



## Full wwPDB EM Validation Report ⓘ

Nov 11, 2025 – 09:44 PM JST

PDB ID : 8ZSL / pdb\_00008zsl  
EMDB ID : EMD-60419  
Title : Complex I from respirasome closed state 1 bound by metformin and CoQ10 (SC-MetC1-i)  
Authors : Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.  
Deposited on : 2024-06-05  
Resolution : 2.88 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

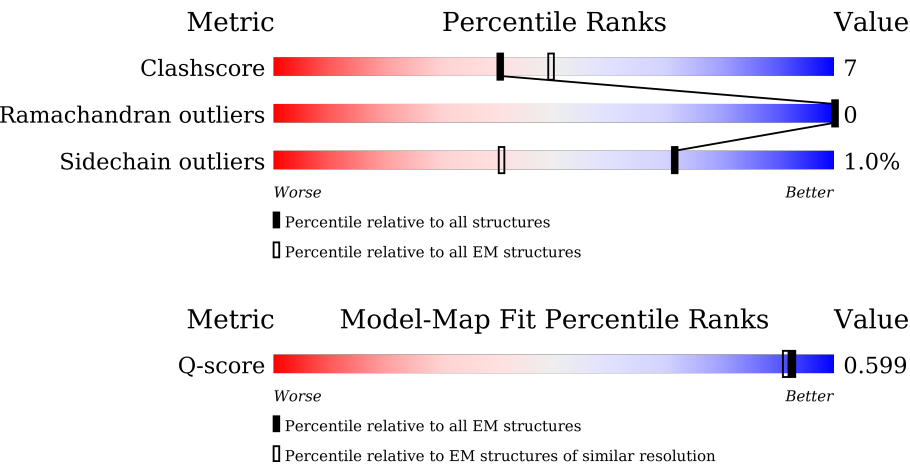
EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	12111 ( 2.38 - 3.38 )

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

Mol	Chain	Length	Quality of chain
1	4L	98	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>73%27%</div></div>
2	A1	70	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>84%14%</div></div>
3	A2	85	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>22%81%19%</div></div>
4	A3	83	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>14%86%14%</div></div>



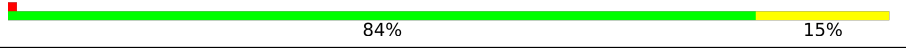




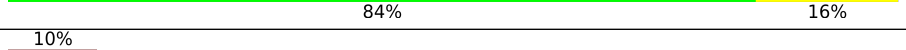
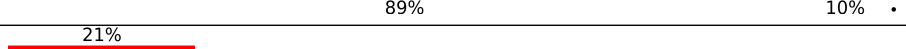
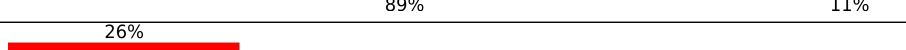

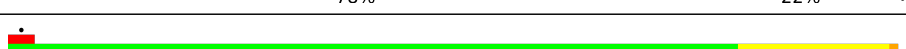


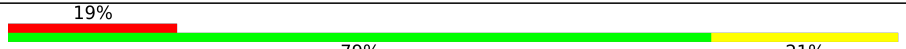

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Mol	Chain	Length	Quality of chain
5	A5	112	
6	A6	114	
7	A7	112	
8	A8	171	
9	A9	341	
10	AB	87	
10	AC	87	
11	AK	321	
12	AL	140	
13	AM	144	
14	AN	142	
15	B1	56	
16	B2	67	
17	B3	80	
18	B4	128	
19	B5	138	
20	B6	126	
21	B7	125	
22	B8	156	
23	B9	178	
24	BK	176	
25	BL	102	
26	CA	49	
27	CB	121	
28	N1	318	

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Mol	Chain	Length	Quality of chain
29	N2	347	
30	N3	115	
31	N4	459	
32	N5	603	
33	N6	174	
34	S1	689	
35	S2	430	
36	S3	208	
37	S4	124	
38	S5	105	
39	S6	96	
40	S7	156	
41	S8	176	
42	V1	431	
43	V2	217	
44	V3	42	

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 69154 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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

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

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

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

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

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

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

- Molecule 7 is a protein called Complex I-B14.5a.

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

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

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

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

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

- Molecule 10 is a protein called Acyl carrier protein.

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

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

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

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

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

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

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

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

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

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.



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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 28 is a protein called NADH-ubiquinone oxidoreductase chain 1.

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

- Molecule 29 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase chain 3.

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

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 6.

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

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

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

- Molecule 36 is a protein called Complex I-30kD.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

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

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

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

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

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

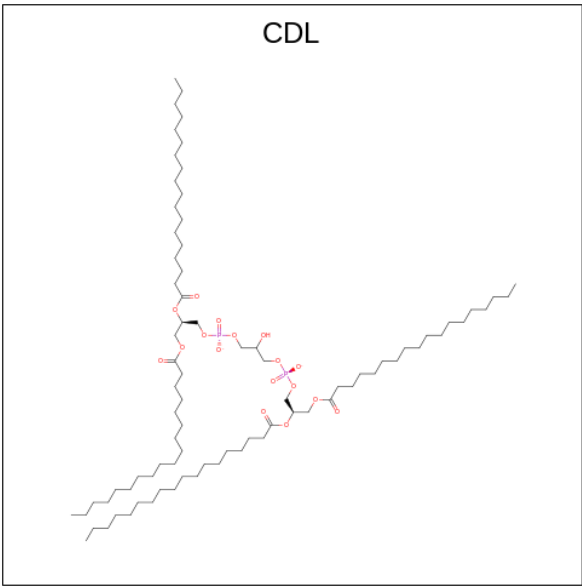
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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

- Molecule 44 is a protein called NADH:ubiquinone oxidoreductase subunit V3.

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

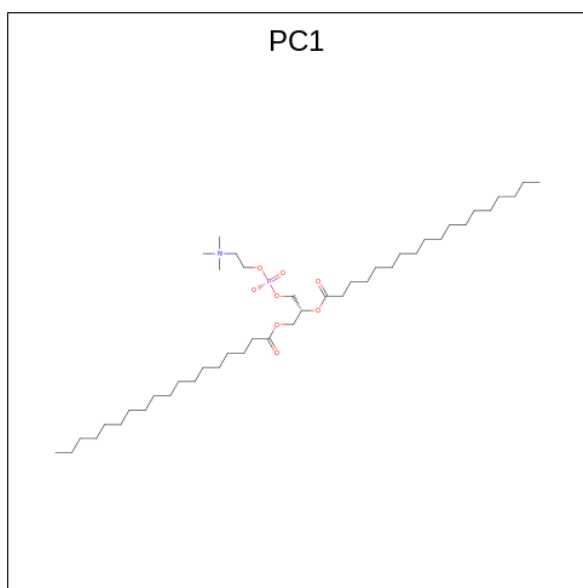
- Molecule 45 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
45	4L	1	Total	C	O	P	0
			91	72	17	2	
45	A1	1	Total	C	O	P	0
			94	75	17	2	
45	A8	1	Total	C	O	P	0
			83	64	17	2	
45	AL	1	Total	C	O	P	0
			94	75	17	2	
45	AL	1	Total	C	O	P	0
			76	57	17	2	
45	B4	1	Total	C	O	P	0
			80	61	17	2	
45	B5	1	Total	C	O	P	0
			100	81	17	2	
45	N1	1	Total	C	O	P	0
			78	59	17	2	
45	N2	1	Total	C	O	P	0
			68	49	17	2	
45	N4	1	Total	C	O	P	0
			100	81	17	2	
45	N4	1	Total	C	O	P	0
			89	70	17	2	
45	N5	1	Total	C	O	P	0
			100	81	17	2	

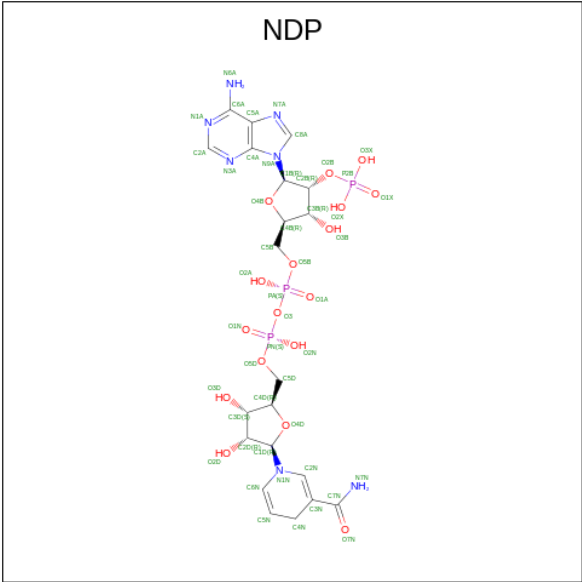
- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1)

(formula:  $C_{44}H_{88}NO_8P$ ).



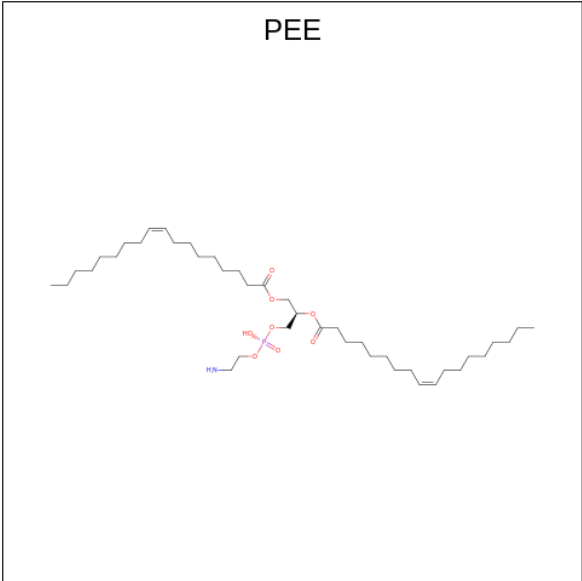
Mol	Chain	Residues	Atoms					AltConf
46	A3	1	Total	C	N	O	P	0
			53	43	1	8	1	
46	A9	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	AN	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	B5	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	N1	1	Total	C	N	O	P	0
			45	35	1	8	1	
46	N1	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	N3	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	N5	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 47 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
47	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C<sub>41</sub>H<sub>78</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
48	A9	1	Total	C	N	O	P	0
			39	29	1	8	1	
48	AL	1	Total	C	N	O	P	0
			36	26	1	8	1	

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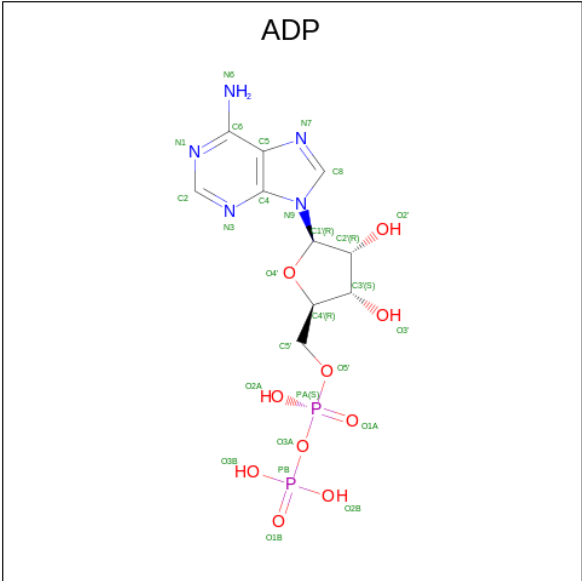
Mol	Chain	Residues	Atoms					AltConf
48	AL	1	Total	C	N	O	P	0
			40	30	1	8	1	
48	AN	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	B4	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	B6	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	N1	1	Total	C	N	O	P	0
			31	21	1	8	1	
48	N1	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	N3	1	Total	C	N	O	P	0
			48	38	1	8	1	
48	N3	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	N3	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	N4	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	N4	1	Total	C	N	O	P	0
			49	39	1	8	1	
48	N5	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	S2	1	Total	C	N	O	P	0
			46	36	1	8	1	

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



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

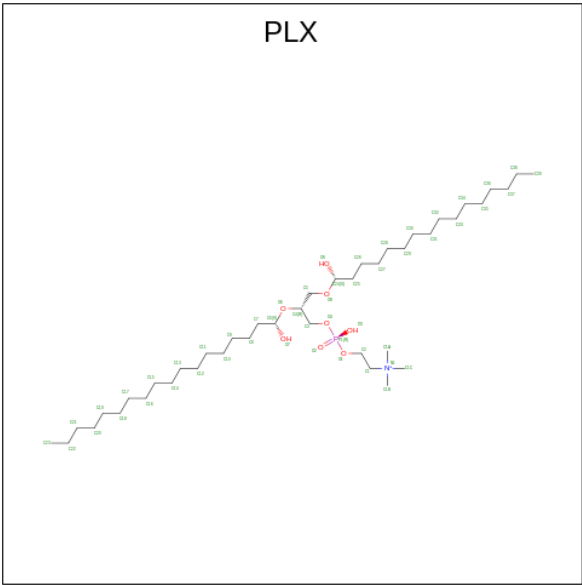
- Molecule 50 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

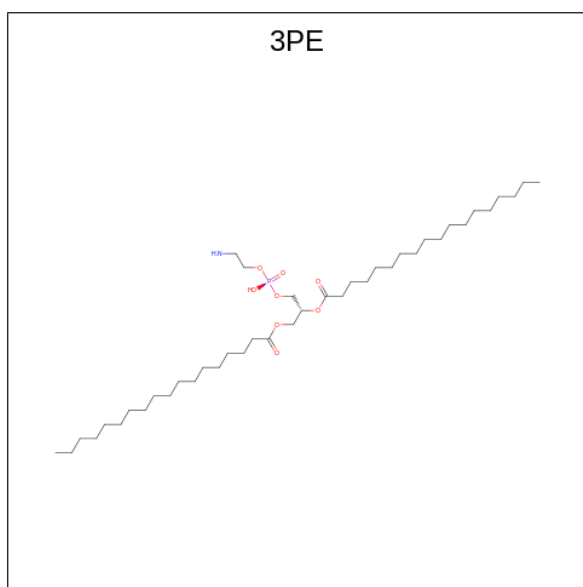


- Molecule 51 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C<sub>42</sub>H<sub>89</sub>NO<sub>8</sub>P).



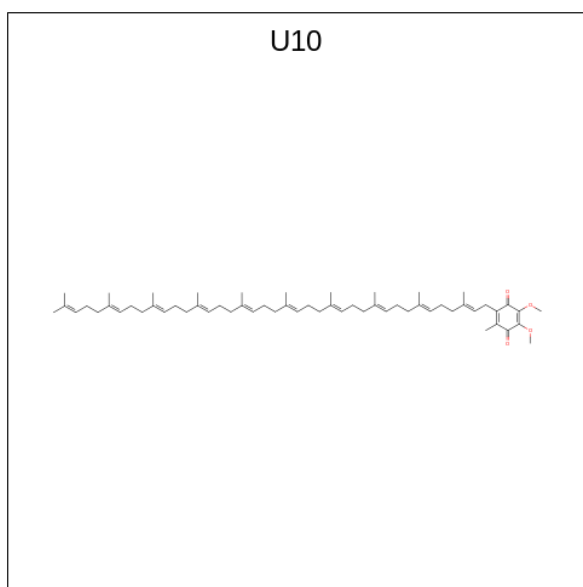
Mol	Chain	Residues	Atoms					AltConf
51	AM	1	Total	C	N	O	P	0
			52	42	1	8	1	
51	B5	1	Total	C	N	O	P	0
			52	42	1	8	1	
51	CB	1	Total	C	N	O	P	0
			52	42	1	8	1	
51	N4	1	Total	C	N	O	P	0
			47	37	1	8	1	
51	N4	1	Total	C	N	O	P	0
			52	42	1	8	1	
51	S7	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 52 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



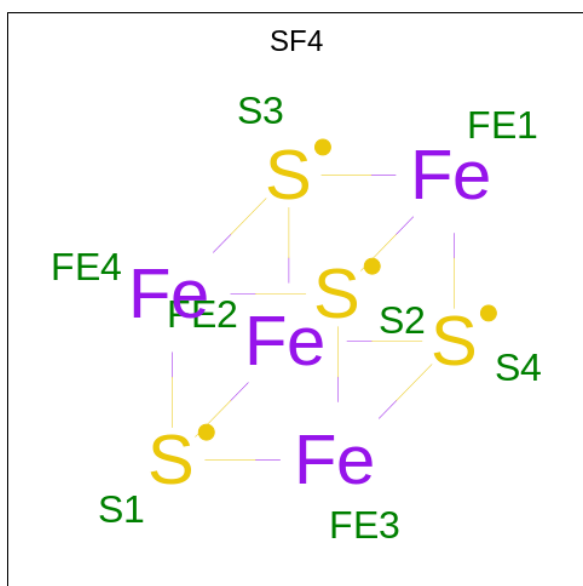
Mol	Chain	Residues	Atoms					AltConf
52	B8	1	Total	C	N	O	P	0
			32	22	1	8	1	
52	CB	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	CB	1	Total	C	N	O	P	0
			46	36	1	8	1	
52	N4	1	Total	C	N	O	P	0
			48	38	1	8	1	
52	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 53 is UBIQUINONE-10 (CCD ID: U10) (formula:  $C_{59}H_{90}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
53	N1	1	Total	C	O	0
			63	59	4	

- Molecule 54 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
54	S1	1	Total	Fe	S	0
			8	4	4	
54	S1	1	Total	Fe	S	0
			8	4	4	

*Continued on next page...*

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

- Molecule 55 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).

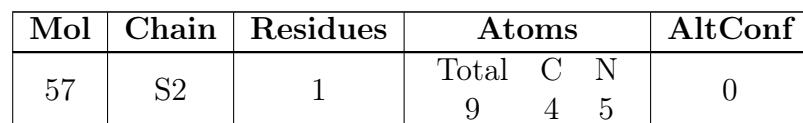


Mol	Chain	Residues	Atoms			AltConf
55	S1	1	Total	Fe	S	0
			4	2	2	
55	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula:  $\text{Mg}$ ) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
56	S1	1	Total	Mg	0
			1	1	

- Molecule 57 is Metformin (CCD ID: MF8) (formula:  $\text{C}_4\text{H}_{11}\text{N}_5$ ) (labeled as "Ligand of Interest" by depositor).



- | Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 58  | S6    | 1        | Total Zn<br>1 1 | 0       |

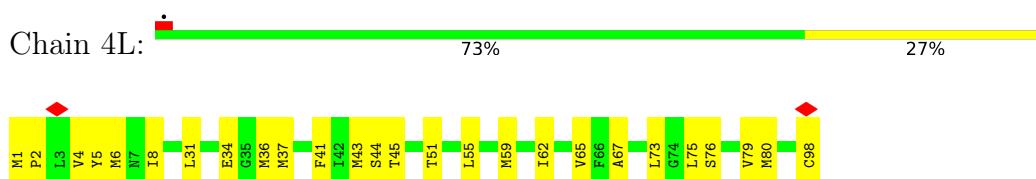
- [illegible]

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

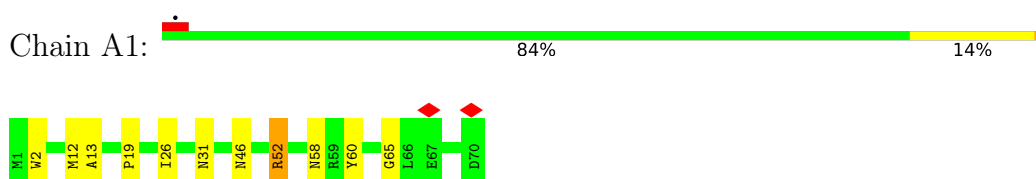
### 3 Residue-property plots

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

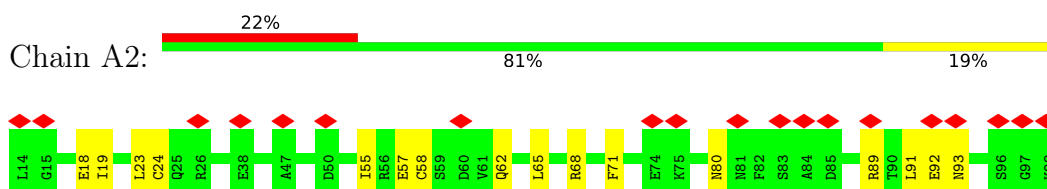
- Molecule 1: NADH-ubiquinone oxidoreductase chain 4L



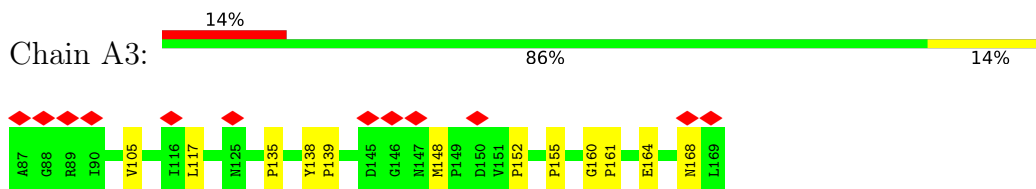
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



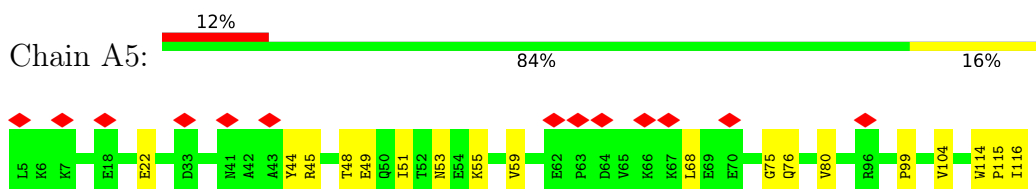
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



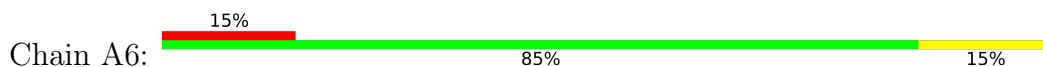
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



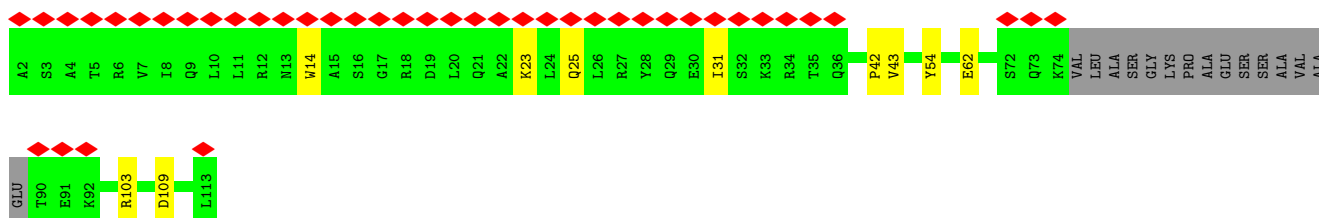
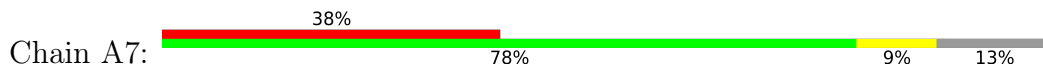
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



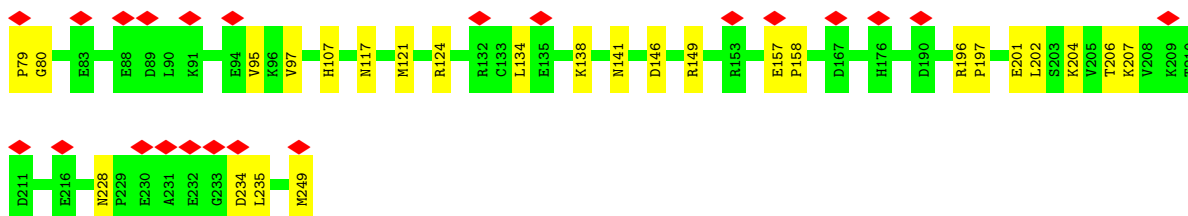
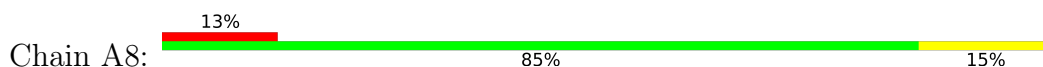
- Molecule 6: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



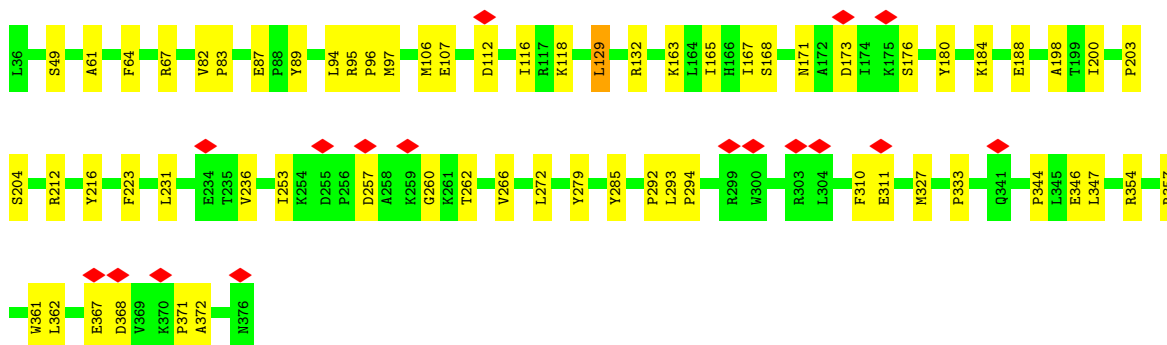
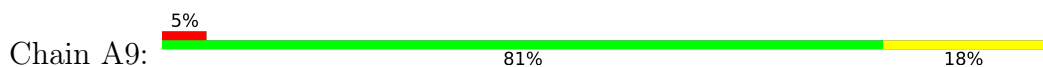
- Molecule 7: Complex I-B14.5a



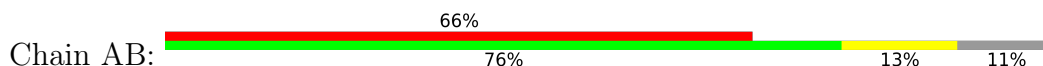
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



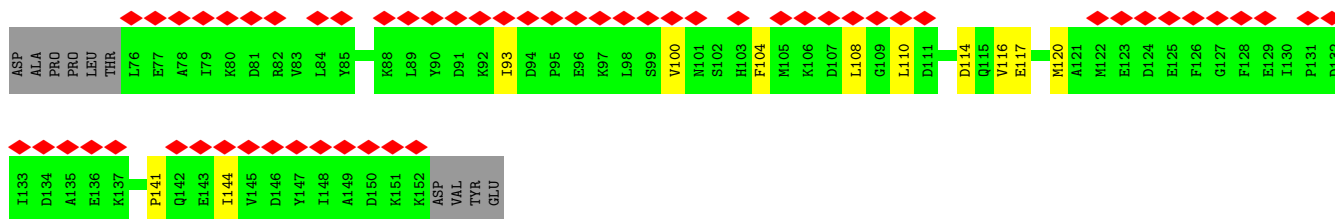
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



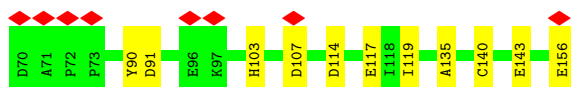
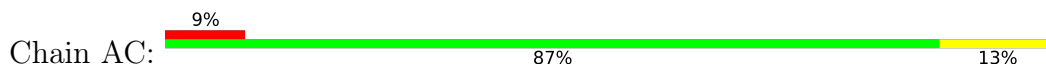
- Molecule 10: Acyl carrier protein



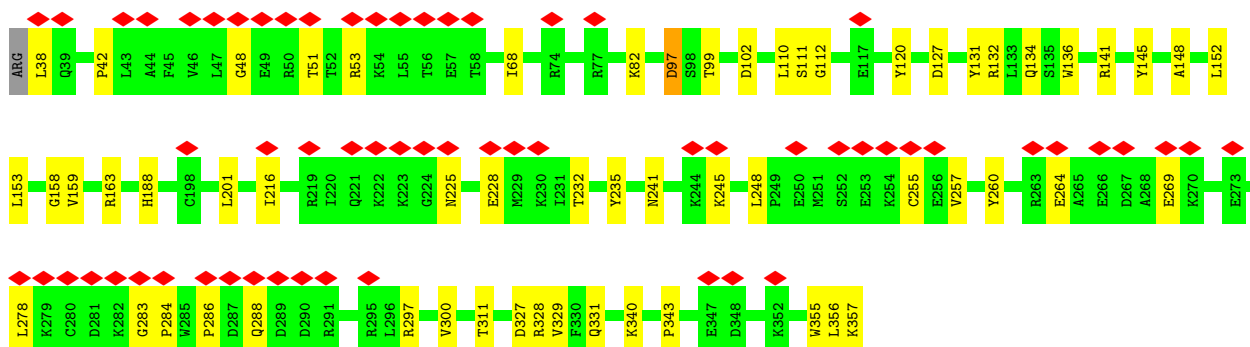
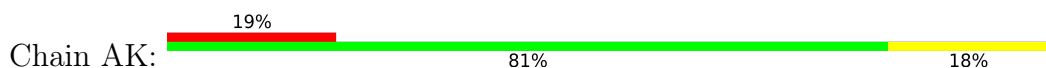




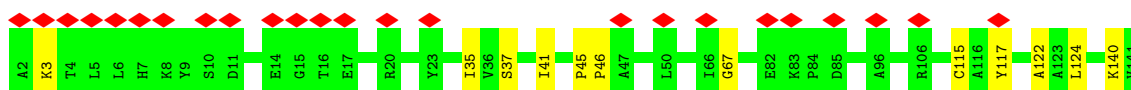
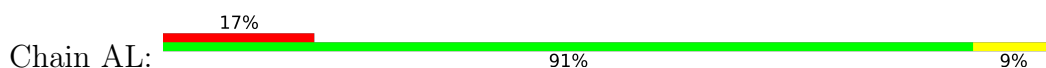
- Molecule 10: Acyl carrier protein



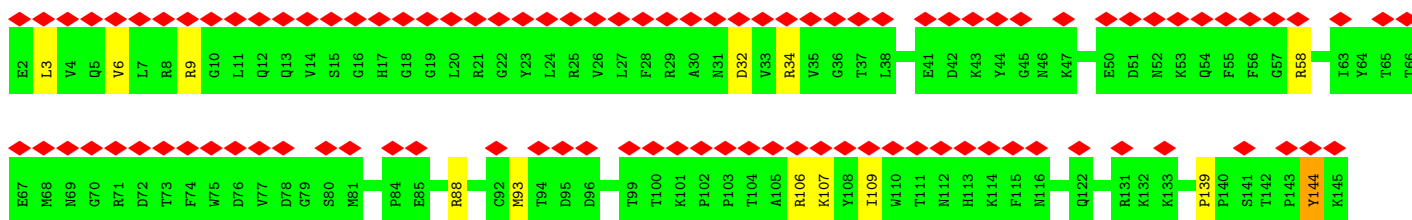
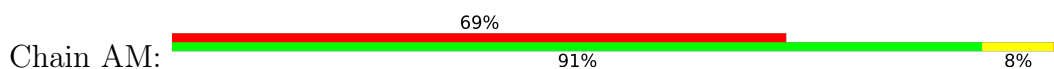
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



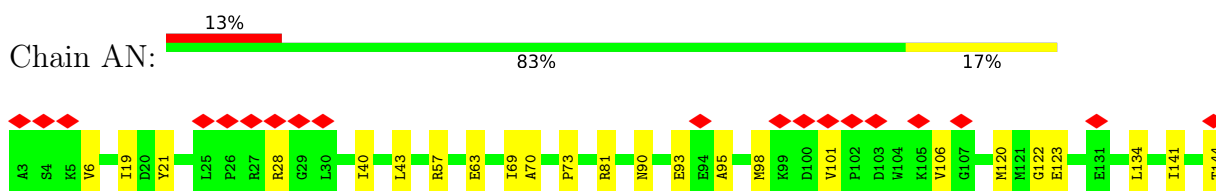
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



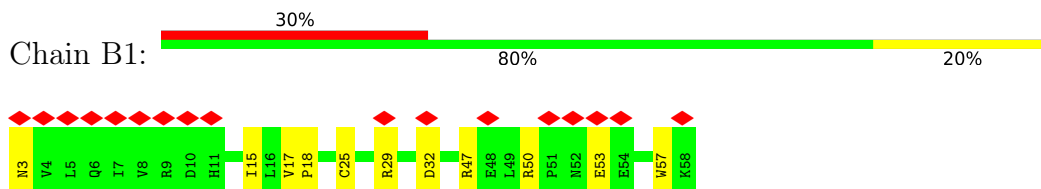
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



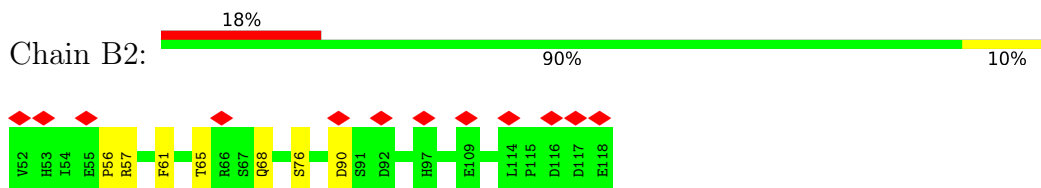
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



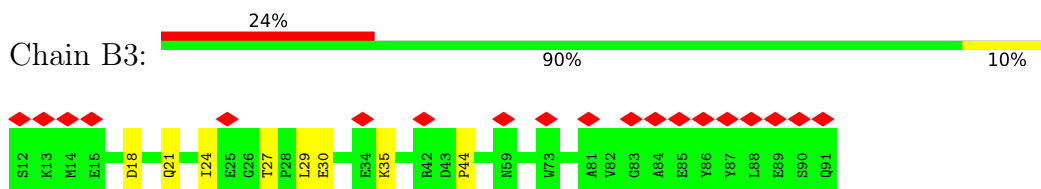
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



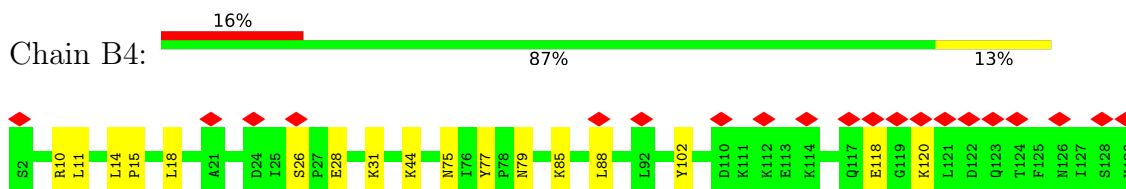
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



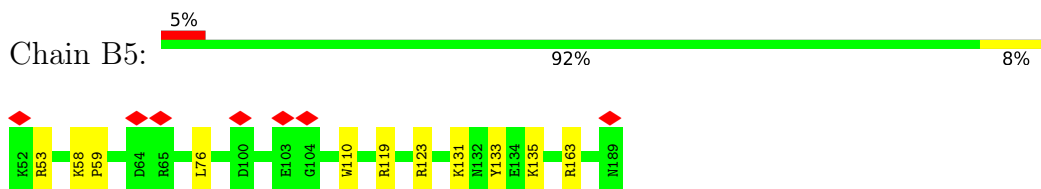
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

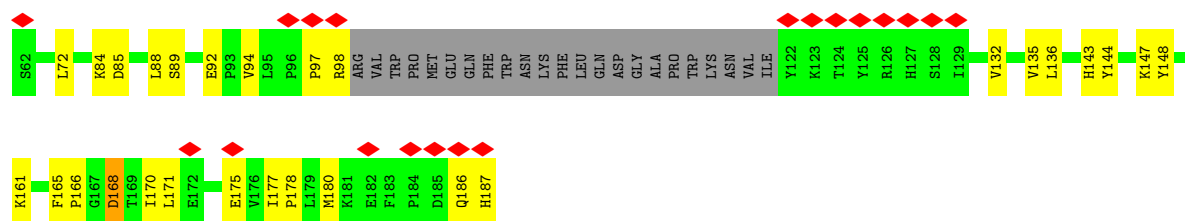


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

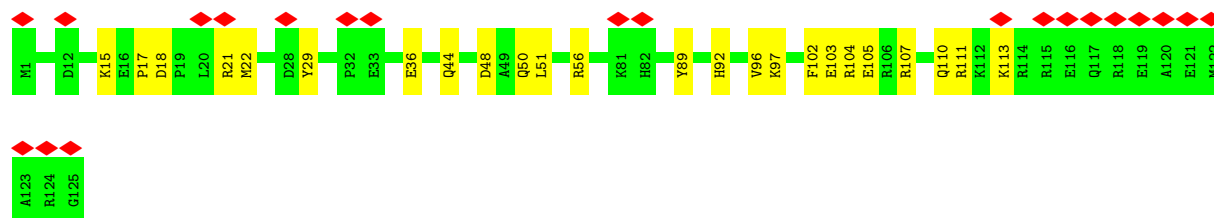
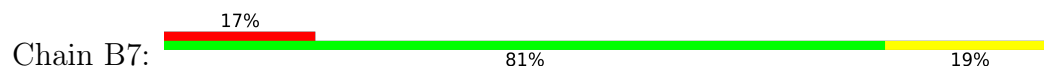


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

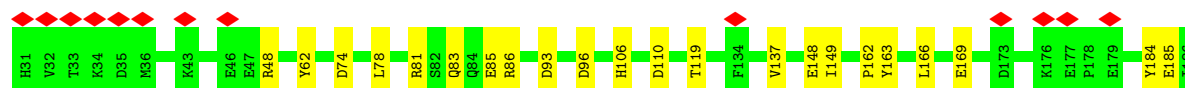




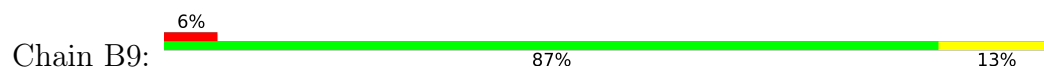
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



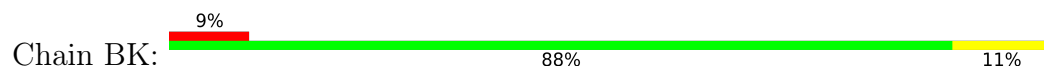
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



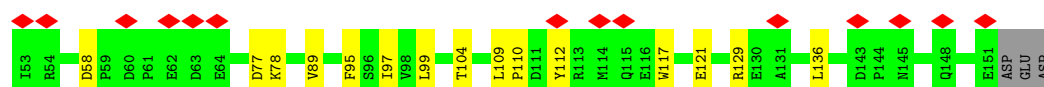
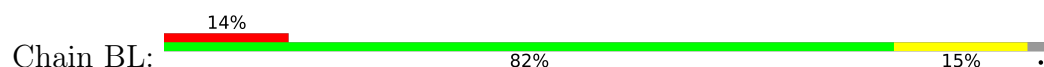
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



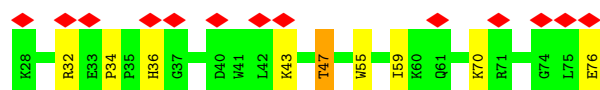
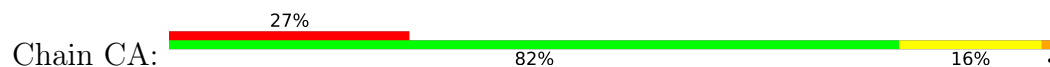
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



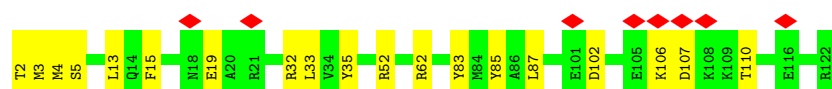
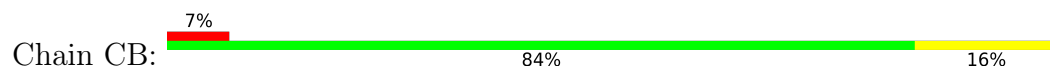
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



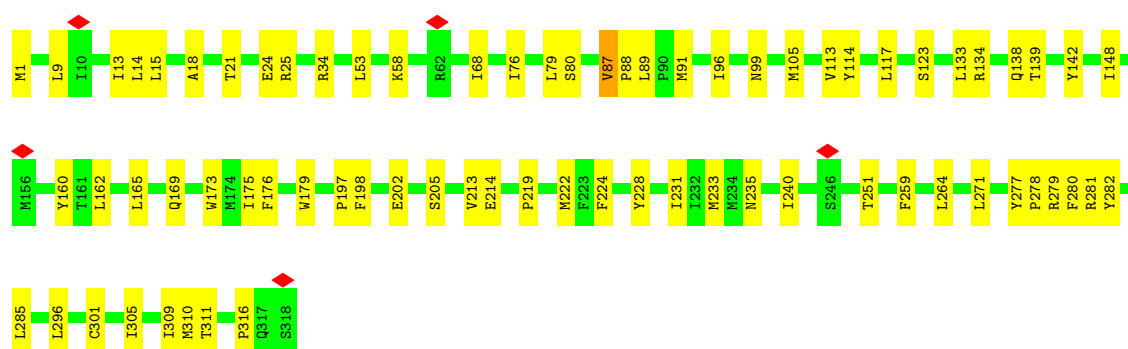
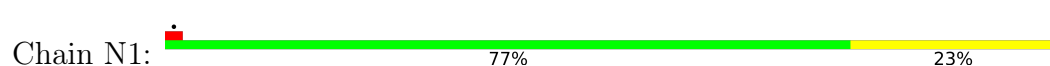
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



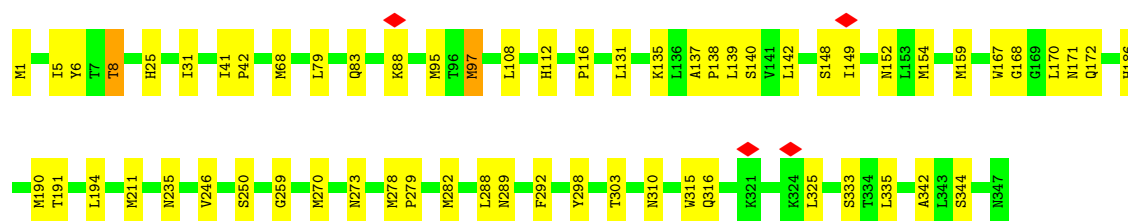
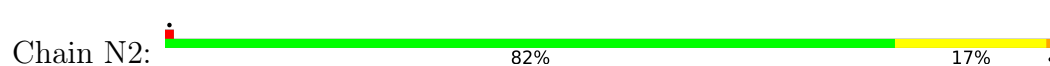
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C2



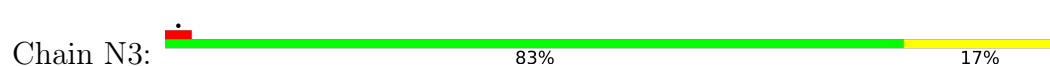
- Molecule 28: NADH-ubiquinone oxidoreductase chain 1



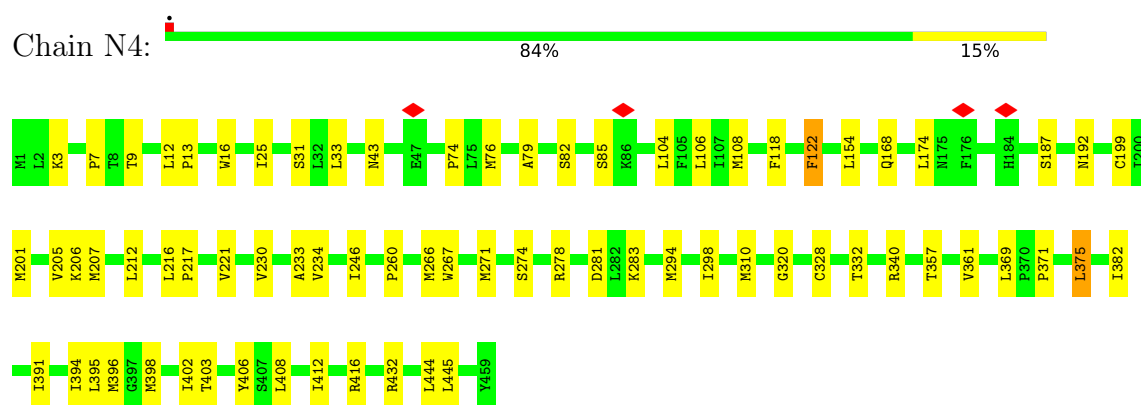
- Molecule 29: NADH-ubiquinone oxidoreductase chain 2



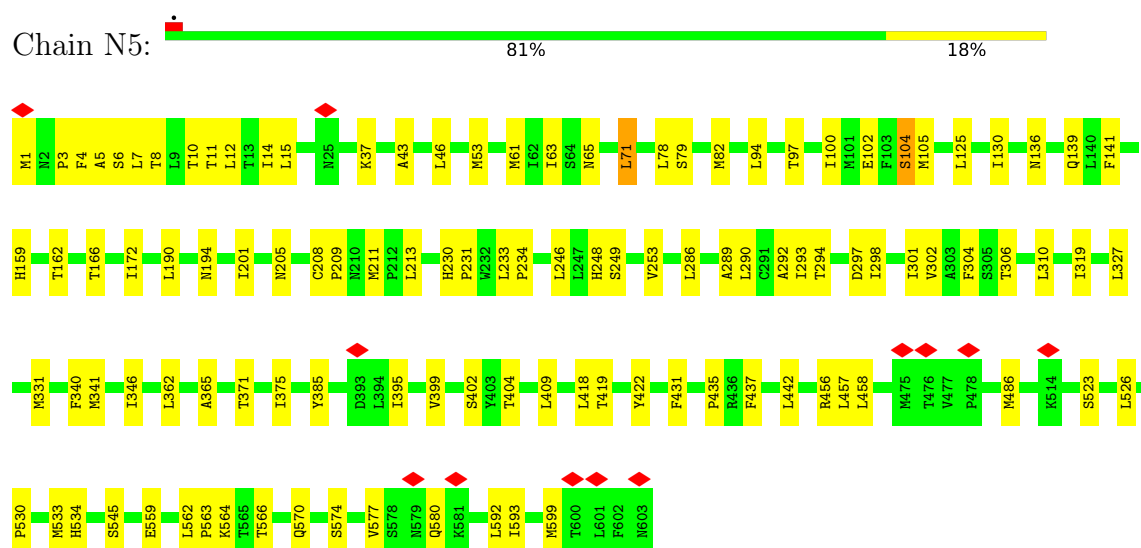
- Molecule 30: NADH-ubiquinone oxidoreductase chain 3



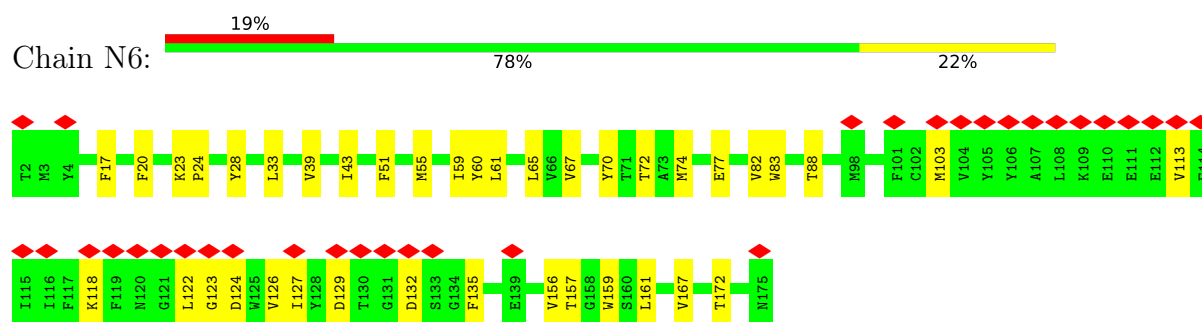
- Molecule 31: NADH-ubiquinone oxidoreductase chain 4



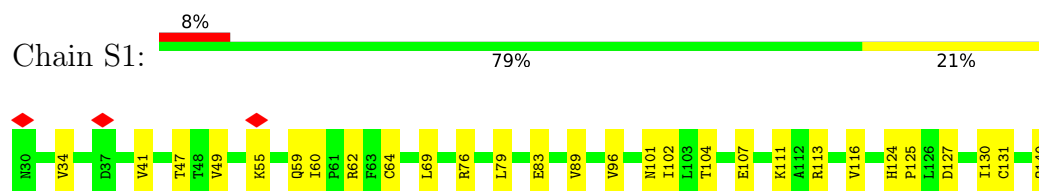
• Molecule 32: NADH-ubiquinone oxidoreductase chain 5

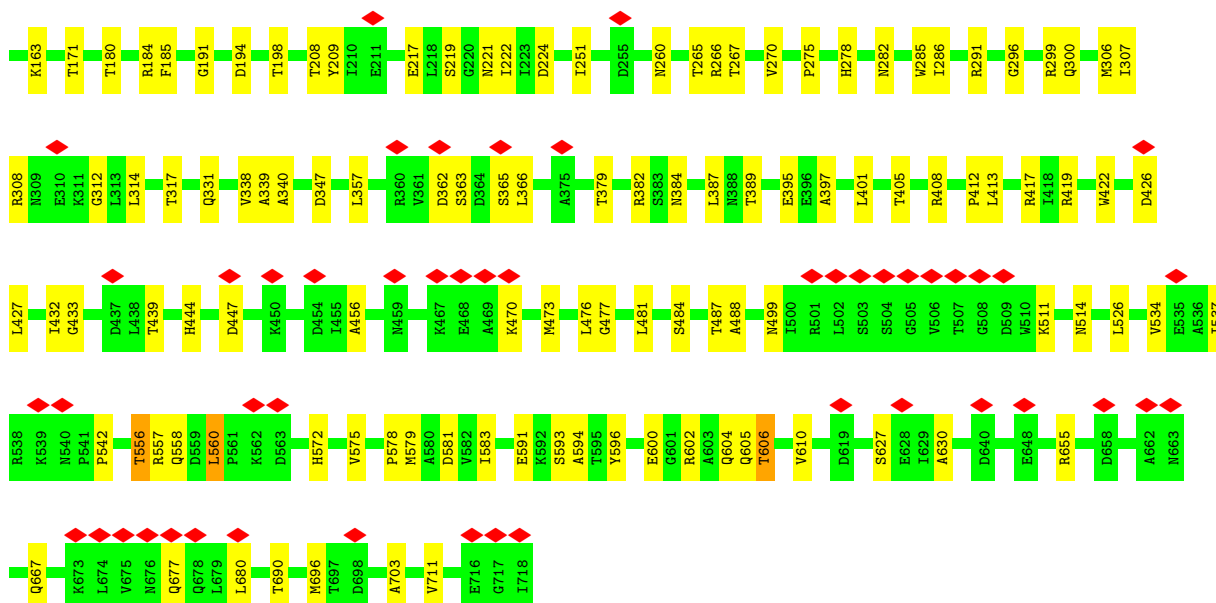


• Molecule 33: NADH-ubiquinone oxidoreductase chain 6

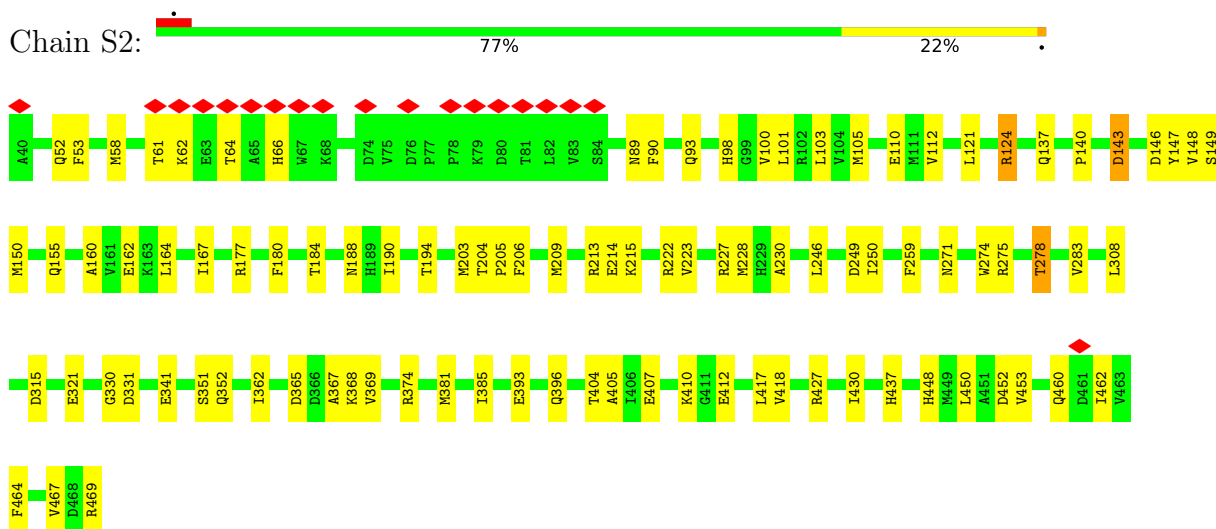


• Molecule 34: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

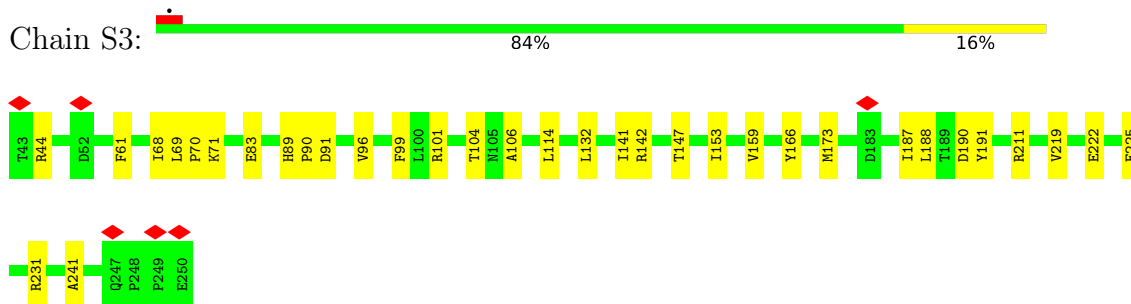




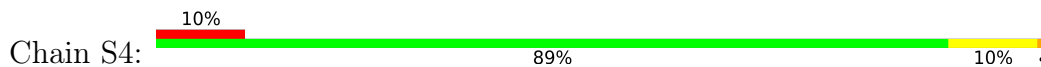
- Molecule 35: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

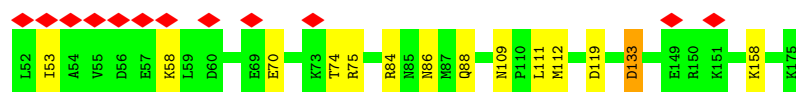


- Molecule 36: Complex I-30kD

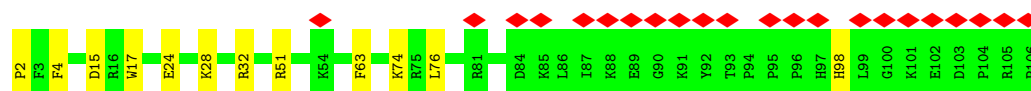
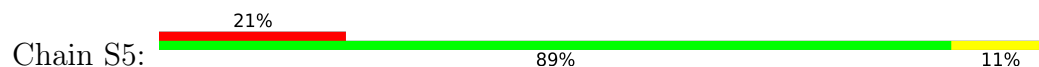


- Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

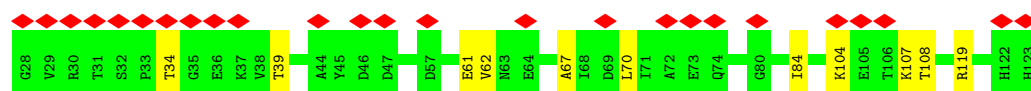




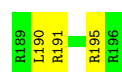
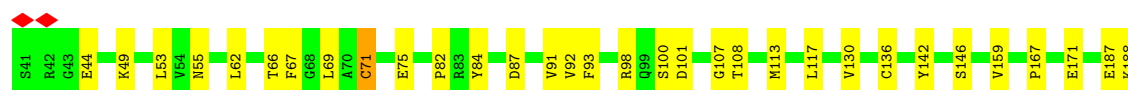
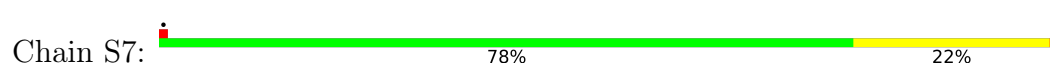
- Molecule 38: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



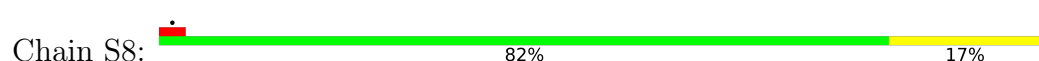
- Molecule 39: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



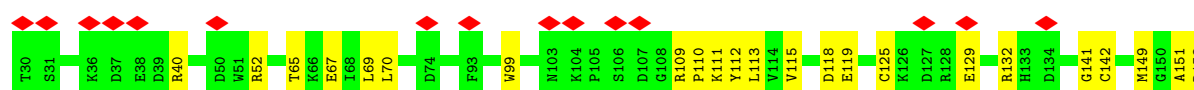
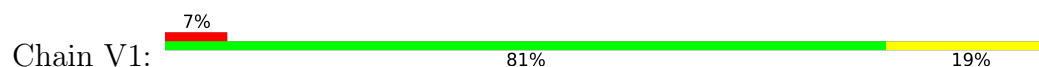
- Molecule 40: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

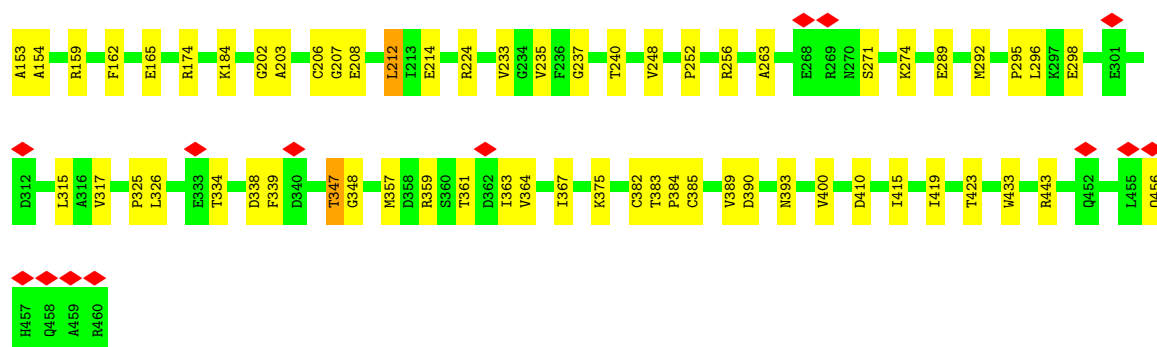


- Molecule 41: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

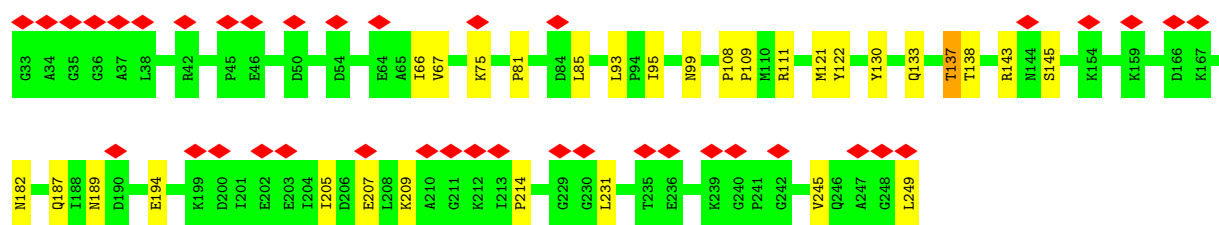
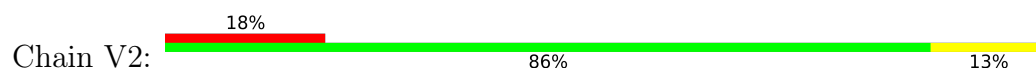


- Molecule 42: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

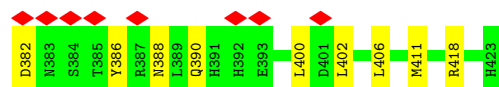
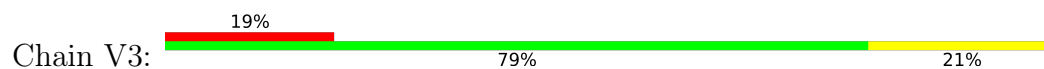




- Molecule 43: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 44: NADH:ubiquinone oxidoreductase subunit V3





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171814	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	43.248	Depositor
Minimum map value	-31.373	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.047	Depositor
Recommended contour level	7	Depositor
Map size (Å)	576.0, 576.0, 576.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.24	0/759	0.32	0/1029
2	A1	0.21	0/577	0.29	0/777
3	A2	0.18	0/697	0.30	0/938
4	A3	0.17	0/664	0.26	0/912
5	A5	0.21	0/929	0.25	0/1258
6	A6	0.23	0/991	0.29	0/1335
7	A7	0.19	0/798	0.30	0/1079
8	A8	0.19	0/1436	0.28	0/1938
9	A9	0.23	0/2820	0.31	0/3823
10	AB	0.12	0/633	0.23	0/851
10	AC	0.24	0/714	0.28	0/965
11	AK	0.20	0/2650	0.31	0/3588
12	AL	0.17	0/1042	0.25	0/1411
13	AM	0.13	0/1245	0.27	0/1694
14	AN	0.22	0/1204	0.27	0/1624
15	B1	0.19	0/491	0.30	0/663
16	B2	0.21	0/610	0.29	0/836
17	B3	0.21	0/660	0.30	0/892
18	B4	0.22	0/1092	0.30	0/1481
19	B5	0.24	0/1184	0.31	0/1603
20	B6	0.23	0/910	0.35	0/1237
21	B7	0.20	0/1092	0.29	0/1459
22	B8	0.23	0/1371	0.30	0/1875
23	B9	0.24	0/1590	0.33	0/2155
24	BK	0.22	0/1489	0.29	0/2008
25	BL	0.22	0/851	0.33	0/1155
26	CA	0.17	0/430	0.24	0/581
27	CB	0.22	0/1031	0.28	0/1394
28	N1	0.27	0/2581	0.40	0/3529
29	N2	0.26	0/2773	0.37	0/3768
30	N3	0.24	0/938	0.34	0/1281
31	N4	0.26	0/3723	0.38	0/5078

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	N5	0.25	0/4914	0.38	0/6683
33	N6	0.21	0/1364	0.34	0/1850
34	S1	0.25	0/5378	0.37	0/7287
35	S2	0.28	0/3538	0.35	0/4796
36	S3	0.27	0/1789	0.33	0/2436
37	S4	0.24	0/1030	0.34	0/1391
38	S5	0.19	0/889	0.26	0/1190
39	S6	0.20	0/755	0.30	0/1018
40	S7	0.28	0/1279	0.35	0/1730
41	S8	0.28	0/1443	0.32	0/1952
42	V1	0.24	0/3391	0.34	0/4583
43	V2	0.21	0/1711	0.35	0/2328
44	V3	0.16	0/365	0.30	0/493
All	All	0.23	0/67821	0.33	0/91954

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4L	748	0	799	21	0
2	A1	562	0	557	9	0
3	A2	686	0	699	10	0
4	A3	643	0	642	11	0
5	A5	910	0	950	13	0
6	A6	967	0	972	13	0
7	A7	780	0	808	11	0
8	A8	1398	0	1372	22	0
9	A9	2743	0	2762	36	0
10	AB	624	0	625	8	0
10	AC	702	0	694	9	0
11	AK	2590	0	2553	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	AL	1021	0	1025	11	0
13	AM	1204	0	1162	10	0
14	AN	1173	0	1166	22	0
15	B1	479	0	486	8	0
16	B2	584	0	529	5	0
17	B3	641	0	620	7	0
18	B4	1062	0	1072	13	0
19	B5	1151	0	1164	10	0
20	B6	882	0	899	23	0
21	B7	1068	0	1041	16	0
22	B8	1315	0	1208	17	0
23	B9	1534	0	1470	18	0
24	BK	1456	0	1426	17	0
25	BL	828	0	788	12	0
26	CA	417	0	422	6	0
27	CB	1000	0	994	18	0
28	N1	2508	0	2607	60	0
29	N2	2710	0	2874	46	0
30	N3	914	0	951	22	0
31	N4	3631	0	3839	59	0
32	N5	4785	0	4933	78	0
33	N6	1329	0	1326	36	0
34	S1	5290	0	5321	91	0
35	S2	3459	0	3396	68	0
36	S3	1738	0	1693	23	0
37	S4	1007	0	1008	8	0
38	S5	867	0	871	12	0
39	S6	741	0	701	8	0
40	S7	1248	0	1254	30	0
41	S8	1412	0	1363	23	0
42	V1	3316	0	3272	53	0
43	V2	1671	0	1673	17	0
44	V3	355	0	329	7	0
45	4L	91	0	132	7	0
45	A1	94	0	141	10	0
45	A8	83	0	113	4	0
45	AL	170	0	237	11	0
45	B4	80	0	107	1	0
45	B5	100	0	156	6	0
45	N1	78	0	103	2	0
45	N2	68	0	80	1	0
45	N4	189	0	284	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	N5	100	0	156	1	0
46	A3	53	0	83	2	0
46	A9	54	0	88	2	0
46	AN	54	0	88	4	0
46	B5	54	0	88	4	0
46	N1	99	0	155	4	0
46	N3	54	0	88	2	0
46	N5	54	0	88	10	0
47	A9	48	0	26	0	0
48	A9	39	0	52	0	0
48	AL	76	0	103	3	0
48	AN	51	0	82	2	0
48	B4	51	0	82	7	0
48	B6	46	0	69	2	0
48	N1	82	0	118	7	0
48	N3	150	0	237	13	0
48	N4	100	0	157	10	0
48	N5	51	0	82	4	0
48	S2	46	0	66	0	0
49	AB	36	0	47	2	0
49	AC	36	0	47	3	0
50	AK	27	0	12	4	0
51	AM	52	0	88	5	0
51	B5	52	0	88	9	0
51	CB	52	0	88	6	0
51	N4	99	0	163	8	0
51	S7	52	0	88	6	0
52	B8	32	0	38	1	0
52	CB	97	0	151	4	0
52	N4	48	0	73	5	0
52	N5	46	0	69	5	0
53	N1	63	0	90	8	0
54	S1	16	0	0	1	0
54	S7	8	0	0	1	0
54	S8	16	0	0	0	0
54	V1	8	0	0	1	0
55	S1	4	0	0	0	0
55	V2	4	0	0	0	0
56	S1	1	0	0	0	0
57	S2	9	0	0	0	0
58	S6	1	0	0	0	0
59	V1	31	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	69154	0	70638	955	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 (955) 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)
24:BK:140:GLN:O	24:BK:144:SER:HB2	1.62	1.00
1:4L:37:MET:HG2	1:4L:67:ALA:HB2	1.56	0.86
28:N1:21:THR:HG21	53:N1:405:U10:H303	1.58	0.84
29:N2:88:LYS:HG3	29:N2:148:SER:HB3	1.64	0.80
45:AL:203:CDL:H772	45:AL:203:CDL:H392	1.63	0.79
45:N4:505:CDL:H792	45:N4:505:CDL:H412	1.64	0.79
29:N2:140:SER:HB2	38:S5:2:PRO:HA	1.65	0.78
34:S1:282:ASN:ND2	34:S1:285:TRP:O	2.19	0.76
8:A8:141:ASN:OD1	14:AN:81:ARG:NH2	2.19	0.75
12:AL:140:LYS:H	29:N2:273:ASN:HD22	1.35	0.75
34:S1:487:THR:HB	34:S1:677:GLN:HE21	1.54	0.73
51:CB:201:PLX:H342	29:N2:342:ALA:HB3	1.70	0.73
31:N4:371:PRO:HD2	45:N4:507:CDL:H391	1.69	0.73
22:B8:137:VAL:HG21	46:N5:701:PC1:H2A1	1.69	0.73
12:AL:140:LYS:O	29:N2:273:ASN:ND2	2.22	0.72
45:A1:101:CDL:H152	45:A1:101:CDL:H842	1.71	0.72
21:B7:18:ASP:OD2	21:B7:21:ARG:NH1	2.23	0.72
28:N1:53:LEU:HD11	51:S7:302:PLX:H192	1.71	0.72
45:A1:101:CDL:H781	45:A1:101:CDL:H612	1.70	0.72
21:B7:29:TYR:O	21:B7:104:ARG:NH2	2.23	0.72
35:S2:374:ARG:NH2	41:S8:165:ASP:OD1	2.23	0.72
28:N1:176:PHE:HE2	46:N1:403:PC1:H261	1.55	0.71
9:A9:94:LEU:HD23	9:A9:97:MET:HE3	1.72	0.71
31:N4:391:ILE:HG23	31:N4:394:ILE:HD12	1.72	0.71
35:S2:61:THR:H	35:S2:64:THR:HG1	1.37	0.71
7:A7:109:ASP:OD2	14:AN:21:TYR:OH	2.07	0.71
30:N3:37:TYR:OH	35:S2:93:GLN:NE2	2.24	0.70
20:B6:88:LEU:HD22	20:B6:92:GLU:HG2	1.71	0.70
34:S1:83:GLU:HB2	34:S1:101:ASN:HB3	1.72	0.70
34:S1:433:GLY:HA2	34:S1:447:ASP:HA	1.74	0.69
43:V2:182:ASN:HB3	43:V2:194:GLU:HB3	1.73	0.69
12:AL:67:GLY:HA2	45:AL:201:CDL:H221	1.74	0.69
17:B3:27:THR:HG22	17:B3:29:LEU:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:S4:109:ASN:ND2	37:S4:111:LEU:O	2.26	0.69
18:B4:15:PRO:HG2	18:B4:18:LEU:HB2	1.74	0.69
21:B7:97:LYS:NZ	22:B8:185:GLU:OE1	2.26	0.68
45:A8:301:CDL:H112	27:CB:32:ARG:HG2	1.76	0.68
45:B5:202:CDL:H212	45:N4:507:CDL:H632	1.74	0.68
34:S1:433:GLY:O	34:S1:444:HIS:NE2	2.22	0.68
42:V1:235:VAL:HG12	42:V1:240:THR:HG21	1.76	0.68
32:N5:5:ALA:HB2	32:N5:61:MET:HE1	1.75	0.68
13:AM:106:ARG:HB2	13:AM:109:ILE:HG13	1.76	0.68
32:N5:211:MET:HA	52:N5:704:3PE:H322	1.77	0.67
10:AC:114:ASP:OD1	23:B9:87:ARG:NH2	2.27	0.67
42:V1:40:ARG:NH1	42:V1:289:GLU:O	2.28	0.67
45:4L:201:CDL:H521	33:N6:88:THR:HG23	1.74	0.67
22:B8:62:TYR:OH	22:B8:74:ASP:O	2.12	0.66
25:BL:95:PHE:O	25:BL:99:LEU:HB2	1.95	0.66
34:S1:456:ALA:O	34:S1:499:ASN:ND2	2.28	0.66
30:N3:38:GLU:HG2	35:S2:89:ASN:HB2	1.76	0.66
9:A9:212:ARG:NH1	9:A9:311:GLU:OE2	2.28	0.66
42:V1:109:ARG:NH1	42:V1:237:GLY:O	2.29	0.66
3:A2:24:CYS:N	3:A2:58:CYS:SG	2.69	0.66
34:S1:426:ASP:OD2	44:V3:418:ARG:NH2	2.29	0.66
36:S3:89:HIS:ND1	36:S3:91:ASP:OD1	2.28	0.66
32:N5:533:MET:HG3	46:N5:701:PC1:H2G1	1.77	0.65
11:AK:145:TYR:OH	11:AK:201:LEU:O	2.13	0.65
13:AM:34:ARG:NH2	41:S8:89:GLU:OE2	2.29	0.65
3:A2:65:LEU:HD11	3:A2:91:LEU:HD13	1.78	0.65
36:S3:83:GLU:OE1	36:S3:142:ARG:NH2	2.30	0.65
32:N5:399:VAL:HG12	32:N5:409:LEU:HD13	1.78	0.65
34:S1:149:ASP:HB2	35:S2:367:ALA:HB3	1.79	0.64
49:AC:201:ZMP:H14	23:B9:102:ALA:HB1	1.79	0.64
35:S2:222:ARG:NH1	35:S2:249:ASP:OD2	2.15	0.64
51:AM:201:PLX:H72	51:AM:201:PLX:H252	1.80	0.64
11:AK:48:GLY:O	11:AK:53:ARG:NH2	2.30	0.64
18:B4:88:LEU:HB3	48:B4:201:PEE:H19	1.78	0.64
32:N5:530:PRO:O	32:N5:534:HIS:HB2	1.98	0.64
46:AN:202:PC1:O12	28:N1:99:ASN:N	2.23	0.63
31:N4:199:CYS:HB3	31:N4:246:ILE:HD13	1.81	0.63
29:N2:298:TYR:O	29:N2:303:THR:OG1	2.15	0.63
32:N5:100:ILE:HG21	32:N5:246:LEU:HB2	1.79	0.63
40:S7:188:LYS:HB2	40:S7:191:ARG:HB2	1.80	0.63
30:N3:96:ILE:HG21	48:N3:203:PEE:H34	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:V2:95:ILE:O	43:V2:99:ASN:ND2	2.32	0.63
34:S1:593:SER:HA	34:S1:606:THR:O	1.98	0.63
25:BL:129:ARG:NH1	25:BL:136:LEU:O	2.28	0.62
5:A5:44:TYR:O	5:A5:48:THR:HG22	1.99	0.62
10:AB:93:ILE:HD12	10:AB:108:LEU:HD13	1.80	0.62
13:AM:88:ARG:HD3	41:S8:200:GLU:HG3	1.81	0.62
23:B9:147:ASP:HB3	23:B9:164:ARG:HH12	1.65	0.62
32:N5:97:THR:HG21	32:N5:125:LEU:HD22	1.81	0.62
46:N5:701:PC1:H392	52:N5:704:3PE:H261	1.82	0.62
30:N3:70:ALA:HB2	33:N6:59:ILE:HD11	1.81	0.62
45:A1:101:CDL:H531	45:A1:101:CDL:H732	1.81	0.62
22:B8:148:GLU:HG2	46:N5:701:PC1:H152	1.82	0.62
35:S2:308:LEU:HB2	35:S2:407:GLU:HB2	1.82	0.62
28:N1:87:VAL:HG11	30:N3:6:THR:HG21	1.81	0.61
29:N2:108:LEU:HD11	29:N2:191:THR:HG21	1.82	0.61
13:AM:32:ASP:OD2	13:AM:58:ARG:NH2	2.32	0.61
40:S7:55:ASN:ND2	40:S7:187:GLU:O	2.33	0.61
11:AK:82:LYS:HZ3	11:AK:269:GLU:HG2	1.65	0.61
37:S4:75:ARG:NH1	37:S4:119:ASP:OD1	2.30	0.61
15:B1:47:ARG:NH2	15:B1:53:GLU:OE2	2.33	0.61
34:S1:60:ILE:O	34:S1:62:ARG:NH1	2.34	0.61
34:S1:251:ILE:HG12	34:S1:606:THR:HG22	1.83	0.61
30:N3:79:SER:HA	30:N3:87:MET:HE2	1.83	0.60
34:S1:488:ALA:HB2	34:S1:677:GLN:HG3	1.83	0.60
18:B4:75:ASN:OD1	18:B4:79:ASN:ND2	2.33	0.60
45:B5:202:CDL:H662	32:N5:12:LEU:HB3	1.83	0.60
25:BL:78:LYS:NZ	31:N4:85:SER:OG	2.33	0.60
31:N4:122:PHE:HE1	31:N4:206:LYS:HG3	1.66	0.60
34:S1:124:HIS:HD2	35:S2:381:MET:HE2	1.66	0.60
34:S1:534:VAL:HG22	34:S1:537:ILE:HB	1.83	0.60
45:A1:101:CDL:H762	45:A1:101:CDL:H591	1.82	0.60
18:B4:26:SER:OG	18:B4:28:GLU:OE1	2.18	0.60
34:S1:387:LEU:HD12	34:S1:514:ASN:HB3	1.84	0.60
41:S8:63:TRP:HB3	41:S8:66:LEU:HD12	1.83	0.60
21:B7:56:ARG:HH22	24:BK:120:SER:HB3	1.67	0.60
1:4L:79:VAL:HG12	33:N6:74:MET:HE3	1.82	0.60
34:S1:419:ARG:NH1	34:S1:439:THR:O	2.33	0.60
29:N2:142:LEU:HB3	29:N2:194:LEU:HD21	1.83	0.59
1:4L:31:LEU:HD21	33:N6:67:VAL:HG11	1.83	0.59
9:A9:188:GLU:HG3	9:A9:200:ILE:HD13	1.85	0.59
14:AN:98:MET:HE3	14:AN:101:VAL:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:S1:405:THR:HB	34:S1:477:GLY:HA3	1.84	0.59
35:S2:101:LEU:HB2	35:S2:464:PHE:CZ	2.38	0.59
8:A8:201:GLU:HA	8:A8:204:LYS:HD3	1.85	0.59
34:S1:163:LYS:O	34:S1:171:THR:OG1	2.20	0.59
20:B6:143:HIS:HD2	24:BK:45:VAL:HG21	1.68	0.58
6:A6:66:TYR:O	6:A6:86:ARG:NH1	2.36	0.58
20:B6:143:HIS:CD2	24:BK:45:VAL:HG21	2.37	0.58
48:N3:204:PEE:H78	33:N6:156:VAL:HG12	1.84	0.58
35:S2:124:2MR:O	40:S7:146:SER:OG	2.20	0.58
8:A8:228:ASN:OD1	38:S5:51:ARG:NH1	2.33	0.58
46:AN:202:PC1:H132	46:AN:202:PC1:H12	1.85	0.58
42:V1:338:ASP:OD1	42:V1:339:PHE:N	2.36	0.58
34:S1:299:ARG:NH1	34:S1:703:ALA:O	2.36	0.58
34:S1:64:CYS:O	34:S1:184:ARG:NH2	2.25	0.58
35:S2:90:PHE:HB3	35:S2:103:LEU:HB3	1.86	0.58
51:B5:201:PLX:H331	48:N4:501:PEE:H73	1.86	0.58
45:AL:203:CDL:OA7	29:N2:152:ASN:ND2	2.37	0.58
45:N4:505:CDL:H411	45:N4:505:CDL:H362	1.84	0.58
34:S1:49:VAL:HG13	34:S1:102:ILE:HD13	1.84	0.58
42:V1:119:GLU:HA	59:V1:502:FMN:HM71	1.86	0.58
42:V1:111:LYS:HB2	42:V1:151:ALA:HA	1.86	0.58
2:A1:2:TRP:HH2	45:A1:101:CDL:H342	1.68	0.57
29:N2:131:LEU:O	29:N2:135:LYS:HG2	2.04	0.57
32:N5:102:GLU:OE1	32:N5:456:ARG:NH2	2.35	0.57
5:A5:75:GLY:O	7:A7:103:ARG:NH2	2.37	0.57
12:AL:140:LYS:H	29:N2:273:ASN:ND2	2.00	0.57
48:N5:703:PEE:H82	52:N5:704:3PE:H3C1	1.87	0.57
28:N1:160:TYR:OH	30:N3:73:LEU:O	2.23	0.57
34:S1:275:PRO:HG3	34:S1:286:ILE:HG12	1.86	0.57
28:N1:139:THR:HA	28:N1:142:TYR:CE2	2.40	0.57
29:N2:170:LEU:HD11	29:N2:288:LEU:HD22	1.85	0.57
3:A2:89:ARG:O	3:A2:93:ASN:ND2	2.37	0.57
19:B5:163:ARG:NH1	27:CB:102:ASP:OD2	2.32	0.57
22:B8:78:LEU:HD12	22:B8:106:HIS:HA	1.87	0.56
45:A1:101:CDL:H112	45:A1:101:CDL:H521	1.88	0.56
7:A7:62:GLU:OE2	36:S3:44:ARG:NH2	2.30	0.56
28:N1:176:PHE:CE2	46:N1:403:PC1:H261	2.40	0.56
34:S1:340:ALA:HB3	34:S1:366:LEU:HD23	1.86	0.56
36:S3:187:ILE:HG23	36:S3:188:LEU:HG	1.86	0.56
46:A3:201:PC1:H332	48:N1:406:PEE:H30	1.87	0.56
11:AK:127:ASP:O	11:AK:132:ARG:NH1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:N4:361:VAL:HG13	45:N4:507:CDL:H351	1.88	0.56
46:N5:701:PC1:H321	48:N5:703:PEE:H44	1.86	0.56
29:N2:289:ASN:HA	29:N2:292:PHE:CE2	2.41	0.56
45:B5:202:CDL:H642	45:N4:507:CDL:H273	1.86	0.56
32:N5:162:THR:O	32:N5:166:THR:HG23	2.06	0.56
32:N5:290:LEU:O	32:N5:523:SER:OG	2.23	0.56
45:4L:201:CDL:H842	32:N5:592:LEU:HD11	1.88	0.56
9:A9:87:GLU:HG3	9:A9:89:TYR:H	1.71	0.56
29:N2:97:MET:HG2	32:N5:599:MET:HE1	1.87	0.56
31:N4:82:SER:HB2	31:N4:432:ARG:NH1	2.21	0.56
15:B1:32:ASP:OD1	19:B5:135:LYS:NZ	2.33	0.55
45:AL:201:CDL:H521	45:AL:201:CDL:H562	1.88	0.55
19:B5:123:ARG:NH2	46:B5:203:PC1:O14	2.39	0.55
21:B7:44:GLN:NE2	21:B7:48:ASP:OD1	2.38	0.55
14:AN:144:THR:HB	28:N1:96:ILE:HG23	1.88	0.55
16:B2:90:ASP:O	32:N5:385:TYR:OH	2.15	0.55
52:CB:202:3PE:H381	29:N2:325:LEU:H	1.71	0.55
29:N2:246:VAL:HG11	45:N4:505:CDL:H382	1.87	0.55
42:V1:110:PRO:HB3	42:V1:152:ARG:HD3	1.87	0.55
42:V1:364:VAL:HG12	42:V1:400:VAL:HG12	1.89	0.55
45:4L:201:CDL:H451	45:4L:201:CDL:H401	1.88	0.55
5:A5:55:LYS:HE3	36:S3:104:THR:HG21	1.89	0.55
11:AK:120:TYR:OH	50:AK:401:ADP:O2'	2.11	0.55
20:B6:166:PRO:HG2	20:B6:180:MET:HG3	1.88	0.55
22:B8:149:ILE:HD12	52:B8:201:3PE:H12	1.88	0.55
34:S1:347:ASP:OD1	34:S1:347:ASP:N	2.40	0.55
45:A8:301:CDL:H762	52:CB:203:3PE:H282	1.89	0.55
28:N1:117:LEU:HD11	33:N6:65:LEU:HD12	1.88	0.55
43:V2:85:LEU:HD13	44:V3:400:LEU:HD22	1.88	0.55
20:B6:165:PHE:O	20:B6:168:ASP:HB2	2.07	0.55
31:N4:16:TRP:CZ2	45:N4:505:CDL:H471	2.42	0.55
36:S3:132:LEU:HB2	36:S3:141:ILE:HG22	1.88	0.55
28:N1:148:ILE:HD11	30:N3:69:ILE:HG22	1.90	0.54
35:S2:146:ASP:OD2	35:S2:149:SER:OG	2.24	0.54
14:AN:90:ASN:ND2	14:AN:123:GLU:O	2.39	0.54
42:V1:263:ALA:HA	42:V1:271:SER:HB3	1.89	0.54
1:4L:65:VAL:HG11	33:N6:157:THR:HG23	1.89	0.54
5:A5:49:GLU:O	5:A5:53:ASN:ND2	2.34	0.54
13:AM:144:TYR:OH	34:S1:581:ASP:OD1	2.23	0.54
42:V1:203:ALA:HB3	42:V1:206:CYS:HB2	1.88	0.54
43:V2:133:GLN:OE1	43:V2:187:GLN:NE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A9:236:VAL:HG22	9:A9:272:LEU:HD23	1.89	0.54
11:AK:225:ASN:HB3	11:AK:228:GLU:HG2	1.89	0.54
20:B6:92:GLU:O	20:B6:94:VAL:N	2.40	0.54
42:V1:382:CYS:HB3	42:V1:384:PRO:HD2	1.90	0.54
1:4L:1:MET:HE3	29:N2:79:LEU:HD21	1.87	0.54
28:N1:34:ARG:HG2	40:S7:82:PRO:HA	1.89	0.54
40:S7:53:LEU:HD22	51:S7:302:PLX:H342	1.89	0.54
31:N4:82:SER:HB2	31:N4:432:ARG:CZ	2.38	0.54
28:N1:24:GLU:HA	28:N1:271:LEU:HD13	1.90	0.54
53:N1:405:U10:H253	40:S7:92:VAL:HG11	1.90	0.54
31:N4:205:VAL:HG22	31:N4:212:LEU:HD13	1.89	0.54
35:S2:393:GLU:OE2	35:S2:396:GLN:NE2	2.41	0.54
9:A9:212:ARG:O	9:A9:216:TYR:N	2.33	0.54
14:AN:120:MET:HG2	14:AN:123:GLU:HG3	1.90	0.54
18:B4:102:TYR:OH	52:N4:506:3PE:O14	2.26	0.54
35:S2:190:ILE:HG23	35:S2:209:MET:HB3	1.90	0.54
9:A9:354:ARG:NH1	9:A9:362:LEU:O	2.39	0.54
27:CB:62:ARG:HG3	52:CB:202:3PE:H221	1.90	0.54
34:S1:191:GLY:HA3	34:S1:439:THR:HB	1.90	0.54
2:A1:46:ASN:ND2	33:N6:132:ASP:OD2	2.41	0.53
29:N2:42:PRO:HG2	33:N6:167:VAL:HG22	1.91	0.53
29:N2:42:PRO:HG3	33:N6:167:VAL:HG13	1.90	0.53
35:S2:62:LYS:O	35:S2:66:HIS:ND1	2.36	0.53
42:V1:52:ARG:HH21	44:V3:390:GLN:HG2	1.72	0.53
1:4L:73:LEU:HD21	29:N2:41:ILE:HG13	1.90	0.53
45:A1:101:CDL:H552	45:A1:101:CDL:H751	1.90	0.53
31:N4:375:LEU:HD11	32:N5:141:PHE:HE2	1.74	0.53
34:S1:389:THR:OG1	34:S1:511:LYS:O	2.26	0.53
42:V1:274:LYS:HD3	42:V1:292:MET:HE1	1.90	0.53
2:A1:31:ASN:OD1	2:A1:60:TYR:OH	2.18	0.53
15:B1:29:ARG:NH2	51:B5:201:PLX:O2	2.41	0.53
32:N5:100:ILE:O	32:N5:104:SER:OG	2.25	0.53
35:S2:274:TRP:O	35:S2:278:THR:OG1	2.23	0.53
14:AN:93:GLU:HG3	38:S5:98:HIS:CD2	2.43	0.53
18:B4:14:LEU:HD12	18:B4:15:PRO:HD2	1.90	0.53
20:B6:89:SER:HB2	20:B6:92:GLU:HB2	1.90	0.53
24:BK:142:ARG:NH1	24:BK:143:TYR:OH	2.42	0.53
48:N3:201:PEE:H41	48:N3:203:PEE:H22	1.91	0.53
35:S2:162:GLU:OE2	35:S2:177:ARG:NH2	2.37	0.53
6:A6:66:TYR:CE2	6:A6:86:ARG:HD3	2.44	0.53
12:AL:124:LEU:HD11	48:N4:502:PEE:H70	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:N1:228:TYR:HA	28:N1:231:ILE:HD12	1.91	0.53
28:N1:219:PRO:HA	28:N1:222:MET:HE3	1.91	0.53
31:N4:233:ALA:HA	31:N4:320:GLY:HA2	1.91	0.53
36:S3:173:MET:HE3	36:S3:188:LEU:HB2	1.90	0.53
3:A2:18:GLU:HG2	3:A2:68:ARG:HB3	1.90	0.53
28:N1:231:ILE:O	28:N1:235:ASN:ND2	2.42	0.52
11:AK:141:ARG:NH2	50:AK:401:ADP:N7	2.56	0.52
42:V1:174:ARG:HA	44:V3:406:LEU:HD21	1.91	0.52
42:V1:357:MET:HB3	42:V1:361:THR:HG21	1.91	0.52
1:4L:41:PHE:O	1:4L:45:THR:HG22	2.09	0.52
45:4L:201:CDL:H391	45:4L:201:CDL:H262	1.92	0.52
6:A6:90:ARG:NH2	10:AB:117:GLU:OE2	2.42	0.52
9:A9:95:ARG:HH22	41:S8:179:THR:HG22	1.74	0.52
9:A9:285:TYR:OH	9:A9:368:ASP:OD2	2.27	0.52
30:N3:66:ASP:O	30:N3:69:ILE:HG12	2.08	0.52
21:B7:17:PRO:HB3	21:B7:105:GLU:HG2	1.91	0.52
21:B7:103:GLU:O	21:B7:107:ARG:HG2	2.09	0.52
32:N5:249:SER:HA	32:N5:306:THR:HG21	1.91	0.52
35:S2:150:MET:SD	35:S2:228:MET:HB2	2.48	0.52
42:V1:235:VAL:H	42:V1:240:THR:HG21	1.74	0.52
2:A1:12:MET:HE3	28:N1:264:LEU:HD22	1.91	0.52
51:B5:201:PLX:H211	46:B5:203:PC1:H2E2	1.91	0.52
46:N3:202:PC1:H3I2	51:S7:302:PLX:H202	1.92	0.52
43:V2:108:PRO:HB2	43:V2:111:ARG:HG2	1.91	0.52
2:A1:52:ARG:NH1	2:A1:58:ASN:OD1	2.42	0.52
20:B6:132:VAL:O	20:B6:136:LEU:HB3	2.10	0.52
32:N5:4:PHE:HD2	32:N5:61:MET:HE2	1.75	0.52
22:B8:85:GLU:OE2	22:B8:119:THR:OG1	2.24	0.52
13:AM:139:PRO:HG3	34:S1:306:MET:HE1	1.91	0.52
31:N4:106:LEU:HD13	31:N4:234:VAL:HG11	1.90	0.52
32:N5:566:THR:O	32:N5:570:GLN:HG2	2.10	0.52
34:S1:306:MET:HB2	34:S1:583:ILE:HB	1.92	0.52
3:A2:57:GLU:O	34:S1:655:ARG:NH2	2.42	0.52
6:A6:111:LYS:HA	6:A6:114:MET:HE2	1.91	0.52
51:B5:201:PLX:H392	48:N4:501:PEE:H36	1.91	0.52
30:N3:35:SER:O	40:S7:98:ARG:NH2	2.43	0.52
32:N5:362:LEU:HA	32:N5:365:ALA:HB3	1.91	0.52
35:S2:140:PRO:HB2	40:S7:142:TYR:CE2	2.45	0.52
36:S3:101:ARG:HE	36:S3:159:VAL:HG13	1.75	0.52
7:A7:14:TRP:O	14:AN:28:ARG:NH1	2.43	0.51
14:AN:141:ILE:HA	46:AN:202:PC1:H141	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:S1:331:GLN:NE2	34:S1:630:ALA:O	2.40	0.51
48:N3:203:PEE:H61	48:N3:203:PEE:H71	1.91	0.51
34:S1:219:SER:O	34:S1:222:ILE:HG12	2.09	0.51
9:A9:173:ASP:HB3	9:A9:176:SER:HB2	1.91	0.51
12:AL:3:LYS:NZ	45:AL:203:CDL:OA4	2.42	0.51
32:N5:341:MET:HE2	32:N5:457:LEU:HD12	1.92	0.51
40:S7:44:GLU:OE2	40:S7:195:ARG:NH1	2.42	0.51
42:V1:112:TYR:HB2	42:V1:240:THR:HG22	1.91	0.51
9:A9:293:LEU:HD12	9:A9:294:PRO:HD2	1.93	0.51
52:CB:202:3PE:H362	52:CB:202:3PE:H222	1.92	0.51
34:S1:69:LEU:O	37:S4:158:LYS:NZ	2.32	0.51
34:S1:251:ILE:HD13	34:S1:604:GLN:HB2	1.91	0.51
42:V1:65:THR:O	42:V1:69:LEU:HG	2.10	0.51
11:AK:51:THR:HG21	11:AK:153:LEU:HD22	1.93	0.51
31:N4:403:THR:HA	31:N4:406:TYR:CE2	2.46	0.51
11:AK:110:LEU:HD23	11:AK:329:VAL:HG13	1.93	0.51
28:N1:89:LEU:HD22	28:N1:240:ILE:HD12	1.93	0.51
28:N1:173:TRP:HE1	46:N1:403:PC1:H121	1.75	0.51
34:S1:266:ARG:HD2	34:S1:267:THR:HG23	1.92	0.51
35:S2:194:THR:HB	35:S2:206:PHE:HA	1.93	0.51
24:BK:107:GLN:HE22	32:N5:194:ASN:HD22	1.57	0.51
35:S2:227:ARG:NH1	40:S7:75:GLU:OE1	2.43	0.51
42:V1:295:PRO:HG2	42:V1:298:GLU:HB3	1.92	0.51
5:A5:59:VAL:HG23	5:A5:68:LEU:HD21	1.93	0.51
51:N4:503:PLX:H81	51:N4:503:PLX:H312	1.92	0.51
35:S2:112:VAL:HG21	35:S2:453:VAL:HG21	1.92	0.51
45:4L:201:CDL:OB9	33:N6:23:LYS:NZ	2.44	0.51
28:N1:18:ALA:HB2	53:N1:405:U10:H38	1.93	0.51
31:N4:416:ARG:HG2	32:N5:159:HIS:HB3	1.91	0.51
32:N5:346:ILE:HD11	32:N5:431:PHE:CZ	2.46	0.51
21:B7:92:HIS:O	21:B7:96:VAL:HG13	2.11	0.51
34:S1:556:THR:HG23	34:S1:558:GLN:HG2	1.92	0.50
42:V1:113:LEU:O	42:V1:154:ALA:HA	2.10	0.50
42:V1:256:ARG:HG3	43:V2:245:VAL:HG23	1.92	0.50
28:N1:173:TRP:HB3	28:N1:175:ILE:HG22	1.93	0.50
34:S1:667:GLN:OE1	34:S1:667:GLN:N	2.41	0.50
40:S7:62:LEU:O	40:S7:91:VAL:HA	2.11	0.50
19:B5:133:TYR:OH	24:BK:87:GLU:OE1	2.18	0.50
28:N1:310:MET:HG3	28:N1:311:THR:HG23	1.92	0.50
32:N5:248:HIS:O	32:N5:253:VAL:HG22	2.11	0.50
36:S3:147:THR:HB	36:S3:153:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:A1:101:CDL:H131	13:AM:3:LEU:HD11	1.94	0.50
4:A3:139:PRO:HD3	14:AN:69:ILE:HD13	1.93	0.50
5:A5:45:ARG:O	5:A5:49:GLU:HB2	2.11	0.50
30:N3:65:PHE:O	30:N3:69:ILE:HG23	2.12	0.50
30:N3:104:TYR:HB2	48:N3:203:PEE:H57	1.92	0.50
31:N4:201:MET:HE1	31:N4:212:LEU:HD11	1.94	0.50
13:AM:6:VAL:HG22	13:AM:9:ARG:HH21	1.76	0.50
31:N4:207:MET:HE3	31:N4:294:MET:HE3	1.93	0.50
36:S3:190:ASP:OD1	36:S3:191:TYR:N	2.45	0.50
1:4L:98:CYS:HB3	32:N5:580:GLN:HB2	1.93	0.50
11:AK:152:LEU:HD12	11:AK:158:GLY:HA2	1.94	0.50
22:B8:110:ASP:HB3	31:N4:278:ARG:NH1	2.27	0.50
28:N1:197:PRO:HB2	28:N1:280:PHE:HD1	1.77	0.50
31:N4:369:LEU:HD23	45:N4:507:CDL:H371	1.93	0.50
20:B6:186:GLN:HG3	21:B7:89:TYR:HE2	1.75	0.50
31:N4:281:ASP:OD1	31:N4:340:ARG:HB3	2.12	0.50
42:V1:326:LEU:HD22	42:V1:363:ILE:HD11	1.94	0.50
46:A3:201:PC1:H3B2	14:AN:40:ILE:HG21	1.93	0.50
26:CA:43:LYS:O	26:CA:47:THR:OG1	2.28	0.50
31:N4:79:ALA:O	31:N4:82:SER:HB3	2.11	0.50
31:N4:260:PRO:HA	52:N4:506:3PE:H342	1.93	0.50
34:S1:600:GLU:OE2	34:S1:602:ARG:NH2	2.36	0.50
6:A6:78:LEU:HD23	6:A6:126:ARG:HD3	1.94	0.49
35:S2:155:GLN:NE2	35:S2:315:ASP:OD2	2.38	0.49
6:A6:127:THR:HG23	36:S3:219:VAL:O	2.12	0.49
27:CB:13:LEU:HD21	38:S5:4:PHE:HB3	1.94	0.49
39:S6:39:THR:HG22	39:S6:62:VAL:HG22	1.93	0.49
48:B6:201:PEE:H12	48:B6:201:PEE:H2	1.93	0.49
29:N2:112:HIS:O	29:N2:116:PRO:HD2	2.12	0.49
34:S1:389:THR:HG21	34:S1:473:MET:HE2	1.93	0.49
35:S2:53:PHE:CD1	35:S2:58:MET:HE1	2.47	0.49
42:V1:113:LEU:HD13	42:V1:149:MET:HE1	1.95	0.49
27:CB:35:TYR:OH	29:N2:335:LEU:O	2.28	0.49
32:N5:402:SER:HB2	32:N5:404:THR:HG23	1.94	0.49
40:S7:84:TYR:CE1	40:S7:171:GLU:HG3	2.48	0.49
10:AB:116:VAL:HG12	10:AB:120:MET:HE2	1.95	0.49
19:B5:76:LEU:HD21	45:N4:507:CDL:H581	1.94	0.49
37:S4:84:ARG:NH1	37:S4:88:GLN:O	2.45	0.49
1:4L:75:LEU:O	1:4L:79:VAL:HG13	2.13	0.49
29:N2:211:MET:HG2	29:N2:333:SER:HB2	1.93	0.49
45:N4:505:CDL:H191	45:N4:505:CDL:H422	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AC:201:ZMP:H1	23:B9:113:PHE:HA	1.95	0.49
34:S1:306:MET:HE2	34:S1:314:LEU:HB3	1.95	0.49
11:AK:357:LYS:HD3	26:CA:36:HIS:O	2.12	0.49
31:N4:408:LEU:HD12	32:N5:172:ILE:HG21	1.94	0.49
32:N5:37:LYS:HD3	32:N5:105:MET:HE1	1.94	0.49
42:V1:423:THR:HB	54:V1:501:SF4:S2	2.52	0.49
31:N4:445:LEU:HD22	45:N4:507:CDL:H401	1.95	0.49
40:S7:108:THR:HA	40:S7:136:CYS:HB3	1.94	0.49
34:S1:130:ILE:HG23	41:S8:114:ILE:HD12	1.95	0.49
42:V1:214:GLU:OE2	42:V1:224:ARG:NE	2.45	0.49
45:A8:301:CDL:H542	45:A8:301:CDL:H182	1.95	0.48
46:AN:202:PC1:H3H2	30:N3:4:MET:HB3	1.94	0.48
27:CB:106:LYS:NZ	27:CB:107:ASP:OD1	2.29	0.48
41:S8:100:GLU:O	41:S8:170:GLY:N	2.41	0.48
13:AM:107:LYS:HE2	39:S6:70:LEU:HD22	1.93	0.48
24:BK:2:PRO:O	24:BK:7:LYS:NZ	2.42	0.48
35:S2:418:VAL:HB	35:S2:427:ARG:HB3	1.94	0.48
42:V1:375:LYS:NZ	42:V1:390:ASP:OD1	2.46	0.48
10:AB:104:PHE:HD1	10:AB:108:LEU:HD12	1.78	0.48
28:N1:68:ILE:HG21	45:N1:401:CDL:HA31	1.95	0.48
31:N4:216:LEU:HB3	31:N4:217:PRO:HD3	1.94	0.48
34:S1:224:ASP:OD2	34:S1:291:ARG:NH2	2.45	0.48
9:A9:171:ASN:HA	9:A9:327:MET:HE2	1.95	0.48
33:N6:51:PHE:CZ	33:N6:55:MET:HE3	2.48	0.48
9:A9:64:PHE:O	9:A9:67:ARG:HG2	2.13	0.48
24:BK:107:GLN:HE22	32:N5:194:ASN:ND2	2.11	0.48
35:S2:140:PRO:HB2	40:S7:142:TYR:HE2	1.78	0.48
5:A5:48:THR:HA	5:A5:51:ILE:HG12	1.96	0.48
19:B5:53:ARG:NH2	20:B6:89:SER:O	2.47	0.48
32:N5:65:ASN:HD21	32:N5:78:LEU:HD23	1.78	0.48
35:S2:230:ALA:O	41:S8:98:ARG:NH2	2.47	0.48
38:S5:24:GLU:OE1	38:S5:28:LYS:NZ	2.44	0.48
12:AL:117:TYR:HB3	48:AL:204:PEE:H29	1.94	0.48
28:N1:296:LEU:HD13	48:N1:406:PEE:H19	1.96	0.48
31:N4:12:LEU:HB2	31:N4:13:PRO:HD3	1.95	0.48
31:N4:260:PRO:HG3	52:N4:506:3PE:H241	1.94	0.48
35:S2:405:ALA:HB1	35:S2:412:GLU:HG3	1.96	0.48
36:S3:61:PHE:HZ	36:S3:106:ALA:HB2	1.78	0.48
43:V2:137:THR:HG22	43:V2:138:THR:H	1.78	0.48
14:AN:43:LEU:HG	28:N1:179:TRP:HE1	1.79	0.48
28:N1:25:ARG:NH2	40:S7:87:ASP:OD1	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:N1:114:TYR:OH	33:N6:61:LEU:O	2.31	0.48
34:S1:217:GLU:HG3	34:S1:412:PRO:HB3	1.94	0.48
34:S1:357:LEU:HD13	34:S1:627:SER:HB3	1.96	0.48
36:S3:114:LEU:HB3	36:S3:166:TYR:HB3	1.94	0.48
42:V1:296:LEU:HD21	42:V1:317:VAL:HG11	1.95	0.48
11:AK:355:TRP:CE3	11:AK:356:LEU:HG	2.49	0.48
4:A3:161:PRO:HD2	8:A8:204:LYS:HG2	1.96	0.48
20:B6:148:TYR:CE1	24:BK:49:ARG:HG2	2.49	0.48
28:N1:309:ILE:HD11	30:N3:87:MET:HE1	1.94	0.48
31:N4:221:VAL:HA	31:N4:283:LYS:HD3	1.95	0.48
34:S1:185:PHE:CZ	34:S1:221:ASN:HB2	2.48	0.48
36:S3:231:ARG:NH2	41:S8:128:ILE:O	2.47	0.48
42:V1:118:ASP:HA	42:V1:159:ARG:HB3	1.96	0.48
43:V2:207:GLU:HB2	43:V2:214:PRO:HG3	1.95	0.48
9:A9:180:TYR:O	9:A9:184:LYS:HG2	2.13	0.47
28:N1:224:PHE:CE2	53:N1:405:U10:H262	2.49	0.47
36:S3:211:ARG:NH2	36:S3:222:GLU:OE2	2.47	0.47
5:A5:104:VAL:HG23	36:S3:71:LYS:HG2	1.95	0.47
31:N4:398:MET:HG2	48:N5:703:PEE:H78	1.96	0.47
32:N5:233:LEU:HB3	32:N5:234:PRO:HD3	1.95	0.47
35:S2:147:TYR:CB	40:S7:71:CYS:HB3	2.44	0.47
42:V1:118:ASP:HB3	42:V1:207:GLY:HA2	1.96	0.47
10:AC:119:ILE:HG21	10:AC:135:ALA:HB1	1.95	0.47
34:S1:127:ASP:O	34:S1:131:CYS:HB2	2.13	0.47
39:S6:108:THR:HG22	39:S6:119:ARG:HD3	1.95	0.47
41:S8:205:ILE:O	41:S8:209:TYR:HB3	2.14	0.47
42:V1:326:LEU:HD23	42:V1:367:ILE:HD11	1.97	0.47
4:A3:164:GLU:O	4:A3:168:ASN:ND2	2.47	0.47
6:A6:90:ARG:NH2	10:AB:114:ASP:OD1	2.35	0.47
45:AL:201:CDL:H372	48:AL:204:PEE:H28	1.96	0.47
51:CB:201:PLX:H331	51:CB:201:PLX:H361	1.72	0.47
21:B7:29:TYR:OH	21:B7:111:ARG:NH2	2.47	0.47
22:B8:162:PRO:HB2	22:B8:163:TYR:CD2	2.50	0.47
27:CB:2:THR:O	27:CB:2:THR:OG1	2.31	0.47
31:N4:122:PHE:CE1	31:N4:206:LYS:HG3	2.49	0.47
33:N6:77:GLU:N	33:N6:77:GLU:OE1	2.48	0.47
11:AK:99:THR:O	26:CA:32:ARG:NH1	2.48	0.47
48:B4:201:PEE:H32	48:B4:201:PEE:H26	1.46	0.47
35:S2:214:GLU:OE2	35:S2:227:ARG:NH2	2.47	0.47
10:AC:117:GLU:OE2	23:B9:62:TYR:OH	2.32	0.47
10:AC:156:GLU:OE2	20:B6:84:LYS:NZ	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:88:ARG:HG3	13:AM:93:MET:HB2	1.97	0.47
15:B1:17:VAL:HG13	31:N4:7:PRO:HB3	1.96	0.47
28:N1:58:LYS:NZ	40:S7:100:SER:O	2.47	0.47
29:N2:1:MET:HE3	29:N2:6:TYR:HD1	1.79	0.47
48:N3:201:PEE:H30	48:N3:201:PEE:H36	1.60	0.47
51:N4:503:PLX:H122	52:N4:506:3PE:H362	1.96	0.47
34:S1:47:THR:O	34:S1:96:VAL:HG22	2.14	0.47
34:S1:696:MET:HG2	34:S1:711:VAL:HG21	1.96	0.47
35:S2:190:ILE:HG21	35:S2:213:ARG:HG3	1.97	0.47
42:V1:141:GLY:HA2	42:V1:252:PRO:HD3	1.97	0.47
42:V1:347:THR:HG22	42:V1:348:GLY:H	1.80	0.47
20:B6:97:PRO:O	20:B6:98:ARG:NE	2.36	0.47
29:N2:154:MET:HE2	29:N2:191:THR:HB	1.97	0.47
39:S6:61:GLU:OE2	41:S8:192:ASN:ND2	2.36	0.47
1:4L:4:VAL:O	1:4L:8:ILE:HG12	2.14	0.47
8:A8:196:ARG:NH2	14:AN:63:GLU:OE2	2.47	0.47
9:A9:346:GLU:HG2	9:A9:371:PRO:HB3	1.97	0.47
24:BK:74:ILE:HG23	24:BK:156:LEU:HD22	1.97	0.47
32:N5:327:LEU:O	32:N5:331:MET:HG2	2.14	0.47
36:S3:89:HIS:CG	36:S3:90:PRO:HD2	2.50	0.47
37:S4:133:ASP:N	37:S4:133:ASP:OD1	2.47	0.47
3:A2:89:ARG:O	3:A2:92:GLU:HG2	2.15	0.47
12:AL:37:SER:O	12:AL:41:ILE:HG12	2.15	0.47
20:B6:135:VAL:HG13	32:N5:46:LEU:HD11	1.96	0.47
26:CA:70:LYS:HD3	26:CA:76:GLU:HB2	1.96	0.47
28:N1:15:LEU:HD11	53:N1:405:U10:H511	1.97	0.47
35:S2:341:GLU:HG2	41:S8:39:LYS:HD2	1.97	0.47
35:S2:464:PHE:HA	35:S2:467:VAL:HB	1.97	0.47
42:V1:112:TYR:O	42:V1:240:THR:HA	2.15	0.47
44:V3:386:TYR:CZ	44:V3:388:ASN:HB3	2.49	0.47
27:CB:4:MET:HE1	27:CB:87:LEU:HB3	1.96	0.46
29:N2:167:TRP:HB3	32:N5:574:SER:HA	1.97	0.46
32:N5:15:LEU:HD11	32:N5:94:LEU:HD21	1.97	0.46
42:V1:67:GLU:OE1	42:V1:67:GLU:N	2.48	0.46
42:V1:129:GLU:OE2	42:V1:132:ARG:NH2	2.49	0.46
5:A5:22:GLU:OE1	5:A5:22:GLU:N	2.38	0.46
34:S1:124:HIS:CG	34:S1:125:PRO:HD2	2.51	0.46
34:S1:145:MET:HE3	36:S3:241:ALA:HB2	1.96	0.46
35:S2:160:ALA:HA	35:S2:404:THR:HG21	1.97	0.46
8:A8:107:HIS:HB3	8:A8:197:PRO:HD2	1.97	0.46
21:B7:22:MET:HE1	21:B7:102:PHE:CD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:N4:505:CDL:H401	45:N4:505:CDL:H261	1.98	0.46
35:S2:98:HIS:HB2	35:S2:464:PHE:HE2	1.81	0.46
42:V1:115:VAL:HG21	42:V1:142:CYS:SG	2.56	0.46
29:N2:250:SER:O	29:N2:259:GLY:HA3	2.16	0.46
32:N5:297:ASP:O	32:N5:301:ILE:HG13	2.16	0.46
34:S1:395:GLU:OE2	34:S1:417:ARG:NH1	2.46	0.46
40:S7:108:THR:OG1	40:S7:136:CYS:SG	2.68	0.46
43:V2:67:VAL:HG13	43:V2:75:LYS:HG3	1.97	0.46
9:A9:279:TYR:HB2	9:A9:372:ALA:HB2	1.98	0.46
11:AK:42:PRO:HB2	45:N2:401:CDL:HB61	1.97	0.46
21:B7:22:MET:HE1	21:B7:102:PHE:HD2	1.81	0.46
32:N5:562:LEU:HB2	32:N5:563:PRO:HD3	1.96	0.46
34:S1:556:THR:OG1	34:S1:557:ARG:N	2.48	0.46
39:S6:104:LYS:HE3	39:S6:107:LYS:HD3	1.96	0.46
1:4L:55:LEU:HD13	38:S5:17:TRP:HE3	1.80	0.46
2:A1:19:PRO:HB3	28:N1:9:LEU:HD12	1.97	0.46
10:AC:140:CYS:HB3	10:AC:143:GLU:HG3	1.98	0.46
45:N4:505:CDL:H442	45:N4:505:CDL:H831	1.97	0.46
33:N6:82:VAL:HG22	33:N6:83:TRP:H	1.80	0.46
6:A6:51:MET:HE1	6:A6:105:VAL:HG21	1.98	0.46
9:A9:112:ASP:O	9:A9:116:ILE:HG13	2.15	0.46
9:A9:344:PRO:HG2	9:A9:347:LEU:HD13	1.97	0.46
11:AK:297:ARG:HA	11:AK:300:VAL:HG22	1.98	0.46
48:B4:201:PEE:H58	48:B4:201:PEE:H53	1.60	0.46
23:B9:181:GLN:NE2	23:B9:198:PRO:O	2.47	0.46
31:N4:274:SER:O	32:N5:545:SER:HB3	2.15	0.46
9:A9:61:ALA:HB3	9:A9:82:VAL:HG13	1.97	0.46
11:AK:97:ASP:N	11:AK:97:ASP:OD1	2.48	0.46
18:B4:10:ARG:HG3	18:B4:11:LEU:HG	1.97	0.46
20:B6:147:LYS:HE3	20:B6:148:TYR:CZ	2.51	0.46
29:N2:139:LEU:HD13	29:N2:190:MET:HE1	1.97	0.46
31:N4:187:SER:O	31:N4:192:ASN:ND2	2.39	0.46
34:S1:308:ARG:NH1	34:S1:312:GLY:O	2.47	0.46
34:S1:556:THR:HA	34:S1:579:MET:HE1	1.98	0.46
21:B7:107:ARG:HA	21:B7:110:GLN:HG2	1.96	0.46
23:B9:147:ASP:HB3	23:B9:164:ARG:NH1	2.29	0.46
29:N2:270:MET:HE3	29:N2:279:PRO:HG3	1.97	0.46
30:N3:56:PHE:O	33:N6:70:TYR:OH	2.32	0.46
41:S8:47:SER:O	41:S8:56:ARG:NH2	2.49	0.46
41:S8:137:ASP:OD1	41:S8:137:ASP:N	2.45	0.46
4:A3:105:VAL:HA	48:N3:201:PEE:H62	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:N3:68:GLU:HG2	33:N6:161:LEU:HD13	1.98	0.46
9:A9:204:SER:HB2	9:A9:266:VAL:HG12	1.97	0.45
19:B5:58:LYS:HG2	23:B9:221:MET:HE2	1.98	0.45
28:N1:213:VAL:HG13	28:N1:214:GLU:HG2	1.98	0.45
28:N1:301:CYS:O	28:N1:305:ILE:HG13	2.16	0.45
32:N5:375:ILE:HD12	32:N5:458:LEU:HD11	1.97	0.45
34:S1:338:VAL:O	34:S1:365:SER:HB2	2.17	0.45
42:V1:325:PRO:HG3	42:V1:433:TRP:HB3	1.97	0.45
8:A8:202:LEU:HD13	14:AN:70:ALA:HB2	1.98	0.45
14:AN:95:ALA:HA	14:AN:106:VAL:HG11	1.98	0.45
17:B3:18:ASP:O	17:B3:21:GLN:HG2	2.16	0.45
33:N6:129:ASP:HB2	38:S5:32:ARG:NH1	2.31	0.45
34:S1:251:ILE:HG21	34:S1:604:GLN:HB3	1.99	0.45
9:A9:357:ARG:HD3	9:A9:361:TRP:O	2.16	0.45
32:N5:6:SER:O	32:N5:10:THR:OG1	2.22	0.45
33:N6:122:LEU:HG	33:N6:123:GLY:H	1.81	0.45
42:V1:112:TYR:CD1	42:V1:153:ALA:HB3	2.52	0.45
31:N4:76:MET:SD	31:N4:230:VAL:HB	2.57	0.45
42:V1:233:VAL:HG13	42:V1:237:GLY:HA2	1.98	0.45
42:V1:410:ASP:OD1	42:V1:443:ARG:NH2	2.35	0.45
11:AK:340:LYS:O	27:CB:52:ARG:NH2	2.50	0.45
28:N1:169:GLN:NE2	28:N1:240:ILE:O	2.44	0.45
28:N1:277:TYR:HE2	48:N1:406:PEE:H62	1.81	0.45
31:N4:207:MET:HG2	31:N4:298:ILE:CG1	2.46	0.45
32:N5:486:MET:HE3	32:N5:486:MET:HB2	1.83	0.45
34:S1:296:GLY:O	34:S1:572:HIS:NE2	2.40	0.45
35:S2:203:MET:O	35:S2:206:PHE:HB3	2.16	0.45
35:S2:430:ILE:HB	35:S2:469:ARG:HD2	1.98	0.45
4:A3:160:GLY:HA3	8:A8:204:LYS:HE3	1.98	0.45
8:A8:157:GLU:HB2	8:A8:158:PRO:HD3	1.97	0.45
45:B4:202:CDL:HB32	45:B4:202:CDL:H1	1.98	0.45
20:B6:186:GLN:O	20:B6:187:HIS:ND1	2.49	0.45
28:N1:205:SER:HB2	28:N1:279:ARG:HH12	1.81	0.45
29:N2:168:GLY:O	29:N2:172:GLN:HG2	2.16	0.45
35:S2:283:VAL:HG22	35:S2:331:ASP:HB3	1.97	0.45
37:S4:112:MET:HG3	41:S8:184:LEU:HD23	1.99	0.45
1:4L:2:PRO:HG3	33:N6:127:ILE:HD13	1.99	0.45
45:AL:201:CDL:H532	32:N5:577:VAL:HA	1.99	0.45
33:N6:113:VAL:HG13	33:N6:118:LYS:HG2	1.98	0.45
40:S7:107:GLY:HA2	54:S7:301:SF4:S4	2.57	0.45
45:AL:201:CDL:H151	45:AL:201:CDL:H362	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:B5:201:PLX:H391	25:BL:97:ILE:HG13	1.98	0.45
29:N2:270:MET:HE1	29:N2:282:MET:SD	2.56	0.45
48:N3:201:PEE:H27	48:N3:201:PEE:H22	1.50	0.45
32:N5:8:THR:HB	32:N5:82:MET:HE3	1.99	0.45
32:N5:136:ASN:ND2	32:N5:139:GLN:H	2.15	0.45
34:S1:382:ARG:C	34:S1:384:ASN:H	2.25	0.45
35:S2:140:PRO:HA	35:S2:143:ASP:HB2	1.99	0.45
49:AC:201:ZMP:H5A	23:B9:109:ALA:HB1	1.97	0.45
45:B5:202:CDL:H672	32:N5:130:ILE:HG13	1.99	0.45
22:B8:110:ASP:HB3	31:N4:278:ARG:HH11	1.82	0.45
28:N1:91:MET:HE3	28:N1:259:PHE:HE2	1.82	0.45
51:N4:503:PLX:H142	52:N4:506:3PE:H272	1.99	0.45
32:N5:293:ILE:HD11	45:N5:702:CDL:H721	1.99	0.45
34:S1:542:PRO:HD2	34:S1:560:LEU:HD12	1.99	0.45
40:S7:69:LEU:HB2	40:S7:107:GLY:HA3	1.99	0.45
9:A9:49:SER:HB2	36:S3:225:GLU:HG2	1.98	0.45
20:B6:170:ILE:HB	20:B6:175:GLU:HB3	1.99	0.45
34:S1:401:LEU:HD11	34:S1:432:ILE:HG13	1.98	0.45
34:S1:594:ALA:O	34:S1:605:GLN:HA	2.17	0.45
8:A8:249:MET:HE2	45:A8:301:CDL:HA32	1.97	0.44
9:A9:310:PHE:CE2	46:A9:403:PC1:H11	2.53	0.44
51:AM:201:PLX:H1C2	51:S7:302:PLX:H252	2.00	0.44
19:B5:59:PRO:HD3	23:B9:141:VAL:HG11	2.00	0.44
48:N1:404:PEE:H48	48:N1:404:PEE:H55	1.54	0.44
33:N6:39:VAL:O	33:N6:43:ILE:HG13	2.17	0.44
34:S1:251:ILE:HD11	34:S1:596:TYR:HB2	1.99	0.44
1:4L:76:SER:O	1:4L:79:VAL:HG22	2.17	0.44
5:A5:99:PRO:O	36:S3:70:PRO:HD2	2.17	0.44
8:A8:134:LEU:O	8:A8:138:LYS:HG2	2.17	0.44
9:A9:262:THR:O	9:A9:333:PRO:HD2	2.17	0.44
14:AN:19:ILE:HD12	35:S2:351:SER:HB2	1.98	0.44
51:B5:201:PLX:H212	46:B5:203:PC1:H272	1.99	0.44
25:BL:89:VAL:HG21	31:N4:25:ILE:HG23	2.00	0.44
28:N1:87:VAL:HG22	28:N1:88:PRO:HD3	1.99	0.44
31:N4:31:SER:HB3	31:N4:74:PRO:HD3	1.99	0.44
31:N4:445:LEU:HB3	45:N4:507:CDL:H452	1.98	0.44
40:S7:67:PHE:CE2	40:S7:117:LEU:HD12	2.52	0.44
11:AK:232:THR:HG23	11:AK:235:TYR:H	1.83	0.44
48:N4:501:PEE:H26	48:N4:501:PEE:H19	1.64	0.44
48:N4:501:PEE:H35	48:N4:501:PEE:H30	1.61	0.44
32:N5:213:LEU:HD23	32:N5:213:LEU:HA	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:N5:559:GLU:O	32:N5:564:LYS:HB2	2.17	0.44
34:S1:339:ALA:HA	34:S1:365:SER:HB2	2.00	0.44
34:S1:575:VAL:C	34:S1:578:PRO:HD2	2.42	0.44
35:S2:194:THR:HG21	35:S2:209:MET:HB2	1.98	0.44
6:A6:88:LYS:HD2	6:A6:92:MET:HE2	2.00	0.44
16:B2:56:PRO:HB3	32:N5:442:LEU:HD23	1.99	0.44
51:B5:201:PLX:H351	51:B5:201:PLX:H381	1.52	0.44
45:B5:202:CDL:H832	51:N4:504:PLX:H131	1.99	0.44
29:N2:137:ALA:HB3	29:N2:138:PRO:HD3	2.00	0.44
51:N4:503:PLX:H1A3	51:N4:503:PLX:H21	1.80	0.44
32:N5:292:ALA:HB2	32:N5:304:PHE:HB3	1.98	0.44
32:N5:298:ILE:O	32:N5:302:VAL:HG23	2.16	0.44
35:S2:167:ILE:HD13	35:S2:369:VAL:HG11	2.00	0.44
1:4L:44:SER:OG	1:4L:59:MET:SD	2.69	0.44
10:AB:93:ILE:HD11	10:AB:110:LEU:HD11	1.99	0.44
11:AK:355:TRP:H	11:AK:355:TRP:CD1	2.35	0.44
22:B8:96:ASP:OD1	22:B8:96:ASP:N	2.47	0.44
24:BK:171:LYS:NZ	24:BK:172:GLU:OE2	2.51	0.44
30:N3:68:GLU:HG3	30:N3:98:LEU:HD13	2.00	0.44
48:N3:203:PEE:H20	48:N3:203:PEE:H14	1.74	0.44
48:N3:203:PEE:H49	48:N3:203:PEE:H7	1.77	0.44
32:N5:419:THR:HA	32:N5:422:TYR:CE2	2.52	0.44
46:N5:701:PC1:H291	46:N5:701:PC1:H2F1	1.99	0.44
33:N6:124:ASP:O	33:N6:127:ILE:HG12	2.17	0.44
1:4L:55:LEU:HD23	1:4L:55:LEU:HA	1.80	0.44
7:A7:14:TRP:HE1	46:N1:402:PC1:H133	1.81	0.44
7:A7:54:TYR:CZ	35:S2:368:LYS:HD2	2.52	0.44
8:A8:146:ASP:OD1	8:A8:149:ARG:NH2	2.51	0.44
9:A9:129:LEU:HD23	9:A9:167:ILE:HG13	1.99	0.44
16:B2:57:ARG:NH1	16:B2:61:PHE:O	2.50	0.44
48:B4:201:PEE:H22	48:B4:201:PEE:H27	1.44	0.44
48:B4:201:PEE:H73	48:B4:201:PEE:H78	1.73	0.44
48:N3:201:PEE:H44	48:N3:203:PEE:H27	2.00	0.44
31:N4:33:LEU:HD13	48:N4:501:PEE:H70	2.00	0.44
35:S2:164:LEU:HD12	35:S2:417:LEU:HD23	1.98	0.44
35:S2:374:ARG:NH1	41:S8:162:CYS:O	2.47	0.44
11:AK:131:TYR:OH	11:AK:188:HIS:ND1	2.33	0.44
14:AN:57:ARG:HB3	28:N1:316:PRO:HG3	1.99	0.44
28:N1:123:SER:HB3	28:N1:214:GLU:HG3	2.00	0.44
31:N4:398:MET:O	31:N4:402:ILE:HG13	2.17	0.44
40:S7:66:THR:HG22	40:S7:93:PHE:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:V2:130:TYR:HA	43:V2:189:ASN:HD21	1.82	0.44
10:AC:103:HIS:N	10:AC:107:ASP:OD1	2.50	0.44
14:AN:122:GLY:HA3	33:N6:126:VAL:HG13	1.99	0.44
22:B8:83:GLN:HA	22:B8:86:ARG:HG3	2.00	0.44
28:N1:198:PHE:CD1	28:N1:285:LEU:HD13	2.53	0.44
29:N2:186:HIS:O	29:N2:190:MET:HG3	2.18	0.44
46:N5:701:PC1:H3A1	46:N5:701:PC1:H32	1.99	0.44
34:S1:150:ARG:NH1	35:S2:365:ASP:OD1	2.50	0.44
35:S2:149:SER:HA	35:S2:184:THR:HG22	1.98	0.44
41:S8:115:ALA:HB2	41:S8:142:THR:HG23	2.00	0.44
7:A7:23:LYS:HG3	35:S2:259:PHE:CD1	2.53	0.44
45:B5:202:CDL:HB62	51:N4:504:PLX:H21	2.00	0.44
20:B6:144:TYR:OH	24:BK:49:ARG:NH1	2.46	0.44
32:N5:289:ALA:O	32:N5:293:ILE:HG23	2.17	0.44
34:S1:55:LYS:HE2	34:S1:55:LYS:HB2	1.81	0.44
34:S1:76:ARG:O	34:S1:116:VAL:HG21	2.18	0.44
40:S7:49:LYS:HE3	51:S7:302:PLX:H302	2.00	0.44
3:A2:19:ILE:HD13	3:A2:91:LEU:HD11	1.99	0.43
8:A8:95:VAL:HG12	8:A8:97:VAL:HG22	2.00	0.43
23:B9:146:LEU:HD21	23:B9:160:TYR:HE2	1.82	0.43
25:BL:117:TRP:CZ2	25:BL:121:GLU:HG3	2.53	0.43
51:CB:201:PLX:H111	51:CB:201:PLX:H81	1.71	0.43
51:CB:201:PLX:H1A2	38:S5:2:PRO:HD2	1.99	0.43
28:N1:14:LEU:HB3	53:N1:405:U10:H412	2.00	0.43
48:N1:406:PEE:H55	48:N1:406:PEE:H60	1.52	0.43
34:S1:198:THR:HG21	34:S1:209:TYR:HB2	2.00	0.43
34:S1:260:ASN:HD21	34:S1:278:HIS:HD2	1.65	0.43
38:S5:15:ASP:OD1	38:S5:15:ASP:N	2.50	0.43
4:A3:155:PRO:O	8:A8:204:LYS:NZ	2.37	0.43
9:A9:168:SER:O	9:A9:203:PRO:HD2	2.18	0.43
28:N1:197:PRO:HB3	28:N1:278:PRO:O	2.18	0.43
34:S1:591:GLU:HG2	34:S1:610:VAL:HG23	1.99	0.43
51:B5:201:PLX:H1A3	51:B5:201:PLX:H22	1.65	0.43
35:S2:188:ASN:OD1	35:S2:410:LYS:NZ	2.50	0.43
8:A8:117:ASN:HB3	14:AN:73:PRO:HG2	2.01	0.43
19:B5:110:TRP:O	19:B5:119:ARG:HG2	2.18	0.43
22:B8:166:LEU:HB3	22:B8:169:GLU:HB2	1.99	0.43
27:CB:15:PHE:HB2	51:CB:201:PLX:H72	1.99	0.43
31:N4:328:CYS:O	31:N4:332:THR:HG23	2.19	0.43
42:V1:99:TRP:N	42:V1:99:TRP:CD1	2.85	0.43
43:V2:93:LEU:HD12	43:V2:122:TYR:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AB:141:PRO:HA	10:AB:144:ILE:HD12	2.01	0.43
11:AK:112:GLY:HA2	11:AK:136:TRP:CD2	2.53	0.43
28:N1:162:LEU:O	28:N1:165:LEU:HB2	2.17	0.43
28:N1:281:ARG:NH1	35:S2:452:ASP:OD1	2.51	0.43
48:N4:502:PEE:H67	48:N4:502:PEE:H28	2.00	0.43
37:S4:70:GLU:O	37:S4:74:THR:OG1	2.30	0.43
42:V1:315:LEU:HB2	42:V1:359:ARG:HA	1.99	0.43
7:A7:42:PRO:HG3	14:AN:6:VAL:HG11	2.01	0.43
28:N1:233:MET:HE3	28:N1:233:MET:HB3	1.82	0.43
31:N4:382:ILE:HG12	31:N4:396:MET:HG2	2.00	0.43
43:V2:66:ILE:HG21	43:V2:81:PRO:HB2	2.00	0.43
31:N4:168:GLN:HB2	31:N4:174:LEU:HG	2.01	0.43
45:N4:505:CDL:H772	45:N4:505:CDL:H801	1.84	0.43
32:N5:7:LEU:O	32:N5:11:THR:HG23	2.19	0.43
39:S6:84:ILE:HD12	39:S6:84:ILE:HA	1.81	0.43
11:AK:241:ASN:HB3	11:AK:245:LYS:HE2	1.99	0.43
18:B4:77:TYR:CZ	32:N5:564:LYS:HG2	2.54	0.43
28:N1:142:TYR:CD1	28:N1:142:TYR:C	2.95	0.43
53:N1:405:U10:H222	40:S7:92:VAL:HG11	2.01	0.43
51:N4:504:PLX:H362	51:N4:504:PLX:H392	1.81	0.43
34:S1:140:GLN:HG2	35:S2:385:ILE:HG23	1.99	0.43
35:S2:228:MET:SD	40:S7:167:PRO:HG3	2.58	0.43
1:4L:5:TYR:HB3	1:4L:43:MET:HE1	2.00	0.43
1:4L:34:GLU:O	33:N6:60:TYR:OH	2.27	0.43
3:A2:71:PHE:CE1	34:S1:362:ASP:HB2	2.53	0.43
7:A7:31:ILE:H	7:A7:31:ILE:HG13	1.61	0.43
11:AK:111:SER:OG	29:N2:316:GLN:NE2	2.51	0.43
48:AL:204:PEE:H58	48:AL:204:PEE:H53	1.68	0.43
51:B5:201:PLX:H182	25:BL:104:THR:HG23	2.00	0.43
45:N4:507:CDL:H642	45:N4:507:CDL:H602	2.01	0.43
32:N5:395:ILE:O	32:N5:399:VAL:HG23	2.19	0.43
33:N6:24:PRO:HG3	33:N6:83:TRP:CE2	2.54	0.43
42:V1:208:GLU:O	42:V1:212:LEU:HB2	2.19	0.43
4:A3:117:LEU:HD22	48:AN:201:PEE:H62	2.01	0.43
11:AK:148:ALA:HB1	11:AK:159:VAL:HG21	2.01	0.43
11:AK:328:ARG:HH21	25:BL:58:ASP:CG	2.26	0.43
29:N2:235:ASN:O	29:N2:315:TRP:NE1	2.52	0.43
31:N4:205:VAL:HG21	48:N4:502:PEE:H42	2.00	0.43
32:N5:304:PHE:CZ	32:N5:526:LEU:HD22	2.54	0.43
34:S1:107:GLU:HG3	34:S1:111:LYS:HZ3	1.84	0.43
34:S1:180:THR:N	54:S1:802:SF4:S4	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:V1:149:MET:HB2	42:V1:149:MET:HE2	1.81	0.43
27:CB:15:PHE:HE1	51:CB:201:PLX:H261	1.84	0.42
28:N1:88:PRO:HG2	28:N1:105:MET:HE2	2.01	0.42
30:N3:33:LYS:O	40:S7:98:ARG:NH1	2.46	0.42
31:N4:118:PHE:O	31:N4:122:PHE:HB3	2.18	0.42
31:N4:278:ARG:HG3	32:N5:545:SER:HB2	2.00	0.42
33:N6:17:PHE:HA	33:N6:20:PHE:CE2	2.53	0.42
35:S2:460:GLN:HB3	35:S2:462:ILE:HD13	2.01	0.42
6:A6:89:VAL:HG22	49:AB:201:ZMP:H2	2.01	0.42
7:A7:25:GLN:O	35:S2:215:LYS:NZ	2.41	0.42
25:BL:110:PRO:HB2	25:BL:112:TYR:CD1	2.54	0.42
28:N1:133:LEU:HD11	33:N6:72:THR:HG21	2.01	0.42
53:N1:405:U10:H121	53:N1:405:U10:H101	1.58	0.42
33:N6:24:PRO:HG2	33:N6:28:TYR:HB2	2.00	0.42
34:S1:299:ARG:NH2	34:S1:300:GLN:HE21	2.17	0.42
8:A8:234:ASP:OD1	8:A8:235:LEU:N	2.52	0.42
9:A9:257:ASP:OD1	9:A9:257:ASP:N	2.52	0.42
48:AN:201:PEE:H67	48:AN:201:PEE:H22	2.01	0.42
34:S1:476:LEU:HD21	34:S1:481:LEU:HD21	2.01	0.42
42:V1:129:GLU:CD	42:V1:132:ARG:HH21	2.28	0.42
3:A2:23:LEU:HD21	3:A2:55:ILE:HG23	2.01	0.42
3:A2:62:GLN:HB3	3:A2:80:ASN:HB2	2.00	0.42
9:A9:83:PRO:HA	9:A9:106:MET:O	2.18	0.42
9:A9:132:ARG:HD3	9:A9:132:ARG:HA	1.66	0.42
11:AK:327:ASP:O	11:AK:331:GLN:HG2	2.19	0.42
15:B1:50:ARG:HB2	15:B1:53:GLU:HG2	2.01	0.42
24:BK:99:ASP:OD2	24:BK:142:ARG:NH1	2.53	0.42
27:CB:107:ASP:OD1	27:CB:107:ASP:N	2.52	0.42
32:N5:293:ILE:HG21	32:N5:418:LEU:HD22	2.02	0.42
41:S8:196:LYS:HE3	41:S8:197:TRP:NE1	2.34	0.42
7:A7:54:TYR:CE2	35:S2:368:LYS:HD2	2.55	0.42
46:B5:203:PC1:H281	46:B5:203:PC1:H2C2	2.00	0.42
22:B8:48:ARG:HE	22:B8:48:ARG:HB3	1.70	0.42
23:B9:94:LYS:HE2	23:B9:94:LYS:HB3	1.84	0.42
30:N3:96:ILE:HG23	48:N3:203:PEE:H26	2.02	0.42
31:N4:310:MET:HE1	32:N5:71:LEU:HD12	2.01	0.42
32:N5:63:ILE:O	32:N5:79:SER:HA	2.20	0.42
46:N5:701:PC1:H2F1	46:N5:701:PC1:H2C1	1.69	0.42
48:N5:703:PEE:H46	52:N5:704:3PE:H2A1	2.02	0.42
34:S1:470:LYS:HD2	34:S1:470:LYS:HA	1.79	0.42
42:V1:415:ILE:O	42:V1:419:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:135:PRO:HB2	14:AN:69:ILE:HD11	2.02	0.42
4:A3:138:TYR:CE2	8:A8:121:MET:HG3	2.55	0.42
12:AL:45:PRO:HA	12:AL:46:PRO:HD3	1.92	0.42
45:AL:201:CDL:H241	45:AL:201:CDL:H472	2.01	0.42
14:AN:134:LEU:HD23	14:AN:134:LEU:HA	1.87	0.42
16:B2:76:SER:OG	32:N5:371:THR:OG1	2.26	0.42
24:BK:78:GLU:HA	27:CB:110:THR:HA	2.01	0.42
27:CB:33:LEU:HD23	27:CB:33:LEU:HA	1.85	0.42
28:N1:9:LEU:O	28:N1:13:ILE:HG12	2.19	0.42
28:N1:138:GLN:HG3	28:N1:285:LEU:HD21	2.01	0.42
31:N4:104:LEU:HG	31:N4:108:MET:HE2	2.02	0.42
51:N4:504:PLX:H1A3	51:N4:504:PLX:H22	1.67	0.42
32:N5:435:PRO:HB3	32:N5:437:PHE:CE2	2.54	0.42
35:S2:271:ASN:O	35:S2:275:ARG:HG3	2.18	0.42
42:V1:385:CYS:O	42:V1:389:VAL:HB	2.20	0.42
45:A1:101:CDL:H341	45:A1:101:CDL:H122	2.02	0.42
4:A3:148:MET:O	8:A8:207:LYS:NZ	2.44	0.42
12:AL:122:ALA:HA	45:AL:201:CDL:H452	2.01	0.42
16:B2:65:THR:HB	16:B2:68:GLN:HG2	2.01	0.42
48:N1:406:PEE:H28	48:N1:406:PEE:H33	1.80	0.42
31:N4:266:MET:HB3	31:N4:395:LEU:HD13	2.01	0.42
35:S2:121:LEU:HD23	40:S7:113:MET:SD	2.60	0.42
39:S6:104:LYS:HE2	39:S6:104:LYS:HB2	1.77	0.42
40:S7:130:VAL:HB	40:S7:159:VAL:HA	2.01	0.42
41:S8:150:THR:HG21	41:S8:180:HIS:CD2	2.54	0.42
43:V2:143:ARG:O	43:V2:145:SER:N	2.52	0.42
10:AC:90:TYR:CE1	17:B3:44:PRO:HB2	2.55	0.42
17:B3:24:ILE:O	17:B3:30:GLU:HB3	2.20	0.42
20:B6:72:LEU:HD23	20:B6:72:LEU:HA	1.85	0.42
20:B6:161:LYS:HG3	21:B7:50:GLN:NE2	2.35	0.42
31:N4:357:THR:O	31:N4:361:VAL:HG23	2.20	0.42
34:S1:408:ARG:HD2	34:S1:439:THR:HG23	2.02	0.42
35:S2:321:GLU:O	35:S2:352:GLN:NE2	2.52	0.42
2:A1:26:ILE:HG23	28:N1:1:MET:HG3	2.01	0.42
5:A5:116:ILE:HD12	5:A5:116:ILE:HA	1.88	0.42
11:AK:68:ILE:O	11:AK:216:ILE:HD12	2.20	0.42
23:B9:143:GLU:O	23:B9:164:ARG:NH2	2.53	0.42
27:CB:85:TYR:CZ	29:N2:344:SER:HB3	2.54	0.42
28:N1:24:GLU:OE1	28:N1:228:TYR:OH	2.14	0.42
11:AK:127:ASP:OD1	11:AK:127:ASP:N	2.52	0.42
20:B6:147:LYS:NZ	24:BK:42:ASP:OD1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:N2:171:ASN:ND2	35:S2:58:MET:O	2.53	0.42
32:N5:457:LEU:HD23	32:N5:457:LEU:HA	1.88	0.42
2:A1:13:ALA:HB2	28:N1:264:LEU:HD11	2.01	0.41
9:A9:223:PHE:CD1	46:A9:403:PC1:H2D1	2.55	0.41
11:AK:283:GLY:O	11:AK:286:PRO:HD2	2.21	0.41
34:S1:484:SER:HB2	34:S1:680:LEU:HD11	2.01	0.41
35:S2:204:THR:N	35:S2:205:PRO:HD2	2.35	0.41
35:S2:246:LEU:O	35:S2:250:ILE:HG13	2.19	0.41
35:S2:283:VAL:HA	35:S2:330:GLY:O	2.20	0.41
1:4L:6:MET:HE3	33:N6:103:MET:HB3	2.02	0.41
15:B1:18:PRO:HG3	48:N4:501:PEE:H71	2.02	0.41
23:B9:178:GLU:OE2	23:B9:209:TRP:NE1	2.52	0.41
28:N1:79:LEU:HD22	28:N1:222:MET:HG2	2.02	0.41
28:N1:113:VAL:CG1	28:N1:139:THR:HG21	2.50	0.41
30:N3:53:MET:HE1	33:N6:70:TYR:CD1	2.54	0.41
32:N5:14:ILE:HD11	32:N5:43:ALA:HA	2.01	0.41
35:S2:137:GLN:O	40:S7:142:TYR:OH	2.39	0.41
22:B8:81:ARG:NH1	22:B8:85:GLU:OE1	2.53	0.41
48:N1:406:PEE:H54	41:S8:66:LEU:HD13	2.02	0.41
45:N4:505:CDL:H422	45:N4:505:CDL:H221	2.03	0.41
32:N5:294:THR:O	32:N5:294:THR:OG1	2.38	0.41
34:S1:59:GLN:HG3	34:S1:62:ARG:HH22	1.85	0.41
35:S2:180:PHE:CZ	35:S2:223:VAL:HG11	2.55	0.41
42:V1:112:TYR:HD1	42:V1:153:ALA:HB3	1.84	0.41
42:V1:202:GLY:N	43:V2:121:MET:HG3	2.36	0.41
4:A3:152:PRO:HG2	8:A8:206:THR:HG22	2.02	0.41
18:B4:44:LYS:HE3	22:B8:93:ASP:OD1	2.21	0.41
32:N5:201:ILE:O	32:N5:205:ASN:ND2	2.41	0.41
34:S1:379:THR:HG21	34:S1:526:LEU:HD22	2.03	0.41
38:S5:74:LYS:HE3	38:S5:74:LYS:HB3	1.90	0.41
1:4L:36:MET:HE3	29:N2:68:MET:HG2	2.03	0.41
1:4L:62:ILE:HG21	29:N2:31:ILE:HD11	2.03	0.41
51:AM:201:PLX:H12	51:S7:302:PLX:H52	2.02	0.41
27:CB:2:THR:HB	27:CB:5:SER:HB3	2.02	0.41
34:S1:338:VAL:HB	34:S1:363:SER:CB	2.50	0.41
39:S6:67:ALA:HB2	41:S8:111:GLU:HG3	2.02	0.41
42:V1:184:LYS:HE2	44:V3:411:MET:HE1	2.01	0.41
43:V2:66:ILE:HD11	44:V3:400:LEU:HD23	2.01	0.41
5:A5:114:TRP:CD2	5:A5:115:PRO:HA	2.55	0.41
6:A6:115:GLU:OE2	49:AB:201:ZMP:H5A	2.20	0.41
10:AC:91:ASP:HB2	17:B3:44:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B4:77:TYR:OH	32:N5:564:LYS:HG2	2.21	0.41
29:N2:159:MET:HG2	29:N2:278:MET:HE1	2.02	0.41
30:N3:97:LEU:HD23	30:N3:97:LEU:HA	1.88	0.41
42:V1:162:PHE:HB3	42:V1:165:GLU:HB2	2.02	0.41
18:B4:85:LYS:HB2	48:B4:201:PEE:H2	2.03	0.41
48:B6:201:PEE:H58	48:B6:201:PEE:H53	1.90	0.41
23:B9:66:LEU:HD23	23:B9:66:LEU:HA	1.87	0.41
25:BL:77:ASP:OD1	25:BL:78:LYS:N	2.53	0.41
32:N5:559:GLU:HG3	32:N5:564:LYS:HD3	2.02	0.41
34:S1:79:LEU:HA	34:S1:89:VAL:O	2.20	0.41
42:V1:375:LYS:HD2	42:V1:393:ASN:ND2	2.35	0.41
20:B6:177:ILE:HA	20:B6:178:PRO:HD3	1.94	0.41
21:B7:15:LYS:HG2	21:B7:113:LYS:HG3	2.03	0.41
24:BK:168:LYS:O	24:BK:172:GLU:HG2	2.21	0.41
28:N1:134:ARG:NH2	35:S2:110:GLU:OE2	2.36	0.41
29:N2:190:MET:HB3	29:N2:190:MET:HE2	1.73	0.41
32:N5:3:PRO:HB2	32:N5:53:MET:HE1	2.03	0.41
32:N5:253:VAL:HG23	32:N5:310:LEU:HD21	2.03	0.41
5:A5:76:GLN:O	5:A5:80:VAL:HG23	2.20	0.41
6:A6:49:ARG:HA	37:S4:53:ILE:HG21	2.03	0.41
6:A6:62:TYR:OH	10:AB:117:GLU:OE2	2.36	0.41
9:A9:163:LYS:NZ	9:A9:253:ILE:O	2.47	0.41
11:AK:134:GLN:HE22	50:AK:401:ADP:HN62	1.68	0.41
11:AK:141:ARG:HH21	50:AK:401:ADP:HN61	1.69	0.41
51:AM:201:PLX:H342	51:AM:201:PLX:H311	1.81	0.41
17:B3:35:LYS:HB3	17:B3:35:LYS:HE2	1.82	0.41
18:B4:118:GLU:OE1	18:B4:120:LYS:HE2	2.20	0.41
48:B4:201:PEE:H23	48:B4:201:PEE:H18	1.64	0.41
26:CA:55:TRP:O	26:CA:59:ILE:HG12	2.21	0.41
46:N3:202:PC1:H222	40:S7:190:LEU:HD22	2.03	0.41
31:N4:267:TRP:O	31:N4:271:MET:HG2	2.21	0.41
32:N5:230:HIS:N	32:N5:231:PRO:HD3	2.36	0.41
46:N5:701:PC1:H2A2	46:N5:701:PC1:H2E2	2.03	0.41
34:S1:422:TRP:HA	34:S1:427:LEU:HB3	2.02	0.41
35:S2:105:MET:HE1	35:S2:450:LEU:HD13	2.03	0.41
36:S3:68:ILE:HG21	36:S3:99:PHE:CE1	2.56	0.41
8:A8:124:ARG:HD2	8:A8:124:ARG:HA	1.85	0.41
9:A9:94:LEU:HA	9:A9:97:MET:HG3	2.03	0.41
11:AK:248:LEU:HD22	11:AK:257:VAL:HG11	2.03	0.41
11:AK:284:PRO:O	11:AK:288:GLN:HG2	2.21	0.41
25:BL:110:PRO:HB2	25:BL:112:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:N2:83:GLN:NE2	38:S5:63:PHE:HE2	2.19	0.41
31:N4:201:MET:HG3	48:N4:502:PEE:H34	2.02	0.41
32:N5:208:CYS:HA	32:N5:209:PRO:HD3	1.84	0.41
33:N6:124:ASP:OD1	33:N6:124:ASP:N	2.54	0.41
35:S2:437:HIS:HB2	35:S2:462:ILE:HD11	2.03	0.41
36:S3:61:PHE:CZ	36:S3:106:ALA:HB2	2.56	0.41
43:V2:108:PRO:HA	43:V2:109:PRO:HD3	1.97	0.41
1:4L:80:MET:HE3	33:N6:172:THR:HA	2.03	0.40
45:4L:201:CDL:H191	32:N5:593:ILE:HD11	2.03	0.40
8:A8:79:PRO:HB2	8:A8:80:GLY:H	1.69	0.40
11:AK:102:ASP:OD1	11:AK:102:ASP:N	2.52	0.40
21:B7:36:GLU:HA	22:B8:184:TYR:HA	2.02	0.40
28:N1:76:ILE:O	28:N1:80:SER:OG	2.36	0.40
29:N2:5:ILE:O	29:N2:8:THR:HG22	2.21	0.40
29:N2:25:HIS:HB2	38:S5:15:ASP:HB2	2.02	0.40
31:N4:9:THR:O	31:N4:13:PRO:HD3	2.21	0.40
34:S1:307:ILE:HG23	34:S1:317:THR:HG21	2.03	0.40
36:S3:69:LEU:HD13	36:S3:96:VAL:HG22	2.03	0.40
42:V1:141:GLY:HA3	42:V1:248:VAL:O	2.20	0.40
9:A9:95:ARG:HB2	9:A9:96:PRO:HD3	2.03	0.40
9:A9:107:GLU:O	9:A9:118:LYS:NZ	2.49	0.40
12:AL:35:ILE:HD12	45:AL:201:CDL:H811	2.03	0.40
18:B4:31:LYS:HE3	18:B4:31:LYS:HB2	1.90	0.40
23:B9:114:TRP:O	23:B9:117:GLN:HG2	2.21	0.40
45:N4:507:CDL:H261	32:N5:78:LEU:HD11	2.03	0.40
34:S1:104:THR:O	34:S1:113:ARG:NH2	2.51	0.40
34:S1:397:ALA:HB2	34:S1:473:MET:HE3	2.04	0.40
41:S8:101:HIS:ND1	41:S8:149:MET:HE1	2.36	0.40
2:A1:65:GLY:HA2	8:A8:97:VAL:HG12	2.03	0.40
9:A9:198:ALA:O	9:A9:260:GLY:HA2	2.20	0.40
11:AK:343:PRO:HB2	26:CA:34:PRO:HB3	2.03	0.40
25:BL:109:LEU:HD22	31:N4:43:ASN:HB2	2.04	0.40
29:N2:95:MET:HE2	29:N2:149:ILE:HA	2.02	0.40
31:N4:394:ILE:HG12	52:N5:704:3PE:H3B2	2.04	0.40
31:N4:412:ILE:HA	31:N4:416:ARG:HD2	2.03	0.40
32:N5:533:MET:SD	46:N5:701:PC1:H2E1	2.62	0.40
34:S1:265:THR:HG22	34:S1:270:VAL:HA	2.02	0.40
34:S1:347:ASP:CB	34:S1:594:ALA:HB1	2.52	0.40
35:S2:448:HIS:HB3	35:S2:452:ASP:HB2	2.04	0.40
41:S8:86:TYR:CG	41:S8:87:PRO:HA	2.57	0.40
45:4L:201:CDL:H181	45:4L:201:CDL:H211	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:A1:101:CDL:H141	45:A1:101:CDL:H172	1.86	0.40
10:AC:90:TYR:HE1	17:B3:44:PRO:HB2	1.86	0.40
51:AM:201:PLX:H141	51:AM:201:PLX:H111	1.93	0.40
15:B1:25:CYS:SG	31:N4:3:LYS:HE3	2.62	0.40
20:B6:85:ASP:OD2	23:B9:167:TRP:NE1	2.36	0.40
45:N1:401:CDL:H512	33:N6:83:TRP:HZ3	1.86	0.40
48:N3:203:PEE:H70	33:N6:159:TRP:CZ3	2.57	0.40
34:S1:34:VAL:HG11	34:S1:96:VAL:HB	2.03	0.40
34:S1:194:ASP:O	34:S1:208:THR:HG23	2.21	0.40
9:A9:231:LEU:HD13	9:A9:292:PRO:HG3	2.03	0.40
11:AK:260:TYR:HB3	11:AK:264:GLU:HB2	2.04	0.40
11:AK:311:THR:HG22	29:N2:310:ASN:HB2	2.03	0.40
15:B1:57:TRP:CE3	19:B5:131:LYS:HG3	2.56	0.40
23:B9:166:GLN:HG2	23:B9:169:ARG:HH22	1.87	0.40
27:CB:3:MET:HE3	27:CB:4:MET:HG3	2.03	0.40
27:CB:19:GLU:OE2	27:CB:83:TYR:OH	2.38	0.40
30:N3:53:MET:HE1	33:N6:70:TYR:CE1	2.55	0.40
31:N4:154:LEU:HA	31:N4:154:LEU:HD23	1.84	0.40
32:N5:319:ILE:HD13	32:N5:399:VAL:HG22	2.04	0.40
43:V2:205:ILE:O	43:V2:209:LYS:HG2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4L	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
2	A1	68/70 (97%)	68 (100%)	0	0	100	100
3	A2	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
4	A3	81/83 (98%)	78 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A5	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
6	A6	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
7	A7	93/112 (83%)	88 (95%)	5 (5%)	0	100	100
8	A8	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
9	A9	339/341 (99%)	324 (96%)	15 (4%)	0	100	100
10	AB	75/87 (86%)	72 (96%)	3 (4%)	0	100	100
10	AC	85/87 (98%)	85 (100%)	0	0	100	100
11	AK	318/321 (99%)	307 (96%)	11 (4%)	0	100	100
12	AL	138/140 (99%)	138 (100%)	0	0	100	100
13	AM	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	AN	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
15	B1	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
16	B2	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
17	B3	78/80 (98%)	77 (99%)	1 (1%)	0	100	100
18	B4	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
19	B5	136/138 (99%)	135 (99%)	1 (1%)	0	100	100
20	B6	99/126 (79%)	95 (96%)	4 (4%)	0	100	100
21	B7	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
22	B8	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
23	B9	176/178 (99%)	174 (99%)	2 (1%)	0	100	100
24	BK	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
25	BL	97/102 (95%)	89 (92%)	8 (8%)	0	100	100
26	CA	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
27	CB	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
28	N1	316/318 (99%)	302 (96%)	14 (4%)	0	100	100
29	N2	345/347 (99%)	335 (97%)	10 (3%)	0	100	100
30	N3	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
31	N4	457/459 (100%)	452 (99%)	5 (1%)	0	100	100
32	N5	601/603 (100%)	576 (96%)	25 (4%)	0	100	100
33	N6	172/174 (99%)	164 (95%)	8 (5%)	0	100	100
34	S1	687/689 (100%)	660 (96%)	27 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	S2	427/430 (99%)	409 (96%)	18 (4%)	0	100	100
36	S3	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
37	S4	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
38	S5	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
39	S6	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
40	S7	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
41	S8	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
42	V1	429/431 (100%)	410 (96%)	19 (4%)	0	100	100
43	V2	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
44	V3	40/42 (95%)	36 (90%)	4 (10%)	0	100	100
All	All	8150/8299 (98%)	7889 (97%)	261 (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%)	84 (99%)	1 (1%)	67	87
2	A1	58/58 (100%)	57 (98%)	1 (2%)	56	81
3	A2	76/76 (100%)	76 (100%)	0	100	100
4	A3	69/69 (100%)	69 (100%)	0	100	100
5	A5	99/99 (100%)	99 (100%)	0	100	100
6	A6	107/107 (100%)	106 (99%)	1 (1%)	75	91
7	A7	87/97 (90%)	86 (99%)	1 (1%)	70	88
8	A8	153/153 (100%)	153 (100%)	0	100	100
9	A9	295/295 (100%)	292 (99%)	3 (1%)	73	90
10	AB	71/80 (89%)	70 (99%)	1 (1%)	62	85
10	AC	80/80 (100%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	AK	283/284 (100%)	278 (98%)	5 (2%)	54	80
12	AL	101/101 (100%)	100 (99%)	1 (1%)	73	90
13	AM	130/130 (100%)	129 (99%)	1 (1%)	79	92
14	AN	123/123 (100%)	123 (100%)	0	100	100
15	B1	53/53 (100%)	51 (96%)	2 (4%)	28	60
16	B2	62/62 (100%)	62 (100%)	0	100	100
17	B3	62/62 (100%)	62 (100%)	0	100	100
18	B4	113/113 (100%)	113 (100%)	0	100	100
19	B5	121/121 (100%)	121 (100%)	0	100	100
20	B6	98/119 (82%)	96 (98%)	2 (2%)	50	78
21	B7	112/112 (100%)	111 (99%)	1 (1%)	75	91
22	B8	141/141 (100%)	141 (100%)	0	100	100
23	B9	159/159 (100%)	159 (100%)	0	100	100
24	BK	155/156 (99%)	155 (100%)	0	100	100
25	BL	91/94 (97%)	91 (100%)	0	100	100
26	CA	45/45 (100%)	44 (98%)	1 (2%)	47	76
27	CB	108/108 (100%)	108 (100%)	0	100	100
28	N1	275/275 (100%)	271 (98%)	4 (2%)	60	84
29	N2	311/311 (100%)	309 (99%)	2 (1%)	84	94
30	N3	100/100 (100%)	99 (99%)	1 (1%)	73	90
31	N4	410/410 (100%)	407 (99%)	3 (1%)	81	93
32	N5	537/537 (100%)	531 (99%)	6 (1%)	70	88
33	N6	140/140 (100%)	138 (99%)	2 (1%)	62	85
34	S1	579/579 (100%)	573 (99%)	6 (1%)	73	90
35	S2	370/370 (100%)	364 (98%)	6 (2%)	58	82
36	S3	190/190 (100%)	190 (100%)	0	100	100
37	S4	112/112 (100%)	109 (97%)	3 (3%)	40	71
38	S5	93/93 (100%)	92 (99%)	1 (1%)	70	88
39	S6	79/79 (100%)	78 (99%)	1 (1%)	65	86
40	S7	132/132 (100%)	130 (98%)	2 (2%)	60	84
41	S8	151/151 (100%)	150 (99%)	1 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	V1	344/344 (100%)	337 (98%)	7 (2%)	50	78
43	V2	183/183 (100%)	180 (98%)	3 (2%)	58	82
44	V3	41/41 (100%)	39 (95%)	2 (5%)	21	50
All	All	7184/7229 (99%)	7113 (99%)	71 (1%)	71	90

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	4L	51	THR
2	A1	52	ARG
6	A6	46	ILE
7	A7	43	VAL
9	A9	129	LEU
9	A9	165	ILE
9	A9	367	GLU
10	AB	100	VAL
11	AK	38	LEU
11	AK	97	ASP
11	AK	163	ARG
11	AK	255	CYS
11	AK	278	LEU
12	AL	115	CYS
13	AM	144	TYR
15	B1	3	ASN
15	B1	15	ILE
20	B6	168	ASP
20	B6	171	LEU
21	B7	51	LEU
26	CA	47	THR
28	N1	87	VAL
28	N1	202	GLU
28	N1	251	THR
28	N1	282	TYR
29	N2	8	THR
29	N2	97	MET
30	N3	69	ILE
31	N4	122	PHE
31	N4	375	LEU
31	N4	444	LEU
32	N5	1	MET
32	N5	71	LEU

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Mol	Chain	Res	Type
32	N5	104	SER
32	N5	190	LEU
32	N5	286	LEU
32	N5	340	PHE
33	N6	33	LEU
33	N6	135	PHE
34	S1	41	VAL
34	S1	413	LEU
34	S1	556	THR
34	S1	560	LEU
34	S1	606	THR
34	S1	690	THR
35	S2	52	GLN
35	S2	100	VAL
35	S2	143	ASP
35	S2	148	VAL
35	S2	278	THR
35	S2	362	ILE
37	S4	58	LYS
37	S4	86	ASN
37	S4	133	ASP
38	S5	76	LEU
39	S6	34	THR
40	S7	71	CYS
40	S7	101	ASP
41	S8	142	THR
42	V1	70	LEU
42	V1	125	CYS
42	V1	212	LEU
42	V1	334	THR
42	V1	347	THR
42	V1	383	THR
42	V1	456	GLN
43	V2	137	THR
43	V2	231	LEU
43	V2	249	LEU
44	V3	382	ASP
44	V3	402	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	4L	57	ASN
3	A2	31	GLN
3	A2	48	ASN
3	A2	73	GLN
3	A2	86	GLN
3	A2	93	ASN
4	A3	156	GLN
4	A3	168	ASN
5	A5	37	GLN
5	A5	50	GLN
5	A5	86	ASN
6	A6	98	HIS
6	A6	152	HIS
7	A7	13	ASN
8	A8	112	GLN
9	A9	37	HIS
9	A9	138	ASN
9	A9	154	GLN
10	AB	142	GLN
11	AK	87	HIS
11	AK	109	GLN
11	AK	134	GLN
11	AK	217	GLN
11	AK	225	ASN
11	AK	324	HIS
13	AM	113	HIS
13	AM	116	ASN
15	B1	11	HIS
15	B1	14	HIS
16	B2	68	GLN
18	B4	79	ASN
19	B5	170	GLN
21	B7	85	HIS
22	B8	56	ASN
22	B8	94	HIS
23	B9	104	GLN
23	B9	108	GLN
23	B9	117	GLN
23	B9	166	GLN
24	BK	107	GLN
25	BL	65	ASN
28	N1	171	HIS
29	N2	221	HIS

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Mol	Chain	Res	Type
29	N2	273	ASN
29	N2	316	GLN
30	N3	10	ASN
31	N4	20	HIS
31	N4	30	HIS
31	N4	175	ASN
31	N4	338	HIS
31	N4	399	ASN
32	N5	59	GLN
32	N5	109	HIS
32	N5	159	HIS
32	N5	170	GLN
32	N5	175	ASN
32	N5	348	HIS
32	N5	400	ASN
32	N5	540	HIS
32	N5	541	ASN
33	N6	46	ASN
33	N6	175	ASN
34	S1	278	HIS
34	S1	540	ASN
34	S1	604	GLN
34	S1	677	GLN
34	S1	705	GLN
35	S2	93	GLN
35	S2	123	HIS
35	S2	166	ASN
35	S2	189	HIS
35	S2	229	HIS
36	S3	63	GLN
36	S3	77	GLN
36	S3	180	ASN
37	S4	86	ASN
38	S5	98	HIS
40	S7	144	HIS
42	V1	57	GLN
42	V1	220	GLN
42	V1	393	ASN
42	V1	456	GLN
43	V2	41	HIS
43	V2	59	ASN
43	V2	89	GLN

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Mol	Chain	Res	Type
43	V2	90	ASN
43	V2	153	GLN
43	V2	187	GLN
44	V3	388	ASN

### 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
35	2MR	S2	124	35	10,12,13	2.41	3 (30%)	5,13,15	0.90	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
35	2MR	S2	124	35	-	3/10/13/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S2	124	2MR	CZ-NH2	4.96	1.44	1.33
35	S2	124	2MR	CZ-NE	4.93	1.44	1.34
35	S2	124	2MR	CQ1-NH1	-2.24	1.41	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	S2	124	2MR	NE-CD-CG-CB
35	S2	124	2MR	CA-CB-CG-CD
35	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
35	S2	124	2MR	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 63 ligands modelled in this entry, 2 are monoatomic - leaving 61 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	$\# Z  > 2$
45	CDL	N5	702	-	99,99,99	0.30	0	105,111,111	0.29	0
48	PEE	B6	201	-	45,45,50	1.37	5 (11%)	48,50,55	1.20	4 (8%)
52	3PE	B8	201	-	31,31,50	0.37	0	34,36,55	0.35	0
46	PC1	B5	203	-	53,53,53	0.29	0	59,61,61	0.29	0
47	NDP	A9	401	-	45,52,52	0.57	0	53,80,80	0.56	1 (1%)
48	PEE	AN	201	-	50,50,50	1.31	5 (10%)	53,55,55	1.18	4 (7%)
46	PC1	A3	201	-	52,52,53	0.29	0	58,60,61	0.28	0
48	PEE	A9	402	-	38,38,50	1.48	5 (13%)	41,43,55	1.24	4 (9%)
48	PEE	AL	204	-	39,39,50	1.46	5 (12%)	41,44,55	1.19	4 (9%)
54	SF4	S8	302	41	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
45	CDL	A1	101	-	93,93,99	0.31	0	99,105,111	0.30	0
51	PLX	AM	201	-	51,51,51	1.10	3 (5%)	55,59,59	0.86	1 (1%)
45	CDL	N1	401	-	77,77,99	0.34	0	83,89,111	0.35	0
54	SF4	S1	801	34	0,12,12	-	-	-	-	-
54	SF4	V1	501	42	0,12,12	-	-	-	-	-
48	PEE	B4	201	-	50,50,50	1.32	5 (10%)	53,55,55	1.16	3 (5%)
59	FMN	V1	502	-	33,33,33	0.37	0	48,50,50	0.52	2 (4%)
51	PLX	B5	201	-	51,51,51	1.10	4 (7%)	55,59,59	0.91	2 (3%)
48	PEE	N1	406	-	50,50,50	1.30	5 (10%)	53,55,55	1.14	2 (3%)
48	PEE	AL	202	-	35,35,50	1.35	4 (11%)	38,40,55	1.12	3 (7%)
51	PLX	N4	503	-	46,46,51	1.16	3 (6%)	50,54,59	0.89	1 (2%)
45	CDL	B5	202	-	99,99,99	0.31	0	105,111,111	0.29	0
45	CDL	A8	301	-	82,82,99	0.33	0	88,94,111	0.37	0
45	CDL	N4	507	-	88,88,99	0.32	0	94,100,111	0.29	0
45	CDL	N2	401	-	67,67,99	0.35	0	73,79,111	0.35	0
46	PC1	AN	202	-	53,53,53	0.30	0	59,61,61	0.30	0
48	PEE	N3	201	-	47,47,50	1.35	5 (10%)	50,52,55	1.17	4 (8%)
48	PEE	S2	501	-	45,45,50	1.36	5 (11%)	48,50,55	1.23	4 (8%)
52	3PE	N4	506	-	47,47,50	0.31	0	50,52,55	0.30	0
52	3PE	N5	704	-	45,45,50	0.32	0	48,50,55	0.33	0
46	PC1	A9	403	-	53,53,53	0.29	0	59,61,61	0.32	0
50	ADP	AK	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.39	4 (13%)
54	SF4	S8	301	41	0,12,12	-	-	-	-	-
51	PLX	CB	201	-	51,51,51	1.08	4 (7%)	55,59,59	0.88	1 (1%)
46	PC1	N1	403	-	53,53,53	0.30	0	59,61,61	0.39	0
48	PEE	N4	501	-	50,50,50	1.31	5 (10%)	53,55,55	1.16	5 (9%)
51	PLX	S7	302	-	51,51,51	1.09	3 (5%)	55,59,59	0.93	2 (3%)
48	PEE	N1	404	-	30,30,50	1.28	3 (10%)	33,35,55	1.12	2 (6%)
45	CDL	AL	201	-	93,93,99	0.30	0	99,105,111	0.32	0
46	PC1	N5	701	-	53,53,53	0.30	0	59,61,61	0.39	0
46	PC1	N3	202	-	53,53,53	0.30	0	59,61,61	0.31	0
53	U10	N1	405	-	63,63,63	2.09	19 (30%)	76,79,79	1.73	21 (27%)
52	3PE	CB	203	-	45,45,50	0.32	0	48,50,55	0.32	0
49	ZMP	AB	201	10	29,35,36	0.77	1 (3%)	34,42,45	0.79	0
55	FES	V2	301	43	0,4,4	-	-	-	-	-
48	PEE	N5	703	-	50,50,50	1.31	5 (10%)	53,55,55	1.21	3 (5%)
48	PEE	N3	203	-	50,50,50	1.32	5 (10%)	53,55,55	1.13	3 (5%)
49	ZMP	AC	201	10	29,35,36	0.71	1 (3%)	34,42,45	0.82	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
55	FES	S1	803	34	0,4,4	-	-	-		
52	3PE	CB	202	-	50,50,50	0.31	0	53,55,55	0.28	0
57	MF8	S2	502	-	7,8,8	0.88	0	7,10,10	1.48	1 (14%)
45	CDL	N4	505	-	99,99,99	0.31	0	105,111,111	0.30	0
51	PLX	N4	504	-	51,51,51	1.11	4 (7%)	55,59,59	0.86	1 (1%)
48	PEE	N3	204	-	50,50,50	1.31	6 (12%)	53,55,55	1.14	4 (7%)
45	CDL	B4	202	-	79,79,99	0.33	0	85,91,111	0.34	0
45	CDL	4L	201	-	90,90,99	0.32	0	96,102,111	0.38	0
46	PC1	N1	402	-	44,44,53	0.32	0	50,52,61	0.30	0
45	CDL	AL	203	-	75,75,99	0.34	0	81,87,111	0.34	0
48	PEE	N4	502	-	48,48,50	1.31	5 (10%)	51,53,55	1.25	4 (7%)
54	SF4	S1	802	34	0,12,12	-	-	-		
54	SF4	S7	301	40	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CDL	N5	702	-	-	21/110/110/110	-
48	PEE	B6	201	-	-	25/49/49/54	-
52	3PE	B8	201	-	-	6/35/35/54	-
46	PC1	B5	203	-	-	15/57/57/57	-
47	NDP	A9	401	-	-	5/30/77/77	0/5/5/5
48	PEE	AN	201	-	-	28/54/54/54	-
46	PC1	A3	201	-	-	13/56/56/57	-
48	PEE	A9	402	-	-	21/42/42/54	-
48	PEE	AL	204	-	-	25/43/43/54	-
54	SF4	S8	302	41	-	-	0/6/5/5
45	CDL	A1	101	-	-	30/104/104/110	-
51	PLX	AM	201	-	-	16/55/55/55	-
45	CDL	N1	401	-	-	24/88/88/110	-
54	SF4	S1	801	34	-	-	0/6/5/5
54	SF4	V1	501	42	-	-	0/6/5/5
48	PEE	B4	201	-	-	29/54/54/54	-
59	FMN	V1	502	-	-	8/18/18/18	0/3/3/3
51	PLX	B5	201	-	-	22/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PEE	N1	406	-	-	26/54/54/54	-
48	PEE	AL	202	-	-	23/39/39/54	-
51	PLX	N4	503	-	-	21/50/50/55	-
45	CDL	B5	202	-	-	17/110/110/110	-
45	CDL	A8	301	-	-	25/93/93/110	-
45	CDL	N4	507	-	-	25/99/99/110	-
45	CDL	N2	401	-	-	19/78/78/110	-
46	PC1	AN	202	-	-	11/57/57/57	-
48	PEE	N3	201	-	-	27/51/51/54	-
48	PEE	S2	501	-	-	19/49/49/54	-
52	3PE	N4	506	-	-	14/51/51/54	-
52	3PE	N5	704	-	-	12/49/49/54	-
46	PC1	A9	403	-	-	17/57/57/57	-
50	ADP	AK	401	-	-	3/12/32/32	0/3/3/3
54	SF4	S8	301	41	-	-	0/6/5/5
51	PLX	CB	201	-	-	27/55/55/55	-
46	PC1	N1	403	-	-	18/57/57/57	-
48	PEE	N4	501	-	-	32/54/54/54	-
51	PLX	S7	302	-	-	21/55/55/55	-
48	PEE	N1	404	-	-	19/34/34/54	-
45	CDL	AL	201	-	-	21/104/104/110	-
46	PC1	N5	701	-	-	20/57/57/57	-
46	PC1	N3	202	-	-	15/57/57/57	-
53	U10	N1	405	-	-	19/63/87/87	0/1/1/1
52	3PE	CB	203	-	-	16/49/49/54	-
49	ZMP	AB	201	10	-	11/40/42/43	-
55	FES	V2	301	43	-	-	0/1/1/1
48	PEE	N5	703	-	-	29/54/54/54	-
48	PEE	N3	203	-	-	25/54/54/54	-
49	ZMP	AC	201	10	-	16/40/42/43	-
55	FES	S1	803	34	-	-	0/1/1/1
52	3PE	CB	202	-	-	11/54/54/54	-
57	MF8	S2	502	-	-	5/8/8/8	-
45	CDL	N4	505	-	-	28/110/110/110	-
51	PLX	N4	504	-	-	23/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PEE	N3	204	-	-	27/54/54/54	-
45	CDL	B4	202	-	-	23/90/90/110	-
45	CDL	4L	201	-	-	23/101/101/110	-
46	PC1	N1	402	-	-	19/48/48/57	-
45	CDL	AL	203	-	-	22/86/86/110	-
48	PEE	N4	502	-	-	34/52/52/54	-
54	SF4	S1	802	34	-	-	0/6/5/5
54	SF4	S7	301	40	-	-	0/6/5/5

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	N1	405	U10	C6-C1	9.99	1.53	1.35
53	N1	405	U10	C4-C3	4.34	1.53	1.36
48	B4	201	PEE	C18-C19	4.06	1.55	1.31
48	N3	203	PEE	C18-C19	4.06	1.55	1.31
48	N5	703	PEE	C18-C19	4.05	1.55	1.31
48	AL	204	PEE	C18-C19	4.04	1.55	1.31
48	B6	201	PEE	C18-C19	4.03	1.55	1.31
48	N1	406	PEE	C18-C19	4.03	1.55	1.31
48	AN	201	PEE	C18-C19	4.02	1.55	1.31
48	N3	204	PEE	C18-C19	4.02	1.55	1.31
48	N4	501	PEE	C18-C19	4.01	1.55	1.31
48	A9	402	PEE	C18-C19	4.00	1.55	1.31
48	N3	201	PEE	C18-C19	4.00	1.54	1.31
48	S2	501	PEE	C18-C19	3.98	1.54	1.31
48	N4	502	PEE	C18-C19	3.95	1.54	1.31
48	N4	501	PEE	C39-C38	3.94	1.54	1.31
48	N4	502	PEE	C39-C38	3.94	1.54	1.31
48	N3	204	PEE	C39-C38	3.93	1.54	1.31
48	N3	203	PEE	C39-C38	3.93	1.54	1.31
48	AN	201	PEE	C39-C38	3.92	1.54	1.31
48	AL	202	PEE	C39-C38	3.92	1.54	1.31
48	N1	406	PEE	C39-C38	3.92	1.54	1.31
48	AL	204	PEE	C39-C38	3.92	1.54	1.31
48	B6	201	PEE	C39-C38	3.91	1.54	1.31
48	N3	201	PEE	C39-C38	3.91	1.54	1.31
48	B4	201	PEE	C39-C38	3.90	1.54	1.31
48	S2	501	PEE	C39-C38	3.89	1.54	1.31
48	N5	703	PEE	C39-C38	3.89	1.54	1.31
48	A9	402	PEE	C39-C38	3.85	1.54	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	AL	202	PEE	O3-C30	3.34	1.43	1.33
48	N3	203	PEE	O3-C30	3.27	1.42	1.33
48	N3	201	PEE	O3-C30	3.25	1.42	1.33
48	N3	204	PEE	O3-C30	3.22	1.42	1.33
48	A9	402	PEE	O3-C30	3.20	1.42	1.33
48	N1	404	PEE	O3-C30	3.20	1.42	1.33
48	AL	204	PEE	O3-C30	3.19	1.42	1.33
48	N5	703	PEE	O3-C30	3.19	1.42	1.33
48	AN	201	PEE	O3-C30	3.17	1.42	1.33
48	N1	406	PEE	O3-C30	3.16	1.42	1.33
48	B4	201	PEE	O3-C30	3.11	1.42	1.33
48	N4	501	PEE	O3-C30	3.10	1.42	1.33
48	S2	501	PEE	O3-C30	3.09	1.42	1.33
48	B6	201	PEE	O3-C30	3.03	1.42	1.33
51	N4	504	PLX	O6-C4	-3.03	1.40	1.44
51	S7	302	PLX	O6-C4	-3.01	1.40	1.44
49	AB	201	ZMP	C9-C10	-2.96	1.47	1.50
48	N4	502	PEE	O3-C30	2.95	1.42	1.33
51	B5	201	PLX	O6-C4	-2.93	1.40	1.44
53	N1	405	U10	C41-C39	2.93	1.57	1.51
51	N4	503	PLX	O6-C4	-2.89	1.40	1.44
48	N4	502	PEE	O2-C2	-2.77	1.39	1.46
51	AM	201	PLX	O6-C4	-2.76	1.40	1.44
48	N3	204	PEE	O2-C10	2.75	1.42	1.34
48	AN	201	PEE	O2-C10	2.73	1.42	1.34
48	N1	406	PEE	O2-C10	2.73	1.42	1.34
48	N3	203	PEE	O2-C10	2.73	1.42	1.34
48	AL	202	PEE	O2-C10	2.70	1.41	1.34
48	B4	201	PEE	O2-C10	2.67	1.41	1.34
51	CB	201	PLX	O6-C4	-2.66	1.41	1.44
48	AL	204	PEE	O2-C10	2.65	1.41	1.34
48	N1	404	PEE	O2-C10	2.61	1.41	1.34
48	N4	501	PEE	O2-C10	2.61	1.41	1.34
48	A9	402	PEE	O2-C10	2.60	1.41	1.34
49	AC	201	ZMP	C9-C10	-2.57	1.48	1.50
48	N3	201	PEE	O2-C10	2.57	1.41	1.34
48	N5	703	PEE	O2-C2	-2.56	1.40	1.46
48	B6	201	PEE	O2-C10	2.56	1.41	1.34
53	N1	405	U10	C31-C29	2.55	1.56	1.51
48	S2	501	PEE	O2-C10	2.54	1.41	1.34
48	S2	501	PEE	O2-C2	-2.54	1.40	1.46
53	N1	405	U10	C26-C24	2.53	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	N1	404	PEE	O2-C2	-2.53	1.40	1.46
48	A9	402	PEE	O2-C2	-2.52	1.40	1.46
53	N1	405	U10	O5-C5	-2.51	1.17	1.23
48	N3	201	PEE	O2-C2	-2.50	1.40	1.46
48	B6	201	PEE	O2-C2	-2.50	1.40	1.46
53	N1	405	U10	C7-C8	2.50	1.54	1.50
53	N1	405	U10	C21-C19	2.49	1.56	1.51
48	N5	703	PEE	O2-C10	2.46	1.41	1.34
53	N1	405	U10	C7-C6	2.44	1.55	1.51
48	B4	201	PEE	O2-C2	-2.44	1.40	1.46
53	N1	405	U10	O2-C2	-2.44	1.18	1.23
48	N4	501	PEE	O2-C2	-2.43	1.40	1.46
48	N4	502	PEE	O2-C10	2.38	1.41	1.34
53	N1	405	U10	C46-C44	2.35	1.56	1.51
50	AK	401	ADP	C5-C4	2.33	1.47	1.40
53	N1	405	U10	C51-C49	2.31	1.56	1.51
53	N1	405	U10	C36-C34	2.27	1.56	1.51
51	B5	201	PLX	C1B-N1	-2.27	1.43	1.50
51	N4	503	PLX	C1B-N1	-2.27	1.43	1.50
51	N4	504	PLX	C1B-N1	-2.26	1.43	1.50
48	AL	204	PEE	O2-C2	-2.23	1.41	1.46
53	N1	405	U10	O3-C3M	-2.22	1.40	1.45
53	N1	405	U10	C27-C28	2.21	1.57	1.50
48	N3	203	PEE	O2-C2	-2.20	1.41	1.46
48	N3	204	PEE	O2-C2	-2.18	1.41	1.46
51	N4	503	PLX	C1A-N1	-2.18	1.43	1.50
48	N1	406	PEE	O2-C2	-2.16	1.41	1.46
51	S7	302	PLX	C1B-N1	-2.16	1.43	1.50
53	N1	405	U10	C11-C9	2.16	1.55	1.51
51	N4	504	PLX	C1A-N1	-2.15	1.43	1.50
48	AN	201	PEE	O2-C2	-2.15	1.41	1.46
48	AL	202	PEE	O2-C2	-2.15	1.41	1.46
51	AM	201	PLX	P1-O4	2.13	1.67	1.59
51	CB	201	PLX	C1B-N1	-2.11	1.43	1.50
51	AM	201	PLX	C1B-N1	-2.11	1.43	1.50
51	B5	201	PLX	C1A-N1	-2.09	1.43	1.50
53	N1	405	U10	C16-C14	2.09	1.55	1.51
53	N1	405	U10	C6-C5	2.08	1.52	1.46
51	CB	201	PLX	C1A-N1	-2.07	1.44	1.50
51	CB	201	PLX	P1-O3	-2.06	1.45	1.55
53	N1	405	U10	C42-C43	2.05	1.57	1.50
51	S7	302	PLX	C1A-N1	-2.04	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	N3	204	PEE	C11-C10	2.04	1.56	1.50
51	N4	504	PLX	P1-O3	-2.03	1.45	1.55
51	B5	201	PLX	P1-O4	2.00	1.67	1.59

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	N5	703	PEE	O2-C10-C11	4.17	120.50	111.50
48	B4	201	PEE	O2-C10-C11	4.13	120.40	111.50
48	N4	502	PEE	O2-C10-C11	4.07	120.28	111.50
48	N4	501	PEE	O2-C10-C11	4.03	120.19	111.50
48	N1	406	PEE	O2-C10-C11	3.96	120.04	111.50
48	AL	204	PEE	O2-C10-C11	3.95	120.02	111.50
48	N3	201	PEE	O2-C10-C11	3.95	120.00	111.50
48	B6	201	PEE	O2-C10-C11	3.93	119.97	111.50
53	N1	405	U10	C7-C8-C9	-3.91	120.28	126.79
48	N1	404	PEE	O2-C10-C11	3.90	119.91	111.50
48	S2	501	PEE	O2-C10-C11	3.89	119.89	111.50
48	N3	204	PEE	O2-C10-C11	3.84	119.78	111.50
48	AN	201	PEE	O2-C10-C11	3.81	119.72	111.50
48	A9	402	PEE	O2-C10-C11	3.80	119.70	111.50
48	N3	203	PEE	O2-C10-C11	3.76	119.61	111.50
57	S2	502	MF8	C07-N06-C04	3.71	132.67	124.55
50	AK	401	ADP	PA-O3A-PB	-3.68	120.19	132.83
53	N1	405	U10	C15-C14-C16	3.42	121.03	115.27
48	AL	202	PEE	O2-C10-C11	3.27	119.91	110.80
53	N1	405	U10	C40-C39-C41	3.24	120.71	115.27
53	N1	405	U10	C47-C48-C49	-3.16	120.05	127.66
53	N1	405	U10	C42-C43-C44	-3.11	120.17	127.66
53	N1	405	U10	C1M-C1-C6	-3.09	119.36	124.40
50	AK	401	ADP	N3-C2-N1	-3.08	123.87	128.68
53	N1	405	U10	C35-C34-C36	3.04	120.39	115.27
53	N1	405	U10	C25-C24-C26	3.00	120.32	115.27
48	N5	703	PEE	O3-C30-C31	2.93	121.09	111.91
53	N1	405	U10	C22-C23-C24	-2.91	120.64	127.66
53	N1	405	U10	C27-C28-C29	-2.82	120.86	127.66
48	N1	406	PEE	O3-C30-C31	2.82	120.75	111.91
53	N1	405	U10	C10-C9-C11	2.81	120.00	115.27
53	N1	405	U10	C12-C13-C14	-2.79	120.94	127.66
53	N1	405	U10	C30-C29-C31	2.75	119.89	115.27
53	N1	405	U10	C32-C33-C34	-2.73	121.08	127.66
53	N1	405	U10	C45-C44-C46	2.73	119.87	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A9	402	PEE	O3-C30-C31	2.72	120.43	111.91
53	N1	405	U10	C50-C49-C51	2.70	119.82	115.27
48	B6	201	PEE	O3-C30-C31	2.68	120.33	111.91
53	N1	405	U10	C20-C19-C21	2.66	119.75	115.27
48	AN	201	PEE	O3-C30-C31	2.65	120.23	111.91
53	N1	405	U10	C37-C38-C39	-2.62	121.35	127.66
50	AK	401	ADP	C4-C5-N7	-2.61	106.68	109.40
48	N3	203	PEE	O3-C30-C31	2.60	120.08	111.91
48	N4	502	PEE	O3-C30-C31	2.59	120.03	111.91
48	N3	204	PEE	O3-C30-C31	2.56	119.95	111.91
53	N1	405	U10	C17-C18-C19	-2.56	121.50	127.66
48	A9	402	PEE	C37-C38-C39	-2.55	109.51	126.84
48	N4	501	PEE	O3-C30-C31	2.52	119.83	111.91
48	AL	204	PEE	O3-C30-C31	2.52	119.80	111.91
48	B4	201	PEE	O3-C30-C31	2.50	119.76	111.91
48	N3	201	PEE	O3-C30-C31	2.50	119.74	111.91
48	N1	404	PEE	O3-C30-C31	2.48	119.69	111.91
48	S2	501	PEE	O3-C30-C31	2.46	119.64	111.91
48	AL	202	PEE	O3-C30-C31	2.40	119.43	111.91
53	N1	405	U10	C56-C54-C55	2.40	119.90	114.60
51	AM	201	PLX	O3-P1-O2	-2.27	101.04	112.24
47	A9	401	NDP	C5A-C6A-N6A	2.26	123.78	120.35
51	CB	201	PLX	O3-P1-O2	-2.25	101.14	112.24
51	B5	201	PLX	O3-P1-O2	-2.22	101.25	112.24
51	N4	503	PLX	O3-P1-O2	-2.21	101.29	112.24
51	S7	302	PLX	O3-P1-O2	-2.20	101.35	112.24
50	AK	401	ADP	C3'-C2'-C1'	2.19	104.28	100.98
51	N4	504	PLX	O3-P1-O2	-2.18	101.45	112.24
51	S7	302	PLX	C8-C7-C6	-2.18	108.34	113.38
59	V1	502	FMN	P-O5'-C5'	2.18	124.29	118.30
53	N1	405	U10	C52-C53-C54	-2.16	120.37	127.75
48	N4	501	PEE	C40-C39-C38	-2.12	108.45	124.73
48	N4	502	PEE	C20-C19-C18	-2.10	108.58	124.73
48	B4	201	PEE	C40-C39-C38	-2.09	108.66	124.73
48	N3	201	PEE	C20-C19-C18	-2.09	108.69	124.73
48	AN	201	PEE	C17-C18-C19	-2.08	108.74	124.73
48	N4	502	PEE	C17-C18-C19	-2.08	108.77	124.73
49	AC	201	ZMP	O1-C10-C9	-2.08	121.53	123.99
48	B6	201	PEE	C37-C38-C39	-2.07	108.84	124.73
48	S2	501	PEE	C37-C38-C39	-2.07	108.84	124.73
48	S2	501	PEE	C17-C18-C19	-2.06	108.89	124.73
48	N3	203	PEE	C40-C39-C38	-2.06	108.91	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AL	202	PEE	C37-C38-C39	-2.06	108.95	124.73
48	AL	204	PEE	C37-C38-C39	-2.05	109.02	124.73
48	N4	501	PEE	C17-C18-C19	-2.04	109.05	124.73
48	N5	703	PEE	C37-C38-C39	-2.04	109.09	124.73
48	N3	204	PEE	C20-C19-C18	-2.03	109.14	124.73
48	N4	501	PEE	C20-C19-C18	-2.03	109.15	124.73
48	N3	204	PEE	C37-C38-C39	-2.03	109.18	124.73
48	AL	204	PEE	C40-C39-C38	-2.02	109.24	124.73
48	B6	201	PEE	C17-C18-C19	-2.02	109.26	124.73
48	N3	201	PEE	C17-C18-C19	-2.01	109.29	124.73
59	V1	502	FMN	C1'-N10-C9A	-2.01	117.16	120.51
48	A9	402	PEE	C17-C18-C19	-2.01	109.33	124.73
51	B5	201	PLX	C8-C7-C6	-2.00	108.75	113.38
48	AN	201	PEE	C40-C39-C38	-2.00	109.37	124.73

There are no chirality outliers.

All (1051) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	4L	201	CDL	CA2-OA2-PA1-OA3
45	4L	201	CDL	CA2-OA2-PA1-OA4
45	4L	201	CDL	CA2-OA2-PA1-OA5
45	4L	201	CDL	CA3-OA5-PA1-OA2
45	4L	201	CDL	CA3-OA5-PA1-OA3
45	4L	201	CDL	CA3-OA5-PA1-OA4
45	4L	201	CDL	CB2-OB2-PB2-OB4
45	A8	301	CDL	CA2-OA2-PA1-OA3
45	A8	301	CDL	CA2-OA2-PA1-OA4
45	A8	301	CDL	CB2-OB2-PB2-OB3
45	A8	301	CDL	CB2-OB2-PB2-OB4
45	A8	301	CDL	CB2-OB2-PB2-OB5
45	AL	201	CDL	CA3-OA5-PA1-OA3
45	AL	201	CDL	CA3-OA5-PA1-OA4
45	AL	201	CDL	CB2-OB2-PB2-OB3
45	AL	201	CDL	CB2-OB2-PB2-OB4
45	AL	201	CDL	CB2-OB2-PB2-OB5
45	AL	203	CDL	CA2-C1-CB2-OB2
45	AL	203	CDL	CA2-OA2-PA1-OA3
45	AL	203	CDL	CA2-OA2-PA1-OA4
45	AL	203	CDL	OB6-CB4-CB6-OB8
45	B4	202	CDL	CA3-OA5-PA1-OA2
45	B4	202	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
45	B4	202	CDL	CA3-OA5-PA1-OA4
45	B5	202	CDL	CA3-OA5-PA1-OA4
45	B5	202	CDL	CB3-OB5-PB2-OB4
45	N1	401	CDL	CA2-OA2-PA1-OA3
45	N1	401	CDL	CA3-OA5-PA1-OA3
45	N1	401	CDL	CA3-OA5-PA1-OA4
45	N1	401	CDL	CB2-OB2-PB2-OB3
45	N1	401	CDL	CB3-OB5-PB2-OB3
45	N1	401	CDL	OB6-CB4-CB6-OB8
45	N2	401	CDL	CA2-OA2-PA1-OA3
45	N2	401	CDL	CA2-OA2-PA1-OA4
45	N2	401	CDL	CA2-OA2-PA1-OA5
45	N2	401	CDL	CA3-OA5-PA1-OA4
45	N2	401	CDL	CB2-OB2-PB2-OB3
45	N2	401	CDL	CB2-OB2-PB2-OB4
45	N2	401	CDL	CB2-OB2-PB2-OB5
45	N4	505	CDL	CA3-OA5-PA1-OA2
45	N4	505	CDL	CA3-OA5-PA1-OA4
45	N4	505	CDL	CB3-OB5-PB2-OB3
45	N4	507	CDL	CA2-OA2-PA1-OA3
45	N4	507	CDL	CA3-OA5-PA1-OA4
45	N5	702	CDL	CA3-OA5-PA1-OA4
45	N5	702	CDL	CB2-OB2-PB2-OB3
45	N5	702	CDL	CB2-OB2-PB2-OB4
45	N5	702	CDL	CB2-OB2-PB2-OB5
46	A9	403	PC1	C1-O11-P-O12
46	AN	202	PC1	C11-O13-P-O14
46	AN	202	PC1	C11-O13-P-O11
46	AN	202	PC1	C1-O11-P-O12
46	AN	202	PC1	C1-O11-P-O14
46	AN	202	PC1	C1-O11-P-O13
46	B5	203	PC1	C11-O13-P-O14
46	N1	402	PC1	C11-O13-P-O12
46	N1	402	PC1	C1-O11-P-O12
46	N1	402	PC1	C1-O11-P-O14
46	N1	402	PC1	C1-O11-P-O13
46	N1	403	PC1	C11-O13-P-O12
46	N1	403	PC1	C1-O11-P-O12
46	N1	403	PC1	C1-O11-P-O13
46	N1	403	PC1	C12-C11-O13-P
46	N3	202	PC1	C11-O13-P-O12
46	N3	202	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
46	N3	202	PC1	C11-O13-P-O11
46	N5	701	PC1	C11-O13-P-O12
46	N5	701	PC1	C11-O13-P-O14
46	N5	701	PC1	C11-O13-P-O11
46	N5	701	PC1	C1-O11-P-O13
47	A9	401	NDP	C2N-C3N-C7N-N7N
48	A9	402	PEE	C11-C10-O2-C2
48	A9	402	PEE	C1-O3P-P-O1P
48	A9	402	PEE	C1-O3P-P-O4P
48	A9	402	PEE	C4-O4P-P-O3P
48	A9	402	PEE	C4-O4P-P-O2P
48	A9	402	PEE	C4-O4P-P-O1P
48	AL	202	PEE	C11-C10-O2-C2
48	AL	202	PEE	C1-O3P-P-O2P
48	AL	202	PEE	C1-O3P-P-O1P
48	AL	202	PEE	C1-O3P-P-O4P
48	AL	202	PEE	C4-O4P-P-O2P
48	AL	202	PEE	C4-O4P-P-O1P
48	AL	202	PEE	O4P-C4-C5-N
48	AL	204	PEE	C18-C19-C20-C21
48	AL	204	PEE	C11-C10-O2-C2
48	AL	204	PEE	C1-O3P-P-O1P
48	AL	204	PEE	C4-O4P-P-O1P
48	AN	201	PEE	C11-C10-O2-C2
48	AN	201	PEE	C1-C2-O2-C10
48	AN	201	PEE	C4-O4P-P-O2P
48	AN	201	PEE	C4-O4P-P-O1P
48	AN	201	PEE	O4P-C4-C5-N
48	B4	201	PEE	O4-C10-O2-C2
48	B4	201	PEE	O4P-C4-C5-N
48	B6	201	PEE	C4-O4P-P-O3P
48	B6	201	PEE	C4-O4P-P-O2P
48	B6	201	PEE	C4-O4P-P-O1P
48	B6	201	PEE	O4P-C4-C5-N
48	N1	404	PEE	C4-O4P-P-O3P
48	N1	404	PEE	C4-O4P-P-O2P
48	N1	404	PEE	C4-O4P-P-O1P
48	N1	406	PEE	C37-C38-C39-C40
48	N3	201	PEE	C1-O3P-P-O2P
48	N3	201	PEE	C1-O3P-P-O1P
48	N3	201	PEE	C35-C36-C37-C38
48	N3	203	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
48	N3	203	PEE	C37-C38-C39-C40
48	N3	204	PEE	O4P-C4-C5-N
48	N3	204	PEE	O5-C30-O3-C3
48	N4	501	PEE	C11-C10-O2-C2
48	N4	501	PEE	O4P-C4-C5-N
48	N4	502	PEE	C4-O4P-P-O2P
48	N4	502	PEE	O4P-C4-C5-N
48	N4	502	PEE	C37-C38-C39-C40
48	N5	703	PEE	C1-O3P-P-O2P
48	N5	703	PEE	C1-O3P-P-O1P
48	N5	703	PEE	C4-O4P-P-O3P
48	N5	703	PEE	C4-O4P-P-O1P
48	N5	703	PEE	O4P-C4-C5-N
48	S2	501	PEE	O4-C10-O2-C2
49	AC	201	ZMP	C17-C18-C21-O5
49	AC	201	ZMP	N2-C16-C17-O4
49	AC	201	ZMP	S1-C11-C12-N1
49	AC	201	ZMP	O1-C10-S1-C11
49	AC	201	ZMP	C9-C10-S1-C11
49	AC	201	ZMP	C7-C8-C9-C10
50	AK	401	ADP	C5'-O5'-PA-O3A
51	AM	201	PLX	O7-C6-O6-C4
51	AM	201	PLX	C2-O1-P1-O4
51	AM	201	PLX	N1-C1-C2-O1
51	AM	201	PLX	C25-C24-O8-C5
51	B5	201	PLX	O7-C6-C7-C8
51	B5	201	PLX	O7-C6-O6-C4
51	B5	201	PLX	C3-O4-P1-O2
51	B5	201	PLX	C2-O1-P1-O2
51	B5	201	PLX	O9-C24-C25-C26
51	CB	201	PLX	O7-C6-C7-C8
51	CB	201	PLX	C3-C4-O6-C6
51	CB	201	PLX	C3-O4-P1-O2
51	CB	201	PLX	C3-O4-P1-O3
51	N4	503	PLX	O7-C6-O6-C4
51	N4	503	PLX	O6-C4-C5-O8
51	N4	503	PLX	N1-C1-C2-O1
51	N4	503	PLX	O9-C24-C25-C26
51	N4	504	PLX	O7-C6-C7-C8
51	N4	504	PLX	C3-O4-P1-O2
51	N4	504	PLX	C3-O4-P1-O3
51	N4	504	PLX	O9-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
51	S7	302	PLX	O7-C6-C7-C8
51	S7	302	PLX	C2-O1-P1-O2
52	B8	201	3PE	O13-C11-C12-N
52	CB	202	3PE	C11-O13-P-O11
52	CB	203	3PE	C1-O11-P-O12
52	CB	203	3PE	C11-O13-P-O11
52	N4	506	3PE	C11-O13-P-O11
52	N4	506	3PE	C11-O13-P-O12
52	N4	506	3PE	C11-O13-P-O14
52	N5	704	3PE	C11-O13-P-O12
52	N5	704	3PE	C11-O13-P-O14
52	N5	704	3PE	O13-C11-C12-N
53	N1	405	U10	C12-C11-C9-C8
53	N1	405	U10	C12-C11-C9-C10
53	N1	405	U10	C33-C34-C36-C37
53	N1	405	U10	C35-C34-C36-C37
59	V1	502	FMN	N10-C1'-C2'-O2'
59	V1	502	FMN	C5'-O5'-P-O1P
59	V1	502	FMN	C5'-O5'-P-O2P
59	V1	502	FMN	C5'-O5'-P-O3P
48	AL	204	PEE	O5-C30-O3-C3
48	N3	201	PEE	O5-C30-O3-C3
48	N3	203	PEE	O5-C30-O3-C3
48	N4	502	PEE	O5-C30-O3-C3
48	AL	204	PEE	C31-C30-O3-C3
48	N3	201	PEE	C31-C30-O3-C3
48	N3	203	PEE	C31-C30-O3-C3
48	N4	502	PEE	C31-C30-O3-C3
48	A9	402	PEE	O5-C30-O3-C3
48	B6	201	PEE	O5-C30-O3-C3
48	N5	703	PEE	O5-C30-O3-C3
48	A9	402	PEE	O4-C10-O2-C2
48	AL	204	PEE	O4-C10-O2-C2
48	N3	203	PEE	O4-C10-O2-C2
48	N3	204	PEE	O4-C10-O2-C2
48	N4	501	PEE	O4-C10-O2-C2
48	N3	204	PEE	C31-C30-O3-C3
48	N5	703	PEE	C31-C30-O3-C3
48	B4	201	PEE	C11-C10-O2-C2
48	N3	204	PEE	C11-C10-O2-C2
48	S2	501	PEE	C11-C10-O2-C2
53	N1	405	U10	C25-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
48	A9	402	PEE	C31-C30-O3-C3
48	B6	201	PEE	C31-C30-O3-C3
48	N1	404	PEE	C31-C30-O3-C3
48	A9	402	PEE	C17-C18-C19-C20
48	AL	204	PEE	C17-C18-C19-C20
48	B6	201	PEE	C37-C38-C39-C40
48	N1	406	PEE	C17-C18-C19-C20
48	N3	203	PEE	C17-C18-C19-C20
48	N4	502	PEE	C17-C18-C19-C20
48	AL	202	PEE	O4-C10-O2-C2
48	AN	201	PEE	O4-C10-O2-C2
48	N1	404	PEE	O5-C30-O3-C3
48	N5	703	PEE	C11-C10-O2-C2
48	N4	501	PEE	C12-C13-C14-C15
48	B6	201	PEE	C11-C12-C13-C14
53	N1	405	U10	C14-C16-C17-C18
53	N1	405	U10	C24-C26-C27-C28
53	N1	405	U10	C39-C41-C42-C43
53	N1	405	U10	C49-C51-C52-C53
48	N4	501	PEE	C31-C30-O3-C3
48	N3	201	PEE	C17-C18-C19-C20
48	AL	204	PEE	C33-C34-C35-C36
48	N4	501	PEE	O5-C30-O3-C3
48	B4	201	PEE	C31-C30-O3-C3
51	B5	201	PLX	C35-C36-C37-C38
48	N1	406	PEE	C34-C35-C36-C37
48	N5	703	PEE	C33-C34-C35-C36
48	N4	502	PEE	O3P-C1-C2-O2
45	AL	203	CDL	O1-C1-CB2-OB2
53	N1	405	U10	C23-C24-C26-C27
48	B4	201	PEE	C22-C23-C24-C25
45	B4	202	CDL	CA5-C11-C12-C13
45	A1	101	CDL	C72-C73-C74-C75
48	AN	201	PEE	C10-C11-C12-C13
48	B4	201	PEE	C37-C38-C39-C40
48	N3	201	PEE	C37-C38-C39-C40
48	N4	501	PEE	C17-C18-C19-C20
48	N5	703	PEE	C37-C38-C39-C40
48	AL	204	PEE	C12-C13-C14-C15
48	N3	201	PEE	C33-C34-C35-C36
48	B4	201	PEE	C31-C32-C33-C34
45	4L	201	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
46	N3	202	PC1	C31-C32-C33-C34
48	AL	204	PEE	C30-C31-C32-C33
48	N1	404	PEE	C10-C11-C12-C13
52	N5	704	3PE	C21-C22-C23-C24
48	N5	703	PEE	O4-C10-O2-C2
48	AN	201	PEE	C32-C33-C34-C35
46	B5	203	PC1	C11-C12-N-C15
46	N3	202	PC1	C11-C12-N-C15
45	B5	202	CDL	CB7-C71-C72-C73
48	B4	201	PEE	C10-C11-C12-C13
48	N1	404	PEE	C30-C31-C32-C33
48	N3	201	PEE	C10-C11-C12-C13
52	CB	203	3PE	C21-C22-C23-C24
48	B4	201	PEE	O5-C30-O3-C3
53	N1	405	U10	C9-C11-C12-C13
48	B4	201	PEE	C30-C31-C32-C33
52	CB	203	3PE	C31-C32-C33-C34
48	AL	202	PEE	C37-C38-C39-C40
48	N3	204	PEE	C17-C18-C19-C20
51	N4	503	PLX	C31-C32-C33-C34
45	4L	201	CDL	CB2-OB2-PB2-OB5
45	A1	101	CDL	CB2-OB2-PB2-OB5
45	A8	301	CDL	CA2-OA2-PA1-OA5
45	AL	201	CDL	CA3-OA5-PA1-OA2
45	AL	203	CDL	CA2-OA2-PA1-OA5
45	AL	203	CDL	CA3-OA5-PA1-OA2
45	B5	202	CDL	CA3-OA5-PA1-OA2
45	N1	401	CDL	CA2-OA2-PA1-OA5
45	N1	401	CDL	CA3-OA5-PA1-OA2
45	N4	507	CDL	CA2-OA2-PA1-OA5
45	N4	507	CDL	CA3-OA5-PA1-OA2
45	N5	702	CDL	CA3-OA5-PA1-OA2
46	A3	201	PC1	C11-O13-P-O11
46	A3	201	PC1	C1-O11-P-O13
46	A9	403	PC1	C1-O11-P-O13
46	N1	402	PC1	C11-O13-P-O11
46	N1	403	PC1	C11-O13-P-O11
48	AL	202	PEE	C4-O4P-P-O3P
48	AN	201	PEE	C4-O4P-P-O3P
48	N3	201	PEE	C1-O3P-P-O4P
48	N3	203	PEE	C1-O3P-P-O4P
48	N4	502	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
48	N4	502	PEE	C4-O4P-P-O3P
48	N5	703	PEE	C1-O3P-P-O4P
51	B5	201	PLX	C3-O4-P1-O1
51	B5	201	PLX	C2-O1-P1-O4
51	CB	201	PLX	C3-O4-P1-O1
51	N4	504	PLX	C3-O4-P1-O1
51	S7	302	PLX	C2-O1-P1-O4
52	B8	201	3PE	C11-O13-P-O11
52	N5	704	3PE	C1-O11-P-O13
52	N5	704	3PE	C11-O13-P-O11
48	B6	201	PEE	C30-C31-C32-C33
48	N1	406	PEE	O4-C10-O2-C2
46	A9	403	PC1	C11-C12-N-C13
46	A9	403	PC1	C11-C12-N-C15
46	N1	403	PC1	C11-C12-N-C13
46	N1	403	PC1	C11-C12-N-C14
46	N1	403	PC1	C11-C12-N-C15
51	B5	201	PLX	O8-C24-C25-C26
51	N4	503	PLX	O8-C24-C25-C26
48	N4	502	PEE	C39-C40-C41-C42
48	N3	201	PEE	C31-C32-C33-C34
51	B5	201	PLX	C26-C27-C28-C29
51	B5	201	PLX	C29-C30-C31-C32
52	N4	506	3PE	C2D-C2E-C2F-C2G
48	N1	406	PEE	C11-C10-O2-C2
45	N4	505	CDL	C32-C33-C34-C35
48	AN	201	PEE	C22-C23-C24-C25
48	B4	201	PEE	C32-C33-C34-C35
49	AC	201	ZMP	C6-C7-C8-C9
51	N4	503	PLX	C28-C29-C30-C31
45	AL	203	CDL	C34-C35-C36-C37
48	B6	201	PEE	C21-C22-C23-C24
48	N1	406	PEE	C14-C15-C16-C17
48	N3	203	PEE	C31-C32-C33-C34
48	AL	202	PEE	C1-C2-O2-C10
48	N3	203	PEE	C3-C2-O2-C10
48	N5	703	PEE	C30-C31-C32-C33
52	B8	201	3PE	C21-C22-C23-C24
46	N1	402	PC1	C26-C27-C28-C29
48	AL	204	PEE	C14-C15-C16-C17
48	N3	204	PEE	C12-C13-C14-C15
51	N4	504	PLX	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
48	AN	201	PEE	C2-C1-O3P-P
48	AN	201	PEE	C37-C38-C39-C40
48	N3	204	PEE	C40-C41-C42-C43
48	N4	502	PEE	C14-C15-C16-C17
48	N4	502	PEE	C12-C13-C14-C15
48	N5	703	PEE	C14-C15-C16-C17
52	CB	203	3PE	C22-C23-C24-C25
45	A8	301	CDL	O1-C1-CB2-OB2
48	AN	201	PEE	C20-C21-C22-C23
46	N1	402	PC1	C31-C32-C33-C34
46	A9	403	PC1	C28-C29-C2A-C2B
46	N5	701	PC1	C34-C35-C36-C37
48	AN	201	PEE	C21-C22-C23-C24
48	N1	406	PEE	C33-C34-C35-C36
48	N4	502	PEE	C20-C21-C22-C23
49	AC	201	ZMP	C1-C2-C3-C4
52	CB	203	3PE	C39-C3A-C3B-C3C
45	AL	203	CDL	C35-C36-C37-C38
46	N3	202	PC1	C25-C26-C27-C28
48	N3	204	PEE	C14-C15-C16-C17
51	AM	201	PLX	C35-C36-C37-C38
51	B5	201	PLX	C13-C14-C15-C16
45	N4	507	CDL	CB5-C51-C52-C53
48	N4	501	PEE	C30-C31-C32-C33
45	4L	201	CDL	C73-C74-C75-C76
48	AL	204	PEE	C31-C32-C33-C34
48	N3	204	PEE	C13-C14-C15-C16
48	N5	703	PEE	C13-C14-C15-C16
51	S7	302	PLX	C17-C18-C19-C20
51	S7	302	PLX	C30-C31-C32-C33
45	N4	505	CDL	C18-C19-C20-C21
51	B5	201	PLX	C17-C18-C19-C20
52	CB	202	3PE	C2B-C2C-C2D-C2E
45	4L	201	CDL	C72-C73-C74-C75
45	AL	201	CDL	C57-C58-C59-C60
48	B4	201	PEE	C21-C22-C23-C24
51	B5	201	PLX	C27-C28-C29-C30
52	CB	203	3PE	C2A-C2B-C2C-C2D
52	N4	506	3PE	C26-C27-C28-C29
48	AL	202	PEE	C35-C36-C37-C38
48	N1	406	PEE	C35-C36-C37-C38
46	A9	403	PC1	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
48	N4	502	PEE	C30-C31-C32-C33
45	A1	101	CDL	C57-C58-C59-C60
46	A3	201	PC1	C32-C33-C34-C35
48	AL	202	PEE	C33-C34-C35-C36
48	N4	501	PEE	C43-C44-C45-C46
48	S2	501	PEE	C14-C15-C16-C17
49	AB	201	ZMP	C6-C7-C8-C9
49	AC	201	ZMP	C2-C3-C4-C5
51	N4	503	PLX	C26-C27-C28-C29
46	A9	403	PC1	C11-C12-N-C14
46	N1	402	PC1	C11-C12-N-C13
46	N3	202	PC1	C11-C12-N-C13
45	4L	201	CDL	C15-C16-C17-C18
48	B6	201	PEE	C32-C33-C34-C35
48	N3	201	PEE	O4P-C4-C5-N
51	AM	201	PLX	C28-C29-C30-C31
45	N5	702	CDL	C72-C73-C74-C75
51	B5	201	PLX	C32-C33-C34-C35
48	A9	402	PEE	C14-C15-C16-C17
48	N4	501	PEE	C11-C12-C13-C14
51	N4	504	PLX	C15-C16-C17-C18
51	S7	302	PLX	C31-C32-C33-C34
45	A8	301	CDL	C54-C55-C56-C57
48	B6	201	PEE	C12-C13-C14-C15
48	N3	203	PEE	C12-C13-C14-C15
51	AM	201	PLX	C11-C10-C9-C8
45	A8	301	CDL	C32-C33-C34-C35
51	B5	201	PLX	C34-C35-C36-C37
48	N3	201	PEE	C23-C24-C25-C26
51	N4	503	PLX	C34-C35-C36-C37
48	N4	502	PEE	C11-C10-O2-C2
45	N4	505	CDL	C14-C15-C16-C17
48	B4	201	PEE	C12-C13-C14-C15
51	CB	201	PLX	O9-C24-C25-C26
48	B4	201	PEE	C20-C21-C22-C23
48	N3	204	PEE	C42-C43-C44-C45
48	A9	402	PEE	C35-C36-C37-C38
48	AN	201	PEE	C39-C40-C41-C42
48	N4	501	PEE	C39-C40-C41-C42
48	N4	502	PEE	C15-C16-C17-C18
46	N3	202	PC1	C3C-C3D-C3E-C3F
45	N4	505	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
48	N3	203	PEE	C21-C22-C23-C24
46	N1	402	PC1	C21-C22-C23-C24
45	N2	401	CDL	C72-C73-C74-C75
48	N5	703	PEE	C22-C23-C24-C25
48	N4	502	PEE	O4-C10-O2-C2
45	4L	201	CDL	C79-C80-C81-C82
45	B4	202	CDL	C13-C14-C15-C16
48	N3	203	PEE	C33-C34-C35-C36
45	N5	702	CDL	C39-C40-C41-C42
46	B5	203	PC1	C11-C12-N-C14
48	B6	201	PEE	C10-C11-C12-C13
45	A8	301	CDL	C16-C17-C18-C19
48	AL	202	PEE	C31-C32-C33-C34
48	S2	501	PEE	C31-C30-O3-C3
45	N2	401	CDL	C31-C32-C33-C34
45	N4	507	CDL	C37-C38-C39-C40
48	N3	204	PEE	C21-C22-C23-C24
45	B4	202	CDL	C76-C77-C78-C79
48	N1	404	PEE	C31-C32-C33-C34
51	CB	201	PLX	C10-C11-C12-C13
51	CB	201	PLX	C7-C8-C9-C10
51	S7	302	PLX	C7-C8-C9-C10
48	A9	402	PEE	C19-C20-C21-C22
48	N3	204	PEE	C35-C36-C37-C38
45	N5	702	CDL	CB5-C51-C52-C53
48	N3	203	PEE	C11-C12-C13-C14
51	CB	201	PLX	C30-C31-C32-C33
45	B5	202	CDL	C51-C52-C53-C54
46	N5	701	PC1	C2C-C2D-C2E-C2F
48	N1	406	PEE	C20-C21-C22-C23
51	N4	503	PLX	C7-C8-C9-C10
46	B5	203	PC1	C36-C37-C38-C39
51	N4	504	PLX	C32-C33-C34-C35
45	N4	505	CDL	C63-C64-C65-C66
45	AL	201	CDL	CB7-C71-C72-C73
46	A3	201	PC1	C33-C34-C35-C36
46	N1	402	PC1	C2C-C2D-C2E-C2F
48	A9	402	PEE	C11-C12-C13-C14
48	N1	404	PEE	C12-C13-C14-C15
48	N4	502	PEE	C11-C12-C13-C14
52	N5	704	3PE	C3B-C3C-C3D-C3E
45	B5	202	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
46	N3	202	PC1	O21-C2-C3-O31
45	4L	201	CDL	C23-C24-C25-C26
45	4L	201	CDL	C42-C43-C44-C45
48	N4	501	PEE	C33-C34-C35-C36
46	B5	203	PC1	C11-C12-N-C13
46	N3	202	PC1	C11-C12-N-C14
48	AL	204	PEE	C35-C36-C37-C38
48	AN	201	PEE	C35-C36-C37-C38
48	N1	406	PEE	C19-C20-C21-C22
48	N3	203	PEE	C15-C16-C17-C18
48	N4	501	PEE	C15-C16-C17-C18
48	N4	502	PEE	C19-C20-C21-C22
48	B6	201	PEE	C22-C23-C24-C25
50	AK	401	ADP	O4'-C4'-C5'-O5'
48	N1	406	PEE	C41-C42-C43-C44
49	AB	201	ZMP	C5-C6-C7-C8
49	AC	201	ZMP	C22-C23-C24-C25
45	N4	505	CDL	C77-C78-C79-C80
51	S7	302	PLX	C34-C35-C36-C37
48	S2	501	PEE	O5-C30-O3-C3
45	B4	202	CDL	CB3-OB5-PB2-OB2
45	B5	202	CDL	CB3-OB5-PB2-OB2
46	B5	203	PC1	C11-O13-P-O11
48	AL	204	PEE	C4-O4P-P-O3P
48	N1	406	PEE	C4-O4P-P-O3P
48	S2	501	PEE	C20-C21-C22-C23
45	A1	101	CDL	OA5-CA3-CA4-CA6
45	N4	507	CDL	OB5-CB3-CB4-CB6
46	N1	403	PC1	O11-C1-C2-C3
51	AM	201	PLX	O4-C3-C4-C5
49	AC	201	ZMP	C3-C4-C5-C6
45	N5	702	CDL	C40-C41-C42-C43
48	A9	402	PEE	C15-C16-C17-C18
48	B4	201	PEE	C35-C36-C37-C38
48	N5	703	PEE	C35-C36-C37-C38
48	N1	406	PEE	C13-C14-C15-C16
45	AL	201	CDL	C52-C53-C54-C55
46	N1	403	PC1	C24-C25-C26-C27
48	AL	204	PEE	C13-C14-C15-C16
48	N4	501	PEE	C34-C35-C36-C37
49	AB	201	ZMP	C4-C5-C6-C7
45	N5	702	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
45	AL	203	CDL	CB3-CB4-CB6-OB8
46	N3	202	PC1	C1-C2-C3-O31
48	AL	204	PEE	C11-C12-C13-C14
48	B4	201	PEE	C41-C42-C43-C44
48	B6	201	PEE	C1-C2-C3-O3
48	S2	501	PEE	C1-C2-C3-O3
51	AM	201	PLX	C10-C11-C12-C13
51	N4	503	PLX	C3-C4-C5-O8
52	N4	506	3PE	C1-C2-C3-O31
51	S7	302	PLX	C14-C15-C16-C17
48	N1	406	PEE	C22-C23-C24-C25
51	N4	504	PLX	C10-C11-C12-C13
52	CB	202	3PE	C38-C39-C3A-C3B
52	N4	506	3PE	C35-C36-C37-C38
48	AL	202	PEE	C30-C31-C32-C33
51	S7	302	PLX	O6-C6-C7-C8
49	AB	201	ZMP	O3-C16-C17-O4
49	AC	201	ZMP	O3-C16-C17-O4
51	S7	302	PLX	C33-C34-C35-C36
48	N1	406	PEE	C39-C40-C41-C42
48	N3	204	PEE	C19-C20-C21-C22
48	N4	501	PEE	C35-C36-C37-C38
48	N4	502	PEE	C35-C36-C37-C38
48	S2	501	PEE	C35-C36-C37-C38
45	B4	202	CDL	CB5-C51-C52-C53
45	N5	702	CDL	C12-C13-C14-C15
46	N1	402	PC1	C33-C34-C35-C36
46	AN	202	PC1	C21-C22-C23-C24
48	N4	502	PEE	C10-C11-C12-C13
45	N4	507	CDL	C20-C21-C22-C23
48	AL	204	PEE	C1-C2-O2-C10
48	N3	204	PEE	C3-C2-O2-C10
48	B4	201	PEE	C11-C12-C13-C14
51	N4	504	PLX	C25-C26-C27-C28
45	N5	702	CDL	C11-C12-C13-C14
48	A9	402	PEE	C34-C35-C36-C37
45	B5	202	CDL	OB5-CB3-CB4-OB6
48	AL	202	PEE	O3P-C1-C2-O2
46	N1	402	PC1	C11-C12-N-C15
45	N4	505	CDL	CB5-C51-C52-C53
51	N4	503	PLX	C30-C31-C32-C33
46	A3	201	PC1	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
46	A9	403	PC1	C32-C33-C34-C35
48	N4	501	PEE	C14-C15-C16-C17
45	A8	301	CDL	C11-C12-C13-C14
45	A1	101	CDL	OB6-CB4-CB6-OB8
48	AL	202	PEE	O2-C2-C3-O3
45	N5	702	CDL	C56-C57-C58-C59
48	N5	703	PEE	C12-C13-C14-C15
51	CB	201	PLX	C26-C27-C28-C29
46	N1	402	PC1	C22-C23-C24-C25
48	S2	501	PEE	C38-C39-C40-C41
46	A9	403	PC1	C35-C36-C37-C38
48	N3	203	PEE	C43-C44-C45-C46
51	B5	201	PLX	C36-C37-C38-C39
47	A9	401	NDP	PN-O3-PA-O1A
48	N5	703	PEE	C31-C32-C33-C34
49	AB	201	ZMP	C22-C23-C24-C25
51	CB	201	PLX	C16-C17-C18-C19
48	N4	502	PEE	C22-C23-C24-C25
51	S7	302	PLX	C25-C26-C27-C28
51	AM	201	PLX	C30-C31-C32-C33
46	N3	202	PC1	C2D-C2E-C2F-C2G
48	AN	201	PEE	C41-C42-C43-C44
48	B6	201	PEE	C15-C16-C17-C18
48	B4	201	PEE	C17-C18-C19-C20
48	S2	501	PEE	C17-C18-C19-C20
46	A9	403	PC1	O11-C1-C2-C3
46	N1	402	PC1	O11-C1-C2-C3
48	N3	201	PEE	O3P-C1-C2-C3
48	N4	502	PEE	O3P-C1-C2-C3
48	B6	201	PEE	C31-C32-C33-C34
48	N1	404	PEE	O4P-C4-C5-N
48	N1	406	PEE	O4P-C4-C5-N
51	CB	201	PLX	C25-C26-C27-C28
51	N4	504	PLX	C12-C13-C14-C15
48	N4	501	PEE	C23-C24-C25-C26
51	CB	201	PLX	C14-C15-C16-C17
59	V1	502	FMN	O2'-C2'-C3'-C4'
51	B5	201	PLX	C16-C17-C18-C19
51	S7	302	PLX	C26-C27-C28-C29
45	N1	401	CDL	CB7-C71-C72-C73
48	N4	501	PEE	C41-C42-C43-C44
45	AL	201	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
45	AL	203	CDL	CB4-CB3-OB5-PB2
51	N4	504	PLX	C4-C3-O4-P1
46	N3	202	PC1	C2F-C2G-C2H-C2I
48	S2	501	PEE	C40-C41-C42-C43
48	B4	201	PEE	C13-C14-C15-C16
45	A1	101	CDL	CB3-CB4-CB6-OB8
48	AL	202	PEE	C1-C2-C3-O3
52	CB	203	3PE	C26-C27-C28-C29
49	AB	201	ZMP	N2-C16-C17-C18
46	N1	402	PC1	C11-C12-N-C14
46	N3	202	PC1	C2A-C2B-C2C-C2D
48	N4	502	PEE	C24-C25-C26-C27
51	B5	201	PLX	C5-C4-O6-C6
45	A1	101	CDL	C76-C77-C78-C79
48	N4	501	PEE	C24-C25-C26-C27
45	AL	203	CDL	C15-C16-C17-C18
45	AL	203	CDL	C74-C75-C76-C77
46	N1	403	PC1	O11-C1-C2-O21
46	N5	701	PC1	O11-C1-C2-O21
48	N3	203	PEE	O3P-C1-C2-O2
48	B6	201	PEE	C33-C34-C35-C36
48	N3	201	PEE	C21-C22-C23-C24
45	N4	505	CDL	C81-C82-C83-C84
48	B6	201	PEE	O2-C2-C3-O3
51	CB	201	PLX	O6-C4-C5-O8
52	CB	203	3PE	O21-C2-C3-O31
48	N1	406	PEE	C18-C19-C20-C21
48	AN	201	PEE	C12-C13-C14-C15
45	A8	301	CDL	CA2-C1-CB2-OB2
45	N1	401	CDL	CA2-C1-CB2-OB2
45	N4	505	CDL	C41-C42-C43-C44
45	N1	401	CDL	C75-C76-C77-C78
48	N4	501	PEE	C40-C41-C42-C43
48	B4	201	PEE	C33-C34-C35-C36
45	AL	203	CDL	C1-CB2-OB2-PB2
45	B4	202	CDL	C1-CA2-OA2-PA1
46	N1	402	PC1	C2-C1-O11-P
45	AL	201	CDL	C54-C55-C56-C57
45	N4	505	CDL	C22-C23-C24-C25
51	AM	201	PLX	C20-C21-C22-C23
45	N4	507	CDL	C23-C24-C25-C26
48	B4	201	PEE	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
51	N4	504	PLX	C7-C8-C9-C10
51	CB	201	PLX	O6-C6-C7-C8
51	N4	504	PLX	O8-C24-C25-C26
45	B5	202	CDL	OA5-CA3-CA4-CA6
48	N4	501	PEE	O3P-C1-C2-C3
45	A8	301	CDL	C21-C22-C23-C24
48	N4	502	PEE	C21-C22-C23-C24
48	N3	204	PEE	C22-C23-C24-C25
45	4L	201	CDL	C40-C41-C42-C43
53	N1	405	U10	C13-C14-C16-C17
48	N3	203	PEE	C30-C31-C32-C33
45	N1	401	CDL	CB3-CB4-CB6-OB8
45	N4	507	CDL	CB4-CB3-OB5-PB2
48	AL	204	PEE	C2-C1-O3P-P
48	B4	201	PEE	C1-C2-C3-O3
52	CB	202	3PE	C2-C1-O11-P
45	B5	202	CDL	OA5-CA3-CA4-OA6
46	A9	403	PC1	O11-C1-C2-O21
46	N1	402	PC1	O11-C1-C2-O21
48	N1	404	PEE	O3P-C1-C2-O2
48	N3	201	PEE	O3P-C1-C2-O2
52	CB	203	3PE	O11-C1-C2-O21
57	S2	502	MF8	N06-C04-N02-C01
45	N4	505	CDL	C57-C58-C59-C60
51	N4	503	PLX	C6-C7-C8-C9
45	A1	101	CDL	C61-C62-C63-C64
48	N4	501	PEE	C31-C32-C33-C34
45	N4	505	CDL	C79-C80-C81-C82
45	N4	505	CDL	OA6-CA4-CA6-OA8
48	B4	201	PEE	O2-C2-C3-O3
52	N4	506	3PE	O21-C2-C3-O31
48	N3	201	PEE	C22-C23-C24-C25
51	CB	201	PLX	C27-C28-C29-C30
45	A1	101	CDL	C51-C52-C53-C54
48	AN	201	PEE	C15-C16-C17-C18
53	N1	405	U10	C15-C14-C16-C17
45	N4	507	CDL	C13-C14-C15-C16
46	N5	701	PC1	C26-C27-C28-C29
45	N4	507	CDL	C15-C16-C17-C18
45	N4	507	CDL	C56-C57-C58-C59
48	N5	703	PEE	C20-C21-C22-C23
46	B5	203	PC1	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
48	AN	201	PEE	C17-C18-C19-C20
48	B6	201	PEE	C35-C36-C37-C38
45	B4	202	CDL	CA2-OA2-PA1-OA5
45	N1	401	CDL	CB3-OB5-PB2-OB2
45	N2	401	CDL	CA3-OA5-PA1-OA2
48	N1	404	PEE	C1-O3P-P-O4P
48	N4	501	PEE	C4-O4P-P-O3P
51	CB	201	PLX	C2-O1-P1-O4
51	N4	504	PLX	C2-O1-P1-O4
52	B8	201	3PE	C1-O11-P-O13
45	AL	201	CDL	C44-C45-C46-C47
51	S7	302	PLX	C32-C33-C34-C35
45	AL	201	CDL	CA4-CA3-OA5-PA1
45	N1	401	CDL	C1-CA2-OA2-PA1
46	N1	403	PC1	C2-C1-O11-P
48	B4	201	PEE	C14-C15-C16-C17
48	N1	404	PEE	C14-C15-C16-C17
45	A1	101	CDL	CB2-OB2-PB2-OB3
45	AL	203	CDL	CA3-OA5-PA1-OA3
45	AL	203	CDL	CA3-OA5-PA1-OA4
45	AL	203	CDL	CB2-OB2-PB2-OB3
45	B4	202	CDL	CB3-OB5-PB2-OB3
45	B5	202	CDL	CA3-OA5-PA1-OA3
45	B5	202	CDL	CB3-OB5-PB2-OB3
45	N1	401	CDL	CA2-OA2-PA1-OA4
45	N1	401	CDL	CB2-OB2-PB2-OB4
45	N2	401	CDL	CA3-OA5-PA1-OA3
45	N4	505	CDL	CA3-OA5-PA1-OA3
45	N4	507	CDL	CA2-OA2-PA1-OA4
46	A3	201	PC1	C11-O13-P-O14
46	A3	201	PC1	C1-O11-P-O14
46	A9	403	PC1	C1-O11-P-O14
46	N1	402	PC1	C11-O13-P-O14
46	N1	403	PC1	C1-O11-P-O14
46	N5	701	PC1	C1-O11-P-O12
48	AL	204	PEE	C4-O4P-P-O2P
48	N1	406	PEE	C4-O4P-P-O2P
48	N1	406	PEE	C4-O4P-P-O1P
48	N3	201	PEE	C4-O4P-P-O2P
48	N3	203	PEE	C1-O3P-P-O1P
48	N4	502	PEE	C1-O3P-P-O2P
48	N4	502	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
48	N4	502	PEE	C4-O4P-P-O1P
50	AK	401	ADP	C5'-O5'-PA-O2A
51	B5	201	PLX	C3-O4-P1-O3
51	CB	201	PLX	C2-C1-N1-C1C
52	B8	201	3PE	C11-O13-P-O12
52	B8	201	3PE	C11-O13-P-O14
52	CB	202	3PE	C11-O13-P-O12
52	CB	203	3PE	C1-O11-P-O14
52	CB	203	3PE	C11-O13-P-O12
52	N5	704	3PE	C1-O11-P-O14
51	CB	201	PLX	C33-C34-C35-C36
48	AL	202	PEE	O3P-C1-C2-C3
48	N1	404	PEE	O3P-C1-C2-C3
48	N3	203	PEE	O3P-C1-C2-C3
51	N4	503	PLX	O4-C3-C4-C5
49	AC	201	ZMP	C14-C15-N2-C16
45	A1	101	CDL	C80-C81-C82-C83
48	B4	201	PEE	C23-C24-C25-C26
48	S2	501	PEE	C37-C38-C39-C40
45	N2	401	CDL	C12-C13-C14-C15
46	A3	201	PC1	C12-C11-O13-P
46	N5	701	PC1	C12-C11-O13-P
48	B6	201	PEE	C5-C4-O4P-P
48	N1	404	PEE	C5-C4-O4P-P
48	N3	201	PEE	C5-C4-O4P-P
51	CB	201	PLX	C25-C24-O8-C5
52	CB	202	3PE	C12-C11-O13-P
48	N3	204	PEE	C24-C25-C26-C27
51	N4	504	PLX	C16-C17-C18-C19
48	S2	501	PEE	C11-C12-C13-C14
51	S7	302	PLX	C11-C10-C9-C8
53	N1	405	U10	C40-C39-C41-C42
45	N1	401	CDL	OA5-CA3-CA4-OA6
45	N4	505	CDL	OB5-CB3-CB4-OB6
45	N4	507	CDL	OB5-CB3-CB4-OB6
48	N4	501	PEE	O3P-C1-C2-O2
51	AM	201	PLX	O4-C3-C4-O6
51	N4	503	PLX	O4-C3-C4-O6
59	V1	502	FMN	N10-C1'-C2'-C3'
48	AN	201	PEE	C24-C25-C26-C27
45	N4	505	CDL	C19-C20-C21-C22
51	N4	504	PLX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
45	N4	505	CDL	C75-C76-C77-C78
46	N5	701	PC1	C11-C12-N-C13
51	CB	201	PLX	C2-C1-N1-C1A
46	B5	203	PC1	C3B-C3C-C3D-C3E
52	N5	704	3PE	C3A-C3B-C3C-C3D
45	A8	301	CDL	C38-C39-C40-C41
45	N2	401	CDL	C11-C12-C13-C14
46	A3	201	PC1	O13-C11-C12-N
46	N1	403	PC1	O13-C11-C12-N
46	N5	701	PC1	O13-C11-C12-N
48	N4	502	PEE	C1-C2-C3-O3
45	B4	202	CDL	OB6-CB4-CB6-OB8
48	N4	502	PEE	O2-C2-C3-O3
48	S2	501	PEE	O2-C2-C3-O3
51	CB	201	PLX	C13-C14-C15-C16
51	N4	503	PLX	C11-C10-C9-C8
48	B6	201	PEE	C14-C15-C16-C17
48	N1	406	PEE	C11-C12-C13-C14
52	CB	202	3PE	C24-C25-C26-C27
45	N4	505	CDL	CB4-CB3-OB5-PB2
46	B5	203	PC1	C2-C1-O11-P
51	N4	503	PLX	C14-C15-C16-C17
45	AL	203	CDL	CA5-C11-C12-C13
51	N4	503	PLX	O6-C6-C7-C8
45	AL	203	CDL	C31-C32-C33-C34
48	S2	501	PEE	C33-C34-C35-C36
45	N4	505	CDL	C33-C34-C35-C36
45	N4	507	CDL	C61-C62-C63-C64
51	N4	503	PLX	O7-C6-C7-C8
52	CB	202	3PE	C26-C27-C28-C29
49	AC	201	ZMP	C19-C18-C21-O5
49	AC	201	ZMP	C20-C18-C21-O5
48	A9	402	PEE	C33-C34-C35-C36
45	B4	202	CDL	C77-C78-C79-C80
45	4L	201	CDL	CA6-CA4-OA6-CA5
48	N1	406	PEE	C3-C2-O2-C10
45	AL	201	CDL	OB5-CB3-CB4-CB6
45	B5	202	CDL	OB5-CB3-CB4-CB6
46	N5	701	PC1	O11-C1-C2-C3
48	N1	406	PEE	O3P-C1-C2-C3
45	A8	301	CDL	C18-C19-C20-C21
45	N1	401	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
45	N2	401	CDL	C1-CA2-OA2-PA1
52	CB	203	3PE	C2-C1-O11-P
45	A1	101	CDL	C71-C72-C73-C74
45	A1	101	CDL	OA5-CA3-CA4-OA6
52	N5	704	3PE	C32-C33-C34-C35
48	B4	201	PEE	C15-C16-C17-C18
45	B4	202	CDL	C72-C73-C74-C75
45	B4	202	CDL	C72-C71-CB7-OB8
45	AL	201	CDL	CB3-OB5-PB2-OB2
45	N1	401	CDL	CB2-OB2-PB2-OB5
45	N4	505	CDL	CB3-OB5-PB2-OB2
45	N4	507	CDL	CB2-OB2-PB2-OB5
46	A9	403	PC1	C11-O13-P-O11
48	N3	204	PEE	C4-O4P-P-O3P
51	S7	302	PLX	C3-O4-P1-O1
52	CB	202	3PE	C1-O11-P-O13
52	CB	203	3PE	C1-O11-P-O13
45	B4	202	CDL	CB3-CB4-CB6-OB8
45	N4	505	CDL	CA3-CA4-CA6-OA8
48	N1	404	PEE	C32-C33-C34-C35
52	N4	506	3PE	C25-C26-C27-C28
46	AN	202	PC1	C11-C12-N-C14
52	N5	704	3PE	C28-C29-C2A-C2B
45	A1	101	CDL	C1-CB2-OB2-PB2
45	N4	505	CDL	C1-CA2-OA2-PA1
48	N1	404	PEE	C34-C35-C36-C37
51	N4	504	PLX	C13-C14-C15-C16
57	S2	502	MF8	N08-C07-N06-C04
59	V1	502	FMN	O2'-C2'-C3'-O3'
48	N5	703	PEE	C15-C16-C17-C18
45	A8	301	CDL	C55-C56-C57-C58
48	AL	204	PEE	C38-C39-C40-C41
46	N5	701	PC1	C11-C12-N-C15
48	AL	204	PEE	O3P-C1-C2-C3
52	CB	203	3PE	O11-C1-C2-C3
47	A9	401	NDP	O4D-C1D-N1N-C6N
45	A1	101	CDL	C21-C22-C23-C24
46	A3	201	PC1	C23-C24-C25-C26
45	A1	101	CDL	OB5-CB3-CB4-OB6
57	S2	502	MF8	N06-C04-N02-C03
52	N4	506	3PE	C33-C34-C35-C36
49	AB	201	ZMP	O3-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
45	A1	101	CDL	C81-C82-C83-C84
51	N4	504	PLX	C6-C7-C8-C9
45	N4	507	CDL	OB6-CB4-CB6-OB8
51	N4	504	PLX	C36-C37-C38-C39
48	AL	202	PEE	C2-C1-O3P-P
51	B5	201	PLX	C4-C3-O4-P1
59	V1	502	FMN	C4'-C5'-O5'-P
48	N3	203	PEE	C44-C45-C46-C47
51	S7	302	PLX	C15-C16-C17-C18
51	CB	201	PLX	C2-C1-N1-C1B
49	AB	201	ZMP	C1-C2-C3-C4
45	A1	101	CDL	C52-C53-C54-C55
45	N4	507	CDL	C55-C56-C57-C58
48	N3	201	PEE	C15-C16-C17-C18
53	N1	405	U10	C20-C19-C21-C22
45	B4	202	CDL	C35-C36-C37-C38
51	S7	302	PLX	C9-C10-C11-C12
48	AN	201	PEE	C44-C45-C46-C47
49	AB	201	ZMP	C2-C3-C4-C5
45	N4	507	CDL	CB3-CB4-CB6-OB8
51	CB	201	PLX	C3-C4-C5-O8
48	N3	201	PEE	C32-C33-C34-C35
48	N3	203	PEE	C14-C15-C16-C17
49	AB	201	ZMP	C3-C4-C5-C6
48	N5	703	PEE	C3-C2-O2-C10
48	N4	502	PEE	C32-C33-C34-C35
46	N5	701	PC1	C11-C12-N-C14
51	B5	201	PLX	C3-C4-O6-C6
57	S2	502	MF8	N05-C04-N02-C01
47	A9	401	NDP	C2D-C1D-N1N-C6N
46	A9	403	PC1	C26-C27-C28-C29
46	A3	201	PC1	C2A-C2B-C2C-C2D
45	A1	101	CDL	C20-C21-C22-C23
48	S2	501	PEE	C13-C14-C15-C16
48	AL	202	PEE	C44-C45-C46-C47
45	N4	505	CDL	OB5-CB3-CB4-CB6
48	B4	201	PEE	C36-C37-C38-C39
48	B6	201	PEE	C23-C24-C25-C26
51	AM	201	PLX	C16-C17-C18-C19
48	N3	203	PEE	C22-C23-C24-C25
51	AM	201	PLX	C27-C28-C29-C30
45	A8	301	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
47	A9	401	NDP	O4B-C4B-C5B-O5B
45	N4	507	CDL	C32-C33-C34-C35
49	AB	201	ZMP	C1-C22-C23-C24
45	AL	201	CDL	C32-C31-CA7-OA8
46	N5	701	PC1	C2B-C2C-C2D-C2E
45	N4	507	CDL	OA6-CA4-CA6-OA8
48	N5	703	PEE	C44-C45-C46-C47
48	N4	501	PEE	C37-C38-C39-C40
45	B5	202	CDL	CB2-C1-CA2-OA2
48	N3	203	PEE	C20-C21-C22-C23
46	B5	203	PC1	C35-C36-C37-C38
45	N5	702	CDL	C55-C56-C57-C58
45	AL	201	CDL	C52-C51-CB5-OB6
46	B5	203	PC1	O31-C31-C32-C33
52	N4	506	3PE	C37-C38-C39-C3A
51	AM	201	PLX	C17-C18-C19-C20
48	N1	406	PEE	C12-C13-C14-C15
48	N3	201	PEE	C38-C39-C40-C41
48	S2	501	PEE	C16-C17-C18-C19
45	AL	201	CDL	OB5-CB3-CB4-OB6
52	N4	506	3PE	O11-C1-C2-O21
49	AC	201	ZMP	S1-C10-C9-C8
45	A1	101	CDL	CB5-C51-C52-C53
51	N4	504	PLX	O6-C6-C7-C8
46	A9	403	PC1	C38-C39-C3A-C3B
45	A1	101	CDL	OB5-CB3-CB4-CB6
45	A8	301	CDL	OA5-CA3-CA4-CA6
45	B4	202	CDL	OA5-CA3-CA4-CA6
53	N1	405	U10	C29-C31-C32-C33
48	AL	202	PEE	C38-C39-C40-C41
45	N2	401	CDL	C13-C14-C15-C16
45	A8	301	CDL	C32-C31-CA7-OA8
51	N4	503	PLX	C12-C13-C14-C15
48	AL	204	PEE	C1-O3P-P-O4P
53	N1	405	U10	C38-C39-C41-C42
48	N3	204	PEE	C41-C42-C43-C44
45	AL	201	CDL	C41-C42-C43-C44
45	N1	401	CDL	C14-C15-C16-C17
51	CB	201	PLX	C31-C32-C33-C34
51	AM	201	PLX	C31-C32-C33-C34
45	N5	702	CDL	C12-C11-CA5-OA6
48	N3	201	PEE	O2-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
48	N4	501	PEE	C38-C39-C40-C41
48	N5	703	PEE	C16-C17-C18-C19
46	N1	403	PC1	C1-C2-O21-C21
48	N5	703	PEE	C1-C2-O2-C10
46	N1	403	PC1	C33-C34-C35-C36
45	A1	101	CDL	C52-C51-CB5-OB6
45	A1	101	CDL	C72-C71-CB7-OB8
45	AL	203	CDL	C72-C71-CB7-OB8
48	AL	204	PEE	O2-C10-C11-C12
52	N4	506	3PE	O21-C21-C22-C23
53	N1	405	U10	C44-C46-C47-C48
48	N3	204	PEE	C36-C37-C38-C39
46	B5	203	PC1	C39-C3A-C3B-C3C
46	AN	202	PC1	C2-C1-O11-P
45	4L	201	CDL	C75-C76-C77-C78
45	A8	301	CDL	OA5-CA3-CA4-OA6
48	N1	406	PEE	O3P-C1-C2-O2
45	N2	401	CDL	C72-C71-CB7-OB8
45	N5	702	CDL	C72-C71-CB7-OB8
45	N2	401	CDL	C35-C36-C37-C38
51	S7	302	PLX	C6-C7-C8-C9
46	A3	201	PC1	C22-C23-C24-C25
48	A9	402	PEE	C18-C19-C20-C21
48	N3	204	PEE	C16-C17-C18-C19
48	N5	703	PEE	C38-C39-C40-C41
48	S2	501	PEE	C18-C19-C20-C21
45	N1	401	CDL	O1-C1-CB2-OB2
48	N4	502	PEE	O2-C10-C11-C12
46	A9	403	PC1	C3B-C3C-C3D-C3E
46	N5	701	PC1	O21-C21-C22-C23
48	AN	201	PEE	O2-C10-C11-C12
48	N3	201	PEE	O3-C30-C31-C32
48	N3	204	PEE	O2-C10-C11-C12
46	B5	203	PC1	C37-C38-C39-C3A
45	A1	101	CDL	OA6-CA4-CA6-OA8
46	N1	402	PC1	O21-C2-C3-O31
48	N4	501	PEE	C10-C11-C12-C13
45	4L	201	CDL	C12-C11-CA5-OA6
48	AN	201	PEE	O3-C30-C31-C32
48	B6	201	PEE	O3-C30-C31-C32
51	S7	302	PLX	O9-C24-C25-C26
46	N5	701	PC1	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
45	N1	401	CDL	C12-C11-CA5-OA6
45	B5	202	CDL	C74-C75-C76-C77
48	N5	703	PEE	C32-C33-C34-C35
48	AL	202	PEE	O2-C10-C11-C12
46	B5	203	PC1	C2E-C2F-C2G-C2H
48	A9	402	PEE	C12-C13-C14-C15
45	N4	507	CDL	C12-C11-CA5-OA6
45	A1	101	CDL	C72-C71-CB7-OB9
45	B4	202	CDL	C79-C80-C81-C82
45	B5	202	CDL	C23-C24-C25-C26
45	B4	202	CDL	CB7-C71-C72-C73
48	N4	501	PEE	O2-C10-C11-C12
48	N4	502	PEE	C34-C35-C36-C37
46	B5	203	PC1	C28-C29-C2A-C2B
45	A1	101	CDL	C52-C51-CB5-OB7
45	A8	301	CDL	C32-C31-CA7-OA9
46	A9	403	PC1	C33-C34-C35-C36
45	N2	401	CDL	C72-C71-CB7-OB9
48	N3	201	PEE	O4-C10-C11-C12
45	A1	101	CDL	C58-C59-C60-C61
52	CB	203	3PE	C1-C2-C3-O31
45	N5	702	CDL	C12-C11-CA5-OA7
48	N4	502	PEE	O4-C10-C11-C12
48	N5	703	PEE	C2-C3-O3-C30
45	AL	201	CDL	C42-C43-C44-C45
48	N1	404	PEE	O4-C10-O2-C2
45	N5	702	CDL	CA4-CA3-OA5-PA1
46	N5	701	PC1	C2-C1-O11-P
45	4L	201	CDL	C12-C11-CA5-OA7
48	B6	201	PEE	O5-C30-C31-C32
46	N1	403	PC1	C2E-C2F-C2G-C2H
45	A1	101	CDL	C33-C34-C35-C36
45	A8	301	CDL	CA3-OA5-PA1-OA3
45	B4	202	CDL	CB3-OB5-PB2-OB4
45	B5	202	CDL	CA2-OA2-PA1-OA3
45	N4	505	CDL	CA2-OA2-PA1-OA3
46	AN	202	PC1	C11-C12-N-C15
48	B4	201	PEE	C1-O3P-P-O1P
48	B4	201	PEE	C4-O4P-P-O1P
48	N1	404	PEE	C1-O3P-P-O1P
48	N3	204	PEE	C1-O3P-P-O1P
48	N3	204	PEE	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
48	N4	501	PEE	C4-O4P-P-O1P
48	S2	501	PEE	C1-O3P-P-O1P
51	N4	503	PLX	C2-O1-P1-O3
51	N4	504	PLX	C2-O1-P1-O2
46	N3	202	PC1	C2C-C2D-C2E-C2F
51	CB	201	PLX	C15-C16-C17-C18
45	AL	203	CDL	C72-C71-CB7-OB9
45	N5	702	CDL	C72-C71-CB7-OB9
48	AL	204	PEE	O4-C10-C11-C12
48	AN	201	PEE	O4-C10-C11-C12
48	N3	204	PEE	O4-C10-C11-C12
45	N1	401	CDL	OB5-CB3-CB4-CB6
45	N4	507	CDL	C21-C22-C23-C24
52	CB	202	3PE	C25-C26-C27-C28
57	S2	502	MF8	N09-C07-N06-C04
45	AL	203	CDL	C11-C12-C13-C14
48	N4	501	PEE	O4-C10-C11-C12
52	N4	506	3PE	O22-C21-C22-C23
51	N4	504	PLX	C27-C28-C29-C30
45	B4	202	CDL	C73-C74-C75-C76
52	CB	202	3PE	C29-C2A-C2B-C2C
48	AN	201	PEE	C23-C24-C25-C26
46	AN	202	PC1	C12-C11-O13-P
48	A9	402	PEE	C5-C4-O4P-P
48	N3	204	PEE	C5-C4-O4P-P
51	S7	302	PLX	C25-C24-O8-C5
52	N5	704	3PE	C12-C11-O13-P
48	AN	201	PEE	O5-C30-C31-C32
45	A8	301	CDL	C72-C73-C74-C75
46	A3	201	PC1	C39-C3A-C3B-C3C
45	N2	401	CDL	C33-C34-C35-C36
46	AN	202	PC1	C11-C12-N-C13
48	AN	201	PEE	C38-C39-C40-C41
45	N5	702	CDL	C52-C51-CB5-OB6
48	N1	406	PEE	O2-C10-C11-C12
45	B4	202	CDL	C83-C84-C85-C86
48	N5	703	PEE	C24-C25-C26-C27
45	A1	101	CDL	C32-C31-CA7-OA8
45	N1	401	CDL	C12-C11-CA5-OA7
48	N3	201	PEE	O5-C30-C31-C32
45	AL	201	CDL	C78-C79-C80-C81
48	N3	203	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
48	N3	203	PEE	C2-C1-O3P-P
53	N1	405	U10	C18-C19-C21-C22
45	4L	201	CDL	C32-C31-CA7-OA9
46	N5	701	PC1	O22-C21-C22-C23
48	N4	501	PEE	O5-C30-C31-C32
45	N4	505	CDL	C31-C32-C33-C34
48	N4	501	PEE	O3-C30-C31-C32
45	A8	301	CDL	C34-C35-C36-C37
48	N3	204	PEE	C33-C34-C35-C36
45	4L	201	CDL	C32-C31-CA7-OA8
45	N4	507	CDL	C12-C11-CA5-OA7
45	A8	301	CDL	C58-C59-C60-C61
45	N5	702	CDL	C71-C72-C73-C74
51	CB	201	PLX	C6-C7-C8-C9
48	A9	402	PEE	O2-C10-C11-C12
45	A1	101	CDL	C32-C31-CA7-OA9
48	N3	201	PEE	C36-C37-C38-C39
48	N1	406	PEE	O4-C10-C11-C12
45	4L	201	CDL	C52-C51-CB5-OB6
46	N1	403	PC1	O21-C21-C22-C23

There are no ring outliers.

51 monomers are involved in 188 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	N5	702	CDL	1	0
48	B6	201	PEE	2	0
52	B8	201	3PE	1	0
46	B5	203	PC1	4	0
48	AN	201	PEE	2	0
46	A3	201	PC1	2	0
48	AL	204	PEE	3	0
45	A1	101	CDL	10	0
51	AM	201	PLX	5	0
45	N1	401	CDL	2	0
54	V1	501	SF4	1	0
48	B4	201	PEE	7	0
59	V1	502	FMN	1	0
51	B5	201	PLX	9	0
48	N1	406	PEE	6	0
51	N4	503	PLX	4	0
45	B5	202	CDL	6	0

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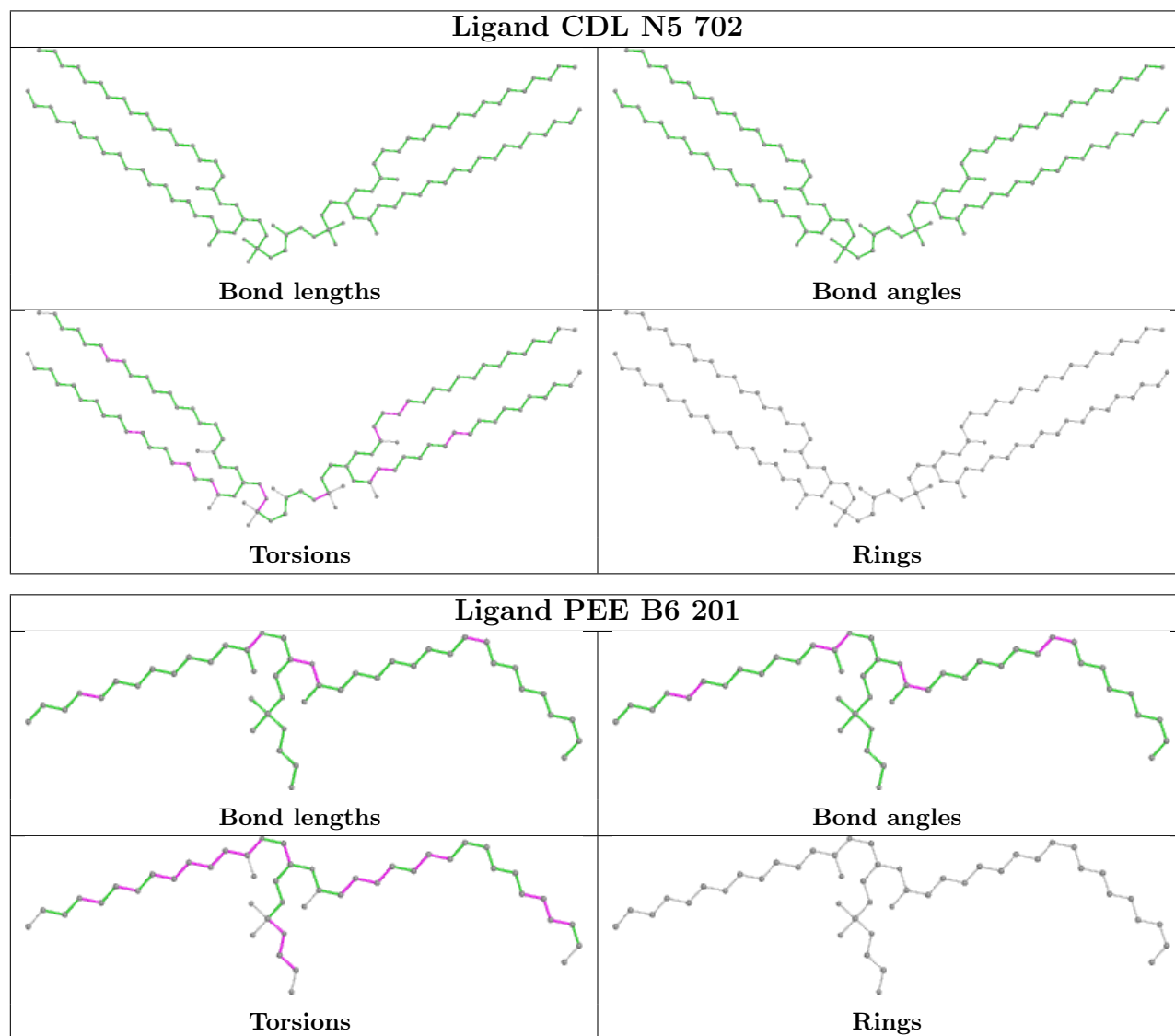


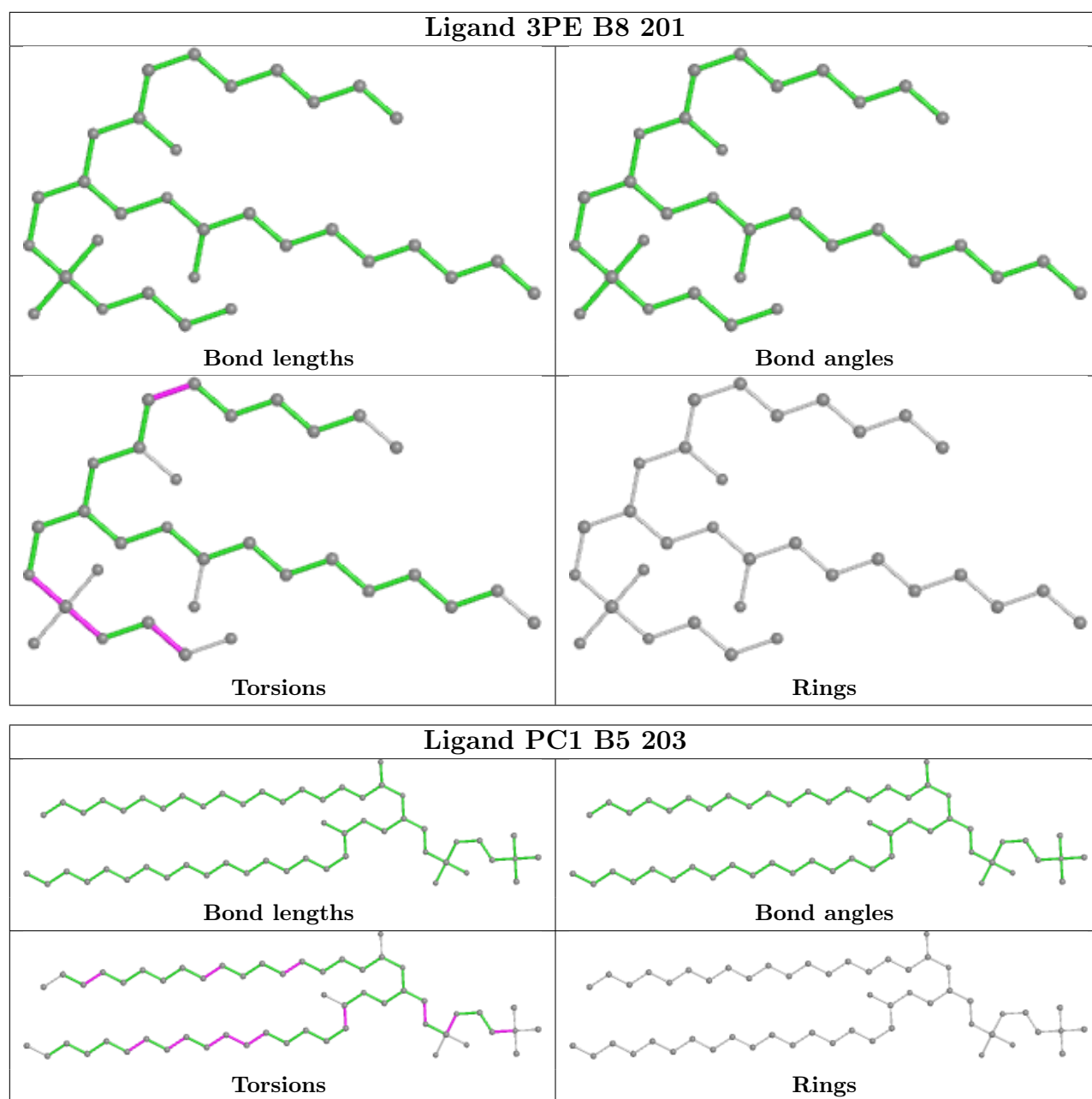
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	A8	301	CDL	4	0
45	N4	507	CDL	10	0
45	N2	401	CDL	1	0
46	AN	202	PC1	4	0
48	N3	201	PEE	5	0
52	N4	506	3PE	5	0
52	N5	704	3PE	5	0
46	A9	403	PC1	2	0
50	AK	401	ADP	4	0
51	CB	201	PLX	6	0
46	N1	403	PC1	3	0
48	N4	501	PEE	6	0
51	S7	302	PLX	6	0
48	N1	404	PEE	1	0
45	AL	201	CDL	8	0
46	N5	701	PC1	10	0
46	N3	202	PC1	2	0
53	N1	405	U10	8	0
52	CB	203	3PE	1	0
49	AB	201	ZMP	2	0
48	N5	703	PEE	4	0
48	N3	203	PEE	9	0
49	AC	201	ZMP	3	0
52	CB	202	3PE	3	0
45	N4	505	CDL	9	0
51	N4	504	PLX	4	0
48	N3	204	PEE	1	0
45	B4	202	CDL	1	0
45	4L	201	CDL	7	0
46	N1	402	PC1	1	0
45	AL	203	CDL	3	0
48	N4	502	PEE	4	0
54	S1	802	SF4	1	0
54	S7	301	SF4	1	0

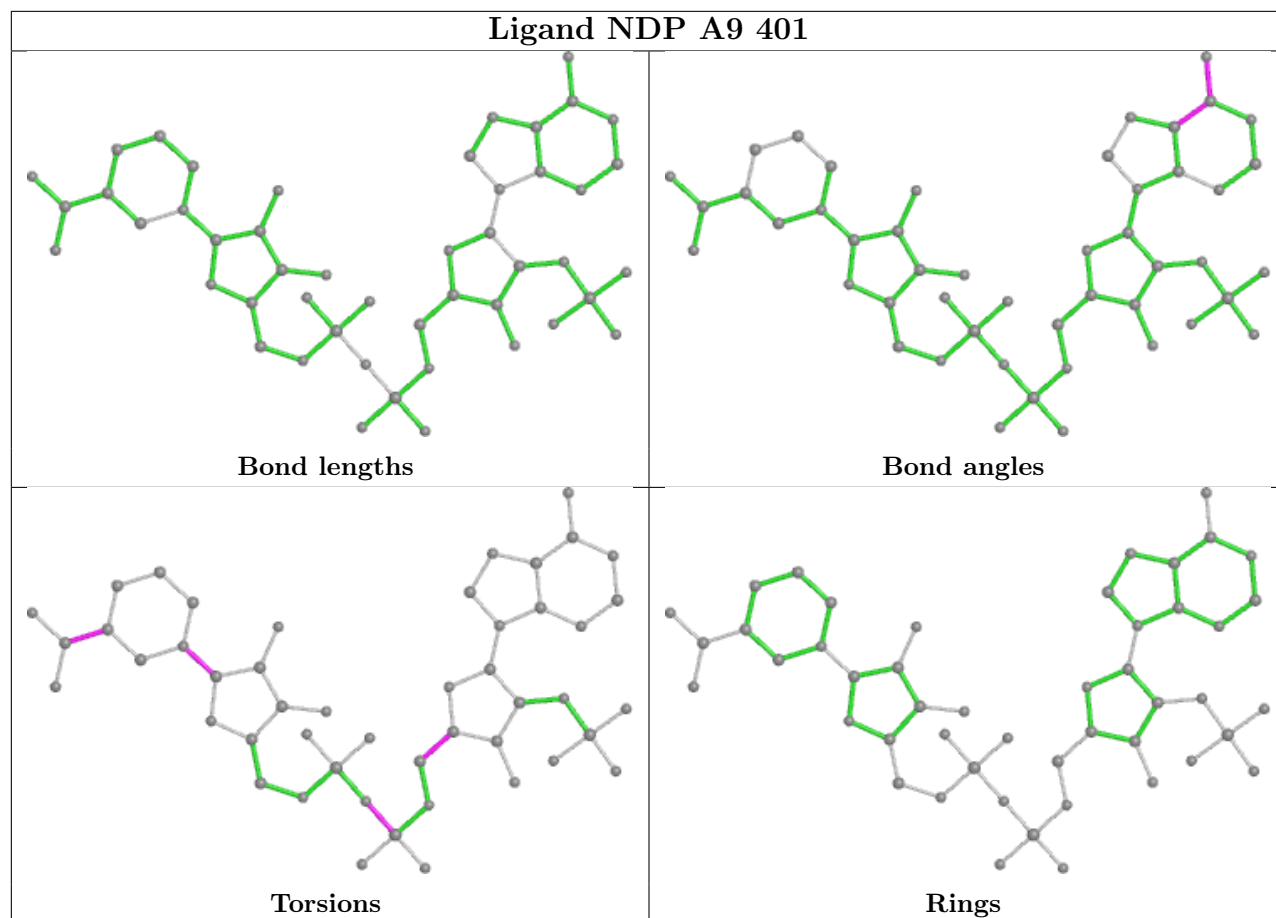
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

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

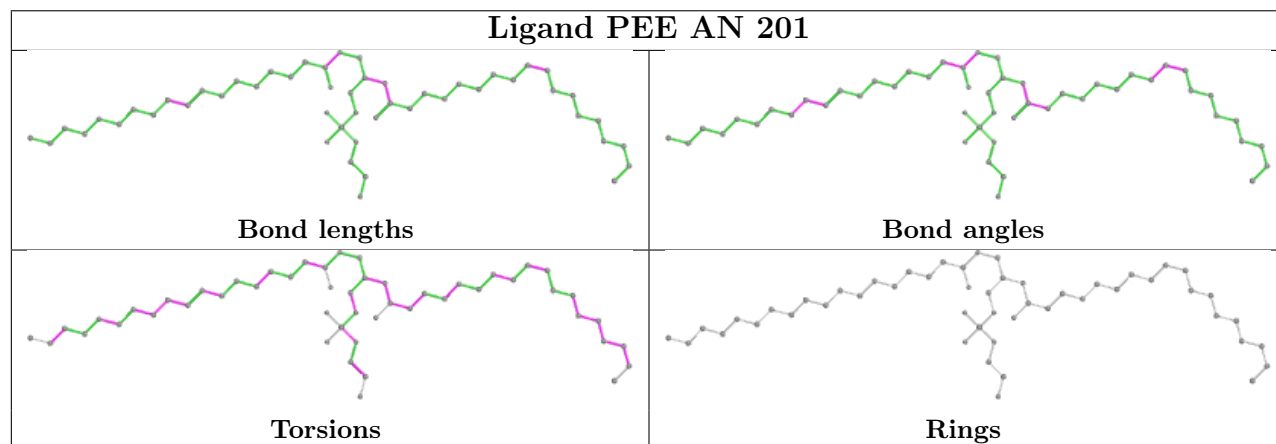


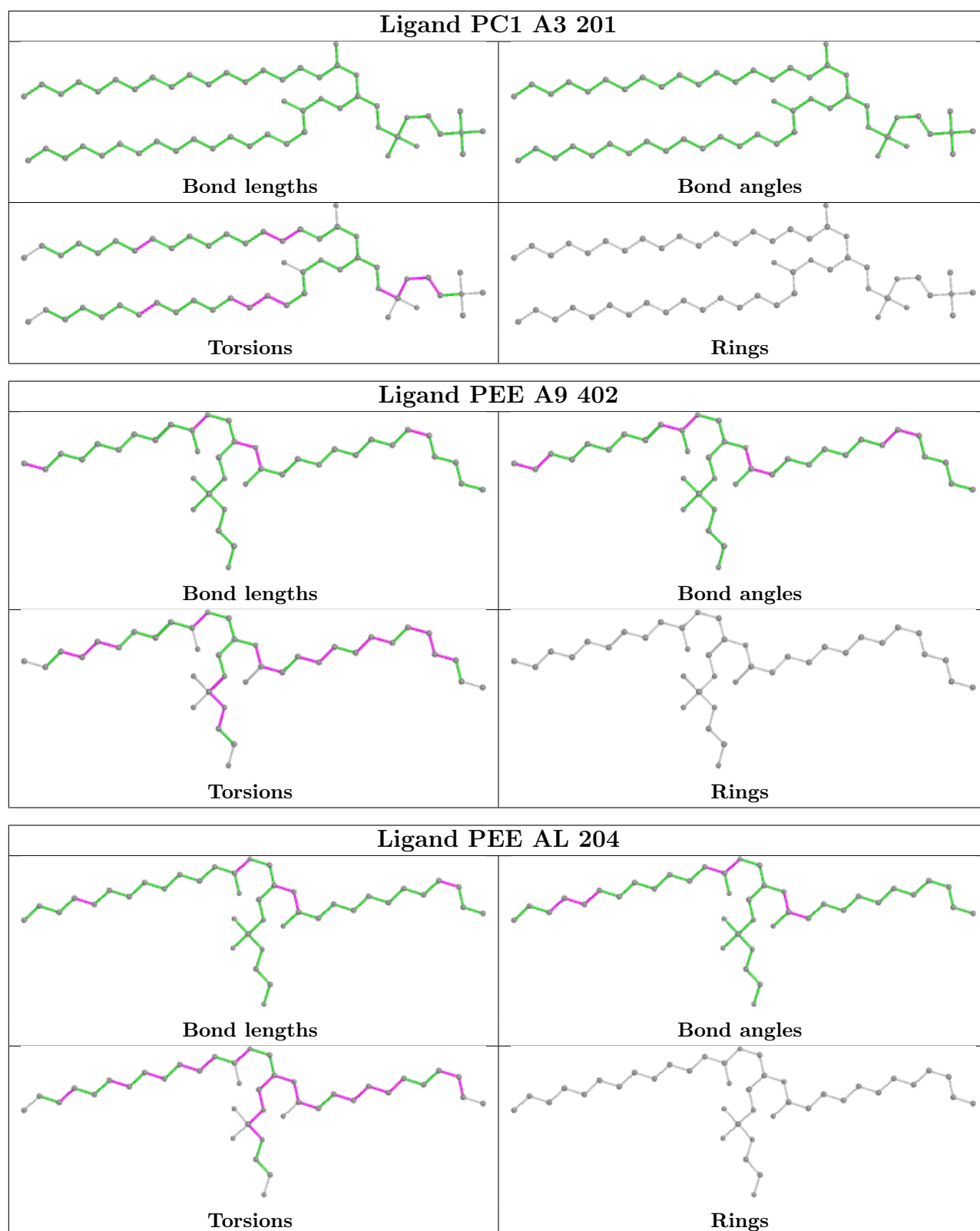


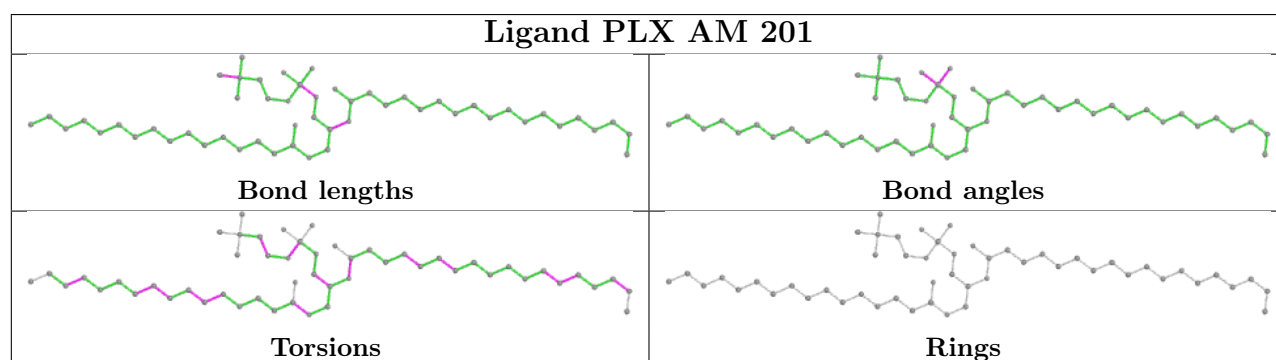
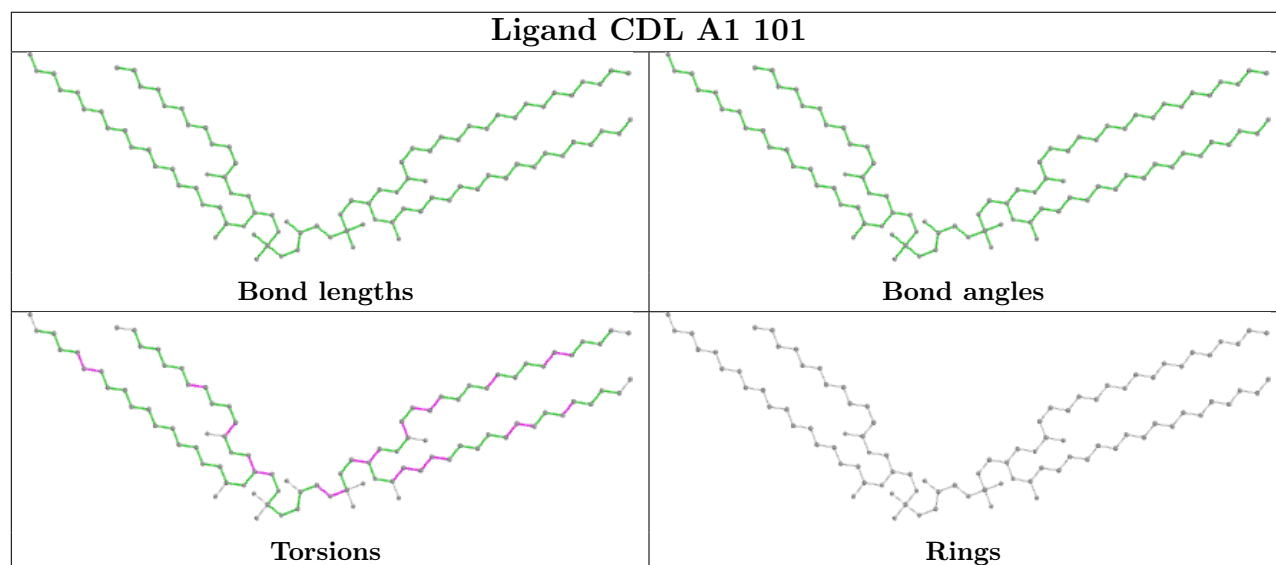
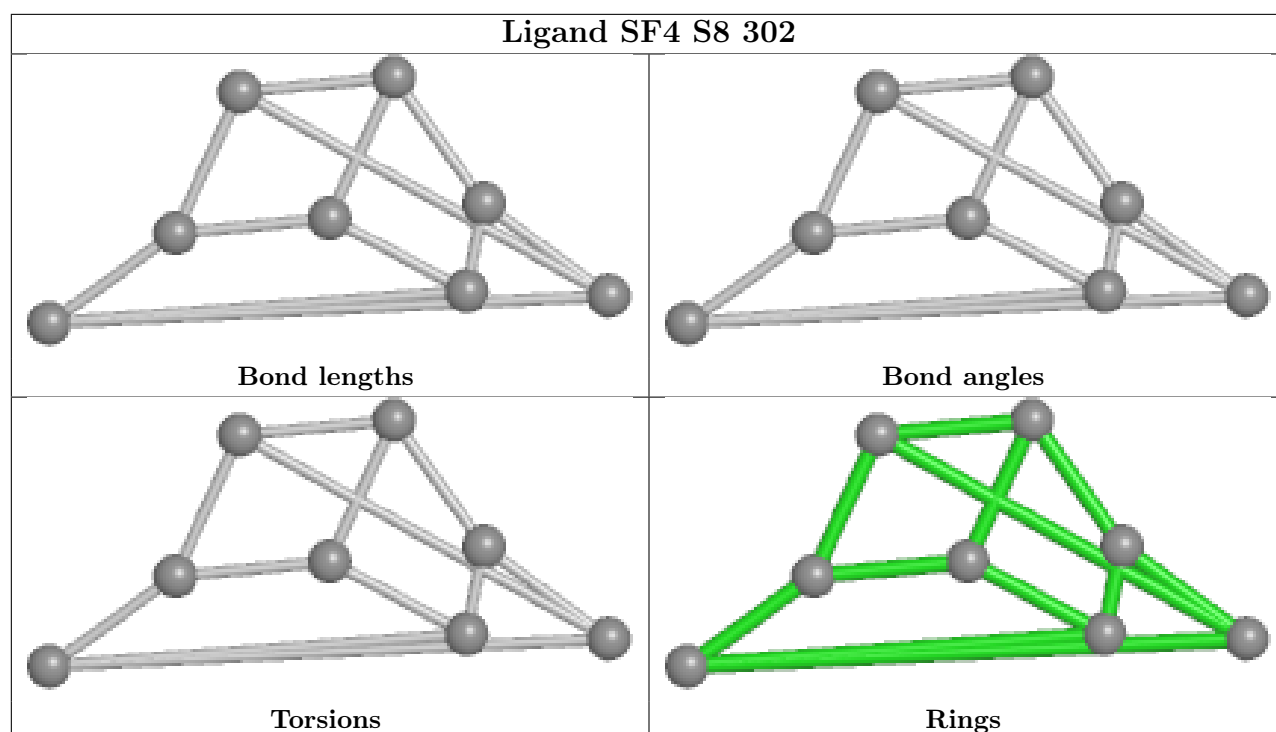
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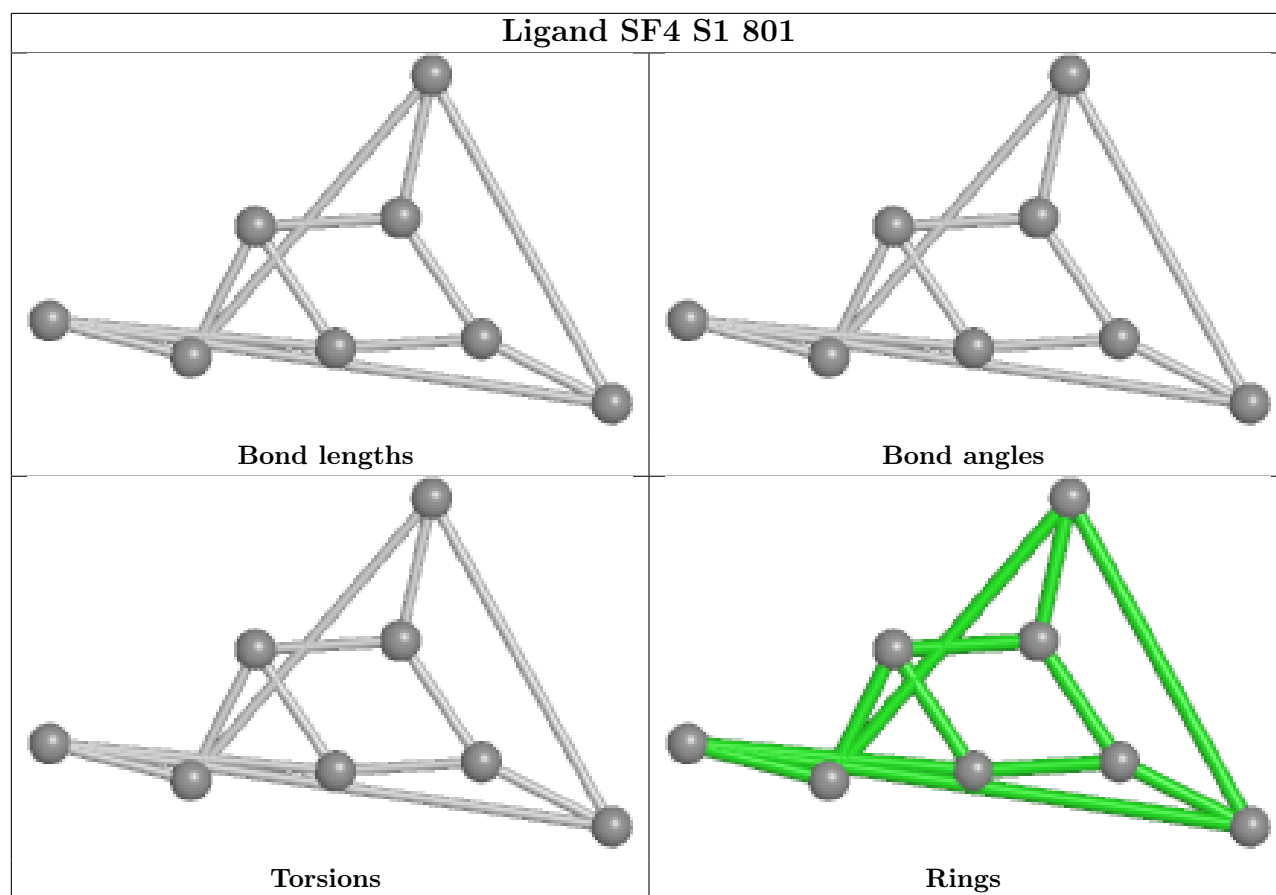
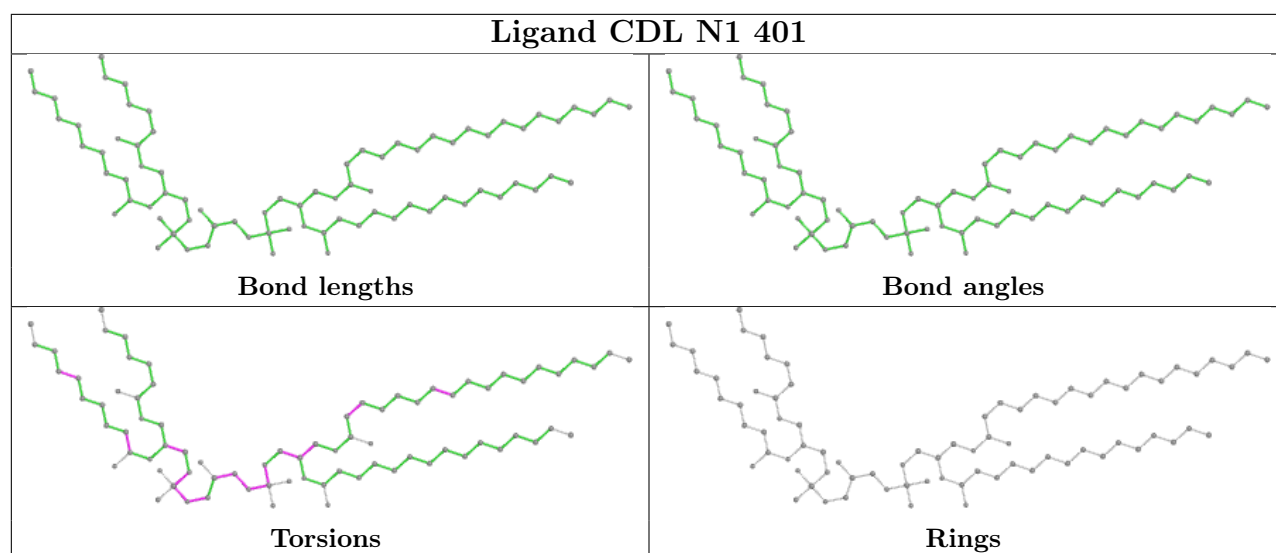


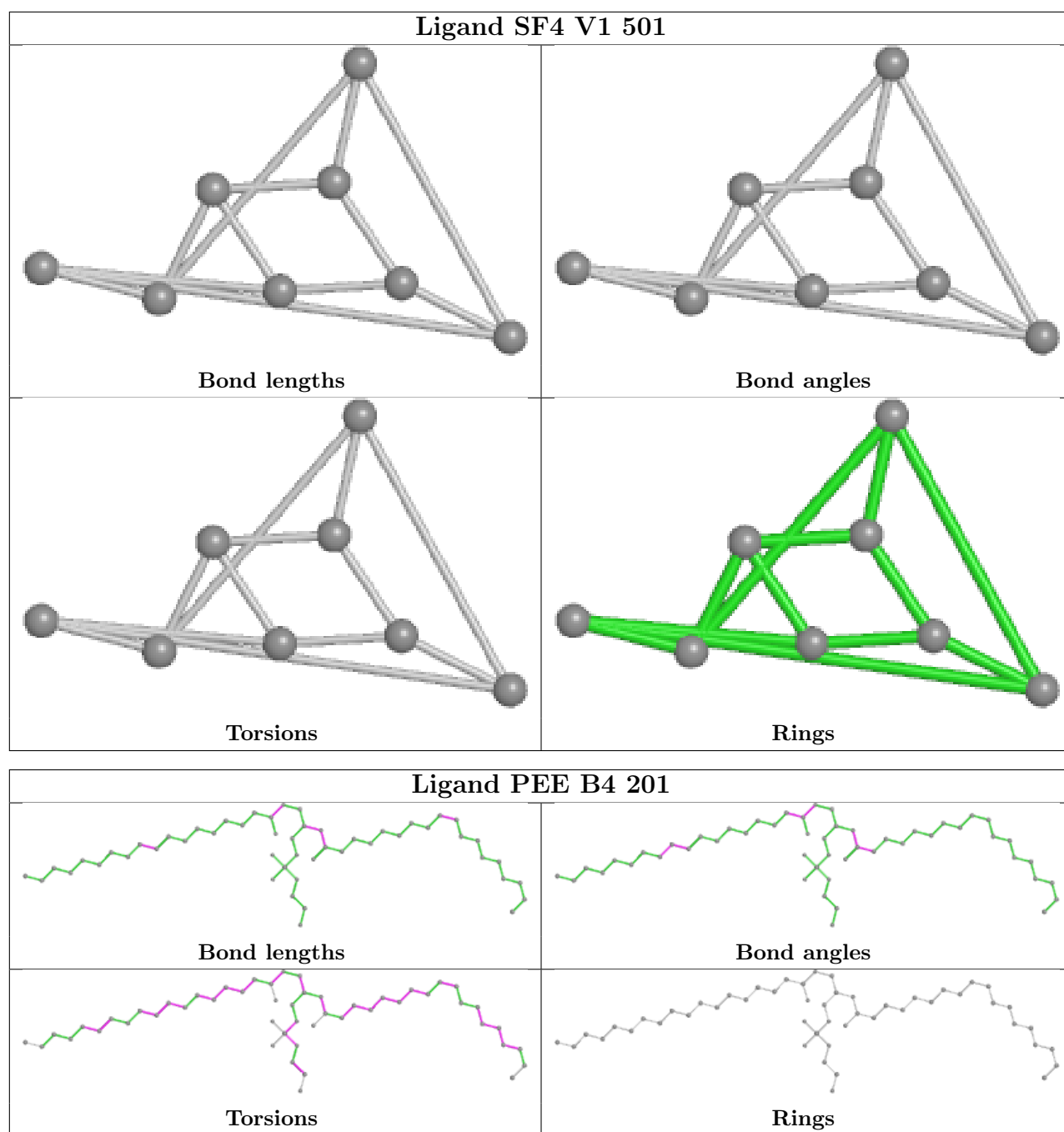
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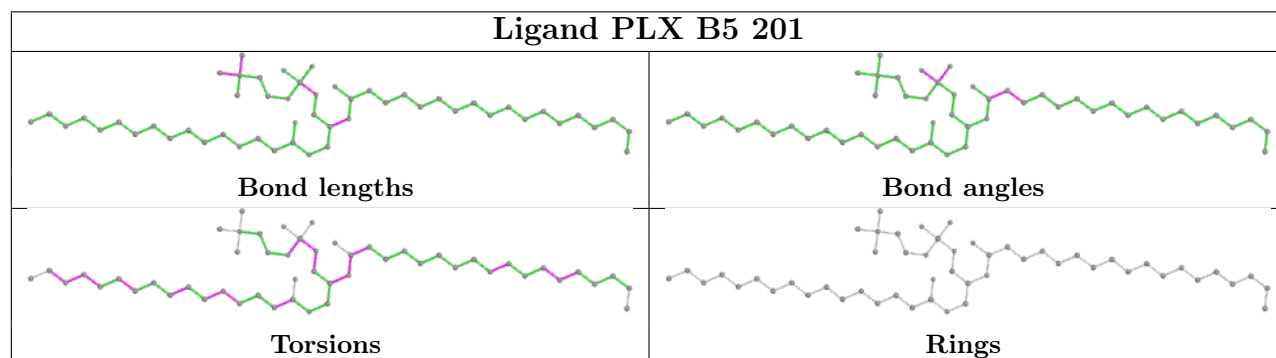
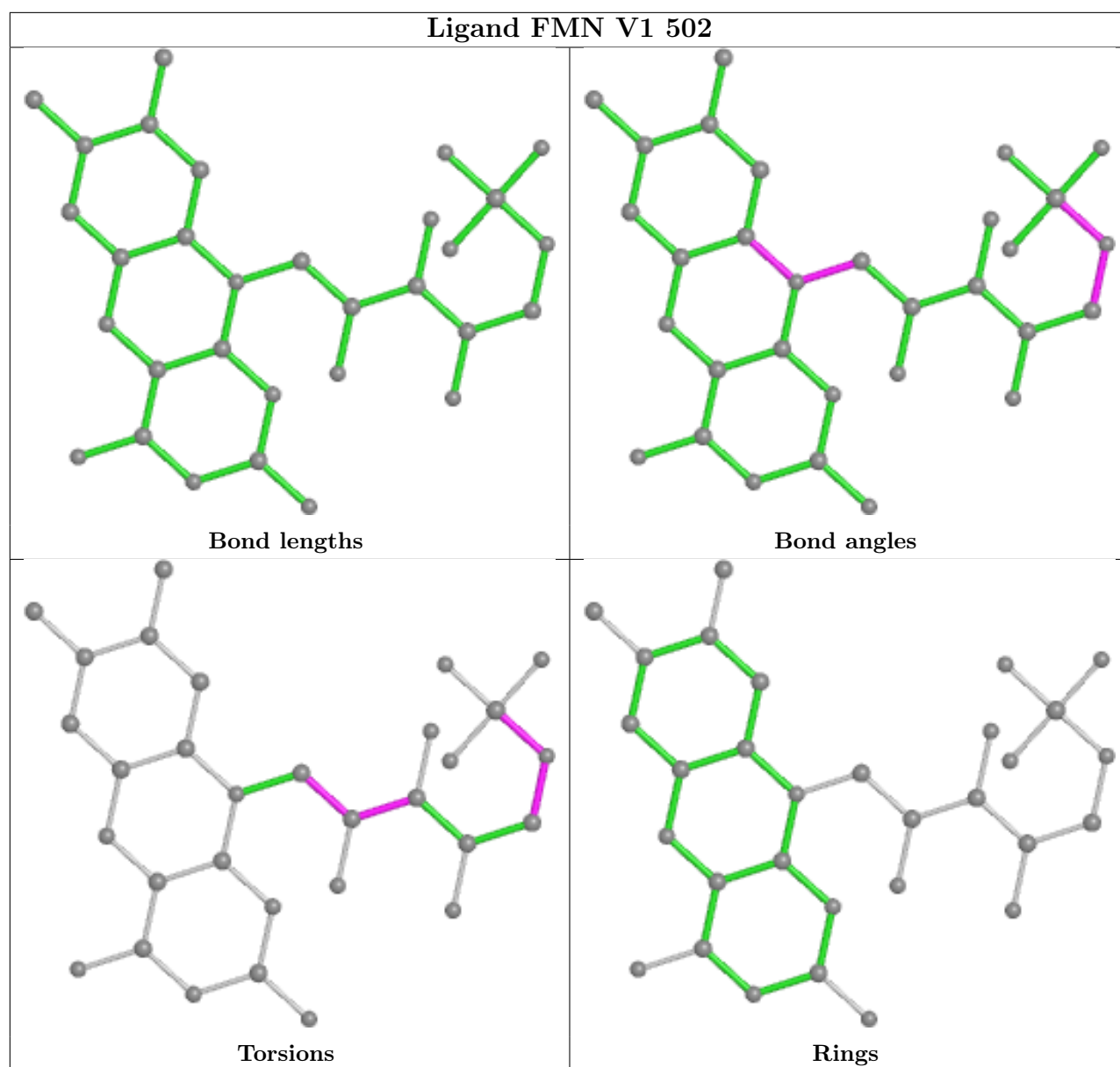


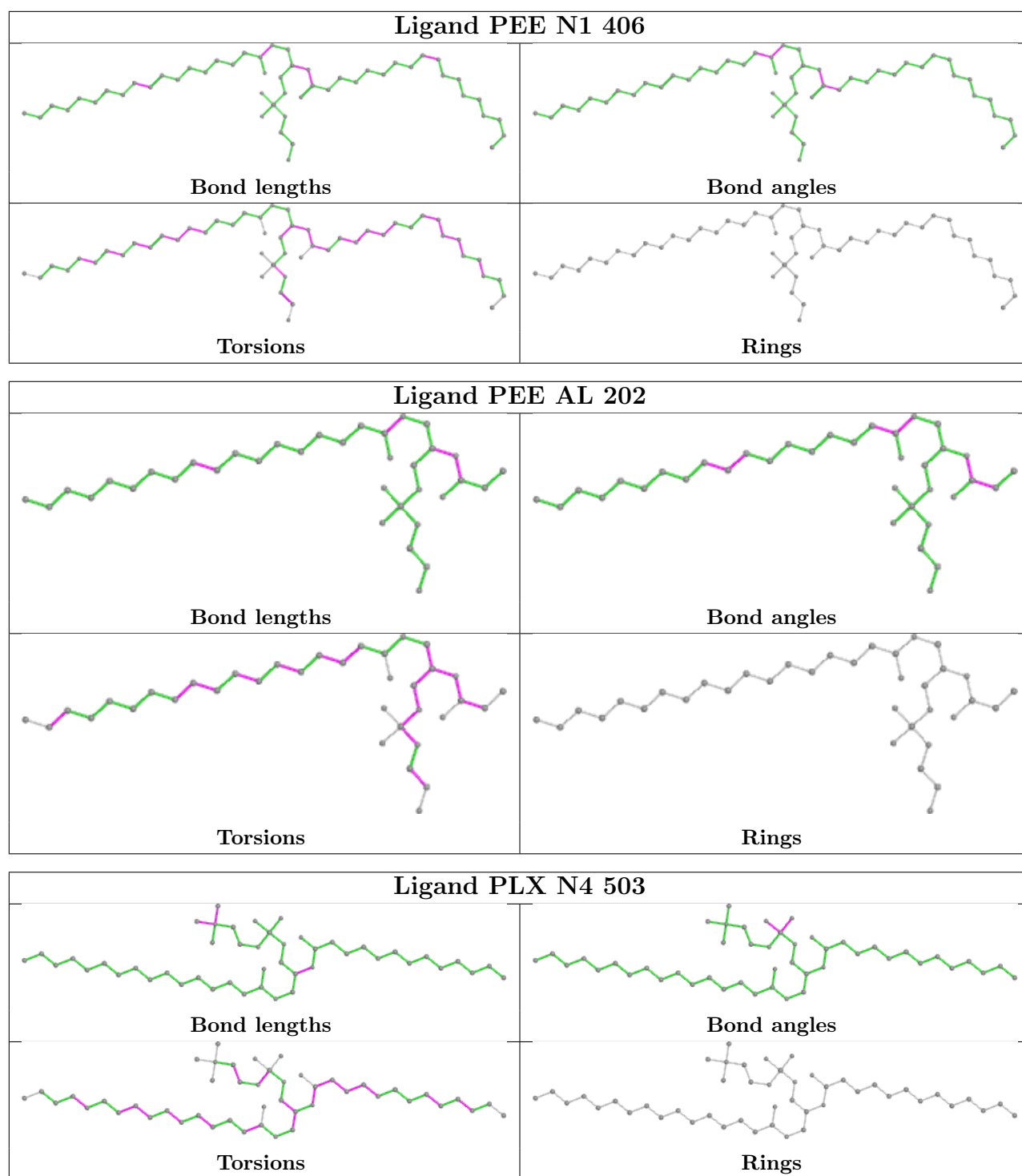


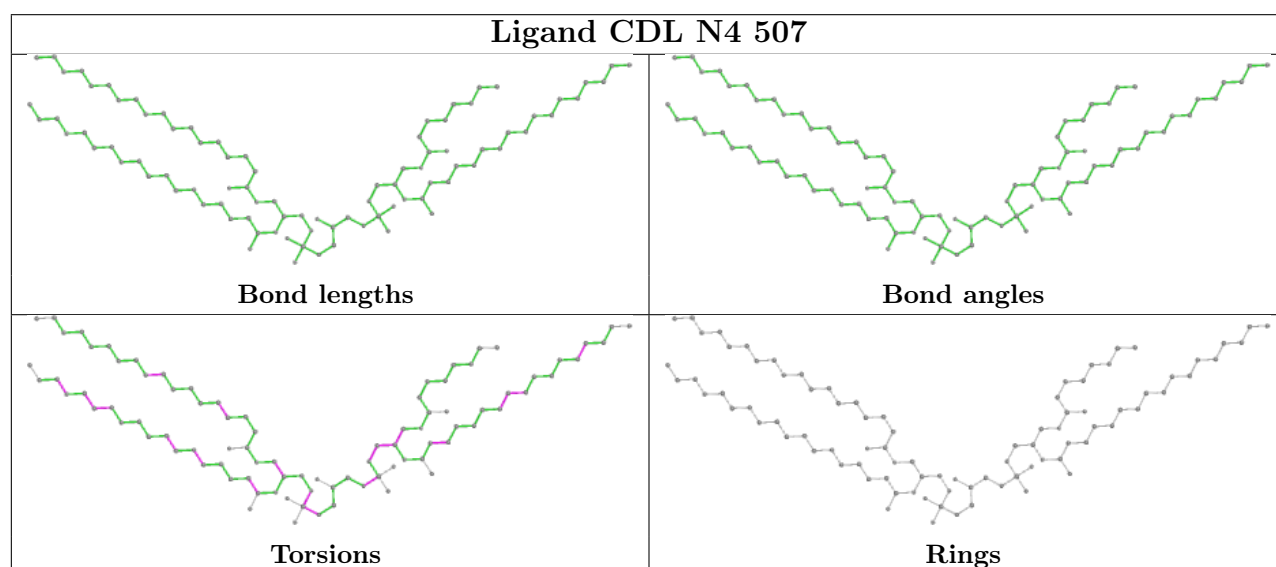
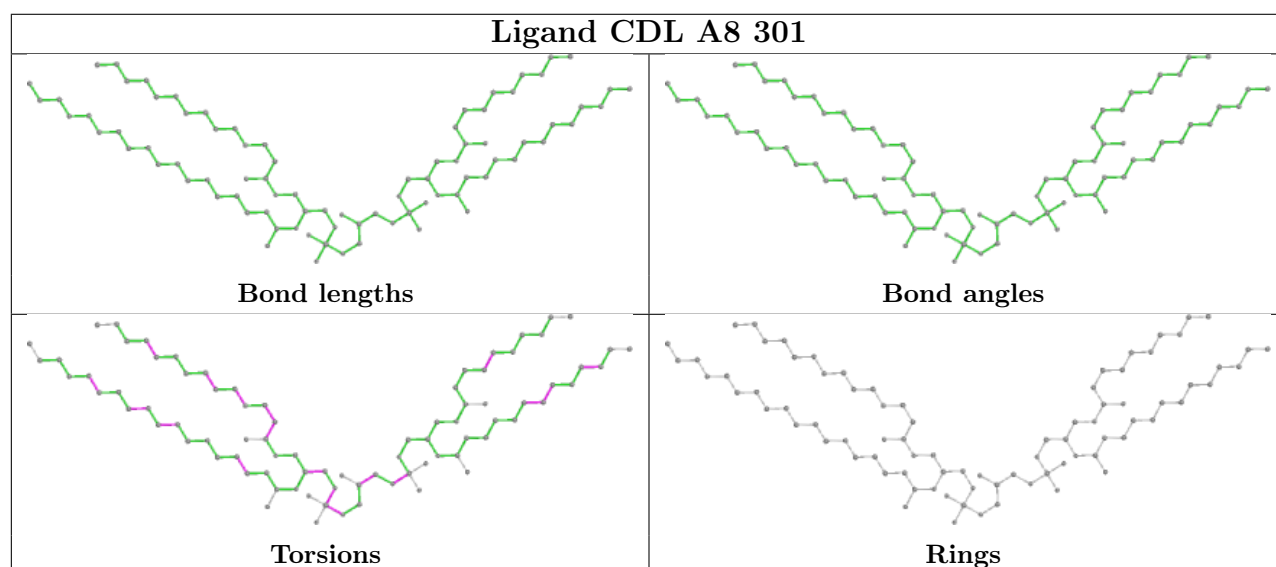
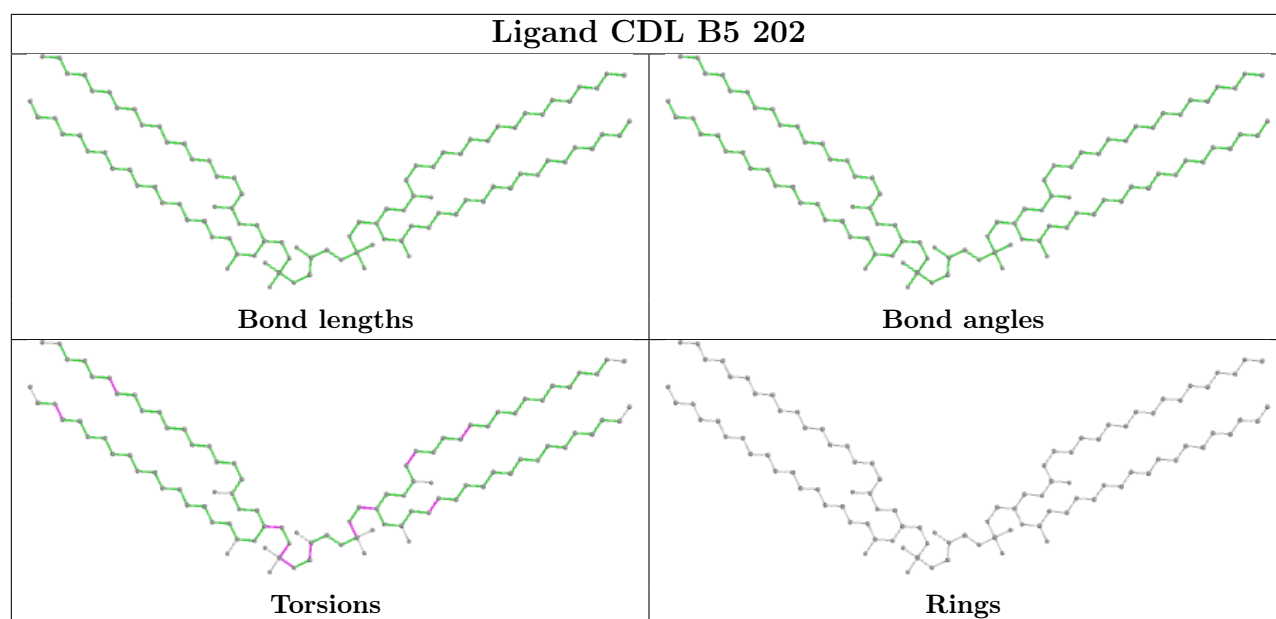


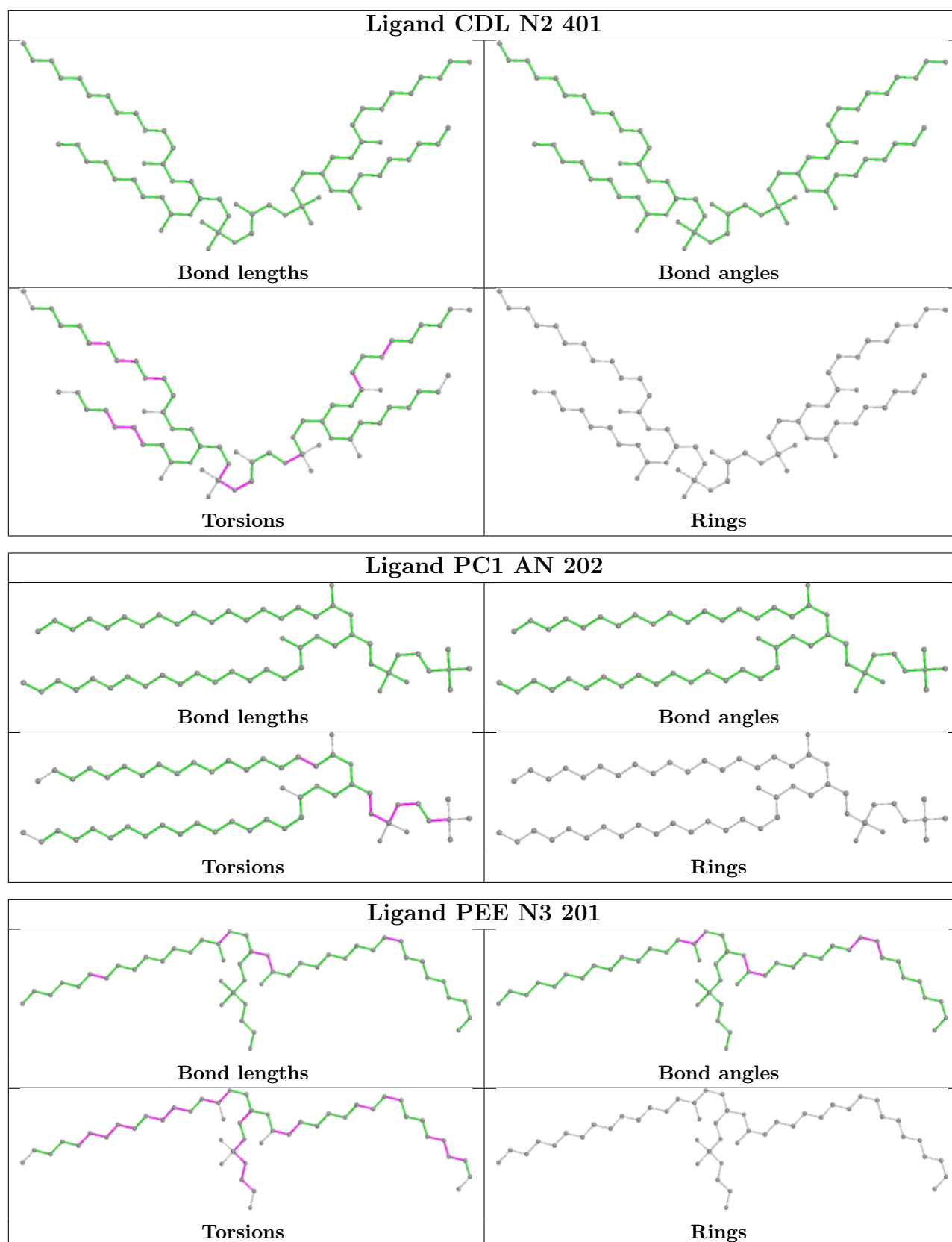


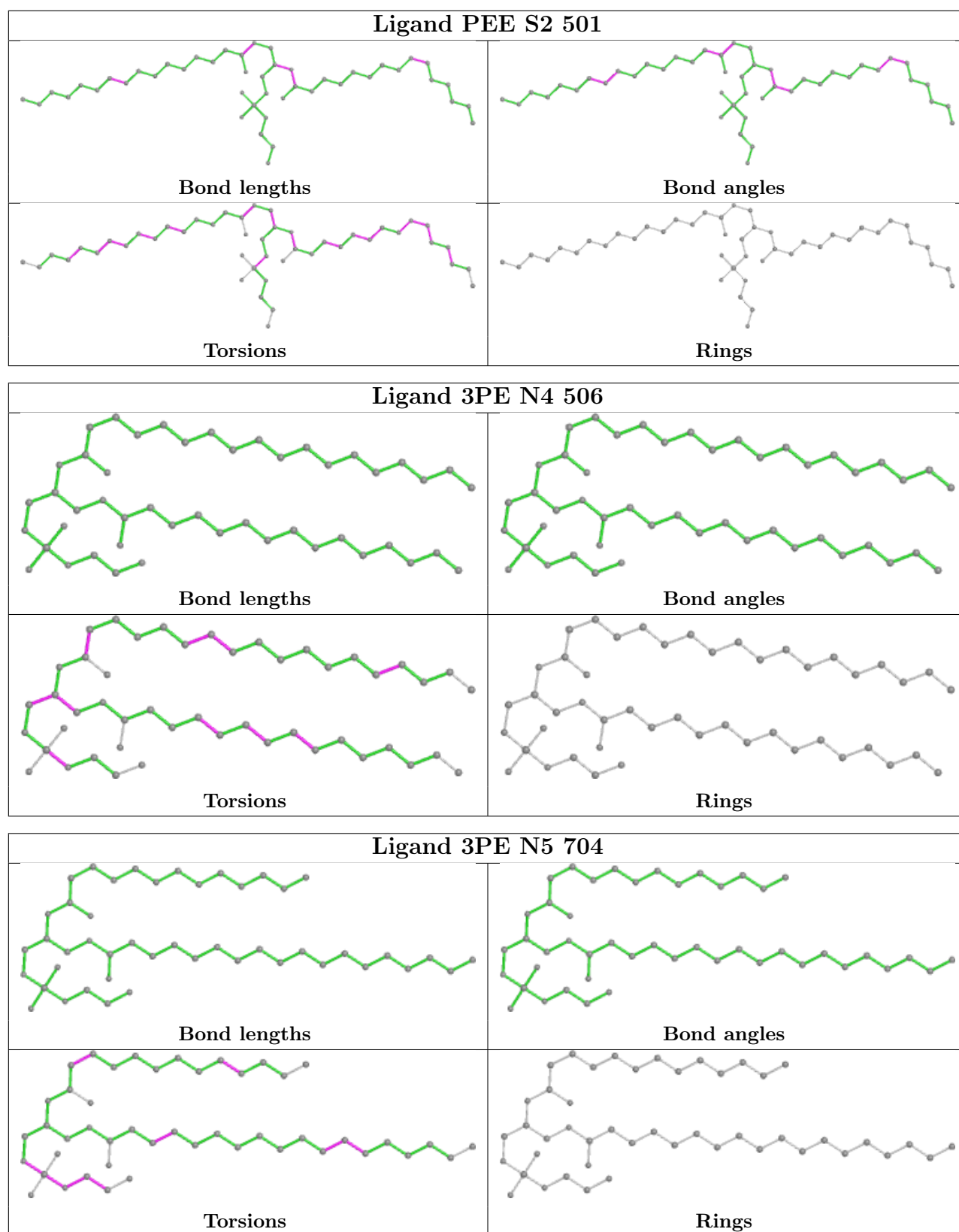


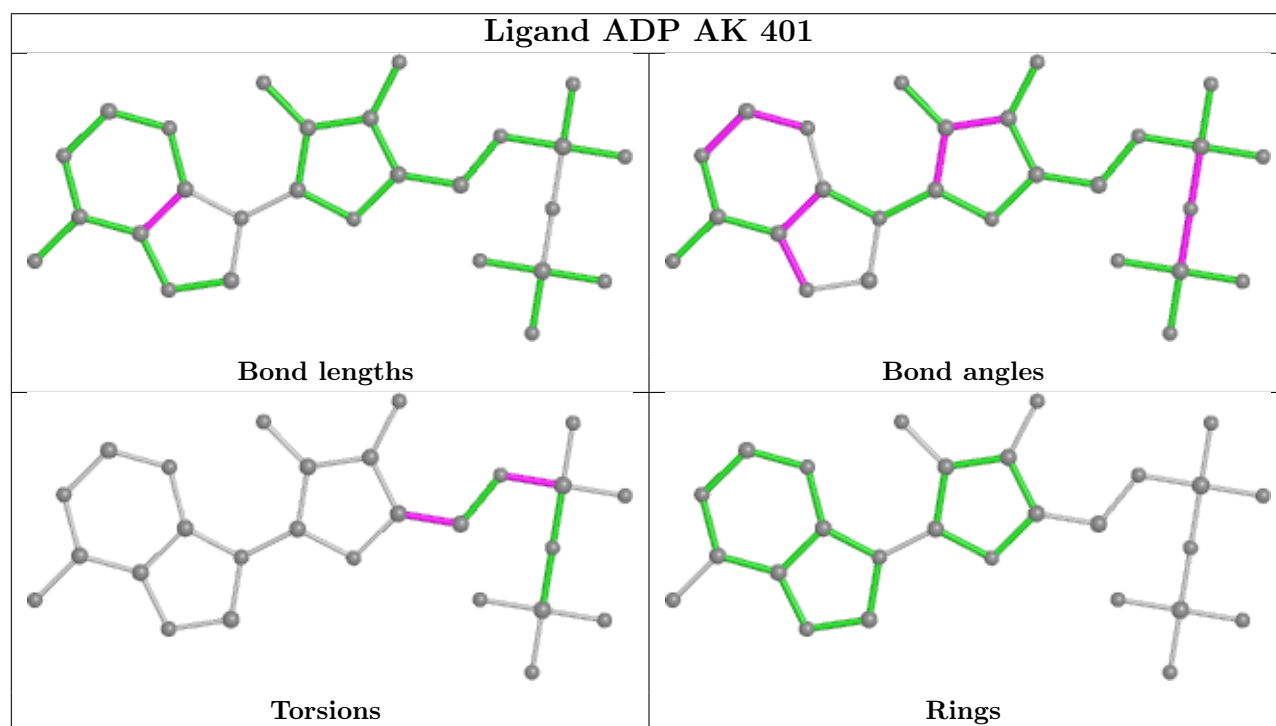
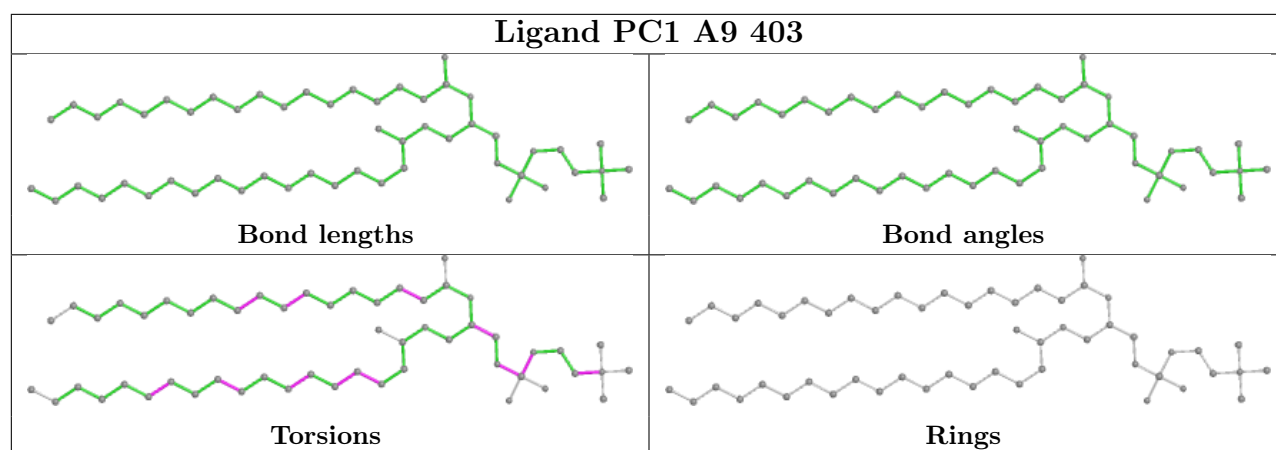


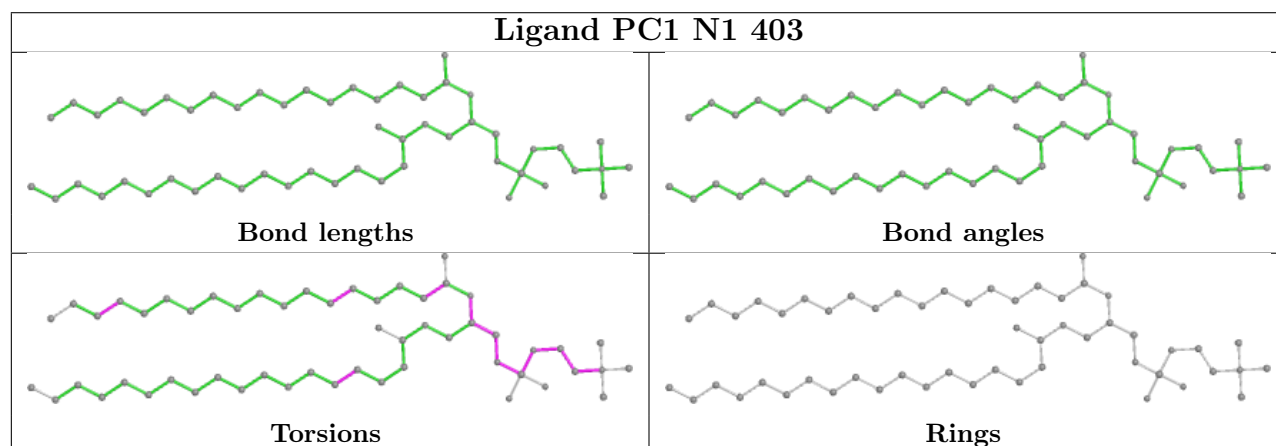
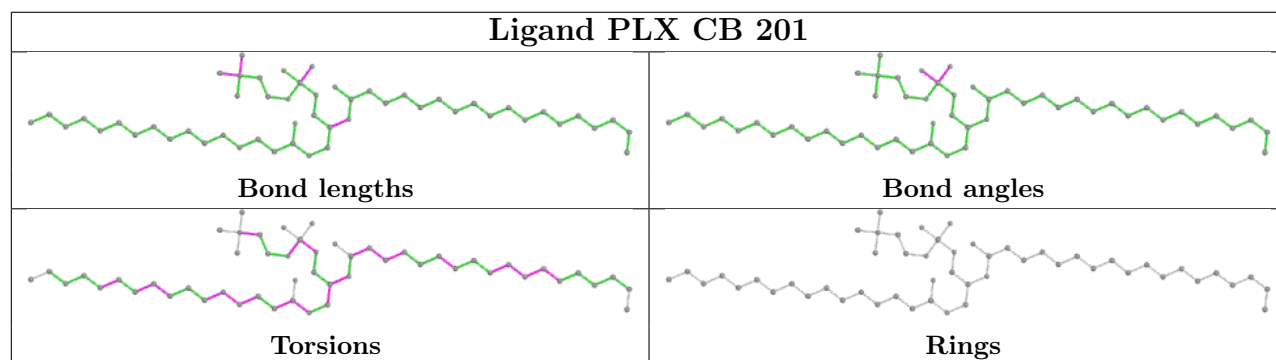
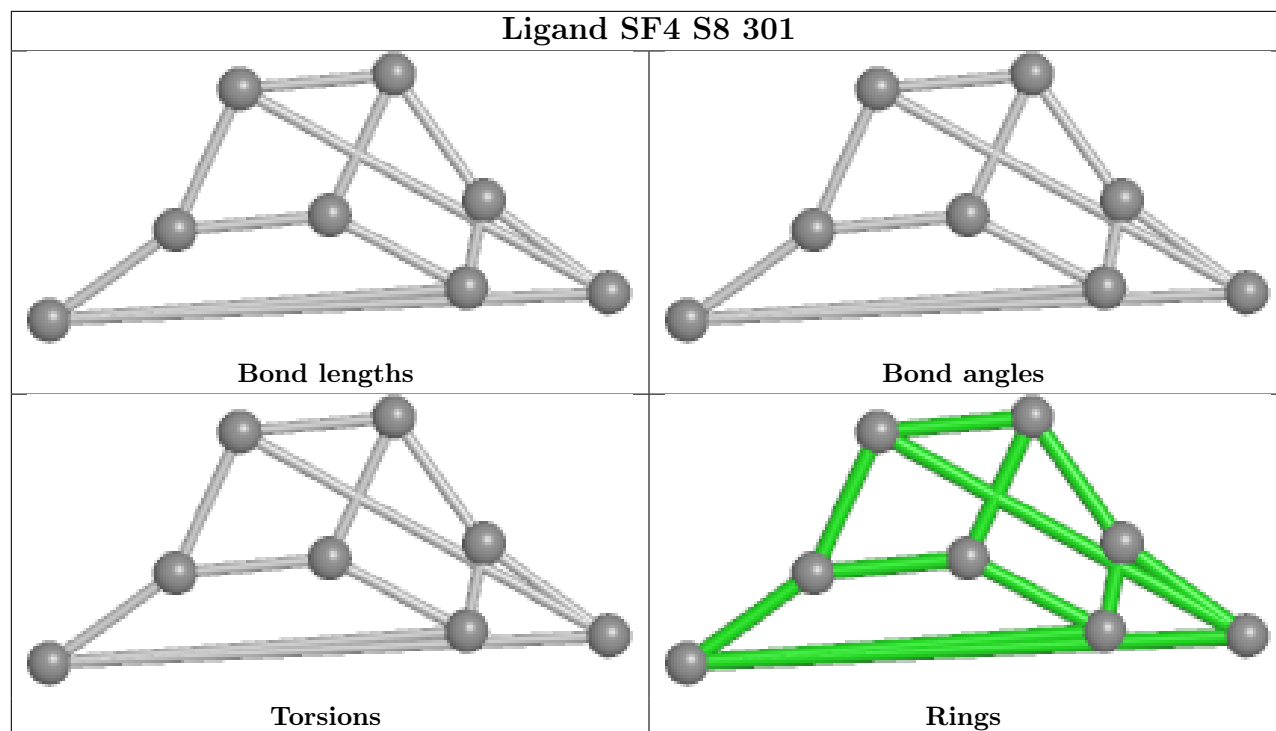


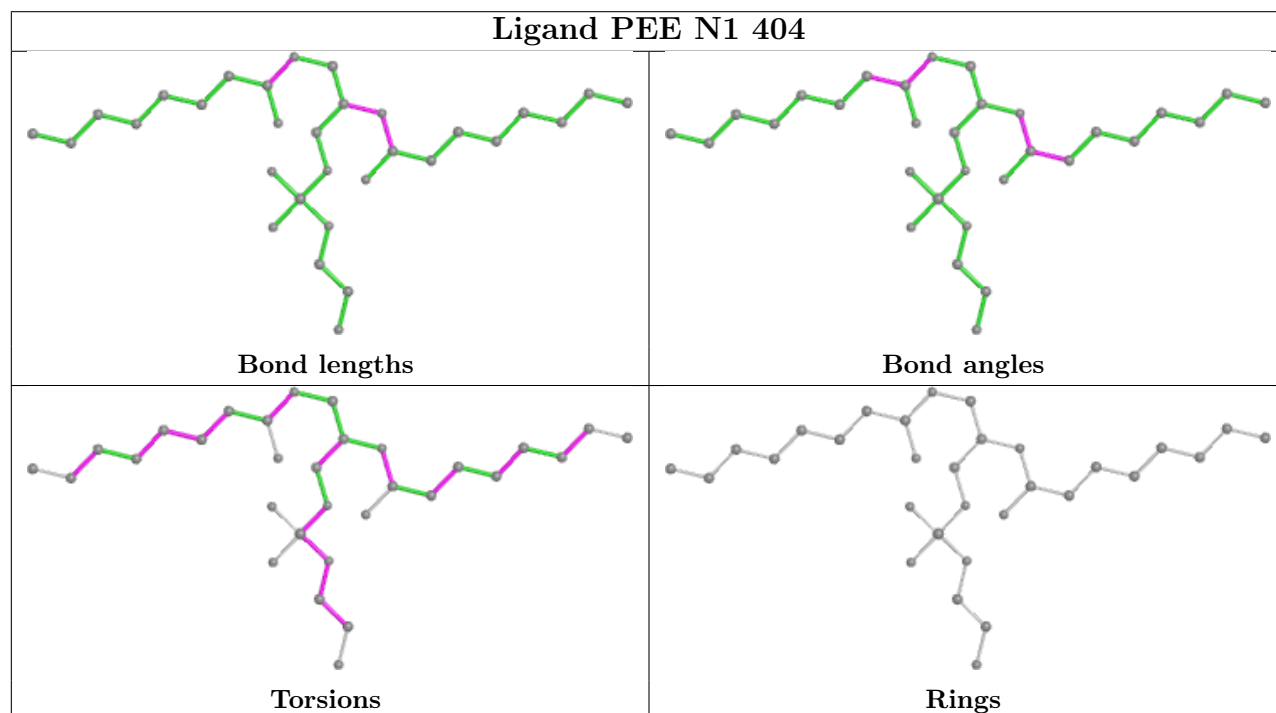
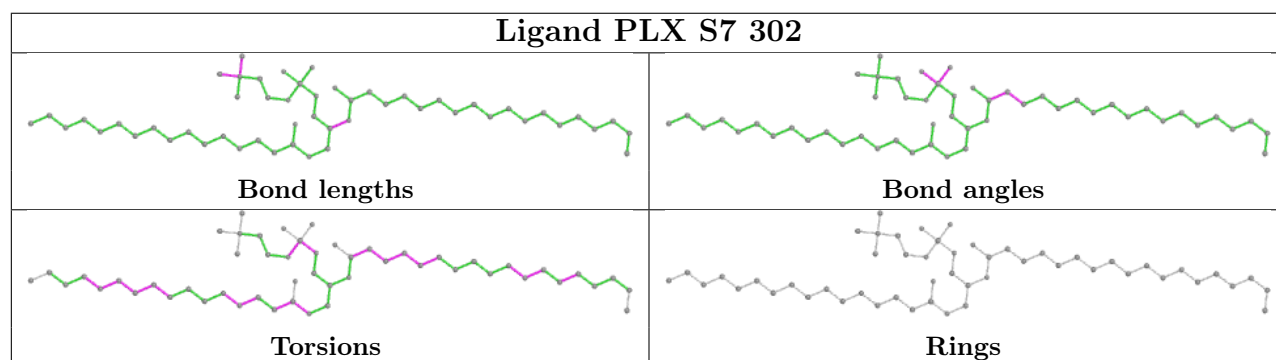
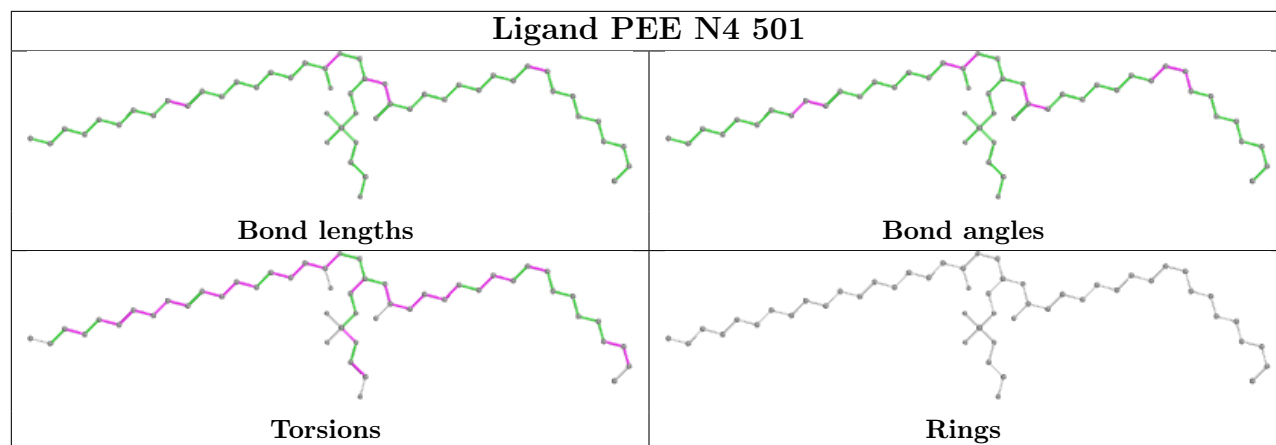




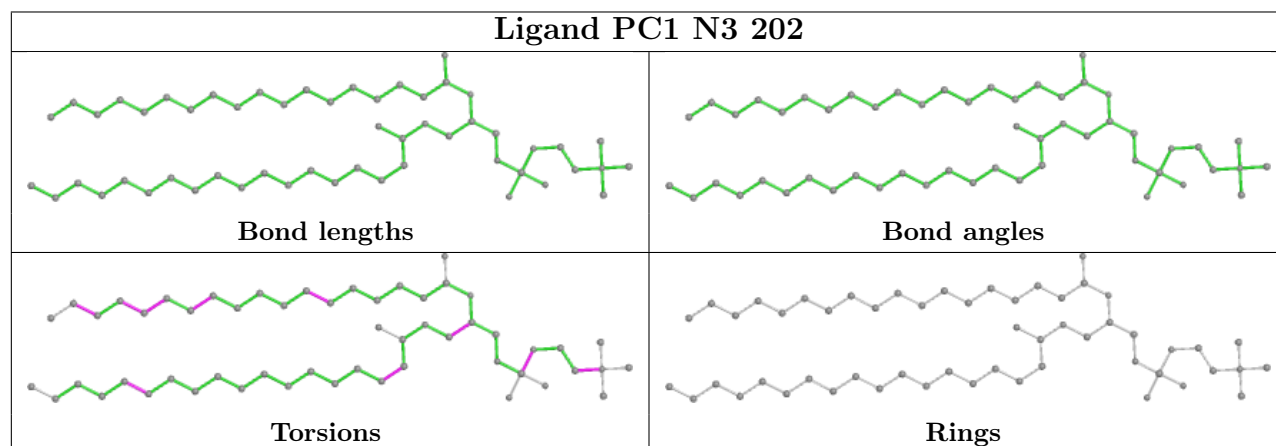
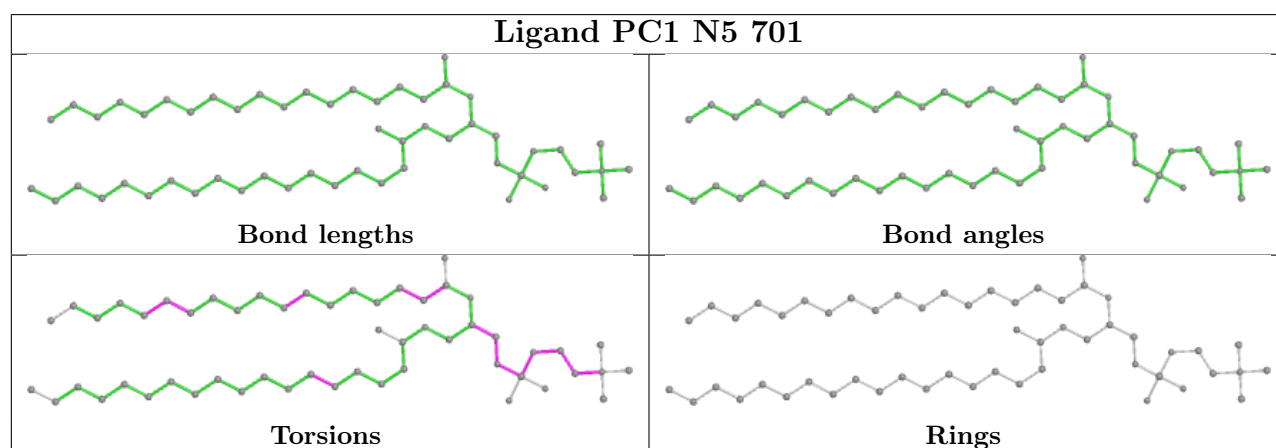
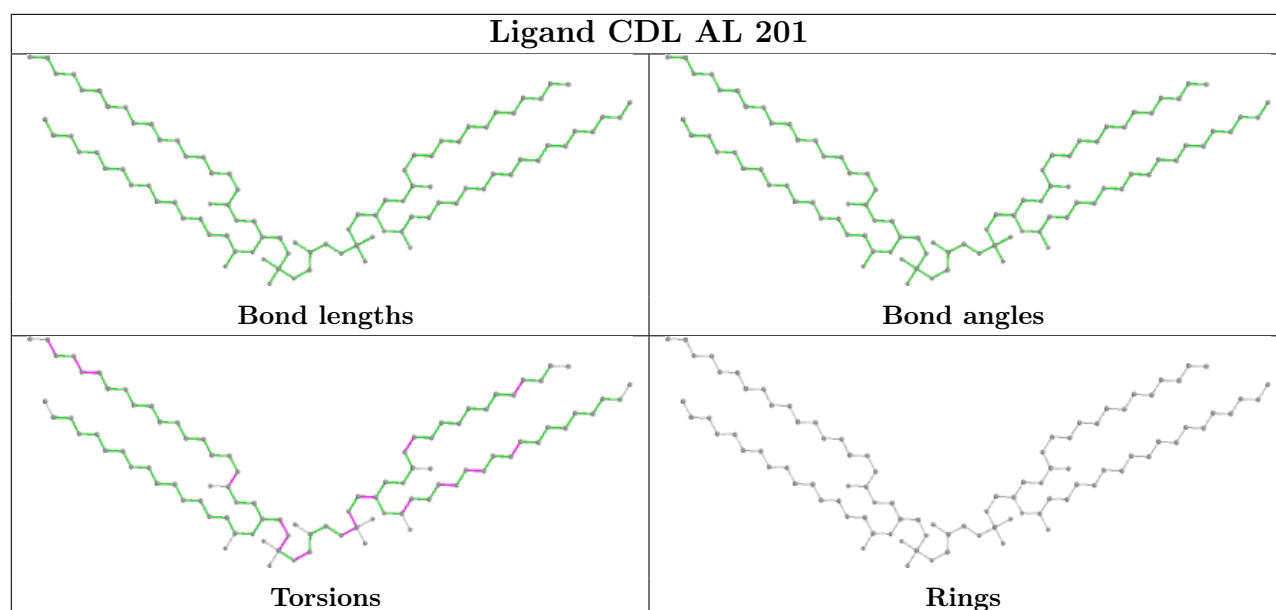


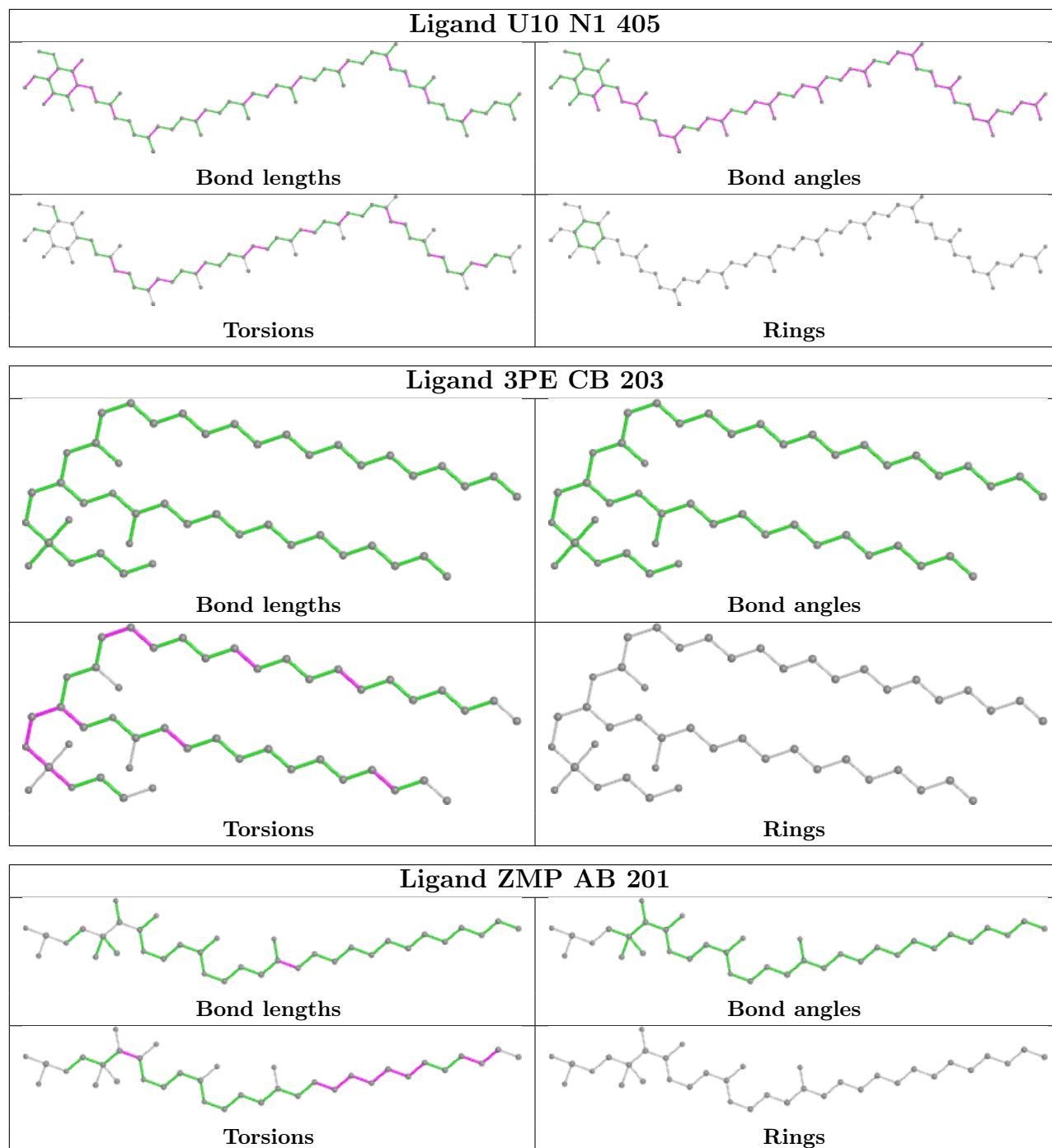


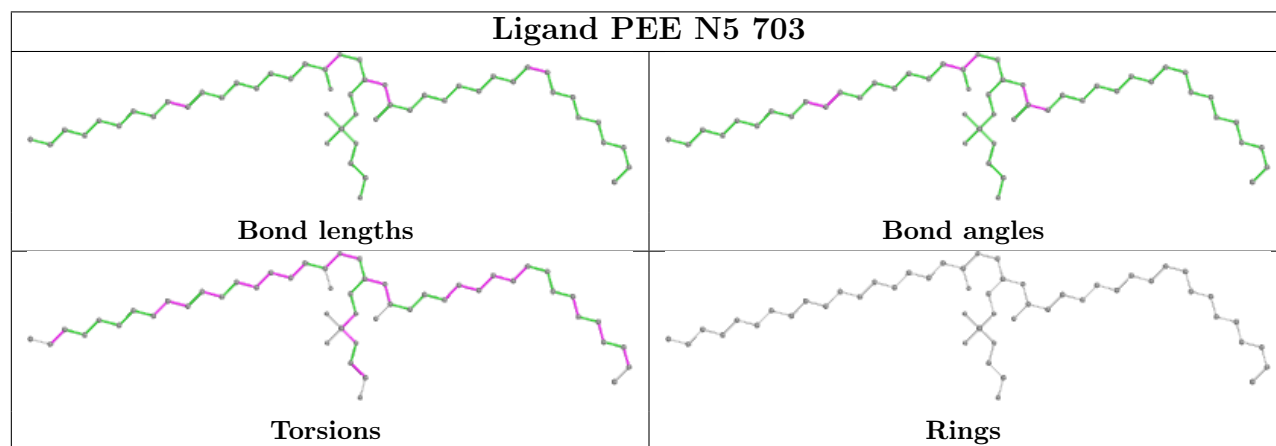
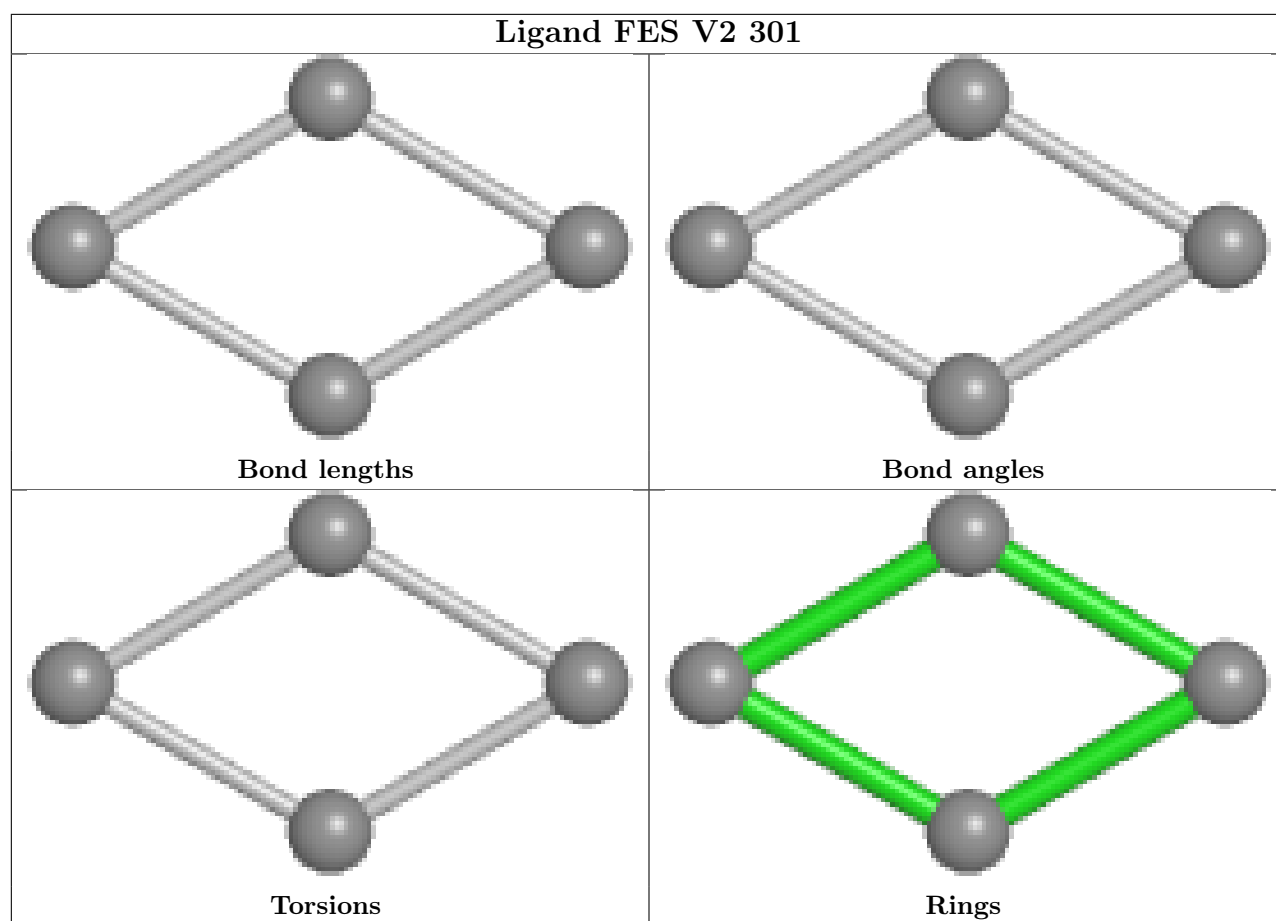


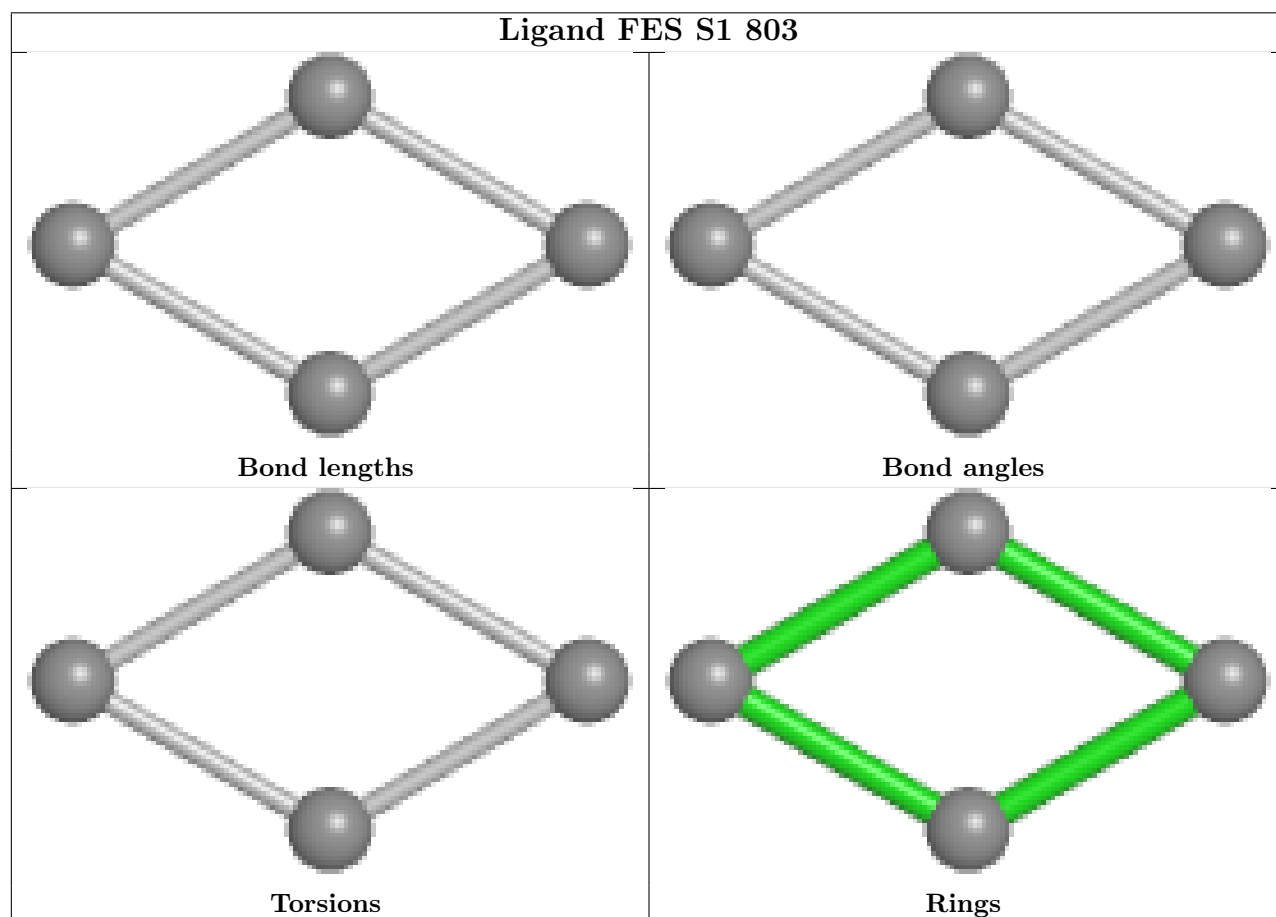
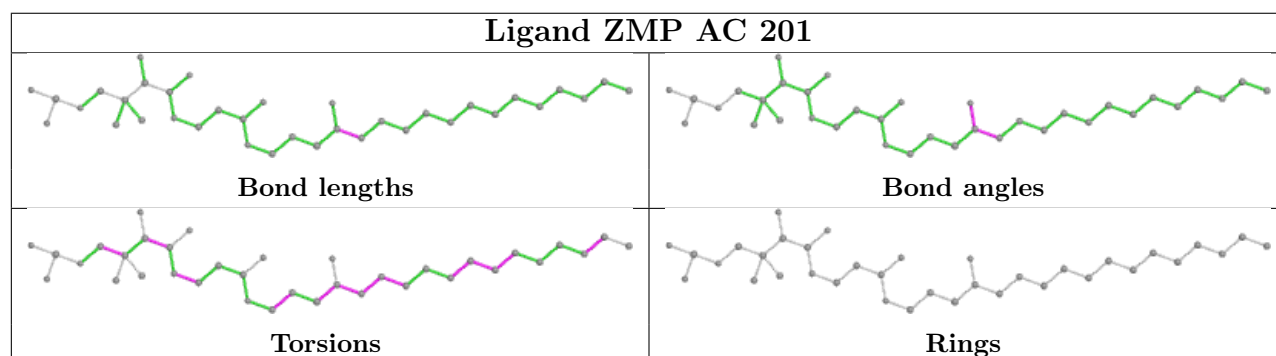
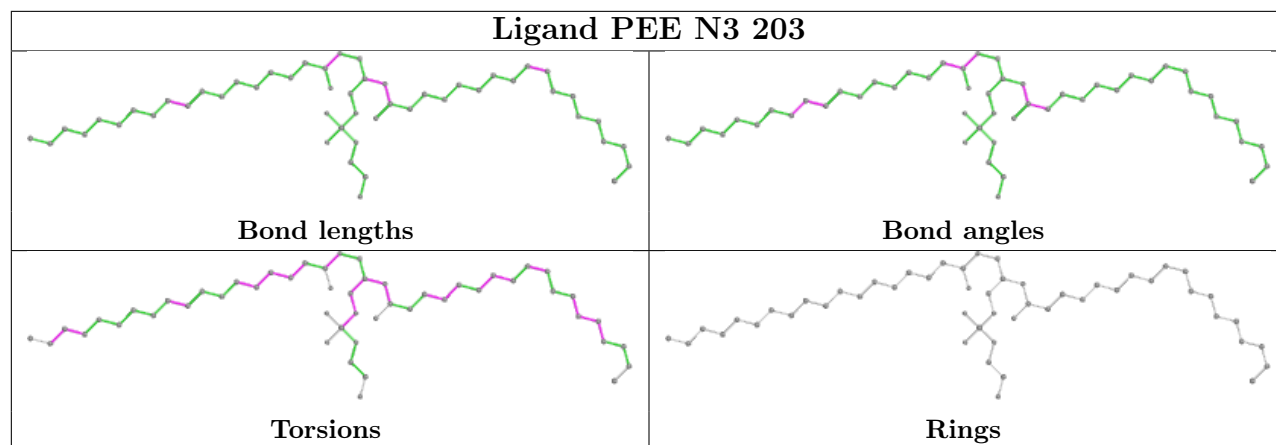


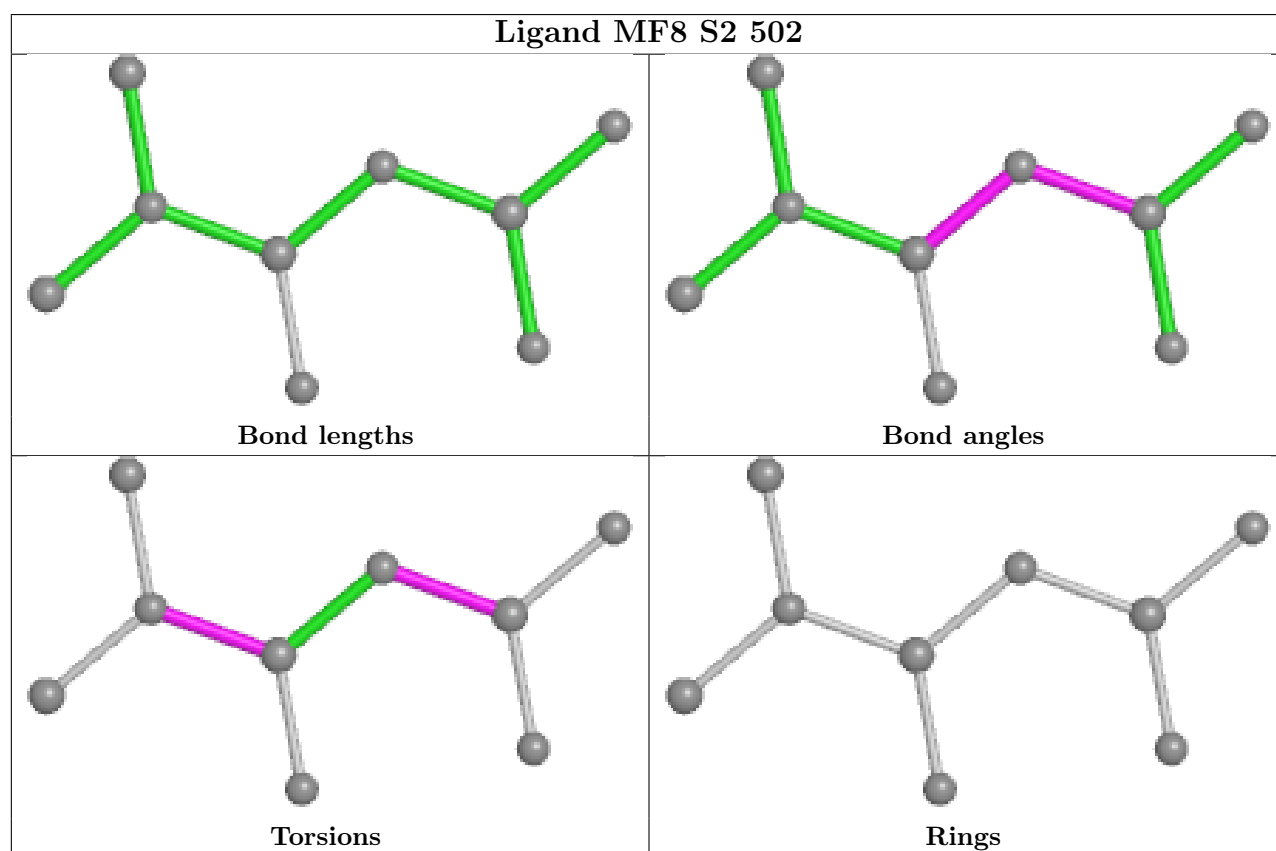
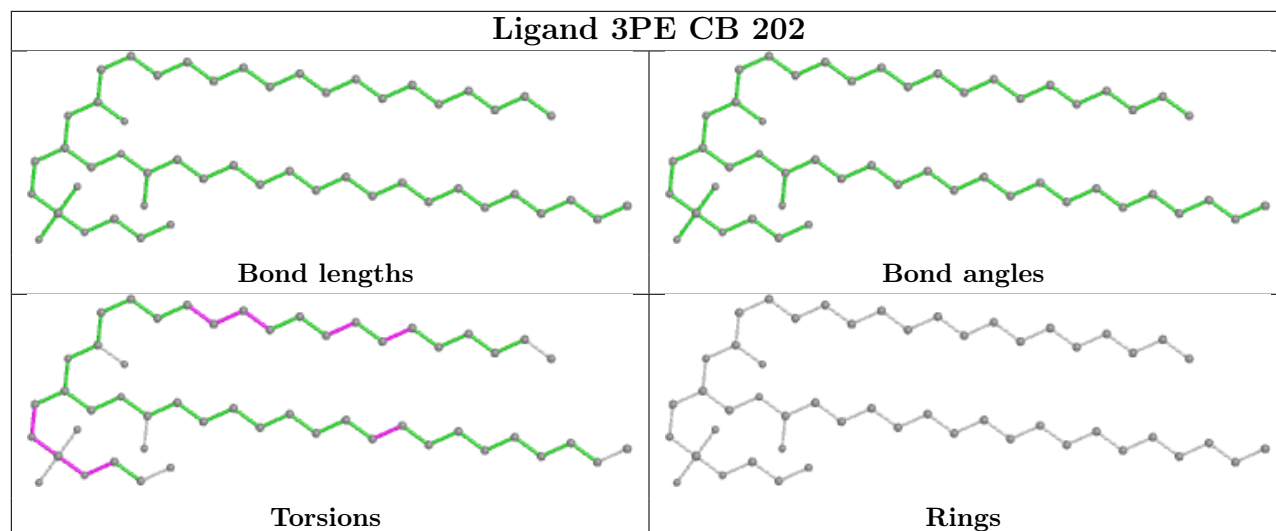


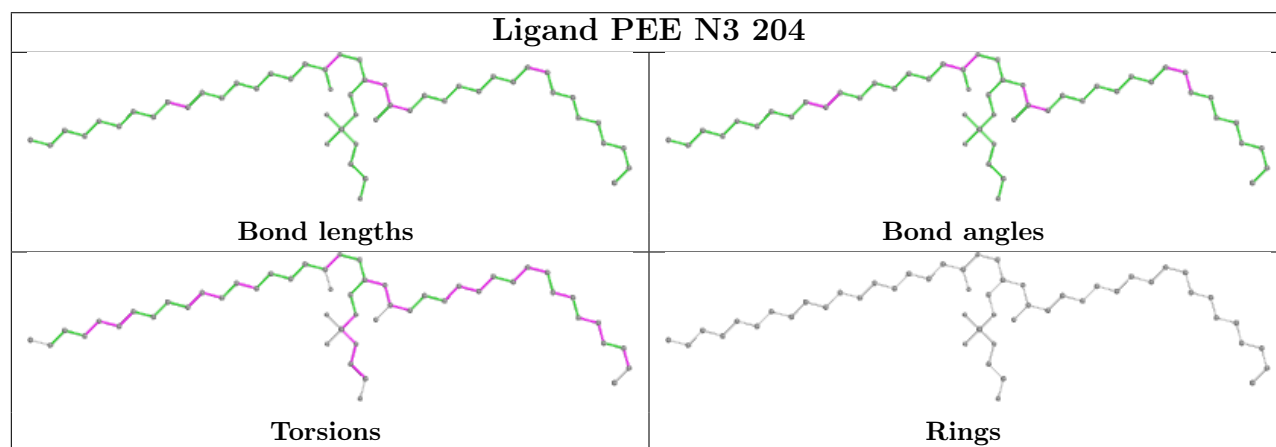
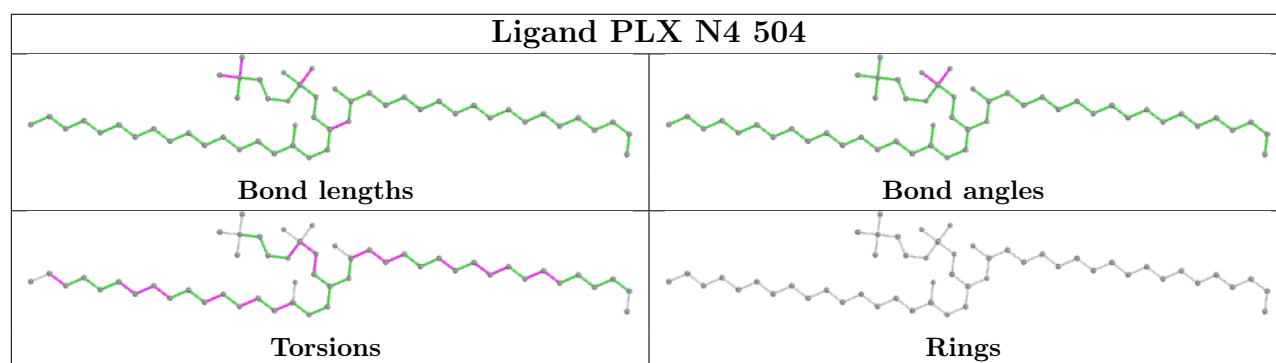
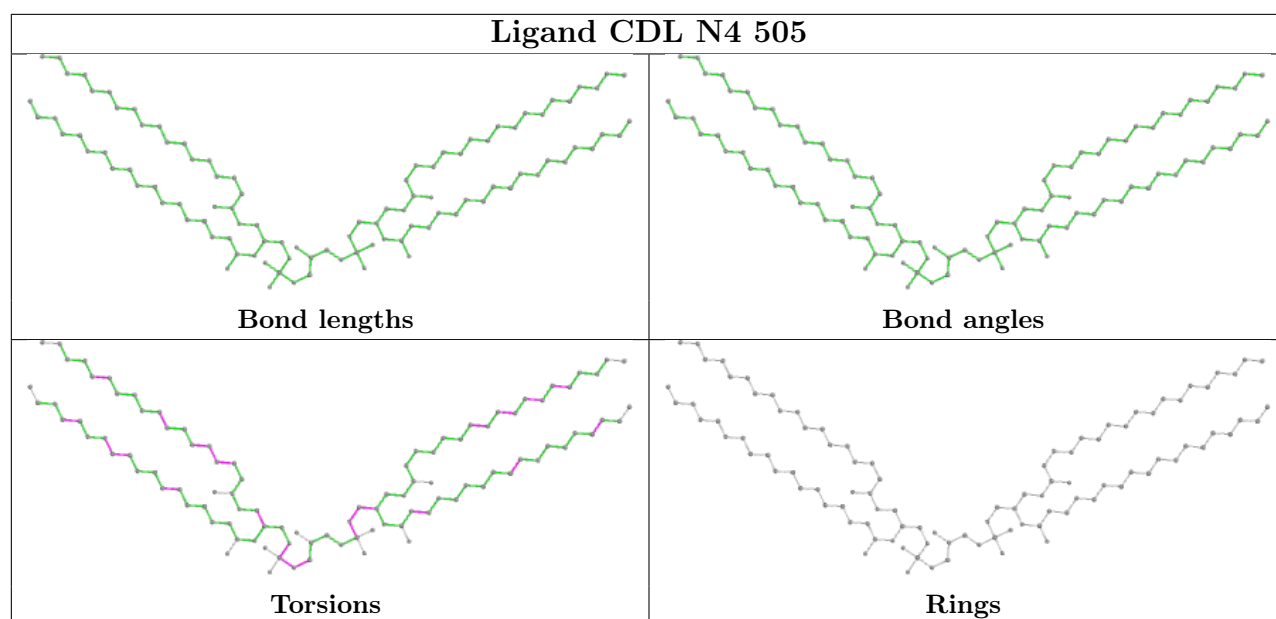


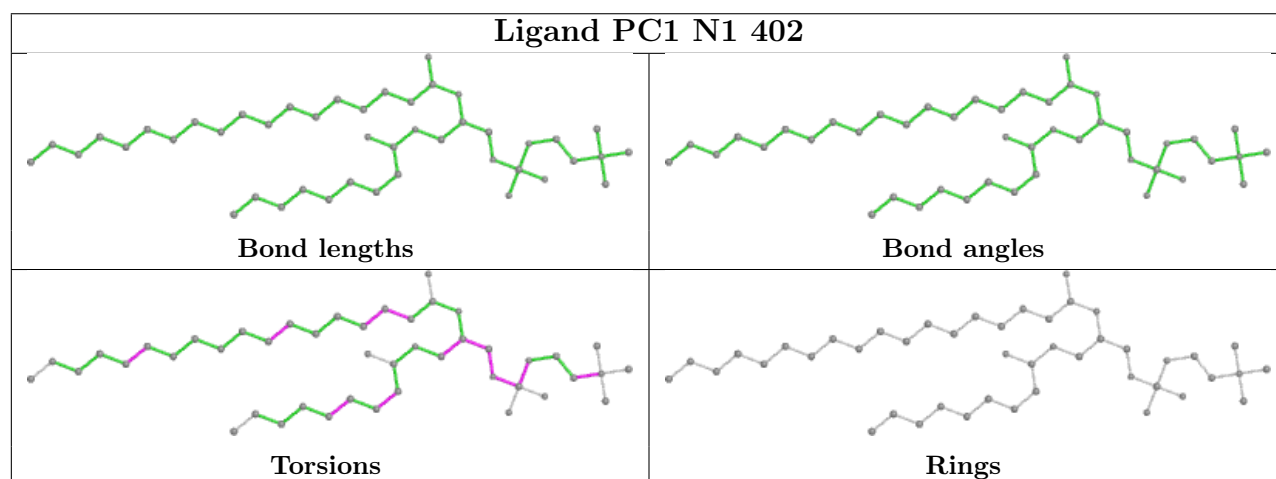
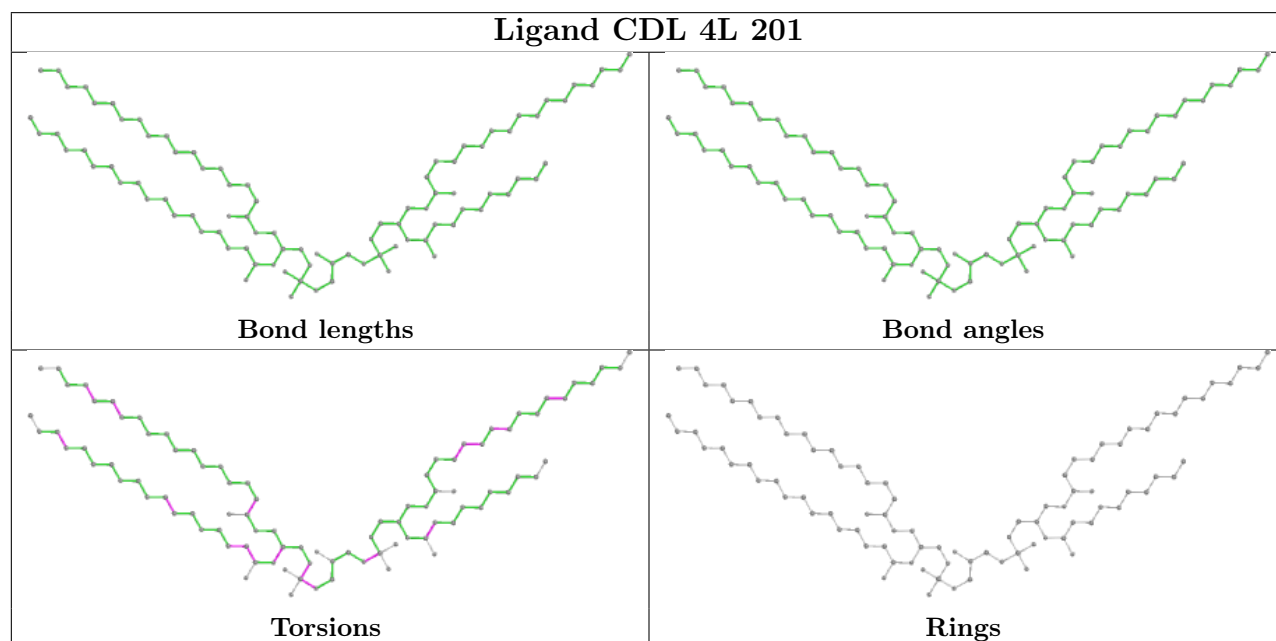
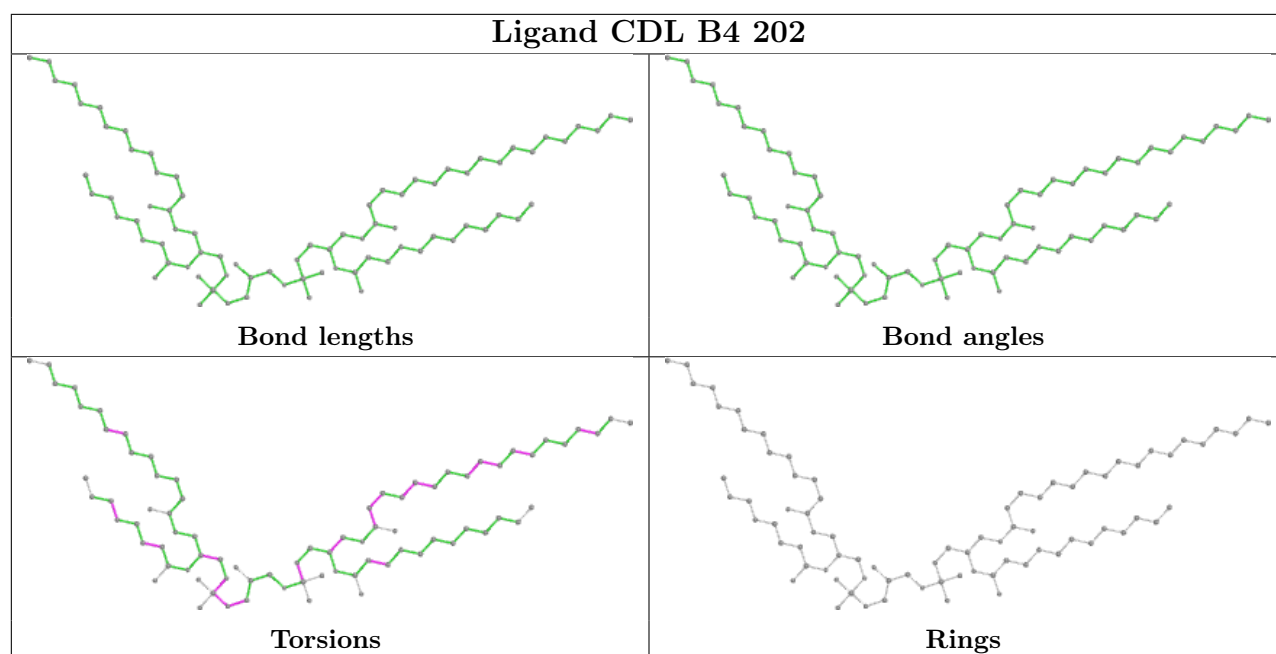


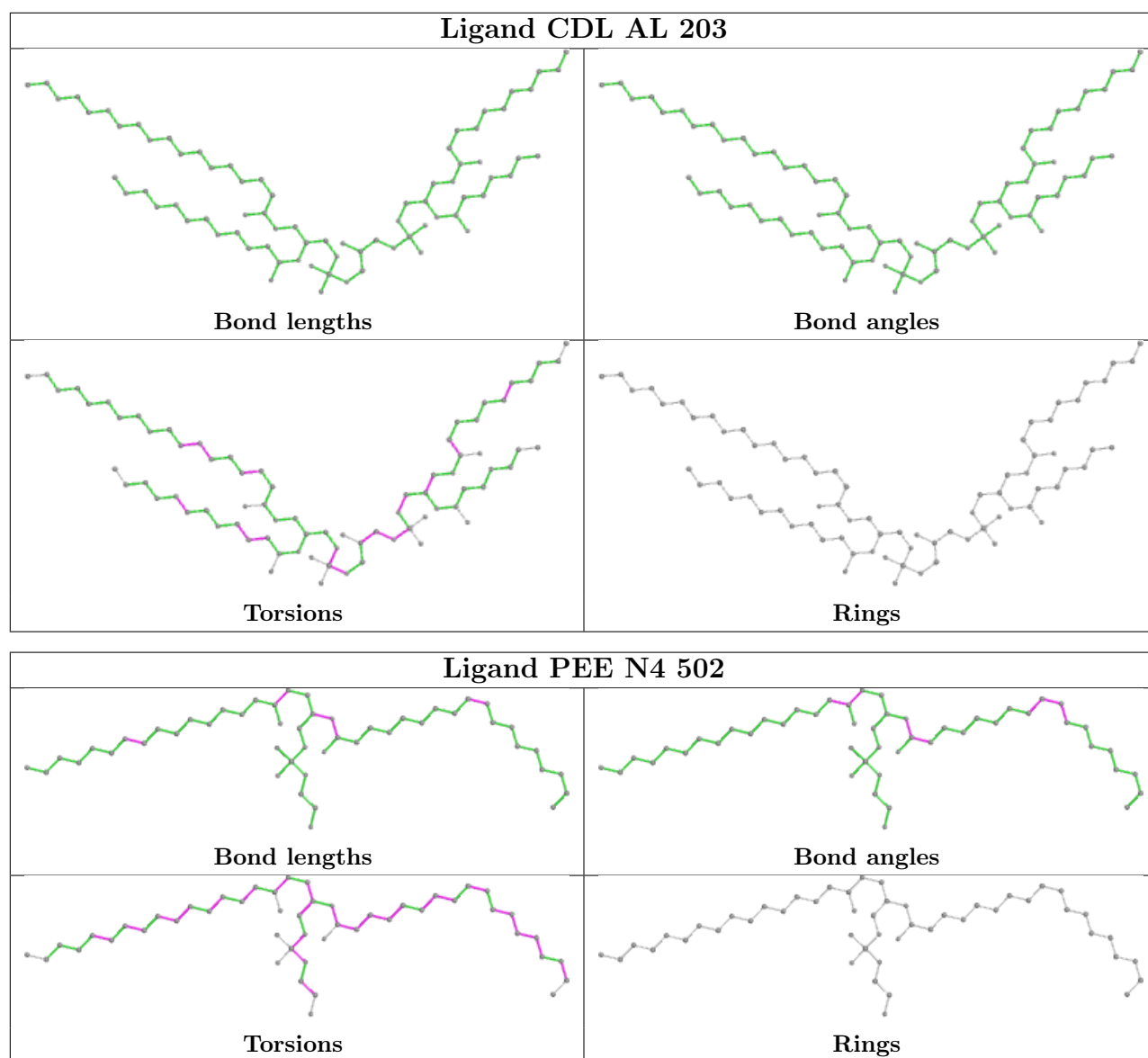




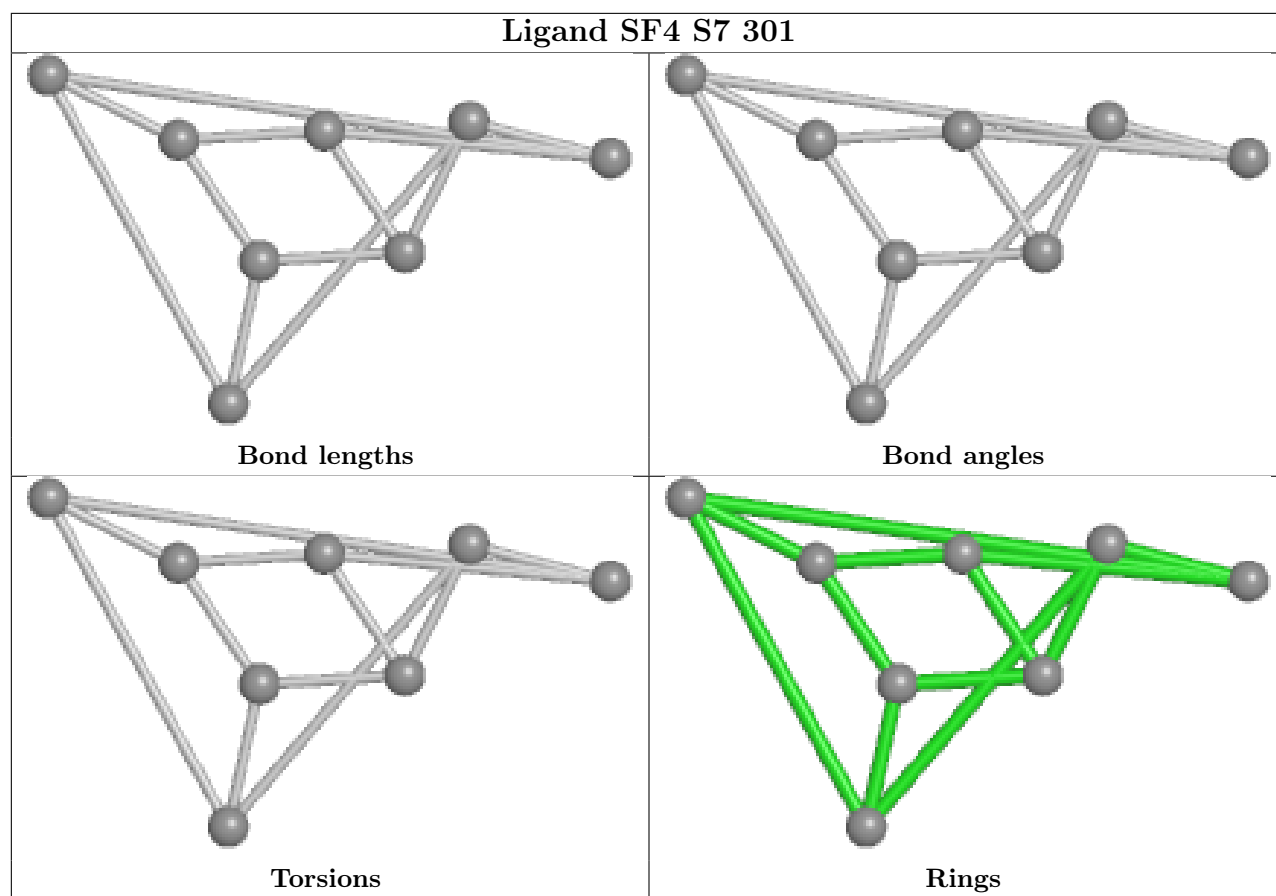
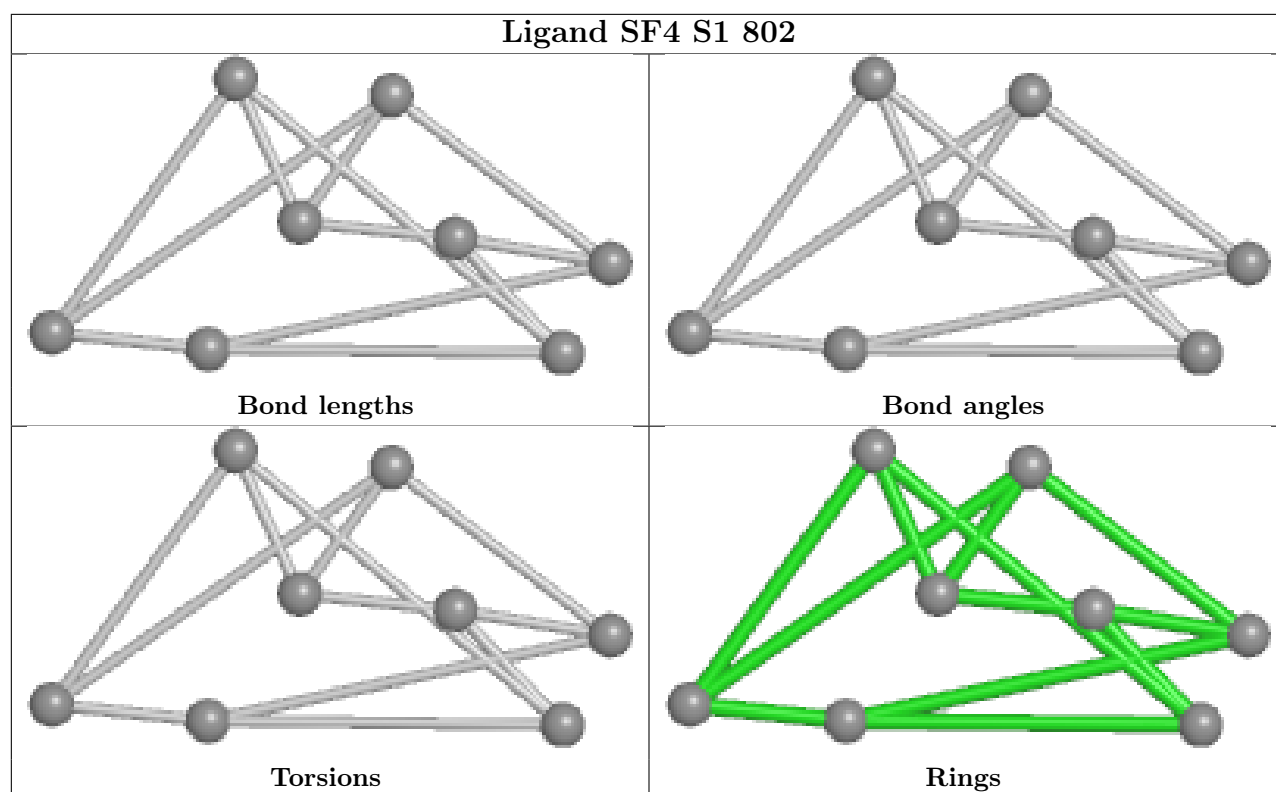












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

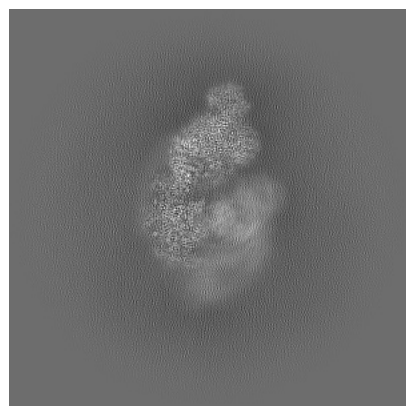
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60419. These allow visual inspection of the internal detail of the map and identification of artifacts.

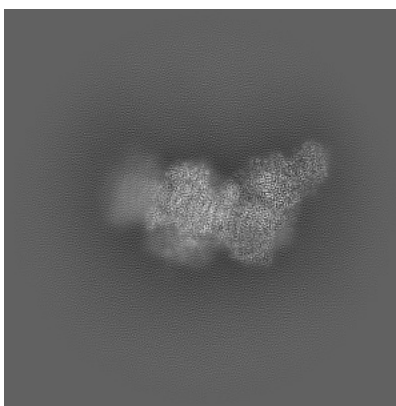
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

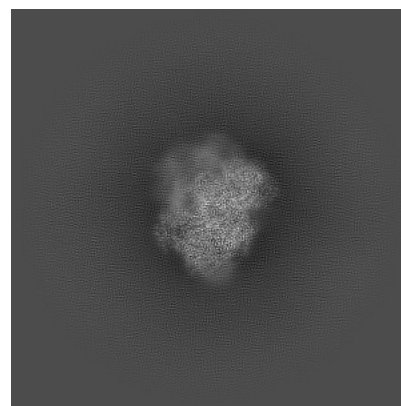
#### 6.1.1 Primary map



X

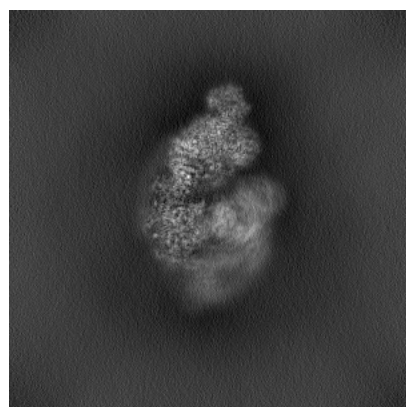


Y

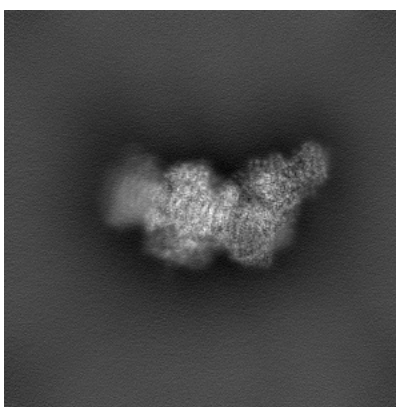


Z

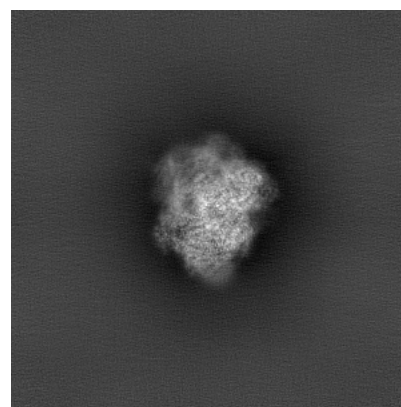
#### 6.1.2 Raw map



X



Y

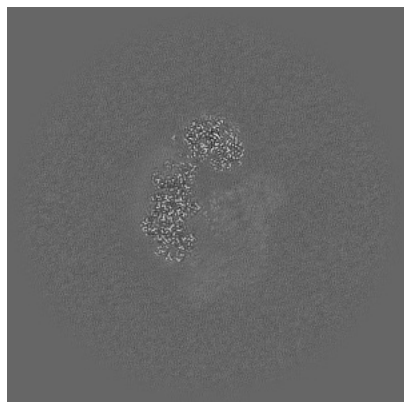


Z

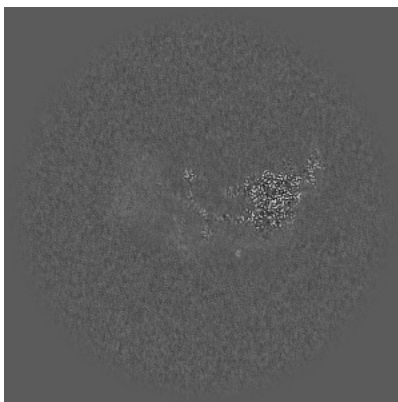
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

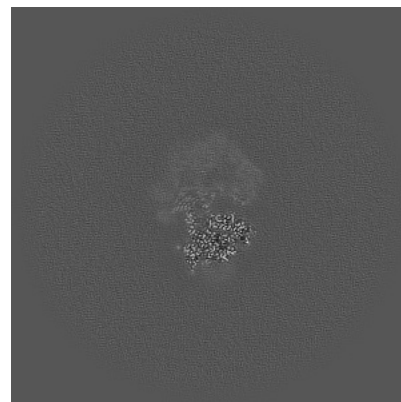
### 6.2.1 Primary map



X Index: 240

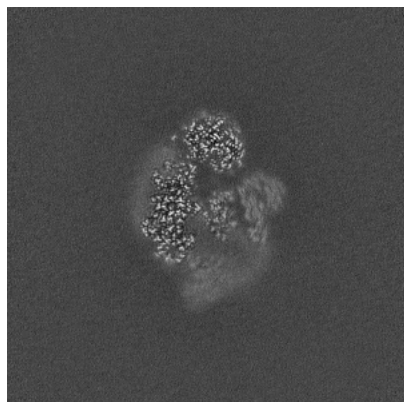


Y Index: 240

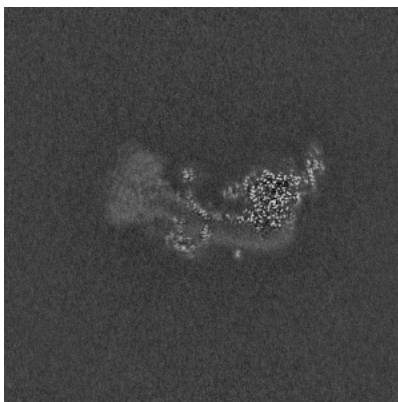


Z Index: 240

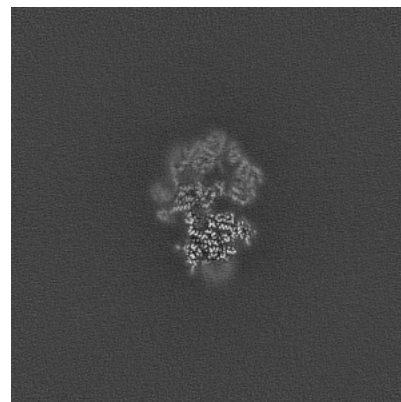
### 6.2.2 Raw map



X Index: 240



Y Index: 240

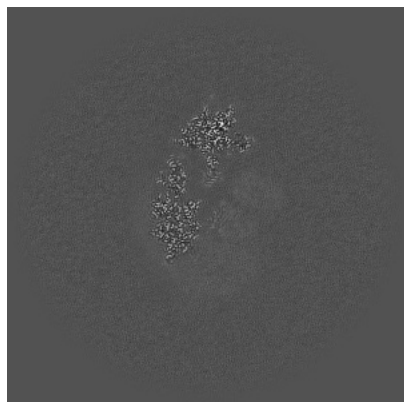


Z Index: 240

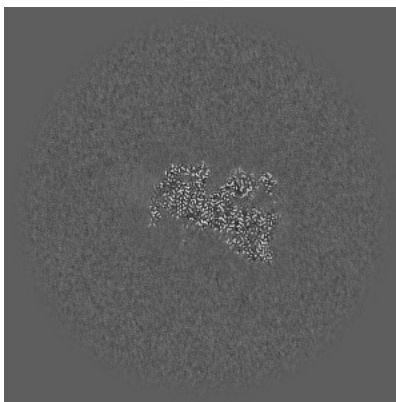
The images above show central slices of the map in three orthogonal directions.

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

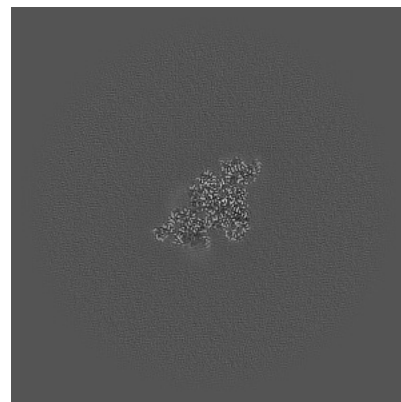
### 6.3.1 Primary map



X Index: 256

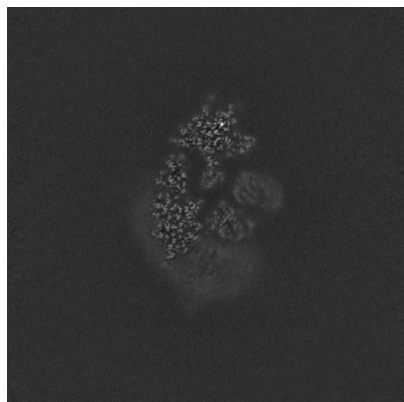


Y Index: 206

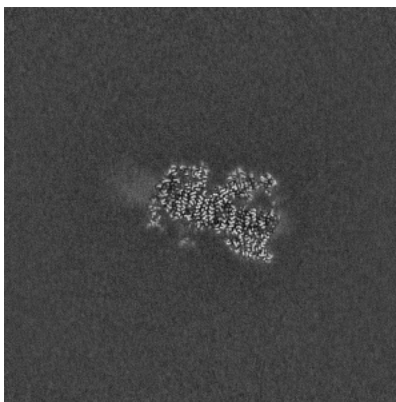


Z Index: 315

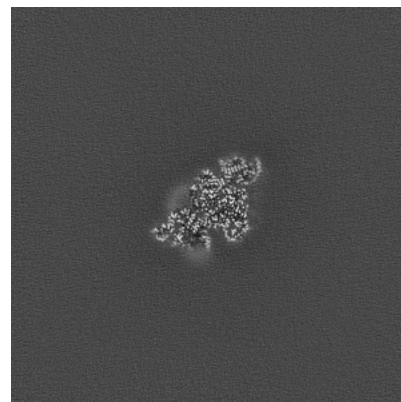
### 6.3.2 Raw map



X Index: 256



Y Index: 205



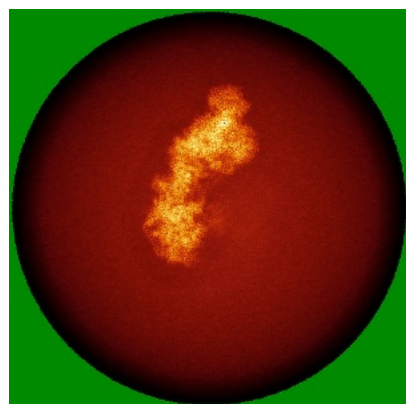
Z Index: 314

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

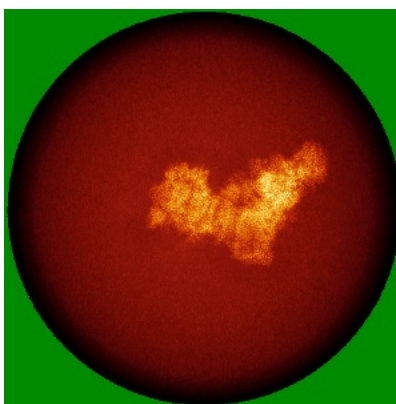


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

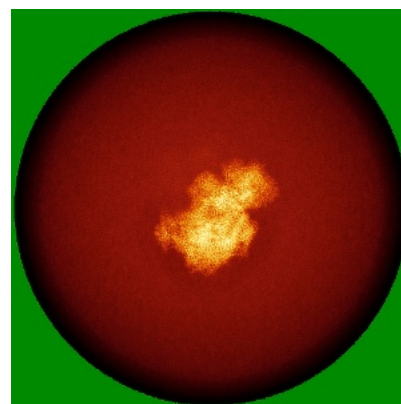
### 6.4.1 Primary map



X

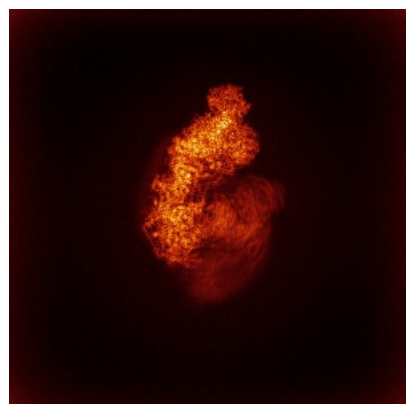


Y

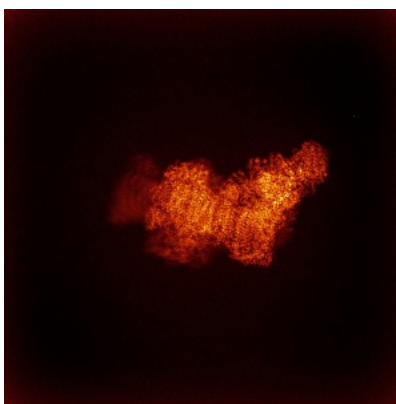


Z

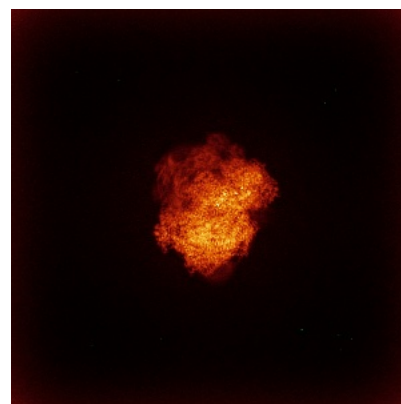
### 6.4.2 Raw map



X



Y



Z

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

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

### 6.5.1 Primary map



X



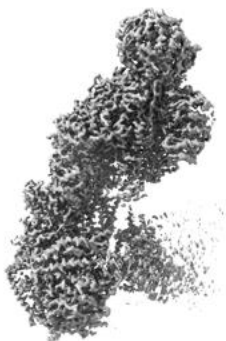
Y



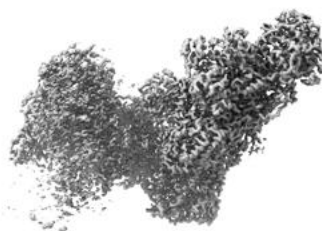
Z

The images above show the 3D surface view of the map at the recommended contour level 7.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

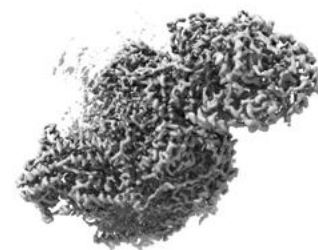
### 6.5.2 Raw map



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.

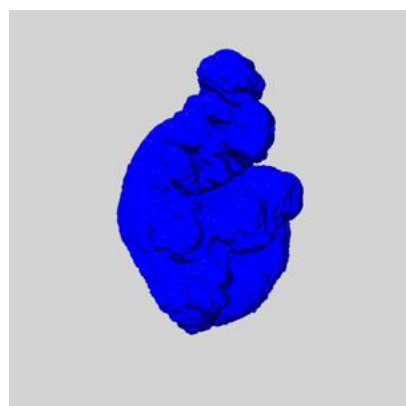
## 6.6 Mask visualisation [i](#)

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

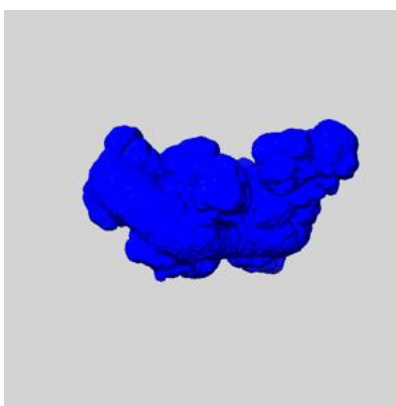
A mask typically either:

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

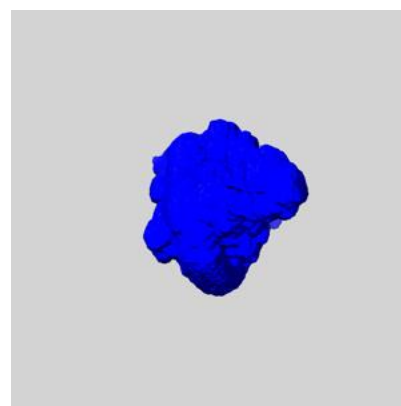
### 6.6.1 emd\_60419\_msk\_1.map [i](#)



X



Y



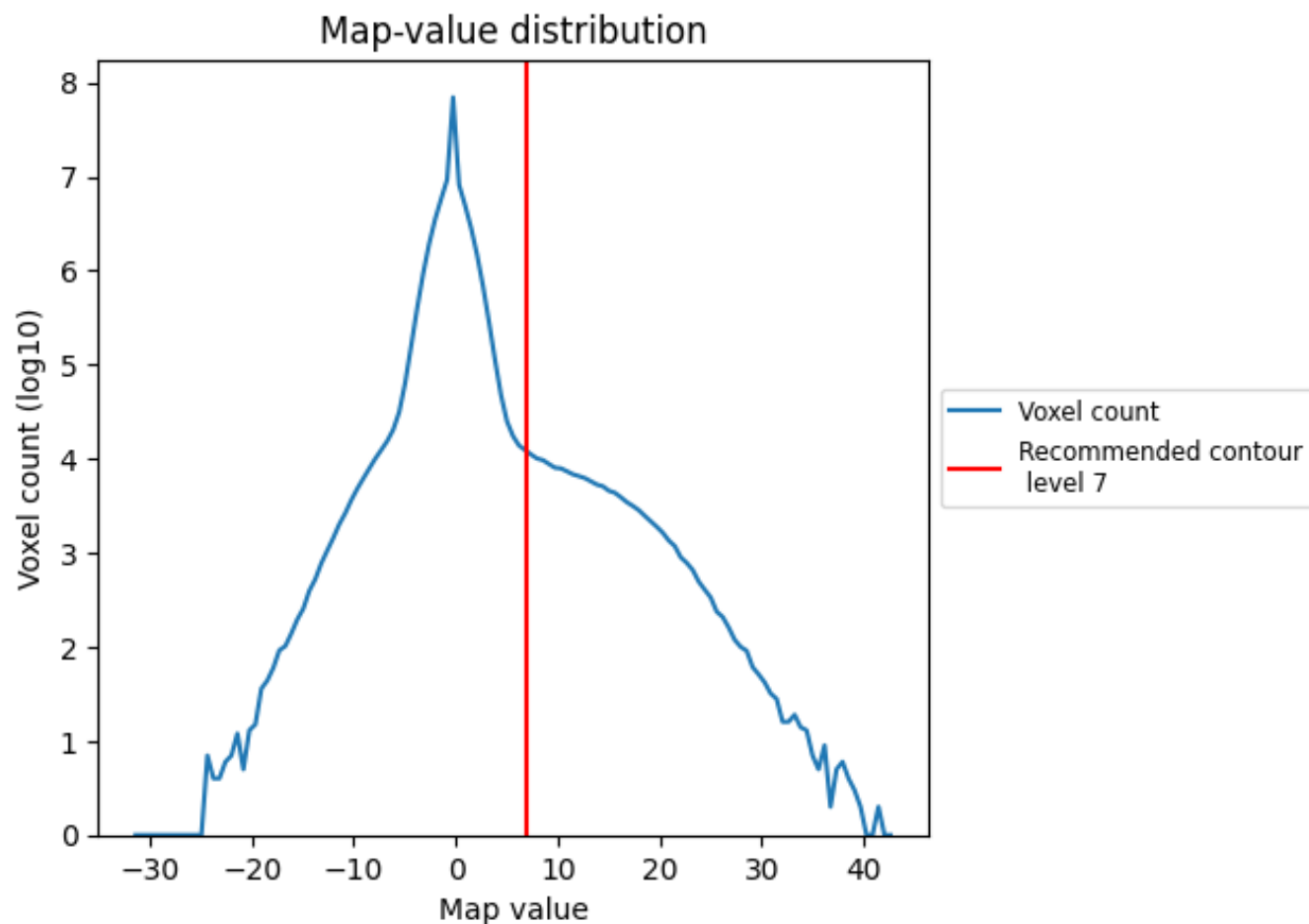
Z



## 7 Map analysis [i](#)

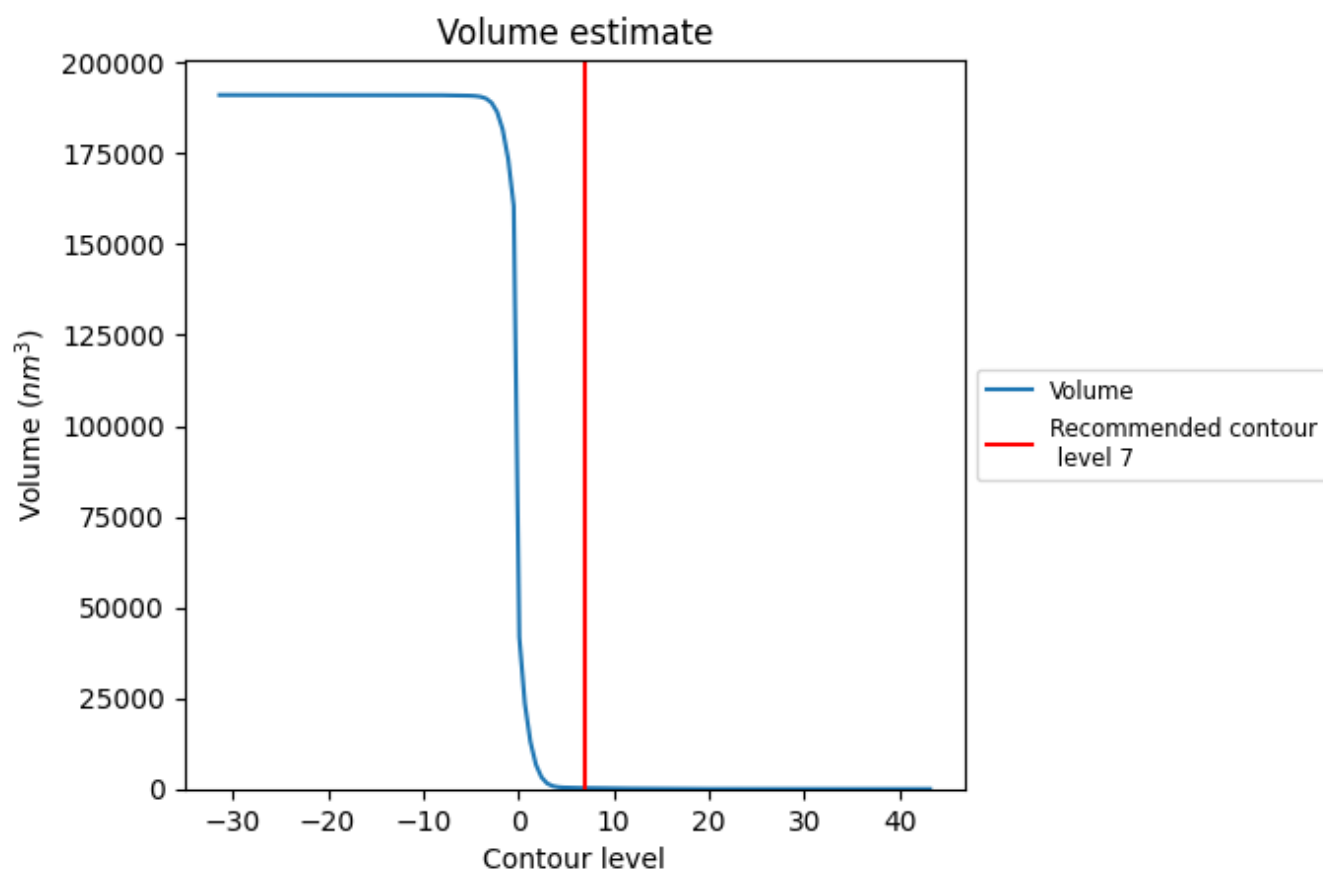
This section contains the results of statistical analysis of the map.

### 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.

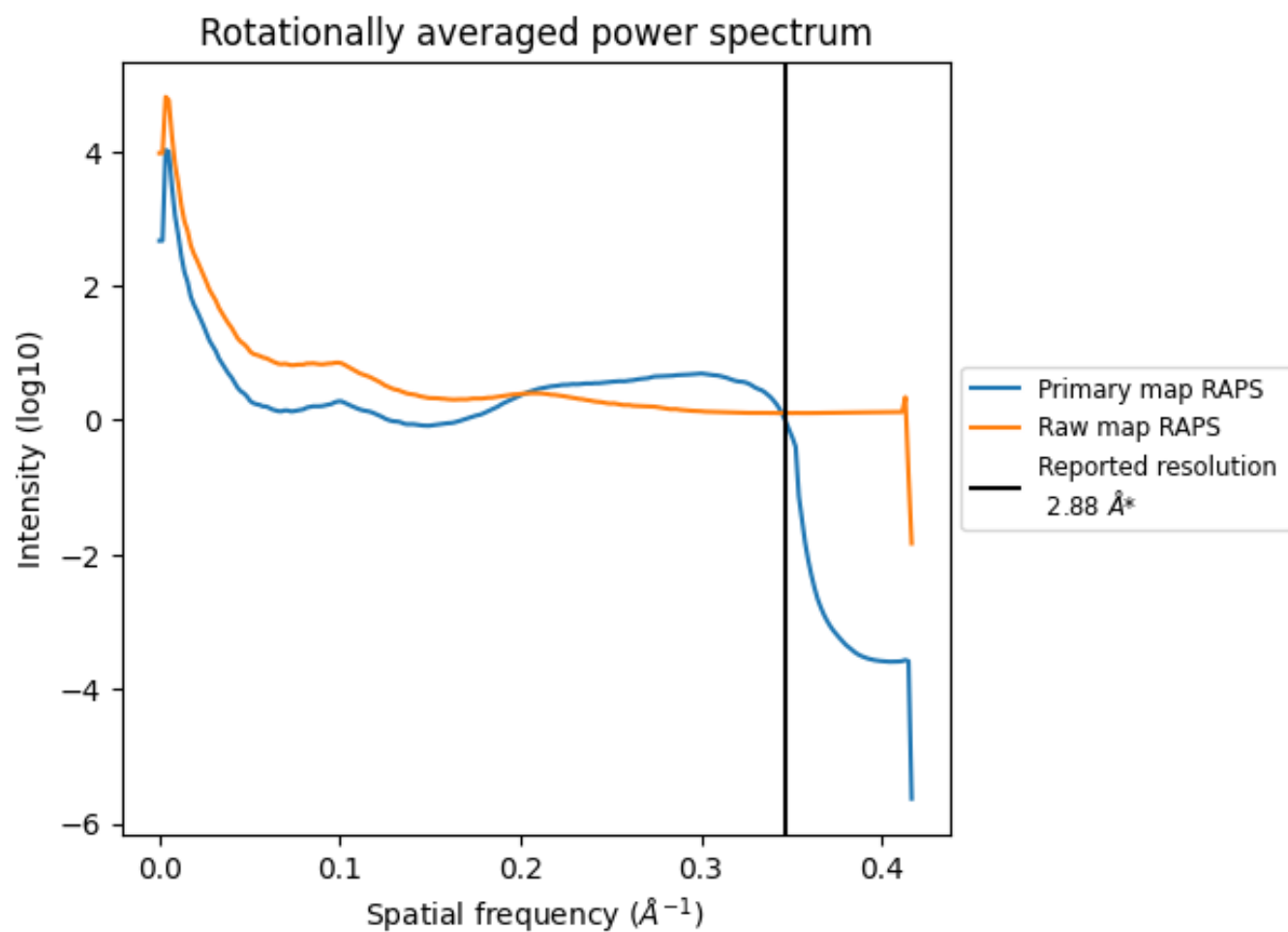
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 251  $\text{nm}^3$ ; this corresponds to an approximate mass of 226 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

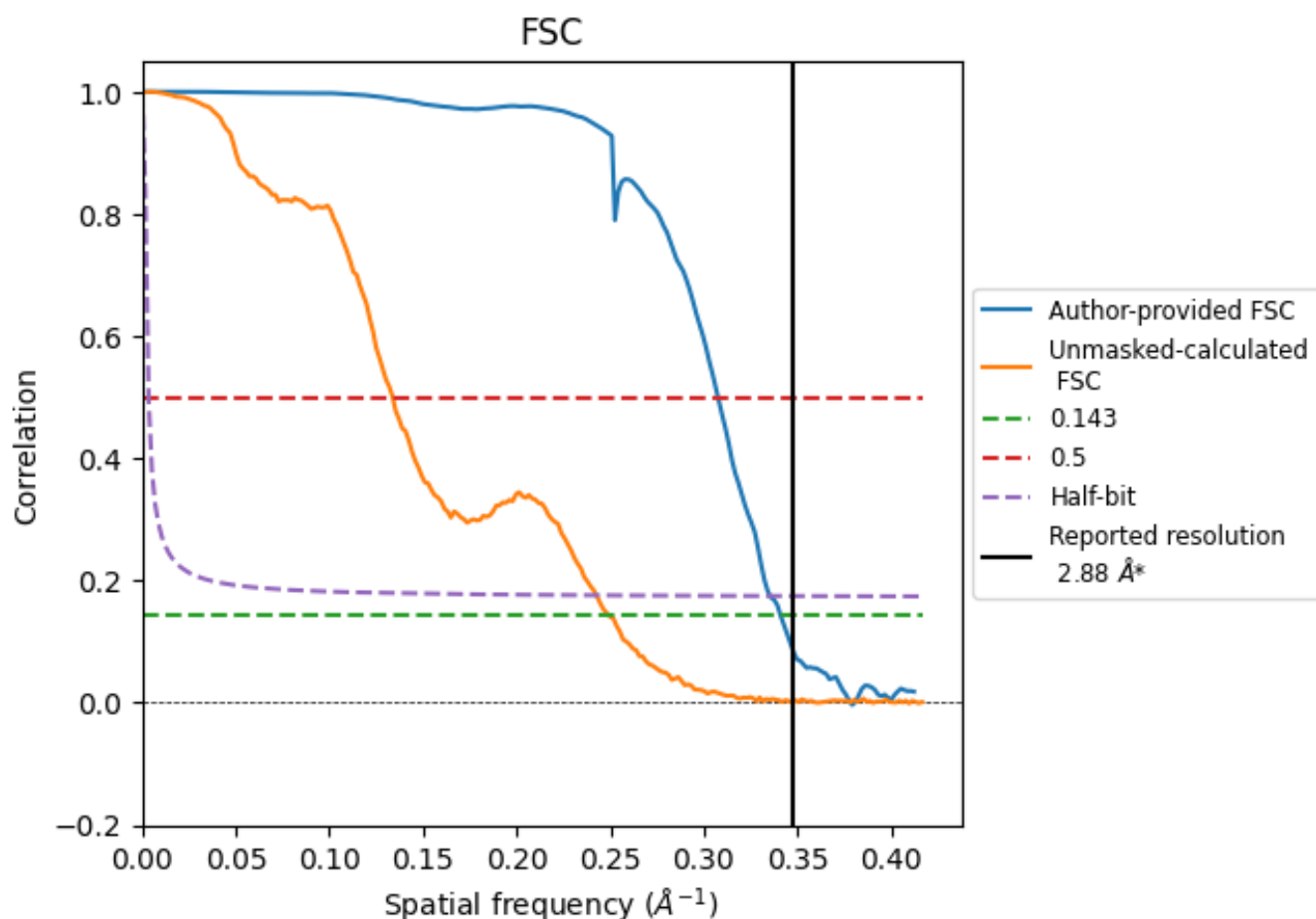


\*Reported resolution corresponds to spatial frequency of 0.347  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



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

## 8.2 Resolution estimates [i](#)

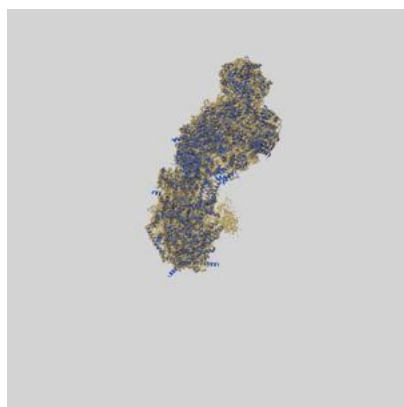
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.93	3.25	2.98
Unmasked-calculated*	4.01	7.47	4.12

\*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 4.01 differs from the reported value 2.88 by more than 10 %

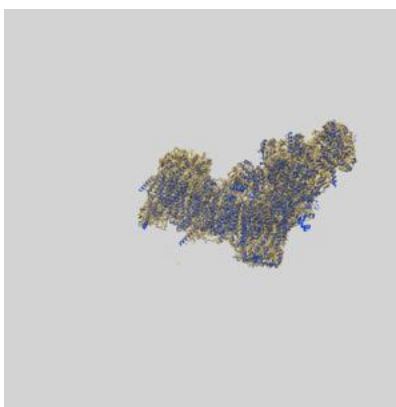
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60419 and PDB model 8ZSL. Per-residue inclusion information can be found in section [3](#) on page [23](#).

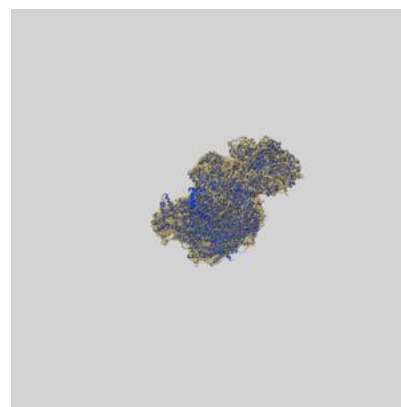
### 9.1 Map-model overlay [i](#)



X



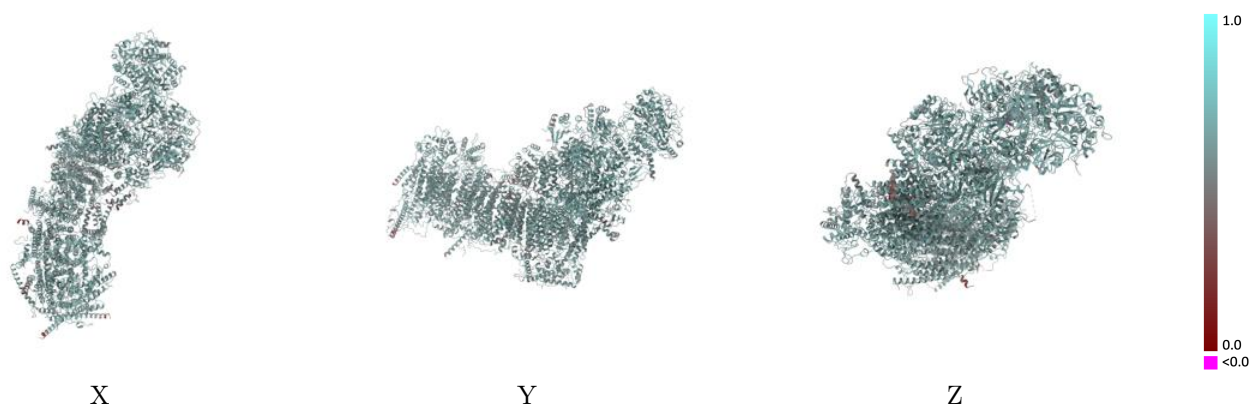
Y



Z

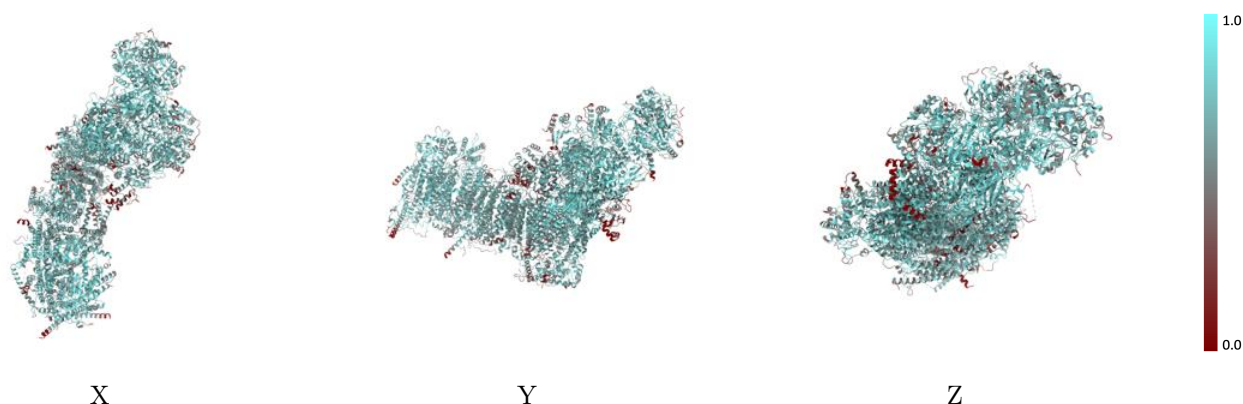
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



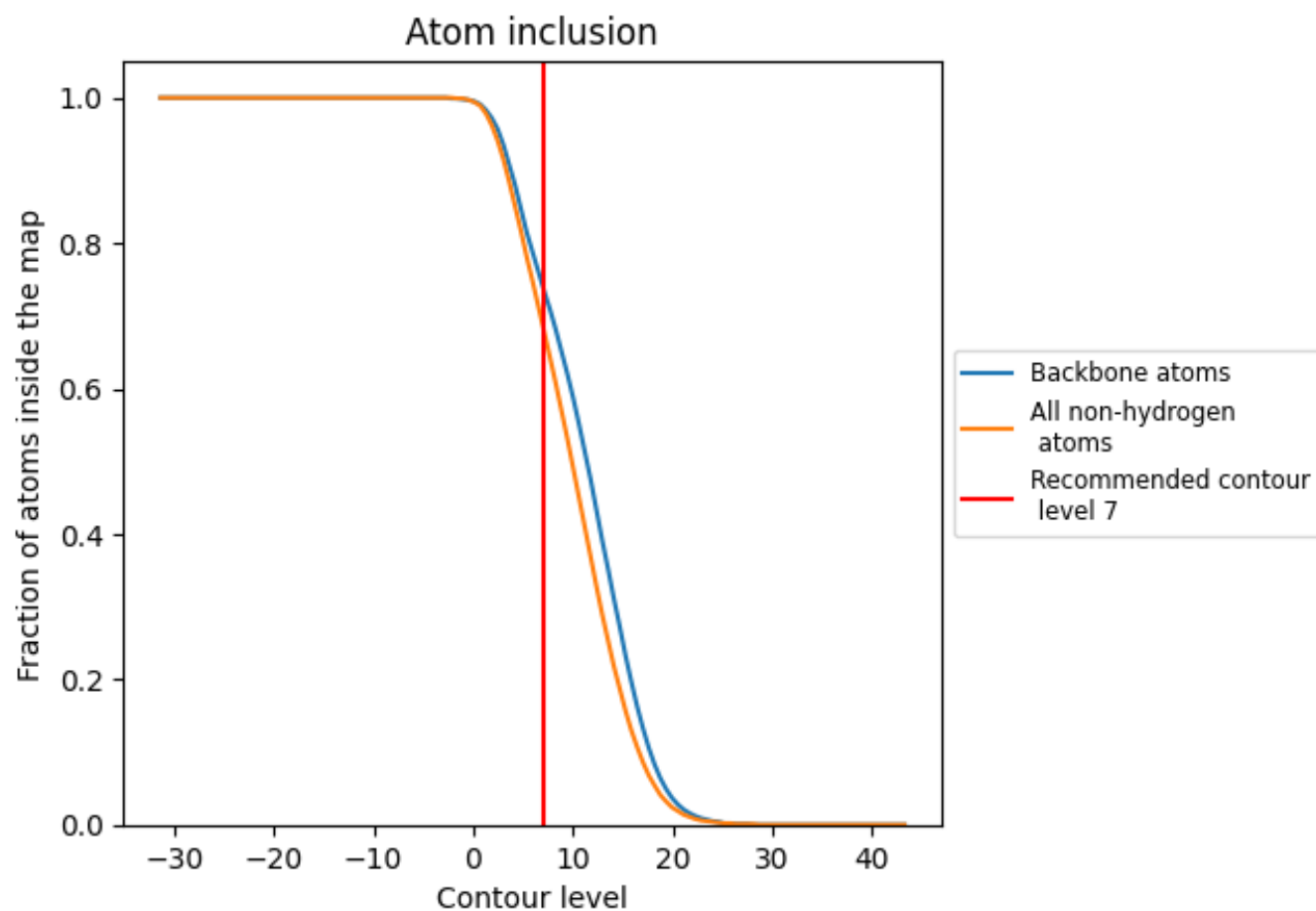
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 74% of all backbone atoms, 68% 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 (7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6850	 0.5990
4L	 0.6850	 0.6040
A1	 0.6270	 0.5850
A2	 0.5880	 0.5770
A3	 0.5810	 0.5870
A5	 0.6690	 0.6010
A6	 0.6660	 0.6010
A7	 0.4430	 0.5460
A8	 0.6590	 0.5960
A9	 0.7260	 0.6150
AB	 0.2900	 0.5020
AC	 0.7350	 0.6020
AK	 0.6040	 0.5720
AL	 0.4930	 0.5790
AM	 0.2710	 0.5580
AN	 0.6280	 0.5880
B1	 0.5560	 0.5470
B2	 0.6700	 0.5900
B3	 0.6020	 0.5650
B4	 0.5910	 0.5920
B5	 0.7030	 0.6070
B6	 0.6070	 0.5610
B7	 0.6630	 0.5780
B8	 0.7250	 0.6040
B9	 0.7560	 0.6100
BK	 0.6920	 0.5920
BL	 0.6780	 0.5950
CA	 0.5440	 0.5780
CB	 0.6650	 0.6030
N1	 0.6980	 0.6010
N2	 0.7500	 0.6110
N3	 0.6410	 0.6060
N4	 0.7460	 0.6150
N5	 0.7430	 0.6090
N6	 0.6120	 0.5640



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
S1	 0.7340	 0.6040
S2	 0.7880	 0.6200
S3	 0.8230	 0.6330
S4	 0.7350	 0.6150
S5	 0.6020	 0.5810
S6	 0.6190	 0.6030
S7	 0.8090	 0.6260
S8	 0.8340	 0.6300
V1	 0.7220	 0.6040
V2	 0.6530	 0.5920
V3	 0.5610	 0.5960