	C4	201	PC1	C24-C25-C26-C27
71	8B	101	PEE	C15-C16-C17-C18
71	AN	202	PEE	C21-C22-C23-C24
71	AN	202	PEE	C42-C43-C44-C45
80	QC	401	HEM	C3D-CAD-CBD-CGD
70	N4	502	PC1	C2C-C2D-C2E-C2F
74	AB	201	ZMP	C1-C2-C3-C4
68	AL	201	CDL	CA3-CA4-CA6-OA8
68	AN	201	CDL	CB3-CB4-CB6-OB8
68	C1	607	CDL	CA3-CA4-CA6-OA8
68	QD	402	CDL	CA3-CA4-CA6-OA8
68	Qh	102	CDL	CB3-CB4-CB6-OB8
70	6A	101	PC1	C1-C2-C3-O31
70	7C	101	PC1	C1-C2-C3-O31
70	C3	304	PC1	C1-C2-C3-O31
71	A3	201	PEE	C1-C2-C3-O3
71	QC	403	PEE	C1-C2-C3-O3
71	QE	302	PEE	C1-C2-C3-O3
71	Qh	101	PEE	C1-C2-C3-O3
76	BL	202	PLX	C3-C4-C5-O8
76	S7	302	PLX	C3-C4-C5-O8
70	N1	401	PC1	C3F-C3G-C3H-C3I
70	N5	705	PC1	C31-C32-C33-C34
70	B7	201	PC1	C2F-C2G-C2H-C2I
71	6A	102	PEE	C34-C35-C36-C37
74	AB	201	ZMP	N2-C16-C17-C18
71	QE	302	PEE	C11-C12-C13-C14
68	A8	301	CDL	C23-C24-C25-C26
71	BL	201	PEE	C21-C22-C23-C24
71	N5	701	PEE	C34-C35-C36-C37
68	B5	201	CDL	CA3-OA5-PA1-OA2
68	Qh	102	CDL	CB2-OB2-PB2-OB5
68	Qh	102	CDL	CB3-OB5-PB2-OB2
68	Qj	101	CDL	CB2-OB2-PB2-OB5
70	N6	201	PC1	C11-O13-P-O11
70	QB	503	PC1	C1-O11-P-O13
70	Qb	501	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
72	Qc	401	3PE	C1-O11-P-O13
76	B1	101	PLX	C5-C4-O6-C6
76	BL	202	PLX	C5-C4-O6-C6
76	C2	301	PLX	C3-C4-O6-C6
76	AM	201	PLX	C19-C20-C21-C22
76	AM	201	PLX	O7-C6-C7-C8
76	AM	201	PLX	O9-C24-C25-C26
68	N5	703	CDL	C52-C53-C54-C55
72	7B	101	3PE	C2B-C2C-C2D-C2E
68	A8	301	CDL	OA5-CA3-CA4-OA6
68	QD	402	CDL	OA5-CA3-CA4-OA6
68	Qc	411	CDL	OB5-CB3-CB4-OB6
70	Qb	501	PC1	O11-C1-C2-O21
70	S8	304	PC1	O11-C1-C2-O21
71	Qh	101	PEE	O3P-C1-C2-O2
72	Qc	406	3PE	O11-C1-C2-O21
76	AL	205	PLX	O4-C3-C4-O6
76	BL	202	PLX	O4-C3-C4-O6
76	B1	101	PLX	C15-C16-C17-C18
71	S8	303	PEE	C15-C16-C17-C18
68	B5	201	CDL	CA7-C31-C32-C33
71	N5	704	PEE	C30-C31-C32-C33
71	Qc	403	PEE	C24-C25-C26-C27
71	Qh	101	PEE	C31-C32-C33-C34
72	CA	101	3PE	C2C-C2D-C2E-C2F
68	B4	201	CDL	OA6-CA4-CA6-OA8
70	7C	101	PC1	O21-C2-C3-O31
70	B7	201	PC1	O21-C2-C3-O31
71	Qb	503	PEE	O2-C2-C3-O3
76	B1	101	PLX	O6-C4-C5-O8
71	Qc	408	PEE	C12-C13-C14-C15
68	N5	702	CDL	CB2-C1-CA2-OA2
70	C1	610	PC1	C33-C34-C35-C36
70	C4	201	PC1	C23-C24-C25-C26
71	A3	201	PEE	C34-C35-C36-C37
76	BL	202	PLX	C33-C34-C35-C36
68	A8	301	CDL	CA4-CA3-OA5-PA1
68	B5	201	CDL	CB4-CB3-OB5-PB2
68	QC	406	CDL	C1-CA2-OA2-PA1
70	B8	201	PC1	C2-C1-O11-P
70	Qc	409	PC1	C2-C1-O11-P
72	CB	202	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
76	BL	202	PLX	C4-C3-O4-P1
71	Qb	503	PEE	C15-C16-C17-C18
71	Qc	408	PEE	C40-C41-C42-C43
68	N5	703	CDL	C39-C40-C41-C42
70	6A	101	PC1	C33-C34-C35-C36
70	N1	401	PC1	C25-C26-C27-C28
71	A3	201	PEE	C41-C42-C43-C44
71	N5	704	PEE	C33-C34-C35-C36
71	QE	302	PEE	C16-C17-C18-C19
68	N4	501	CDL	CA7-C31-C32-C33
83	QH	101	PX2	C17-C18-C19-C20
68	Qj	101	CDL	C73-C74-C75-C76
71	QC	404	PEE	C18-C19-C20-C21
71	QC	405	PEE	C31-C32-C33-C34
76	QE	301	PLX	O6-C6-C7-C8
71	C1	609	PEE	C17-C18-C19-C20
68	A8	301	CDL	OA5-CA3-CA4-CA6
68	AL	204	CDL	OB5-CB3-CB4-CB6
68	N4	501	CDL	OA5-CA3-CA4-CA6
68	QB	501	CDL	OB5-CB3-CB4-CB6
68	QC	407	CDL	OA5-CA3-CA4-CA6
68	QD	402	CDL	OA5-CA3-CA4-CA6
70	6A	101	PC1	O11-C1-C2-C3
70	C1	608	PC1	O11-C1-C2-C3
70	C4	201	PC1	O11-C1-C2-C3
70	N6	201	PC1	O11-C1-C2-C3
71	C3	303	PEE	O3P-C1-C2-C3
72	Qc	406	3PE	O11-C1-C2-C3
68	A7	201	CDL	C72-C71-CB7-OB8
76	N3	201	PLX	C19-C20-C21-C22
68	QC	406	CDL	C41-C42-C43-C44
71	S8	303	PEE	C34-C35-C36-C37
70	Qc	412	PC1	C22-C21-O21-C2
68	N5	702	CDL	C37-C38-C39-C40
70	C3	301	PC1	C21-C22-C23-C24
71	Qc	403	PEE	C2-C3-O3-C30
68	N4	501	CDL	C42-C43-C44-C45
71	N5	704	PEE	C21-C22-C23-C24
71	C3	302	PEE	C13-C14-C15-C16
76	QE	301	PLX	C15-C16-C17-C18
71	6A	103	PEE	C3-C2-O2-C10
68	Qj	101	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
71	BL	201	PEE	C41-C42-C43-C44
72	CA	101	3PE	C27-C28-C29-C2A
70	S8	304	PC1	C29-C2A-C2B-C2C
76	AL	205	PLX	C29-C30-C31-C32
71	CB	203	PEE	C19-C20-C21-C22
70	Qb	501	PC1	C21-C22-C23-C24
68	B4	201	CDL	C1-CB2-OB2-PB2
68	B4	201	CDL	CB3-CB4-CB6-OB8
68	C1	607	CDL	C1-CB2-OB2-PB2
68	QC	407	CDL	CA4-CA3-OA5-PA1
68	QD	402	CDL	CB3-CB4-CB6-OB8
68	Qb	502	CDL	CA3-CA4-CA6-OA8
68	Qc	411	CDL	CA4-CA3-OA5-PA1
68	Qj	101	CDL	CB4-CB3-OB5-PB2
71	AL	206	PEE	C2-C1-O3P-P
71	CB	203	PEE	C1-C2-C3-O3
71	CB	203	PEE	C2-C1-O3P-P
71	QC	405	PEE	C2-C1-O3P-P
71	Qb	503	PEE	C1-C2-C3-O3
72	CB	202	3PE	C1-C2-C3-O31
68	A7	201	CDL	OB5-CB3-CB4-OB6
68	QB	501	CDL	OB5-CB3-CB4-OB6
68	Qh	102	CDL	OA5-CA3-CA4-OA6
68	Qj	101	CDL	OA5-CA3-CA4-OA6
70	6A	101	PC1	O11-C1-C2-O21
70	7A	101	PC1	O11-C1-C2-O21
70	C1	608	PC1	O11-C1-C2-O21
70	C4	201	PC1	O11-C1-C2-O21
70	QJ	101	PC1	O11-C1-C2-O21
71	6A	103	PEE	O3P-C1-C2-O2
71	C1	609	PEE	O3P-C1-C2-O2
71	QH	102	PEE	O3P-C1-C2-O2
76	QI	102	PLX	O4-C3-C4-O6
83	QH	101	PX2	O4-C1-C2-O7
76	N3	201	PLX	C6-C7-C8-C9
76	S7	302	PLX	C6-C7-C8-C9
71	AL	203	PEE	C42-C43-C44-C45
68	A8	301	CDL	CA2-C1-CB2-OB2
68	Qh	102	CDL	O1-C1-CA2-OA2
74	AB	201	ZMP	C16-C17-C18-C19
71	C3	303	PEE	O5-C30-O3-C3
68	Qj	101	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
68	AN	203	CDL	OB6-CB4-CB6-OB8
68	C1	607	CDL	OA6-CA4-CA6-OA8
68	N5	703	CDL	OB6-CB4-CB6-OB8
68	Qh	102	CDL	OB6-CB4-CB6-OB8
70	N5	705	PC1	O21-C2-C3-O31
71	6A	103	PEE	O2-C2-C3-O3
71	AL	203	PEE	O2-C2-C3-O3
71	AN	202	PEE	O2-C2-C3-O3
76	AM	201	PLX	O6-C4-C5-O8
76	QI	102	PLX	O6-C4-C5-O8
70	QB	502	PC1	C26-C27-C28-C29
68	Qj	101	CDL	C33-C34-C35-C36
76	CB	201	PLX	C32-C33-C34-C35
76	CB	201	PLX	C2-C1-N1-C1C
71	QC	404	PEE	C33-C34-C35-C36
71	N5	704	PEE	C19-C20-C21-C22
71	Qc	408	PEE	C19-C20-C21-C22
71	BL	201	PEE	C10-C11-C12-C13
70	N4	502	PC1	C39-C3A-C3B-C3C
76	QI	102	PLX	C6-C7-C8-C9
70	Qh	103	PC1	C36-C37-C38-C39
68	N5	702	CDL	C18-C19-C20-C21
70	7A	101	PC1	C2B-C2C-C2D-C2E
73	A9	401	NDP	PN-O3-PA-O1A
70	Qh	103	PC1	C3D-C3E-C3F-C3G
71	Qc	403	PEE	C14-C15-C16-C17
71	6A	103	PEE	C32-C33-C34-C35
68	Qc	411	CDL	C31-C32-C33-C34
71	Qc	408	PEE	C44-C45-C46-C47
68	AL	202	CDL	C35-C36-C37-C38
71	S8	303	PEE	C11-C12-C13-C14
76	C2	301	PLX	C24-C25-C26-C27
71	BL	201	PEE	C19-C20-C21-C22
71	S8	303	PEE	C35-C36-C37-C38
68	A7	201	CDL	CA3-OA5-PA1-OA2
68	A7	201	CDL	CB2-OB2-PB2-OB5
68	A8	301	CDL	CA3-OA5-PA1-OA2
68	AN	201	CDL	CA3-OA5-PA1-OA2
68	Qh	102	CDL	CA2-OA2-PA1-OA5
70	B7	201	PC1	C1-O11-P-O13
70	QJ	101	PC1	C1-O11-P-O13
70	Qc	410	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
71	6A	103	PEE	C1-O3P-P-O4P
72	Qc	401	3PE	C11-O13-P-O11
76	N3	201	PLX	C2-O1-P1-O4
76	CB	201	PLX	C26-C27-C28-C29
68	AL	202	CDL	O1-C1-CA2-OA2
76	BL	202	PLX	C10-C11-C12-C13
76	S7	302	PLX	C9-C10-C11-C12
68	N2	401	CDL	CA4-CA3-OA5-PA1
71	N5	701	PEE	C2-C1-O3P-P
72	Qc	401	3PE	C2-C1-O11-P
83	QH	101	PX2	C2-C1-O4-P1
70	Qc	412	PC1	C34-C35-C36-C37
76	CB	201	PLX	C10-C11-C12-C13
68	4L	101	CDL	CB3-OB5-PB2-OB4
68	A7	201	CDL	CA3-OA5-PA1-OA4
68	A7	201	CDL	CB2-OB2-PB2-OB4
68	A7	201	CDL	CB3-OB5-PB2-OB3
68	A8	301	CDL	CA3-OA5-PA1-OA3
68	A8	301	CDL	CB2-OB2-PB2-OB3
68	AL	201	CDL	CB2-OB2-PB2-OB4
68	AL	204	CDL	CA3-OA5-PA1-OA3
68	AN	201	CDL	CB3-OB5-PB2-OB3
68	AN	203	CDL	CA2-OA2-PA1-OA4
68	AN	203	CDL	CB2-OB2-PB2-OB3
68	AN	203	CDL	CB3-OB5-PB2-OB3
68	B4	201	CDL	CA2-OA2-PA1-OA4
68	B5	201	CDL	CA2-OA2-PA1-OA4
68	B5	201	CDL	CB3-OB5-PB2-OB3
68	C1	607	CDL	CB3-OB5-PB2-OB4
68	N4	501	CDL	CB3-OB5-PB2-OB3
68	N5	702	CDL	CA3-OA5-PA1-OA4
68	N5	702	CDL	CB2-OB2-PB2-OB3
68	N5	703	CDL	CA2-OA2-PA1-OA3
68	N5	703	CDL	CB3-OB5-PB2-OB4
68	QB	501	CDL	CB2-OB2-PB2-OB3
68	QB	501	CDL	CB2-OB2-PB2-OB4
68	QB	501	CDL	CB3-OB5-PB2-OB4
68	QC	406	CDL	CA2-OA2-PA1-OA3
68	QC	406	CDL	CA2-OA2-PA1-OA4
68	QC	406	CDL	CA3-OA5-PA1-OA3
68	QC	406	CDL	CB2-OB2-PB2-OB4
68	QC	407	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
68	QD	402	CDL	CA2-OA2-PA1-OA4
68	QD	402	CDL	CA3-OA5-PA1-OA4
68	Qb	502	CDL	CA3-OA5-PA1-OA3
68	Qc	402	CDL	CB3-OB5-PB2-OB3
68	Qc	411	CDL	CB2-OB2-PB2-OB4
68	Qh	102	CDL	CB2-OB2-PB2-OB4
68	Qj	101	CDL	CA2-OA2-PA1-OA3
68	Qj	101	CDL	CB2-OB2-PB2-OB4
70	6A	101	PC1	C1-O11-P-O12
70	7A	101	PC1	C1-O11-P-O14
70	B8	201	PC1	C11-O13-P-O12
70	C1	606	PC1	C11-O13-P-O12
70	C3	301	PC1	C1-O11-P-O12
70	C3	304	PC1	C1-O11-P-O12
70	N1	401	PC1	C11-O13-P-O14
70	N1	401	PC1	C1-O11-P-O14
70	N4	502	PC1	C1-O11-P-O14
70	N5	705	PC1	C11-O13-P-O14
70	N6	201	PC1	C1-O11-P-O12
70	N6	201	PC1	C1-O11-P-O14
70	QB	502	PC1	C11-O13-P-O12
70	QB	502	PC1	C1-O11-P-O12
70	QB	503	PC1	C11-C12-N-C14
70	Qb	501	PC1	C11-O13-P-O12
70	Qc	407	PC1	C1-O11-P-O14
70	Qc	409	PC1	C1-O11-P-O12
70	Qc	409	PC1	C1-O11-P-O14
70	Qd	402	PC1	C11-O13-P-O14
70	Qh	103	PC1	C11-O13-P-O12
70	Qh	103	PC1	C11-O13-P-O14
71	A3	201	PEE	C1-O3P-P-O2P
71	AN	202	PEE	C1-O3P-P-O2P
71	AN	202	PEE	C1-O3P-P-O1P
71	AN	202	PEE	C4-O4P-P-O1P
71	BL	201	PEE	C1-O3P-P-O2P
71	BL	201	PEE	C4-O4P-P-O2P
71	C1	609	PEE	C4-O4P-P-O2P
71	C1	609	PEE	C4-O4P-P-O1P
71	C3	302	PEE	C4-O4P-P-O2P
71	C3	303	PEE	C1-O3P-P-O1P
71	N5	706	PEE	C1-O3P-P-O1P
71	N5	706	PEE	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
71	QC	404	PEE	C1-O3P-P-O1P
71	QE	302	PEE	C1-O3P-P-O1P
71	QH	102	PEE	C4-O4P-P-O2P
71	QH	102	PEE	C4-O4P-P-O1P
71	Qc	403	PEE	C1-O3P-P-O2P
71	Qe	302	PEE	C4-O4P-P-O1P
71	Qh	101	PEE	C1-O3P-P-O1P
71	Qh	101	PEE	C4-O4P-P-O2P
71	Qh	101	PEE	C4-O4P-P-O1P
72	7B	101	3PE	C1-O11-P-O12
72	Qc	406	3PE	C1-O11-P-O14
75	AK	401	ADP	C5'-O5'-PA-O2A
76	CB	201	PLX	C2-C1-N1-C1A
76	QE	301	PLX	C2-O1-P1-O3
76	S7	302	PLX	C3-O4-P1-O2
68	Qh	102	CDL	C79-C80-C81-C82
71	C1	609	PEE	C14-C15-C16-C17
68	C1	607	CDL	OB5-CB3-CB4-CB6
70	Qc	409	PC1	O11-C1-C2-C3
71	6A	103	PEE	O3P-C1-C2-C3
71	QC	403	PEE	O3P-C1-C2-C3
71	QC	405	PEE	O3P-C1-C2-C3
71	QH	102	PEE	O3P-C1-C2-C3
68	Qj	101	CDL	C52-C53-C54-C55
70	7A	101	PC1	C22-C23-C24-C25
70	B5	202	PC1	C29-C2A-C2B-C2C
76	S7	302	PLX	C17-C18-C19-C20
71	A7	202	PEE	C11-C12-C13-C14
71	6A	103	PEE	C37-C38-C39-C40
77	C1	603	HEA	C20-C21-C22-C23
68	AN	201	CDL	C15-C16-C17-C18
70	B7	201	PC1	C12-C11-O13-P
70	B8	201	PC1	C12-C11-O13-P
70	C1	608	PC1	C12-C11-O13-P
71	6A	103	PEE	C5-C4-O4P-P
71	Qc	408	PEE	C5-C4-O4P-P
76	AL	205	PLX	C1-C2-O1-P1
76	B1	101	PLX	C1-C2-O1-P1
76	BL	202	PLX	C25-C24-O8-C5
76	CB	201	PLX	C25-C24-O8-C5
76	N3	201	PLX	C25-C24-O8-C5
71	N5	706	PEE	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
76	CB	201	PLX	C14-C15-C16-C17
76	QI	102	PLX	C16-C17-C18-C19
71	QH	102	PEE	C15-C16-C17-C18
68	AN	201	CDL	CA7-C31-C32-C33
68	N5	703	CDL	C76-C77-C78-C79
71	Qe	302	PEE	C41-C42-C43-C44
68	AN	203	CDL	OB5-CB3-CB4-OB6
68	N2	401	CDL	OB5-CB3-CB4-OB6
68	QC	406	CDL	OA5-CA3-CA4-OA6
68	QC	407	CDL	OA5-CA3-CA4-OA6
70	Qc	407	PC1	O11-C1-C2-O21
71	A3	201	PEE	O3P-C1-C2-O2
71	C3	303	PEE	O3P-C1-C2-O2
71	QC	404	PEE	O3P-C1-C2-O2
85	V1	502	FMN	N10-C1'-C2'-C3'
71	N5	701	PEE	C24-C25-C26-C27
76	AM	201	PLX	C31-C32-C33-C34
71	BL	201	PEE	O3-C30-C31-C32
71	6A	103	PEE	C12-C13-C14-C15
71	QE	302	PEE	C31-C32-C33-C34
76	S7	302	PLX	C7-C8-C9-C10
68	N4	501	CDL	C34-C35-C36-C37
70	C3	301	PC1	C11-C12-N-C15
70	C3	304	PC1	C11-C12-N-C15
70	Qb	501	PC1	C11-C12-N-C13
70	Qc	410	PC1	C11-C12-N-C13
76	QI	102	PLX	C29-C30-C31-C32
76	S7	302	PLX	C29-C30-C31-C32
70	6A	101	PC1	O13-C11-C12-N
70	7A	101	PC1	O13-C11-C12-N
70	B7	201	PC1	O13-C11-C12-N
70	B8	201	PC1	O13-C11-C12-N
70	C1	606	PC1	O13-C11-C12-N
70	C1	608	PC1	O13-C11-C12-N
70	C3	301	PC1	O13-C11-C12-N
70	C3	304	PC1	O13-C11-C12-N
70	C4	201	PC1	O13-C11-C12-N
70	N1	401	PC1	C39-C3A-C3B-C3C
70	N5	705	PC1	C1-C2-C3-O31
70	QB	502	PC1	O13-C11-C12-N
70	QI	101	PC1	O13-C11-C12-N
70	QJ	101	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
70	Qc	407	PC1	O13-C11-C12-N
70	Qc	409	PC1	O13-C11-C12-N
70	Qc	410	PC1	O13-C11-C12-N
70	S8	304	PC1	O13-C11-C12-N
71	AN	202	PEE	C1-C2-C3-O3
71	N5	704	PEE	C1-C2-C3-O3
72	CA	101	3PE	C2B-C2C-C2D-C2E
76	AM	201	PLX	N1-C1-C2-O1
76	B1	101	PLX	N1-C1-C2-O1
76	QI	102	PLX	C3-C4-C5-O8
76	S7	302	PLX	N1-C1-C2-O1
68	QD	402	CDL	OA6-CA4-CA6-OA8
68	Qc	411	CDL	OA6-CA4-CA6-OA8
71	QE	302	PEE	O2-C2-C3-O3
71	Qc	403	PEE	O2-C2-C3-O3
76	BL	202	PLX	O6-C4-C5-O8
72	7B	101	3PE	C34-C35-C36-C37
68	AN	201	CDL	C35-C36-C37-C38
70	QI	101	PC1	C32-C33-C34-C35
70	B5	202	PC1	C3E-C3F-C3G-C3H
70	B7	201	PC1	C2-C1-O11-P
70	QJ	101	PC1	O31-C31-C32-C33
71	QC	405	PEE	C34-C35-C36-C37
71	QE	302	PEE	C12-C13-C14-C15
72	CB	202	3PE	C32-C33-C34-C35
68	B4	201	CDL	CA5-C11-C12-C13
71	A3	201	PEE	C12-C13-C14-C15
71	N5	704	PEE	C24-C25-C26-C27
76	AL	205	PLX	O8-C24-C25-C26
76	BL	202	PLX	O8-C24-C25-C26
76	N3	201	PLX	O6-C6-C7-C8
70	N6	201	PC1	C38-C39-C3A-C3B
74	AC	201	ZMP	O3-C16-C17-O4
70	B8	201	PC1	C22-C23-C24-C25
72	Qc	406	3PE	C35-C36-C37-C38
68	Qc	411	CDL	C72-C71-CB7-OB8
76	BL	202	PLX	O9-C24-C25-C26
76	CB	201	PLX	O7-C6-C7-C8
76	N3	201	PLX	O7-C6-C7-C8
70	N4	502	PC1	C33-C34-C35-C36
71	N5	704	PEE	C22-C23-C24-C25
70	Qh	103	PC1	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
70	Qd	402	PC1	C38-C39-C3A-C3B
71	6A	102	PEE	C37-C38-C39-C40
70	C3	304	PC1	C2A-C2B-C2C-C2D
76	C2	301	PLX	C25-C26-C27-C28
72	CB	202	3PE	C31-C32-C33-C34
70	B5	202	PC1	C27-C28-C29-C2A
70	C1	606	PC1	C27-C28-C29-C2A
70	C1	608	PC1	C22-C23-C24-C25
70	Qd	402	PC1	C2A-C2B-C2C-C2D
70	N3	202	PC1	C24-C25-C26-C27
72	7B	101	3PE	C25-C26-C27-C28
76	S7	302	PLX	C15-C16-C17-C18
70	QB	502	PC1	C3-C2-O21-C21
71	C3	302	PEE	C3-C2-O2-C10
71	CB	203	PEE	C3-C2-O2-C10
71	QC	404	PEE	C1-C2-O2-C10
70	7C	101	PC1	O11-C1-C2-C3
76	BL	202	PLX	O4-C3-C4-C5
71	N5	704	PEE	C13-C14-C15-C16
68	QC	406	CDL	C32-C33-C34-C35
70	Qc	410	PC1	C33-C34-C35-C36
71	6A	103	PEE	C23-C24-C25-C26
71	N5	704	PEE	C16-C17-C18-C19
68	A8	301	CDL	C1-CA2-OA2-PA1
68	AL	204	CDL	CB4-CB3-OB5-PB2
68	AN	203	CDL	CA4-CA3-OA5-PA1
71	Qe	302	PEE	C2-C3-O3-C30
71	AN	202	PEE	O5-C30-O3-C3
68	N4	501	CDL	OA5-CA3-CA4-OA6
70	C1	606	PC1	O11-C1-C2-O21
76	C2	301	PLX	O4-C3-C4-O6
71	Qc	408	PEE	C37-C38-C39-C40
70	C3	304	PC1	C11-C12-N-C14
76	CB	201	PLX	C2-C1-N1-C1B
68	Qh	102	CDL	C11-C12-C13-C14
70	QB	502	PC1	C38-C39-C3A-C3B
70	7A	101	PC1	C21-C22-C23-C24
71	N5	704	PEE	C18-C19-C20-C21
71	Qc	408	PEE	O2-C2-C3-O3
83	QH	101	PX2	O7-C2-C3-O5
70	N4	502	PC1	C34-C35-C36-C37
68	AL	202	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
68	N2	401	CDL	CA3-OA5-PA1-OA2
68	N4	501	CDL	CA2-OA2-PA1-OA5
68	Qc	411	CDL	CA3-OA5-PA1-OA2
70	6A	101	PC1	C11-O13-P-O11
70	B8	201	PC1	C1-O11-P-O13
70	C1	608	PC1	C1-O11-P-O13
70	C3	301	PC1	C11-O13-P-O11
70	QI	101	PC1	C1-O11-P-O13
71	C1	609	PEE	C1-O3P-P-O4P
71	QC	403	PEE	C1-O3P-P-O4P
72	Qc	406	3PE	C1-O11-P-O13
76	AM	201	PLX	C3-O4-P1-O1
76	AM	201	PLX	C2-O1-P1-O4
76	BL	202	PLX	C2-O1-P1-O4
76	CB	201	PLX	C2-O1-P1-O4
76	S7	302	PLX	C2-O1-P1-O4
71	QC	405	PEE	C13-C14-C15-C16
72	7B	101	3PE	C27-C28-C29-C2A
75	AK	401	ADP	O4'-C4'-C5'-O5'
68	N4	501	CDL	C73-C74-C75-C76
70	C1	610	PC1	C31-C32-C33-C34
70	C1	606	PC1	C29-C2A-C2B-C2C
68	QB	501	CDL	CB3-CB4-CB6-OB8
71	Qc	408	PEE	C1-C2-C3-O3
68	A8	301	CDL	C14-C15-C16-C17
71	6A	102	PEE	C12-C13-C14-C15
70	QI	101	PC1	C3B-C3C-C3D-C3E
70	C1	606	PC1	C11-C12-N-C14
70	QI	101	PC1	C11-C12-N-C13
71	Qh	101	PEE	C34-C35-C36-C37
71	AL	206	PEE	C35-C36-C37-C38
73	A9	401	NDP	O4D-C1D-N1N-C6N
68	Qh	102	CDL	C62-C63-C64-C65
76	B1	101	PLX	C26-C27-C28-C29
71	CB	203	PEE	C13-C14-C15-C16
76	BL	202	PLX	C11-C10-C9-C8
68	4L	101	CDL	CA4-CA3-OA5-PA1
68	Qc	411	CDL	C1-CA2-OA2-PA1
70	7C	101	PC1	C2-C1-O11-P
71	6A	102	PEE	C2-C1-O3P-P
71	6A	102	PEE	C36-C37-C38-C39
71	S8	303	PEE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
70	QI	101	PC1	C2A-C2B-C2C-C2D
71	Qb	503	PEE	C31-C32-C33-C34
76	CB	201	PLX	C6-C7-C8-C9
68	AN	201	CDL	C51-C52-C53-C54
71	Qb	503	PEE	C33-C34-C35-C36
70	N5	705	PC1	C21-C22-C23-C24
71	AN	202	PEE	C31-C30-O3-C3
70	Qc	412	PC1	C2C-C2D-C2E-C2F
71	8B	101	PEE	C35-C36-C37-C38
68	AN	203	CDL	CA7-C31-C32-C33
68	N5	703	CDL	C59-C60-C61-C62
80	Qc	405	HEM	CAD-CBD-CGD-O1D
71	BL	201	PEE	C11-C12-C13-C14
83	QH	101	PX2	C24-C25-C26-C27
70	C3	301	PC1	C11-C12-N-C13
70	QB	502	PC1	C11-C12-N-C14
70	Qb	501	PC1	C11-C12-N-C14
70	Qc	412	PC1	O22-C21-O21-C2
76	AL	205	PLX	O4-C3-C4-C5
71	AL	206	PEE	C13-C14-C15-C16
70	7A	101	PC1	C23-C24-C25-C26
77	C1	603	HEA	C27-C19-C20-C21
71	AL	206	PEE	C15-C16-C17-C18
71	N5	701	PEE	C35-C36-C37-C38
71	S8	303	PEE	C19-C20-C21-C22
74	AB	201	ZMP	O3-C16-C17-C18
68	A7	201	CDL	C73-C74-C75-C76
71	6A	103	PEE	C41-C42-C43-C44
80	Qc	404	HEM	CAA-CBA-CGA-O1A
72	C1	601	3PE	C23-C24-C25-C26
70	Qc	410	PC1	C26-C27-C28-C29
80	QC	401	HEM	CAA-CBA-CGA-O1A
71	BL	201	PEE	O2-C2-C3-O3
71	C1	609	PEE	O2-C2-C3-O3
76	AM	201	PLX	O8-C24-C25-C26
71	QE	302	PEE	C34-C35-C36-C37
68	B4	201	CDL	CA4-CA3-OA5-PA1
71	6A	102	PEE	C40-C41-C42-C43
80	Qc	405	HEM	CAA-CBA-CGA-O1A
70	QB	503	PC1	C11-C12-N-C13
73	A9	401	NDP	C2D-C1D-N1N-C6N
71	QC	405	PEE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
70	B8	201	PC1	C2B-C2C-C2D-C2E
76	N3	201	PLX	C18-C19-C20-C21
77	C1	602	HEA	CAD-CBD-CGD-O1D
71	Qb	503	PEE	C35-C36-C37-C38
68	Qj	101	CDL	CB5-C51-C52-C53
68	AL	201	CDL	C31-C32-C33-C34
68	N2	401	CDL	C11-C12-C13-C14
71	N5	701	PEE	C14-C15-C16-C17
68	QC	406	CDL	C42-C43-C44-C45
77	C1	602	HEA	CAD-CBD-CGD-O2D
77	C1	603	HEA	CAA-CBA-CGA-O1A
80	QC	401	HEM	CAA-CBA-CGA-O2A
68	N5	703	CDL	C73-C74-C75-C76
70	B5	202	PC1	C2C-C2D-C2E-C2F
68	AL	202	CDL	C52-C53-C54-C55
68	AL	204	CDL	CB3-CB4-CB6-OB8
68	N2	401	CDL	CB3-CB4-CB6-OB8
68	N5	703	CDL	CB3-CB4-CB6-OB8
68	Qh	102	CDL	CB2-C1-CA2-OA2
68	Qj	101	CDL	CA3-CA4-CA6-OA8
71	6A	102	PEE	O4-C10-O2-C2
71	AN	202	PEE	O4-C10-O2-C2
80	QC	401	HEM	CAD-CBD-CGD-O1D
80	Qc	404	HEM	CAA-CBA-CGA-O2A
80	Qc	404	HEM	CAD-CBD-CGD-O2D
68	QC	406	CDL	C72-C73-C74-C75
71	Qe	302	PEE	C21-C22-C23-C24
70	N6	201	PC1	C3E-C3F-C3G-C3H
71	QH	102	PEE	C32-C33-C34-C35
80	QC	402	HEM	CAA-CBA-CGA-O2A
80	Qc	405	HEM	CAD-CBD-CGD-O2D
74	AC	201	ZMP	N2-C16-C17-C18
68	B5	201	CDL	C35-C36-C37-C38
71	C3	302	PEE	C39-C40-C41-C42
76	QE	301	PLX	C6-C7-C8-C9
71	QE	302	PEE	C40-C41-C42-C43
71	Qe	302	PEE	C14-C15-C16-C17
68	AL	202	CDL	CB3-CB4-OB6-CB5
68	B5	201	CDL	CB6-CB4-OB6-CB5
68	QB	501	CDL	CA6-CA4-OA6-CA5
68	Qb	502	CDL	CA6-CA4-OA6-CA5
68	Qj	101	CDL	CA6-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
70	Qc	412	PC1	C3-C2-O21-C21
70	S8	304	PC1	C1-C2-O21-C21
71	8B	101	PEE	C3-C2-O2-C10
71	QC	404	PEE	C3-C2-O2-C10
68	Qh	102	CDL	C55-C56-C57-C58
71	A3	201	PEE	C31-C32-C33-C34
70	C3	304	PC1	C11-C12-N-C13
70	Qb	501	PC1	C11-C12-N-C15
68	C1	607	CDL	C32-C31-CA7-OA8
70	6A	101	PC1	O31-C31-C32-C33
71	Qe	302	PEE	C16-C17-C18-C19
71	QE	302	PEE	C21-C22-C23-C24
76	CB	201	PLX	C20-C21-C22-C23
68	N5	703	CDL	C16-C17-C18-C19
72	Qc	406	3PE	C26-C27-C28-C29
70	N4	502	PC1	C1-O11-P-O13
71	QC	404	PEE	C1-O3P-P-O4P
77	C1	602	HEA	CAA-CBA-CGA-O2A
80	Qc	405	HEM	CAA-CBA-CGA-O2A
68	A7	201	CDL	CA4-CA3-OA5-PA1
71	AN	202	PEE	C2-C1-O3P-P
72	CA	101	3PE	O31-C31-C32-C33
77	C1	603	HEA	CAD-CBD-CGD-O2D
80	QC	402	HEM	CAA-CBA-CGA-O1A
76	CB	201	PLX	C18-C19-C20-C21
68	C1	607	CDL	OA5-CA3-CA4-CA6
68	Qc	411	CDL	OB5-CB3-CB4-CB6
70	C1	606	PC1	O11-C1-C2-C3
71	QC	404	PEE	O3P-C1-C2-C3
80	Qc	404	HEM	CAD-CBD-CGD-O1D
68	B5	201	CDL	C71-C72-C73-C74
70	B7	201	PC1	C36-C37-C38-C39
70	N6	201	PC1	C37-C38-C39-C3A
77	C1	603	HEA	CAA-CBA-CGA-O2A
72	7B	101	3PE	C2E-C2F-C2G-C2H
70	C1	608	PC1	C24-C25-C26-C27
68	Qb	502	CDL	CB5-C51-C52-C53
70	C3	301	PC1	C11-C12-N-C14
71	AL	203	PEE	C44-C45-C46-C47
71	N5	704	PEE	C31-C30-O3-C3
71	S8	303	PEE	C31-C32-C33-C34
68	AN	201	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
80	QC	401	HEM	CAD-CBD-CGD-O2D
74	AC	201	ZMP	C5-C6-C7-C8
68	AL	202	CDL	CB2-C1-CA2-OA2
68	AL	202	CDL	CA2-C1-CB2-OB2
70	Qd	402	PC1	C39-C3A-C3B-C3C
76	B1	101	PLX	C24-C25-C26-C27
70	B5	202	PC1	O31-C31-C32-C33
71	A7	202	PEE	O2-C10-C11-C12
71	N5	701	PEE	O5-C30-C31-C32
68	QC	406	CDL	C81-C82-C83-C84
70	N4	502	PC1	C3A-C3B-C3C-C3D
70	QI	101	PC1	C27-C28-C29-C2A
71	A7	202	PEE	O3-C30-C31-C32
76	S7	302	PLX	C13-C14-C15-C16
71	N5	704	PEE	O5-C30-O3-C3
71	6A	102	PEE	C15-C16-C17-C18
68	4L	101	CDL	C21-C22-C23-C24
71	AL	206	PEE	C31-C32-C33-C34
71	C1	609	PEE	C32-C33-C34-C35
70	Qc	412	PC1	C26-C27-C28-C29
76	N3	201	PLX	C3-C4-C5-O8
70	QI	101	PC1	C39-C3A-C3B-C3C
71	N5	701	PEE	C20-C21-C22-C23
71	AN	202	PEE	C11-C10-O2-C2
72	CA	101	3PE	C2A-C2B-C2C-C2D
68	Qh	102	CDL	C74-C75-C76-C77
70	C1	610	PC1	C39-C3A-C3B-C3C
68	AN	201	CDL	C33-C34-C35-C36
70	Qc	409	PC1	O11-C1-C2-O21
71	QE	302	PEE	O3P-C1-C2-O2
72	7B	101	3PE	O11-C1-C2-O21
72	CA	101	3PE	O11-C1-C2-O21
70	C1	610	PC1	C37-C38-C39-C3A
77	C1	603	HEA	CAD-CBD-CGD-O1D
71	A7	202	PEE	C32-C33-C34-C35
72	Qc	406	3PE	C33-C34-C35-C36
76	BL	202	PLX	O6-C6-C7-C8
74	AC	201	ZMP	C1-C22-C23-C24
71	Qc	408	PEE	C13-C14-C15-C16
70	Qb	501	PC1	O11-C1-C2-C3
68	AN	201	CDL	C32-C31-CA7-OA8
71	A3	201	PEE	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
71	C3	302	PEE	C32-C33-C34-C35
71	N5	704	PEE	C40-C41-C42-C43
68	A7	201	CDL	CB4-CB3-OB5-PB2
70	B5	202	PC1	C2-C1-O11-P
71	AL	203	PEE	C2-C1-O3P-P
71	BL	201	PEE	C35-C36-C37-C38
71	Qe	302	PEE	C15-C16-C17-C18
68	AL	204	CDL	OB6-CB4-CB6-OB8
76	QE	301	PLX	O6-C4-C5-O8
68	AL	204	CDL	C31-CA7-OA8-CA6
71	6A	103	PEE	C40-C41-C42-C43
68	AN	203	CDL	C38-C39-C40-C41
70	Qd	402	PC1	C23-C24-C25-C26
68	QB	501	CDL	C32-C31-CA7-OA8
70	B5	202	PC1	C2B-C2C-C2D-C2E
68	N4	501	CDL	C41-C42-C43-C44
68	QC	406	CDL	C83-C84-C85-C86
71	AN	202	PEE	C36-C37-C38-C39
71	C3	303	PEE	C36-C37-C38-C39
71	Qh	101	PEE	C36-C37-C38-C39
68	Qj	101	CDL	C75-C76-C77-C78
70	7A	101	PC1	C39-C3A-C3B-C3C
71	QC	403	PEE	C32-C33-C34-C35
74	AC	201	ZMP	N2-C16-C17-O4
68	AL	202	CDL	C32-C31-CA7-OA8
68	B4	201	CDL	C32-C31-CA7-OA8
70	Qc	407	PC1	O21-C21-C22-C23
68	C1	607	CDL	C76-C77-C78-C79
68	N5	702	CDL	C13-C14-C15-C16
72	7B	101	3PE	C24-C25-C26-C27
72	Qc	406	3PE	C3A-C3B-C3C-C3D
76	B1	101	PLX	C3-O4-P1-O1
68	N5	702	CDL	C60-C61-C62-C63
68	AL	204	CDL	C52-C51-CB5-OB6
68	4L	101	CDL	C73-C74-C75-C76
81	Qd	401	HEC	CAA-CBA-CGA-O2A
76	CB	201	PLX	C29-C30-C31-C32
76	QI	102	PLX	C33-C34-C35-C36
70	7A	101	PC1	O21-C21-C22-C23
70	C1	608	PC1	O31-C31-C32-C33
70	N6	201	PC1	O21-C21-C22-C23
71	AL	203	PEE	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
71	BL	201	PEE	C36-C37-C38-C39
71	QC	405	PEE	C18-C19-C20-C21
71	QE	302	PEE	C18-C19-C20-C21
71	Qc	408	PEE	C18-C19-C20-C21
71	Qc	408	PEE	C38-C39-C40-C41
71	Qe	302	PEE	C36-C37-C38-C39
68	AN	203	CDL	CB6-CB4-OB6-CB5
68	B4	201	CDL	CB3-CB4-OB6-CB5
70	7A	101	PC1	C1-C2-O21-C21
70	C3	301	PC1	C3-C2-O21-C21
70	N3	202	PC1	C1-C2-O21-C21
70	N3	202	PC1	C3-C2-O21-C21
72	Qc	406	3PE	C3-C2-O21-C21
70	Qh	103	PC1	C27-C28-C29-C2A
71	AL	203	PEE	O4-C10-O2-C2
71	6A	103	PEE	C42-C43-C44-C45
72	CB	202	3PE	C37-C38-C39-C3A
68	4L	101	CDL	C12-C11-CA5-OA6
68	AN	201	CDL	C72-C71-CB7-OB8
68	N5	703	CDL	C12-C11-CA5-OA6
68	QD	402	CDL	C72-C71-CB7-OB8
68	Qj	101	CDL	C72-C71-CB7-OB8
71	6A	102	PEE	O2-C10-C11-C12
68	N4	501	CDL	C76-C77-C78-C79
70	Qc	410	PC1	C2C-C2D-C2E-C2F
74	AB	201	ZMP	C13-C14-C15-N2
70	7C	101	PC1	C31-C32-C33-C34
70	QB	502	PC1	C3C-C3D-C3E-C3F
72	CB	202	3PE	C34-C35-C36-C37
68	QC	407	CDL	C72-C71-CB7-OB8
70	C1	606	PC1	O21-C21-C22-C23
71	Qh	101	PEE	O2-C10-C11-C12
72	Qc	401	3PE	O21-C21-C22-C23
70	C1	610	PC1	C26-C27-C28-C29
71	N5	704	PEE	C34-C35-C36-C37
71	C3	302	PEE	C36-C37-C38-C39
71	Qb	503	PEE	C38-C39-C40-C41
68	C1	607	CDL	CB3-CB4-CB6-OB8
70	B7	201	PC1	C1-C2-C3-O31
71	A3	201	PEE	C40-C41-C42-C43
70	7C	101	PC1	O11-C1-C2-O21
68	QC	406	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
70	Qc	410	PC1	O21-C21-C22-C23
71	Qc	403	PEE	O2-C10-C11-C12
72	Qc	401	3PE	O31-C31-C32-C33
70	S8	304	PC1	C11-C12-N-C13
71	S8	303	PEE	C22-C23-C24-C25
76	AL	205	PLX	C10-C11-C12-C13
68	N5	703	CDL	C75-C76-C77-C78
68	4L	101	CDL	C52-C51-CB5-OB6
70	B7	201	PC1	O31-C31-C32-C33
70	N3	202	PC1	O21-C21-C22-C23
71	AL	206	PEE	C16-C17-C18-C19
71	N5	701	PEE	C16-C17-C18-C19
68	AN	201	CDL	O1-C1-CA2-OA2
68	N4	501	CDL	C77-C78-C79-C80
70	QJ	101	PC1	C26-C27-C28-C29
81	QD	401	HEC	CAA-CBA-CGA-O2A
71	QC	404	PEE	O3-C30-C31-C32
71	QC	403	PEE	C20-C21-C22-C23
71	QC	405	PEE	C21-C22-C23-C24
71	Qh	101	PEE	C33-C34-C35-C36
71	C1	609	PEE	C15-C16-C17-C18
71	QC	405	PEE	C19-C20-C21-C22
68	AL	202	CDL	C32-C33-C34-C35
68	AL	202	CDL	C36-C37-C38-C39
70	B7	201	PC1	C35-C36-C37-C38
71	AN	202	PEE	C34-C35-C36-C37
71	6A	102	PEE	C11-C10-O2-C2
68	QC	406	CDL	OA5-CA3-CA4-CA6
68	Qc	402	CDL	OB5-CB3-CB4-CB6
72	7B	101	3PE	O11-C1-C2-C3
68	AN	201	CDL	C14-C15-C16-C17
70	C1	610	PC1	O21-C21-C22-C23
71	AN	202	PEE	O3-C30-C31-C32
68	C1	607	CDL	OB6-CB4-CB6-OB8
68	N2	401	CDL	OB6-CB4-CB6-OB8
72	Qc	401	3PE	O21-C2-C3-O31
71	Qh	101	PEE	C38-C39-C40-C41
68	N5	702	CDL	C12-C11-CA5-OA6
71	8B	101	PEE	O3-C30-C31-C32
71	AN	202	PEE	O2-C10-C11-C12
71	CB	203	PEE	O2-C10-C11-C12
70	Qc	409	PC1	C11-C12-N-C15

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Mol	Chain	Res	Type	Atoms
73	A9	401	NDP	C2B-O2B-P2B-O2X
72	CB	202	3PE	C26-C27-C28-C29
68	N5	703	CDL	C74-C75-C76-C77
70	B5	202	PC1	C3F-C3G-C3H-C3I
70	C1	608	PC1	C28-C29-C2A-C2B
68	AN	203	CDL	C32-C31-CA7-OA8
70	Qc	412	PC1	O21-C21-C22-C23
71	C3	302	PEE	O3-C30-C31-C32
71	S8	303	PEE	C39-C40-C41-C42
76	QI	102	PLX	C20-C21-C22-C23
71	N5	704	PEE	C2-C1-O3P-P
71	BL	201	PEE	O4-C10-O2-C2
71	Qc	408	PEE	C36-C37-C38-C39
71	S8	303	PEE	O2-C10-C11-C12
81	QD	401	HEC	CAD-CBD-CGD-O2D
68	B4	201	CDL	C72-C71-CB7-OB8
71	AL	203	PEE	O2-C10-C11-C12
71	C3	302	PEE	C34-C35-C36-C37
68	Qj	101	CDL	C51-C52-C53-C54
70	7C	101	PC1	C33-C34-C35-C36
70	Qd	402	PC1	C3C-C3D-C3E-C3F
71	BL	201	PEE	C20-C21-C22-C23
73	A9	401	NDP	O4B-C4B-C5B-O5B
72	7B	101	3PE	O31-C31-C32-C33
68	A7	201	CDL	C72-C71-CB7-OB9
76	CB	201	PLX	C25-C26-C27-C28
70	C3	304	PC1	O21-C21-C22-C23
70	N4	502	PC1	O21-C21-C22-C23
74	AB	201	ZMP	C2-C1-C22-C23
71	CB	203	PEE	C18-C19-C20-C21
71	Qb	503	PEE	C16-C17-C18-C19
70	QB	502	PC1	C11-C12-N-C13
70	QI	101	PC1	C11-C12-N-C14
70	QI	101	PC1	C11-C12-N-C15
68	QC	407	CDL	C72-C71-CB7-OB9
68	QD	402	CDL	C72-C71-CB7-OB9
71	C3	302	PEE	C31-C32-C33-C34
70	N4	502	PC1	C25-C26-C27-C28
81	Qd	401	HEC	CAA-CBA-CGA-O1A
68	AL	202	CDL	C32-C31-CA7-OA9
68	N5	703	CDL	C12-C11-CA5-OA7
70	N6	201	PC1	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
70	Qc	407	PC1	C2A-C2B-C2C-C2D
72	Qc	401	3PE	O32-C31-C32-C33
71	C3	302	PEE	C18-C19-C20-C21
71	BL	201	PEE	C12-C13-C14-C15
68	AN	201	CDL	C72-C71-CB7-OB9
68	AN	203	CDL	C32-C31-CA7-OA9
68	B4	201	CDL	C32-C31-CA7-OA9
68	Qj	101	CDL	C72-C71-CB7-OB9
70	C1	606	PC1	O22-C21-C22-C23
70	N3	202	PC1	O22-C21-C22-C23
71	QC	404	PEE	O5-C30-C31-C32
71	Qh	101	PEE	O4-C10-C11-C12
68	A8	301	CDL	C12-C13-C14-C15
68	Qh	102	CDL	C58-C59-C60-C61
68	AL	204	CDL	CA3-CA4-CA6-OA8
70	Qc	410	PC1	C1-C2-C3-O31
71	AL	203	PEE	C1-C2-C3-O3
76	QE	301	PLX	C3-C4-C5-O8
76	AL	205	PLX	C24-C25-C26-C27
70	Qc	409	PC1	C11-O13-P-O11
71	AL	206	PEE	C11-C12-C13-C14
70	Qc	407	PC1	O22-C21-C22-C23
71	6A	102	PEE	O4-C10-C11-C12
68	N5	702	CDL	C32-C33-C34-C35
70	B7	201	PC1	O21-C21-C22-C23
68	AL	202	CDL	C1-CB2-OB2-PB2
70	QB	503	PC1	C31-C32-C33-C34
68	AL	204	CDL	C52-C51-CB5-OB7
68	QB	501	CDL	C32-C31-CA7-OA9
70	C1	608	PC1	O32-C31-C32-C33
70	C1	610	PC1	O22-C21-C22-C23
70	QJ	101	PC1	C27-C28-C29-C2A
68	4L	101	CDL	CA3-OA5-PA1-OA3
68	AN	201	CDL	CA2-OA2-PA1-OA3
68	AN	201	CDL	CA2-OA2-PA1-OA4
68	N2	401	CDL	CA3-OA5-PA1-OA3
68	N5	703	CDL	CA3-OA5-PA1-OA3
68	QC	407	CDL	CA3-OA5-PA1-OA3
68	QC	407	CDL	CA3-OA5-PA1-OA4
68	Qh	102	CDL	CB3-OB5-PB2-OB3
70	6A	101	PC1	C11-O13-P-O12
70	B8	201	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
70	C1	606	PC1	C11-C12-N-C13
70	C1	606	PC1	C11-C12-N-C15
70	C3	301	PC1	C11-O13-P-O12
70	N1	401	PC1	C11-C12-N-C13
70	QB	502	PC1	C11-C12-N-C15
70	QJ	101	PC1	C1-O11-P-O12
70	Qc	409	PC1	C11-O13-P-O14
70	Qc	410	PC1	C11-O13-P-O12
71	C3	302	PEE	C1-O3P-P-O1P
71	N5	704	PEE	C4-O4P-P-O1P
71	Qh	101	PEE	C1-O3P-P-O2P
72	Qc	401	3PE	C1-O11-P-O14
76	CB	201	PLX	C3-O4-P1-O3
76	CB	201	PLX	C2-O1-P1-O2
76	N3	201	PLX	C2-O1-P1-O2
70	B7	201	PC1	O32-C31-C32-C33
71	C3	302	PEE	O5-C30-C31-C32
71	QE	302	PEE	O3P-C1-C2-C3
70	Qc	407	PC1	C27-C28-C29-C2A
71	AL	206	PEE	O4P-C4-C5-N
71	BL	201	PEE	O4P-C4-C5-N
71	N5	706	PEE	O4P-C4-C5-N
68	QC	406	CDL	C32-C31-CA7-OA9
71	Qc	403	PEE	O4-C10-C11-C12
68	AN	203	CDL	C72-C71-CB7-OB8
68	Qc	402	CDL	C71-C72-C73-C74
68	B5	201	CDL	C22-C23-C24-C25
68	N5	703	CDL	C56-C57-C58-C59
70	B8	201	PC1	C24-C25-C26-C27
70	Qc	412	PC1	C37-C38-C39-C3A
71	8B	101	PEE	O5-C30-C31-C32
71	AN	202	PEE	O5-C30-C31-C32
71	S8	303	PEE	O4-C10-C11-C12
72	Qc	401	3PE	O22-C21-C22-C23
71	QH	102	PEE	C16-C17-C18-C19
72	7B	101	3PE	C2D-C2E-C2F-C2G
81	QD	401	HEC	CAD-CBD-CGD-O1D
68	A8	301	CDL	C72-C71-CB7-OB8
70	QB	502	PC1	C3D-C3E-C3F-C3G
71	Qh	101	PEE	C23-C24-C25-C26
71	N5	704	PEE	C37-C38-C39-C40
70	7A	101	PC1	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
71	AN	202	PEE	O4-C10-C11-C12
71	AL	203	PEE	C11-C10-O2-C2
68	QC	406	CDL	C78-C79-C80-C81
71	N5	701	PEE	C13-C14-C15-C16
81	QD	401	HEC	CAA-CBA-CGA-O1A
68	AL	202	CDL	CB6-CB4-OB6-CB5
68	AN	201	CDL	CA3-CA4-OA6-CA5
68	AN	201	CDL	CA6-CA4-OA6-CA5
68	AN	203	CDL	CB3-CB4-OB6-CB5
68	B4	201	CDL	CB6-CB4-OB6-CB5
68	QB	501	CDL	CA3-CA4-OA6-CA5
68	Qc	402	CDL	CA3-CA4-OA6-CA5
68	Qc	402	CDL	CA6-CA4-OA6-CA5
68	Qc	411	CDL	CA3-CA4-OA6-CA5
68	Qc	411	CDL	CA6-CA4-OA6-CA5
70	C1	606	PC1	C12-C11-O13-P
70	C3	301	PC1	C1-C2-O21-C21
70	C3	304	PC1	C12-C11-O13-P
70	C4	201	PC1	C1-C2-O21-C21
70	C4	201	PC1	C3-C2-O21-C21
70	N4	502	PC1	C12-C11-O13-P
70	N5	705	PC1	C12-C11-O13-P
70	QB	502	PC1	C12-C11-O13-P
71	8B	101	PEE	C1-C2-O2-C10
71	A7	202	PEE	C5-C4-O4P-P
71	AL	203	PEE	C5-C4-O4P-P
71	C3	303	PEE	C5-C4-O4P-P
71	QC	404	PEE	C5-C4-O4P-P
71	Qh	101	PEE	C5-C4-O4P-P
72	Qc	406	3PE	C1-C2-O21-C21
74	AC	201	ZMP	O3-C16-C17-C18
77	C1	602	HEA	C4D-C3D-CAD-CBD
68	AL	204	CDL	OA9-CA7-OA8-CA6
68	4L	101	CDL	C12-C11-CA5-OA7
70	Qc	410	PC1	O22-C21-C22-C23
68	Qh	102	CDL	C38-C39-C40-C41
70	QB	503	PC1	O31-C31-C32-C33
76	QI	102	PLX	C9-C10-C11-C12
68	Qj	101	CDL	C18-C19-C20-C21
70	6A	101	PC1	C36-C37-C38-C39
70	C3	301	PC1	C3B-C3C-C3D-C3E
68	N5	702	CDL	C12-C11-CA5-OA7

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Mol	Chain	Res	Type	Atoms
68	AL	202	CDL	C52-C51-CB5-OB6
68	N5	702	CDL	C52-C51-CB5-OB6
68	Qh	102	CDL	C12-C11-CA5-OA6
72	C1	601	3PE	O31-C31-C32-C33
68	A7	201	CDL	C16-C17-C18-C19
68	Qh	102	CDL	C39-C40-C41-C42
70	N1	401	PC1	C3B-C3C-C3D-C3E
70	QJ	101	PC1	C39-C3A-C3B-C3C
70	C4	201	PC1	C22-C23-C24-C25
68	AL	201	CDL	C72-C71-CB7-OB8
68	N4	501	CDL	C72-C71-CB7-OB8
68	AL	204	CDL	C52-C53-C54-C55
76	B1	101	PLX	C14-C15-C16-C17
68	4L	101	CDL	C52-C51-CB5-OB7
70	B7	201	PC1	O22-C21-C22-C23
71	CB	203	PEE	O4-C10-C11-C12
72	7B	101	3PE	O32-C31-C32-C33
68	AL	201	CDL	C38-C39-C40-C41
70	N1	401	PC1	C24-C25-C26-C27
68	AL	202	CDL	CA4-CA3-OA5-PA1
68	Qj	101	CDL	C1-CB2-OB2-PB2
70	N1	401	PC1	C2-C1-O11-P
70	N6	201	PC1	C2-C1-O11-P
76	N3	201	PLX	C35-C36-C37-C38
74	AB	201	ZMP	C16-C17-C18-C21
68	N4	501	CDL	C72-C71-CB7-OB9
68	Qh	102	CDL	C12-C11-CA5-OA7
70	QB	503	PC1	O32-C31-C32-C33
70	N4	502	PC1	C2F-C2G-C2H-C2I
76	BL	202	PLX	C11-C12-C13-C14
68	Qc	402	CDL	C72-C71-CB7-OB8
68	C1	607	CDL	C53-C54-C55-C56
70	C4	201	PC1	O31-C31-C32-C33
70	B7	201	PC1	C3E-C3F-C3G-C3H
72	C1	601	3PE	O32-C31-C32-C33
68	C1	607	CDL	C33-C34-C35-C36
71	N5	706	PEE	C18-C19-C20-C21
68	N4	501	CDL	C60-C61-C62-C63
76	QE	301	PLX	C26-C27-C28-C29
71	N5	704	PEE	C11-C12-C13-C14

There are no ring outliers.

110 monomers are involved in 409 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
71	AN	202	PEE	5	0
70	N5	705	PC1	2	0
68	N5	703	CDL	5	0
84	S8	302	SF4	2	0
68	AL	201	CDL	3	0
77	C1	602	HEA	11	0
71	A7	202	PEE	1	0
70	C3	301	PC1	6	0
76	N3	201	PLX	3	0
71	8B	101	PEE	3	0
74	AB	201	ZMP	2	0
76	CB	201	PLX	4	0
76	S7	302	PLX	9	0
70	Qb	501	PC1	5	0
82	S1	803	FES	1	0
71	QC	404	PEE	1	0
71	QH	102	PEE	4	0
82	QE	303	FES	2	0
76	QE	301	PLX	3	0
72	7B	101	3PE	5	0
70	Qh	103	PC1	5	0
68	A7	201	CDL	5	0
68	AN	201	CDL	3	0
68	N4	501	CDL	10	0
72	Qc	401	3PE	2	0
70	N6	201	PC1	8	0
71	Qc	408	PEE	5	0
70	N1	401	PC1	7	0
71	N5	706	PEE	1	0
81	Qd	401	HEC	3	0
68	AN	203	CDL	7	0
75	AK	401	ADP	3	0
73	A9	401	NDP	2	0
76	BL	202	PLX	6	0
83	QH	101	PX2	1	0
71	Qb	503	PEE	1	0
76	B1	101	PLX	1	0
68	AL	204	CDL	5	0
70	7A	101	PC1	2	0
74	AC	201	ZMP	5	0
68	C1	607	CDL	5	0
70	C4	201	PC1	1	0

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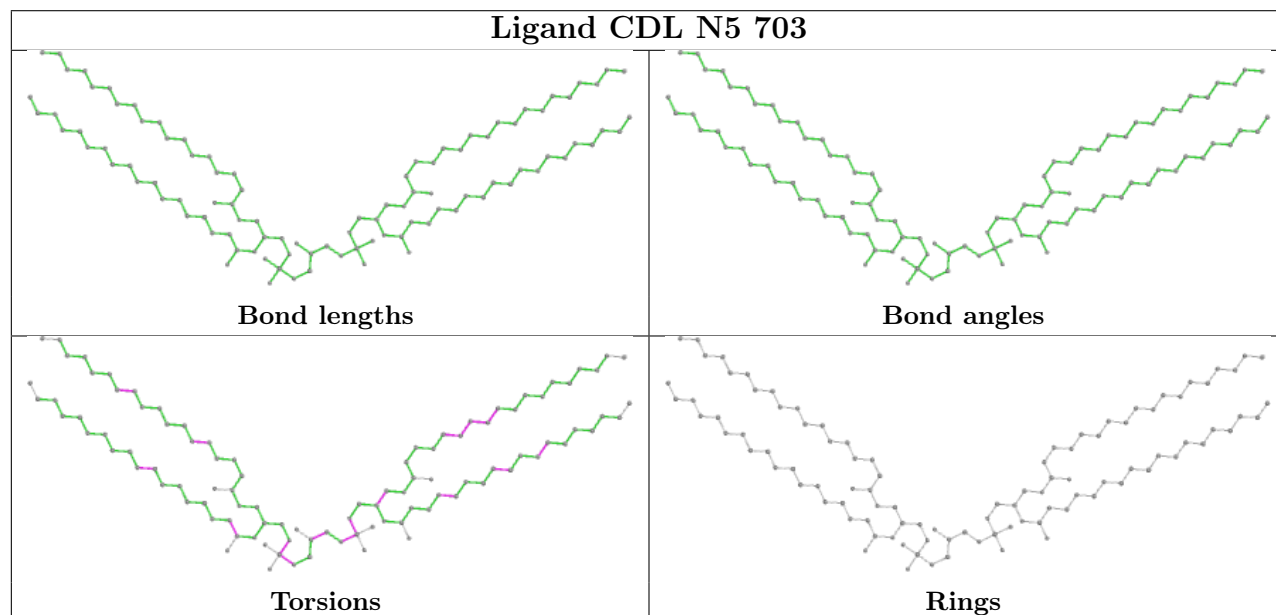
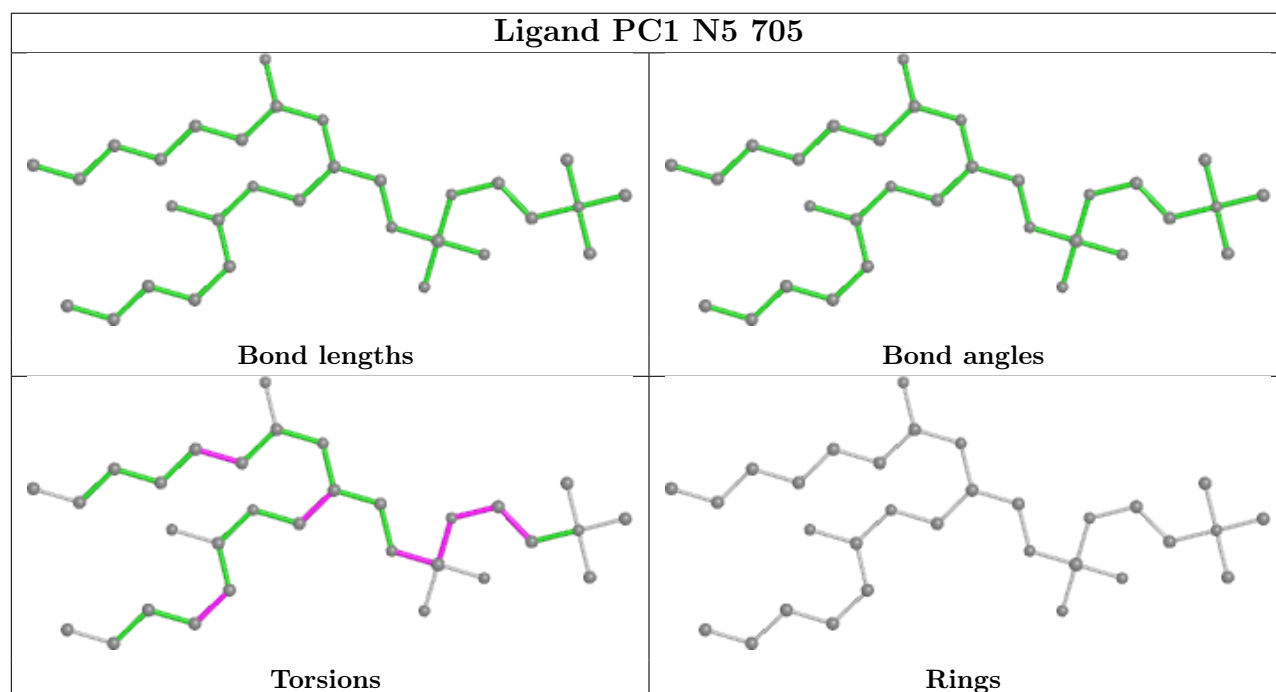
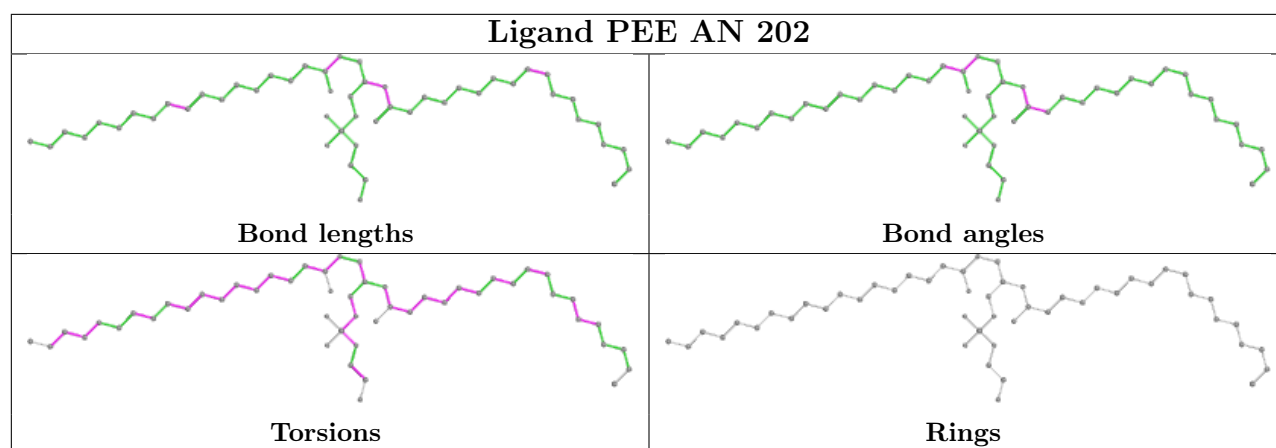
Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	S1	802	SF4	1	0
71	N5	701	PEE	9	0
71	6A	103	PEE	4	0
82	Qe	301	FES	2	0
70	6A	101	PC1	13	0
70	C3	304	PC1	1	0
68	Qb	502	CDL	4	0
71	Qh	101	PEE	3	0
71	Qe	302	PEE	3	0
77	C1	603	HEA	8	0
68	QC	406	CDL	2	0
72	Qc	406	3PE	1	0
71	C3	302	PEE	6	0
72	C1	601	3PE	4	0
71	QC	403	PEE	5	0
80	QC	402	HEM	6	0
70	C1	610	PC1	9	0
71	N5	704	PEE	6	0
68	QC	407	CDL	2	0
70	QJ	101	PC1	4	0
70	Qc	409	PC1	2	0
70	N3	202	PC1	3	0
68	Qj	101	CDL	4	0
76	AL	205	PLX	4	0
70	C1	608	PC1	7	0
70	N4	502	PC1	11	0
68	N2	401	CDL	1	0
68	B5	201	CDL	7	0
80	Qc	405	HEM	8	0
71	Qc	403	PEE	1	0
71	6A	102	PEE	3	0
71	S8	303	PEE	1	0
70	Qd	402	PC1	3	0
80	Qc	404	HEM	2	0
68	A8	301	CDL	7	0
68	Qh	102	CDL	2	0
70	B7	201	PC1	1	0
70	S8	304	PC1	10	0
68	N5	702	CDL	7	0
76	QI	102	PLX	5	0
70	Qc	412	PC1	3	0
76	AM	201	PLX	3	0

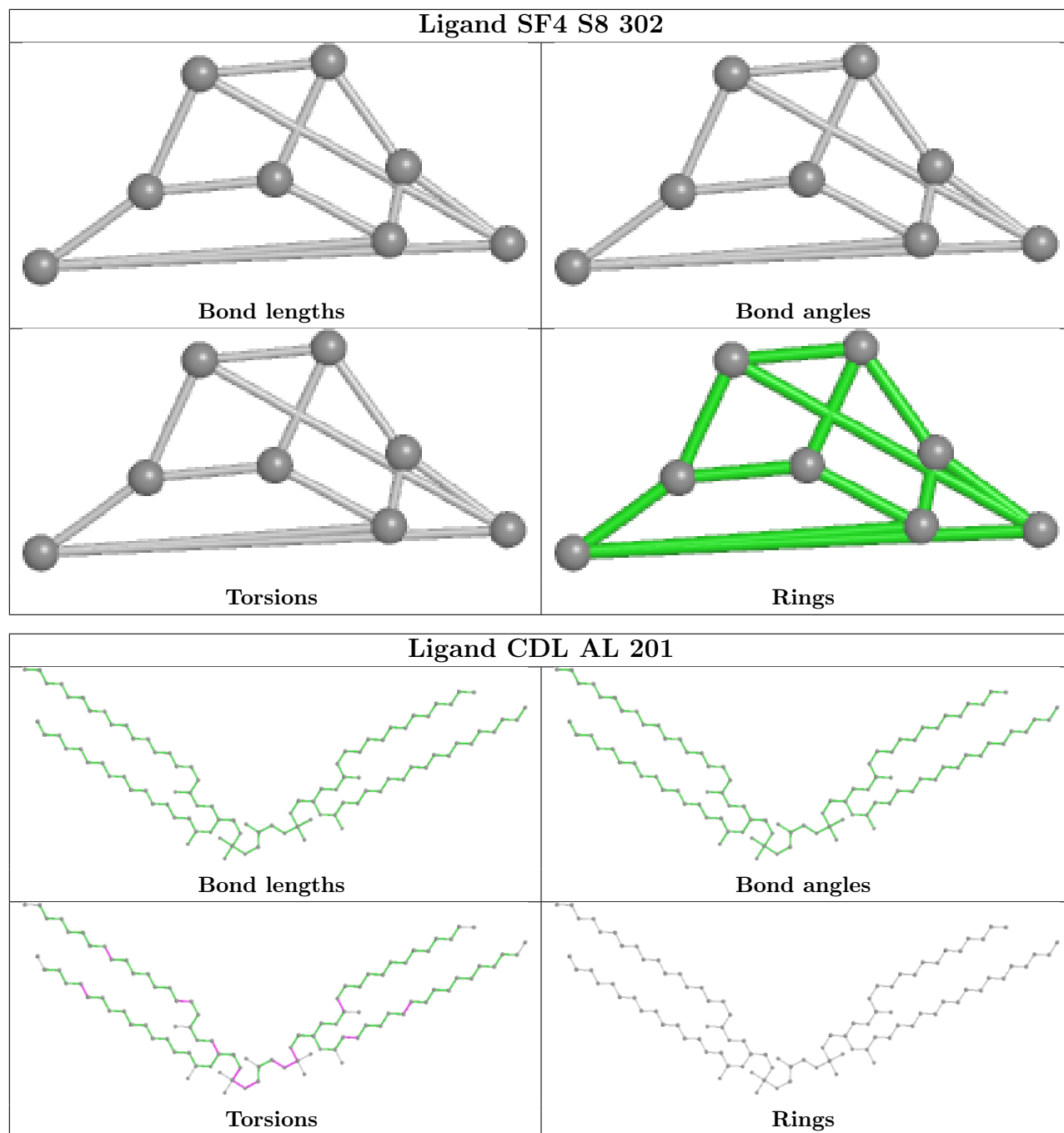
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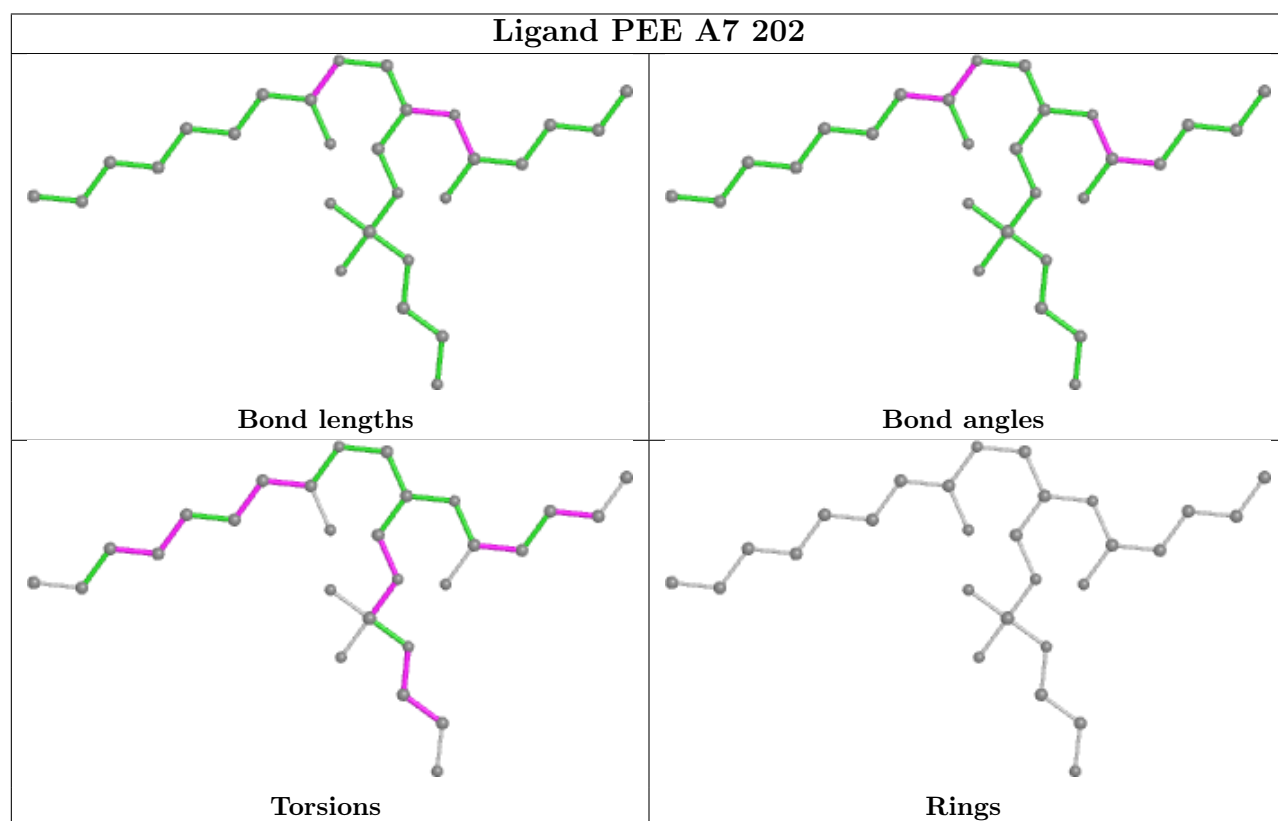
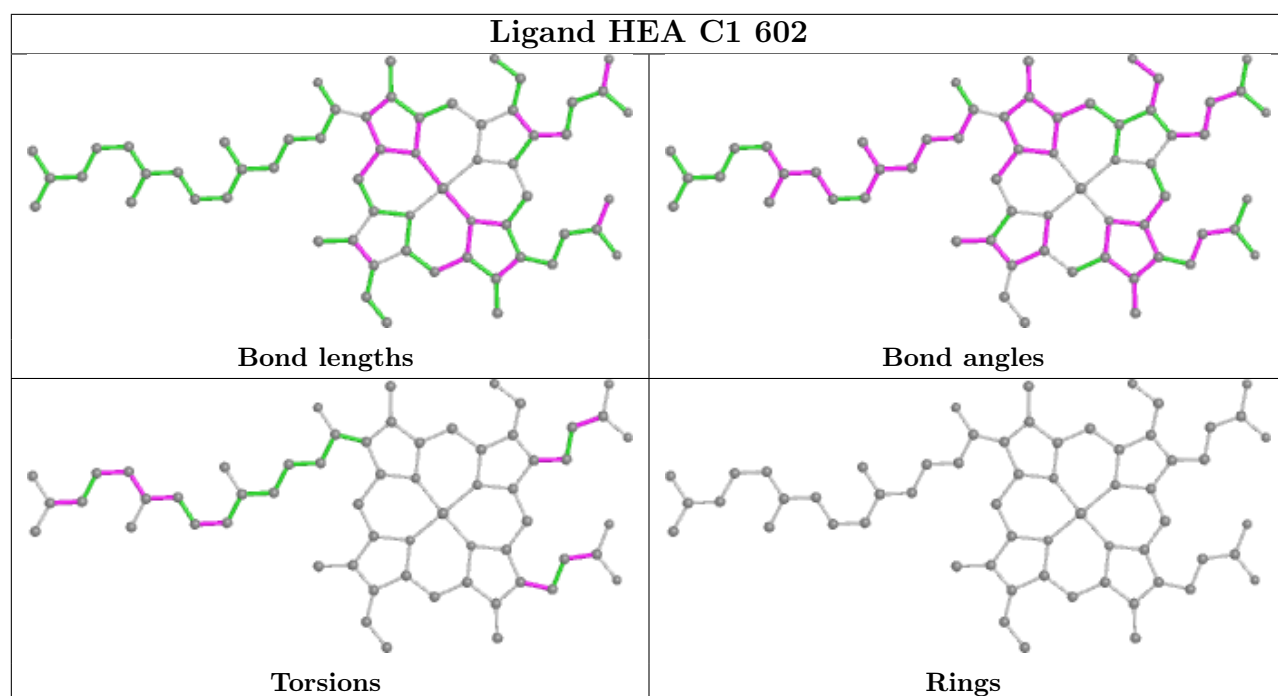
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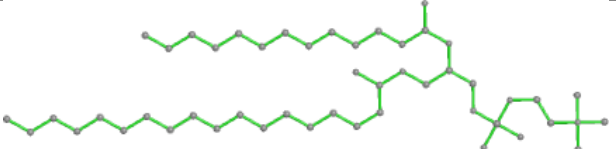
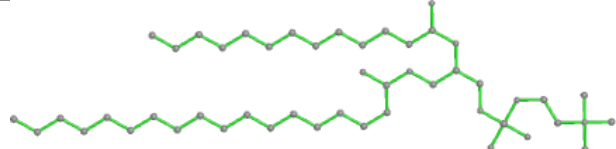
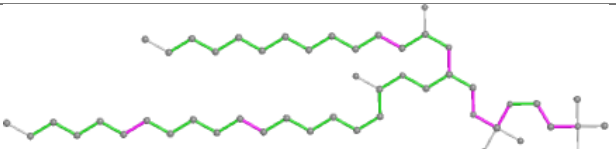
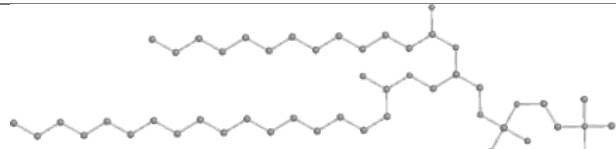
Mol	Chain	Res	Type	Clashes	Symm-Clashes
71	QE	302	PEE	4	0
70	Qc	410	PC1	4	0
80	QC	401	HEM	2	0
68	QD	402	CDL	2	0
70	QI	101	PC1	3	0
71	C3	303	PEE	1	0
71	CB	203	PEE	3	0
85	V1	502	FMN	2	0
72	CA	101	3PE	4	0
68	B4	201	CDL	3	0
68	Qc	411	CDL	7	0
70	QB	502	PC1	11	0
70	B8	201	PC1	1	0
68	QB	501	CDL	10	0
68	4L	101	CDL	3	0
70	Qc	407	PC1	4	0
71	QC	405	PEE	6	0
68	Qc	402	CDL	1	0
71	A3	201	PEE	4	0
68	AL	202	CDL	6	0
70	7C	101	PC1	6	0
71	C1	609	PEE	3	0
70	QB	503	PC1	6	0
81	QD	401	HEC	1	0
71	BL	201	PEE	1	0
76	C2	301	PLX	4	0

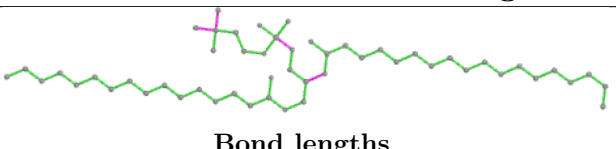
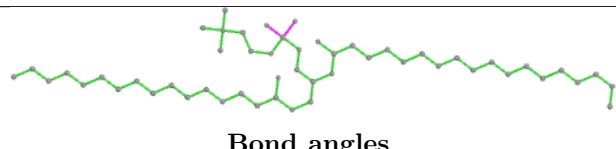
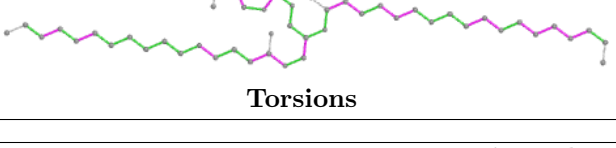

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

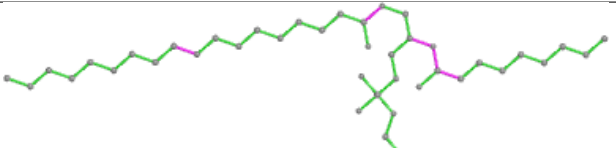
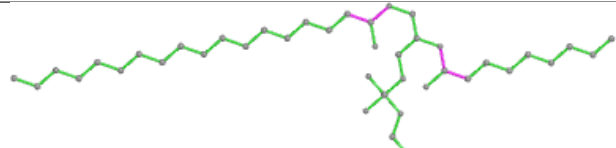
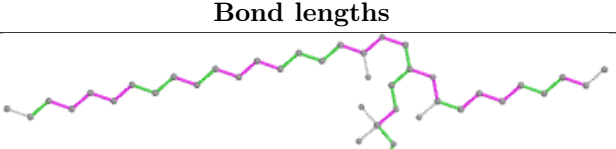
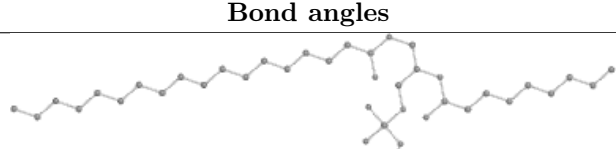


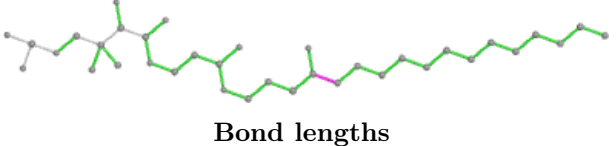
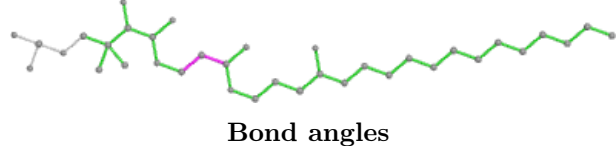
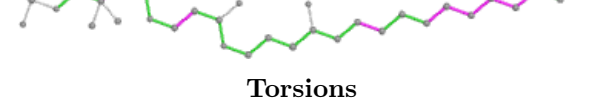



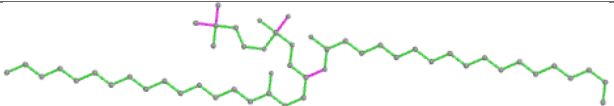
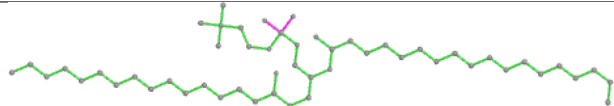
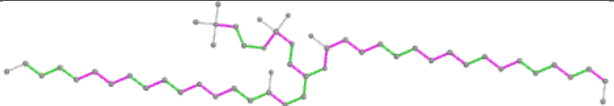
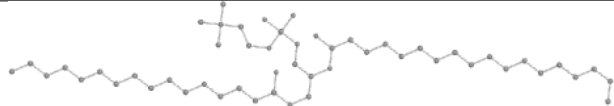


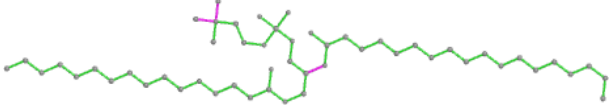
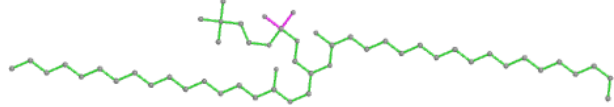
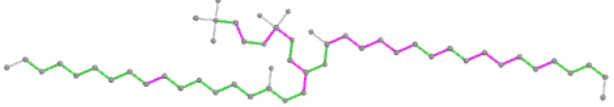
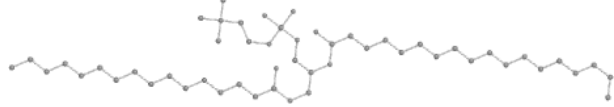
Ligand PC1 C3 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

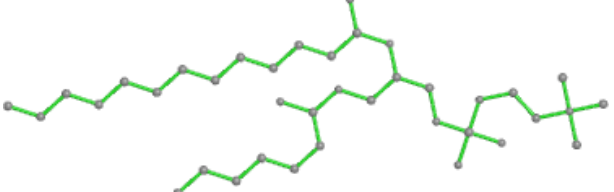
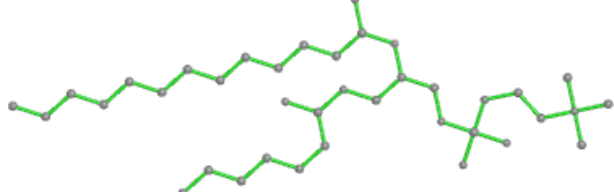
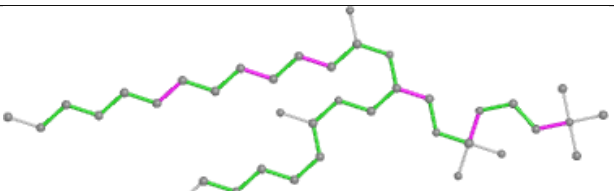
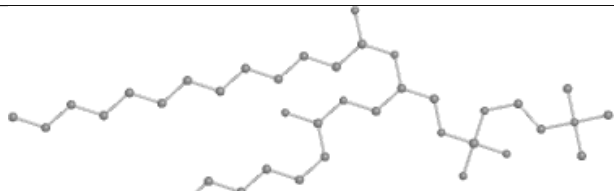
Ligand PLX N3 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

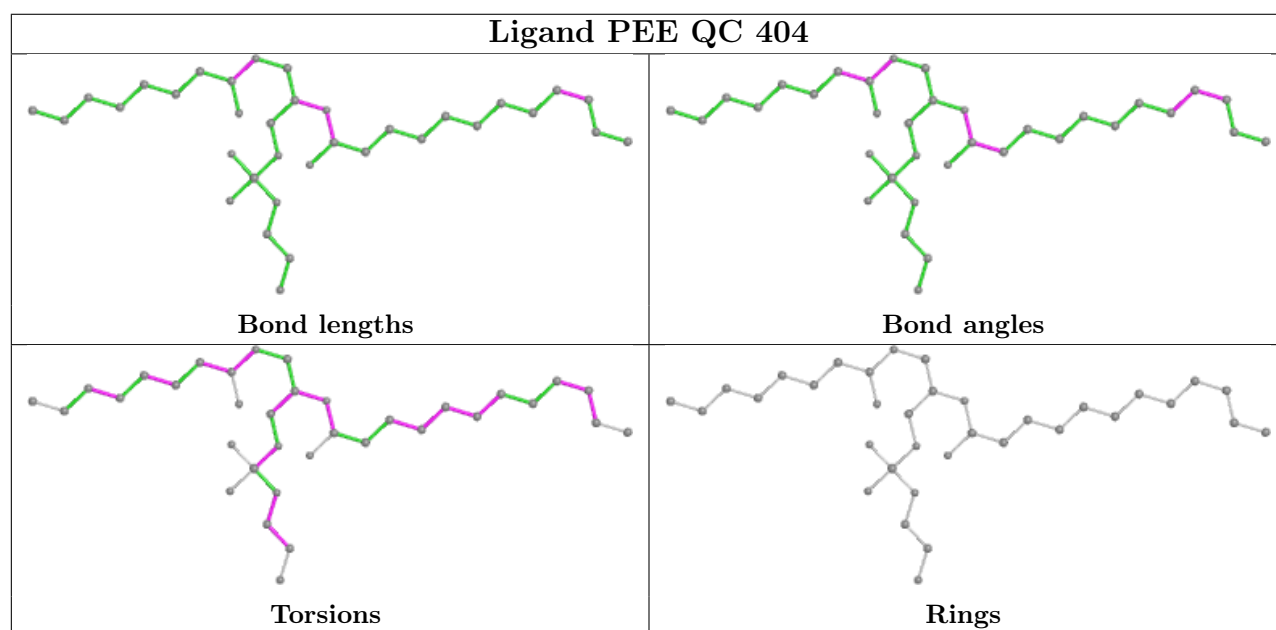
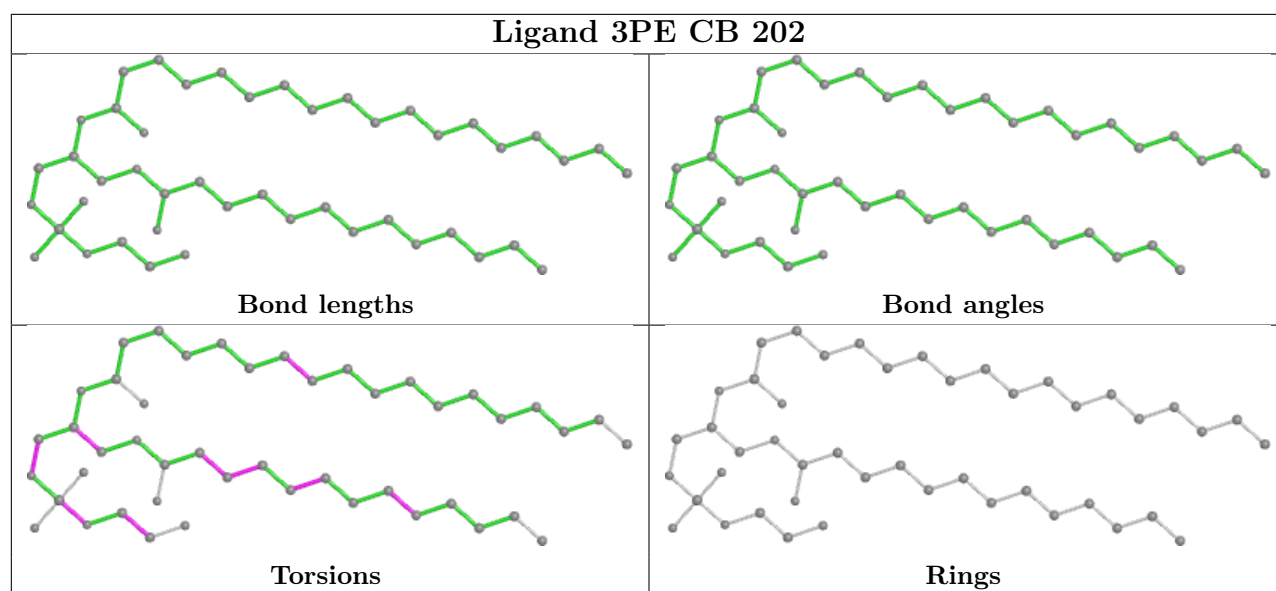
Ligand PEE 8B 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

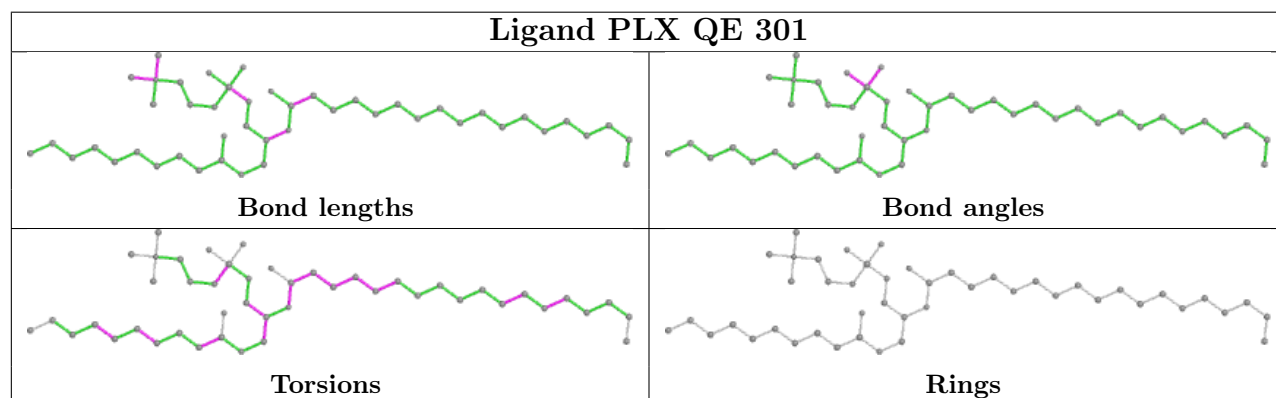
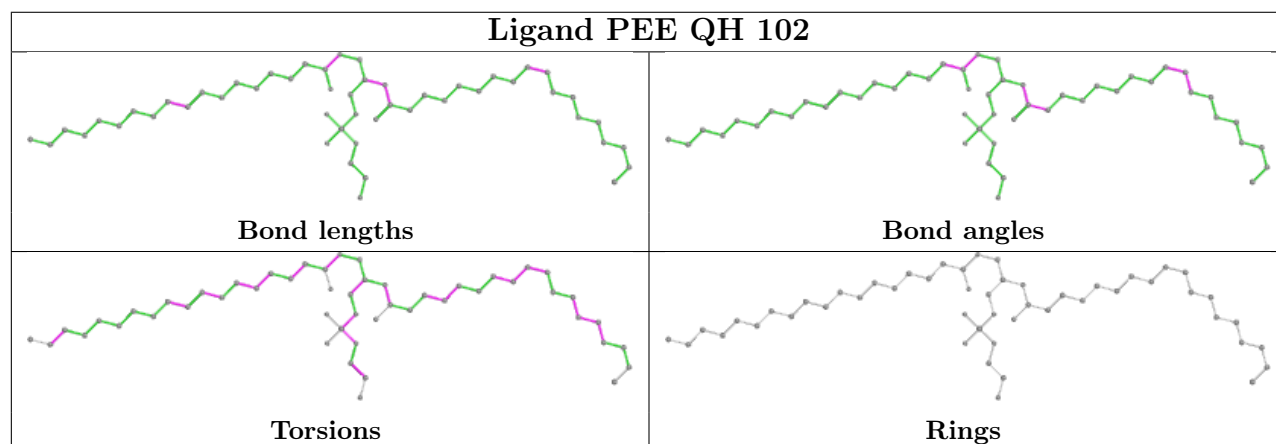
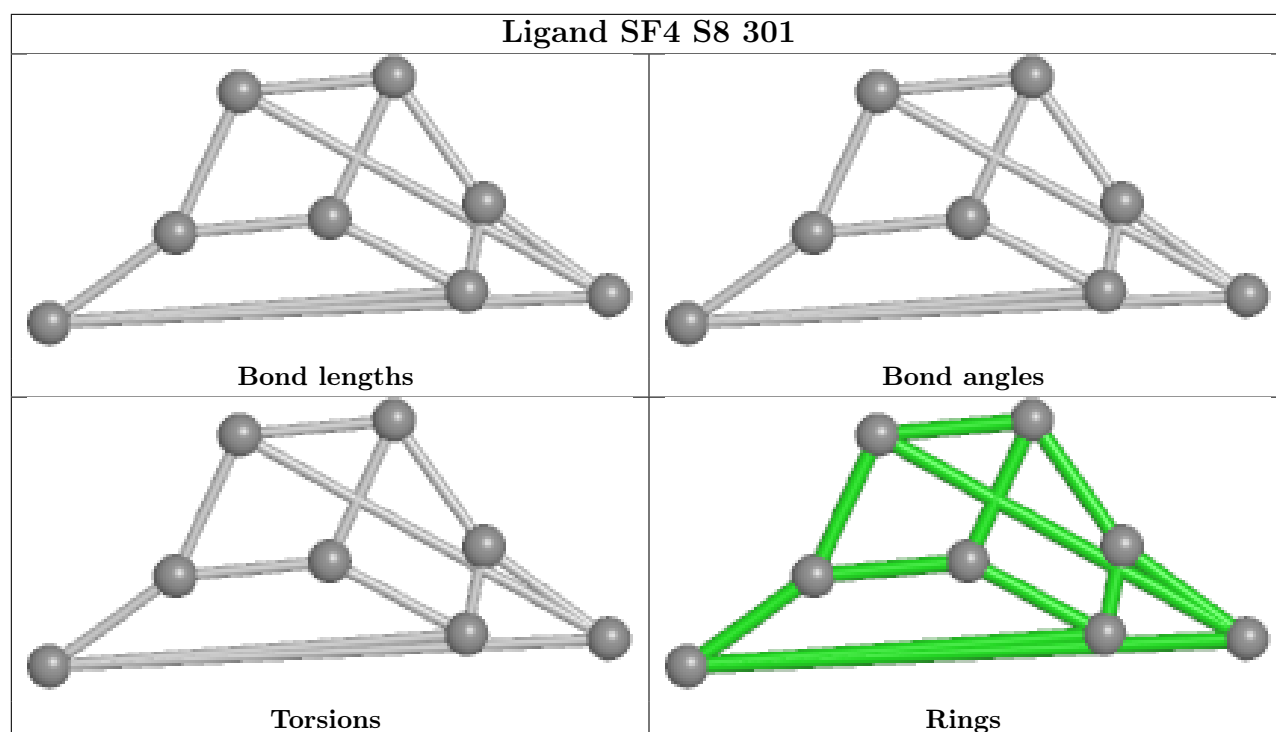
Ligand ZMP AB 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

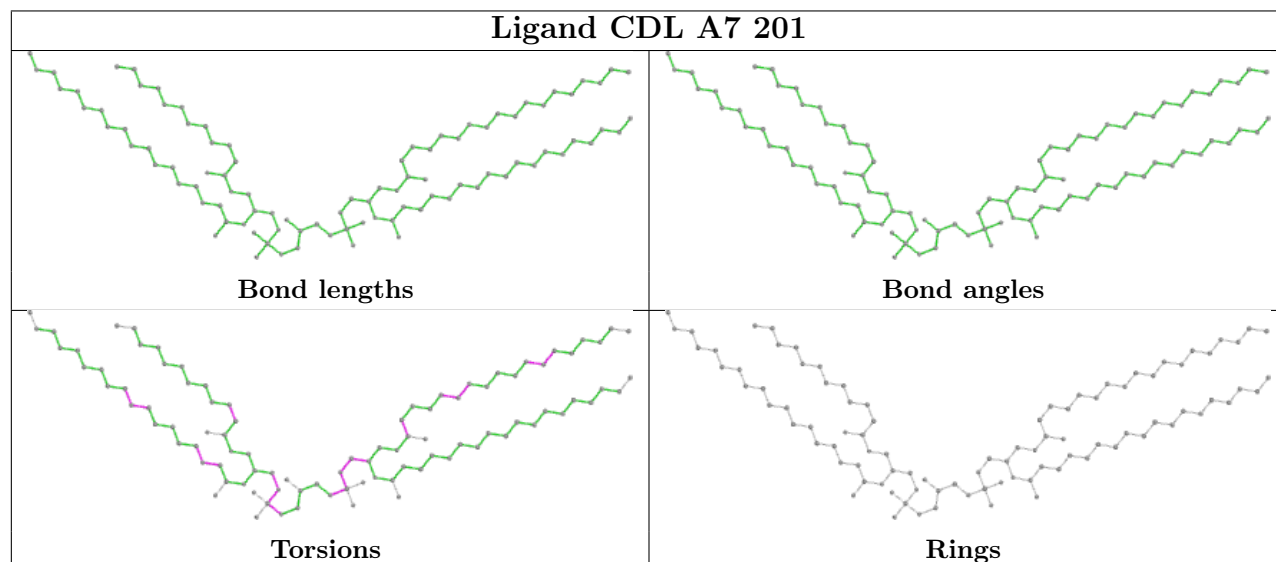
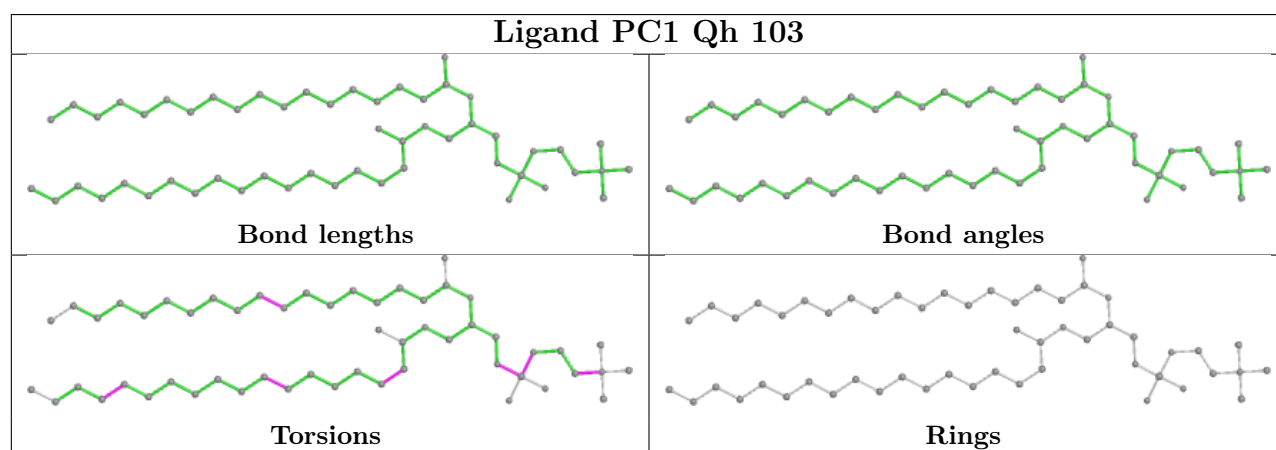
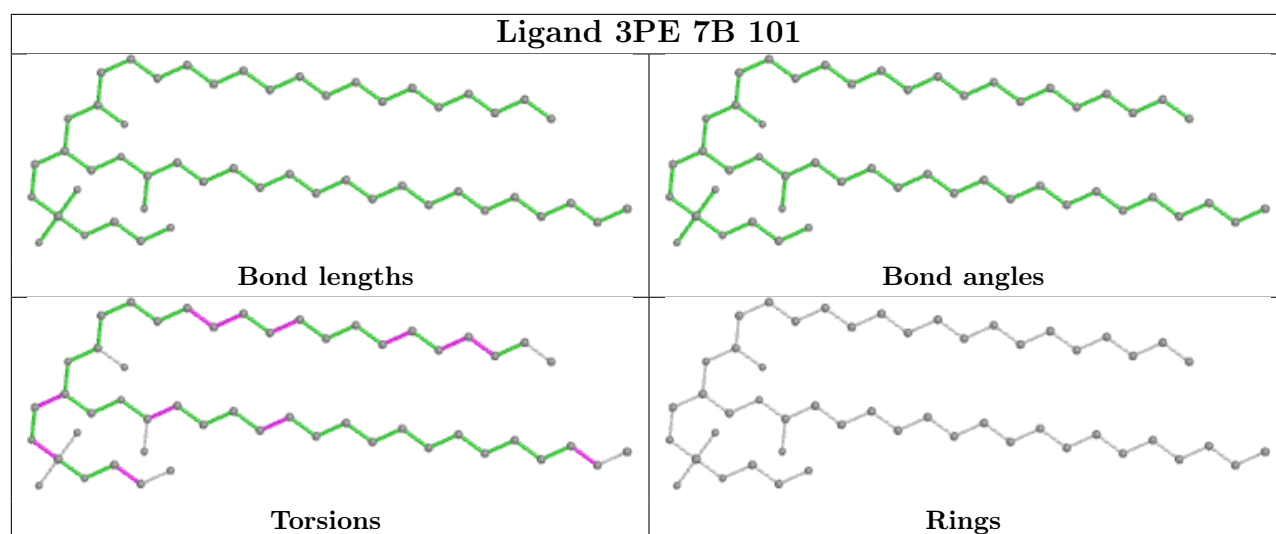
Ligand PLX CB 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

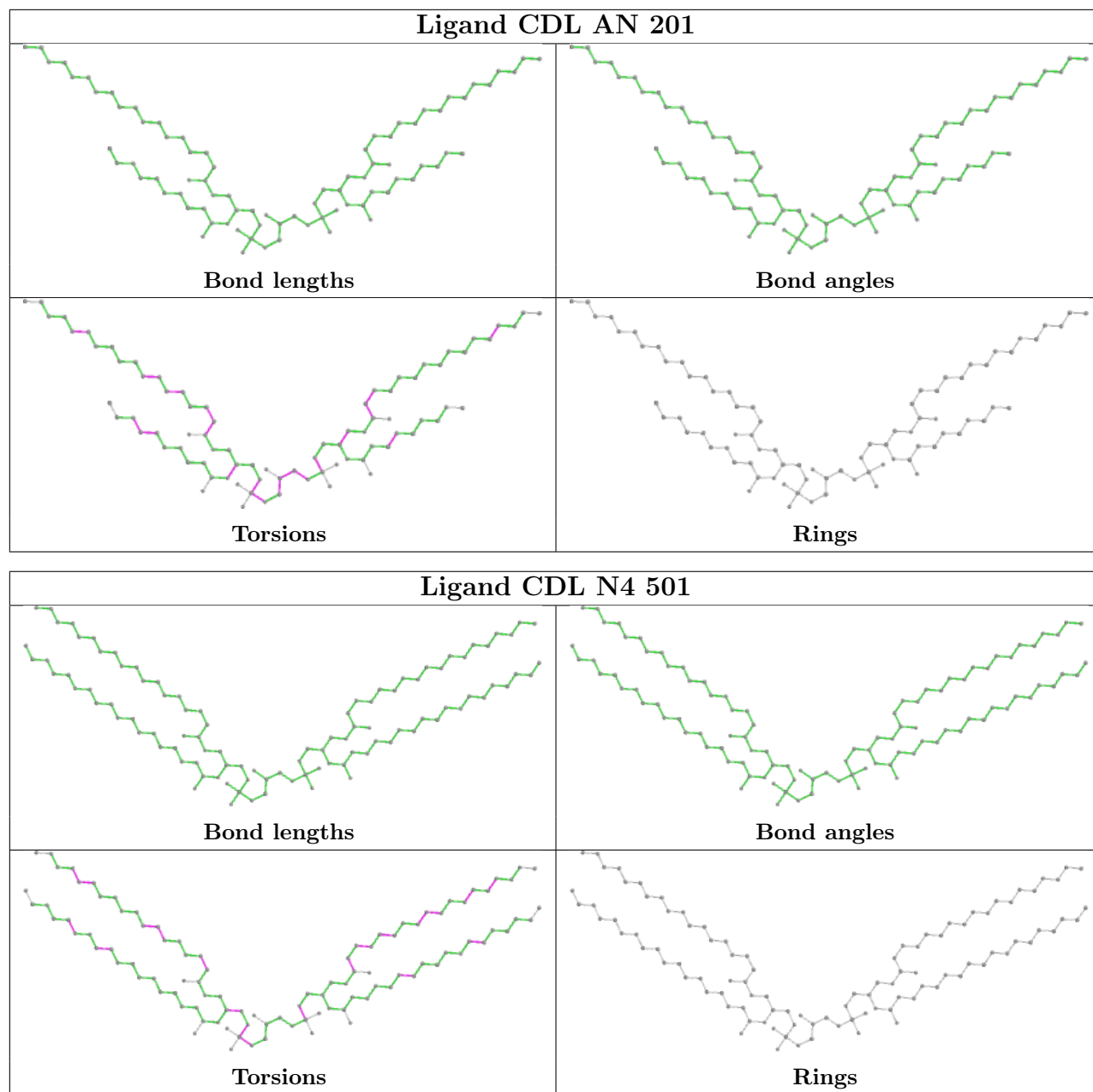
Ligand PLX S7 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

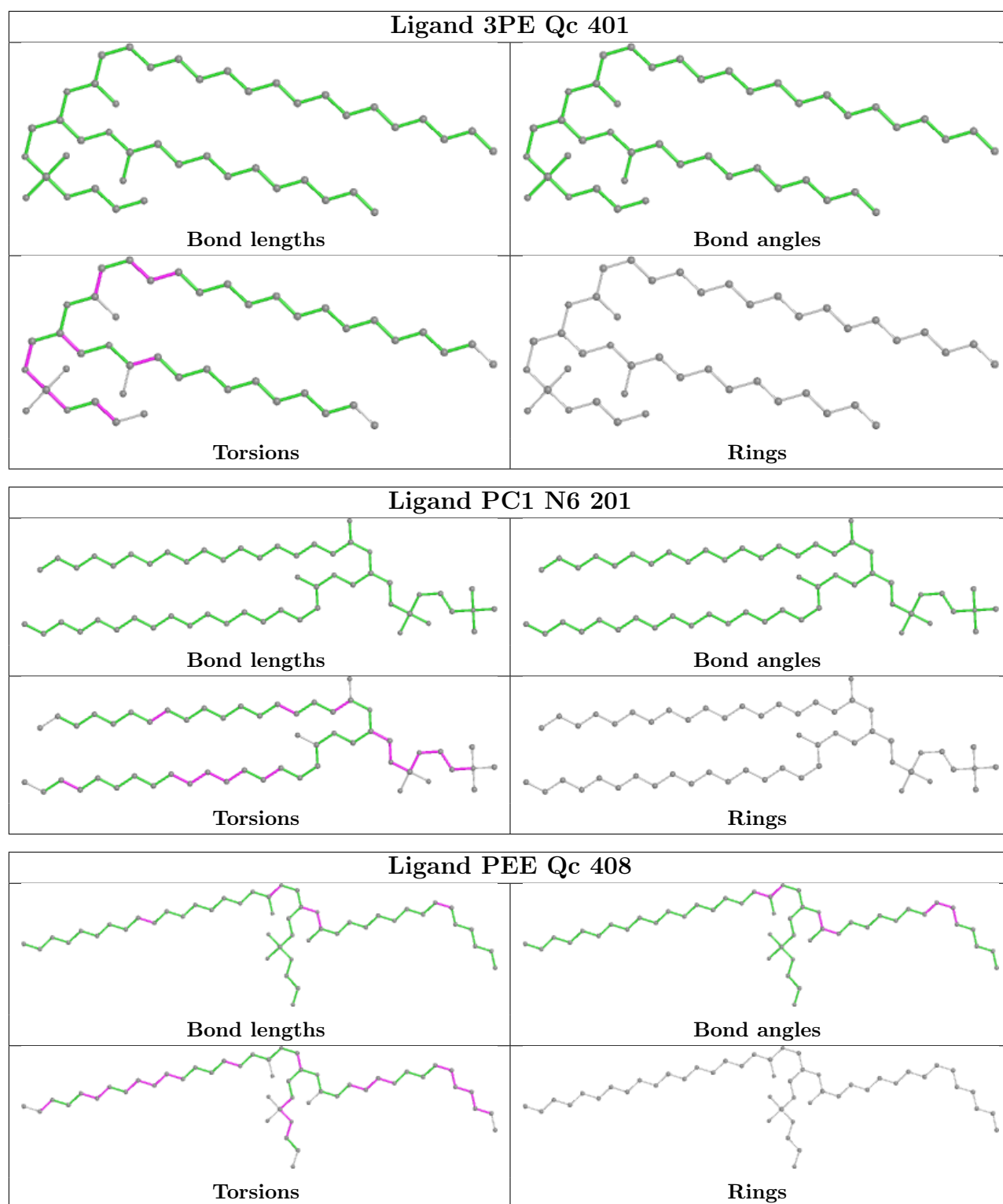
Ligand PC1 Qb 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

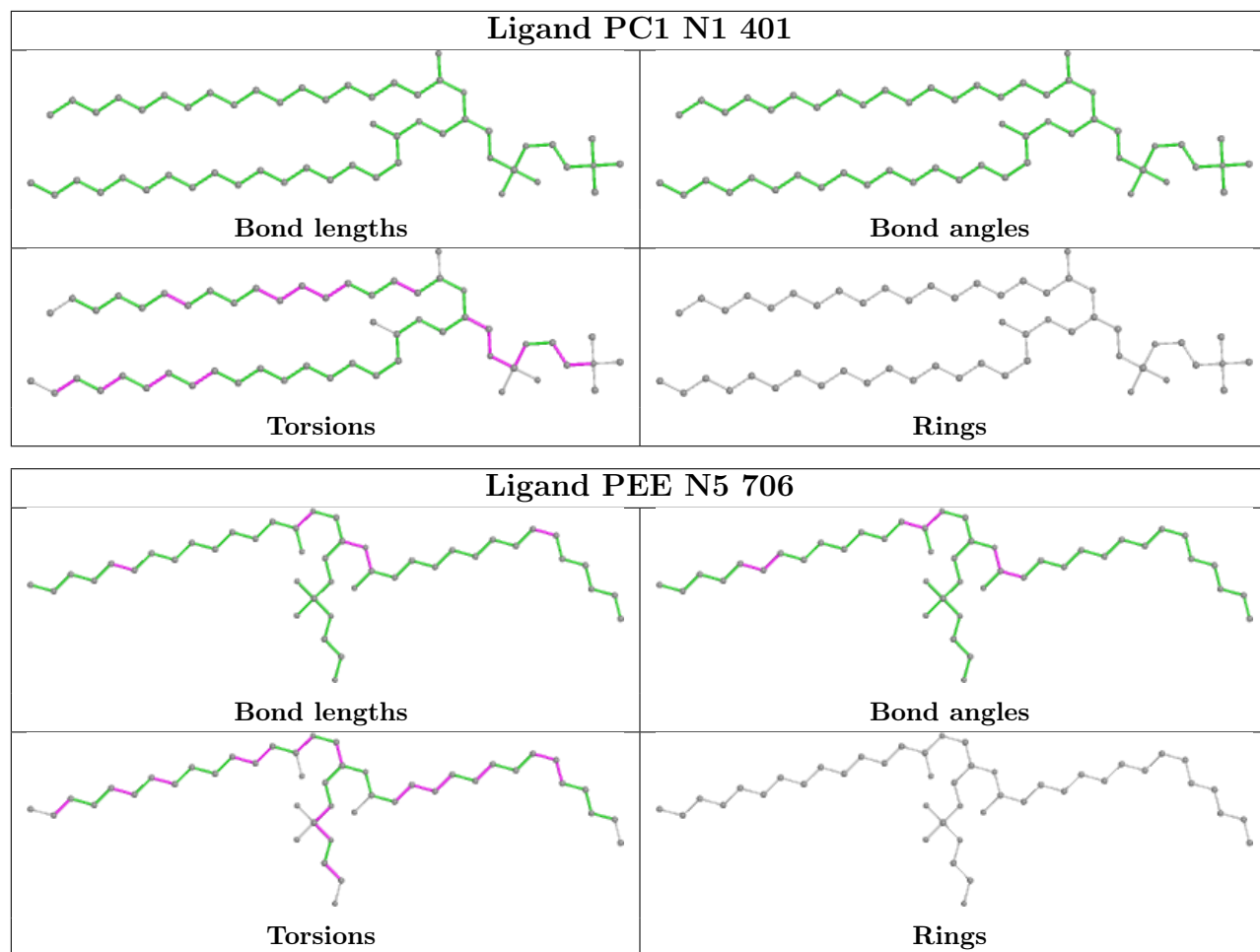


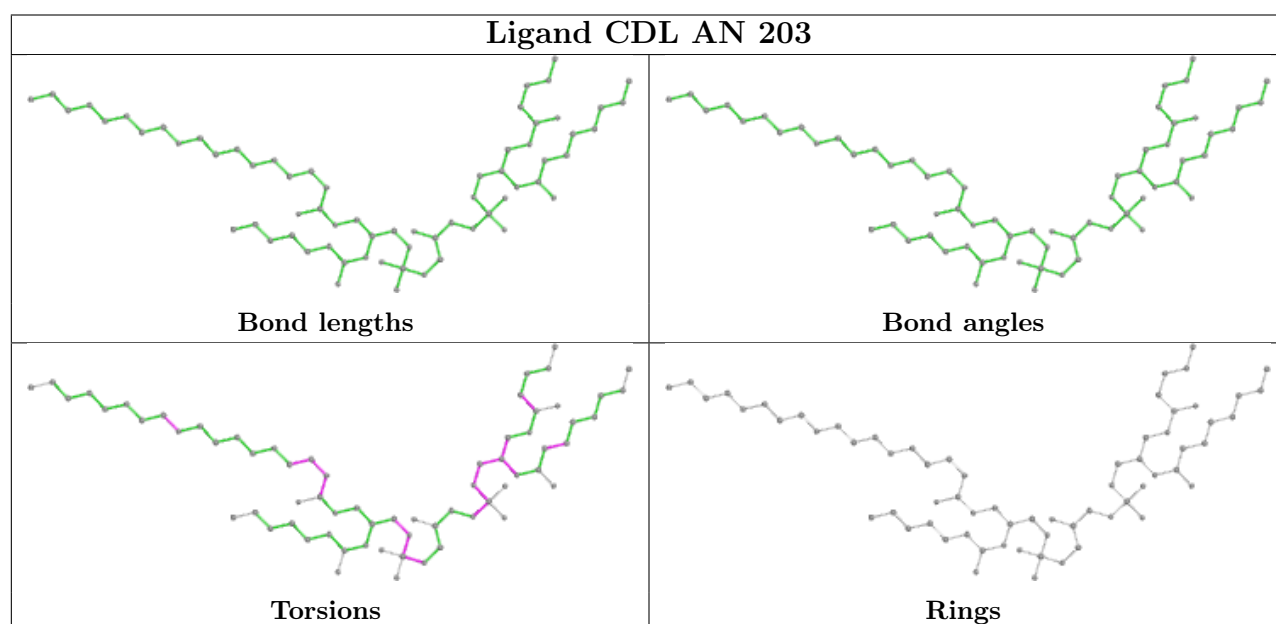
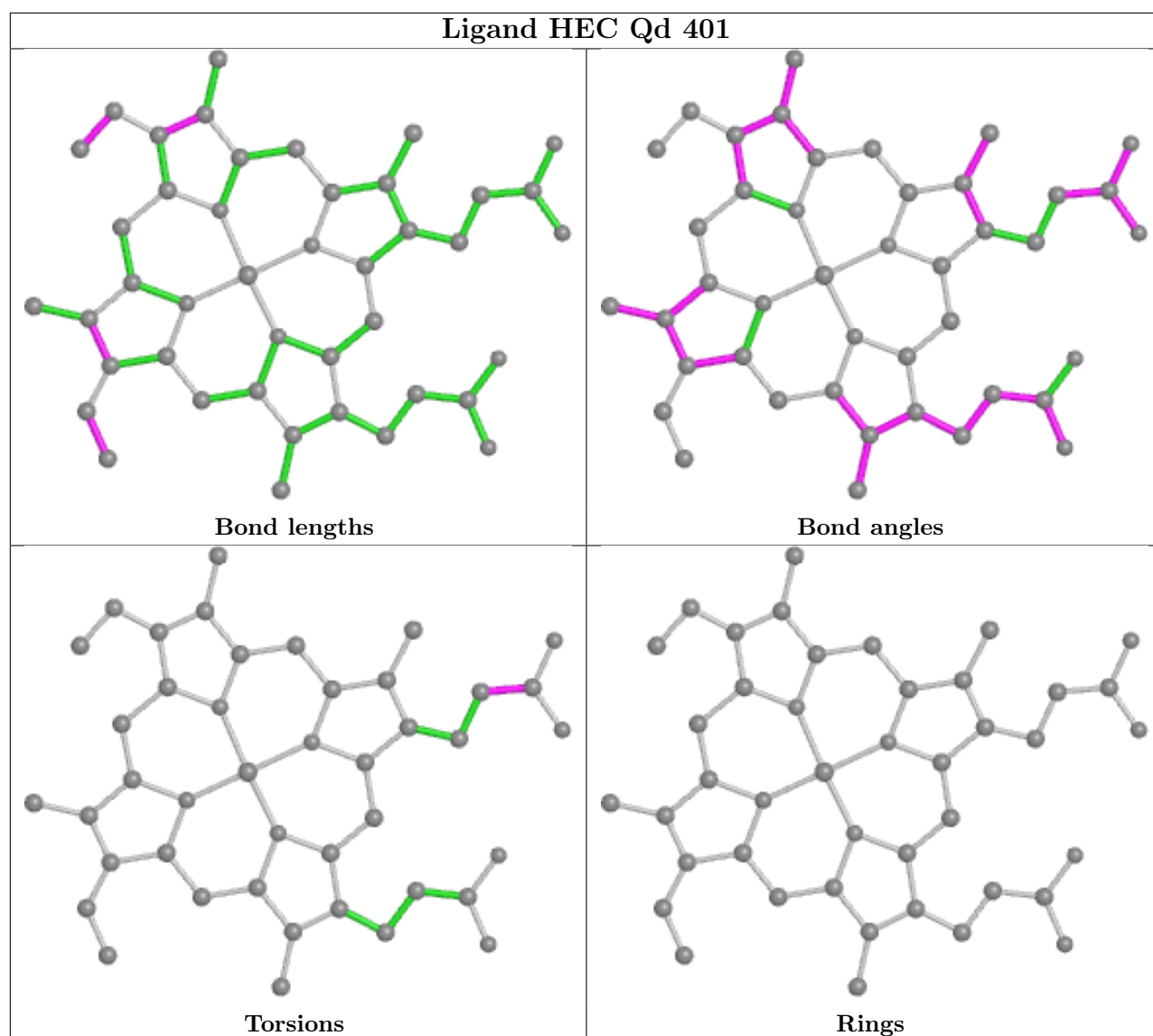


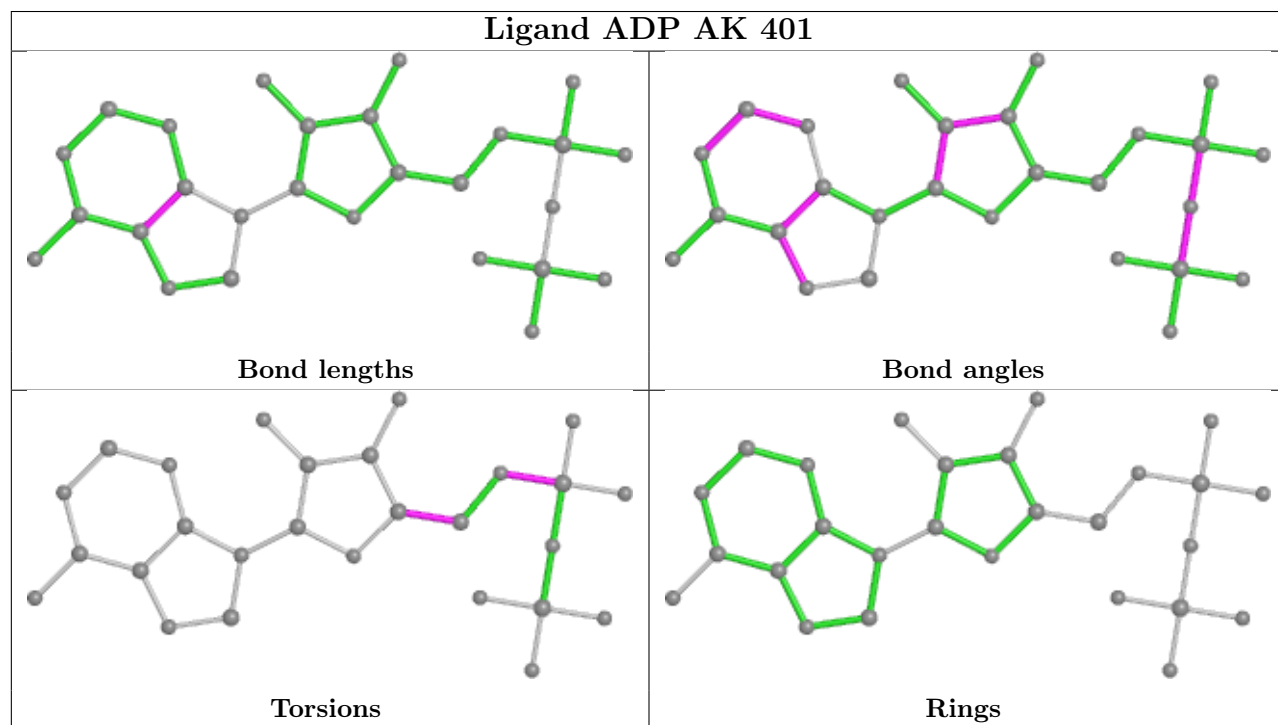
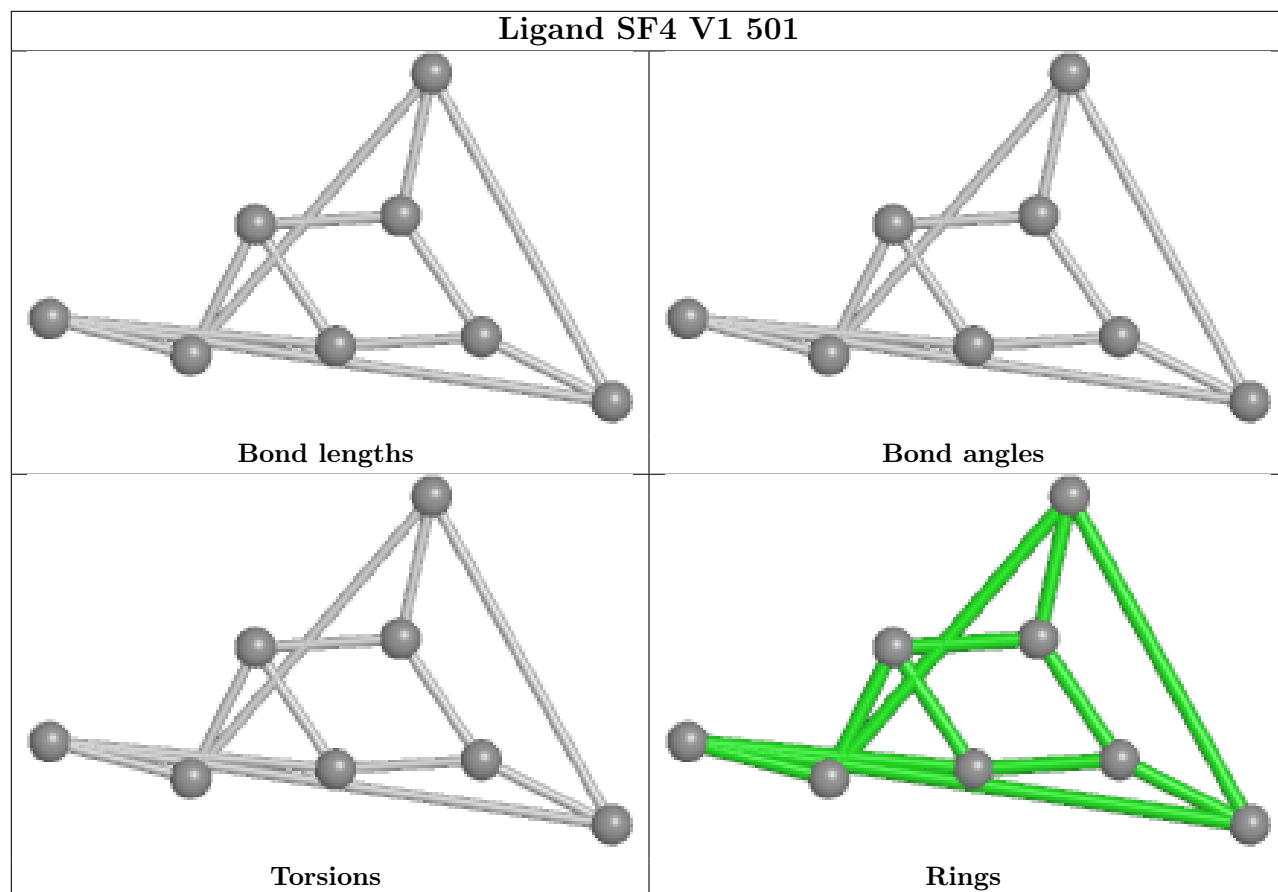




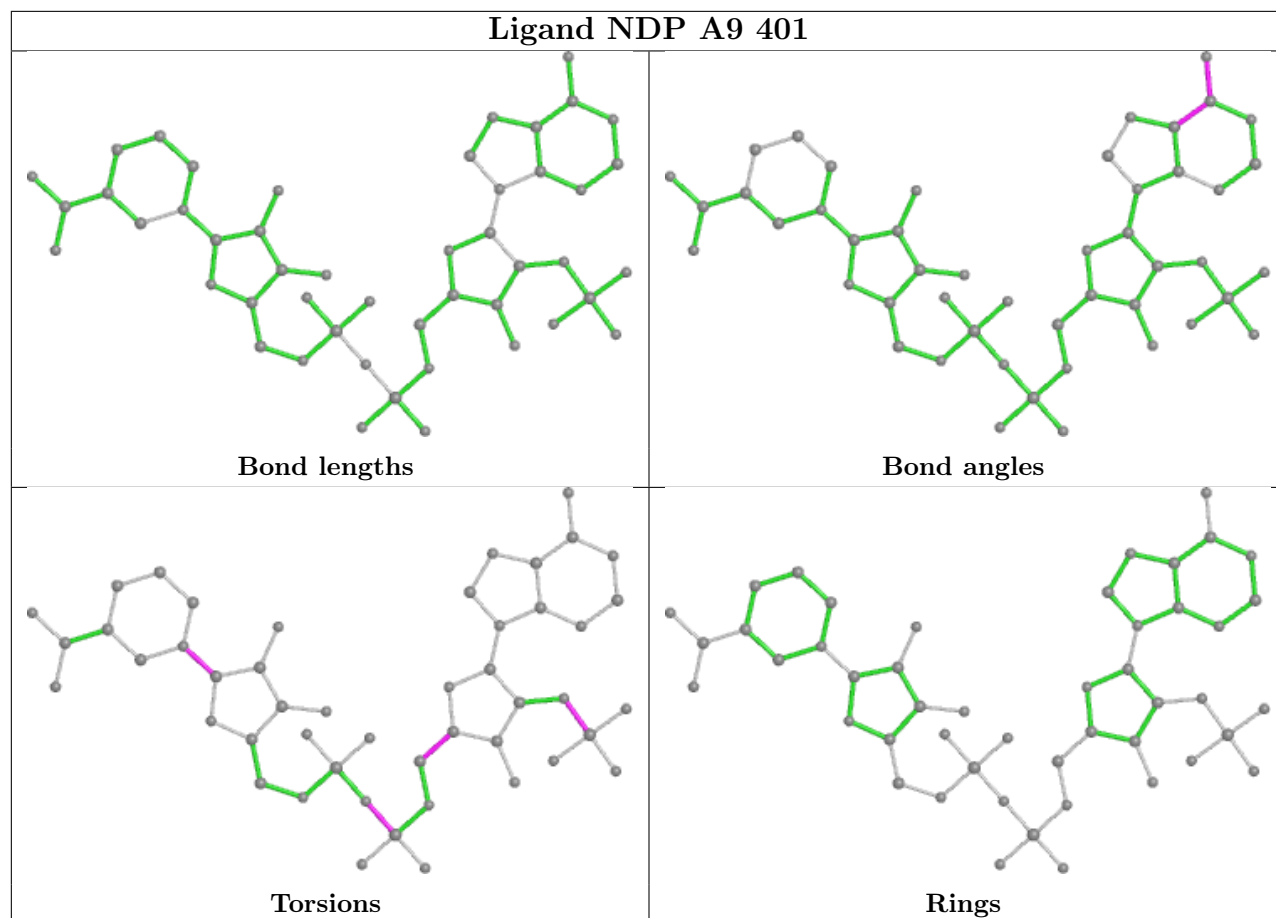




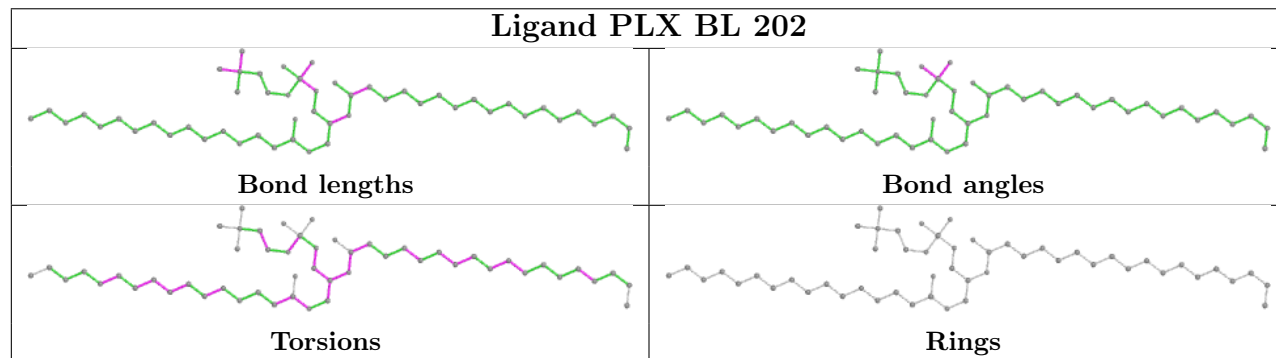


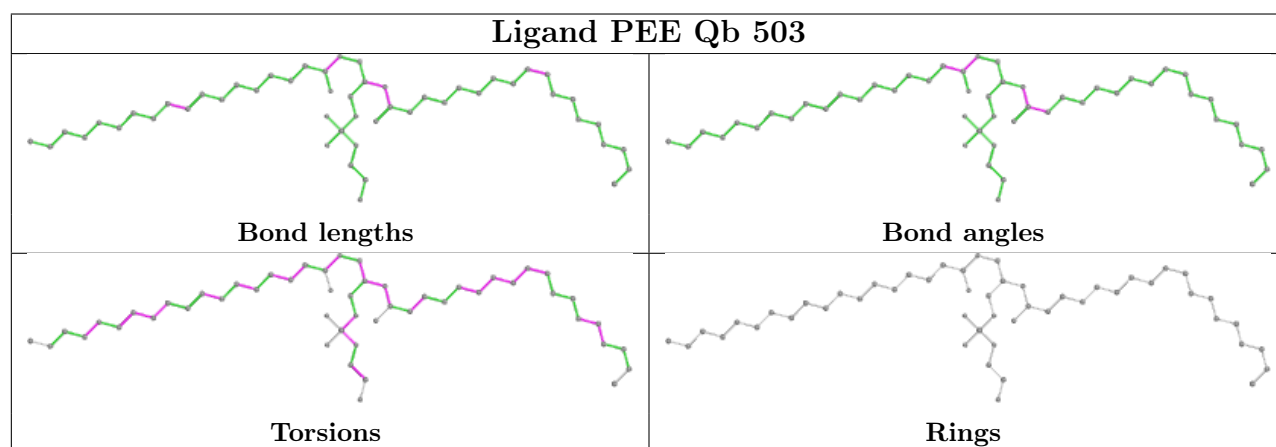
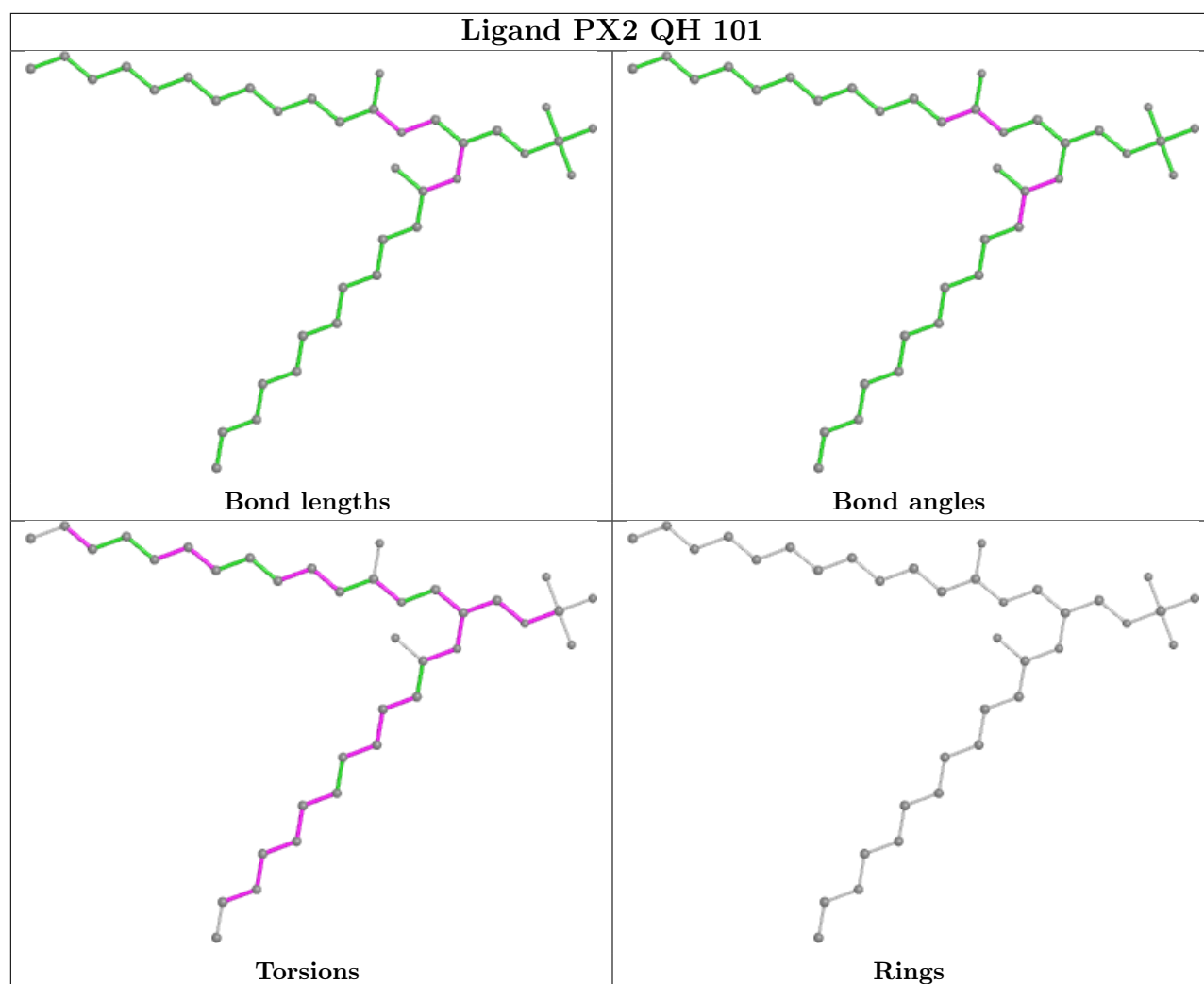


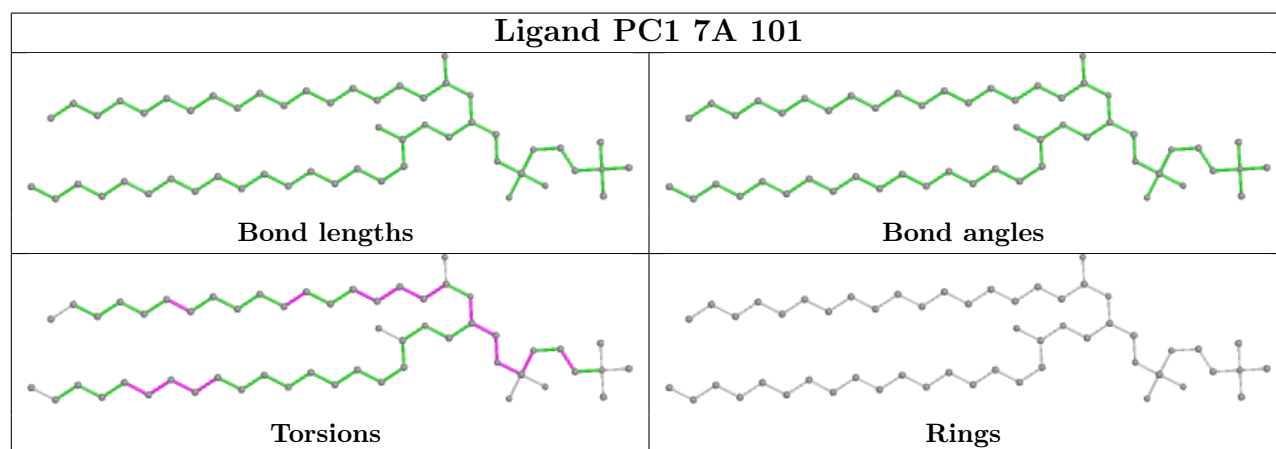
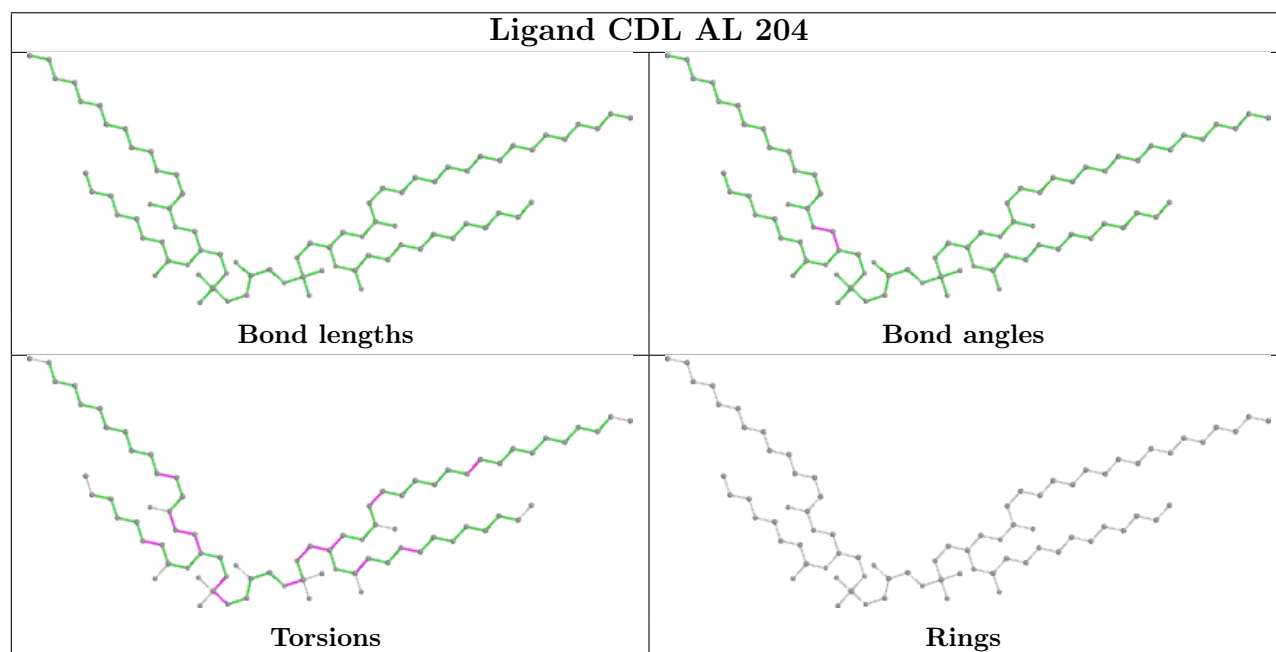
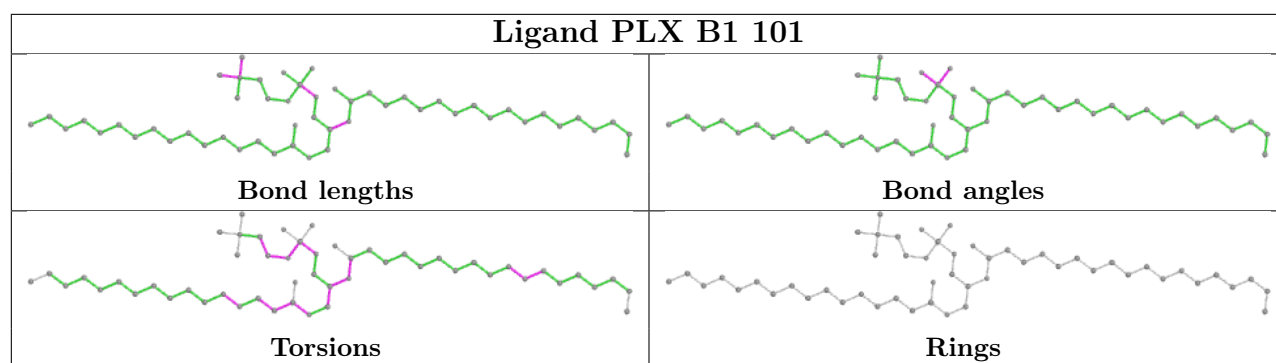
Ligand NDP A9 401

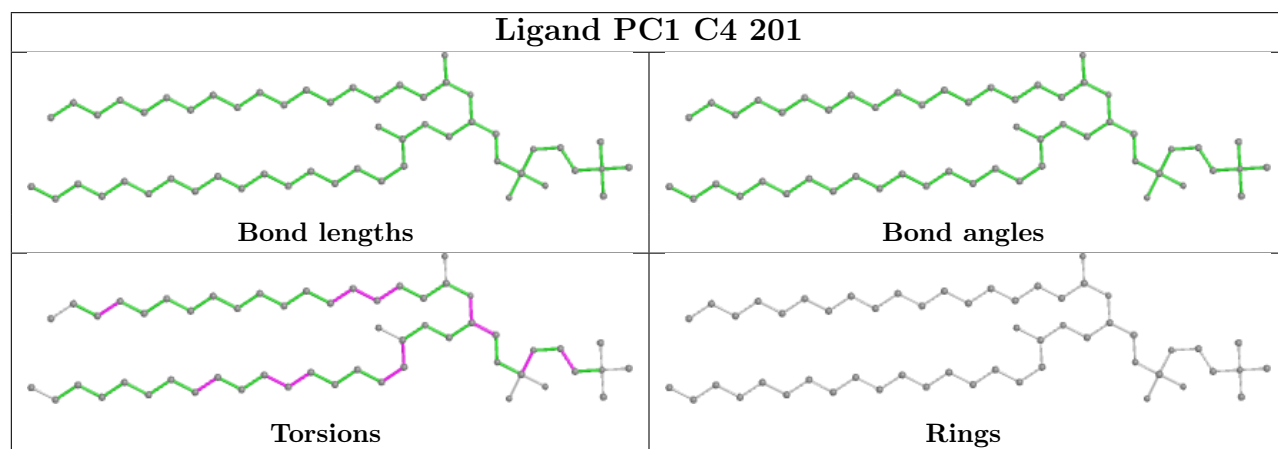
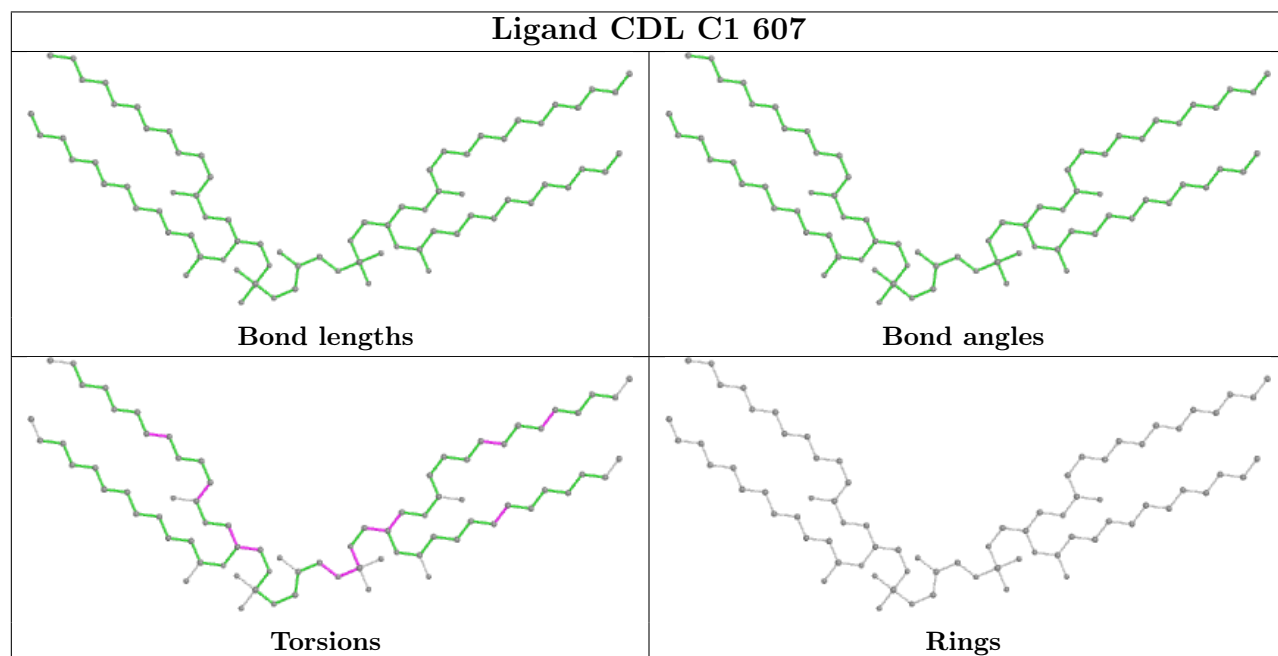
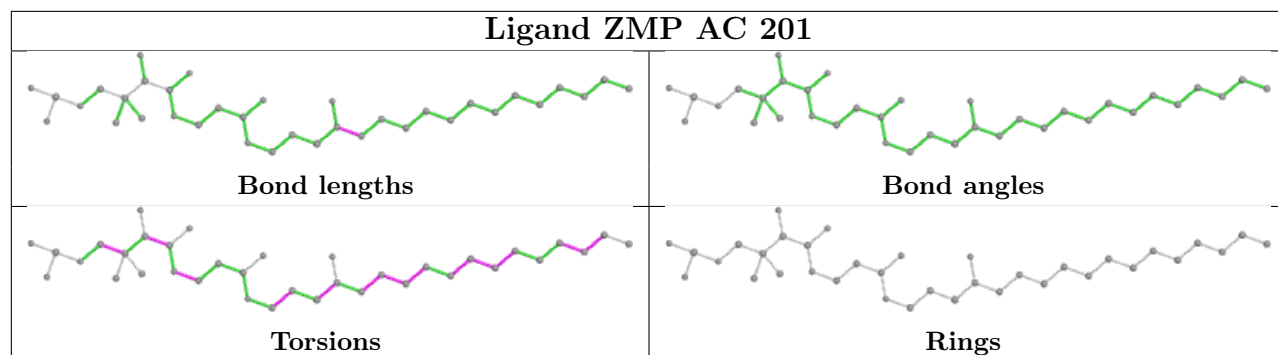


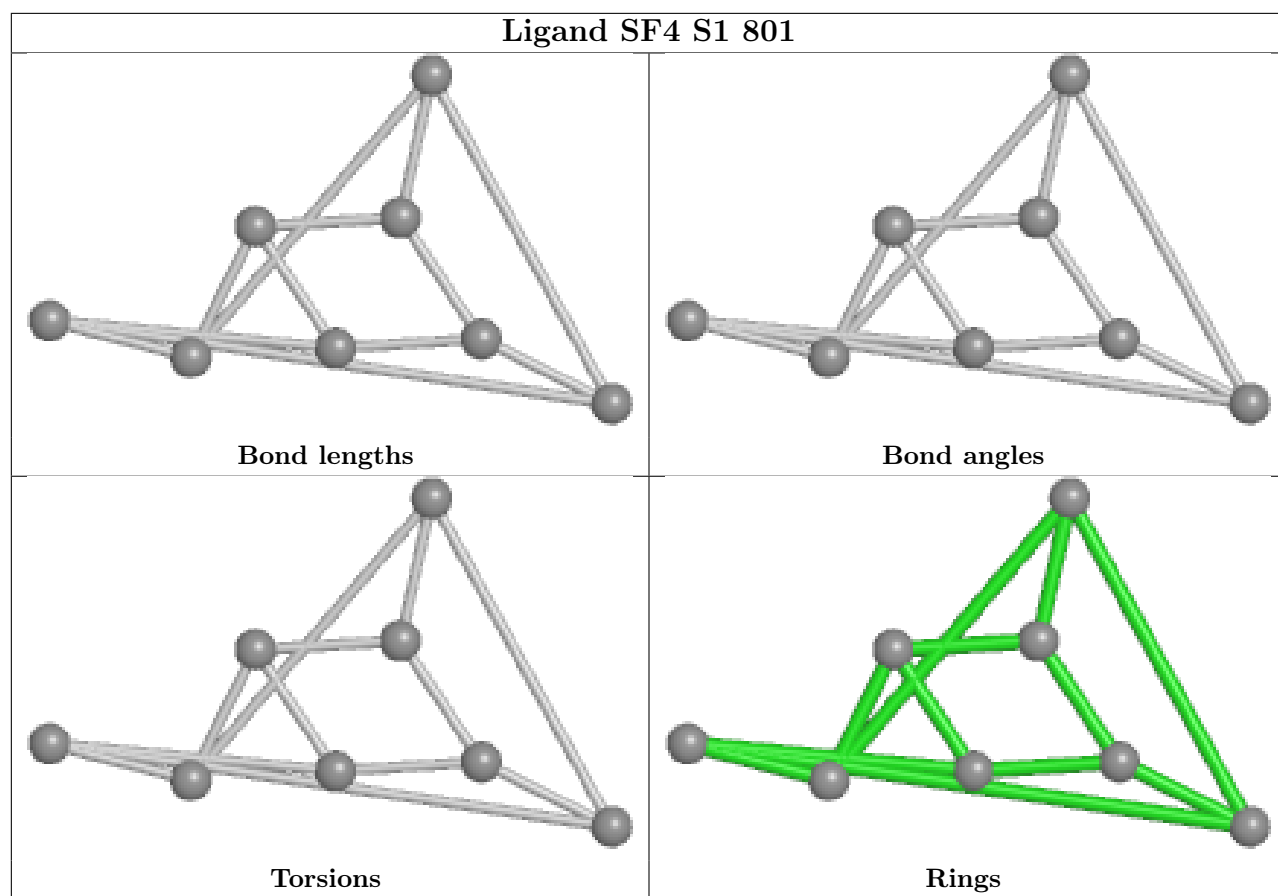
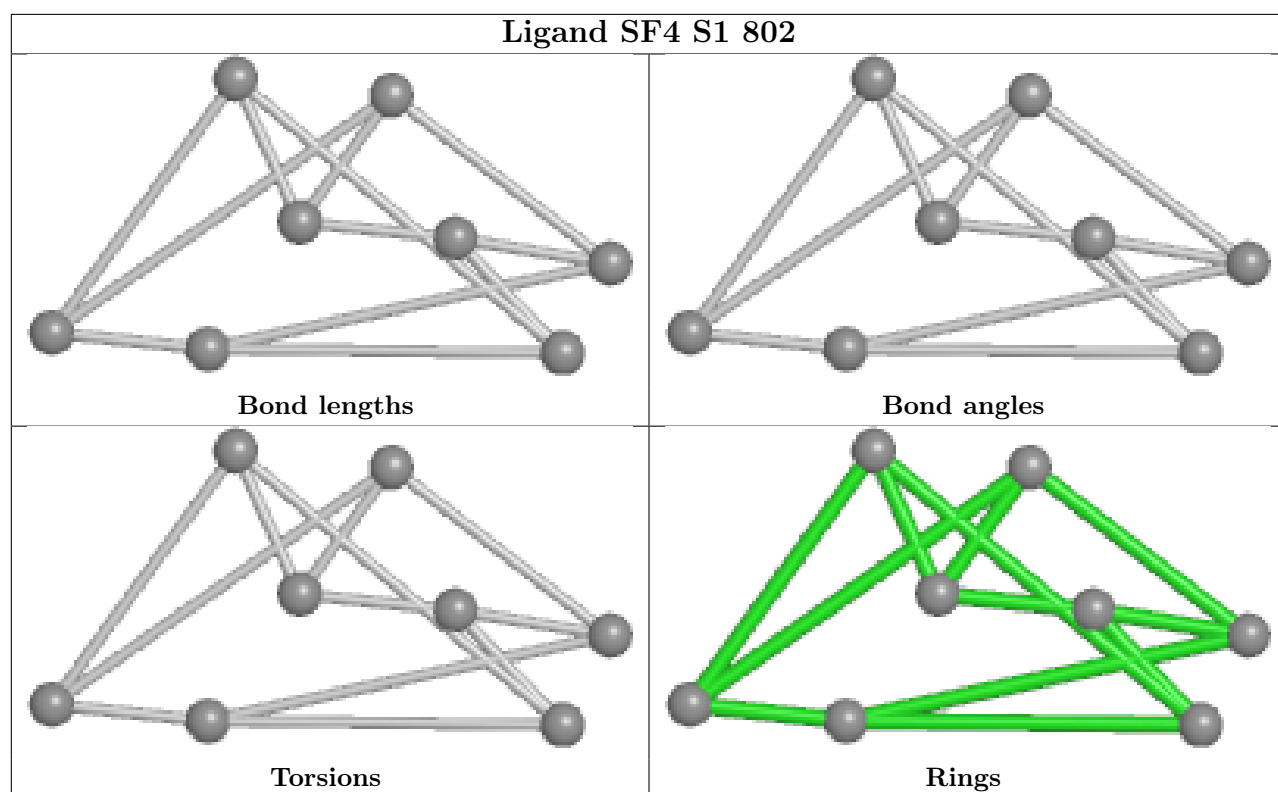
Ligand PLX BL 202

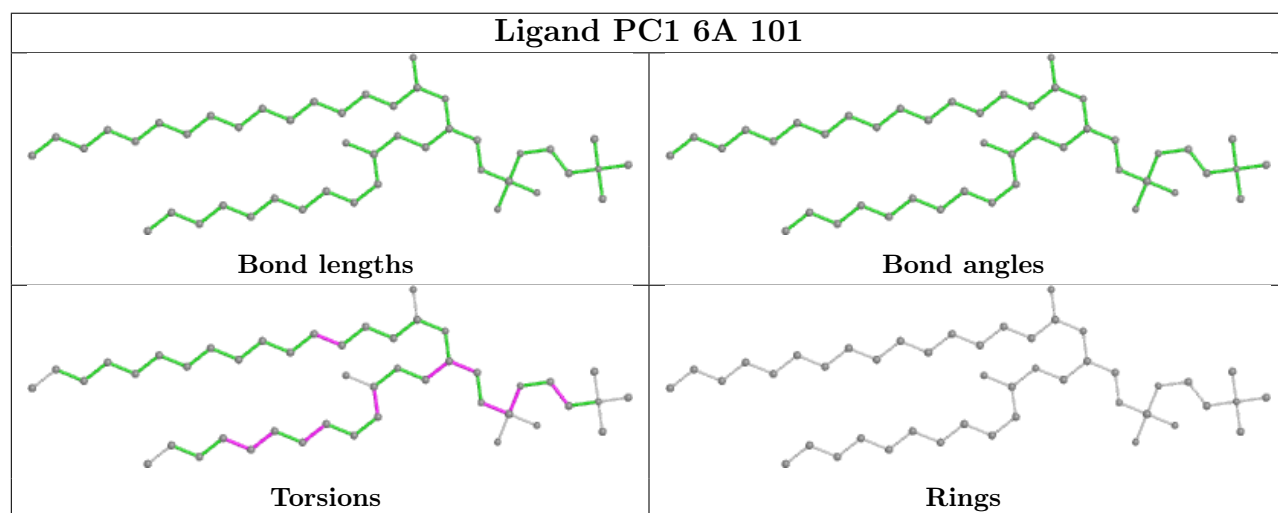
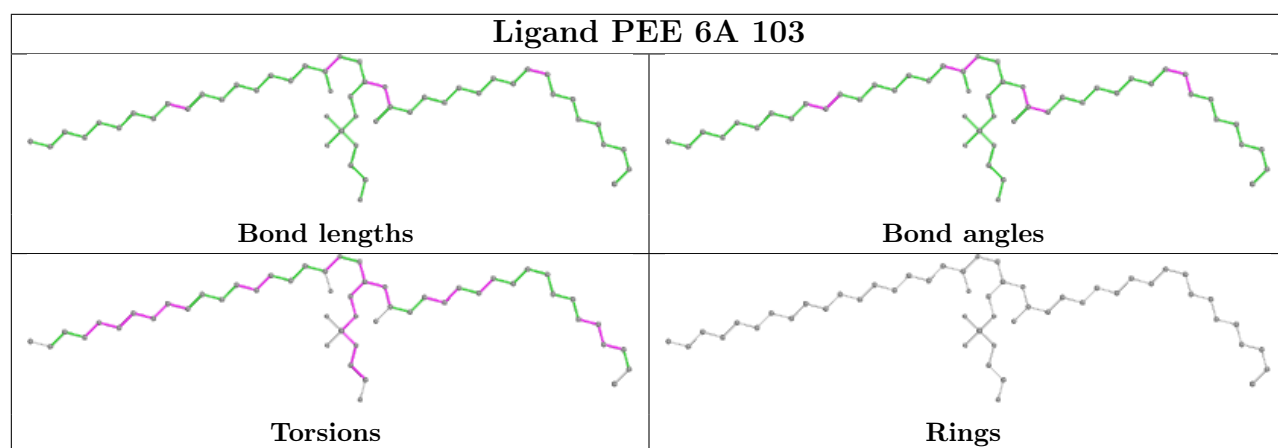
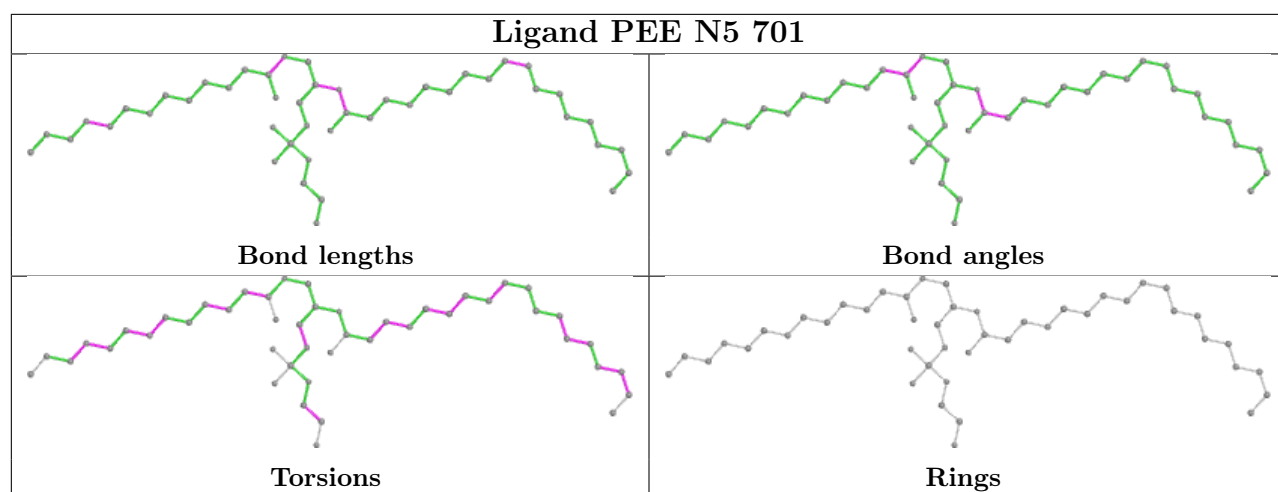


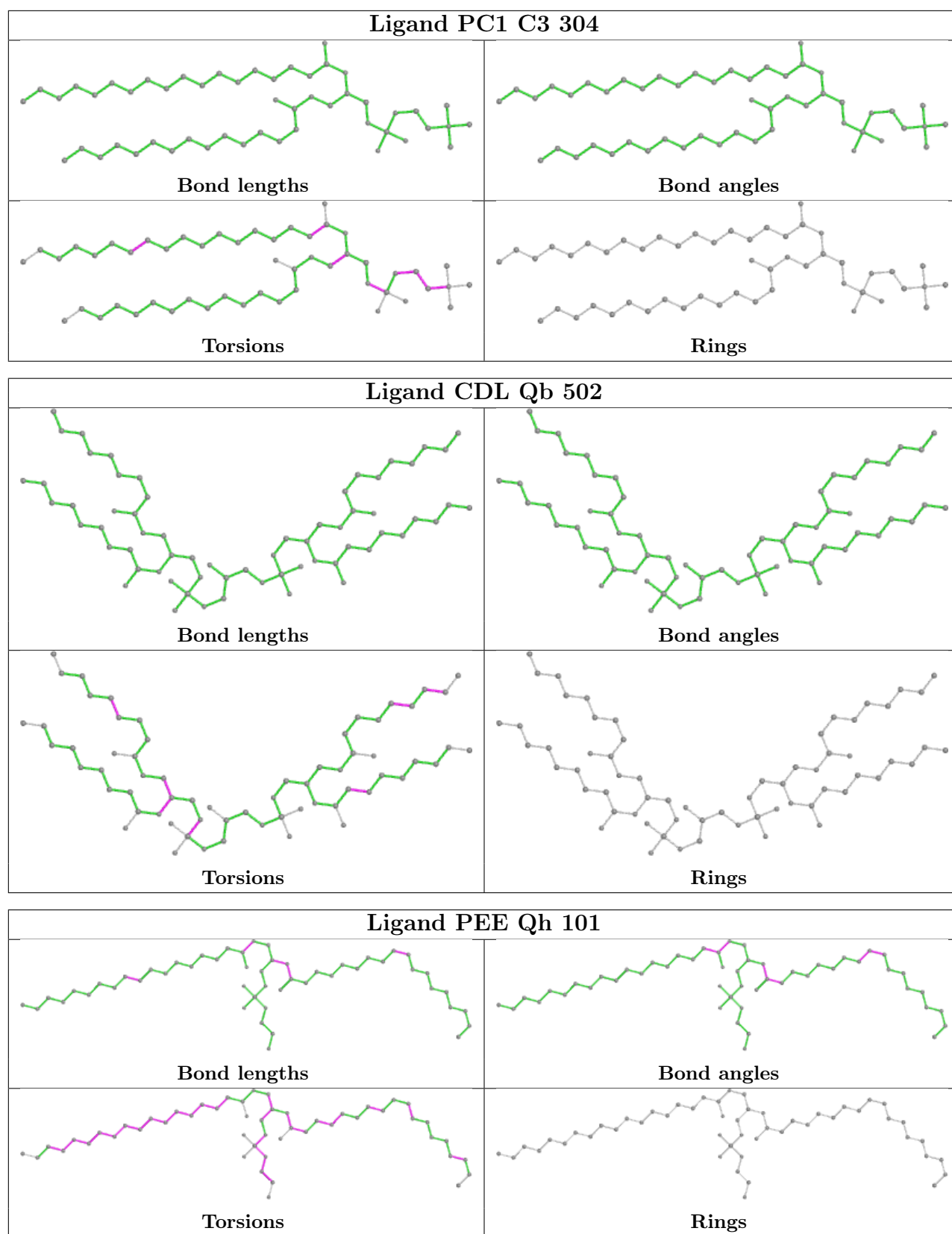


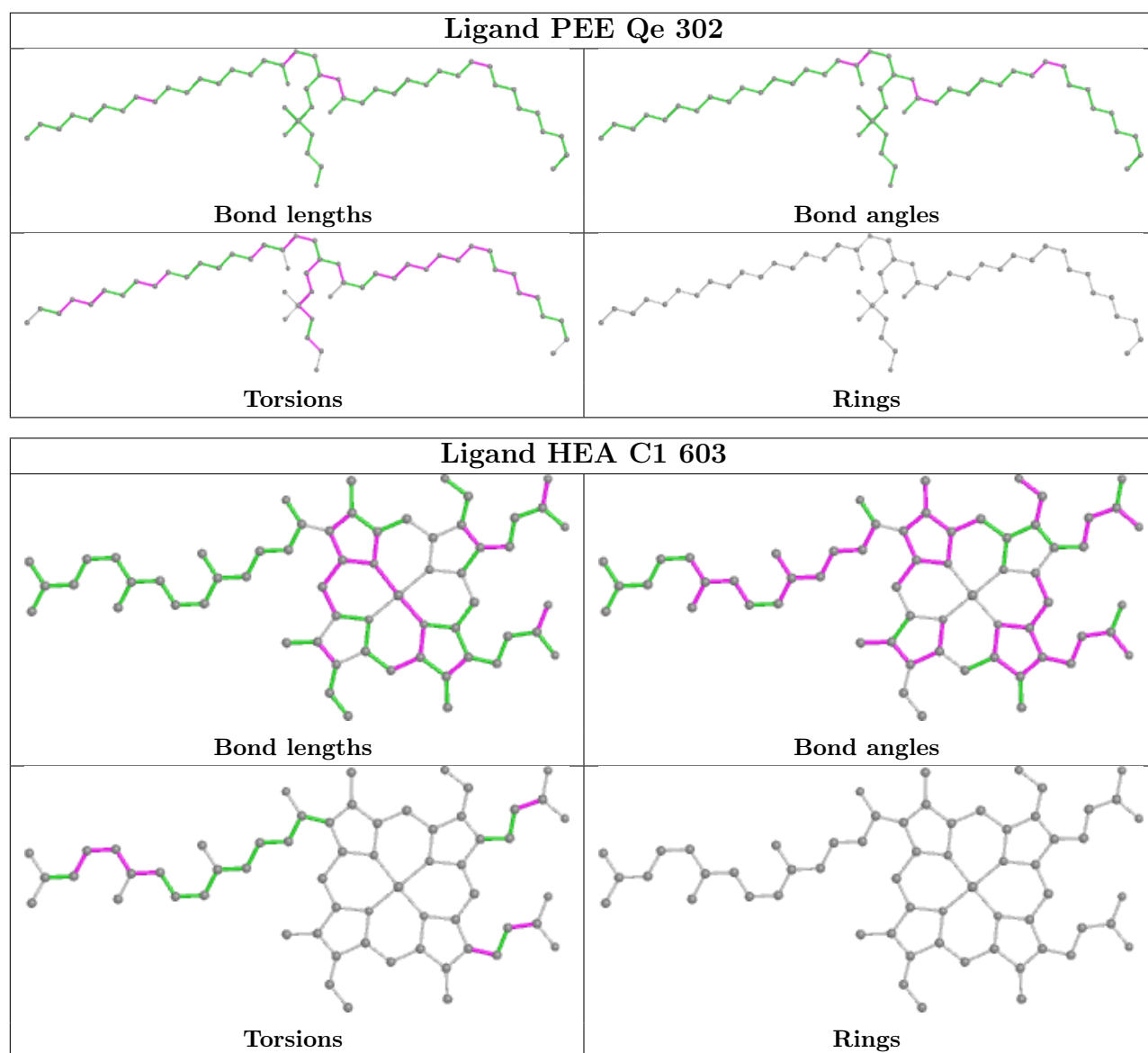


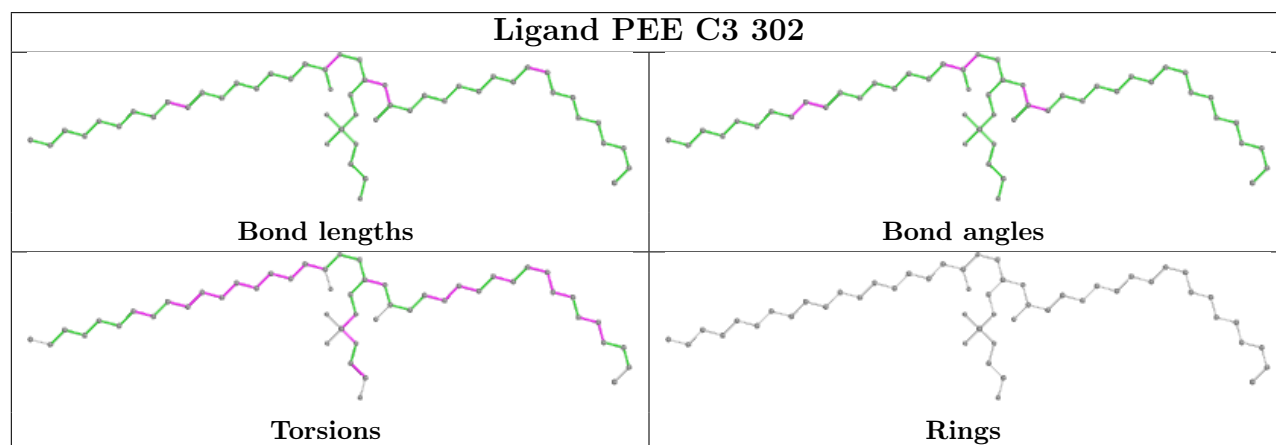
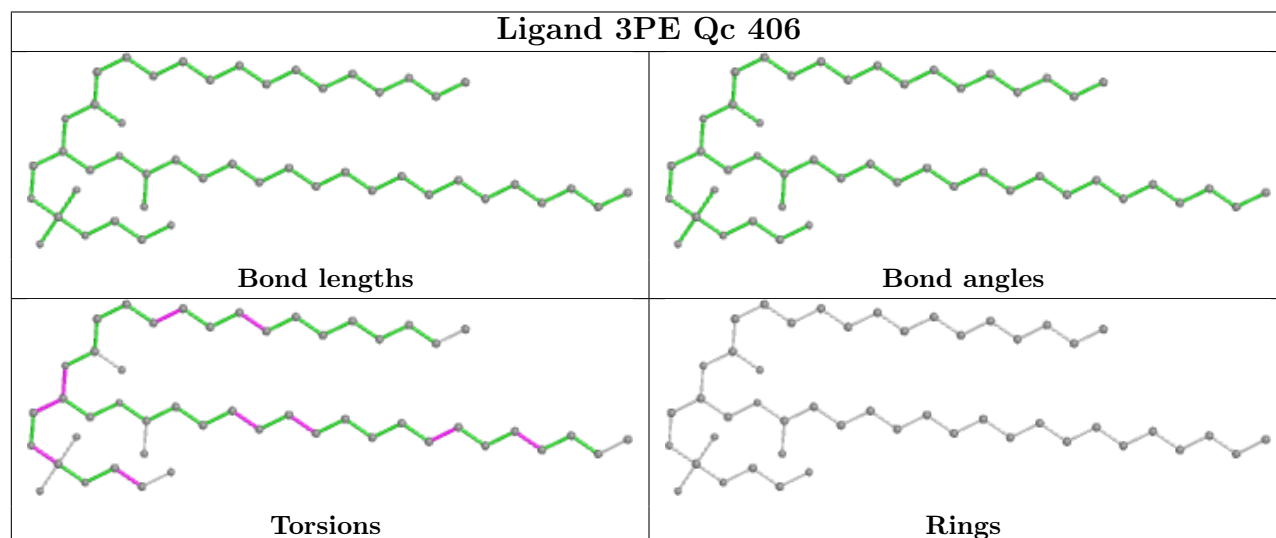
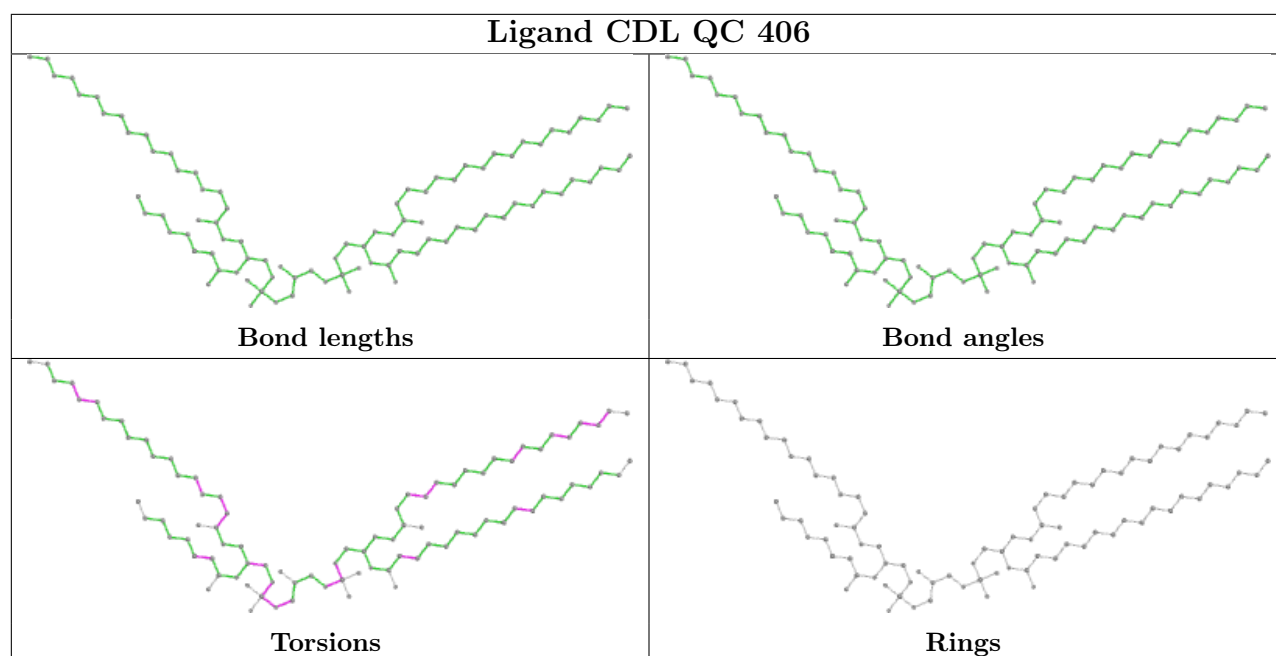


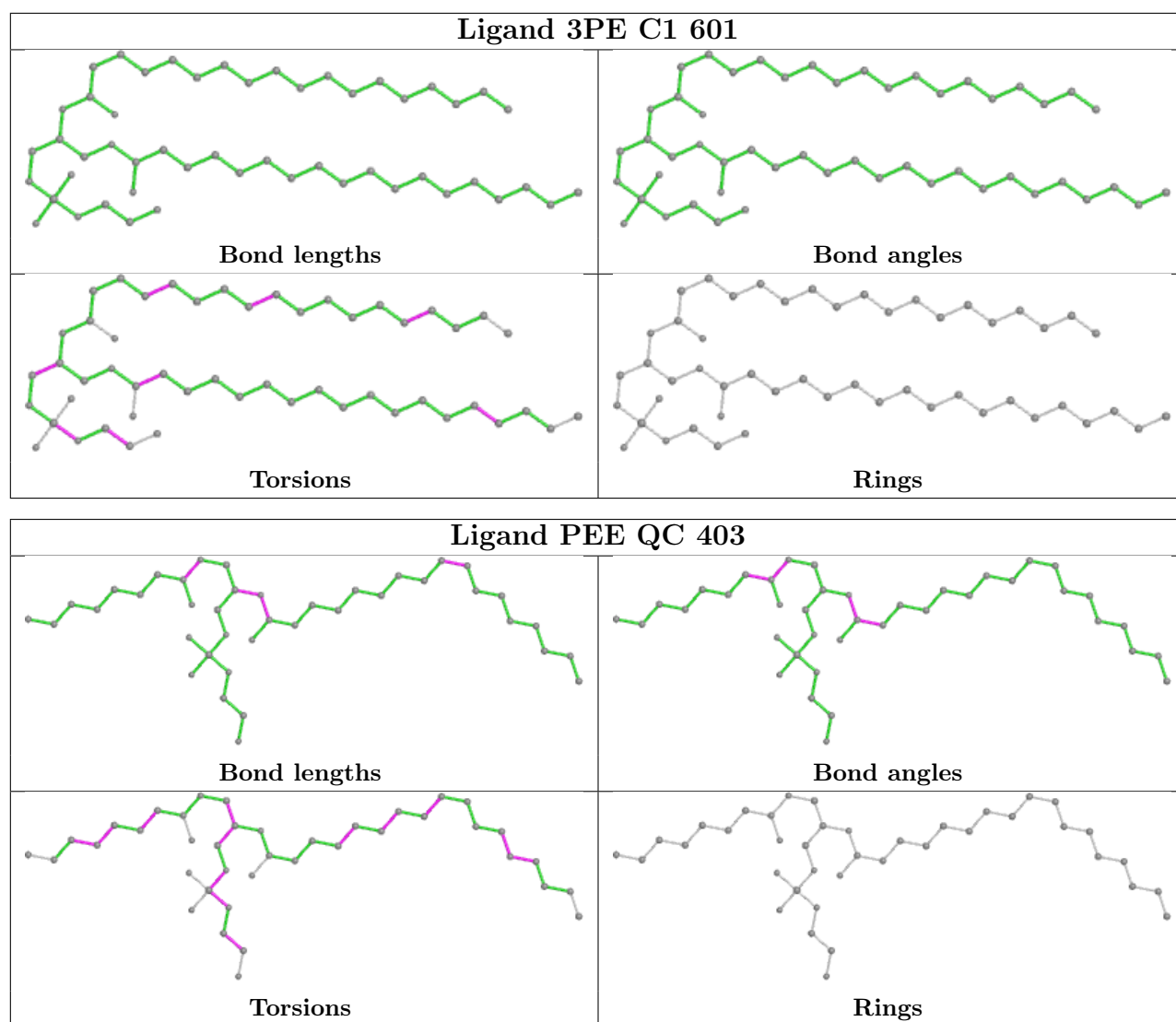




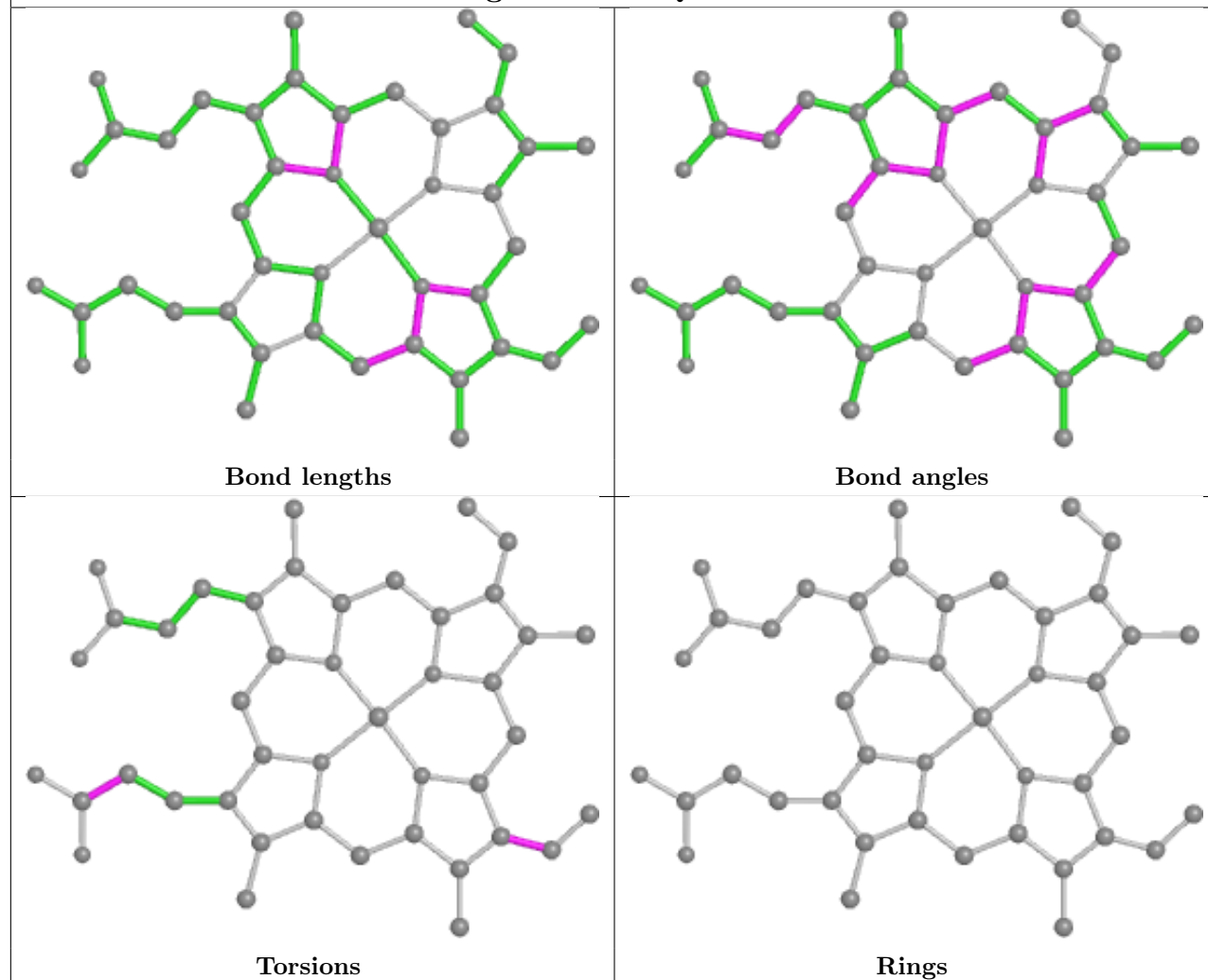




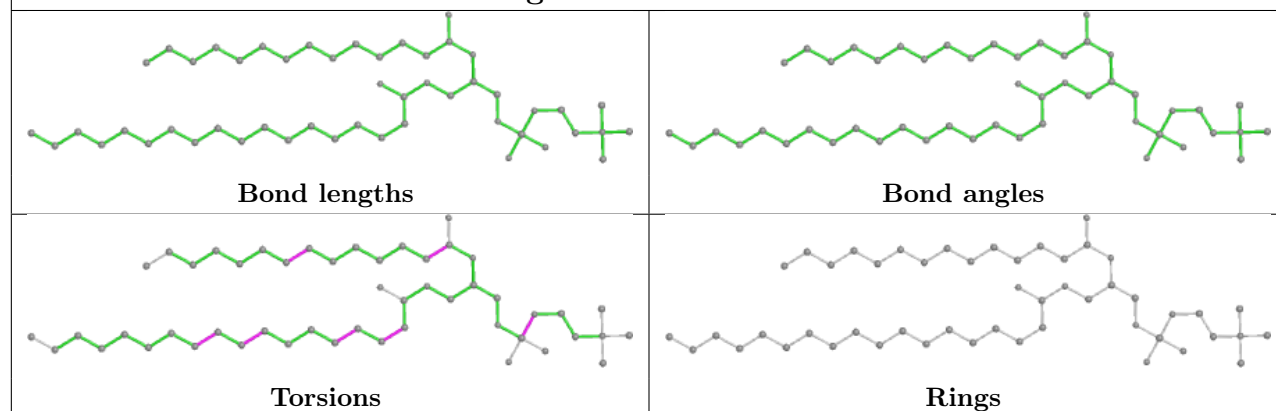


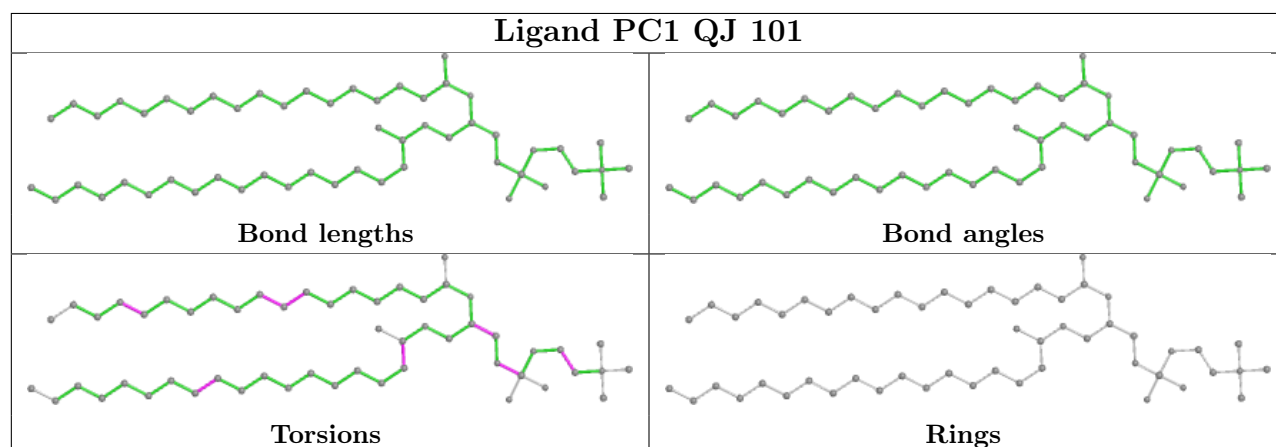
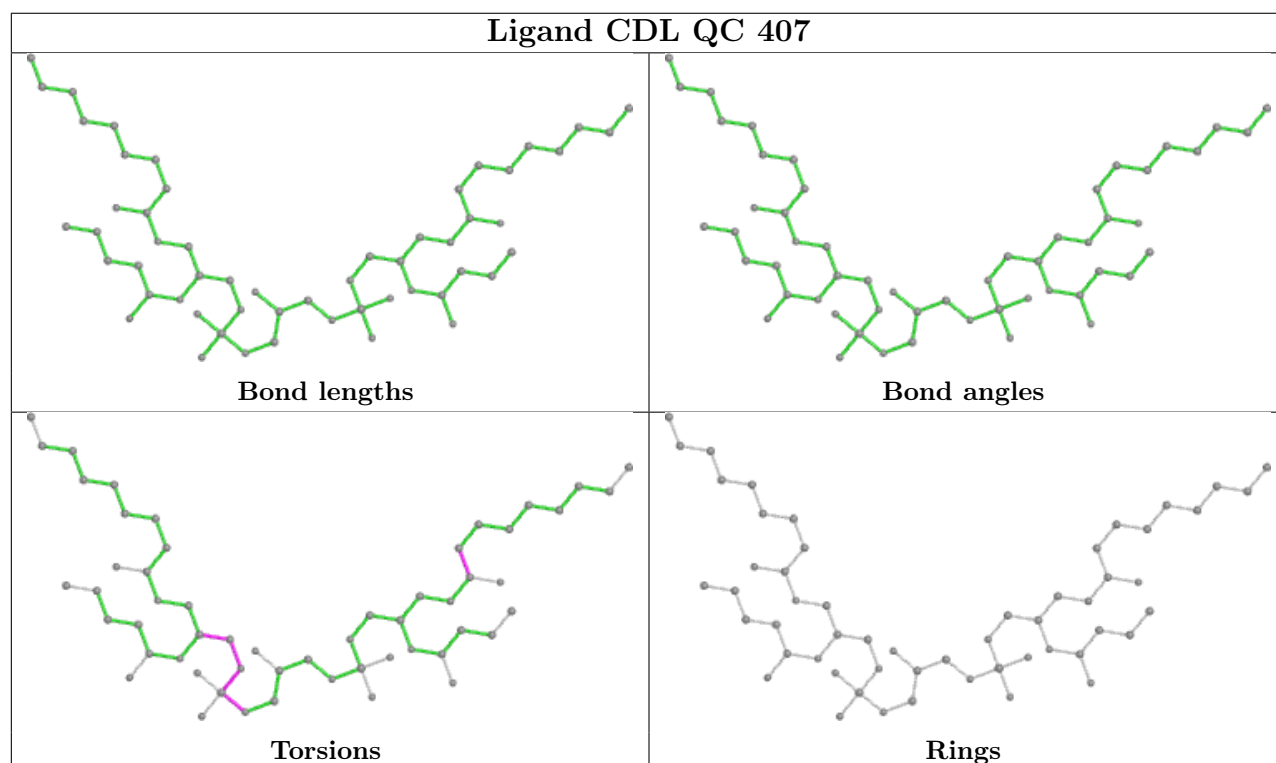
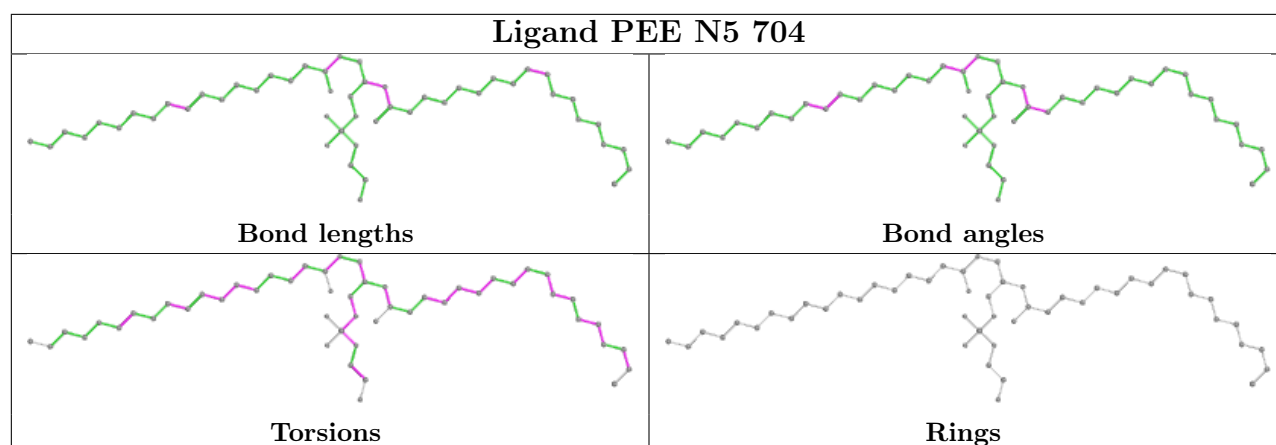


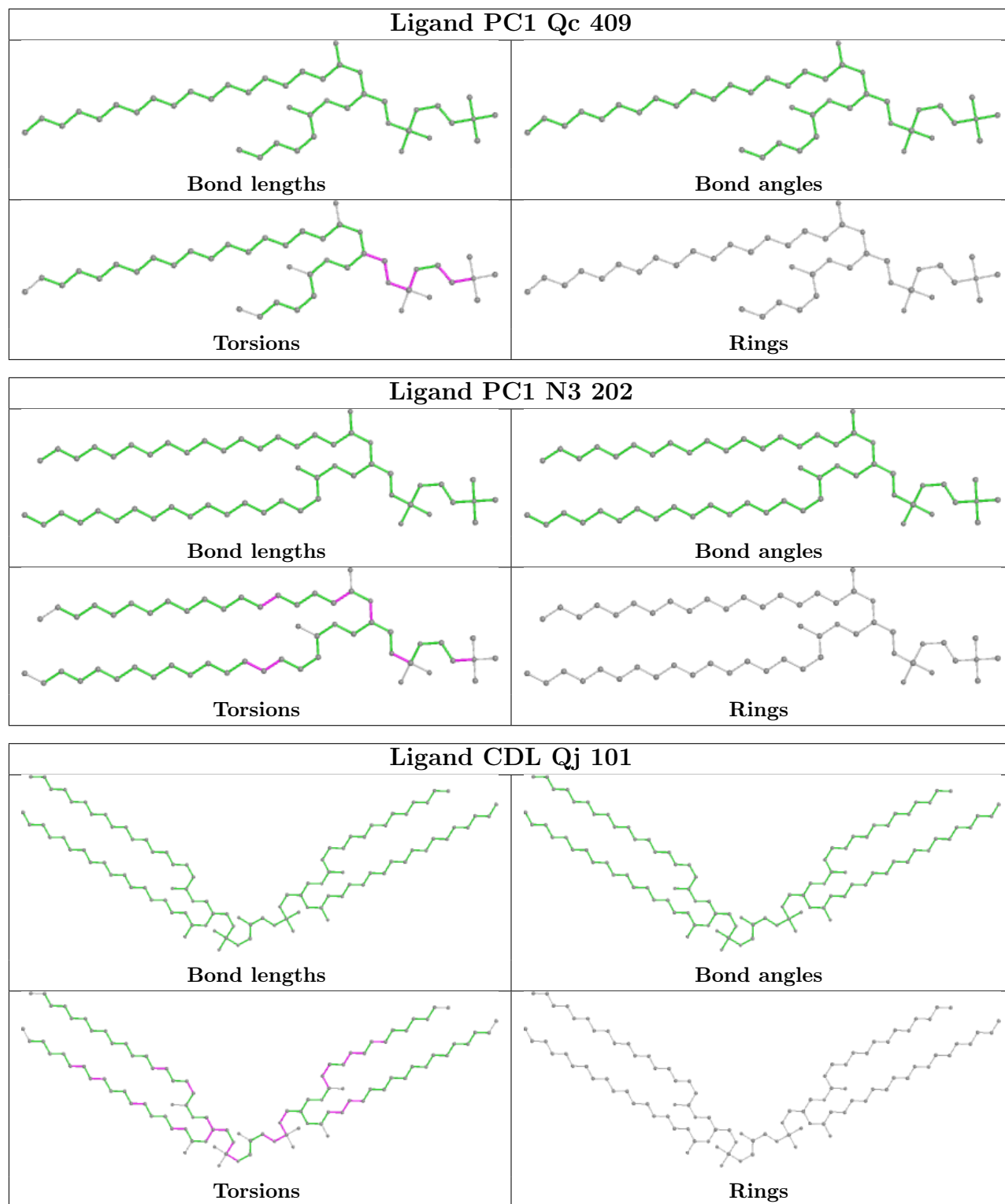
Ligand HEM QC 402

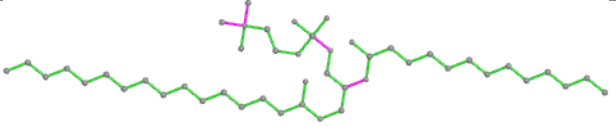
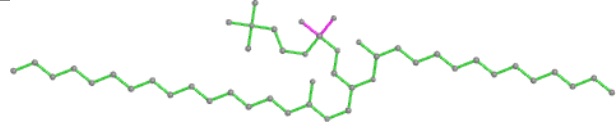
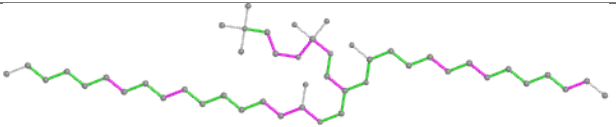
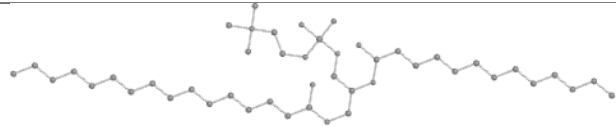


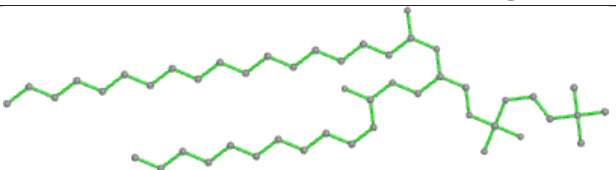
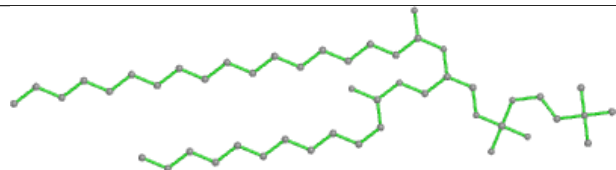
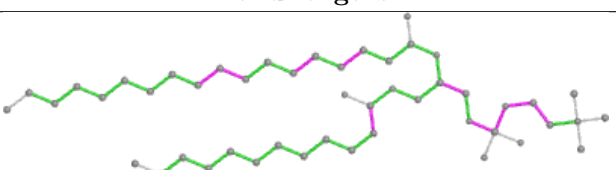
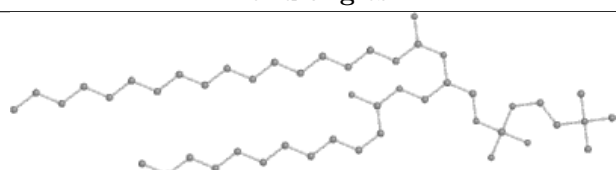
Ligand PC1 C1 610

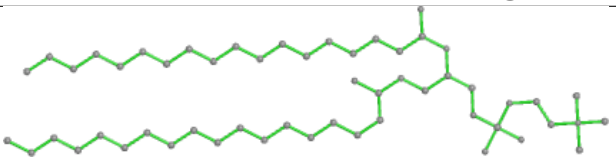
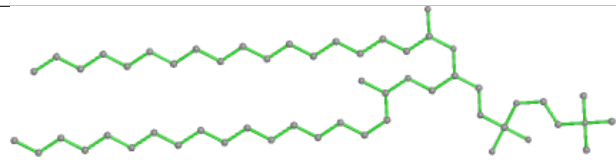
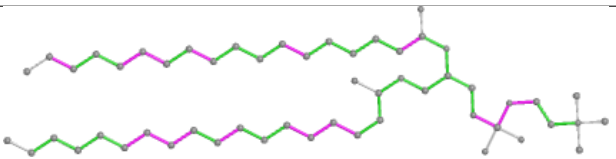
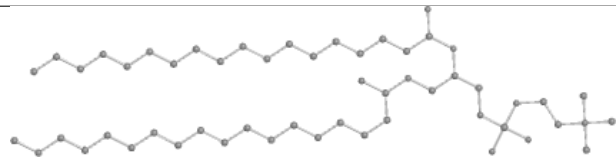


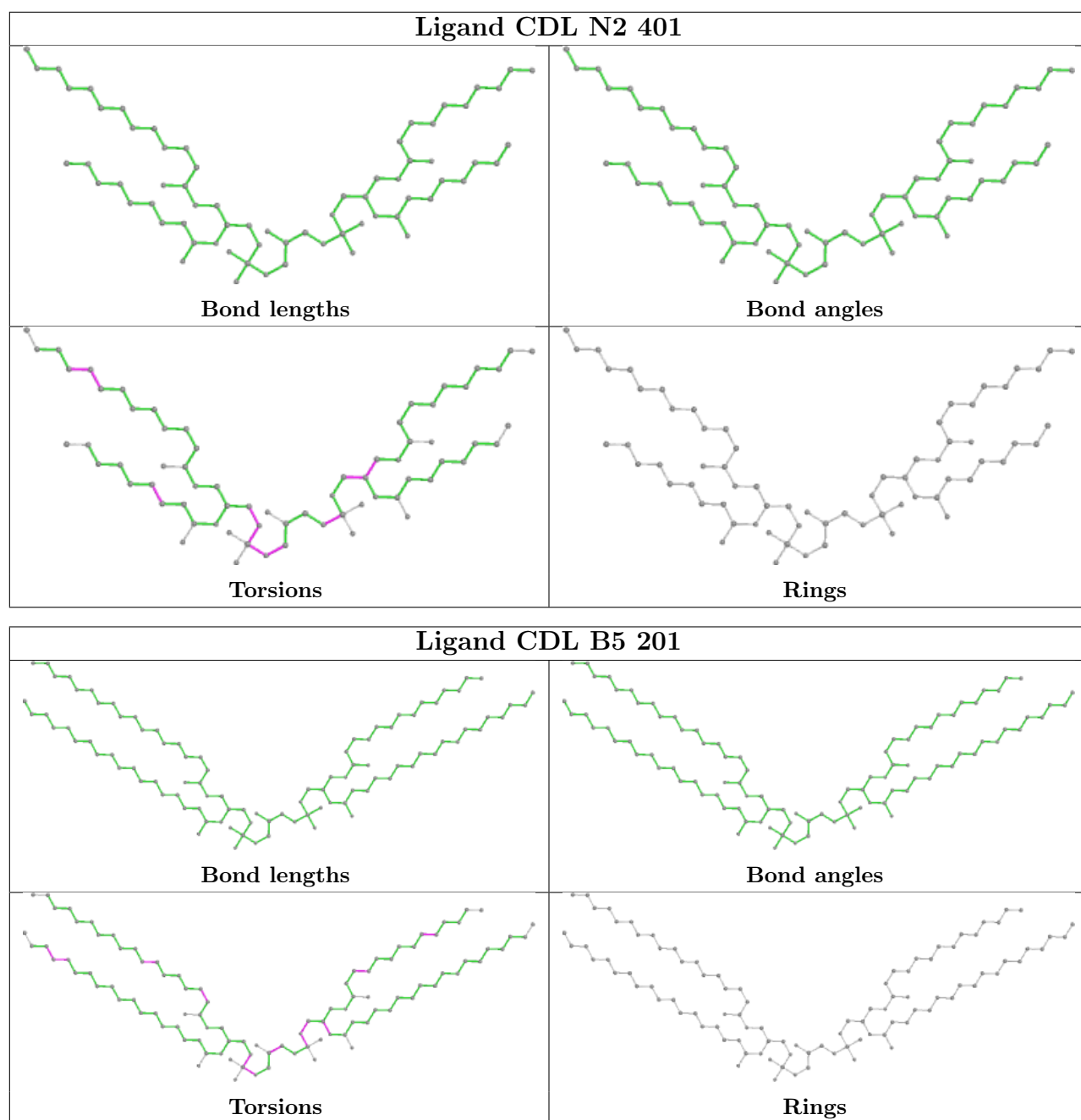


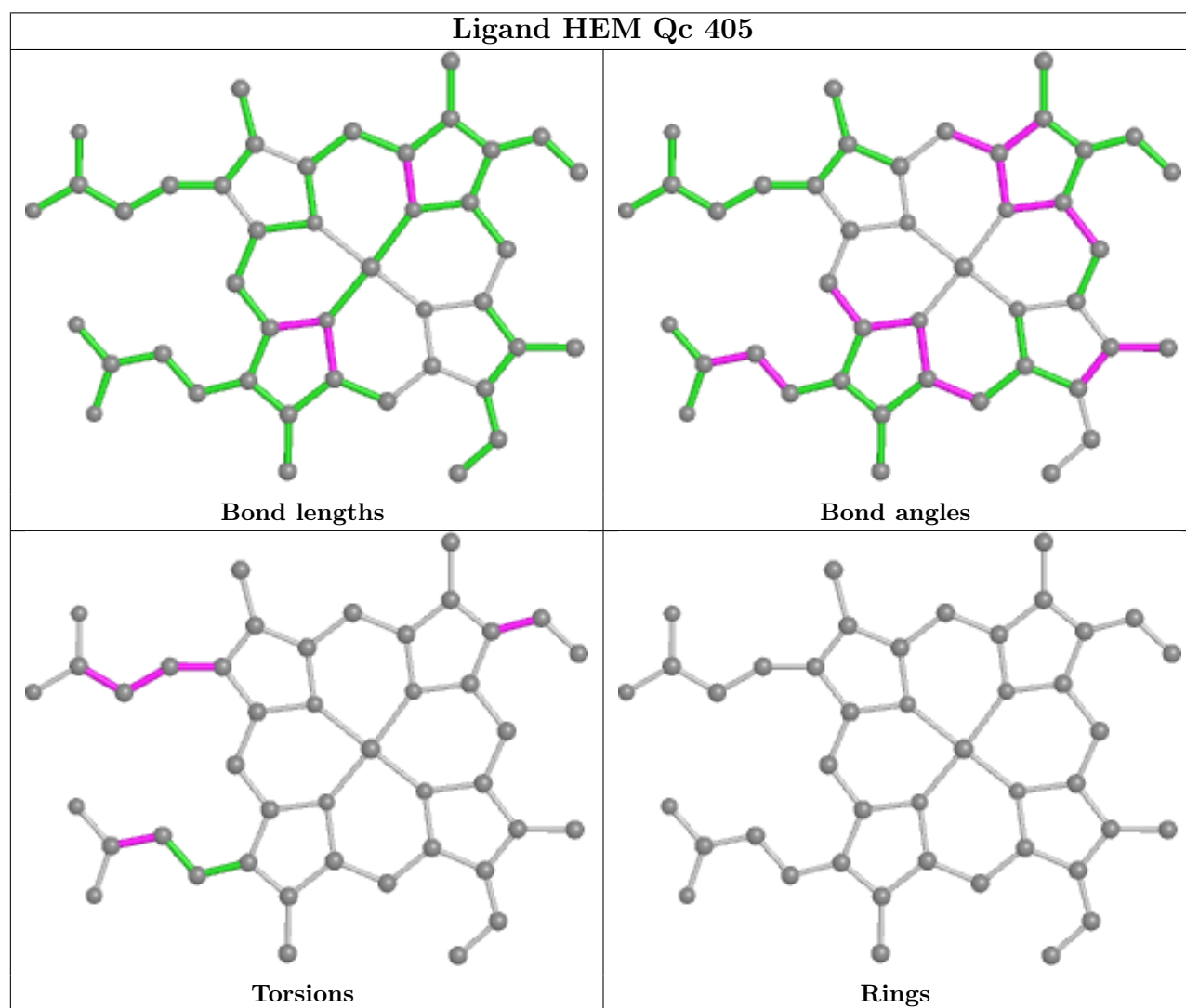
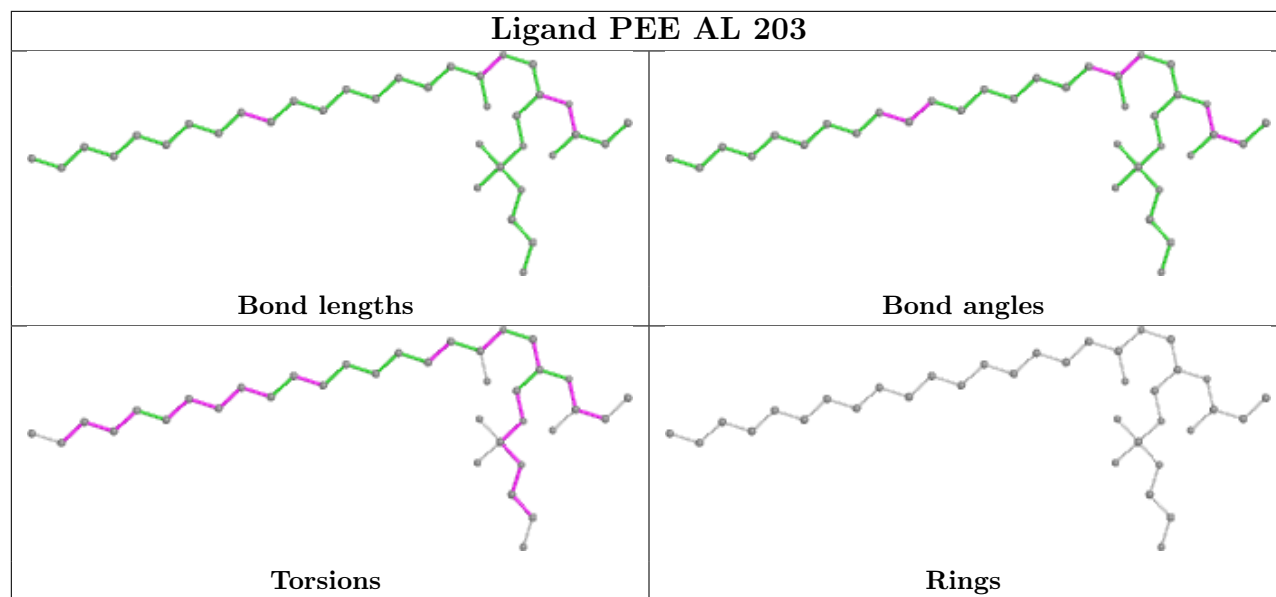


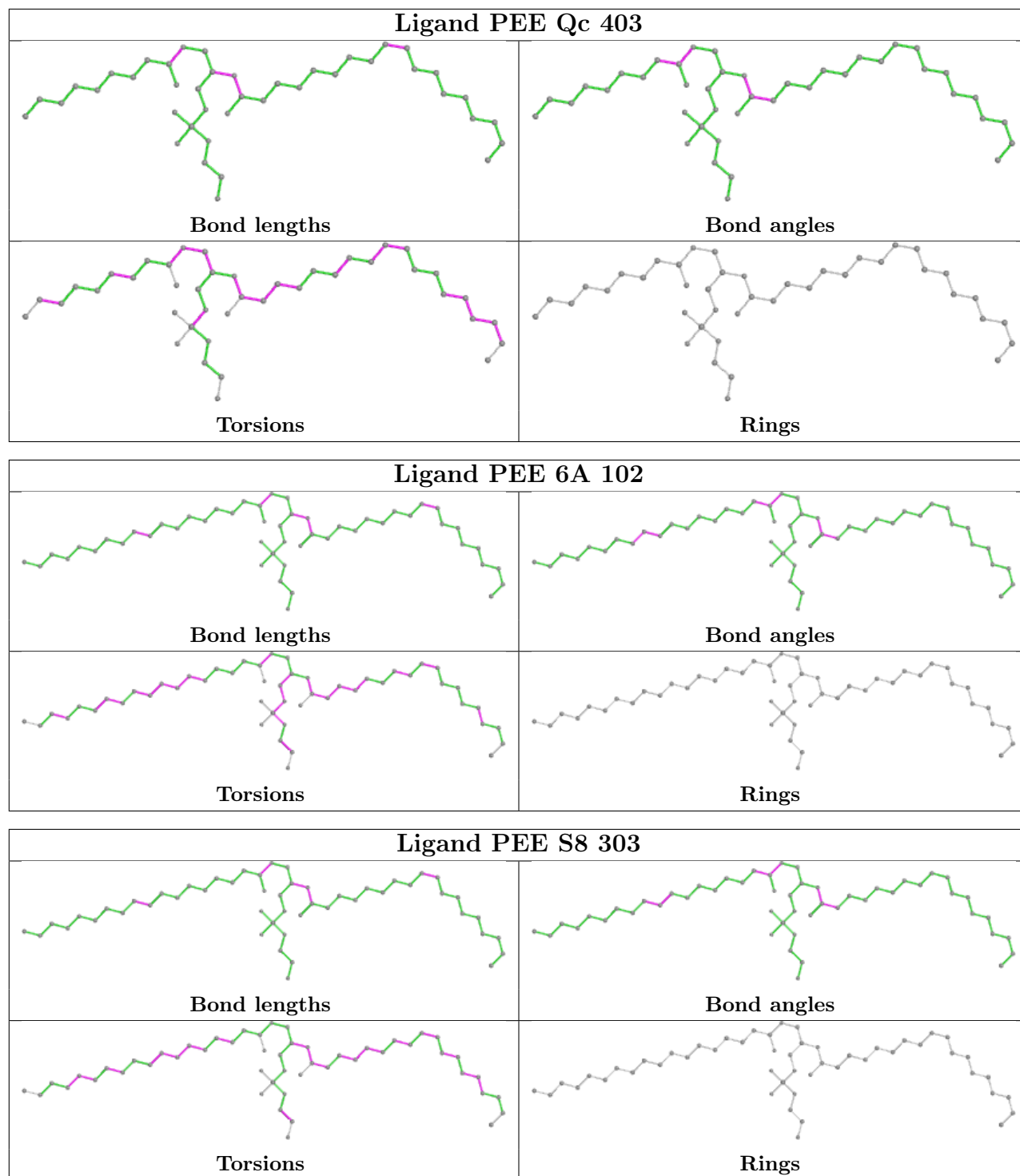
Ligand PLX AL 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

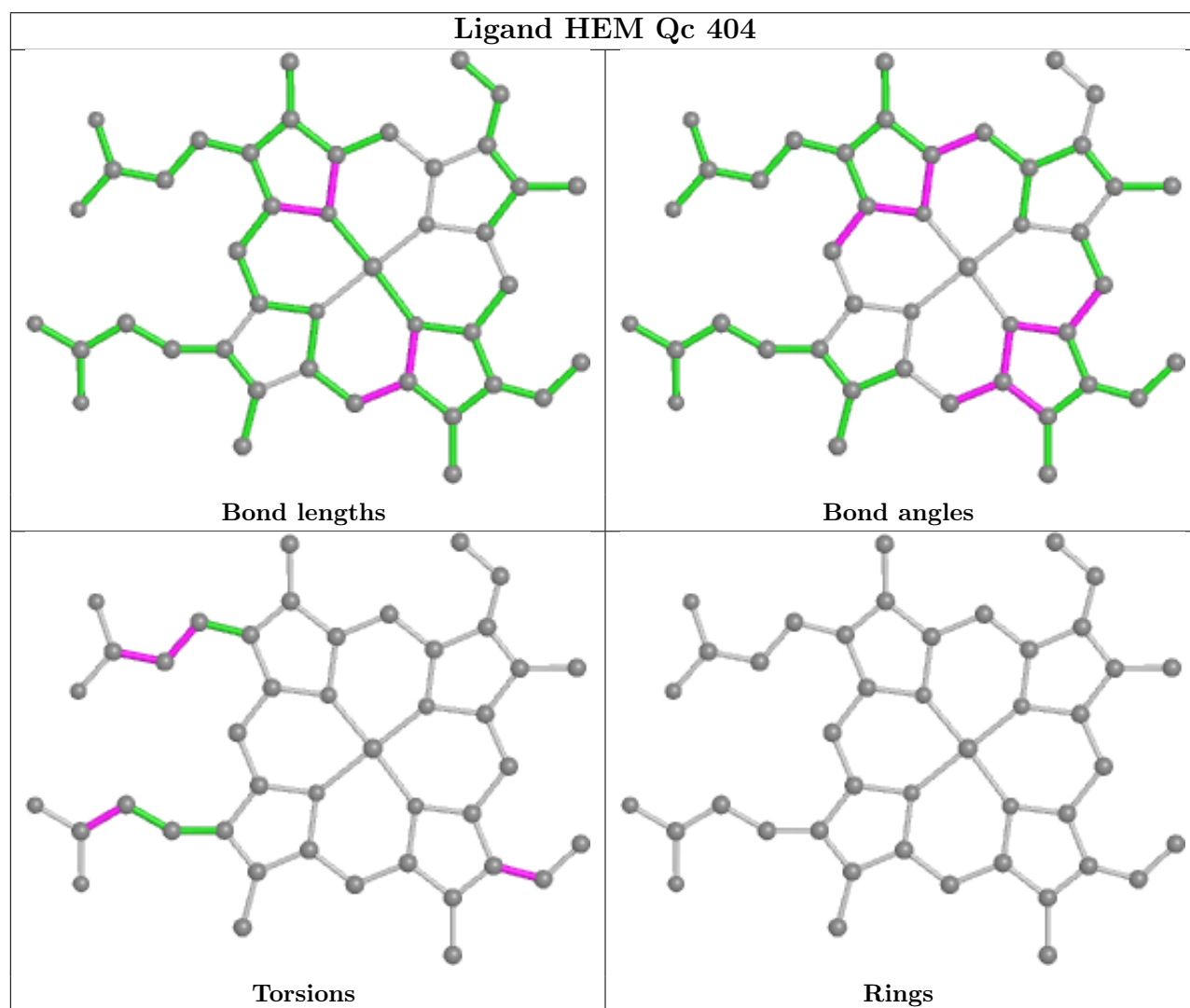
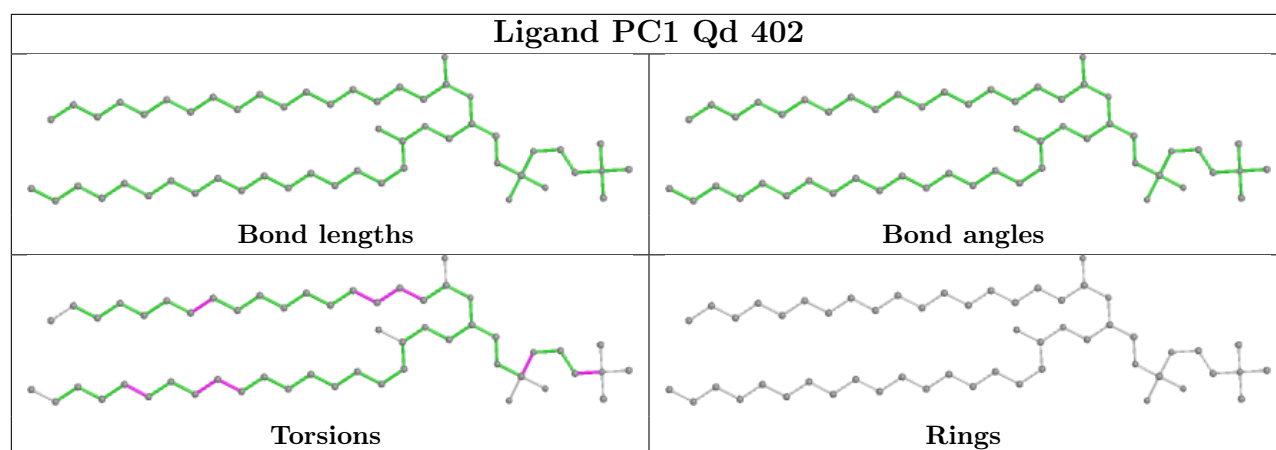
Ligand PC1 C1 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

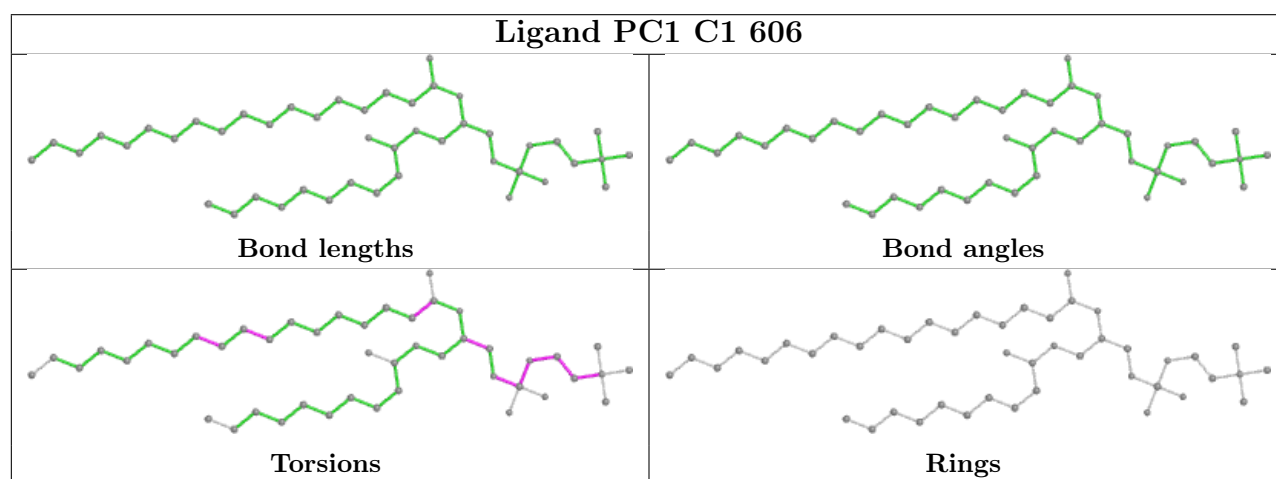
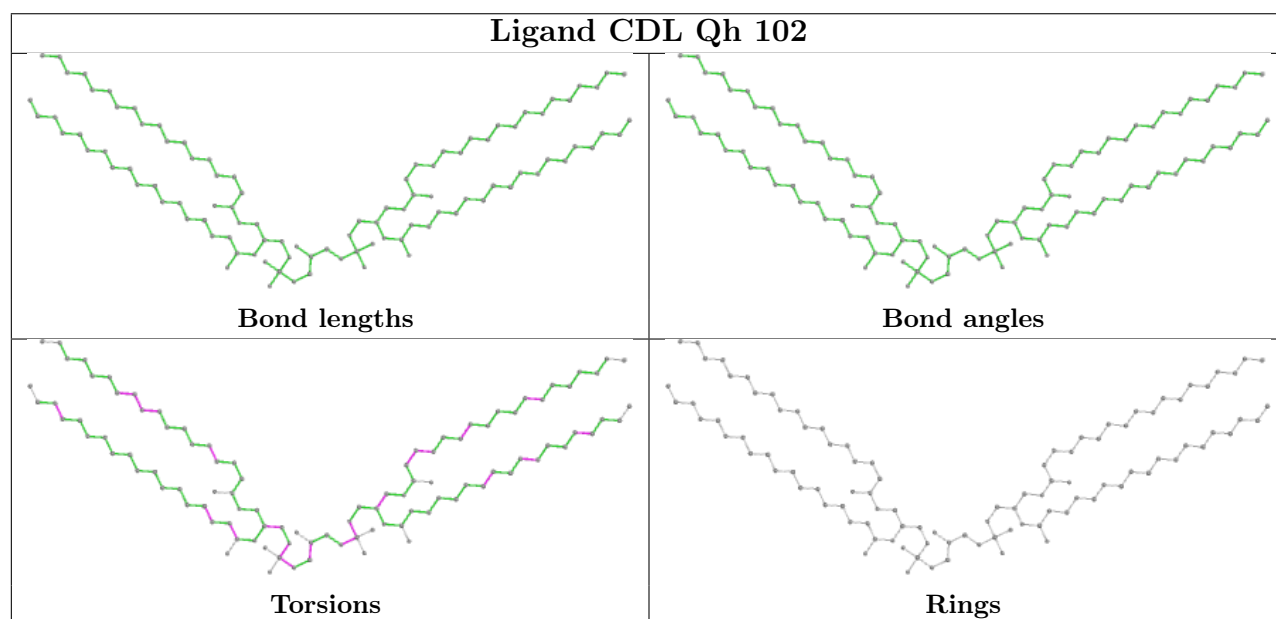
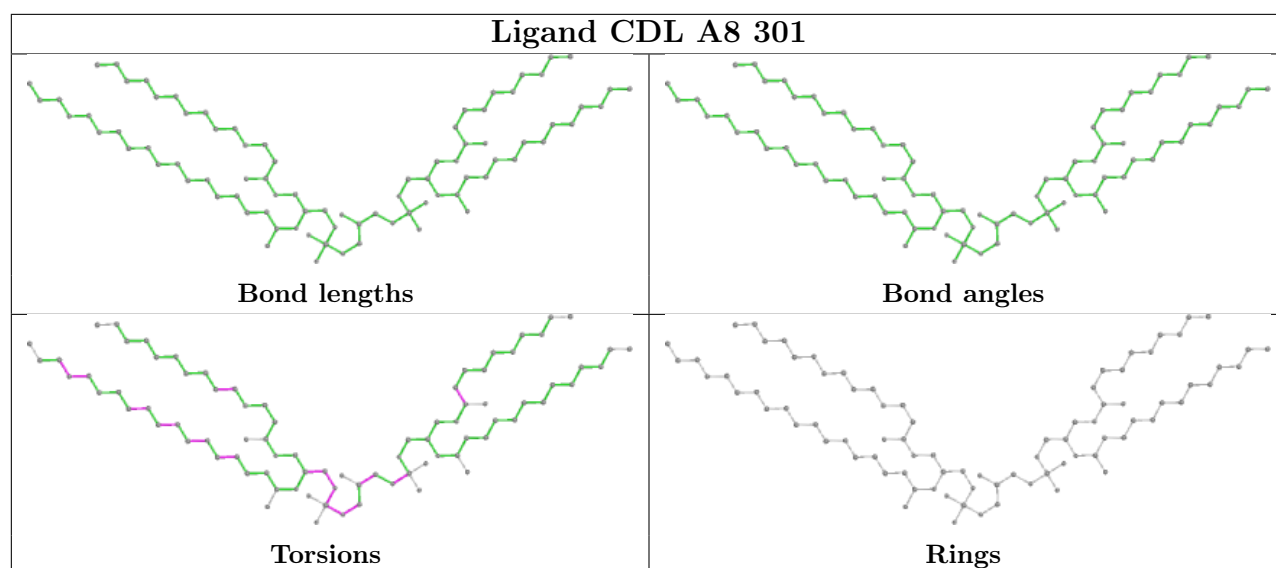
Ligand PC1 N4 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

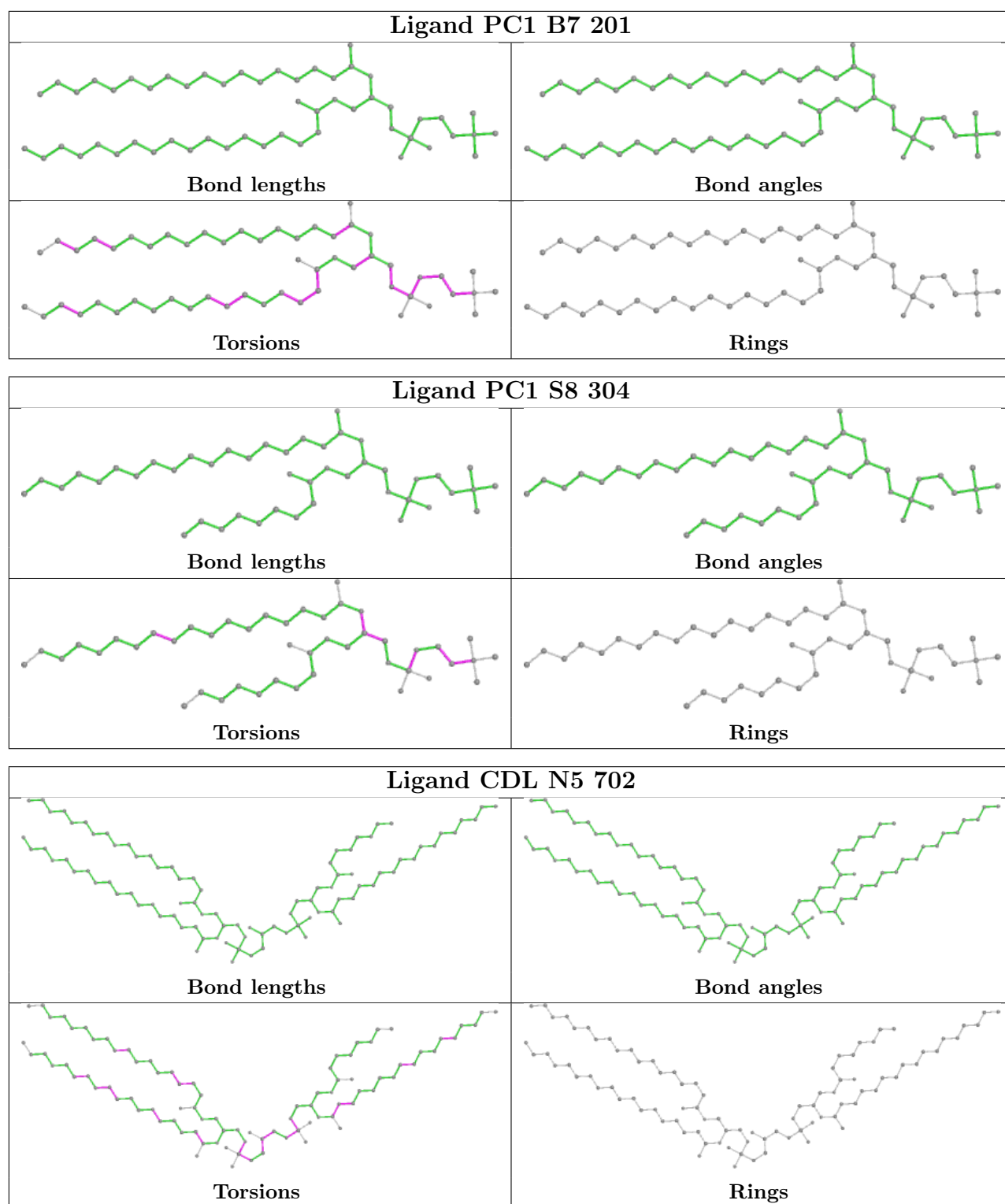


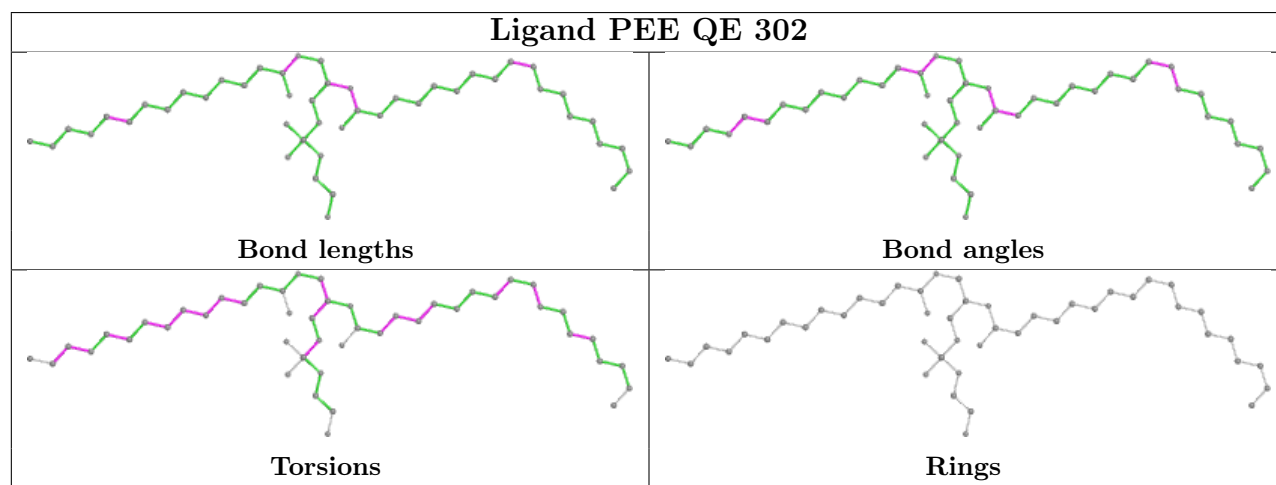
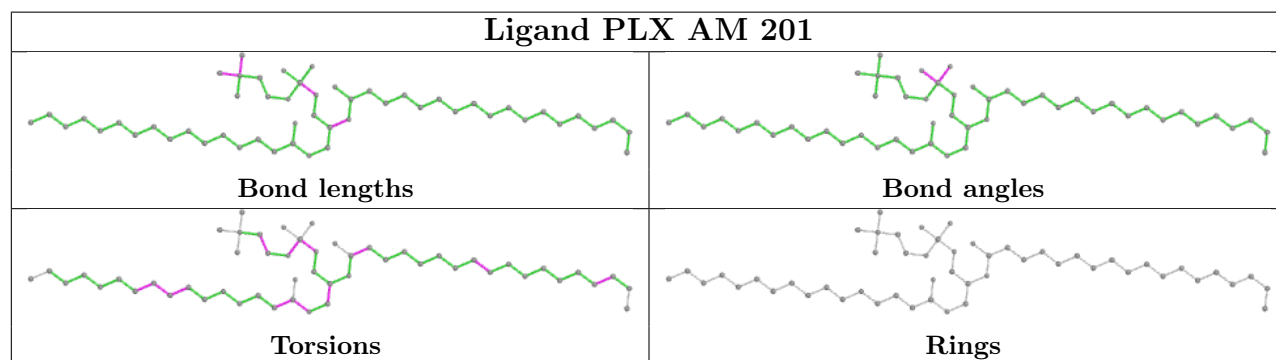
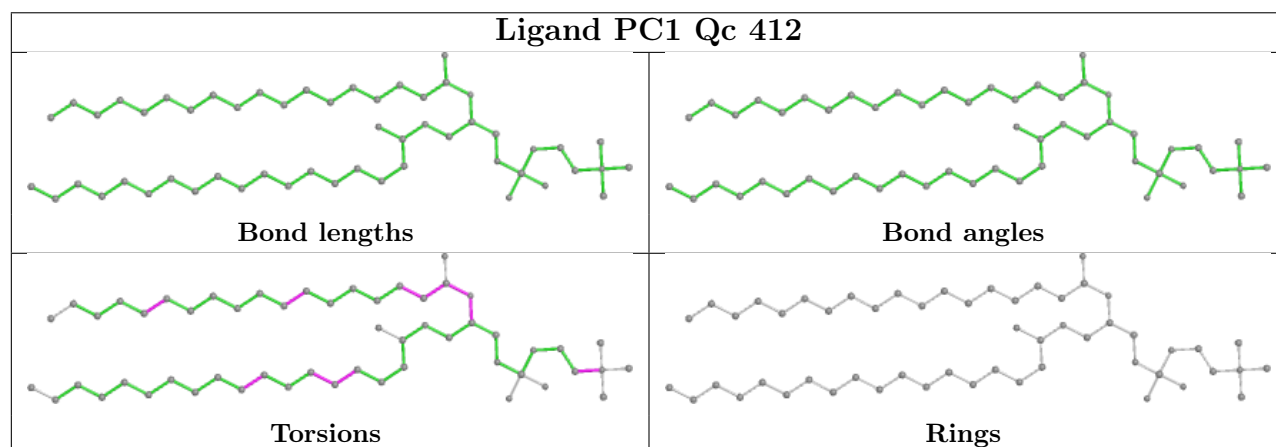
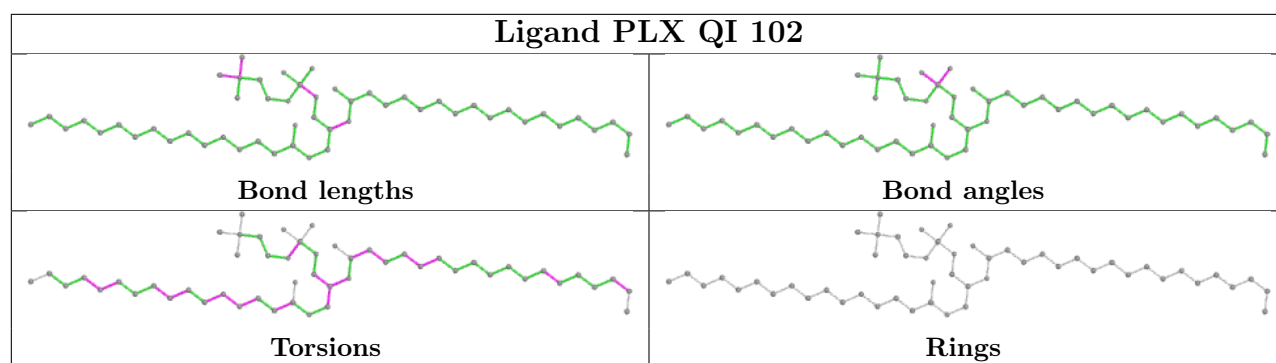


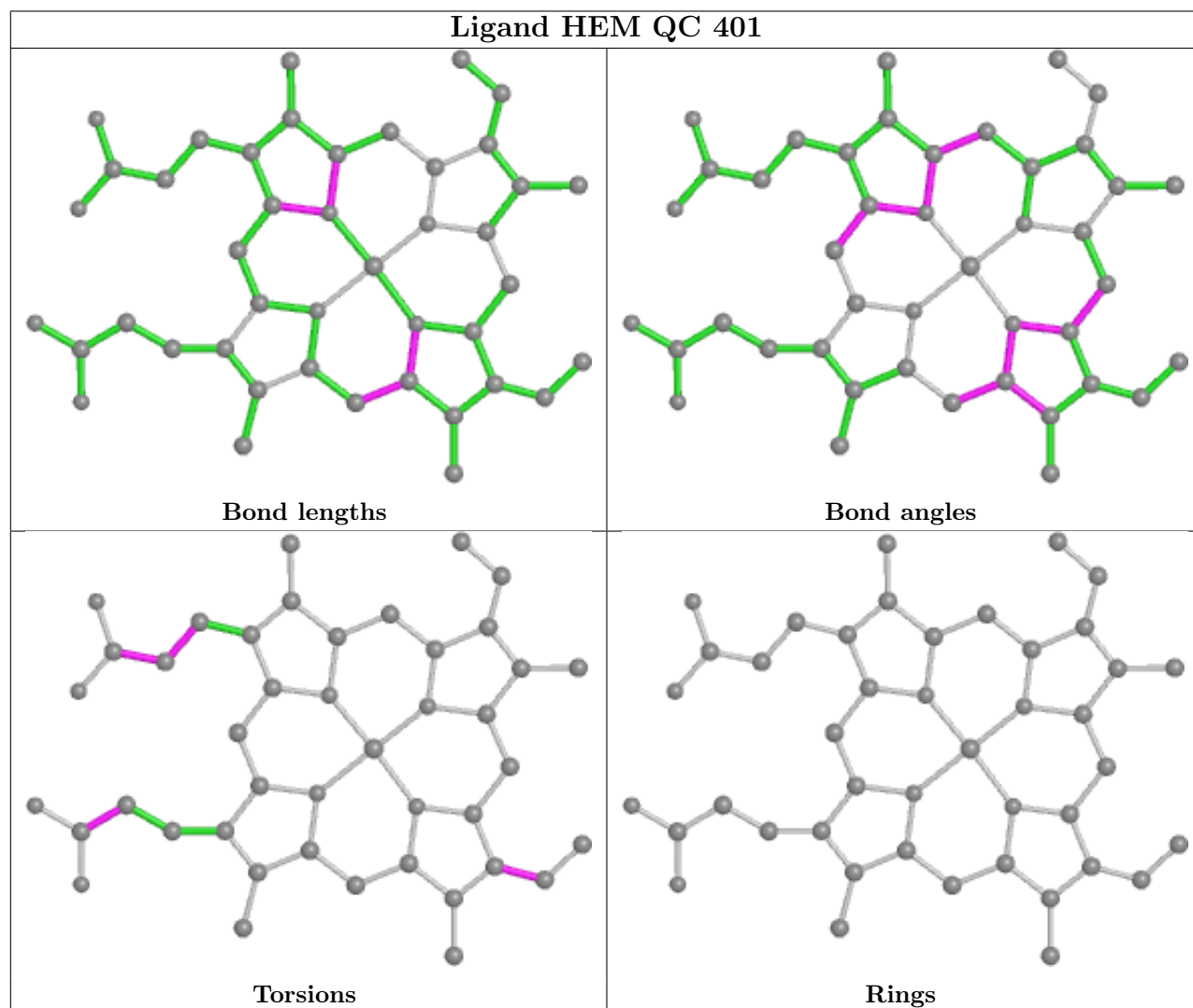
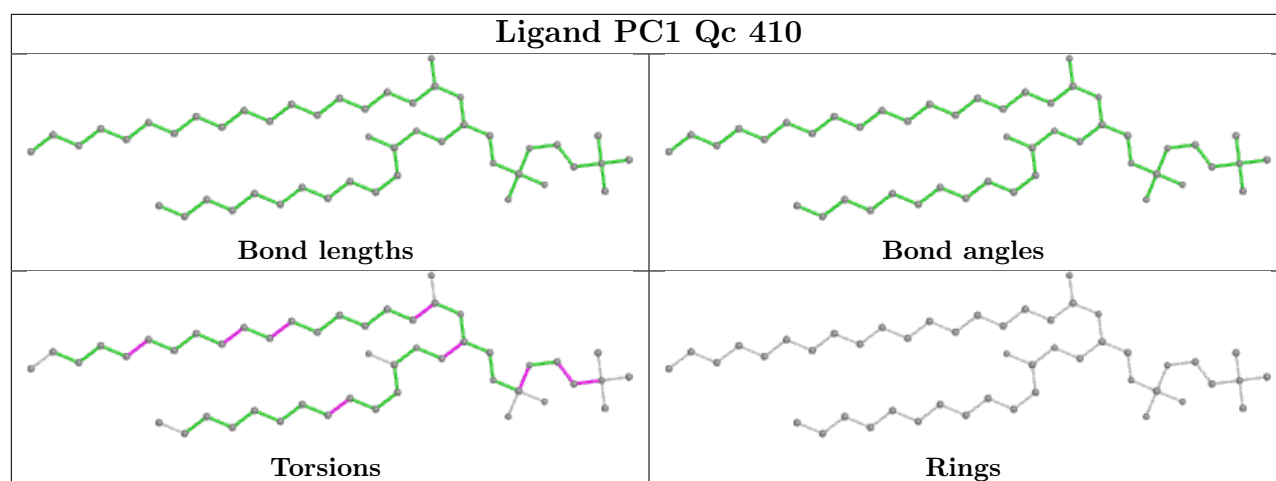


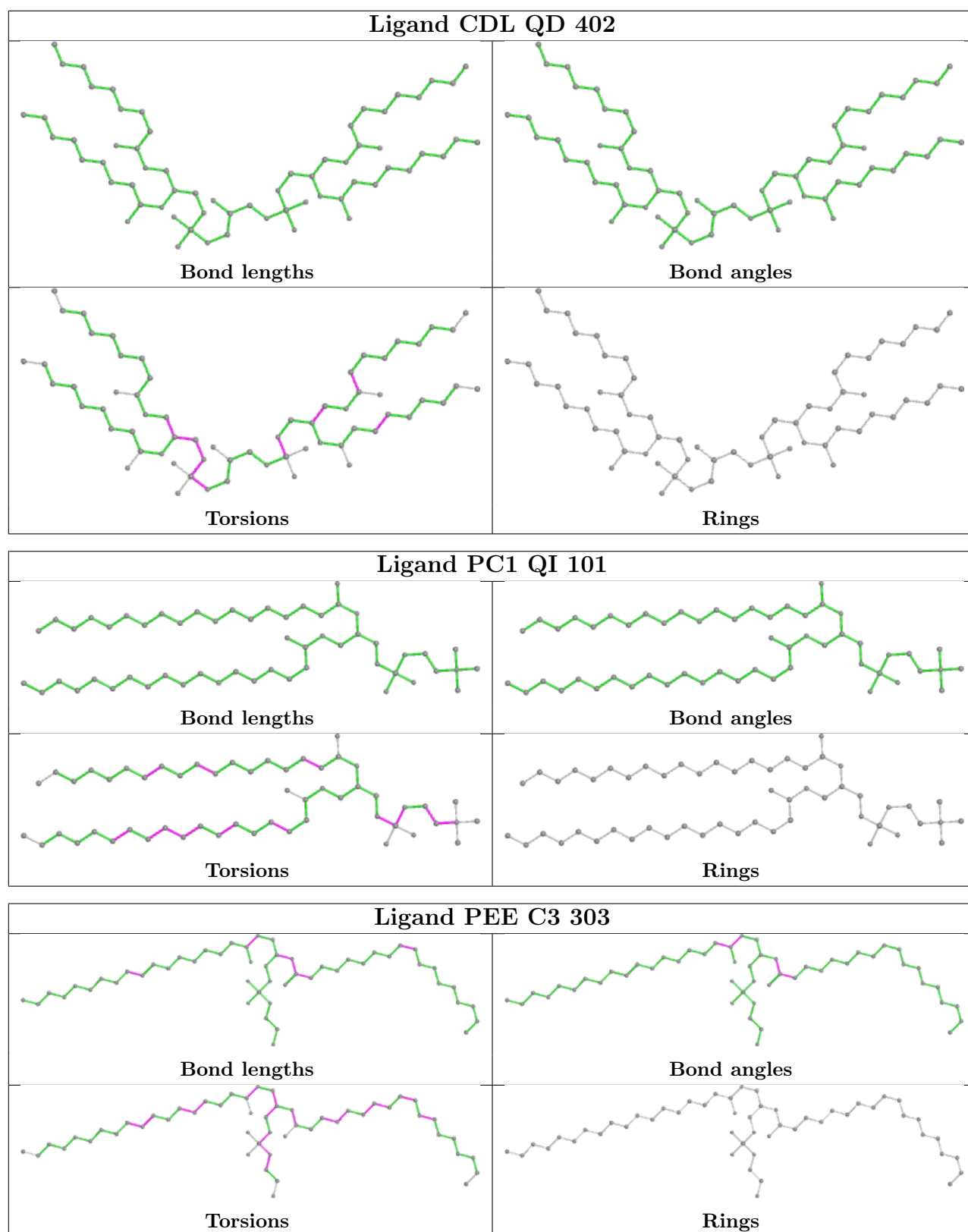


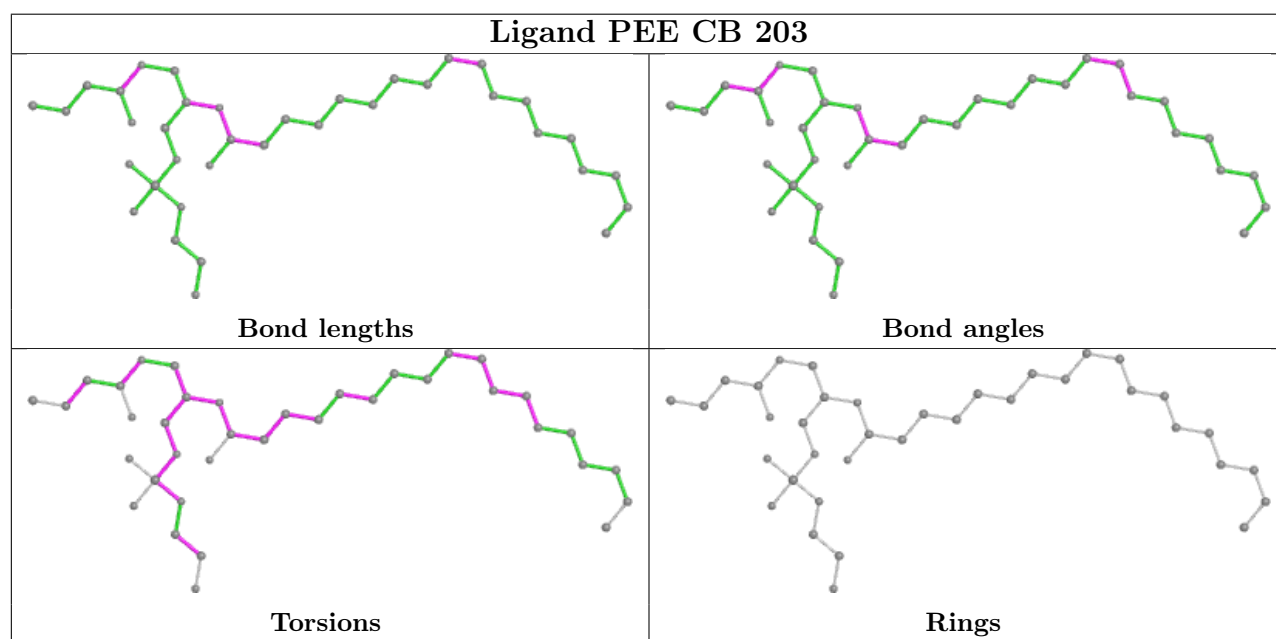
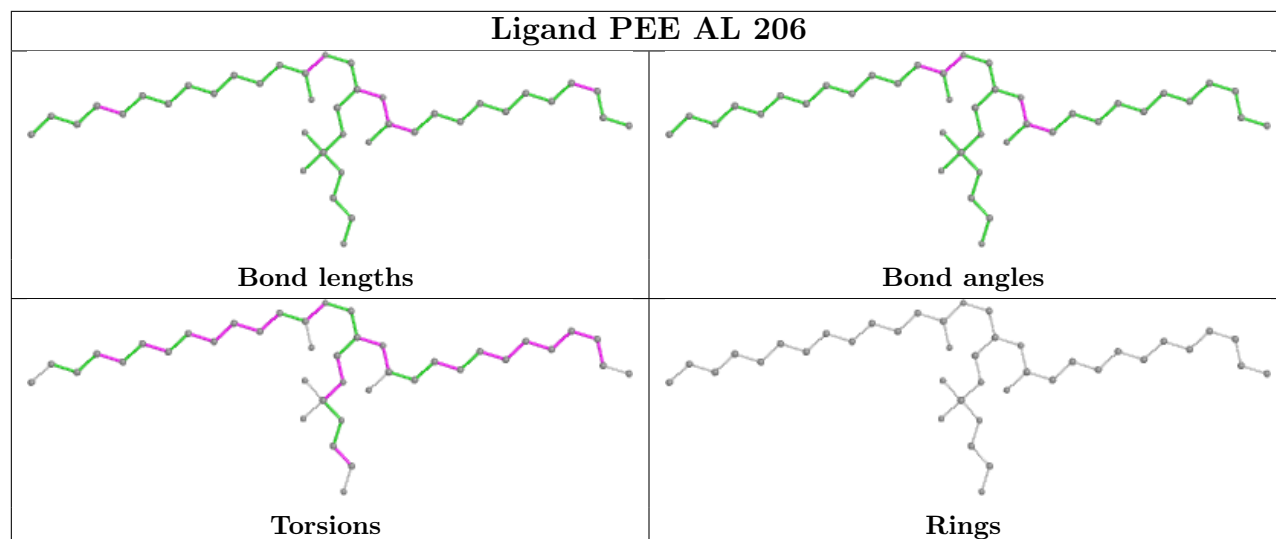


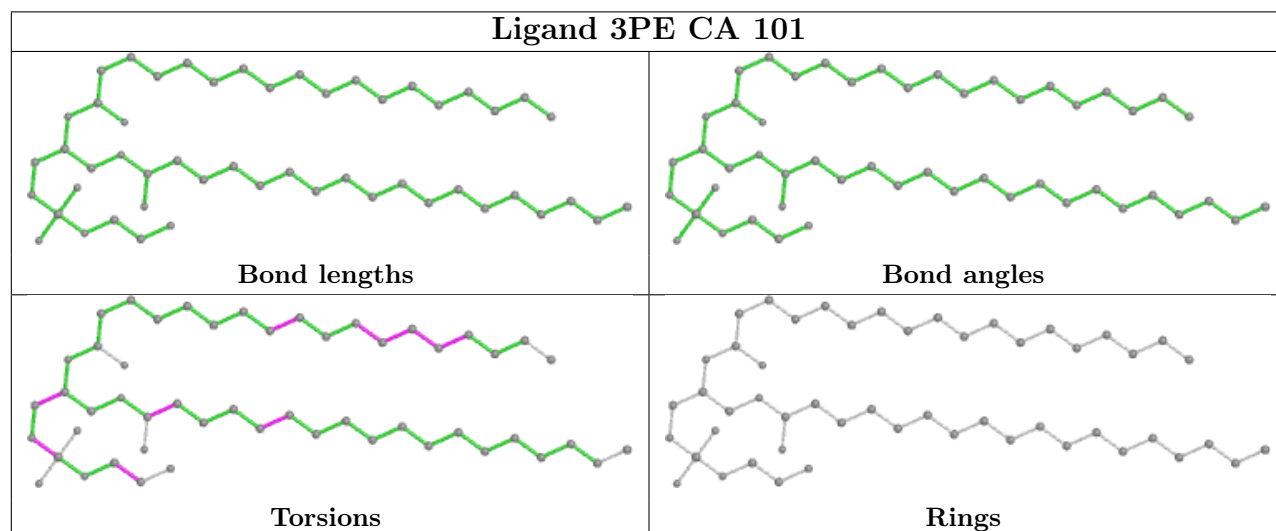
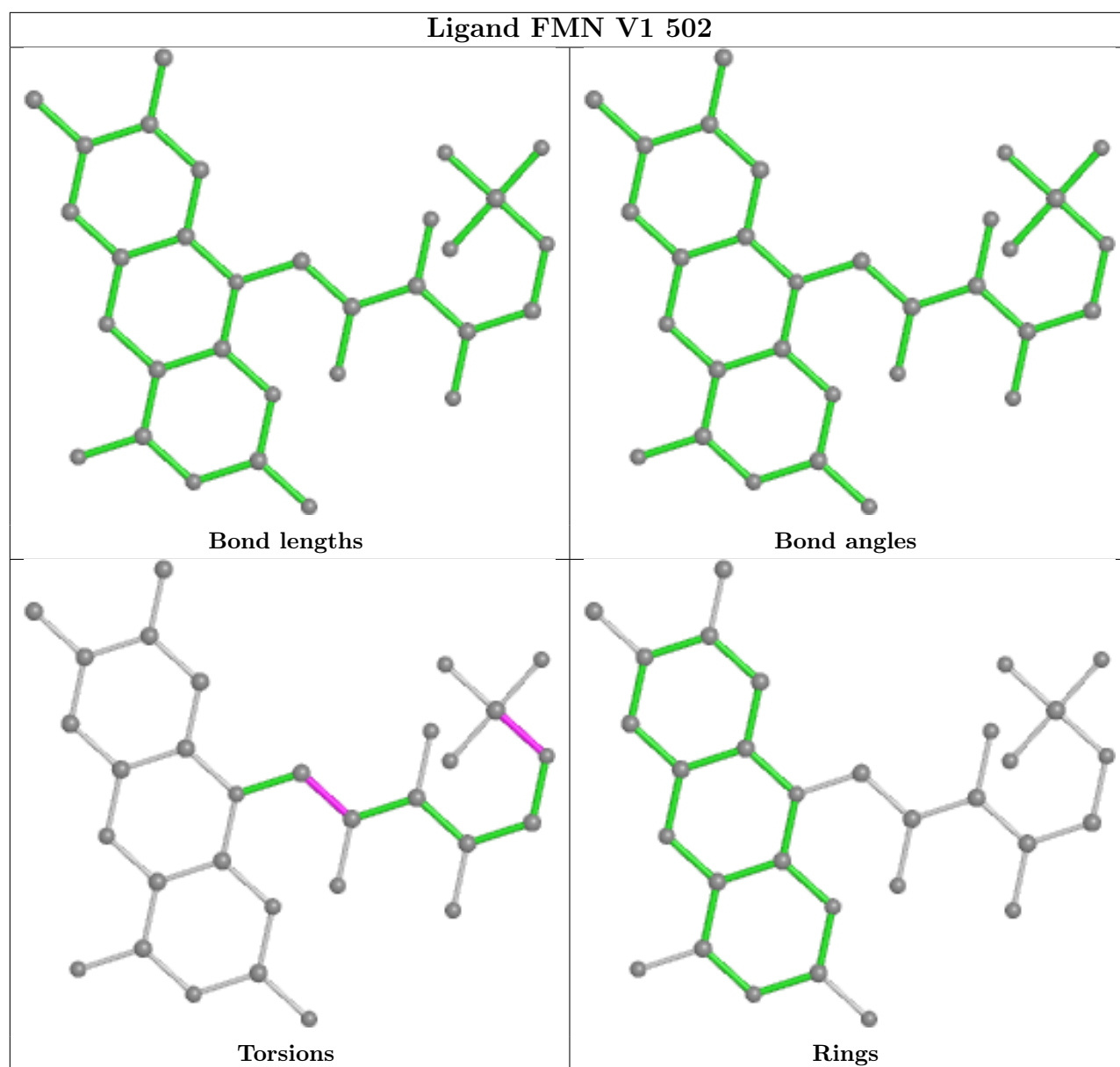


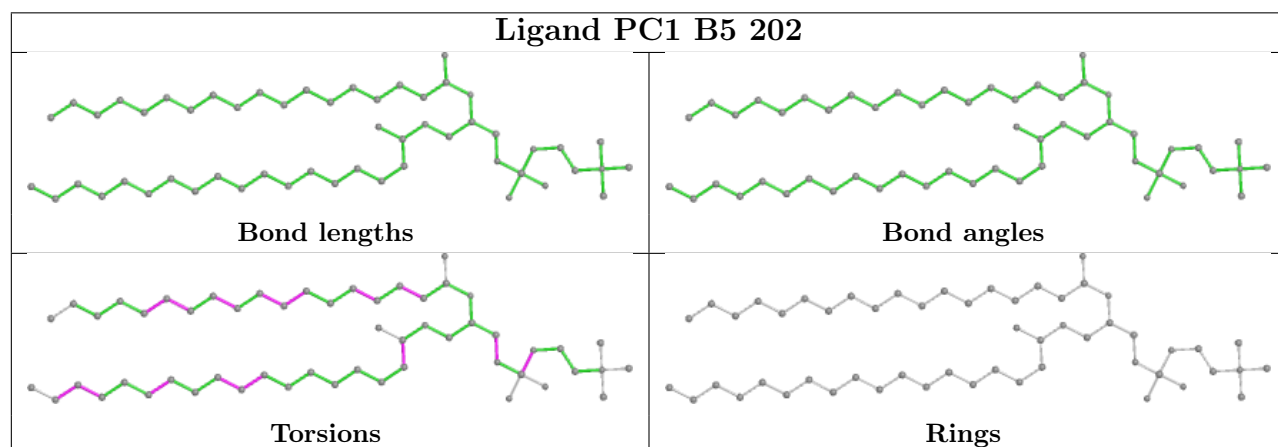
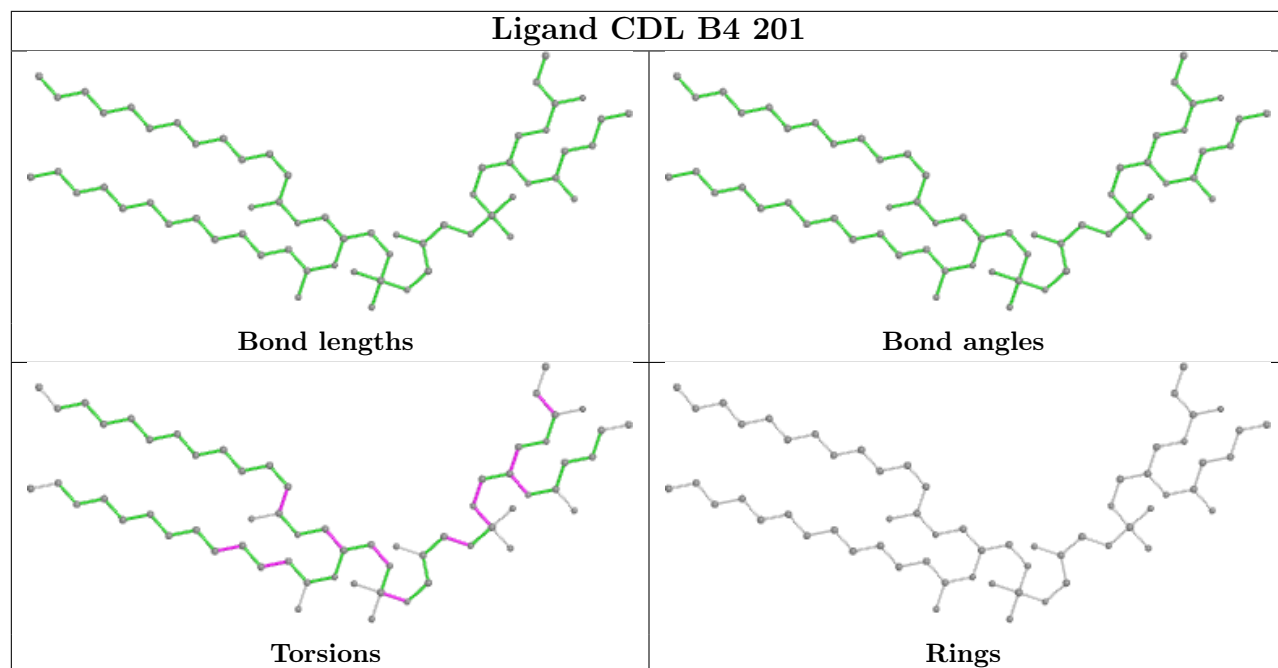


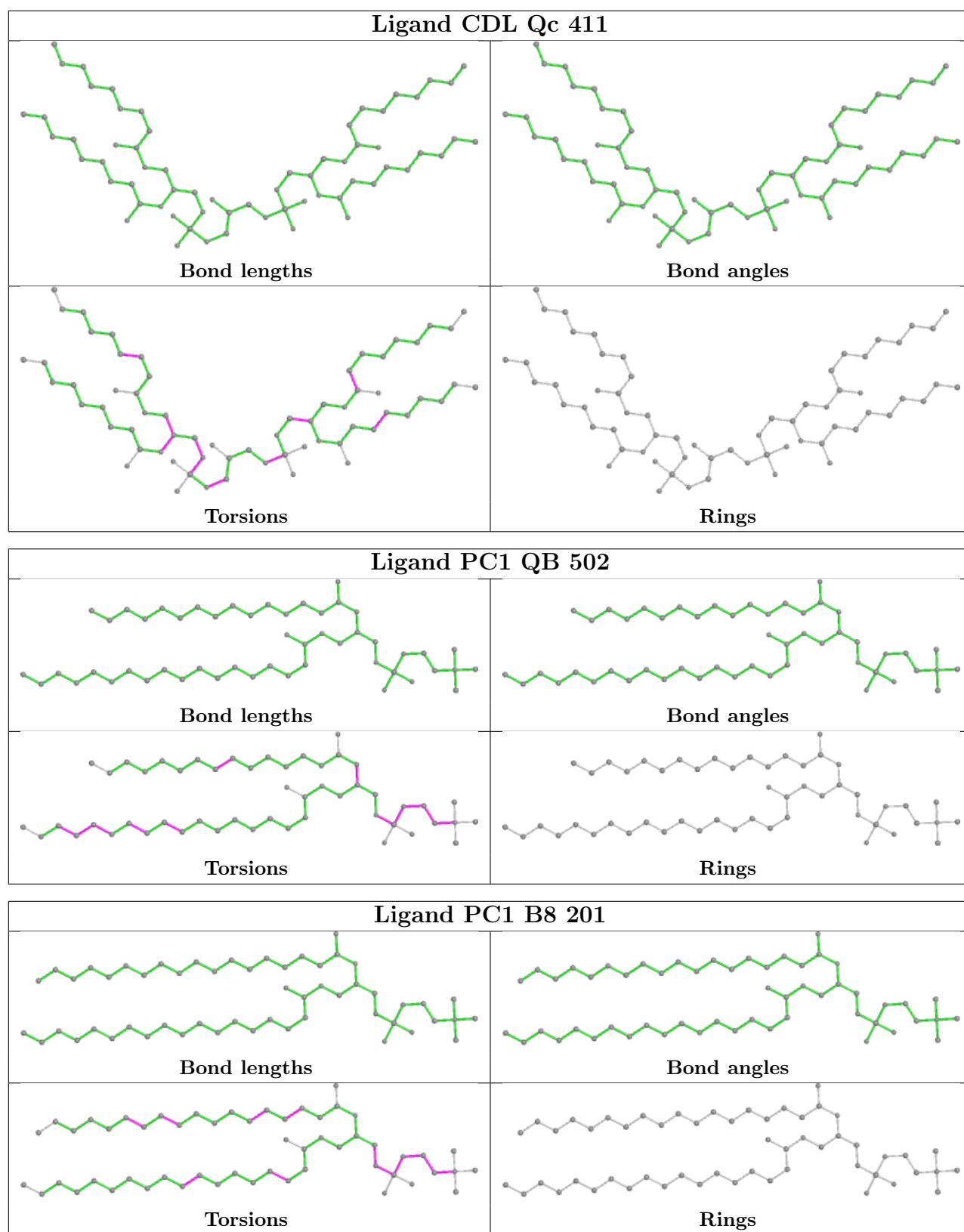


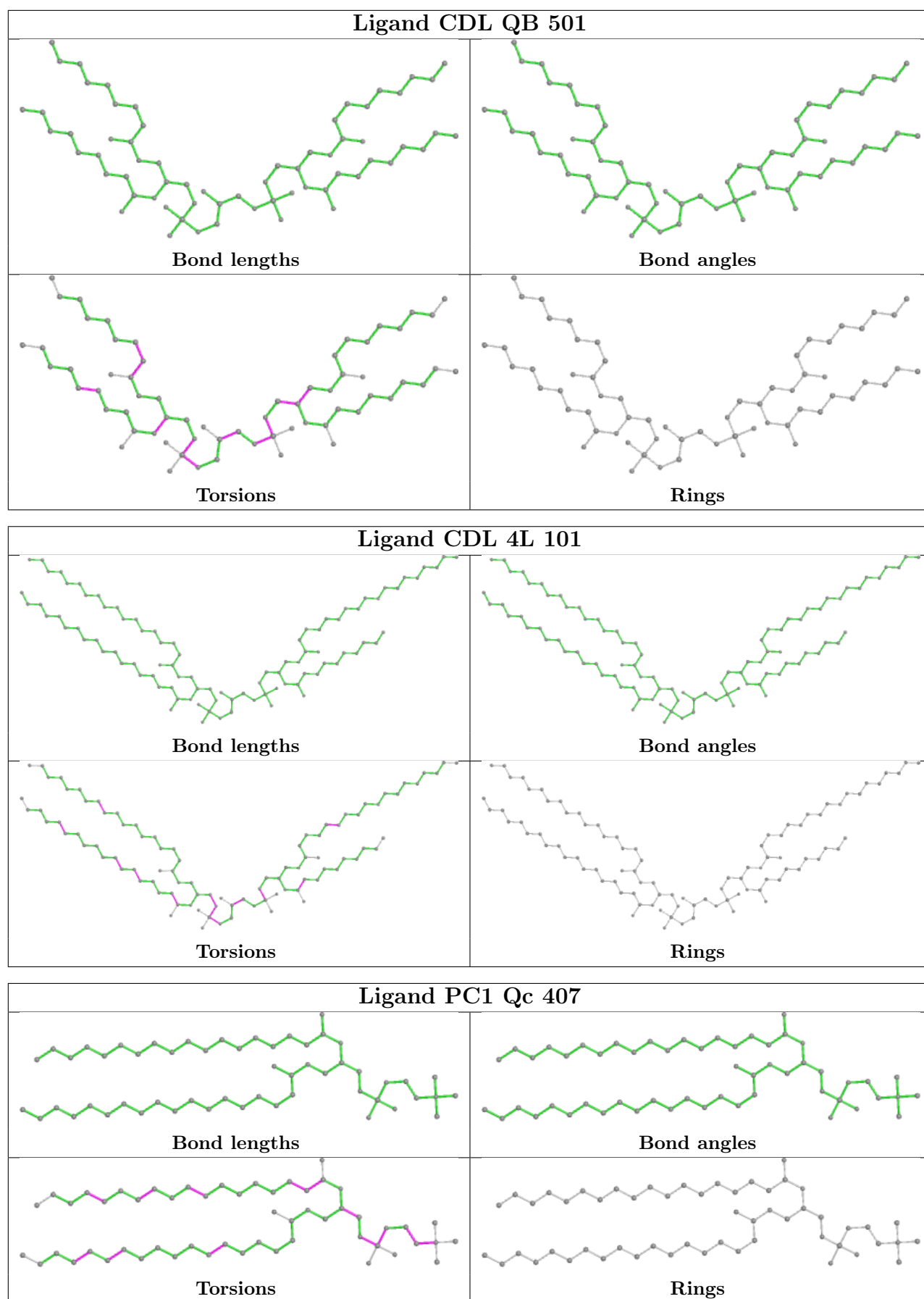


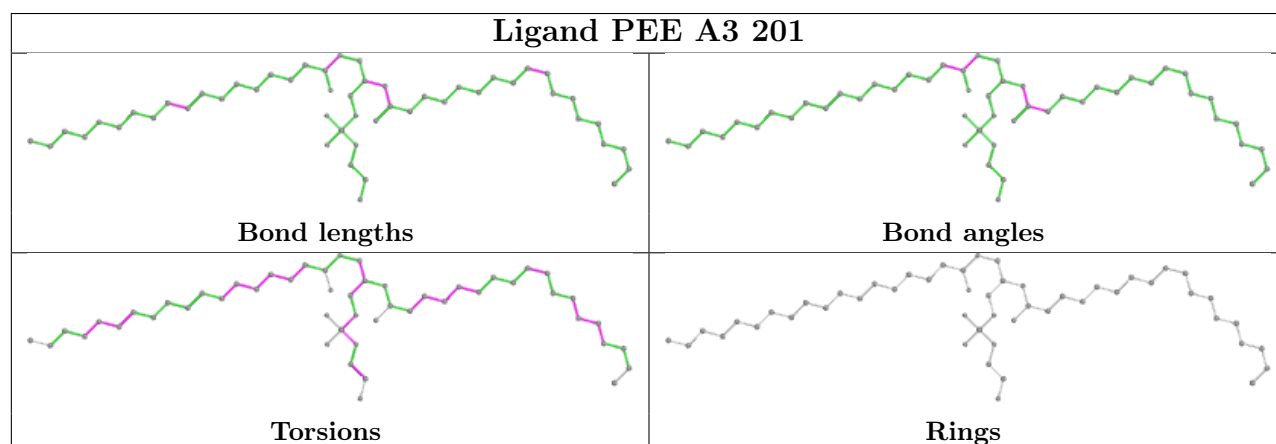
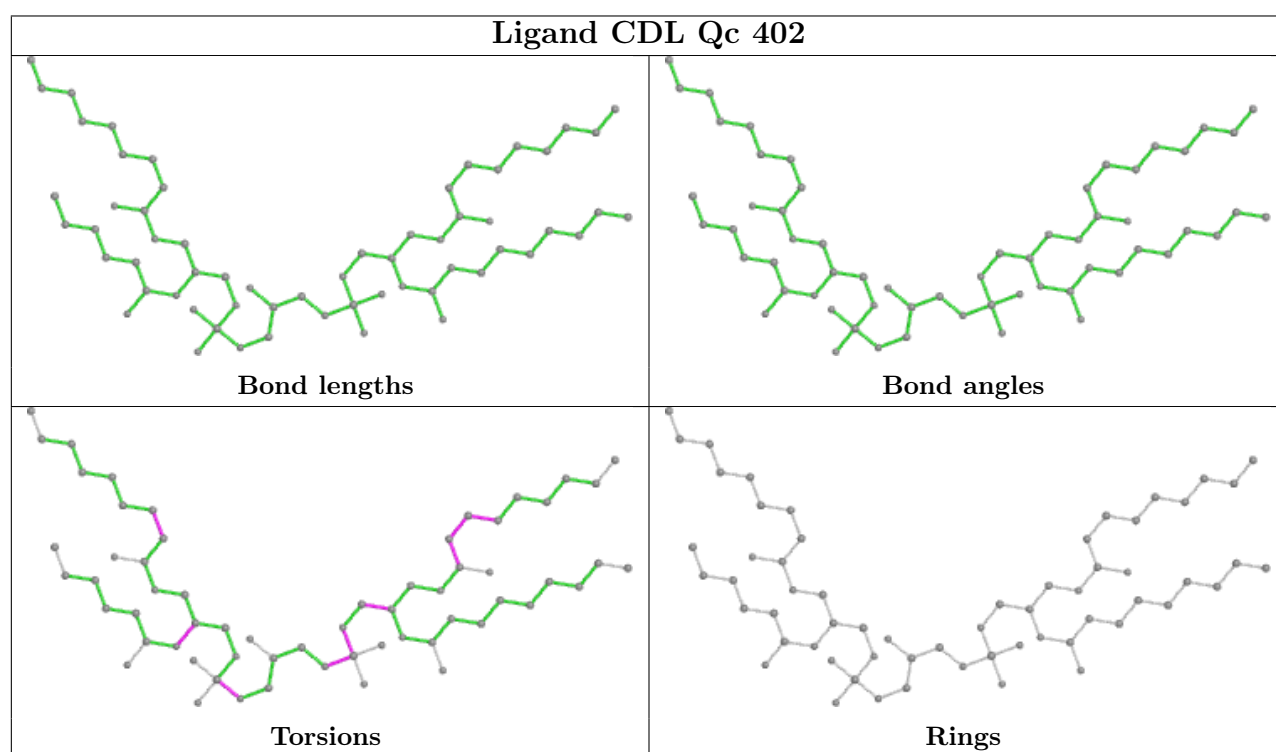
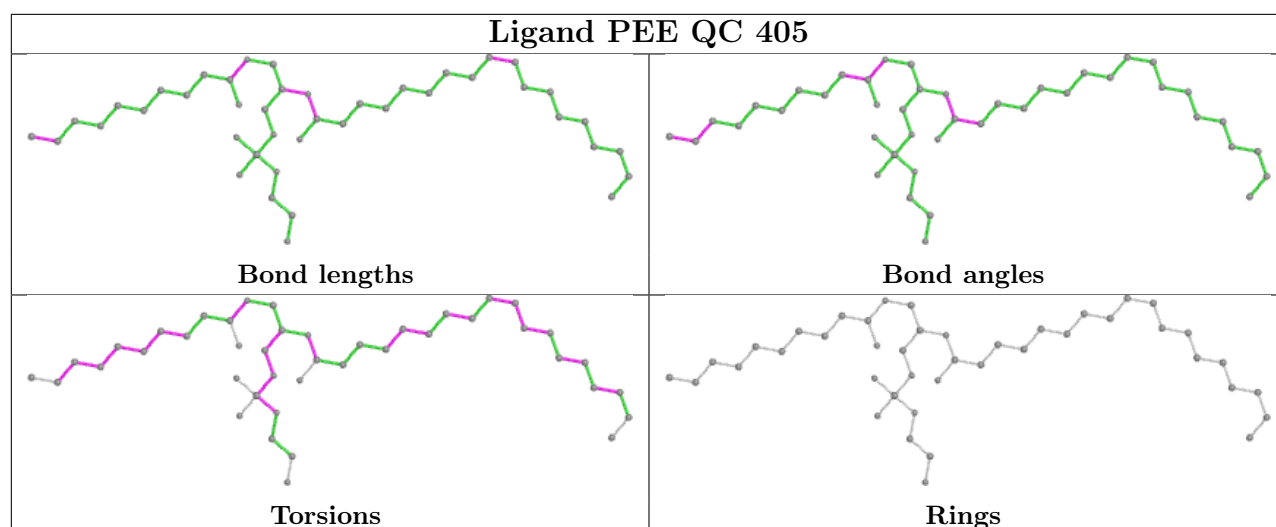


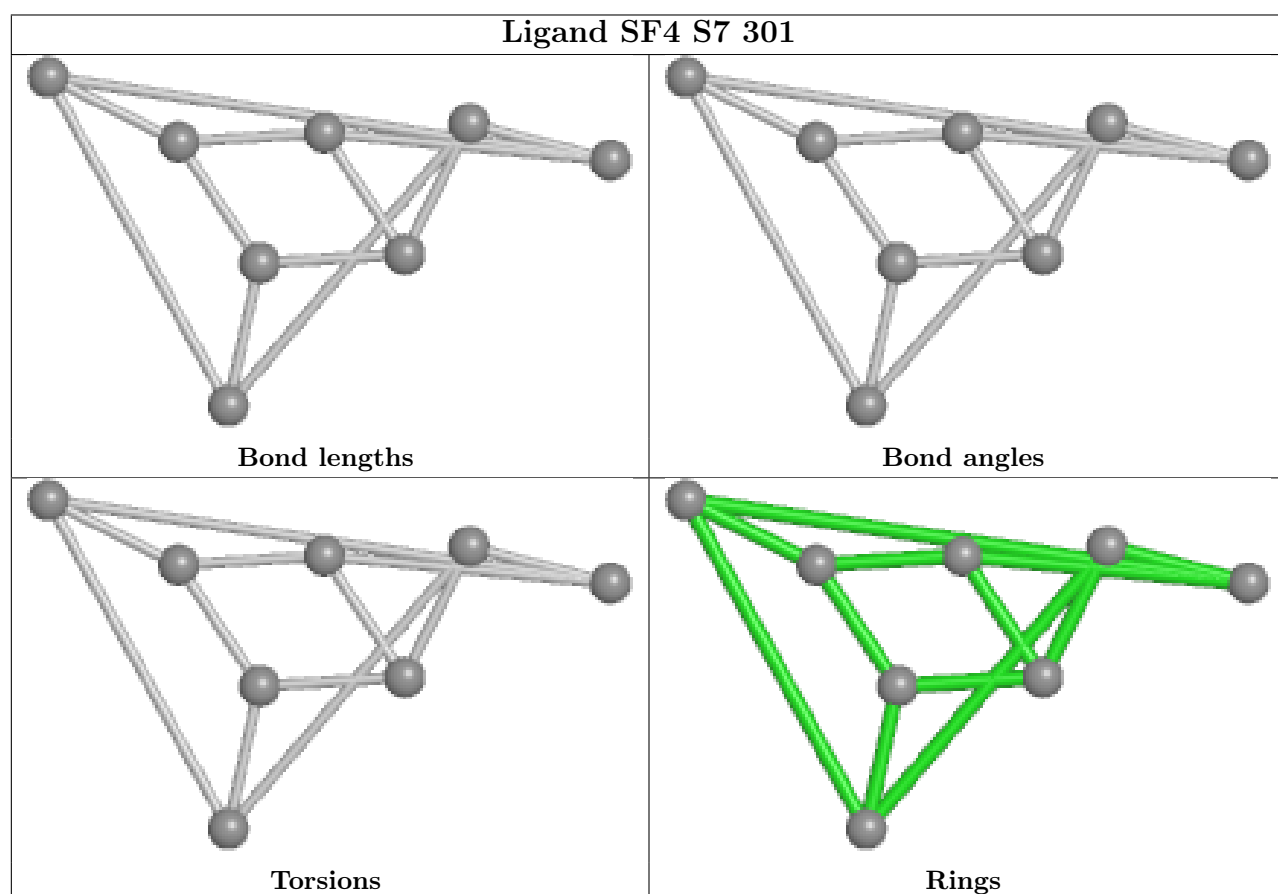
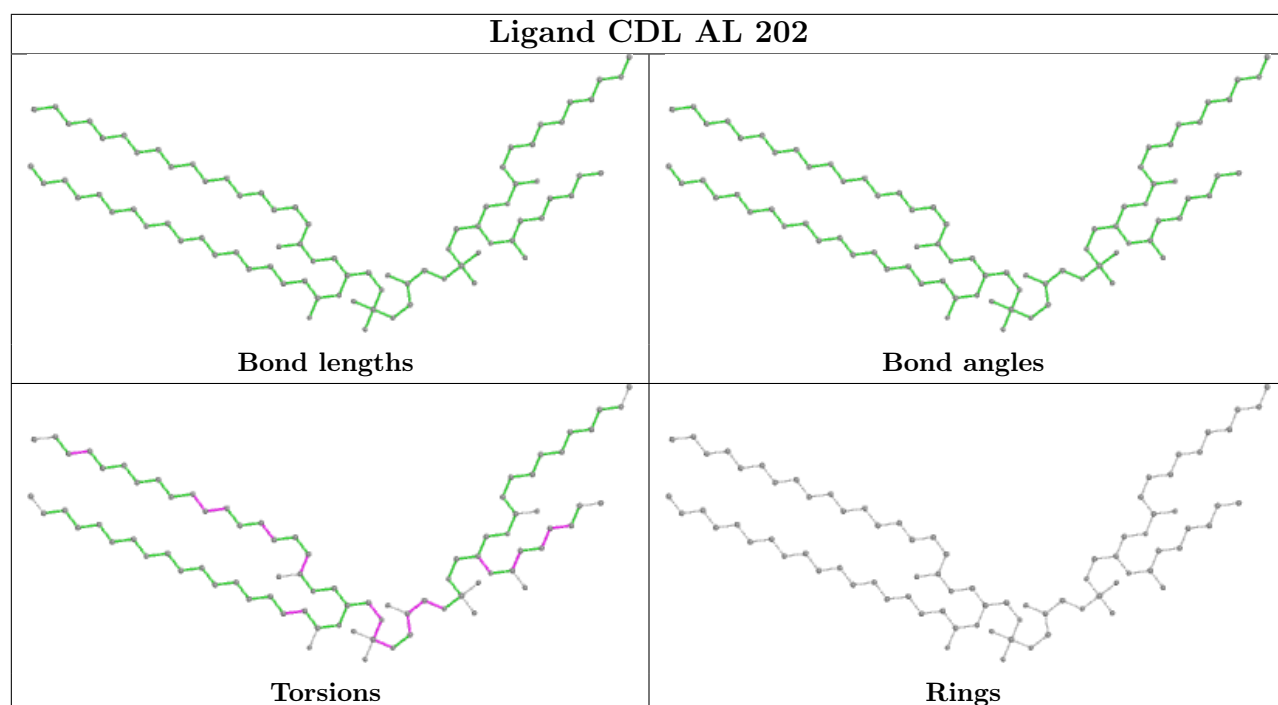


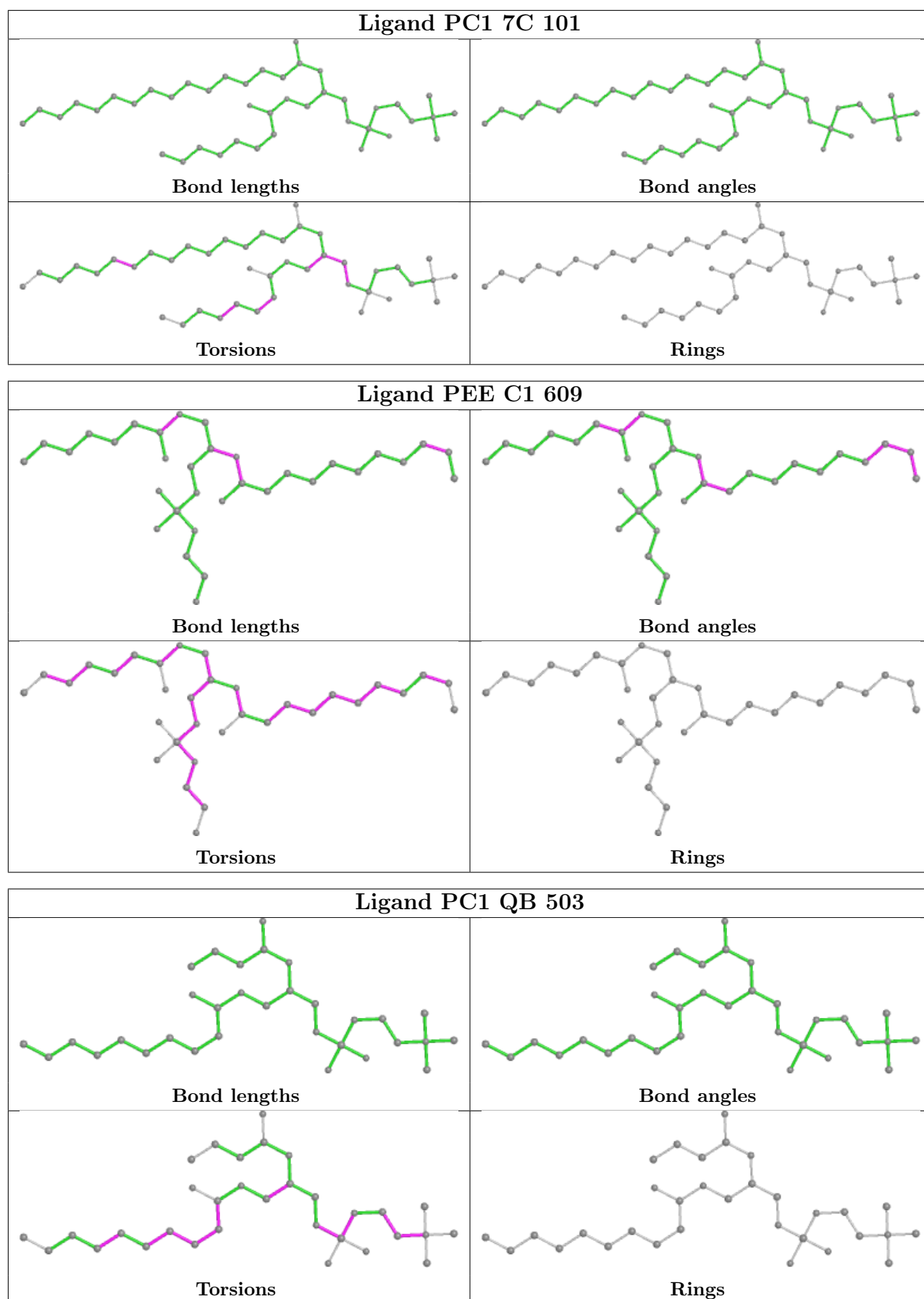




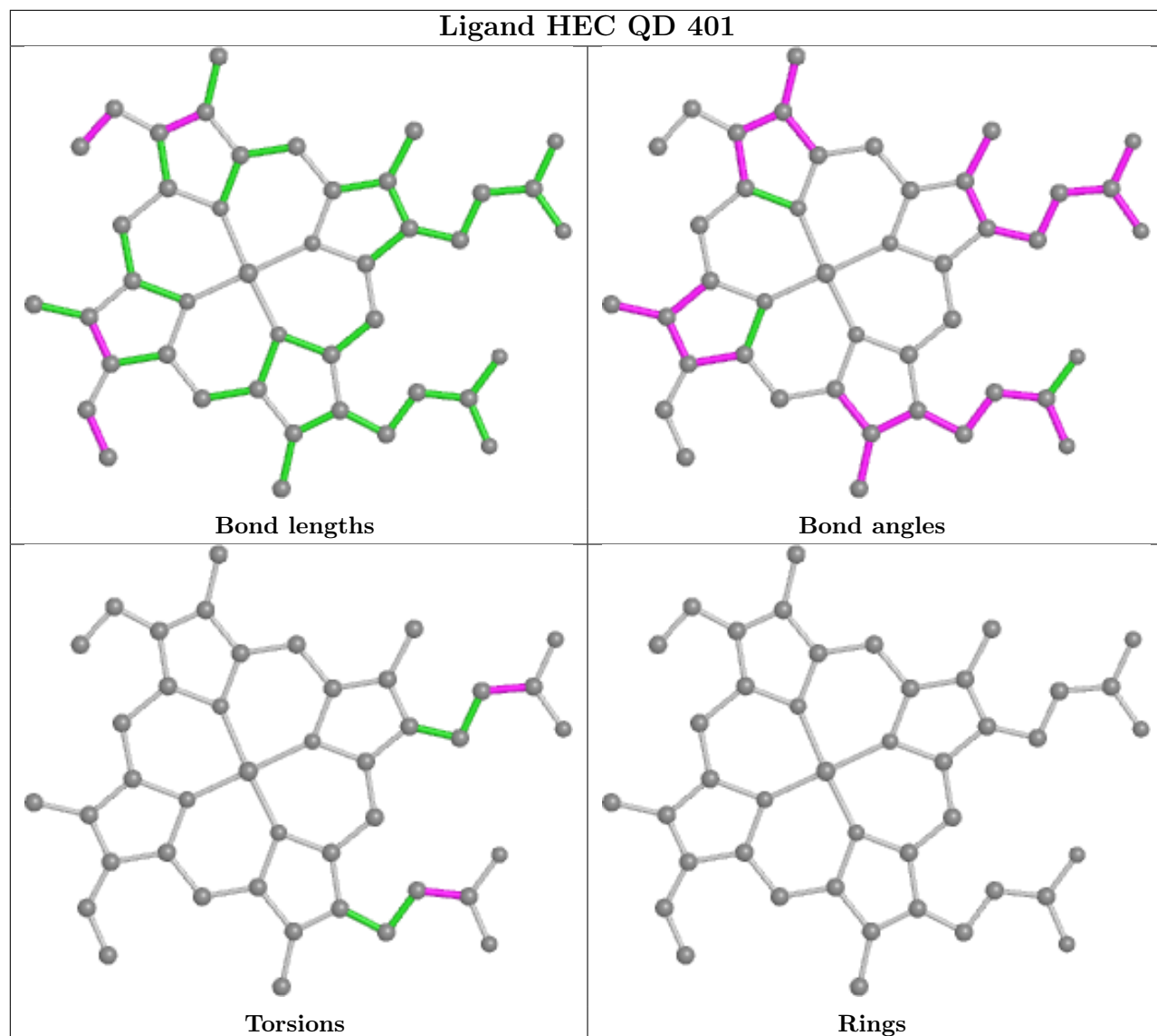




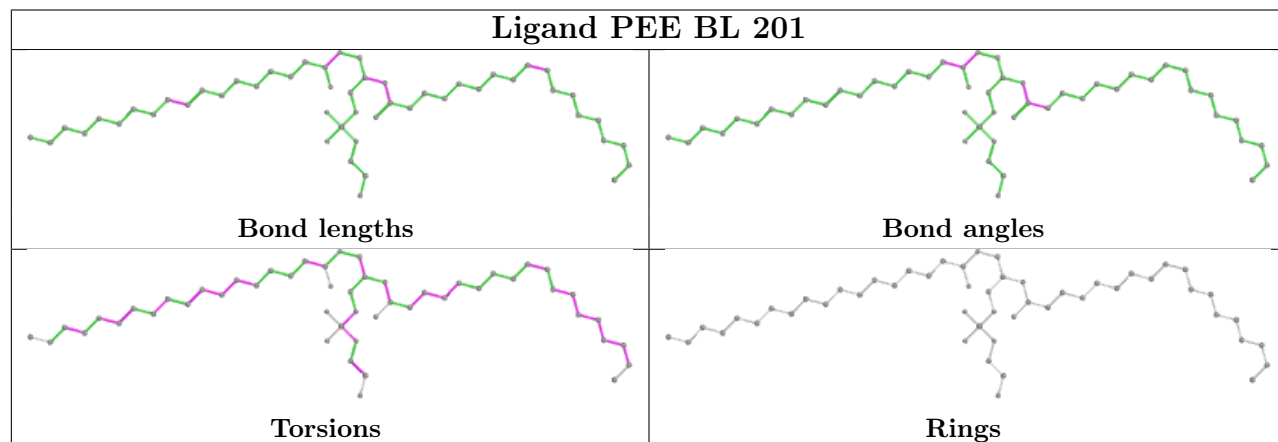


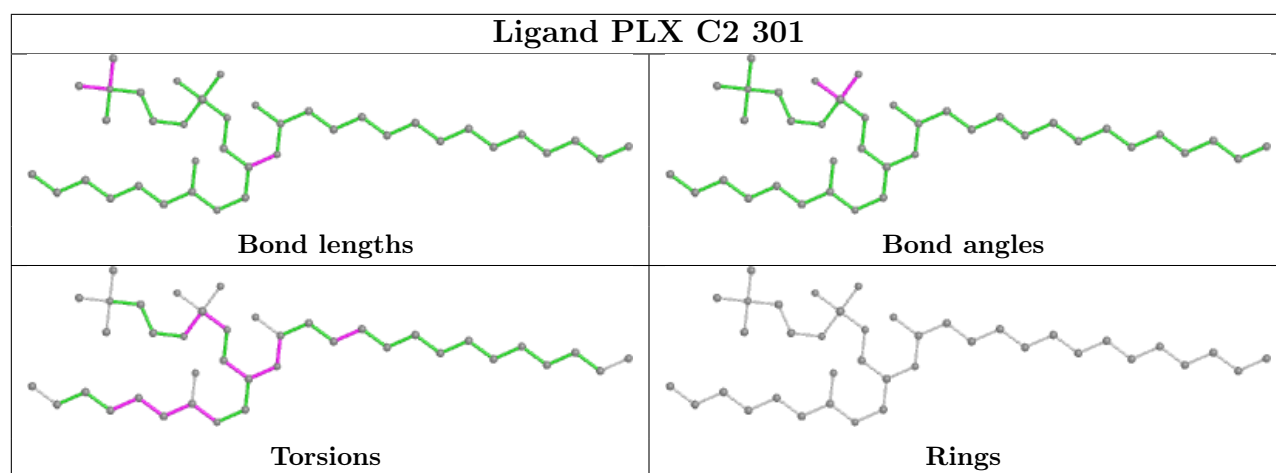


Ligand HEC QD 401



Ligand PEE BL 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.

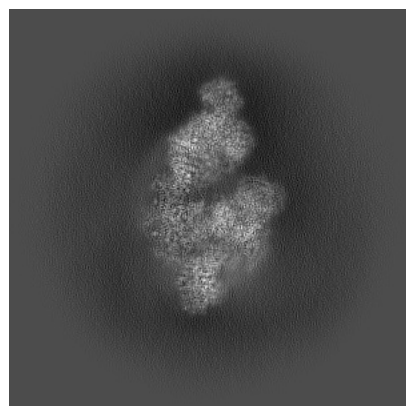
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60319. These allow visual inspection of the internal detail of the map and identification of artifacts.

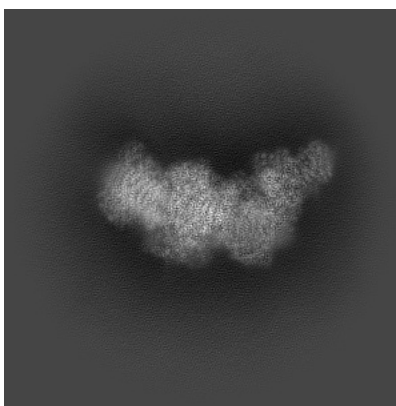
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

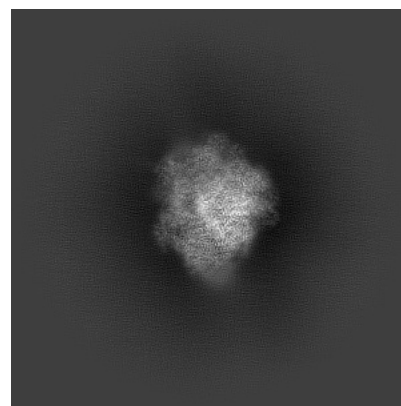
6.1.1 Primary map



X

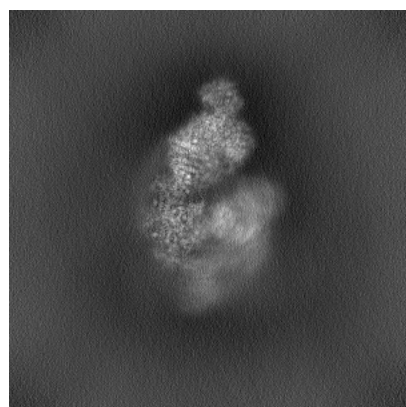


Y

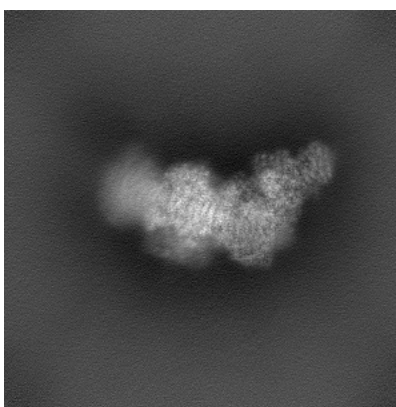


Z

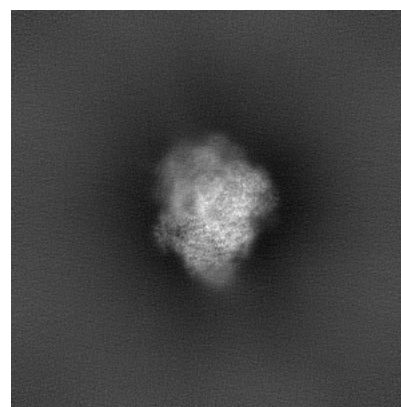
6.1.2 Raw map



X



Y

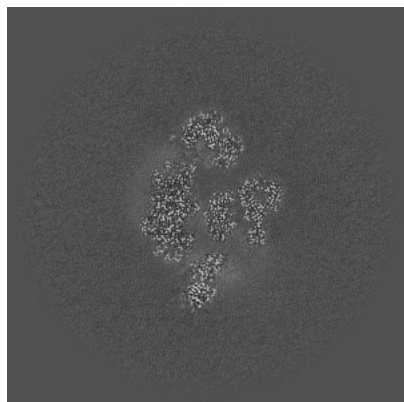


Z

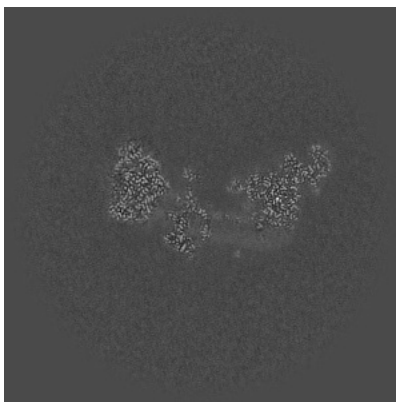
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

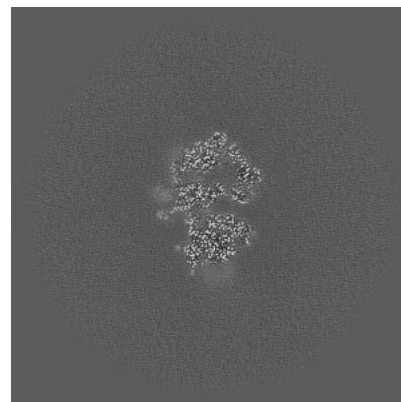
6.2.1 Primary map



X Index: 240

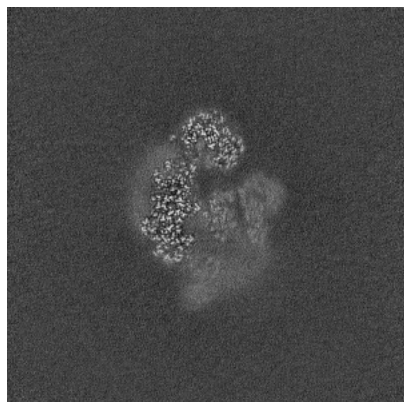


Y Index: 240

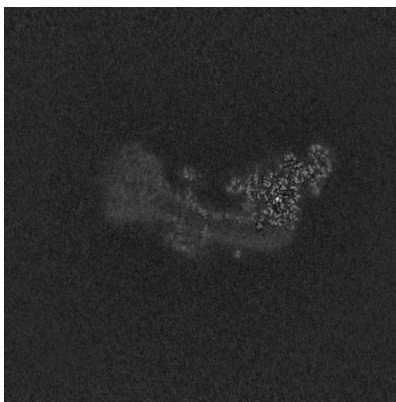


Z Index: 240

6.2.2 Raw map



X Index: 240



Y Index: 240

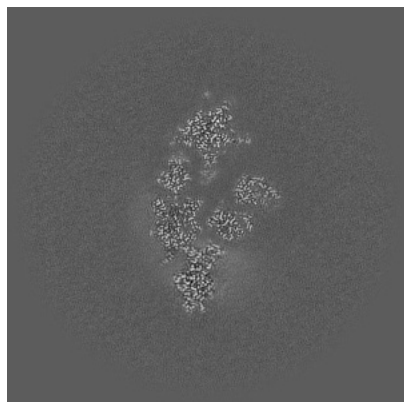


Z Index: 240

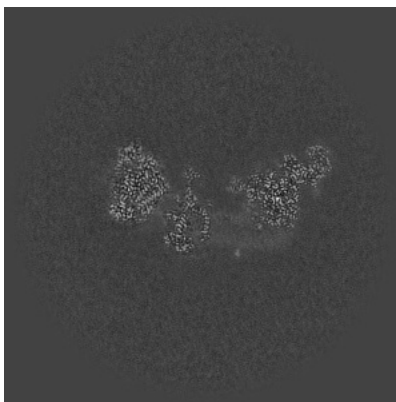
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

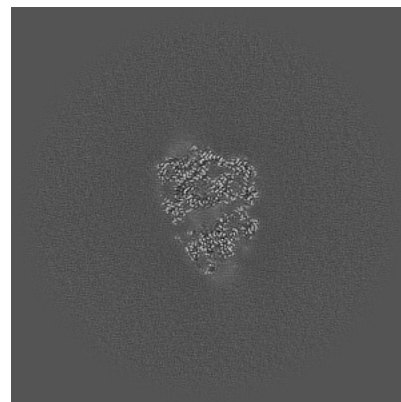
6.3.1 Primary map



X Index: 259

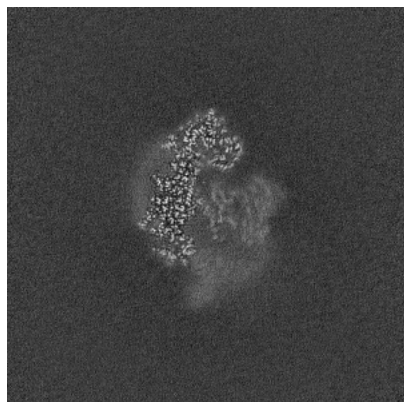


Y Index: 241

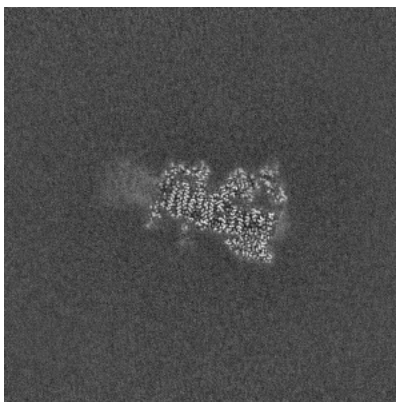


Z Index: 217

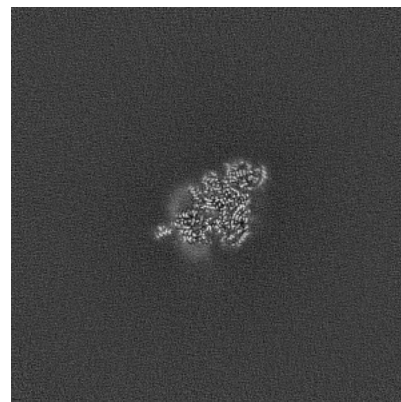
6.3.2 Raw map



X Index: 235



Y Index: 206

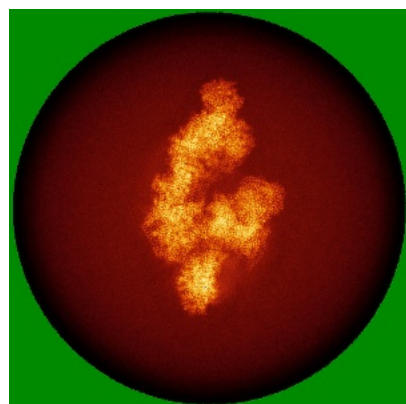


Z Index: 320

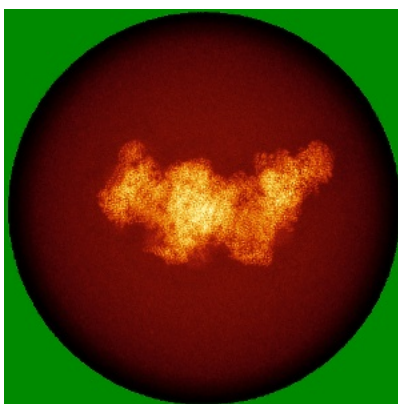
The images above show the largest variance slices of the map in three orthogonal directions.

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

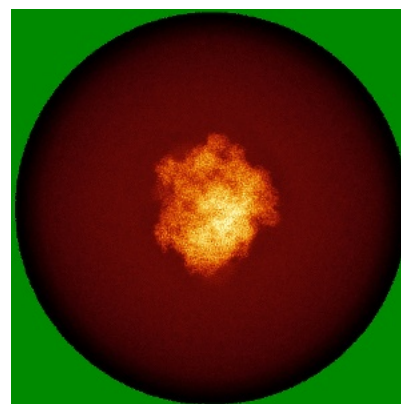
6.4.1 Primary map



X

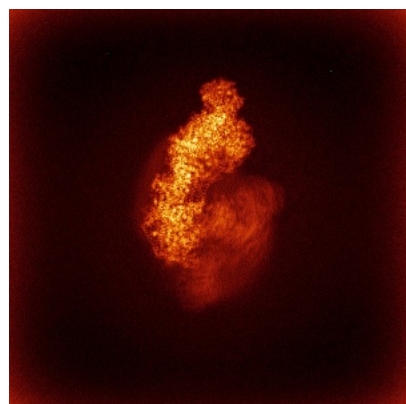


Y

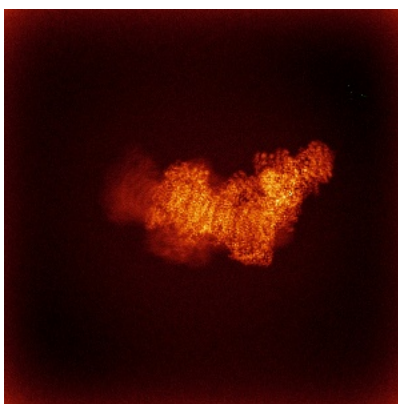


Z

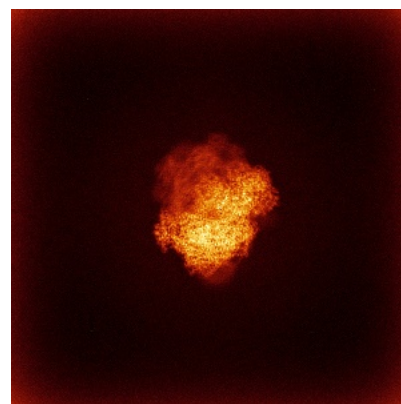
6.4.2 Raw map



X



Y

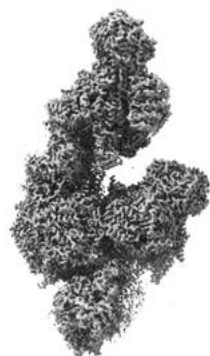


Z

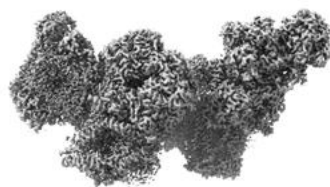
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

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



X



Y



Z

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

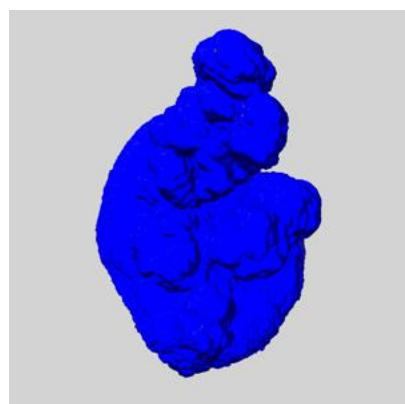
6.6 Mask visualisation [i](#)

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

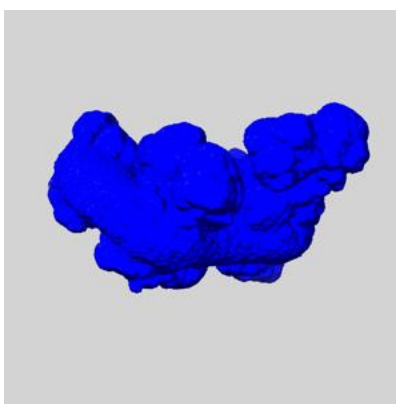
A mask typically either:

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

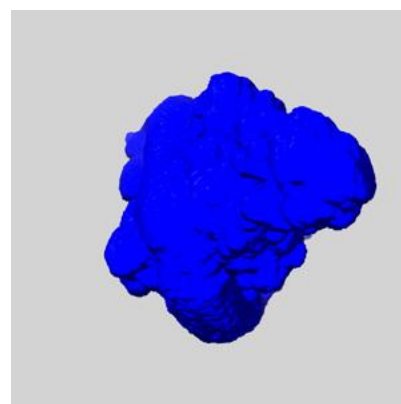
6.6.1 emd_60319_msk_1.map [i](#)



X



Y

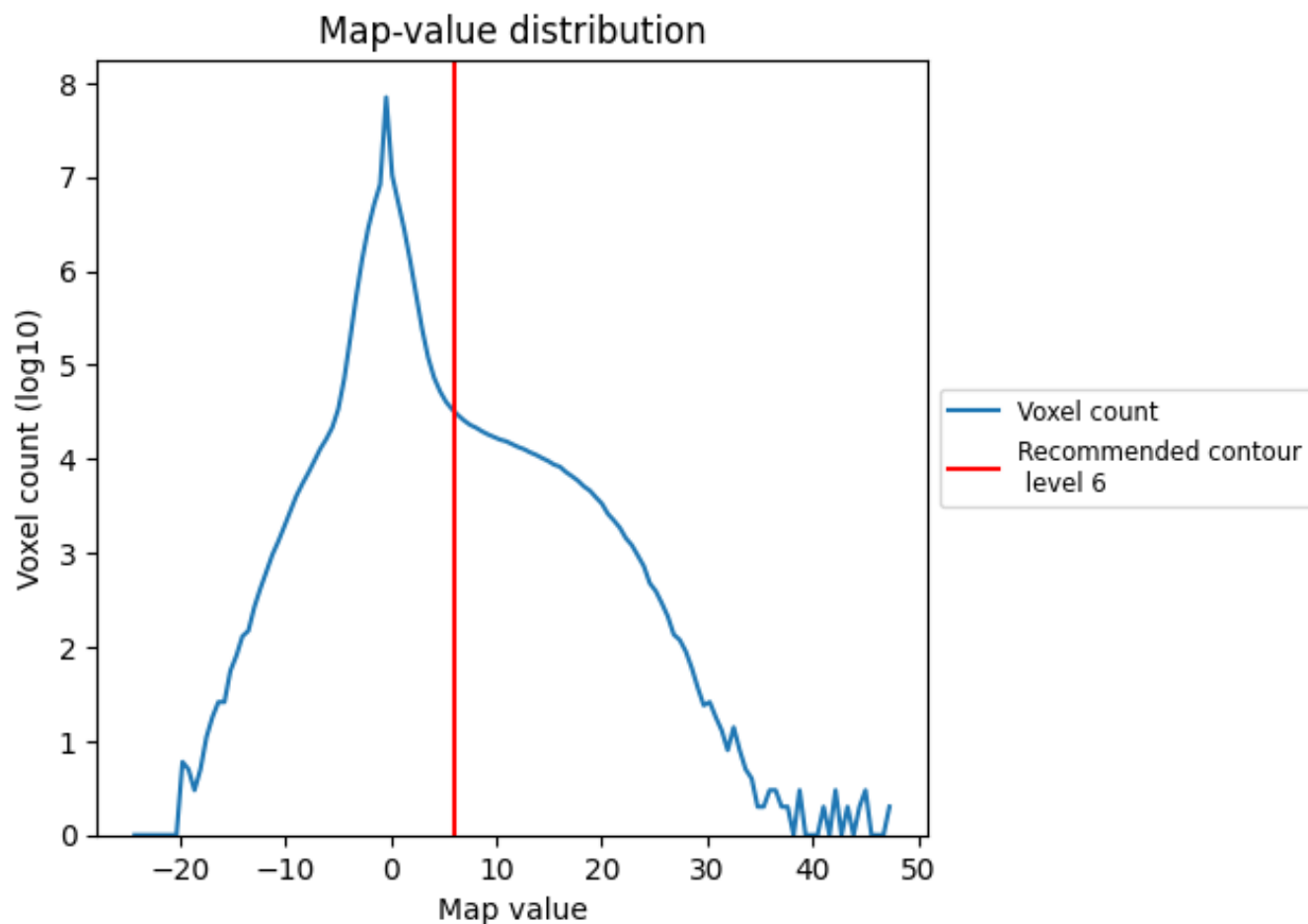


Z

7 Map analysis [i](#)

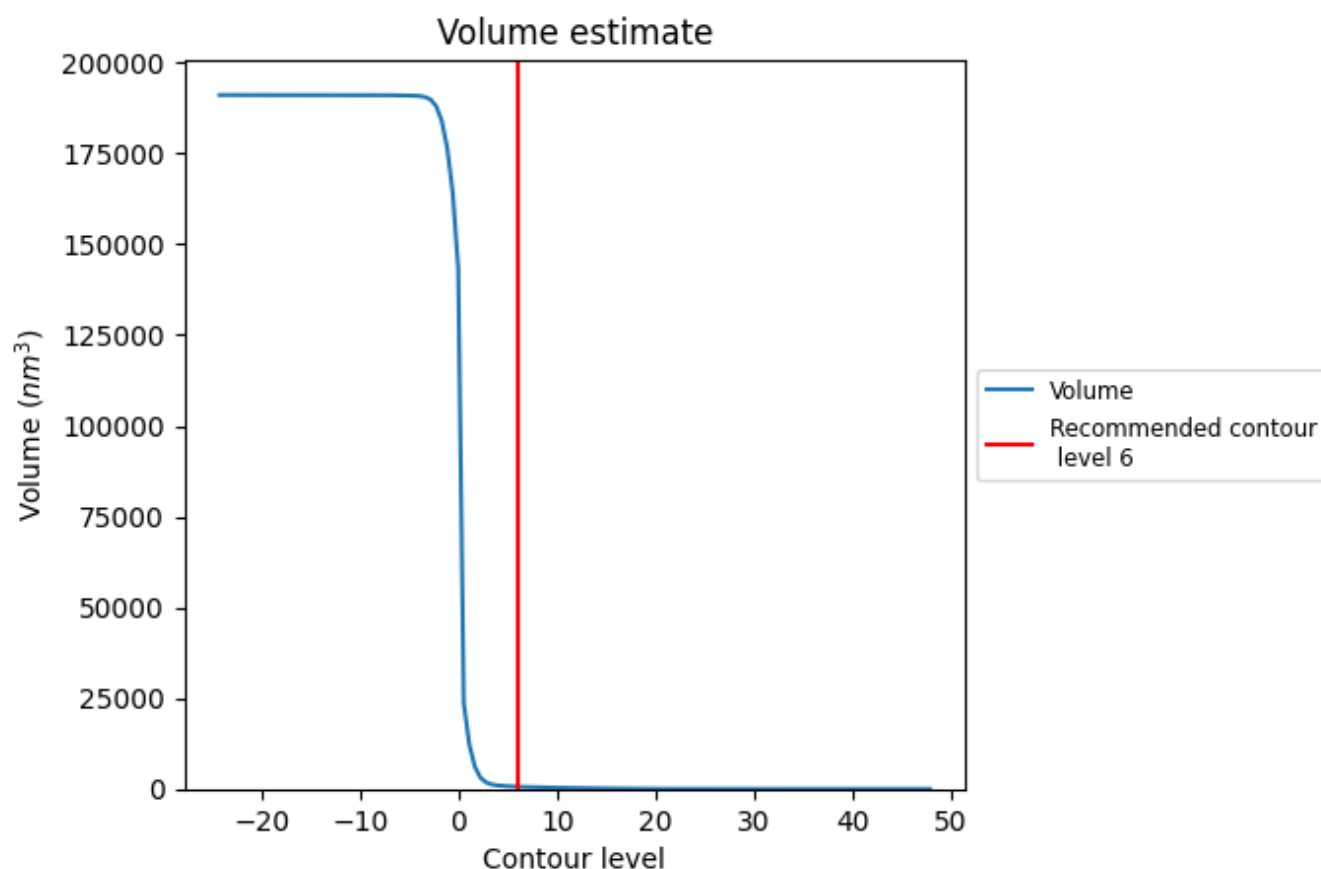
This section contains the results of statistical analysis of the map.

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.

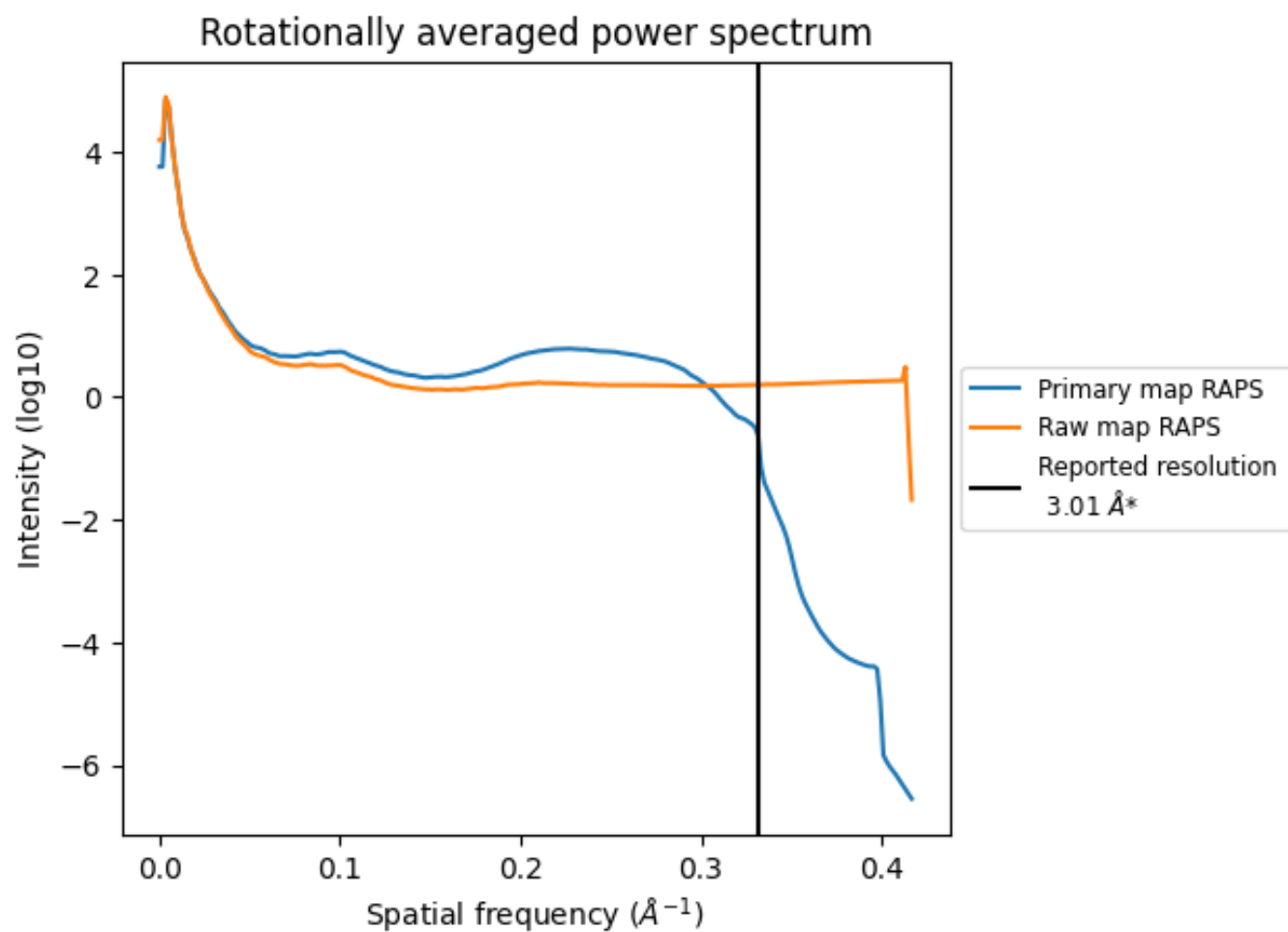
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 621 nm³; this corresponds to an approximate mass of 561 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 ⓘ

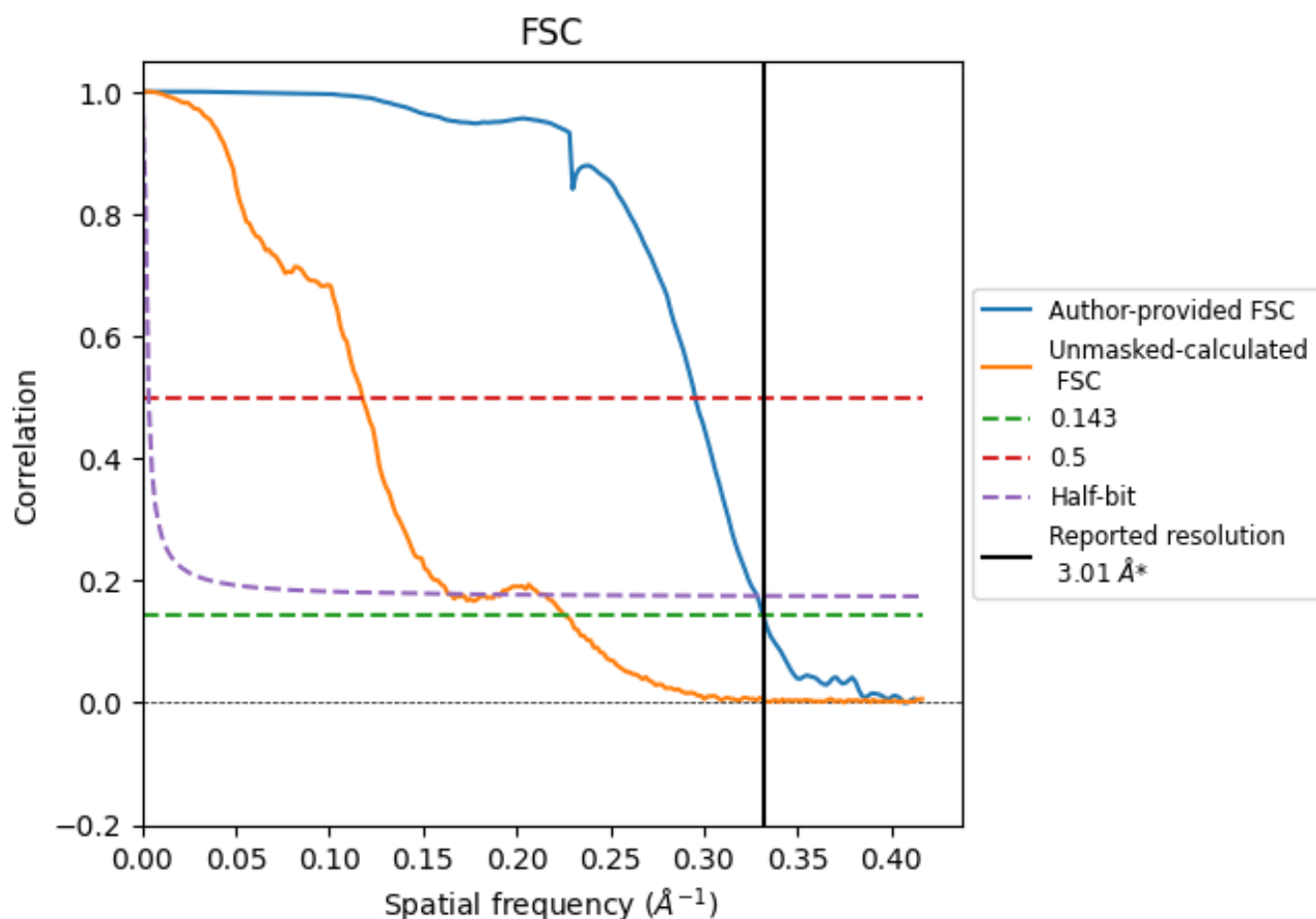


*Reported resolution corresponds to spatial frequency of 0.332 \AA^{-1}

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 0.332 \AA^{-1}

8.2 Resolution estimates [i](#)

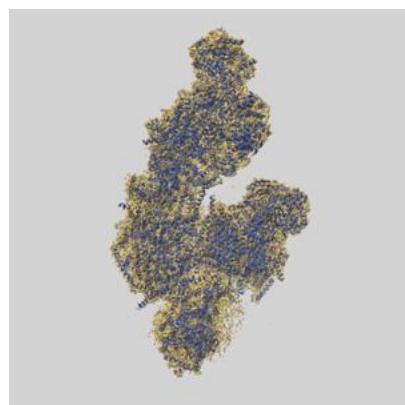
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	3.01	3.38	3.04
Unmasked-calculated*	4.43	8.50	6.09

*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 4.43 differs from the reported value 3.01 by more than 10 %

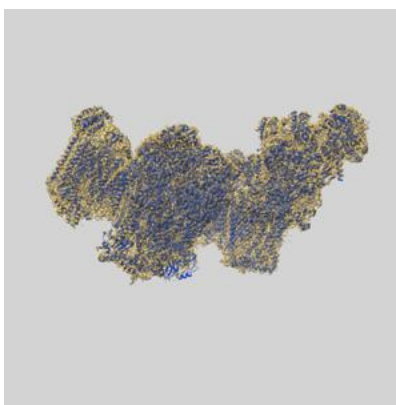
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60319 and PDB model 8ZOU. Per-residue inclusion information can be found in section 3 on page 32.

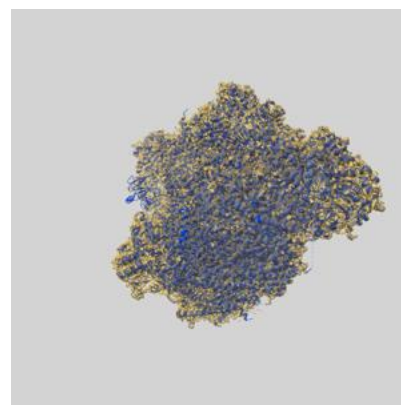
9.1 Map-model overlay [i](#)



X



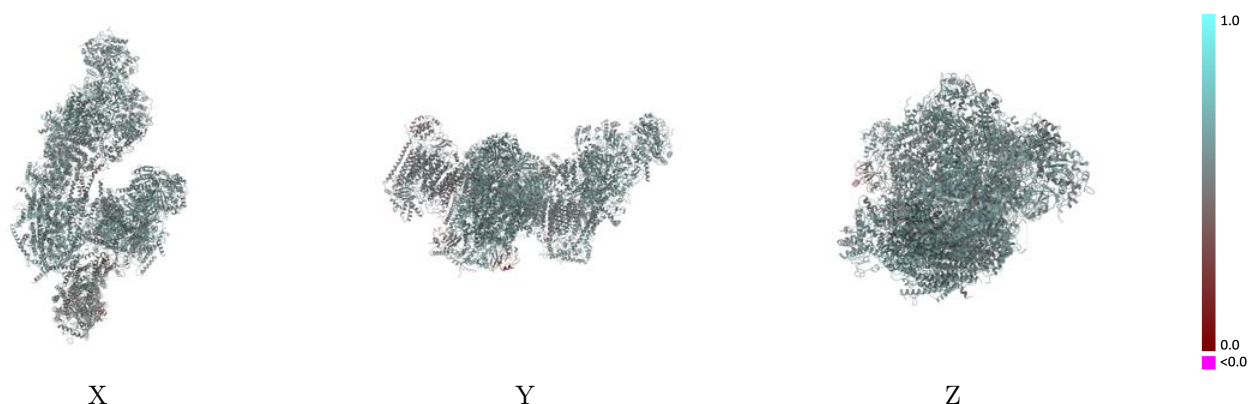
Y



Z

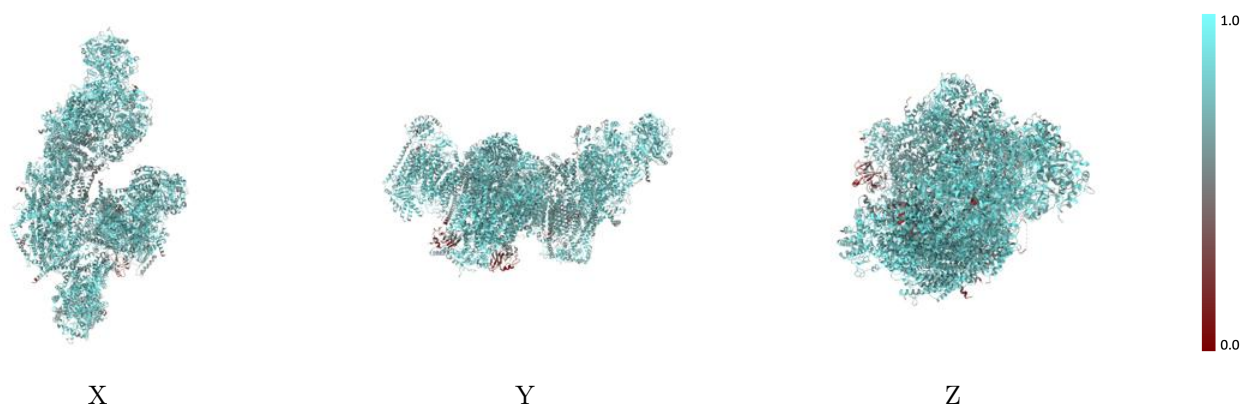
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



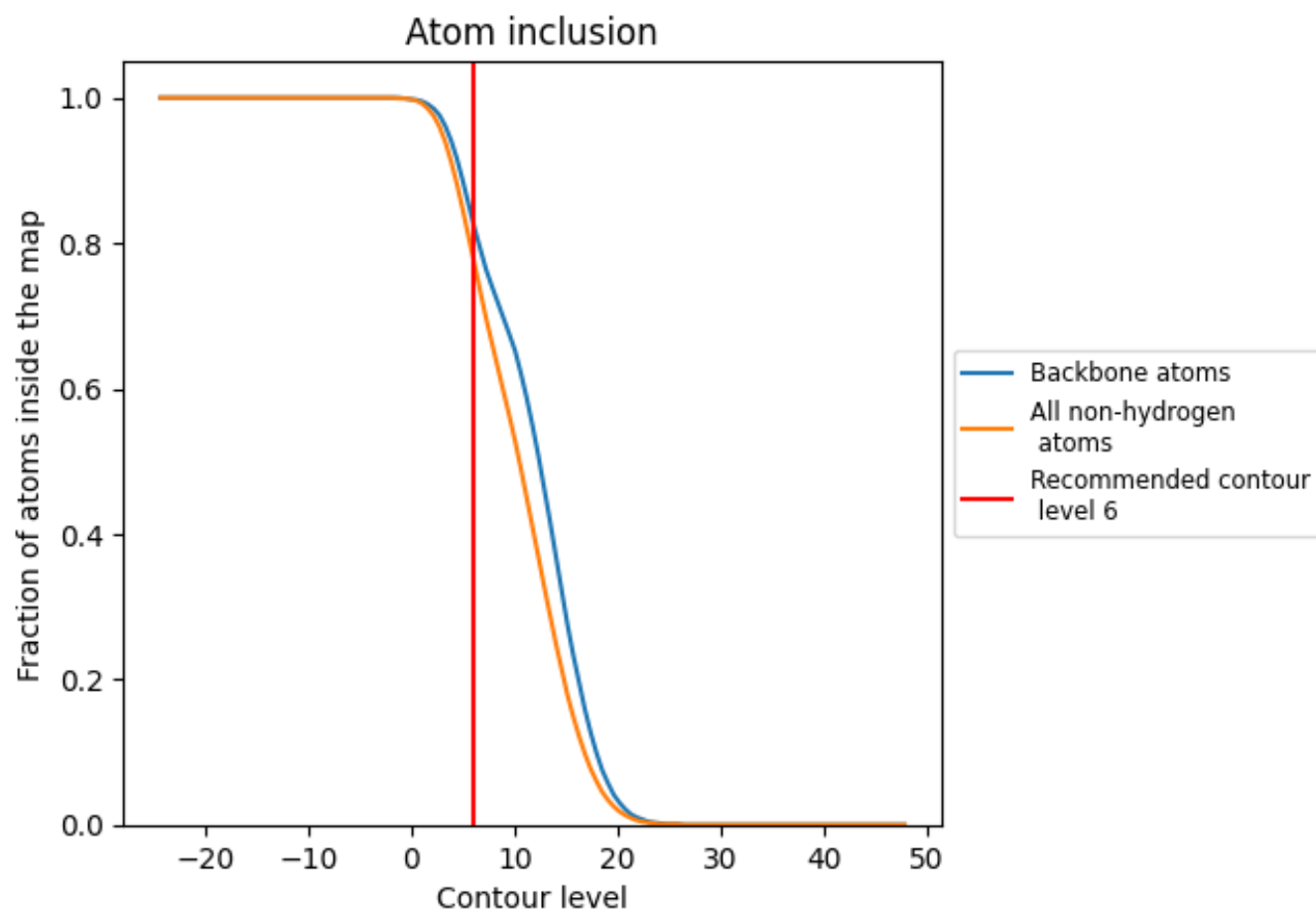
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.7810	 0.5580
4L	 0.7600	 0.5780
5A	 0.7180	 0.4680
5B	 0.7780	 0.4750
6A	 0.7540	 0.4710
6B	 0.8190	 0.4810
6C	 0.6900	 0.4820
7A	 0.6780	 0.4760
7B	 0.5560	 0.4770
7C	 0.8480	 0.5140
8B	 0.7590	 0.5000
A1	 0.8560	 0.5720
A2	 0.7060	 0.5380
A3	 0.8060	 0.5710
A5	 0.7730	 0.5540
A6	 0.7650	 0.5650
A7	 0.6750	 0.5590
A8	 0.8070	 0.5730
A9	 0.7650	 0.5610
AB	 0.5650	 0.4790
AC	 0.7990	 0.5800
AK	 0.7660	 0.5460
AL	 0.6430	 0.5600
AM	 0.7100	 0.5610
AN	 0.7160	 0.5620
B1	 0.7070	 0.5710
B2	 0.7750	 0.5790
B3	 0.7340	 0.5510
B4	 0.7520	 0.5770
B5	 0.8290	 0.5930
B6	 0.7290	 0.5540
B7	 0.7420	 0.5620
B8	 0.8050	 0.5840
B9	 0.8360	 0.5840
BK	 0.7910	 0.5740









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Chain	Atom inclusion	Q-score
BL	 0.7700	 0.5760
C1	 0.8600	 0.5320
C2	 0.8090	 0.5070
C3	 0.8260	 0.5080
C4	 0.7290	 0.4770
CA	 0.7520	 0.5670
CB	 0.8180	 0.5890
N1	 0.8050	 0.5690
N2	 0.8550	 0.5840
N3	 0.7000	 0.5580
N4	 0.8670	 0.5920
N5	 0.8360	 0.5890
N6	 0.6730	 0.5230
QA	 0.8000	 0.5700
QB	 0.8040	 0.5710
QC	 0.8260	 0.5770
QD	 0.8050	 0.5730
QE	 0.4530	 0.4770
QF	 0.6500	 0.5050
QG	 0.7980	 0.5650
QH	 0.7490	 0.5640
QI	 0.7000	 0.5680
QJ	 0.6610	 0.5380
QK	 0.5450	 0.5320
Qa	 0.7830	 0.5680
Qb	 0.7920	 0.5730
Qc	 0.7970	 0.5740
Qd	 0.8270	 0.5800
Qe	 0.3810	 0.4410
Qf	 0.6530	 0.5160
Qg	 0.7810	 0.5610
Qh	 0.6700	 0.5610
Qi	 0.7980	 0.5730
Qj	 0.6660	 0.5400
S1	 0.8170	 0.5670
S2	 0.8560	 0.5860
S3	 0.8890	 0.5960
S4	 0.8120	 0.5780
S5	 0.7720	 0.5600
S6	 0.7820	 0.5680
S7	 0.8550	 0.5830
S8	 0.8830	 0.5940

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Chain	Atom inclusion	Q-score
V1	 0.7980	 0.5570
V2	 0.7490	 0.5470
V3	 0.7620	 0.5520