



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 07:17 PM UTC

PDB ID : 8ZSK / pdb_00008zsk
EMDB ID : EMD-60418
Title : Complex I from respirasome closed state 1 bound by metformin and CoQ10, alternative orientation (SC-MetC1-ii)
Authors : Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.
Deposited on : 2024-06-05
Resolution : 3.09 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

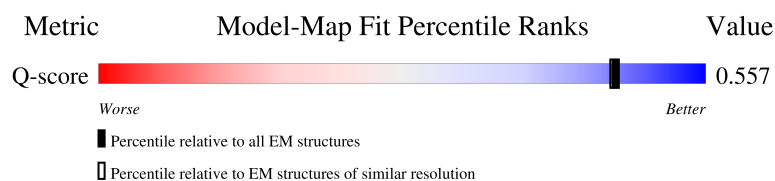
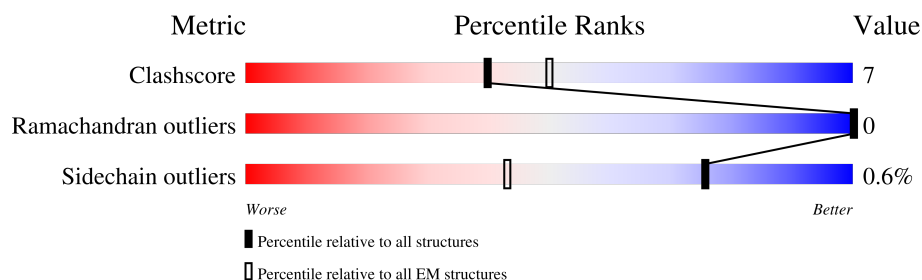
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.09 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14003 (2.59 - 3.59)

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

Mol	Chain	Length	Quality of chain
1	4L	98	
2	A1	70	
3	A2	85	
4	A3	83	

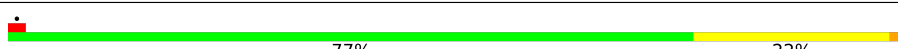
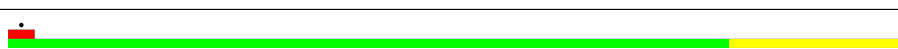
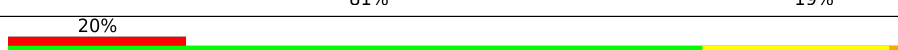
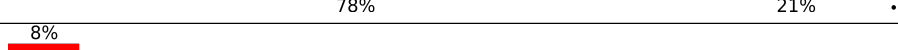
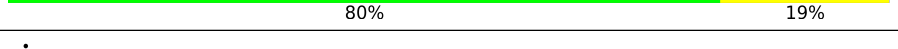
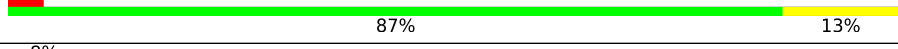
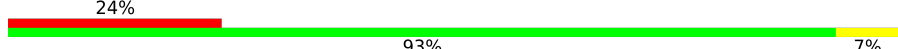
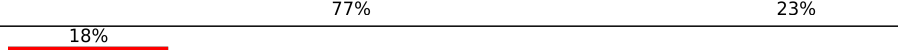
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Mol	Chain	Length	Quality of chain
5	A5	112	
6	A6	115	
7	A7	112	
8	A8	171	
9	A9	341	
10	AB	87	
10	AC	87	
11	AK	321	
12	AL	140	
13	AM	144	
14	AN	142	
15	B1	56	
16	B2	67	
17	B3	80	
18	B4	128	
19	B5	138	
20	B6	126	
21	B7	125	
22	B8	156	
23	B9	178	
24	BK	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	125	
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 60 unique types of molecules in this entry. The entry contains 69125 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	115	Total	C	N	O	S	0	0
			971	619	179	168	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	125	Total	C	N	O	S	0	0
			1016	642	181	190	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		

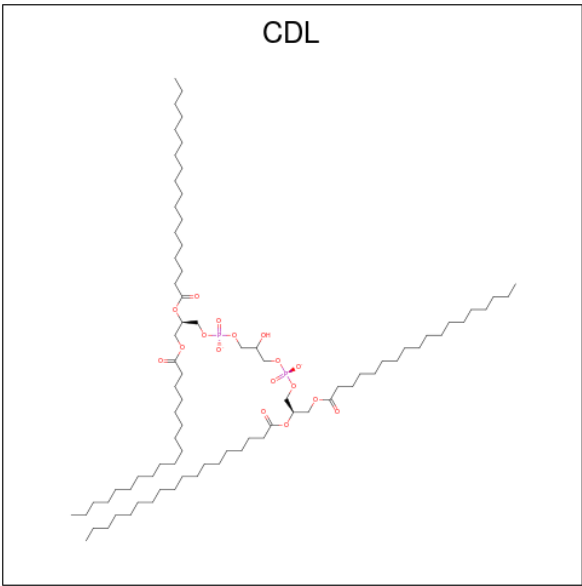
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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.

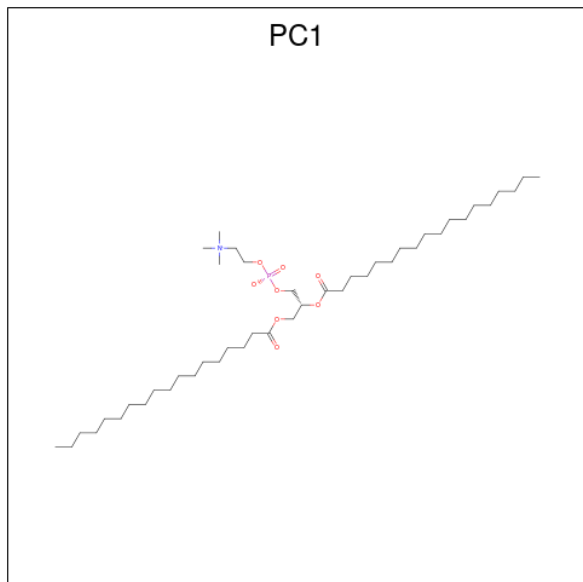
Mol	Chain	Residues	Atoms					AltConf	Trace
44	V3	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

- Molecule 45 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



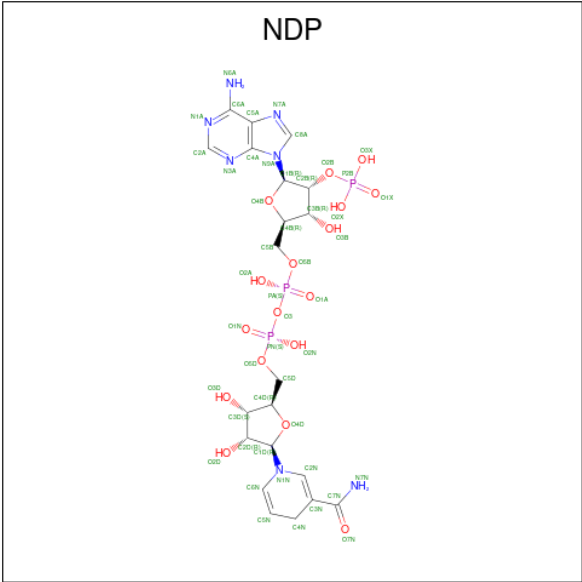
Mol	Chain	Residues	Atoms				AltConf
45	4L	1	Total	C	O	P	0
			92	73	17	2	
45	AL	1	Total	C	O	P	0
			94	75	17	2	
45	AL	1	Total	C	O	P	0
			71	52	17	2	
45	AM	1	Total	C	O	P	0
			88	69	17	2	
45	AN	1	Total	C	O	P	0
			100	81	17	2	
45	B1	1	Total	C	O	P	0
			76	57	17	2	
45	B4	1	Total	C	O	P	0
			80	61	17	2	
45	B5	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	N5	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: $C_{44}H_{88}NO_8P$).



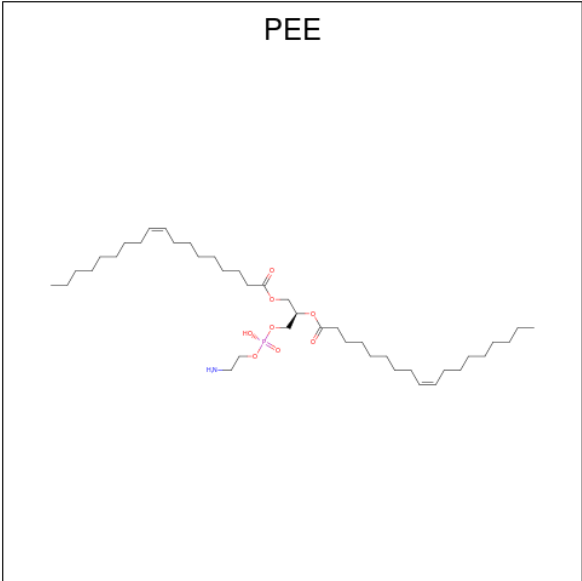
Mol	Chain	Residues	Atoms					AltConf
46	A3	1	Total	C	N	O	P	0
			50	40	1	8	1	
46	A3	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	B4	1	Total	C	N	O	P	0
			52	42	1	8	1	
46	B5	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	B5	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	N1	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	N3	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	N3	1	Total	C	N	O	P	0
			54	44	1	8	1	

- 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: C₄₁H₇₈NO₈P).



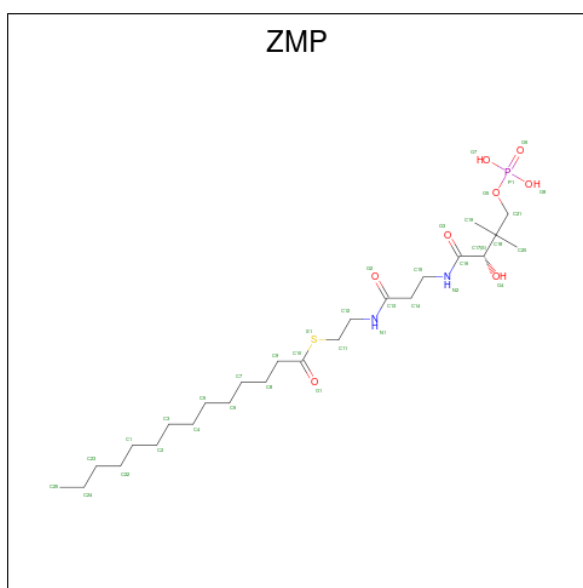
Mol	Chain	Residues	Atoms					AltConf
48	A9	1	Total	C	N	O	P	0
			39	29	1	8	1	
48	AL	1	Total	C	N	O	P	0
			36	26	1	8	1	

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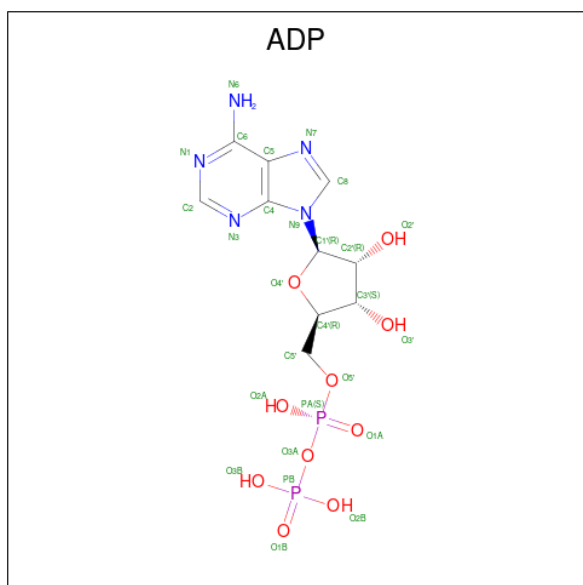
Mol	Chain	Residues	Atoms					AltConf
48	B6	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	BL	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	N1	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	N1	1	Total	C	N	O	P	0
			31	21	1	8	1	
48	N3	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	N4	1	Total	C	N	O	P	0
			49	39	1	8	1	
48	N5	1	Total	C	N	O	P	0
			35	25	1	8	1	
48	N5	1	Total	C	N	O	P	0
			40	30	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
			48	38	1	8	1	
48	S8	1	Total	C	N	O	P	0
			51	41	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: C₂₅H₄₉N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



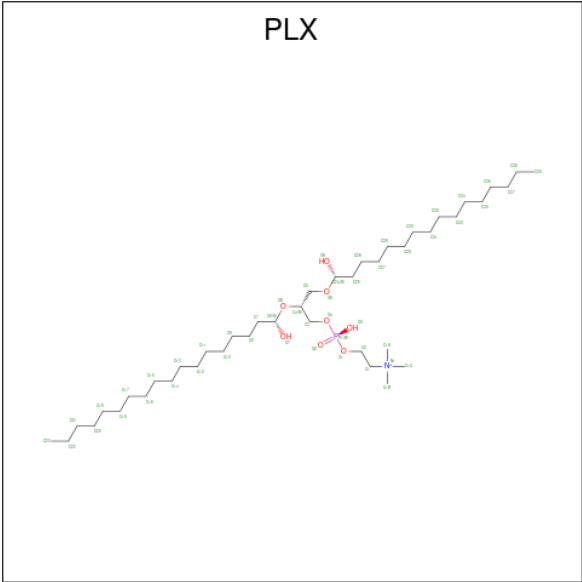
Mol	Chain	Residues	Atoms						AltConf
49	AB	1	Total 36	C 25	N 2	O 7	P 1	S 1	0
49	AC	1	Total 36	C 25	N 2	O 7	P 1	S 1	0

- Molecule 50 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



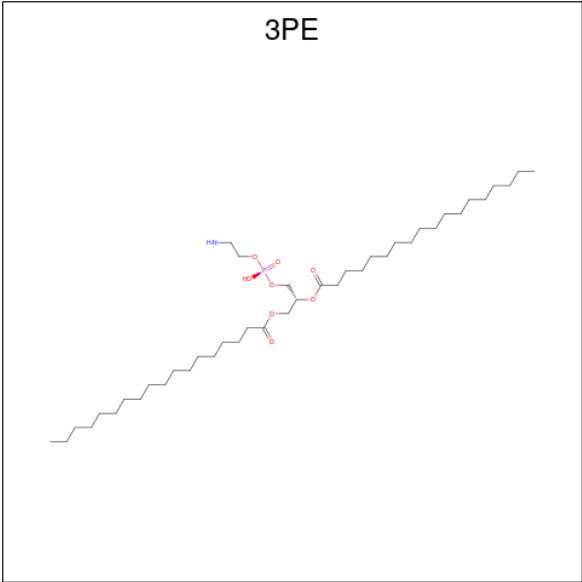
Mol	Chain	Residues	Atoms					AltConf
50	AK	1	Total	C	N	O	P	0
			27	10	5	10	2	

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



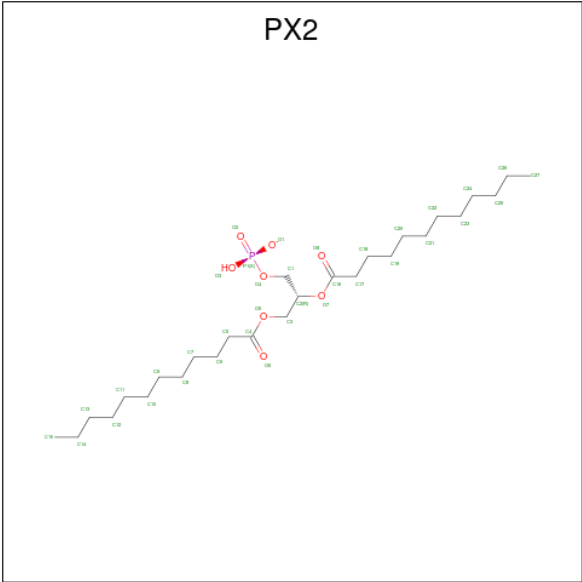
Mol	Chain	Residues	Atoms					AltConf
51	B1	1	Total	C	N	O	P	0
			52	42	1	8	1	
51	BL	1	Total	C	N	O	P	0
			52	42	1	8	1	
51	CB	1	Total	C	N	O	P	0
			52	42	1	8	1	
51	N1	1	Total	C	N	O	P	0
			47	37	1	8	1	
51	N2	1	Total	C	N	O	P	0
			52	42	1	8	1	
51	N4	1	Total	C	N	O	P	0
			47	37	1	8	1	
51	S7	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 52 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



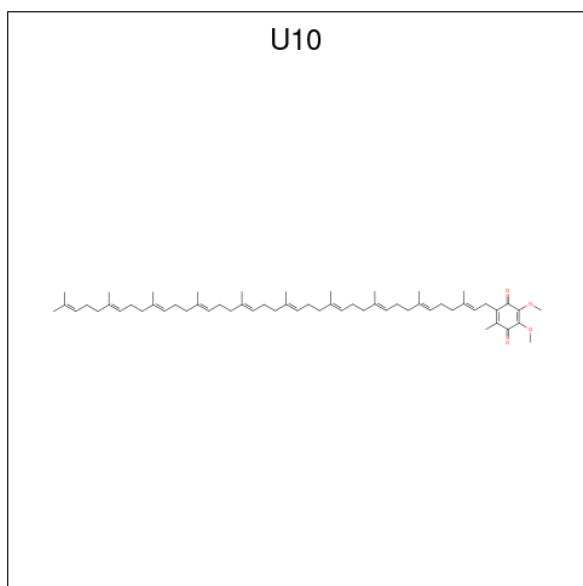
Mol	Chain	Residues	Atoms					AltConf
52	B8	1	Total	C	N	O	P	0
			32	22	1	8	1	
52	CB	1	Total	C	N	O	P	0
			46	36	1	8	1	
52	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 53 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: $C_{27}H_{52}O_8P$).



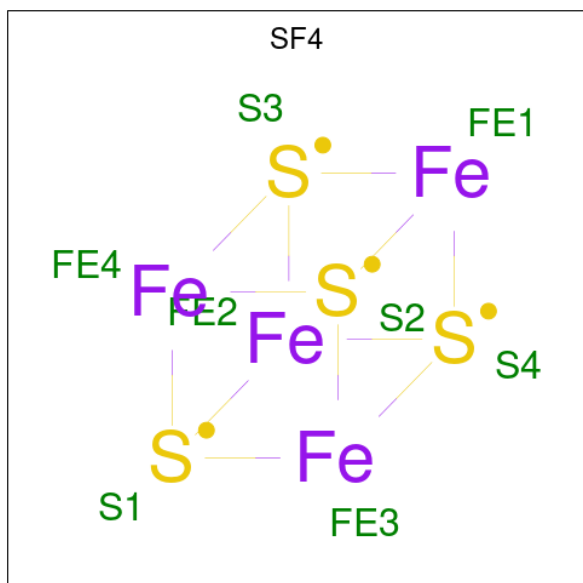
Mol	Chain	Residues	Atoms				AltConf
53	CA	1	Total	C	O	P	0
			36	27	8	1	

- Molecule 54 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



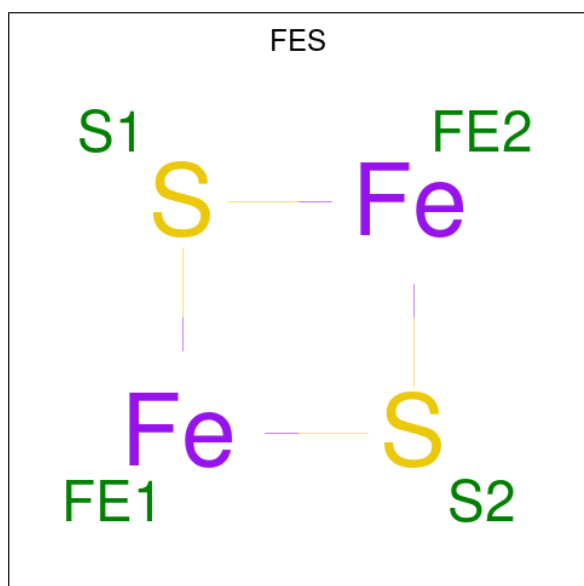
Mol	Chain	Residues	Atoms				AltConf
54	N1	1	Total	C	O		0
			63	59	4		

- Molecule 55 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 56 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

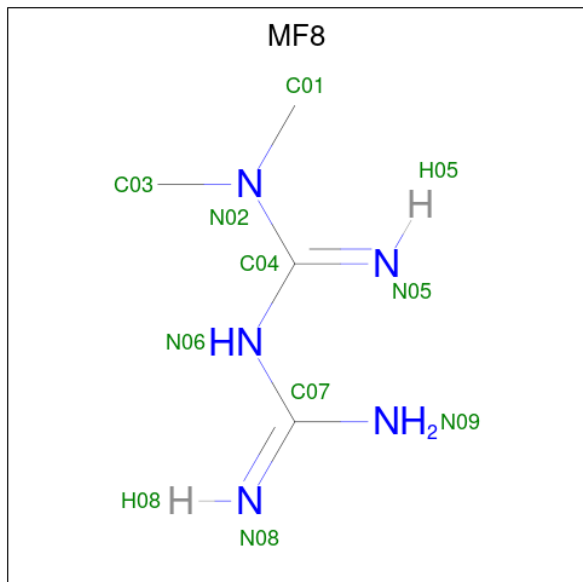


Mol	Chain	Residues	Atoms			AltConf
56	S1	1	Total	Fe	S	0
			4	2	2	
56	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 58 is Metformin (CCD ID: MF8) (formula: $C_4H_{11}N_5$) (labeled as "Ligand of Interest" by depositor).

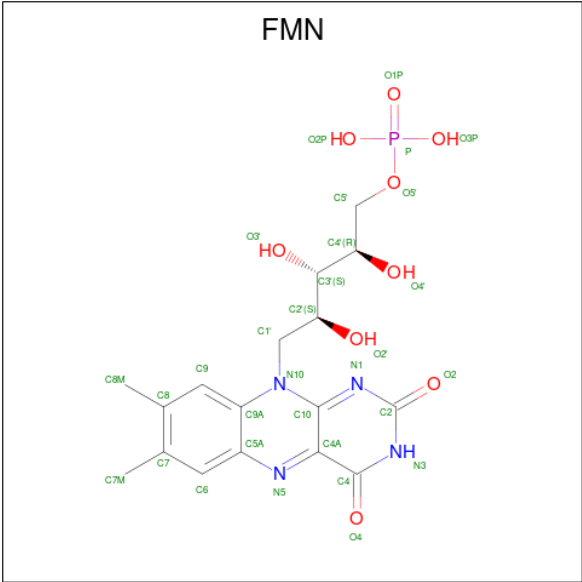


Mol	Chain	Residues	Atoms			AltConf
58	S2	1	Total	C	N	0
			9	4	5	

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	S6	1	Total	Zn	0
			1	1	

- Molecule 60 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).

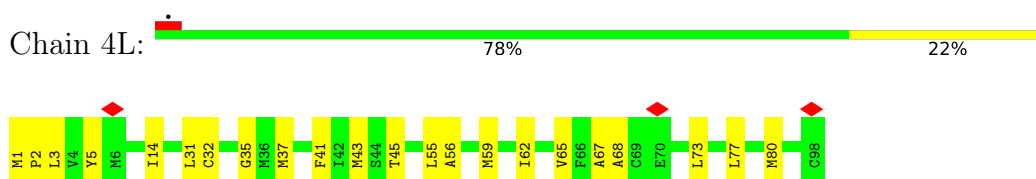


Mol	Chain	Residues	Atoms					AltConf
60	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

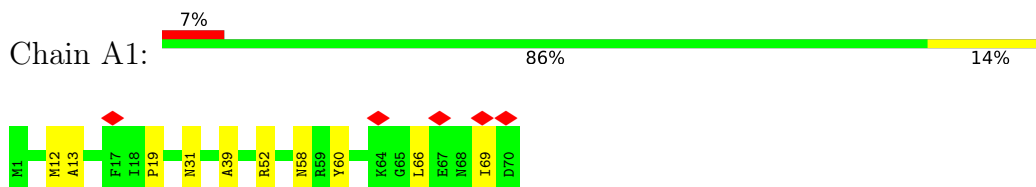
3 Residue-property plots

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.

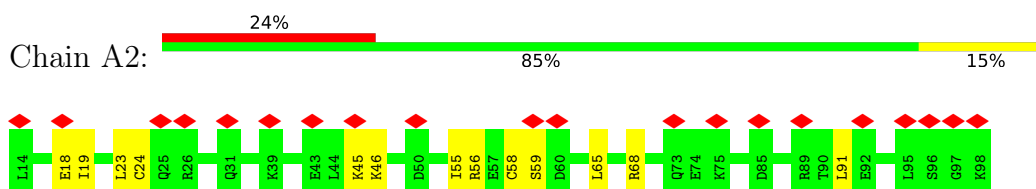
- Molecule 1: NADH-ubiquinone oxidoreductase chain 4L



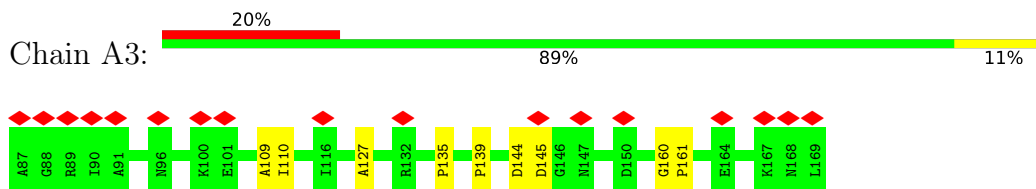
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



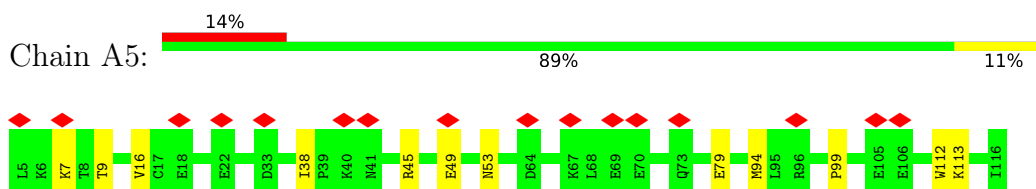
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



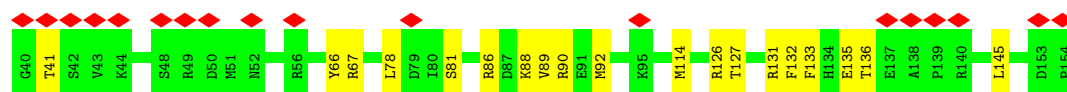
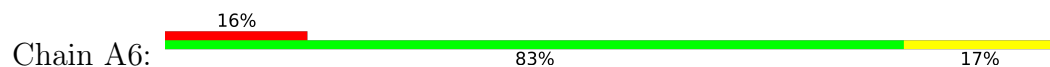
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



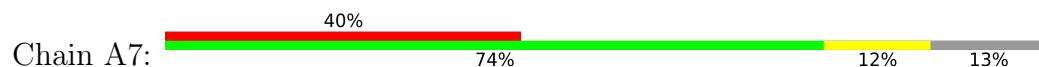
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



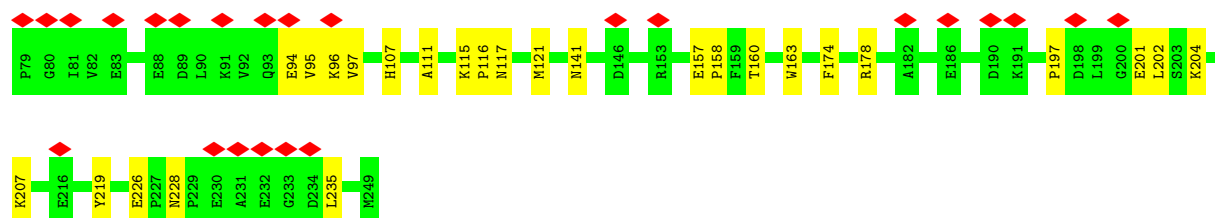
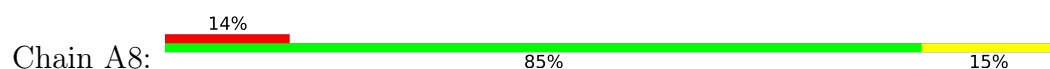
- Molecule 6: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



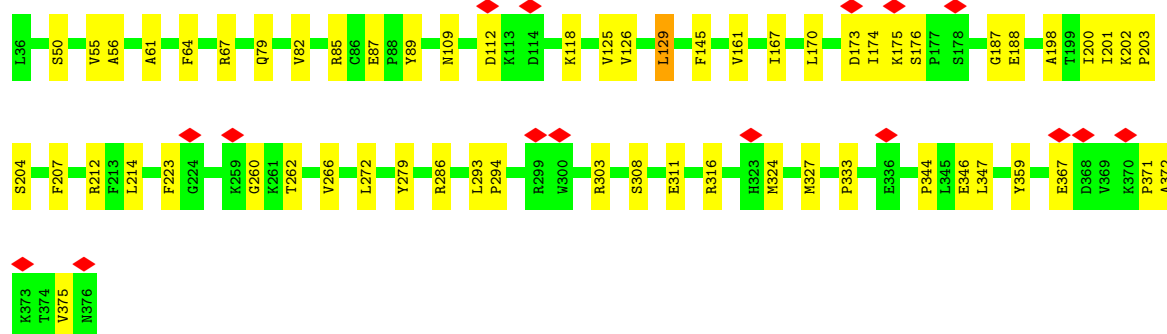
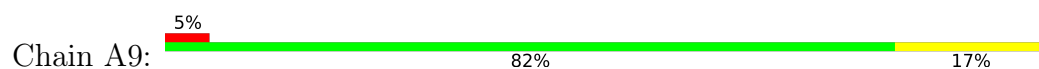
- Molecule 7: Complex I-B14.5a



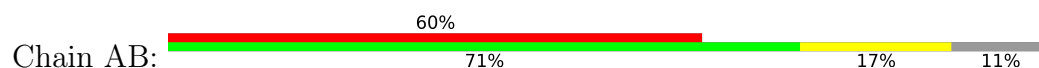
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

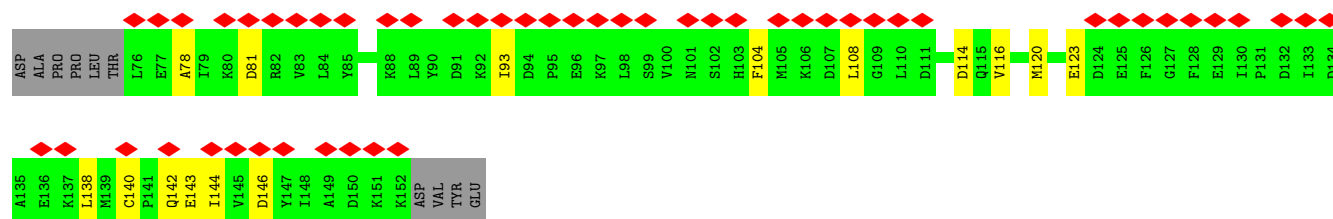


- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

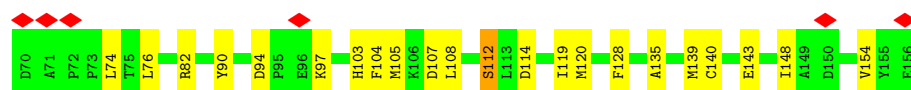
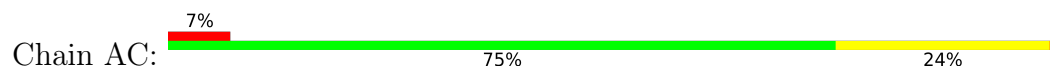


- Molecule 10: Acyl carrier protein

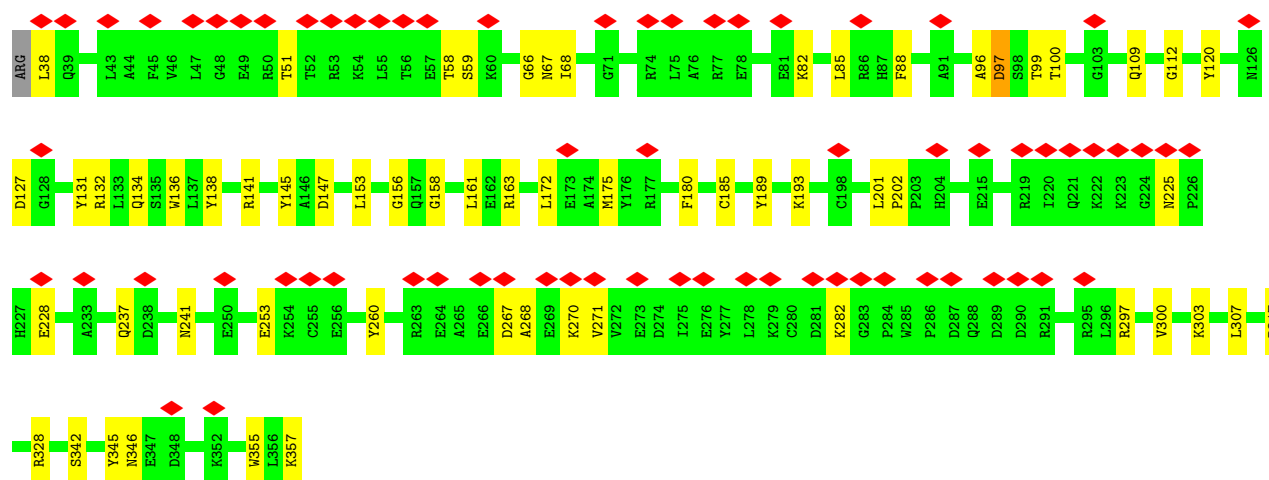
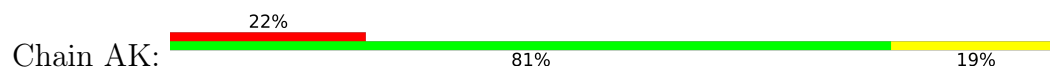




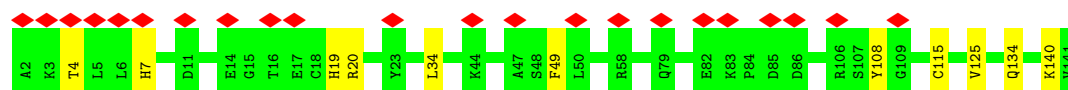
- Molecule 10: Acyl carrier protein



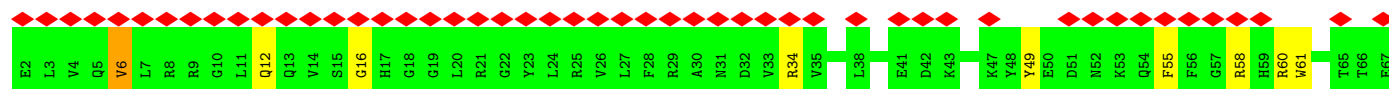
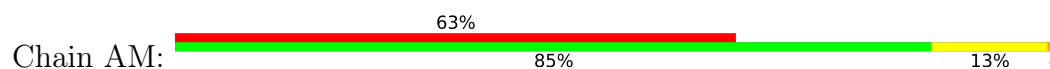
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

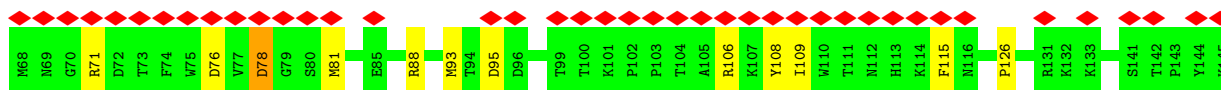


- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

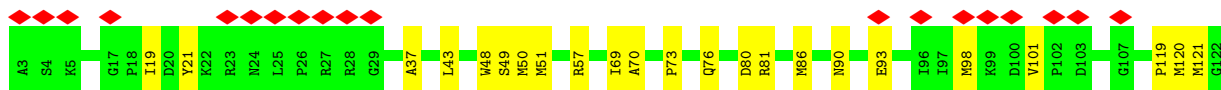
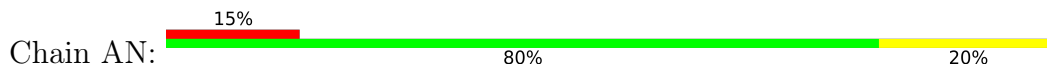


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

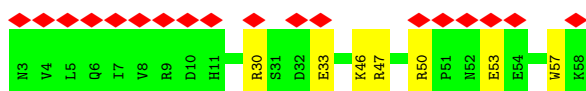
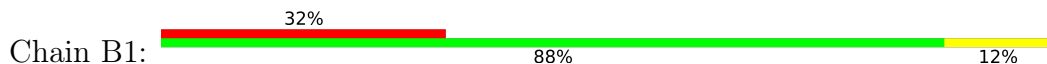




- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



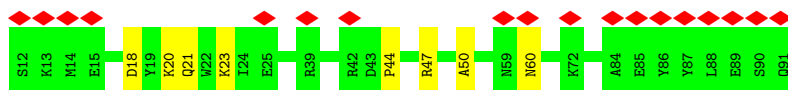
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



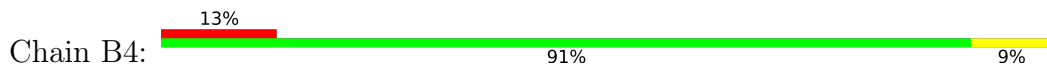
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



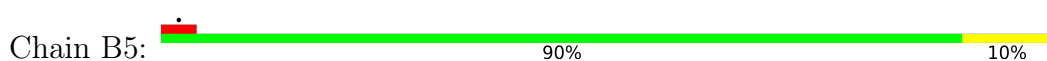
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



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

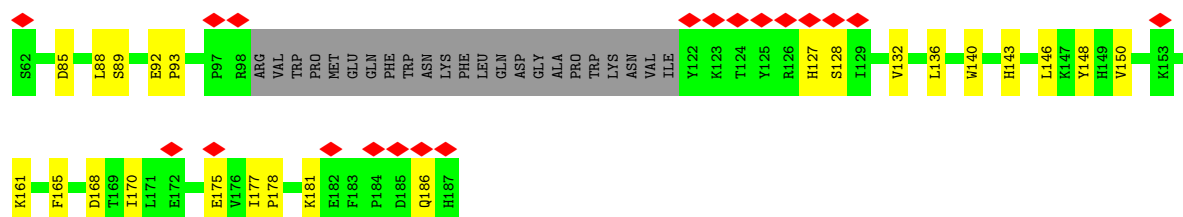


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

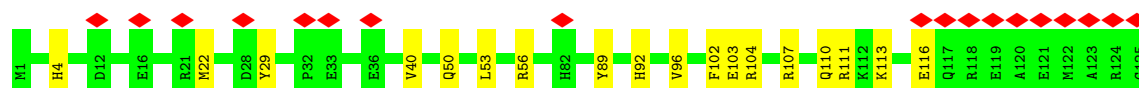
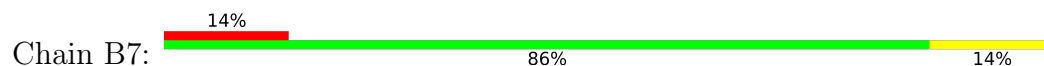




- Molecule 20: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



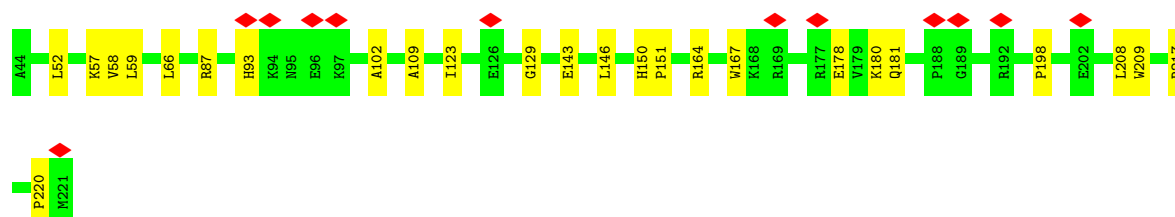
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



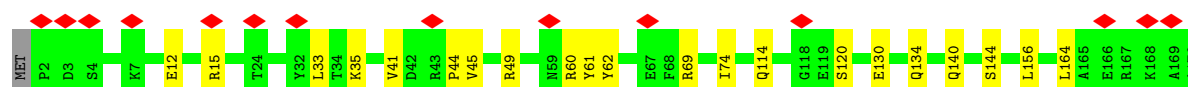
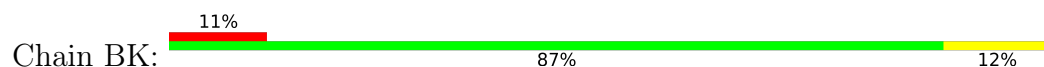
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



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

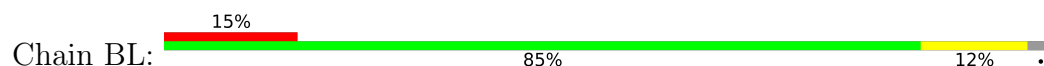


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

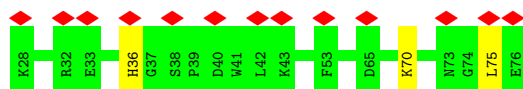




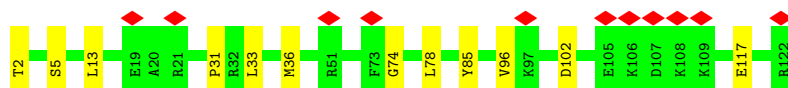
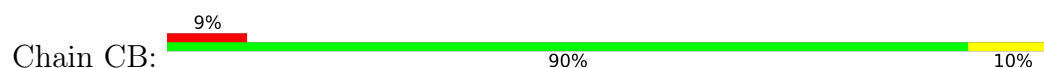
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



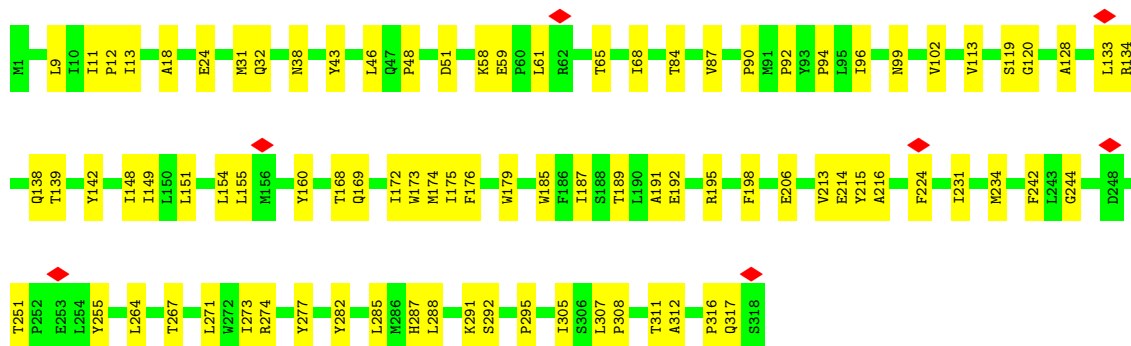
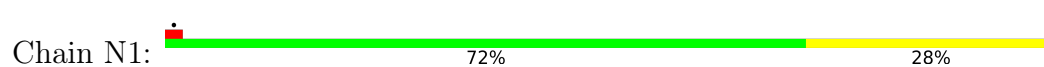
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



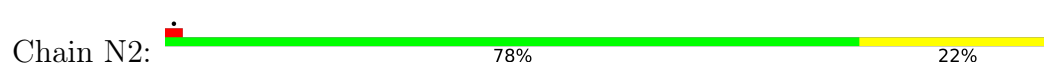
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C2

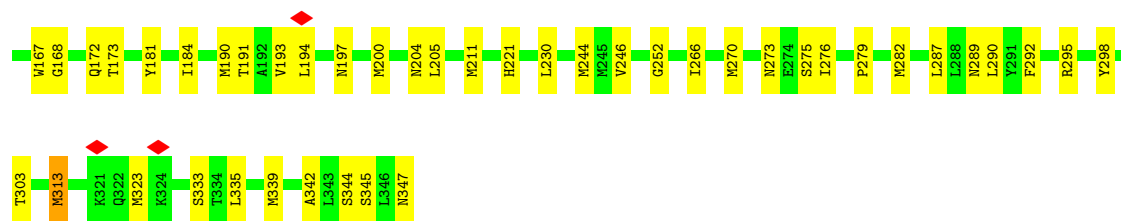


- Molecule 28: NADH-ubiquinone oxidoreductase chain 1

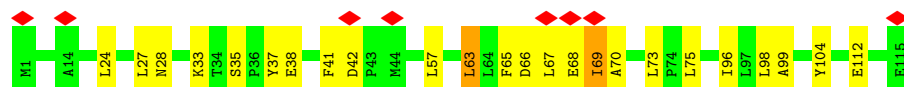
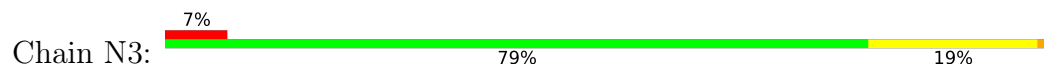


- Molecule 29: NADH-ubiquinone oxidoreductase chain 2

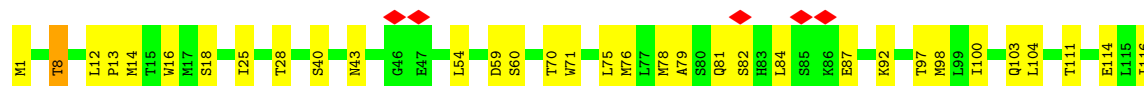
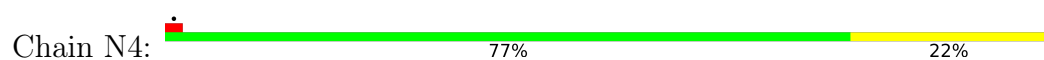




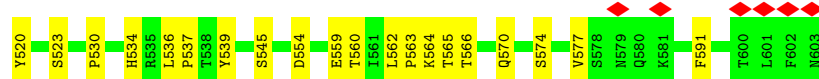
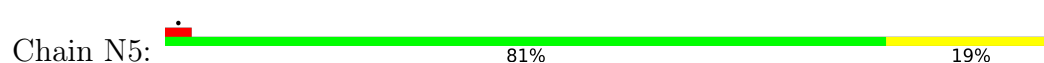
• Molecule 30: NADH-ubiquinone oxidoreductase chain 3



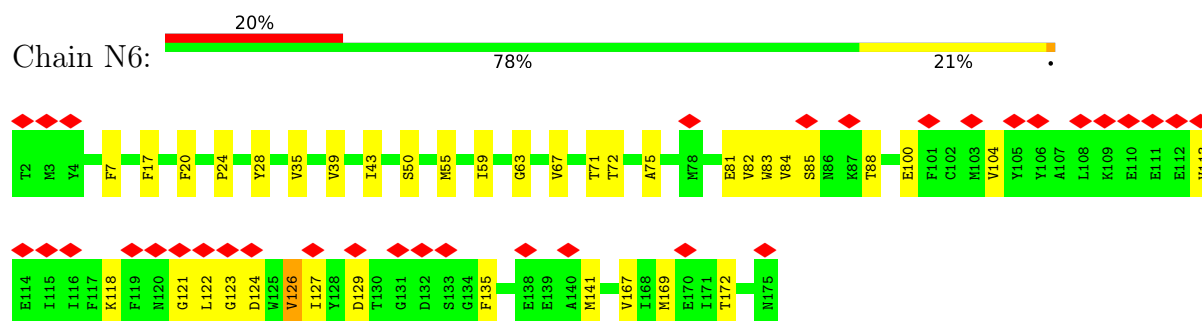
• Molecule 31: NADH-ubiquinone oxidoreductase chain 4



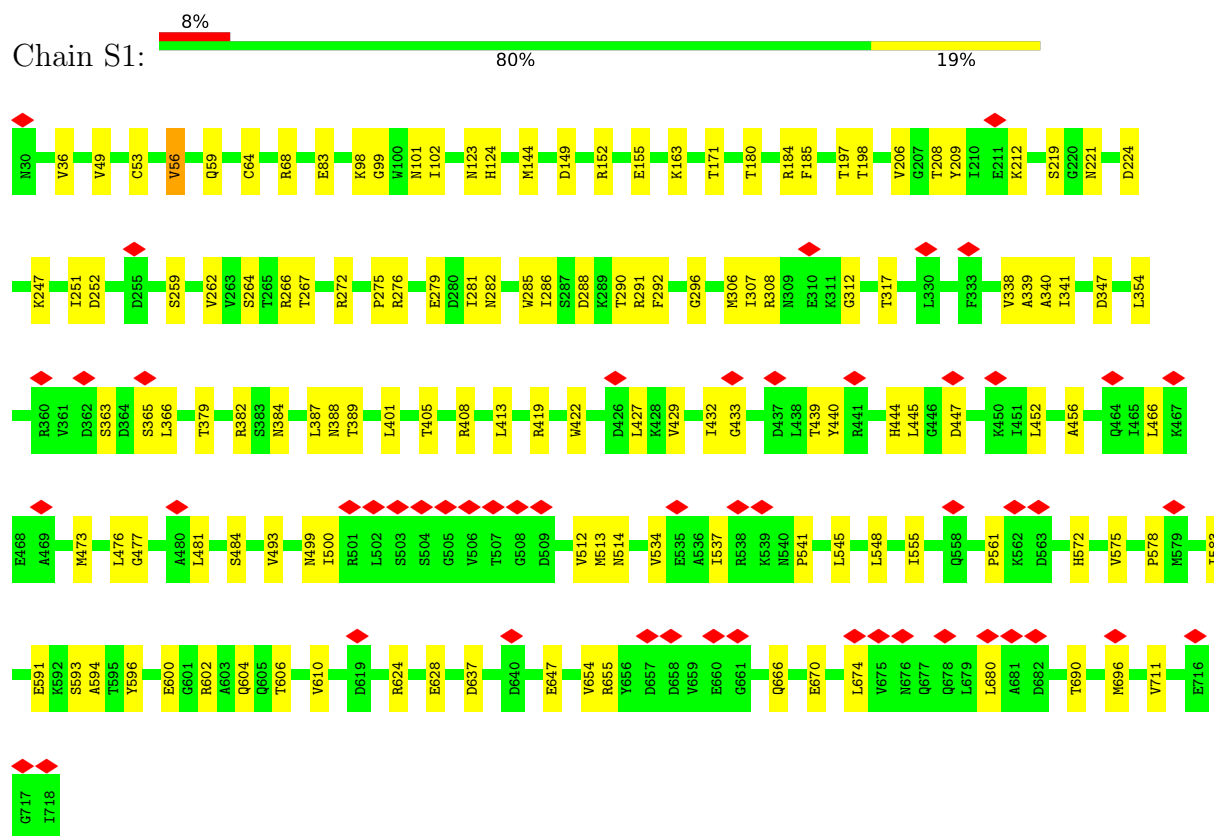
• Molecule 32: NADH-ubiquinone oxidoreductase chain 5



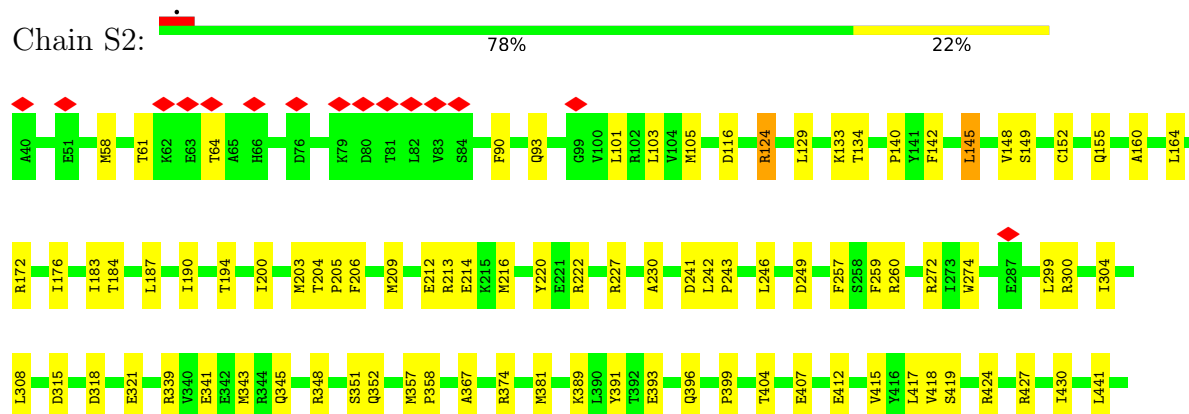
- Molecule 33: NADH-ubiquinone oxidoreductase chain 6

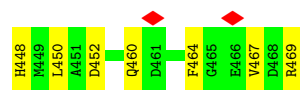


- Molecule 34: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



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





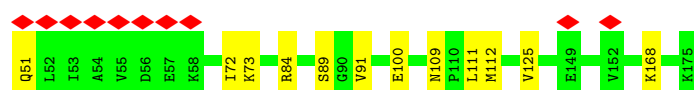
- Molecule 36: Complex I-30kD

Chain S3: 87% 13%



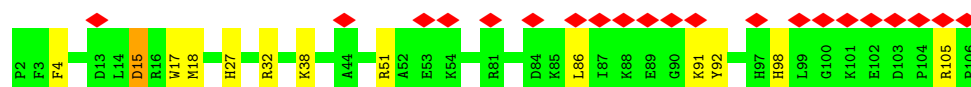
- Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain S4: 8% 90% 10%



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

Chain S5: 20% 88% 11%



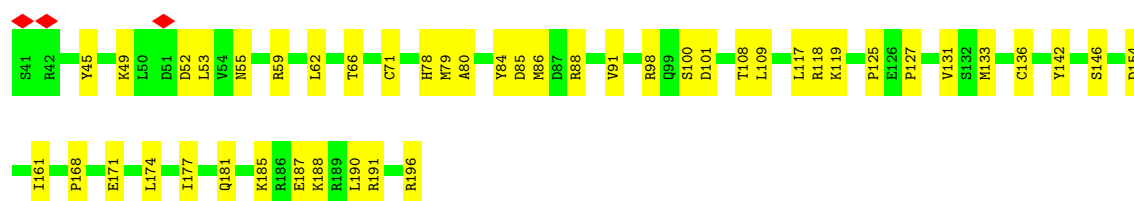
- Molecule 39: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain S6: 24% 93% 7%

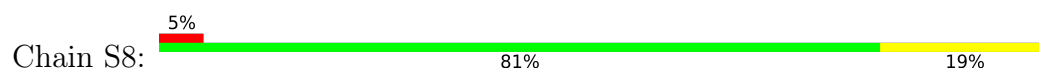


- Molecule 40: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

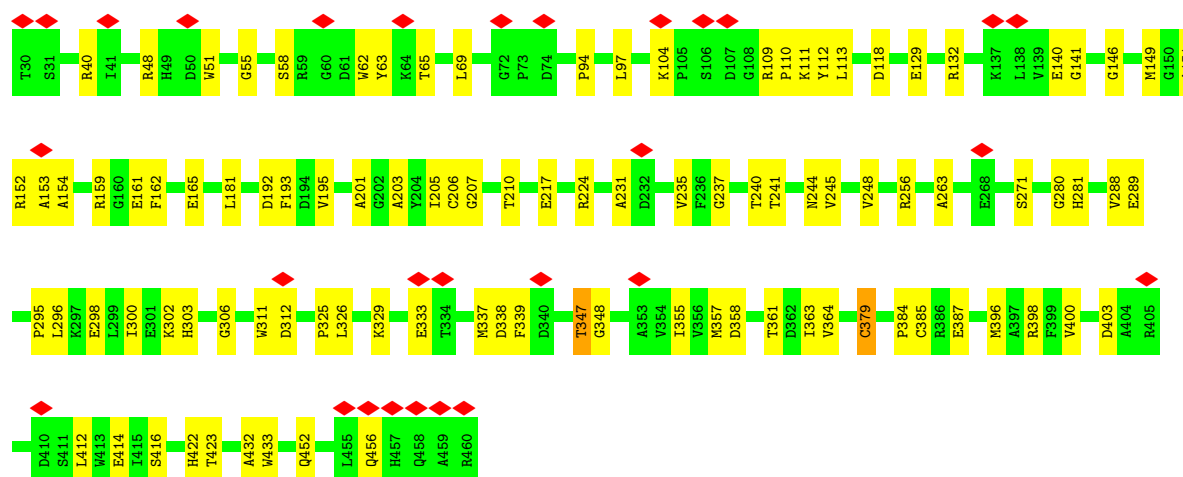
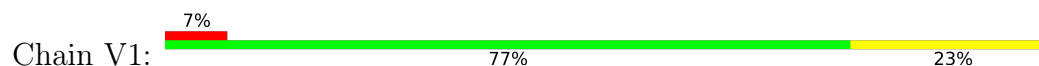
Chain S7: 71% 29%



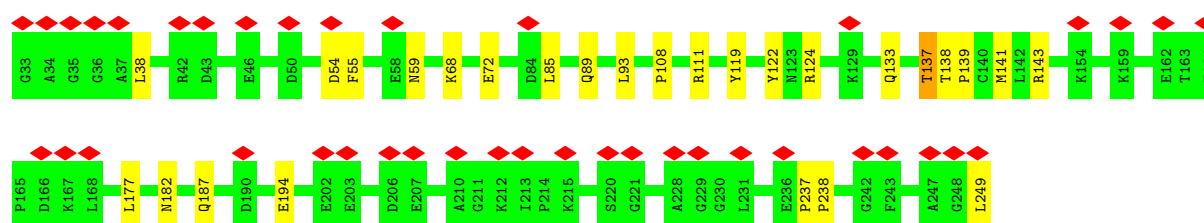
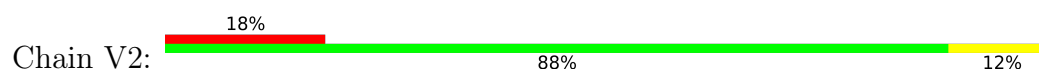
- Molecule 41: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



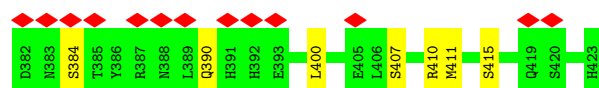
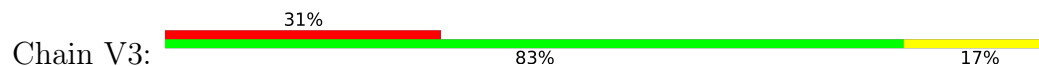
- Molecule 42: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



- 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	30599	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	40.742	Depositor
Minimum map value	-14.815	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.019	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: SF4, MF8, MG, PLX, ADP, CDL, PX2, FMN, PEE, PC1, U10, ZMP, 2MR, ZN, 3PE, FES, NDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	4L	0.14	0/759	0.29	0/1029
2	A1	0.13	0/577	0.25	0/777
3	A2	0.09	0/697	0.23	0/938
4	A3	0.09	0/664	0.22	0/912
5	A5	0.12	0/929	0.21	0/1258
6	A6	0.13	0/995	0.27	0/1340
7	A7	0.11	0/798	0.25	0/1079
8	A8	0.11	0/1436	0.24	0/1938
9	A9	0.13	0/2820	0.26	0/3823
10	AB	0.08	0/633	0.22	0/851
10	AC	0.13	0/714	0.24	0/965
11	AK	0.11	0/2650	0.25	0/3588
12	AL	0.12	0/1042	0.22	0/1411
13	AM	0.10	0/1245	0.22	0/1694
14	AN	0.13	0/1204	0.24	0/1624
15	B1	0.11	0/491	0.24	0/663
16	B2	0.13	0/610	0.27	0/836
17	B3	0.12	0/660	0.23	0/892
18	B4	0.12	0/1092	0.24	0/1481
19	B5	0.13	0/1184	0.26	0/1603
20	B6	0.13	0/910	0.31	0/1237
21	B7	0.12	0/1092	0.23	0/1459
22	B8	0.12	0/1371	0.25	0/1875
23	B9	0.13	0/1590	0.26	0/2155
24	BK	0.12	0/1489	0.23	0/2008
25	BL	0.13	0/851	0.26	0/1155
26	CA	0.10	0/430	0.19	0/581
27	CB	0.12	0/1031	0.24	0/1394
28	N1	0.17	0/2581	0.33	0/3529
29	N2	0.16	0/2773	0.31	0/3768
30	N3	0.15	0/938	0.26	0/1281
31	N4	0.16	0/3723	0.29	0/5078

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	N5	0.15	0/4914	0.33	0/6683
33	N6	0.14	0/1364	0.30	0/1850
34	S1	0.14	0/5378	0.29	0/7287
35	S2	0.16	0/3538	0.28	0/4796
36	S3	0.13	0/1789	0.27	0/2436
37	S4	0.12	0/1039	0.26	0/1403
38	S5	0.11	0/889	0.21	0/1190
39	S6	0.11	0/755	0.25	0/1018
40	S7	0.15	0/1279	0.29	0/1730
41	S8	0.14	0/1443	0.25	0/1952
42	V1	0.14	0/3391	0.28	0/4583
43	V2	0.12	0/1711	0.27	0/2328
44	V3	0.09	0/365	0.25	0/493
All	All	0.14	0/67834	0.27	0/91971

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	24	0
2	A1	562	0	557	7	0
3	A2	686	0	699	7	0
4	A3	643	0	642	9	0
5	A5	910	0	950	8	0
6	A6	971	0	975	19	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	9	0
10	AC	702	0	694	13	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	15	0
14	AN	1173	0	1166	26	0
15	B1	479	0	486	5	0
16	B2	584	0	529	3	0
17	B3	641	0	620	5	0
18	B4	1062	0	1072	10	0
19	B5	1151	0	1164	14	0
20	B6	882	0	899	21	0
21	B7	1068	0	1043	15	0
22	B8	1315	0	1208	10	0
23	B9	1534	0	1470	18	0
24	BK	1456	0	1426	17	0
25	BL	828	0	788	10	0
26	CA	417	0	422	2	0
27	CB	1000	0	994	10	0
28	N1	2508	0	2607	68	0
29	N2	2710	0	2874	60	0
30	N3	914	0	951	26	0
31	N4	3631	0	3839	74	0
32	N5	4785	0	4933	84	0
33	N6	1329	0	1326	39	0
34	S1	5290	0	5321	84	0
35	S2	3459	0	3396	75	0
36	S3	1738	0	1693	21	0
37	S4	1016	0	1016	7	0
38	S5	867	0	871	17	0
39	S6	741	0	701	6	0
40	S7	1248	0	1254	38	0
41	S8	1412	0	1363	29	0
42	V1	3316	0	3272	66	0
43	V2	1671	0	1673	17	0
44	V3	355	0	329	7	0
45	4L	92	0	137	6	0
45	AL	165	0	224	10	0
45	AM	88	0	129	7	0
45	AN	100	0	156	6	0
45	B1	76	0	96	2	0
45	B4	80	0	107	4	0
45	B5	100	0	156	5	0
45	N1	78	0	103	5	0
45	N2	68	0	80	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	N4	100	0	156	10	0
45	N5	189	0	284	14	0
46	A3	104	0	165	6	0
46	B4	52	0	81	4	0
46	B5	108	0	176	2	0
46	N1	54	0	88	7	0
46	N3	108	0	176	10	0
47	A9	48	0	26	0	0
48	A9	39	0	52	2	0
48	AL	36	0	49	0	0
48	B6	46	0	69	2	0
48	BL	51	0	82	1	0
48	N1	82	0	118	8	0
48	N3	51	0	82	6	0
48	N4	49	0	75	5	0
48	N5	126	0	180	5	0
48	S2	48	0	73	3	0
48	S8	51	0	82	9	0
49	AB	36	0	47	2	0
49	AC	36	0	47	5	0
50	AK	27	0	12	4	0
51	B1	52	0	88	3	0
51	BL	52	0	88	4	0
51	CB	52	0	88	0	0
51	N1	47	0	75	2	0
51	N2	52	0	88	2	0
51	N4	47	0	75	4	0
51	S7	52	0	88	11	0
52	B8	32	0	38	0	0
52	CB	46	0	69	0	0
52	N5	46	0	69	3	0
53	CA	36	0	52	0	0
54	N1	63	0	90	9	0
55	S1	16	0	0	1	0
55	S7	8	0	0	0	0
55	S8	16	0	0	2	0
55	V1	8	0	0	0	0
56	S1	4	0	0	0	0
56	V2	4	0	0	0	0
57	S1	1	0	0	0	0
58	S2	9	0	0	1	0
59	S6	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	V1	31	0	19	2	0
All	All	69125	0	70564	998	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 (998) 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	1.79	0.83
1:4L:37:MET:HG2	1:4L:67:ALA:HB2	1.61	0.82
42:V1:235:VAL:HG12	42:V1:240:THR:HG21	1.63	0.79
35:S2:145:LEU:HD21	35:S2:430:ILE:HD13	1.66	0.78
29:N2:335:LEU:HD21	45:N4:503:CDL:H411	1.68	0.76
43:V2:68:LYS:NZ	44:V3:407:SER:OG	2.19	0.75
1:4L:68:ALA:HB3	30:N3:67:LEU:HD11	1.69	0.74
49:AC:201:ZMP:H14	23:B9:102:ALA:HB1	1.69	0.74
20:B6:88:LEU:HD22	20:B6:92:GLU:HG2	1.69	0.72
12:AL:140:LYS:H	29:N2:273:ASN:HD22	1.34	0.72
46:B4:202:PC1:H3I2	48:N5:702:PEE:H57	1.71	0.71
34:S1:149:ASP:HB2	35:S2:367:ALA:HB3	1.73	0.71
29:N2:108:LEU:HD11	29:N2:191:THR:HG21	1.71	0.71
34:S1:338:VAL:O	34:S1:365:SER:HB2	1.91	0.71
9:A9:87:GLU:HG3	9:A9:89:TYR:H	1.57	0.70
34:S1:124:HIS:HD2	35:S2:381:MET:HE2	1.55	0.70
9:A9:174:ILE:HG23	9:A9:175:LYS:HD3	1.74	0.70
18:B4:15:PRO:HG2	18:B4:18:LEU:HB2	1.74	0.70
51:N4:502:PLX:H311	51:N4:502:PLX:H111	1.75	0.69
35:S2:357:MET:HE3	35:S2:358:PRO:HD2	1.73	0.69
29:N2:88:LYS:HG3	29:N2:148:SER:HB3	1.74	0.69
1:4L:3:LEU:HD11	33:N6:121:GLY:HA2	1.75	0.69
35:S2:183:ILE:HG23	35:S2:216:MET:HE2	1.73	0.69
42:V1:205:ILE:HG12	42:V1:379:CYS:HB3	1.74	0.69
12:AL:140:LYS:O	29:N2:273:ASN:ND2	2.25	0.69
42:V1:111:LYS:HB2	42:V1:151:ALA:HA	1.73	0.69
34:S1:433:GLY:HA2	34:S1:447:ASP:HA	1.76	0.68
31:N4:369:LEU:HD23	45:N5:703:CDL:H362	1.76	0.68
1:4L:14:ILE:HG12	45:4L:201:CDL:H791	1.76	0.68
30:N3:37:TYR:OH	35:S2:93:GLN:NE2	2.27	0.68
29:N2:230:LEU:HD11	29:N2:244:MET:HE1	1.76	0.67
9:A9:204:SER:HB2	9:A9:266:VAL:HG12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:S1:456:ALA:O	34:S1:499:ASN:ND2	2.28	0.67
3:A2:24:CYS:N	3:A2:58:CYS:SG	2.68	0.66
45:AN:201:CDL:H161	48:S8:303:PEE:H68	1.76	0.66
34:S1:282:ASN:ND2	34:S1:285:TRP:O	2.27	0.66
9:A9:129:LEU:HD23	9:A9:167:ILE:HG13	1.76	0.66
9:A9:188:GLU:HG3	9:A9:200:ILE:HD13	1.77	0.66
30:N3:73:LEU:HD12	33:N6:55:MET:HE1	1.74	0.66
11:AK:120:TYR:OH	50:AK:401:ADP:O2'	2.14	0.66
20:B6:132:VAL:O	20:B6:136:LEU:HB3	1.95	0.66
25:BL:129:ARG:NH1	25:BL:136:LEU:O	2.29	0.66
34:S1:387:LEU:HD12	34:S1:514:ASN:HB3	1.78	0.65
34:S1:534:VAL:HG22	34:S1:537:ILE:HB	1.76	0.65
6:A6:88:LYS:NZ	6:A6:132:PHE:O	2.27	0.65
17:B3:60:ASN:ND2	32:N5:433:GLY:O	2.29	0.65
54:N1:403:U10:O4	58:S2:502:MF8:N09	2.29	0.65
43:V2:108:PRO:HB2	43:V2:111:ARG:HG2	1.77	0.65
9:A9:173:ASP:HB3	9:A9:176:SER:HB2	1.78	0.65
27:CB:36:MET:HE2	29:N2:339:MET:HE2	1.76	0.65
35:S2:190:ILE:HG23	35:S2:209:MET:HB3	1.79	0.65
11:AK:141:ARG:NH2	50:AK:401:ADP:N7	2.45	0.65
8:A8:107:HIS:HB3	8:A8:197:PRO:HD2	1.78	0.65
13:AM:88:ARG:HD3	41:S8:200:GLU:HG3	1.77	0.65
39:S6:74:GLN:HG3	41:S8:108:SER:HB2	1.78	0.65
22:B8:165:ASP:O	22:B8:170:ARG:NH1	2.30	0.65
14:AN:119:PRO:HB3	14:AN:123:GLU:HB2	1.79	0.64
42:V1:40:ARG:NH1	42:V1:289:GLU:O	2.30	0.64
13:AM:34:ARG:NH2	41:S8:89:GLU:OE2	2.30	0.64
32:N5:362:LEU:HA	32:N5:365:ALA:HB3	1.79	0.64
42:V1:48:ARG:HH21	44:V3:384:SER:HA	1.63	0.64
21:B7:92:HIS:ND1	32:N5:481:THR:OG1	2.26	0.64
35:S2:374:ARG:NH2	41:S8:165:ASP:OD1	2.30	0.64
23:B9:52:LEU:O	23:B9:57:LYS:NZ	2.31	0.63
31:N4:416:ARG:HG3	32:N5:159:HIS:HB3	1.80	0.63
34:S1:405:THR:HB	34:S1:477:GLY:HA3	1.79	0.63
40:S7:188:LYS:HB2	40:S7:191:ARG:HB2	1.79	0.63
20:B6:143:HIS:HD2	24:BK:45:VAL:HG21	1.63	0.63
48:N1:405:PEE:H7	48:N1:405:PEE:H10	1.80	0.63
3:A2:19:ILE:HD11	3:A2:65:LEU:HD11	1.80	0.63
35:S2:469:ARG:NH2	36:S3:169:GLU:OE2	2.31	0.63
42:V1:63:TYR:HB3	42:V1:256:ARG:HD3	1.81	0.63
4:A3:161:PRO:HD2	8:A8:204:LYS:HG2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:N1:174:MET:HB2	28:N1:242:PHE:HA	1.81	0.63
46:A3:202:PC1:H2C1	46:A3:202:PC1:H361	1.81	0.63
45:N4:503:CDL:H792	45:N4:503:CDL:H832	1.81	0.63
51:B1:101:PLX:H181	46:B5:202:PC1:H2D2	1.80	0.63
42:V1:110:PRO:HB3	42:V1:152:ARG:HD3	1.81	0.62
33:N6:113:VAL:HG13	33:N6:118:LYS:HG2	1.80	0.62
31:N4:391:ILE:HG23	31:N4:394:ILE:HD12	1.81	0.62
10:AB:116:VAL:HG12	10:AB:120:MET:HE2	1.81	0.62
45:AN:201:CDL:H141	48:S8:303:PEE:H72	1.81	0.62
42:V1:195:VAL:O	44:V3:410:ARG:NH1	2.31	0.62
49:AC:201:ZMP:H5A	23:B9:109:ALA:HB1	1.82	0.62
19:B5:163:ARG:NH1	27:CB:102:ASP:OD2	2.28	0.62
54:N1:403:U10:H403	46:N3:203:PC1:H3G2	1.81	0.62
41:S8:205:ILE:O	41:S8:209:TYR:HB3	2.00	0.62
34:S1:340:ALA:HB3	34:S1:366:LEU:HD23	1.82	0.62
13:AM:60:ARG:HH22	13:AM:95:ASP:HA	1.64	0.61
34:S1:419:ARG:NH1	34:S1:439:THR:O	2.33	0.61
42:V1:281:HIS:ND1	42:V1:358:ASP:OD1	2.33	0.61
9:A9:50:SER:OG	36:S3:225:GLU:OE2	2.17	0.61
35:S2:90:PHE:HB2	35:S2:105:MET:HE2	1.82	0.61
29:N2:42:PRO:HG2	33:N6:167:VAL:HG22	1.81	0.61
3:A2:59:SER:HB2	34:S1:655:ARG:HD3	1.83	0.61
43:V2:59:ASN:ND2	43:V2:89:GLN:OE1	2.34	0.61
4:A3:127:ALA:HB2	28:N1:312:ALA:HA	1.80	0.61
28:N1:195:ARG:HH11	28:N1:231:ILE:HD13	1.66	0.61
29:N2:289:ASN:HA	29:N2:292:PHE:CE2	2.35	0.61
35:S2:300:ARG:NH2	35:S2:407:GLU:OE2	2.34	0.61
15:B1:47:ARG:NH2	15:B1:53:GLU:OE2	2.34	0.60
32:N5:295:GLN:O	32:N5:425:ARG:NH1	2.34	0.60
34:S1:144:MET:HG3	35:S2:389:LYS:HG3	1.83	0.60
1:4L:31:LEU:HD21	33:N6:67:VAL:HG11	1.83	0.60
11:AK:66:GLY:O	11:AK:163:ARG:NH2	2.34	0.60
10:AB:142:GLN:NE2	10:AB:146:ASP:OD1	2.34	0.60
24:BK:12:GLU:OE2	24:BK:15:ARG:NH2	2.35	0.60
28:N1:138:GLN:NE2	28:N1:191:ALA:O	2.35	0.60
43:V2:182:ASN:HB3	43:V2:194:GLU:HB3	1.82	0.60
20:B6:85:ASP:OD2	23:B9:167:TRP:NE1	2.29	0.60
34:S1:493:VAL:HG23	34:S1:513:MET:HE1	1.83	0.60
1:4L:65:VAL:HA	30:N3:67:LEU:HD22	1.84	0.60
5:A5:49:GLU:O	5:A5:53:ASN:ND2	2.33	0.60
32:N5:530:PRO:O	32:N5:534:HIS:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:109:GLN:OE1	11:AK:328:ARG:NH1	2.34	0.60
8:A8:141:ASN:OD1	14:AN:81:ARG:NH2	2.35	0.59
34:S1:219:SER:OG	34:S1:288:ASP:OD2	2.20	0.59
34:S1:666:GLN:NE2	34:S1:670:GLU:OE2	2.35	0.59
35:S2:155:GLN:NE2	35:S2:315:ASP:OD2	2.34	0.59
30:N3:70:ALA:HB2	33:N6:59:ILE:HD11	1.85	0.59
14:AN:98:MET:HE3	14:AN:101:VAL:HG21	1.85	0.59
28:N1:51:ASP:HB2	54:N1:403:U10:H302	1.84	0.59
28:N1:58:LYS:HE2	40:S7:125:PRO:HG2	1.85	0.59
10:AC:114:ASP:OD1	23:B9:87:ARG:NH2	2.35	0.59
8:A8:219:TYR:OH	19:B5:189:ASN:ND2	2.36	0.59
9:A9:223:PHE:HE2	48:A9:402:PEE:H13	1.67	0.59
11:AK:267:ASP:OD2	11:AK:270:LYS:NZ	2.36	0.59
31:N4:373:ILE:HD11	31:N4:444:LEU:HD12	1.84	0.59
42:V1:263:ALA:HA	42:V1:271:SER:HB3	1.85	0.59
42:V1:338:ASP:OD1	42:V1:339:PHE:N	2.35	0.59
9:A9:212:ARG:NH1	9:A9:311:GLU:OE2	2.36	0.59
12:AL:125:VAL:HA	45:AL:203:CDL:H712	1.84	0.59
21:B7:29:TYR:O	21:B7:104:ARG:NH2	2.35	0.59
32:N5:419:THR:HA	32:N5:422:TYR:CE2	2.38	0.59
35:S2:209:MET:HE1	35:S2:260:ARG:HB3	1.85	0.59
25:BL:95:PHE:O	25:BL:99:LEU:HB2	2.03	0.59
6:A6:81:SER:OG	9:A9:367:GLU:OE2	2.20	0.58
35:S2:187:LEU:HD21	35:S2:216:MET:HB2	1.84	0.58
39:S6:61:GLU:OE2	41:S8:192:ASN:ND2	2.36	0.58
48:A9:402:PEE:H36	46:N3:201:PC1:H2F1	1.85	0.58
32:N5:100:ILE:HG21	32:N5:246:LEU:HB2	1.85	0.58
34:S1:308:ARG:NH1	34:S1:312:GLY:O	2.37	0.58
12:AL:108:TYR:HB2	45:B4:201:CDL:HB32	1.85	0.58
42:V1:118:ASP:HB3	42:V1:207:GLY:HA2	1.86	0.58
14:AN:86:MET:O	14:AN:90:ASN:ND2	2.28	0.58
31:N4:12:LEU:HD13	45:N4:503:CDL:H842	1.86	0.58
9:A9:61:ALA:HB3	9:A9:82:VAL:HG13	1.84	0.58
28:N1:102:VAL:HG11	28:N1:154:LEU:HD11	1.86	0.58
12:AL:140:LYS:H	29:N2:273:ASN:ND2	2.00	0.58
28:N1:160:TYR:OH	30:N3:73:LEU:O	2.21	0.58
25:BL:89:VAL:HG21	31:N4:25:ILE:HG23	1.85	0.57
19:B5:57:ILE:HG23	23:B9:146:LEU:HD13	1.87	0.57
31:N4:403:THR:HA	31:N4:406:TYR:CE2	2.39	0.57
9:A9:308:SER:HB2	46:N3:201:PC1:H221	1.86	0.57
35:S2:222:ARG:NH1	35:S2:249:ASP:OD2	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A8:95:VAL:HG12	8:A8:97:VAL:HG22	1.86	0.57
31:N4:383:THR:HG21	32:N5:190:LEU:HD23	1.85	0.57
45:B1:102:CDL:HB62	27:CB:31:PRO:HB3	1.85	0.57
51:BL:202:PLX:H231	32:N5:23:ASN:HB2	1.86	0.57
45:N1:401:CDL:HB61	33:N6:84:VAL:HG22	1.86	0.57
35:S2:393:GLU:OE2	35:S2:396:GLN:NE2	2.38	0.57
6:A6:66:TYR:O	6:A6:86:ARG:NH1	2.37	0.57
31:N4:303:ILE:HD11	31:N4:308:SER:HB3	1.87	0.56
19:B5:53:ARG:NH2	20:B6:89:SER:O	2.38	0.56
32:N5:249:SER:HA	32:N5:306:THR:HG21	1.87	0.56
34:S1:198:THR:HG21	34:S1:209:TYR:HB2	1.86	0.56
34:S1:433:GLY:O	34:S1:444:HIS:NE2	2.33	0.56
35:S2:430:ILE:HB	35:S2:469:ARG:HD2	1.86	0.56
35:S2:464:PHE:HA	35:S2:467:VAL:HB	1.85	0.56
40:S7:79:MET:HE1	40:S7:177:ILE:HG13	1.87	0.56
31:N4:87:GLU:O	31:N4:92:LYS:NZ	2.30	0.56
32:N5:253:VAL:HG23	32:N5:310:LEU:HD21	1.87	0.56
32:N5:504:LEU:O	32:N5:507:THR:OG1	2.23	0.56
42:V1:104:LYS:NZ	42:V1:231:ALA:O	2.30	0.56
22:B8:57:MET:HE2	22:B8:104:PRO:HG3	1.88	0.56
34:S1:224:ASP:OD2	34:S1:291:ARG:NH2	2.38	0.56
6:A6:88:LYS:HE2	6:A6:92:MET:HE2	1.87	0.56
31:N4:232:ALA:O	31:N4:237:LYS:NZ	2.38	0.56
31:N4:368:ALA:HB1	31:N4:375:LEU:HD23	1.87	0.56
37:S4:109:ASN:ND2	37:S4:111:LEU:O	2.39	0.56
29:N2:221:HIS:HB2	29:N2:323:MET:HE1	1.87	0.55
42:V1:311:TRP:NE1	42:V1:333:GLU:OE1	2.35	0.55
27:CB:2:THR:HB	27:CB:5:SER:HB3	1.88	0.55
42:V1:396:MET:HE1	42:V1:412:LEU:HD21	1.88	0.55
29:N2:96:THR:HG22	29:N2:100:MET:HE2	1.88	0.55
34:S1:251:ILE:HD11	34:S1:596:TYR:HB2	1.88	0.55
31:N4:8:THR:HG22	31:N4:100:ILE:HG23	1.89	0.55
14:AN:50:MET:HG2	28:N1:172:ILE:HD11	1.89	0.55
28:N1:133:LEU:HD11	33:N6:72:THR:HG21	1.88	0.55
29:N2:167:TRP:O	32:N5:574:SER:OG	2.18	0.55
31:N4:114:GLU:HG2	31:N4:116:ILE:HG22	1.87	0.55
35:S2:308:LEU:HB2	35:S2:407:GLU:HB2	1.89	0.55
40:S7:133:MET:HG3	40:S7:168:PRO:HG2	1.88	0.55
10:AC:103:HIS:N	10:AC:107:ASP:OD1	2.39	0.55
36:S3:187:ILE:HG23	36:S3:188:LEU:HG	1.88	0.55
46:B4:202:PC1:H222	51:N4:502:PLX:H82	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A6:67:ARG:NH2	10:AB:123:GLU:OE1	2.40	0.54
27:CB:13:LEU:HD21	38:S5:4:PHE:HB3	1.88	0.54
45:AM:201:CDL:H741	45:AM:201:CDL:H572	1.87	0.54
34:S1:591:GLU:HG2	34:S1:610:VAL:HG23	1.89	0.54
29:N2:270:MET:O	29:N2:275:SER:OG	2.26	0.54
30:N3:63:LEU:HD11	33:N6:63:GLY:HA2	1.89	0.54
2:A1:31:ASN:OD1	2:A1:60:TYR:OH	2.21	0.54
45:AL:201:CDL:H532	32:N5:577:VAL:HG22	1.89	0.54
13:AM:12:GLN:O	13:AM:16:GLY:N	2.36	0.54
18:B4:75:ASN:OD1	18:B4:79:ASN:ND2	2.41	0.54
21:B7:107:ARG:HA	21:B7:110:GLN:HG2	1.89	0.54
28:N1:46:LEU:HD13	51:S7:302:PLX:H121	1.90	0.54
31:N4:392:THR:O	31:N4:396:MET:HG2	2.08	0.54
32:N5:190:LEU:HB2	32:N5:196:TRP:NE1	2.23	0.54
33:N6:17:PHE:HA	33:N6:20:PHE:CE2	2.42	0.54
42:V1:113:LEU:O	42:V1:154:ALA:HA	2.08	0.54
34:S1:401:LEU:HD11	34:S1:432:ILE:HG13	1.90	0.54
31:N4:122:PHE:HE2	31:N4:206:LYS:HG3	1.73	0.53
31:N4:371:PRO:HD2	45:N5:703:CDL:H391	1.90	0.53
34:S1:49:VAL:HG13	34:S1:102:ILE:HD13	1.88	0.53
22:B8:81:ARG:NH1	22:B8:85:GLU:OE1	2.40	0.53
34:S1:163:LYS:O	34:S1:171:THR:OG1	2.27	0.53
32:N5:362:LEU:HD22	32:N5:366:MET:HE2	1.90	0.53
10:AC:105:MET:HE2	10:AC:139:MET:HE1	1.89	0.53
29:N2:173:THR:HG22	35:S2:58:MET:HG2	1.90	0.53
31:N4:266:MET:HA	31:N4:269:MET:HE2	1.90	0.53
9:A9:303:ARG:HB2	9:A9:316:ARG:HD3	1.91	0.53
8:A8:228:ASN:OD1	38:S5:51:ARG:NH1	2.40	0.53
46:N3:203:PC1:H2D1	51:S7:302:PLX:H382	1.90	0.53
42:V1:113:LEU:HD13	42:V1:149:MET:HE1	1.90	0.53
32:N5:126:ILE:HG21	45:N5:703:CDL:H622	1.90	0.53
42:V1:203:ALA:HB3	42:V1:206:CYS:HB2	1.90	0.53
45:AM:201:CDL:H381	45:AM:201:CDL:H271	1.91	0.53
10:AB:104:PHE:HD1	10:AB:108:LEU:HD12	1.74	0.53
28:N1:173:TRP:HB3	28:N1:175:ILE:HG22	1.91	0.52
28:N1:24:GLU:HA	28:N1:271:LEU:HD13	1.91	0.52
31:N4:288:TYR:OH	32:N5:554:ASP:OD2	2.23	0.52
9:A9:293:LEU:HD12	9:A9:294:PRO:HD2	1.91	0.52
32:N5:293:ILE:HD13	32:N5:418:LEU:HD22	1.91	0.52
6:A6:135:GLU:OE1	36:S3:218:ARG:NH2	2.39	0.52
34:S1:266:ARG:HD2	34:S1:267:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A8:160:THR:HA	8:A8:163:TRP:CD1	2.43	0.52
9:A9:279:TYR:HB2	9:A9:372:ALA:HB2	1.90	0.52
45:AN:201:CDL:H552	45:AN:201:CDL:H331	1.90	0.52
16:B2:65:THR:HB	16:B2:68:GLN:HG2	1.91	0.52
29:N2:154:MET:HE3	29:N2:191:THR:HB	1.91	0.52
35:S2:391:TYR:HD1	41:S8:122:VAL:HG21	1.74	0.52
27:CB:117:GLU:OE1	27:CB:117:GLU:N	2.38	0.52
31:N4:1:MET:HE2	31:N4:111:THR:HG21	1.90	0.52
35:S2:272:ARG:NE	41:S8:65:GLU:OE2	2.38	0.52
9:A9:346:GLU:HG2	9:A9:371:PRO:HB3	1.91	0.52
19:B5:152:LYS:HD2	27:CB:96:VAL:HG21	1.92	0.52
34:S1:512:VAL:O	34:S1:514:ASN:ND2	2.43	0.52
10:AC:76:LEU:HD22	10:AC:154:VAL:HG12	1.92	0.52
11:AK:99:THR:HG23	11:AK:100:THR:HG23	1.92	0.52
29:N2:14:MET:HA	29:N2:133:TRP:HE1	1.75	0.52
19:B5:139:ILE:HG23	31:N4:54:LEU:HD23	1.92	0.52
42:V1:140:GLU:OE2	42:V1:256:ARG:NH1	2.32	0.52
45:AM:201:CDL:H422	45:AM:201:CDL:H361	1.92	0.51
24:BK:114:GLN:HG3	32:N5:203:MET:HG2	1.92	0.51
35:S2:194:THR:HG21	35:S2:209:MET:HB2	1.91	0.51
35:S2:321:GLU:O	35:S2:352:GLN:NE2	2.39	0.51
42:V1:347:THR:HG22	42:V1:348:GLY:H	1.75	0.51
43:V2:38:LEU:O	43:V2:124:ARG:NH2	2.36	0.51
7:A7:39:PRO:HG3	41:S8:211:TYR:CZ	2.44	0.51
29:N2:167:TRP:HB3	32:N5:574:SER:HA	1.92	0.51
45:B5:201:CDL:H672	32:N5:12:LEU:HB3	1.91	0.51
28:N1:213:VAL:HG13	28:N1:214:GLU:HG2	1.91	0.51
29:N2:298:TYR:O	29:N2:303:THR:OG1	2.20	0.51
30:N3:28:ASN:O	30:N3:33:LYS:NZ	2.44	0.51
35:S2:90:PHE:HB3	35:S2:103:LEU:HB3	1.91	0.51
11:AK:88:PHE:HB2	11:AK:161:LEU:HD23	1.91	0.51
5:A5:94:MET:SD	5:A5:99:PRO:HG3	2.51	0.51
9:A9:173:ASP:HB2	9:A9:327:MET:HE1	1.91	0.51
28:N1:187:ILE:HD12	48:S8:303:PEE:H52	1.91	0.51
34:S1:593:SER:HA	34:S1:606:THR:O	2.10	0.51
40:S7:98:ARG:HA	40:S7:125:PRO:HD3	1.91	0.51
11:AK:82:LYS:HZ2	11:AK:268:ALA:HB3	1.76	0.51
42:V1:162:PHE:HB3	42:V1:165:GLU:HB2	1.93	0.51
45:AL:201:CDL:H452	45:AL:201:CDL:H412	1.92	0.51
28:N1:59:GLU:HG3	30:N3:27:LEU:HD13	1.93	0.51
29:N2:276:ILE:HG21	48:N4:501:PEE:H14	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:A3:201:PC1:H381	46:A3:201:PC1:H341	1.93	0.51
31:N4:196:TRP:CD1	31:N4:250:LEU:HB3	2.46	0.51
32:N5:290:LEU:O	32:N5:523:SER:OG	2.28	0.51
34:S1:338:VAL:HB	34:S1:363:SER:HB2	1.93	0.51
28:N1:58:LYS:HG3	40:S7:127:PRO:HD2	1.92	0.51
32:N5:5:ALA:HB2	32:N5:61:MET:HE1	1.93	0.51
34:S1:347:ASP:OD1	34:S1:347:ASP:N	2.42	0.51
13:AM:106:ARG:HB2	13:AM:109:ILE:HG13	1.92	0.51
17:B3:20:LYS:O	17:B3:23:LYS:NZ	2.44	0.50
46:N3:203:PC1:H3H1	51:S7:302:PLX:H233	1.93	0.50
40:S7:80:ALA:HA	40:S7:86:MET:HG2	1.93	0.50
11:AK:96:ALA:HA	11:AK:99:THR:HG22	1.93	0.50
28:N1:31:MET:HG2	41:S8:77:LEU:HB2	1.92	0.50
45:N2:401:CDL:H372	45:N2:401:CDL:H171	1.93	0.50
32:N5:248:HIS:O	32:N5:253:VAL:HG22	2.11	0.50
15:B1:50:ARG:HB2	15:B1:53:GLU:HG2	1.93	0.50
45:N4:503:CDL:H352	45:N4:503:CDL:H211	1.92	0.50
3:A2:18:GLU:HG2	3:A2:68:ARG:HB3	1.93	0.50
49:AC:201:ZMP:H12	23:B9:93:HIS:HB3	1.93	0.50
19:B5:179:ILE:HG21	38:S5:38:LYS:HG3	1.93	0.50
28:N1:195:ARG:HH21	28:N1:274:ARG:HD2	1.75	0.50
29:N2:26:TRP:HB3	29:N2:74:ILE:HD13	1.93	0.50
30:N3:35:SER:O	40:S7:98:ARG:NH2	2.44	0.50
30:N3:42:ASP:OD1	40:S7:119:LYS:NZ	2.45	0.50
31:N4:119:TYR:CZ	31:N4:161:LEU:HB2	2.46	0.50
8:A8:94:GLU:OE2	38:S5:105:ARG:NH2	2.45	0.50
11:AK:59:SER:OG	11:AK:156:GLY:O	2.26	0.50
51:B1:101:PLX:H82	31:N4:40:SER:HB3	1.93	0.50
45:N4:503:CDL:H772	45:N4:503:CDL:H262	1.94	0.50
42:V1:288:VAL:HG21	42:V1:303:HIS:CD2	2.47	0.50
1:4L:73:LEU:HD21	29:N2:41:ILE:HG13	1.93	0.50
2:A1:52:ARG:NH1	2:A1:58:ASN:OD1	2.44	0.50
31:N4:408:LEU:HD12	32:N5:172:ILE:HG21	1.93	0.50
42:V1:364:VAL:HG12	42:V1:400:VAL:HG12	1.93	0.50
1:4L:77:LEU:HD13	29:N2:57:THR:HA	1.93	0.50
29:N2:112:HIS:O	29:N2:116:PRO:HD2	2.11	0.50
45:AN:201:CDL:H361	45:AN:201:CDL:H322	1.93	0.50
28:N1:273:ILE:HG23	28:N1:277:TYR:HD2	1.76	0.50
46:N3:203:PC1:H3H2	51:S7:302:PLX:H212	1.93	0.50
31:N4:370:PRO:HG3	31:N4:375:LEU:HG	1.93	0.50
39:S6:38:VAL:HG12	39:S6:44:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4L:56:ALA:HA	38:S5:18:MET:HE3	1.93	0.50
11:AK:134:GLN:HE21	11:AK:175:MET:HE1	1.77	0.50
14:AN:49:SER:HB3	28:N1:172:ILE:HD13	1.94	0.50
46:B4:202:PC1:H241	51:N4:502:PLX:H121	1.92	0.50
21:B7:103:GLU:O	21:B7:107:ARG:HG2	2.12	0.50
28:N1:195:ARG:HD3	28:N1:231:ILE:HD11	1.94	0.50
34:S1:624:ARG:NH1	34:S1:628:GLU:OE1	2.36	0.50
35:S2:241:ASP:OD1	35:S2:242:LEU:N	2.44	0.50
42:V1:210:THR:HB	42:V1:224:ARG:H	1.77	0.50
23:B9:181:GLN:NE2	23:B9:198:PRO:O	2.45	0.49
32:N5:257:VAL:HG21	32:N5:313:MET:HE2	1.94	0.49
32:N5:536:LEU:HB3	32:N5:537:PRO:HD3	1.94	0.49
11:AK:127:ASP:O	11:AK:132:ARG:NH1	2.39	0.49
46:B4:202:PC1:H2F2	46:B4:202:PC1:H3A2	1.93	0.49
29:N2:131:LEU:O	29:N2:135:LYS:HG2	2.12	0.49
32:N5:119:LYS:NZ	45:N5:703:CDL:OA3	2.35	0.49
33:N6:123:GLY:HA3	33:N6:126:VAL:HG13	1.93	0.49
34:S1:68:ARG:HH12	34:S1:279:GLU:HG2	1.77	0.49
35:S2:61:THR:H	35:S2:64:THR:HG1	1.54	0.49
9:A9:201:ILE:HG22	9:A9:203:PRO:HD3	1.94	0.49
12:AL:125:VAL:HG21	48:N5:701:PEE:H37	1.94	0.49
13:AM:88:ARG:HG3	13:AM:93:MET:HB2	1.94	0.49
32:N5:260:LEU:HD22	32:N5:267:MET:HE3	1.92	0.49
34:S1:83:GLU:HB2	34:S1:101:ASN:HB3	1.94	0.49
7:A7:28:TYR:CZ	13:AM:55:PHE:HB3	2.46	0.49
42:V1:112:TYR:HB2	42:V1:240:THR:HG22	1.92	0.49
14:AN:43:LEU:HG	28:N1:179:TRP:HE1	1.78	0.49
20:B6:143:HIS:CD2	24:BK:45:VAL:HG21	2.45	0.49
29:N2:25:HIS:HB2	38:S5:15:ASP:HB2	1.93	0.49
45:N5:703:CDL:H592	45:N5:703:CDL:H192	1.95	0.49
35:S2:140:PRO:HB2	40:S7:142:TYR:CE2	2.48	0.49
20:B6:148:TYR:CE1	24:BK:49:ARG:HG2	2.48	0.49
48:N1:404:PEE:H45	48:N3:202:PEE:H31	1.94	0.49
34:S1:251:ILE:HG21	34:S1:604:GLN:HB3	1.94	0.49
34:S1:452:LEU:HD21	34:S1:493:VAL:HG13	1.95	0.49
42:V1:94:PRO:HB2	42:V1:97:LEU:HB2	1.94	0.49
8:A8:94:GLU:HB2	8:A8:96:LYS:HE2	1.94	0.49
23:B9:178:GLU:OE2	23:B9:209:TRP:NE1	2.45	0.49
24:BK:33:LEU:HD13	32:N5:49:VAL:HG13	1.94	0.49
48:N1:404:PEE:H28	30:N3:99:ALA:HB1	1.94	0.49
30:N3:68:GLU:HG3	30:N3:98:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:S1:155:GLU:OE2	42:V1:398:ARG:NE	2.37	0.49
35:S2:230:ALA:O	41:S8:98:ARG:NH2	2.45	0.49
1:4L:32:CYS:HA	33:N6:20:PHE:HE1	1.77	0.49
6:A6:90:ARG:NH2	10:AB:114:ASP:OD1	2.41	0.49
14:AN:51:MET:HE2	28:N1:311:THR:HB	1.94	0.49
45:B1:102:CDL:HB61	45:B1:102:CDL:HB22	1.94	0.49
41:S8:74:LEU:HD12	41:S8:77:LEU:HD23	1.95	0.49
42:V1:416:SER:HB2	42:V1:432:ALA:HB1	1.94	0.49
28:N1:148:ILE:HD11	30:N3:69:ILE:HG22	1.94	0.49
9:A9:64:PHE:O	9:A9:67:ARG:HG2	2.13	0.49
13:AM:6:VAL:HB	45:AM:201:CDL:H712	1.95	0.49
29:N2:168:GLY:O	29:N2:172:GLN:HG2	2.12	0.49
40:S7:52:ASP:HB3	51:S7:302:PLX:H262	1.94	0.49
45:B5:201:CDL:H782	45:B5:201:CDL:H212	1.95	0.48
45:B5:201:CDL:H821	45:N5:703:CDL:H473	1.94	0.48
28:N1:61:LEU:HD23	40:S7:125:PRO:HB3	1.95	0.48
35:S2:134:THR:HA	35:S2:424:ARG:HG2	1.95	0.48
54:N1:403:U10:H201	54:N1:403:U10:H221	1.63	0.48
35:S2:190:ILE:HG21	35:S2:213:ARG:HG3	1.94	0.48
28:N1:169:GLN:HB3	28:N1:244:GLY:HA3	1.95	0.48
30:N3:104:TYR:HB2	48:N3:202:PEE:H57	1.95	0.48
34:S1:408:ARG:HD2	34:S1:439:THR:HG23	1.94	0.48
42:V1:326:LEU:HD22	42:V1:363:ILE:HD11	1.95	0.48
15:B1:57:TRP:NE1	19:B5:134:GLU:OE1	2.23	0.48
19:B5:94:GLY:O	24:BK:61:TYR:OH	2.30	0.48
36:S3:93:VAL:HG22	36:S3:145:THR:HG21	1.95	0.48
41:S8:117:LYS:NZ	41:S8:130:ILE:O	2.46	0.48
14:AN:93:GLU:OE1	38:S5:92:TYR:OH	2.27	0.48
30:N3:38:GLU:HB3	30:N3:41:PHE:O	2.12	0.48
32:N5:562:LEU:HB2	32:N5:563:PRO:HD3	1.96	0.48
34:S1:275:PRO:HG3	34:S1:286:ILE:HG12	1.96	0.48
36:S3:132:LEU:HB2	36:S3:141:ILE:HG22	1.96	0.48
40:S7:109:LEU:HD13	40:S7:117:LEU:HD13	1.94	0.48
42:V1:112:TYR:O	42:V1:240:THR:HA	2.13	0.48
11:AK:237:GLN:NE2	11:AK:241:ASN:OD1	2.47	0.48
14:AN:120:MET:HG3	14:AN:121:MET:H	1.78	0.48
18:B4:112:LYS:NZ	31:N4:388:TRP:O	2.44	0.48
20:B6:127:HIS:ND1	32:N5:42:TYR:OH	2.37	0.48
31:N4:16:TRP:HB3	45:N4:503:CDL:H512	1.96	0.48
32:N5:97:THR:HG21	32:N5:125:LEU:HD22	1.95	0.48
42:V1:109:ARG:NH1	42:V1:237:GLY:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:V1:312:ASP:OD1	42:V1:312:ASP:N	2.45	0.48
45:4L:201:CDL:H273	12:AL:34:LEU:HD22	1.94	0.48
4:A3:110:ILE:HD11	48:S8:303:PEE:H36	1.96	0.48
29:N2:111:PHE:HA	32:N5:591:PHE:CE1	2.48	0.48
32:N5:566:THR:O	32:N5:570:GLN:HG2	2.13	0.48
34:S1:422:TRP:HA	34:S1:427:LEU:HB3	1.96	0.48
42:V1:357:MET:HB3	42:V1:361:THR:HG21	1.95	0.48
46:A3:201:PC1:H371	48:S8:303:PEE:H32	1.95	0.48
7:A7:8:ILE:HG13	45:AM:201:CDL:HA32	1.95	0.48
9:A9:286:ARG:NH1	45:N1:401:CDL:OA4	2.45	0.48
45:AL:203:CDL:H542	45:AL:203:CDL:OB7	2.13	0.48
32:N5:214:ILE:HG12	32:N5:276:MET:HE1	1.96	0.48
34:S1:247:LYS:NZ	36:S3:234:ASP:OD2	2.46	0.48
34:S1:259:SER:HB3	34:S1:282:ASN:HD22	1.79	0.48
36:S3:89:HIS:CG	36:S3:90:PRO:HD2	2.49	0.48
40:S7:55:ASN:ND2	40:S7:187:GLU:O	2.45	0.48
1:4L:55:LEU:HD13	38:S5:17:TRP:HE3	1.78	0.48
6:A6:66:TYR:CE2	6:A6:86:ARG:HD3	2.48	0.48
45:AL:201:CDL:H612	29:N2:160:LEU:HD11	1.95	0.48
45:AL:203:CDL:H371	45:AL:203:CDL:H321	1.96	0.48
24:BK:130:GLU:O	24:BK:134:GLN:HG2	2.13	0.48
32:N5:383:MET:O	32:N5:389:PHE:HB2	2.14	0.48
32:N5:559:GLU:O	32:N5:564:LYS:HB2	2.13	0.48
52:N5:706:3PE:H3A2	52:N5:706:3PE:H2C1	1.96	0.48
40:S7:79:MET:HE3	40:S7:174:LEU:HD13	1.95	0.48
42:V1:118:ASP:HA	42:V1:159:ARG:HB3	1.95	0.48
6:A6:127:THR:HG22	6:A6:131:ARG:HE	1.79	0.48
43:V2:93:LEU:HD12	43:V2:122:TYR:HB3	1.95	0.48
31:N4:278:ARG:HG3	32:N5:545:SER:HB2	1.96	0.47
32:N5:293:ILE:HD12	45:N5:704:CDL:H521	1.96	0.47
35:S2:172:ARG:NH1	35:S2:358:PRO:O	2.43	0.47
37:S4:72:ILE:HG22	37:S4:73:LYS:HD2	1.96	0.47
3:A2:46:LYS:HD3	34:S1:674:LEU:HD22	1.96	0.47
9:A9:359:TYR:HB2	28:N1:65:THR:HA	1.95	0.47
10:AC:112:SER:HB3	23:B9:59:LEU:HD11	1.96	0.47
11:AK:260:TYR:HE2	11:AK:271:VAL:HG13	1.79	0.47
16:B2:79:MET:SD	32:N5:375:ILE:HG12	2.54	0.47
30:N3:66:ASP:O	30:N3:69:ILE:HG13	2.14	0.47
32:N5:313:MET:HE3	32:N5:329:ILE:HG12	1.96	0.47
6:A6:78:LEU:HD23	6:A6:126:ARG:HD3	1.96	0.47
9:A9:344:PRO:HG2	9:A9:347:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:N2:154:MET:HE2	29:N2:194:LEU:HD23	1.97	0.47
31:N4:282:LEU:HD21	31:N4:359:TRP:HH2	1.79	0.47
34:S1:282:ASN:HA	34:S1:413:LEU:HD23	1.95	0.47
8:A8:115:LYS:HB3	8:A8:116:PRO:HD3	1.95	0.47
31:N4:318:ALA:HB2	31:N4:373:ILE:HG13	1.95	0.47
34:S1:388:ASN:ND2	34:S1:513:MET:O	2.47	0.47
4:A3:160:GLY:HA3	8:A8:204:LYS:HE3	1.97	0.47
17:B3:47:ARG:HA	17:B3:50:ALA:HB3	1.96	0.47
46:N3:201:PC1:H3E1	46:N3:201:PC1:H3A1	1.95	0.47
33:N6:7:PHE:CZ	33:N6:104:VAL:HG23	2.50	0.47
34:S1:262:VAL:HG23	34:S1:276:ARG:HB2	1.96	0.47
34:S1:696:MET:HG2	34:S1:711:VAL:HG21	1.96	0.47
6:A6:136:THR:HG21	36:S3:220:VAL:HG11	1.96	0.47
13:AM:71:ARG:HH21	13:AM:115:PHE:HE1	1.61	0.47
33:N6:124:ASP:O	33:N6:127:ILE:HG12	2.15	0.47
34:S1:347:ASP:HB3	34:S1:594:ALA:HB1	1.97	0.47
35:S2:101:LEU:HB2	35:S2:464:PHE:CZ	2.50	0.47
42:V1:192:ASP:HB3	44:V3:411:MET:SD	2.54	0.47
45:4L:201:CDL:H381	45:4L:201:CDL:H421	1.97	0.47
4:A3:109:ALA:HB2	48:N1:404:PEE:H68	1.97	0.47
11:AK:145:TYR:OH	11:AK:201:LEU:O	2.26	0.47
11:AK:175:MET:HG2	11:AK:180:PHE:HB2	1.96	0.47
51:BL:202:PLX:H1A3	51:BL:202:PLX:H22	1.69	0.47
28:N1:134:ARG:NH1	28:N1:206:GLU:OE1	2.41	0.47
32:N5:49:VAL:HB	32:N5:50:PRO:HD3	1.97	0.47
42:V1:384:PRO:HB2	42:V1:423:THR:HG22	1.97	0.47
16:B2:92:ASP:HB2	16:B2:97:HIS:HB2	1.96	0.47
31:N4:216:LEU:HB3	31:N4:217:PRO:HD3	1.97	0.47
5:A5:9:THR:HG23	5:A5:16:VAL:HG22	1.97	0.47
11:AK:134:GLN:NE2	50:AK:401:ADP:N1	2.61	0.47
14:AN:144:THR:HB	28:N1:96:ILE:HG23	1.96	0.47
31:N4:266:MET:HB3	31:N4:395:LEU:HD13	1.97	0.47
34:S1:64:CYS:O	34:S1:184:ARG:NH2	2.30	0.47
35:S2:160:ALA:HA	35:S2:404:THR:HG21	1.97	0.47
42:V1:244:ASN:OD1	42:V1:245:VAL:N	2.47	0.47
45:4L:201:CDL:H531	45:4L:201:CDL:H172	1.95	0.47
29:N2:270:MET:HE1	29:N2:282:MET:HE1	1.97	0.47
35:S2:448:HIS:HB3	35:S2:452:ASP:HB2	1.97	0.47
9:A9:198:ALA:O	9:A9:260:GLY:HA2	2.14	0.46
11:AK:225:ASN:HB3	11:AK:228:GLU:HG2	1.97	0.46
20:B6:170:ILE:HB	20:B6:175:GLU:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B8:110:ASP:O	22:B8:116:ARG:NH1	2.48	0.46
48:N3:202:PEE:H7	48:N3:202:PEE:H49	1.68	0.46
31:N4:76:MET:SD	31:N4:230:VAL:HB	2.55	0.46
32:N5:331:MET:HB3	32:N5:387:THR:HG22	1.97	0.46
34:S1:123:ASN:ND2	42:V1:387:GLU:OE1	2.28	0.46
40:S7:108:THR:HA	40:S7:136:CYS:HB3	1.97	0.46
43:V2:72:GLU:HB2	44:V3:415:SER:HA	1.97	0.46
1:4L:35:GLY:HA3	33:N6:20:PHE:CZ	2.50	0.46
11:AK:342:SER:HB2	11:AK:345:TYR:HD2	1.80	0.46
45:B5:201:CDL:H442	24:BK:44:PRO:HG3	1.97	0.46
46:N3:203:PC1:H332	40:S7:190:LEU:HD21	1.98	0.46
34:S1:338:VAL:HB	34:S1:363:SER:CB	2.45	0.46
35:S2:412:GLU:OE2	36:S3:140:ARG:NH2	2.48	0.46
8:A8:174:PHE:HB3	8:A8:178:ARG:HH12	1.80	0.46
21:B7:22:MET:HE1	21:B7:102:PHE:HD2	1.79	0.46
29:N2:193:VAL:HG21	29:N2:266:ILE:HG12	1.97	0.46
29:N2:211:MET:HG2	29:N2:333:SER:HB2	1.97	0.46
33:N6:82:VAL:HG12	33:N6:85:SER:HB2	1.96	0.46
35:S2:299:LEU:HD22	35:S2:304:ILE:HD12	1.97	0.46
43:V2:85:LEU:HD13	44:V3:400:LEU:HD22	1.98	0.46
1:4L:35:GLY:HA3	33:N6:20:PHE:HZ	1.79	0.46
4:A3:145:ASP:OD1	4:A3:145:ASP:N	2.45	0.46
14:AN:93:GLU:HG3	38:S5:98:HIS:CD2	2.50	0.46
20:B6:165:PHE:O	20:B6:168:ASP:HB2	2.15	0.46
45:N5:703:CDL:H511	45:N5:703:CDL:HA32	1.97	0.46
37:S4:112:MET:HG3	41:S8:184:LEU:HD23	1.96	0.46
41:S8:153:ILE:HG13	41:S8:155:CYS:HB3	1.98	0.46
4:A3:139:PRO:HD3	14:AN:69:ILE:HD13	1.98	0.46
7:A7:64:MET:HB3	36:S3:80:CYS:SG	2.56	0.46
13:AM:55:PHE:CZ	13:AM:58:ARG:HG3	2.50	0.46
28:N1:113:VAL:HG11	28:N1:139:THR:HG21	1.98	0.46
34:S1:432:ILE:HG12	34:S1:445:LEU:HB2	1.96	0.46
18:B4:10:ARG:HG2	18:B4:11:LEU:HG	1.98	0.46
28:N1:173:TRP:HB2	28:N1:176:PHE:HD2	1.80	0.46
51:N1:402:PLX:H11	51:S7:302:PLX:H52	1.98	0.46
43:V2:54:ASP:OD1	43:V2:55:PHE:N	2.49	0.46
2:A1:12:MET:HE3	28:N1:264:LEU:HD22	1.97	0.46
5:A5:7:LYS:H	5:A5:7:LYS:HD2	1.80	0.46
25:BL:109:LEU:HD22	31:N4:43:ASN:HB2	1.96	0.46
28:N1:317:GLN:NE2	33:N6:141:MET:SD	2.85	0.46
33:N6:7:PHE:HZ	33:N6:104:VAL:HG23	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:S1:197:THR:HG22	34:S1:206:VAL:HG22	1.96	0.46
34:S1:296:GLY:O	34:S1:572:HIS:NE2	2.38	0.46
40:S7:154:ASP:OD1	40:S7:154:ASP:N	2.37	0.46
12:AL:4:THR:HA	12:AL:7:HIS:ND1	2.31	0.46
29:N2:19:LEU:O	29:N2:23:SER:OG	2.30	0.46
29:N2:42:PRO:HG3	33:N6:167:VAL:HG13	1.96	0.46
32:N5:151:SER:HB2	32:N5:252:MET:SD	2.56	0.46
35:S2:341:GLU:O	35:S2:345:GLN:HG2	2.16	0.46
5:A5:112:TRP:CE2	36:S3:87:PHE:HB3	2.51	0.46
11:AK:97:ASP:N	11:AK:97:ASP:OD1	2.49	0.46
51:BL:202:PLX:H351	31:N4:443:PRO:HB3	1.98	0.46
28:N1:18:ALA:HB1	28:N1:48:PRO:HB3	1.98	0.46
29:N2:295:ARG:HD3	35:S2:58:MET:HE3	1.97	0.46
34:S1:36:VAL:HG11	34:S1:56:VAL:HG11	1.97	0.46
9:A9:170:LEU:HA	9:A9:202:LYS:HB3	1.98	0.46
24:BK:74:ILE:HG23	24:BK:156:LEU:HD22	1.98	0.46
34:S1:281:ILE:HD11	34:S1:602:ARG:HD2	1.98	0.46
42:V1:55:GLY:O	42:V1:58:SER:OG	2.23	0.46
15:B1:30:ARG:O	15:B1:33:GLU:HG2	2.15	0.45
29:N2:246:VAL:HG11	45:N4:503:CDL:H392	1.98	0.45
35:S2:214:GLU:OE2	35:S2:227:ARG:NH2	2.42	0.45
46:A3:202:PC1:H272	46:A3:202:PC1:H232	1.98	0.45
8:A8:201:GLU:HA	8:A8:204:LYS:HD3	1.97	0.45
10:AC:119:ILE:HG21	10:AC:135:ALA:HB1	1.97	0.45
13:AM:108:TYR:HE1	41:S8:198:GLU:HG2	1.81	0.45
20:B6:140:TRP:HD1	24:BK:41:VAL:HG13	1.81	0.45
21:B7:22:MET:HE1	21:B7:102:PHE:CD2	2.51	0.45
22:B8:110:ASP:OD1	31:N4:409:TYR:OH	2.34	0.45
30:N3:65:PHE:O	30:N3:69:ILE:HG23	2.16	0.45
46:N3:201:PC1:H3B1	46:N3:201:PC1:H322	1.98	0.45
31:N4:210:TYR:CG	31:N4:268:GLY:HA3	2.51	0.45
35:S2:149:SER:HA	35:S2:184:THR:HG22	1.98	0.45
41:S8:150:THR:HG21	41:S8:180:HIS:CD2	2.52	0.45
2:A1:19:PRO:HB3	28:N1:9:LEU:HD12	1.97	0.45
32:N5:313:MET:HG3	32:N5:328:HIS:HD2	1.81	0.45
32:N5:560:THR:O	32:N5:565:THR:OG1	2.25	0.45
52:N5:706:3PE:H3A1	52:N5:706:3PE:H362	1.99	0.45
35:S2:212:GLU:O	35:S2:216:MET:HG3	2.15	0.45
7:A7:27:ARG:HD2	7:A7:31:ILE:HG21	1.97	0.45
9:A9:207:PHE:HB2	9:A9:214:LEU:HG	1.98	0.45
31:N4:176:PHE:HA	31:N4:179:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:N5:267:MET:O	32:N5:274:GLN:NE2	2.50	0.45
32:N5:375:ILE:HD12	32:N5:458:LEU:HD11	1.99	0.45
40:S7:62:LEU:O	40:S7:91:VAL:HA	2.16	0.45
41:S8:142:THR:O	41:S8:187:LYS:NZ	2.50	0.45
2:A1:66:LEU:O	2:A1:69:ILE:HG13	2.16	0.45
10:AB:138:LEU:HD23	10:AB:144:ILE:HG12	1.99	0.45
25:BL:106:VAL:HG13	31:N4:453:MET:HE3	1.98	0.45
29:N2:190:MET:HE3	29:N2:205:LEU:HB2	1.98	0.45
34:S1:306:MET:HB2	34:S1:583:ILE:HB	1.99	0.45
34:S1:484:SER:HB2	34:S1:680:LEU:HD11	1.99	0.45
43:V2:133:GLN:OE1	43:V2:187:GLN:NE2	2.49	0.45
1:4L:59:MET:HB2	38:S5:18:MET:HE1	1.99	0.45
23:B9:123:ILE:HD13	23:B9:129:GLY:HA3	1.99	0.45
7:A7:23:LYS:HB2	35:S2:259:PHE:CD2	2.52	0.45
17:B3:18:ASP:O	17:B3:21:GLN:HG2	2.16	0.45
19:B5:71:MET:HE3	31:N4:442:LEU:HD11	1.98	0.45
20:B6:146:LEU:HA	20:B6:150:VAL:HB	1.98	0.45
31:N4:198:ALA:HA	48:N4:501:PEE:H34	1.98	0.45
35:S2:176:ILE:HG13	35:S2:357:MET:HE1	1.99	0.45
35:S2:213:ARG:HE	40:S7:78:HIS:CE1	2.35	0.45
6:A6:127:THR:HG23	36:S3:219:VAL:O	2.17	0.45
28:N1:13:ILE:HD13	28:N1:13:ILE:HA	1.81	0.45
31:N4:231:LEU:HD23	31:N4:235:LEU:HD12	1.98	0.45
40:S7:131:VAL:HG22	40:S7:161:ILE:HB	1.97	0.45
29:N2:24:SER:OG	38:S5:15:ASP:OD1	2.32	0.45
32:N5:241:THR:HG21	32:N5:344:GLY:HA3	1.97	0.45
32:N5:292:ALA:HB2	32:N5:304:PHE:HB3	1.99	0.45
40:S7:53:LEU:HB2	51:S7:302:PLX:H321	1.99	0.45
42:V1:141:GLY:HA3	42:V1:248:VAL:O	2.17	0.45
1:4L:2:PRO:HG3	33:N6:127:ILE:HD13	1.99	0.44
8:A8:117:ASN:HB3	14:AN:73:PRO:HG2	1.99	0.44
9:A9:55:VAL:HG13	9:A9:79:GLN:HG2	1.99	0.44
9:A9:85:ARG:HH12	40:S7:196:ARG:HG3	1.83	0.44
45:AL:201:CDL:H521	45:AL:201:CDL:H562	1.98	0.44
28:N1:99:ASN:HB2	46:N1:406:PC1:H142	1.98	0.44
29:N2:323:MET:HE3	29:N2:323:MET:HB2	1.85	0.44
31:N4:82:SER:HB2	31:N4:432:ARG:CZ	2.47	0.44
32:N5:103:PHE:HB2	32:N5:341:MET:HE3	1.99	0.44
35:S2:129:LEU:HD23	36:S3:204:LEU:HD11	1.99	0.44
35:S2:203:MET:O	35:S2:206:PHE:HB3	2.17	0.44
42:V1:325:PRO:HG3	42:V1:433:TRP:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A6:88:LYS:NZ	6:A6:133:PHE:HA	2.32	0.44
11:AK:317:PRO:HB3	25:BL:54:ARG:HA	1.99	0.44
12:AL:19:HIS:CD2	12:AL:20:ARG:HG2	2.52	0.44
45:AN:201:CDL:H742	48:S8:303:PEE:H66	2.00	0.44
28:N1:189:THR:HG22	28:N1:234:MET:HE3	1.98	0.44
29:N2:1:MET:HE3	29:N2:6:TYR:HD1	1.82	0.44
51:N2:402:PLX:H111	51:N2:402:PLX:H142	1.80	0.44
30:N3:33:LYS:O	40:S7:98:ARG:NH1	2.43	0.44
32:N5:534:HIS:CD2	48:N5:705:PEE:H16	2.51	0.44
33:N6:82:VAL:HG22	33:N6:83:TRP:H	1.83	0.44
10:AC:74:LEU:HD21	10:AC:82:ARG:HH21	1.82	0.44
32:N5:15:LEU:HD11	32:N5:94:LEU:HD21	1.99	0.44
34:S1:476:LEU:HD22	34:S1:493:VAL:HG21	2.00	0.44
48:S2:501:PEE:H68	48:S2:501:PEE:H63	1.75	0.44
39:S6:67:ALA:HB2	41:S8:111:GLU:HG3	1.98	0.44
46:A3:202:PC1:H11	14:AN:48:TRP:HB2	1.99	0.44
7:A7:43:VAL:HG22	7:A7:47:HIS:CG	2.53	0.44
10:AC:128:PHE:HZ	10:AC:148:ILE:HG12	1.81	0.44
11:AK:85:LEU:HD22	11:AK:158:GLY:HA3	1.98	0.44
11:AK:172:LEU:HD22	11:AK:189:TYR:CD1	2.52	0.44
18:B4:98:LEU:HD11	45:B4:201:CDL:H861	1.99	0.44
19:B5:179:ILE:HD13	38:S5:38:LYS:HG3	2.00	0.44
28:N1:198:PHE:CE1	28:N1:285:LEU:HD13	2.53	0.44
46:N1:406:PC1:H381	46:N1:406:PC1:H3C2	1.99	0.44
42:V1:62:TRP:CD2	42:V1:181:LEU:HD13	2.52	0.44
1:4L:62:ILE:HG21	29:N2:31:ILE:HD11	2.00	0.44
20:B6:92:GLU:HB3	20:B6:93:PRO:HD3	1.99	0.44
25:BL:90:VAL:HG22	31:N4:28:THR:HG21	1.99	0.44
46:N1:406:PC1:H122	46:N1:406:PC1:H12	1.98	0.44
29:N2:137:ALA:HB3	29:N2:138:PRO:HD3	2.00	0.44
31:N4:200:ILE:O	31:N4:204:MET:HG2	2.18	0.44
34:S1:476:LEU:HD21	34:S1:481:LEU:HD21	2.00	0.44
35:S2:243:PRO:HD2	35:S2:246:LEU:HD22	2.00	0.44
36:S3:118:ASP:OD2	36:S3:125:ARG:NH2	2.48	0.44
41:S8:153:ILE:HG12	55:S8:302:SF4:S1	2.57	0.44
42:V1:112:TYR:CD1	42:V1:153:ALA:HB3	2.52	0.44
9:A9:145:PHE:O	9:A9:187:GLY:HA3	2.18	0.44
23:B9:150:HIS:CD2	23:B9:151:PRO:HD2	2.52	0.44
32:N5:174:TYR:CD2	32:N5:232:TRP:HB3	2.52	0.44
32:N5:186:MET:HG2	32:N5:196:TRP:NE1	2.33	0.44
34:S1:59:GLN:NE2	37:S4:89:SER:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:S4:100:GLU:HG3	37:S4:125:VAL:HG22	1.99	0.44
20:B6:132:VAL:O	20:B6:136:LEU:CB	2.64	0.44
29:N2:313:MET:HE2	29:N2:313:MET:HB2	1.79	0.44
34:S1:307:ILE:HG23	34:S1:317:THR:HG21	1.99	0.44
24:BK:35:LYS:HE3	24:BK:35:LYS:HB3	1.89	0.44
30:N3:24:LEU:HD21	46:N3:203:PC1:H3A2	2.00	0.44
31:N4:448:THR:HG21	45:N5:703:CDL:H411	2.00	0.44
32:N5:208:CYS:HA	32:N5:209:PRO:HD3	1.77	0.44
32:N5:401:MET:HE3	32:N5:482:MET:HE2	2.00	0.44
40:S7:85:ASP:O	40:S7:88:ARG:HG2	2.18	0.44
5:A5:113:LYS:HE2	5:A5:113:LYS:HB3	1.81	0.44
7:A7:113:LEU:HD12	41:S8:41:VAL:HA	2.00	0.44
29:N2:36:ASN:OD1	29:N2:134:GLN:NE2	2.37	0.44
32:N5:297:ASP:O	32:N5:301:ILE:HG13	2.18	0.44
34:S1:185:PHE:CZ	34:S1:221:ASN:HB2	2.53	0.44
34:S1:575:VAL:C	34:S1:578:PRO:HD2	2.42	0.44
48:S8:303:PEE:H41	48:S8:303:PEE:H35	1.63	0.44
23:B9:143:GLU:O	23:B9:164:ARG:NH2	2.50	0.43
24:BK:60:ARG:HE	24:BK:62:TYR:HE1	1.66	0.43
31:N4:225:ILE:HD13	31:N4:331:ASN:HB2	2.00	0.43
32:N5:327:LEU:O	32:N5:331:MET:HG2	2.18	0.43
33:N6:124:ASP:OD1	33:N6:124:ASP:N	2.50	0.43
35:S2:194:THR:HB	35:S2:206:PHE:HA	1.99	0.43
37:S4:84:ARG:HD3	37:S4:91:VAL:HG12	2.00	0.43
51:S7:302:PLX:H1C2	51:S7:302:PLX:H21	1.65	0.43
11:AK:147:ASP:OD1	11:AK:303:LYS:NZ	2.42	0.43
18:B4:10:ARG:NH1	32:N5:539:TYR:OH	2.51	0.43
28:N1:288:LEU:O	28:N1:292:SER:HB2	2.18	0.43
29:N2:112:HIS:HB2	29:N2:184:ILE:HD13	2.00	0.43
29:N2:168:GLY:HA3	29:N2:181:TYR:CE1	2.52	0.43
31:N4:70:THR:HA	31:N4:103:GLN:HE21	1.82	0.43
51:N4:502:PLX:H352	51:N4:502:PLX:H381	1.68	0.43
32:N5:435:PRO:HB3	32:N5:437:PHE:CZ	2.53	0.43
34:S1:208:THR:HG21	34:S1:212:LYS:HB3	2.00	0.43
35:S2:145:LEU:HD12	35:S2:145:LEU:HA	1.85	0.43
49:AC:201:ZMP:H25B	49:AC:201:ZMP:H22	1.43	0.43
11:AK:67:ASN:ND2	11:AK:68:ILE:H	2.16	0.43
51:BL:202:PLX:H352	31:N4:71:TRP:CG	2.53	0.43
31:N4:98:MET:HE1	45:N4:503:CDL:H202	2.00	0.43
10:AC:120:MET:HE1	23:B9:66:LEU:HB3	2.00	0.43
11:AK:355:TRP:H	11:AK:355:TRP:CD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:78:ASP:HB2	13:AM:81:MET:HG3	2.00	0.43
20:B6:186:GLN:HG2	21:B7:89:TYR:CE2	2.53	0.43
23:B9:217:ARG:NH2	23:B9:220:PRO:O	2.52	0.43
34:S1:624:ARG:NH2	34:S1:637:ASP:OD1	2.51	0.43
11:AK:297:ARG:HA	11:AK:300:VAL:HG22	2.00	0.43
19:B5:147:ALA:HB2	31:N4:173:SER:HB2	2.00	0.43
30:N3:96:ILE:HD13	48:N3:202:PEE:H33	2.01	0.43
48:N3:202:PEE:H56	48:N3:202:PEE:H51	1.63	0.43
32:N5:8:THR:HB	32:N5:82:MET:HE2	1.99	0.43
35:S2:399:PRO:HA	35:S2:419:SER:O	2.19	0.43
8:A8:226:GLU:O	38:S5:51:ARG:NH2	2.45	0.43
29:N2:130:LEU:HD12	29:N2:134:GLN:HG3	2.00	0.43
45:N4:503:CDL:H371	45:N4:503:CDL:H791	2.00	0.43
32:N5:289:ALA:O	32:N5:293:ILE:HG23	2.19	0.43
34:S1:389:THR:HG21	34:S1:473:MET:HE2	2.00	0.43
35:S2:149:SER:HB2	35:S2:152:CYS:HB2	2.01	0.43
35:S2:190:ILE:HD11	35:S2:257:PHE:CZ	2.54	0.43
35:S2:441:LEU:HA	35:S2:460:GLN:HE22	1.82	0.43
42:V1:146:GLY:HA3	42:V1:193:PHE:CE1	2.54	0.43
42:V1:452:GLN:O	42:V1:456:GLN:HG2	2.18	0.43
13:AM:76:ASP:OD1	40:S7:185:LYS:HE3	2.18	0.43
14:AN:57:ARG:NH1	28:N1:168:THR:OG1	2.52	0.43
40:S7:84:TYR:CE1	40:S7:171:GLU:HG3	2.54	0.43
1:4L:37:MET:HG2	1:4L:67:ALA:CB	2.40	0.43
45:AM:201:CDL:H541	28:N1:43:TYR:CZ	2.54	0.43
14:AN:19:ILE:HD12	35:S2:351:SER:HB2	2.01	0.43
15:B1:46:LYS:O	24:BK:69:ARG:NH1	2.51	0.43
18:B4:48:LEU:HB3	23:B9:208:LEU:HD13	2.01	0.43
18:B4:87:SER:HB3	45:B4:201:CDL:H571	2.00	0.43
20:B6:181:LYS:HG2	21:B7:40:VAL:HG13	2.00	0.43
48:B6:201:PEE:H22	48:B6:201:PEE:H15	1.68	0.43
28:N1:68:ILE:HG21	45:N1:401:CDL:HA31	2.01	0.43
28:N1:149:ILE:HG21	28:N1:185:TRP:HB2	2.00	0.43
32:N5:184:LEU:HD22	52:N5:706:3PE:H352	1.99	0.43
32:N5:486:MET:HE3	32:N5:486:MET:HB2	1.87	0.43
34:S1:387:LEU:HB3	34:S1:600:GLU:HA	2.01	0.43
51:S7:302:PLX:H262	51:S7:302:PLX:H292	1.73	0.43
31:N4:201:MET:HE1	31:N4:212:LEU:HD11	2.01	0.43
34:S1:466:LEU:HD13	34:S1:500:ILE:HD11	2.01	0.43
35:S2:116:ASP:OD1	36:S3:185:ARG:NH2	2.52	0.43
35:S2:124:2MR:O	40:S7:146:SER:OG	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A8:111:ALA:HB2	8:A8:197:PRO:HG3	2.01	0.43
10:AB:78:ALA:HA	10:AB:81:ASP:OD2	2.19	0.43
13:AM:49:TYR:HB2	13:AM:61:TRP:CE2	2.54	0.43
51:B1:101:PLX:H1C2	51:B1:101:PLX:H21	1.59	0.43
31:N4:14:MET:O	31:N4:18:SER:OG	2.26	0.43
32:N5:96:VAL:O	32:N5:100:ILE:HG12	2.19	0.43
49:AC:201:ZMP:H11	23:B9:58:VAL:HG21	2.01	0.42
28:N1:224:PHE:CE2	54:N1:403:U10:H271	2.54	0.42
45:N2:401:CDL:H151	45:N2:401:CDL:H361	2.00	0.42
30:N3:73:LEU:HA	30:N3:73:LEU:HD23	1.81	0.42
31:N4:8:THR:HB	31:N4:104:LEU:HD13	2.00	0.42
31:N4:84:LEU:HD22	31:N4:87:GLU:HG3	2.01	0.42
33:N6:24:PRO:HG2	33:N6:28:TYR:HB2	2.00	0.42
35:S2:272:ARG:NH1	48:S8:303:PEE:H1	2.34	0.42
40:S7:79:MET:HE2	40:S7:86:MET:HE2	2.00	0.42
1:4L:55:LEU:HD23	1:4L:55:LEU:HA	1.89	0.42
10:AB:93:ILE:HD12	10:AB:108:LEU:HD13	2.01	0.42
10:AC:94:ASP:HB3	10:AC:97:LYS:HG2	2.00	0.42
20:B6:89:SER:HB2	20:B6:92:GLU:HB2	1.99	0.42
20:B6:146:LEU:HD23	20:B6:150:VAL:HG21	2.00	0.42
28:N1:267:THR:O	28:N1:271:LEU:HG	2.19	0.42
28:N1:291:LYS:NZ	30:N3:112:GLU:OE2	2.52	0.42
29:N2:190:MET:HG2	29:N2:204:ASN:HB3	2.01	0.42
48:N3:202:PEE:H65	48:N3:202:PEE:H71	1.79	0.42
31:N4:12:LEU:HB2	31:N4:13:PRO:HD3	2.00	0.42
31:N4:204:MET:O	31:N4:208:PRO:HA	2.19	0.42
31:N4:398:MET:HG2	48:N5:705:PEE:H78	2.01	0.42
33:N6:122:LEU:HG	33:N6:123:GLY:H	1.83	0.42
39:S6:70:LEU:HD13	41:S8:109:GLY:HA3	2.02	0.42
42:V1:65:THR:O	42:V1:69:LEU:HG	2.18	0.42
6:A6:145:LEU:HD12	6:A6:145:LEU:HA	1.89	0.42
8:A8:121:MET:HE2	14:AN:73:PRO:HA	2.01	0.42
9:A9:262:THR:O	9:A9:333:PRO:HD2	2.20	0.42
9:A9:272:LEU:HG	9:A9:375:VAL:HG21	2.02	0.42
11:AK:112:GLY:HA2	11:AK:136:TRP:CD2	2.54	0.42
11:AK:253:GLU:O	11:AK:282:LYS:NZ	2.50	0.42
28:N1:142:TYR:CE1	28:N1:192:GLU:HG2	2.54	0.42
28:N1:273:ILE:HG23	28:N1:277:TYR:CD2	2.54	0.42
31:N4:82:SER:HB2	31:N4:432:ARG:NH1	2.33	0.42
32:N5:264:TYR:CD2	32:N5:265:PRO:HD3	2.53	0.42
33:N6:129:ASP:HB2	38:S5:32:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S2:149:SER:HA	35:S2:184:THR:CG2	2.49	0.42
6:A6:114:MET:SD	36:S3:185:ARG:HA	2.59	0.42
7:A7:95:VAL:O	36:S3:105:ASN:ND2	2.51	0.42
27:CB:33:LEU:HD23	27:CB:33:LEU:HA	1.86	0.42
54:N1:403:U10:H301	54:N1:403:U10:C33	2.49	0.42
29:N2:287:LEU:HD12	48:S2:501:PEE:H64	2.01	0.42
33:N6:141:MET:HE2	38:S5:27:HIS:NE2	2.33	0.42
35:S2:105:MET:HE1	35:S2:450:LEU:HD13	2.01	0.42
35:S2:204:THR:N	35:S2:205:PRO:HD2	2.35	0.42
45:4L:201:CDL:HA61	12:AL:49:PHE:HA	2.01	0.42
6:A6:127:THR:O	6:A6:131:ARG:HG3	2.20	0.42
11:AK:51:THR:HG21	11:AK:153:LEU:HD22	2.01	0.42
45:AN:201:CDL:H871	41:S8:74:LEU:HD13	2.00	0.42
31:N4:78:MET:HA	31:N4:81:GLN:HE21	1.84	0.42
32:N5:414:ILE:HG21	45:N5:704:CDL:H782	2.02	0.42
32:N5:520:TYR:CE1	45:N5:704:CDL:HB22	2.55	0.42
33:N6:39:VAL:O	33:N6:43:ILE:HG13	2.20	0.42
34:S1:541:PRO:HB3	34:S1:561:PRO:HD3	2.00	0.42
35:S2:103:LEU:HG	35:S2:105:MET:HG3	2.00	0.42
42:V1:300:ILE:HG22	42:V1:306:GLY:HA2	2.00	0.42
42:V1:398:ARG:NH1	42:V1:403:ASP:O	2.52	0.42
11:AK:138:TYR:OH	11:AK:193:LYS:HA	2.19	0.42
20:B6:128:SER:O	20:B6:132:VAL:HG12	2.19	0.42
21:B7:4:HIS:NE2	22:B8:155:PRO:HD3	2.35	0.42
32:N5:504:LEU:HD12	45:N5:704:CDL:H511	2.00	0.42
33:N6:123:GLY:O	33:N6:126:VAL:HG22	2.20	0.42
34:S1:98:LYS:HD3	34:S1:99:GLY:N	2.34	0.42
35:S2:200:ILE:HD12	35:S2:274:TRP:CZ3	2.55	0.42
35:S2:339:ARG:O	35:S2:343:MET:HG3	2.20	0.42
35:S2:418:VAL:HB	35:S2:427:ARG:HB3	2.01	0.42
42:V1:201:ALA:HB3	43:V2:119:TYR:CD1	2.54	0.42
9:A9:109:ASN:HB3	9:A9:112:ASP:HB2	2.00	0.42
10:AC:140:CYS:HB3	10:AC:143:GLU:HG3	2.01	0.42
11:AK:134:GLN:HE22	50:AK:401:ADP:HN62	1.68	0.42
11:AK:357:LYS:HD3	26:CA:36:HIS:O	2.19	0.42
14:AN:57:ARG:HB3	28:N1:316:PRO:HG3	2.01	0.42
19:B5:180:ASP:OD2	19:B5:182:SER:OG	2.37	0.42
28:N1:120:GLY:HA2	28:N1:128:ALA:HB1	2.01	0.42
34:S1:180:THR:N	55:S1:802:SF4:S4	2.86	0.42
34:S1:291:ARG:HD2	34:S1:292:PHE:CE2	2.55	0.42
42:V1:280:GLY:O	43:V2:143:ARG:NH1	2.53	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	2.01	0.42
8:A8:157:GLU:HB2	8:A8:158:PRO:HD3	2.02	0.42
8:A8:160:THR:HA	8:A8:163:TRP:NE1	2.35	0.42
9:A9:324:MET:HE3	9:A9:324:MET:HB2	1.89	0.42
45:AL:201:CDL:H582	29:N2:110:PRO:HB3	2.01	0.42
20:B6:161:LYS:HG3	21:B7:50:GLN:NE2	2.35	0.42
28:N1:58:LYS:NZ	40:S7:100:SER:O	2.47	0.42
28:N1:155:LEU:HD21	28:N1:305:ILE:HA	2.01	0.42
31:N4:75:LEU:HD13	31:N4:440:HIS:CE1	2.55	0.42
34:S1:429:VAL:HG11	34:S1:440:TYR:HE1	1.85	0.42
6:A6:88:LYS:HD2	6:A6:88:LYS:HA	1.71	0.42
9:A9:126:VAL:HG23	9:A9:161:VAL:HG11	2.02	0.42
14:AN:76:GLN:NE2	14:AN:80:ASP:OD1	2.53	0.42
21:B7:29:TYR:OH	21:B7:111:ARG:NH2	2.45	0.42
28:N1:151:LEU:HD21	30:N3:75:LEU:HD12	2.01	0.42
28:N1:216:ALA:HB2	40:S7:98:ARG:HB3	2.01	0.42
29:N2:252:GLY:HA3	29:N2:290:LEU:HD13	2.01	0.42
29:N2:270:MET:HB3	29:N2:279:PRO:HG3	2.02	0.42
51:N2:402:PLX:H22	51:N2:402:PLX:H1B2	1.76	0.42
40:S7:59:ARG:HG3	40:S7:181:GLN:HB3	2.02	0.42
42:V1:384:PRO:HG2	42:V1:422:HIS:O	2.18	0.42
3:A2:45:LYS:HA	3:A2:45:LYS:HD2	1.94	0.42
9:A9:56:ALA:HA	9:A9:125:VAL:O	2.20	0.42
10:AB:140:CYS:HB2	10:AB:143:GLU:HG3	2.02	0.42
45:AL:203:CDL:CA7	45:AL:203:CDL:H512	2.50	0.42
22:B8:115:ASN:HA	32:N5:166:THR:HG22	2.02	0.42
45:N2:401:CDL:H142	45:N2:401:CDL:H111	1.92	0.42
32:N5:264:TYR:CG	32:N5:265:PRO:HD3	2.55	0.42
34:S1:152:ARG:NH1	42:V1:414:GLU:OE1	2.53	0.42
34:S1:354:LEU:HD22	34:S1:548:LEU:HD22	2.02	0.42
35:S2:129:LEU:O	35:S2:133:LYS:HG2	2.20	0.42
41:S8:75:SER:O	41:S8:79:ARG:HG3	2.19	0.42
41:S8:85:ASN:HD22	41:S8:88:PHE:HB2	1.85	0.42
42:V1:355:ILE:HD13	43:V2:139:PRO:HG3	2.02	0.42
1:4L:1:MET:HG3	1:4L:5:TYR:HD2	1.84	0.41
6:A6:89:VAL:HG22	49:AB:201:ZMP:H22A	2.01	0.41
14:AN:137:THR:HG23	14:AN:138:TYR:CD2	2.55	0.41
28:N1:58:LYS:NZ	40:S7:101:ASP:OD1	2.43	0.41
28:N1:307:LEU:HB3	28:N1:308:PRO:HD3	2.02	0.41
48:N1:405:PEE:H21	48:N1:405:PEE:H15	1.93	0.41
29:N2:142:LEU:HB3	29:N2:194:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:N4:243:MET:HA	31:N4:246:ILE:HG22	2.02	0.41
48:N4:501:PEE:H29	48:N4:501:PEE:H36	1.73	0.41
32:N5:23:ASN:HD22	45:N5:703:CDL:HB4	1.85	0.41
32:N5:341:MET:SD	32:N5:457:LEU:HD12	2.59	0.41
2:A1:39:ALA:O	46:N1:406:PC1:H131	2.20	0.41
4:A3:144:ASP:HB2	8:A8:207:LYS:HB2	2.02	0.41
10:AC:104:PHE:HD1	10:AC:108:LEU:HD12	1.85	0.41
18:B4:9:SER:OG	18:B4:10:ARG:N	2.53	0.41
24:BK:164:LEU:HD23	25:BL:149:LEU:HD13	2.01	0.41
28:N1:90:PRO:HB3	28:N1:94:PRO:HD3	2.03	0.41
46:N1:406:PC1:O14	33:N6:50:SER:OG	2.35	0.41
35:S2:164:LEU:HD12	35:S2:417:LEU:HD23	2.02	0.41
48:S2:501:PEE:H18	48:S2:501:PEE:H24	1.77	0.41
45:4L:201:CDL:H521	33:N6:88:THR:HG23	2.01	0.41
18:B4:82:PRO:HB2	45:B4:201:CDL:HB4	2.02	0.41
48:B6:201:PEE:H35	48:B6:201:PEE:H29	1.85	0.41
28:N1:287:HIS:O	28:N1:291:LYS:HB2	2.20	0.41
29:N2:270:MET:HG2	29:N2:275:SER:OG	2.21	0.41
31:N4:79:ALA:O	31:N4:82:SER:HB3	2.20	0.41
42:V1:296:LEU:HD13	42:V1:337:MET:HE3	2.02	0.41
43:V2:137:THR:O	43:V2:141:MET:N	2.50	0.41
13:AM:126:PRO:HG3	41:S8:181:GLU:O	2.20	0.41
22:B8:96:ASP:OD1	22:B8:96:ASP:N	2.51	0.41
28:N1:295:PRO:HB3	48:N1:404:PEE:H29	2.03	0.41
31:N4:243:MET:HB3	31:N4:301:ILE:HG21	2.02	0.41
31:N4:357:THR:O	31:N4:361:VAL:HG23	2.21	0.41
34:S1:389:THR:HG22	34:S1:514:ASN:HD21	1.86	0.41
42:V1:302:LYS:HE3	42:V1:302:LYS:HB2	1.92	0.41
1:4L:80:MET:SD	33:N6:172:THR:HA	2.60	0.41
45:N1:401:CDL:H812	45:N1:401:CDL:H751	2.03	0.41
32:N5:457:LEU:HD23	32:N5:457:LEU:HA	1.84	0.41
33:N6:24:PRO:O	33:N6:81:GLU:HB2	2.20	0.41
42:V1:161:GLU:HG2	43:V2:177:LEU:HD22	2.03	0.41
43:V2:137:THR:HG22	43:V2:138:THR:H	1.85	0.41
8:A8:202:LEU:HD13	14:AN:70:ALA:HB2	2.03	0.41
21:B7:113:LYS:O	21:B7:116:GLU:HG3	2.21	0.41
48:N1:404:PEE:H39	48:N1:404:PEE:H47	1.86	0.41
34:S1:341:ILE:HG13	34:S1:545:LEU:HD11	2.02	0.41
34:S1:647:GLU:HB2	34:S1:654:VAL:HG11	2.03	0.41
35:S2:318:ASP:OD1	35:S2:318:ASP:N	2.49	0.41
1:4L:68:ALA:HB3	30:N3:67:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A2:55:ILE:O	3:A2:56:ARG:NH1	2.41	0.41
46:A3:201:PC1:H2C2	14:AN:37:ALA:HA	2.02	0.41
22:B8:113:ILE:HD11	22:B8:116:ARG:HD3	2.01	0.41
23:B9:180:LYS:HE2	23:B9:180:LYS:HB3	1.91	0.41
28:N1:38:ASN:OD1	40:S7:88:ARG:HB2	2.21	0.41
28:N1:119:SER:HB2	28:N1:215:TYR:CE2	2.54	0.41
45:N1:401:CDL:H871	46:N1:406:PC1:H3D1	2.01	0.41
48:N4:501:PEE:H30	48:N4:501:PEE:H68	2.02	0.41
32:N5:11:THR:HG22	32:N5:46:LEU:HB3	2.02	0.41
32:N5:162:THR:O	32:N5:166:THR:HG23	2.21	0.41
33:N6:71:THR:HA	33:N6:75:ALA:HB3	2.01	0.41
33:N6:135:PHE:HD1	33:N6:135:PHE:HA	1.73	0.41
42:V1:51:TRP:NE1	44:V3:390:GLN:OE1	2.38	0.41
42:V1:62:TRP:CE2	42:V1:181:LEU:HD13	2.56	0.41
42:V1:111:LYS:CB	42:V1:151:ALA:HA	2.48	0.41
8:A8:219:TYR:CZ	38:S5:38:LYS:HE2	2.56	0.41
11:AK:131:TYR:CD1	11:AK:185:CYS:HB3	2.55	0.41
30:N3:57:LEU:HD21	33:N6:169:MET:SD	2.60	0.41
33:N6:100:GLU:O	33:N6:104:VAL:HG12	2.20	0.41
34:S1:252:ASP:OD2	34:S1:290:THR:OG1	2.31	0.41
34:S1:264:SER:HB2	34:S1:272:ARG:HB3	2.03	0.41
34:S1:339:ALA:HA	34:S1:365:SER:HB2	2.03	0.41
39:S6:84:ILE:HD12	39:S6:84:ILE:HA	1.95	0.41
42:V1:295:PRO:HG2	42:V1:298:GLU:HB3	2.03	0.41
60:V1:502:FMN:H9	60:V1:502:FMN:H1'2	1.84	0.41
2:A1:13:ALA:HB2	28:N1:264:LEU:HD11	2.02	0.41
5:A5:79:GLU:OE1	36:S3:136:ARG:NH2	2.51	0.41
9:A9:118:LYS:HE2	9:A9:118:LYS:HB3	1.90	0.41
11:AK:201:LEU:HA	11:AK:202:PRO:HD3	1.96	0.41
14:AN:21:TYR:CE2	35:S2:348:ARG:HD2	2.56	0.41
14:AN:141:ILE:O	46:N1:406:PC1:H32	2.21	0.41
21:B7:56:ARG:HH22	24:BK:120:SER:HB3	1.84	0.41
28:N1:92:PRO:HB3	28:N1:255:TYR:CD1	2.56	0.41
51:N1:402:PLX:H302	54:N1:403:U10:H472	2.03	0.41
32:N5:15:LEU:HD23	32:N5:15:LEU:HA	1.93	0.41
33:N6:59:ILE:HD13	33:N6:59:ILE:HA	1.94	0.41
35:S2:93:GLN:NE2	35:S2:93:GLN:O	2.54	0.41
38:S5:86:LEU:HG	38:S5:91:LYS:HD2	2.03	0.41
41:S8:117:LYS:N	55:S8:301:SF4:S1	2.88	0.41
7:A7:3:SER:O	45:AM:201:CDL:O1	2.38	0.41
11:AK:342:SER:O	11:AK:346:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:B5:203:PC1:H232	25:BL:88:ARG:HB3	2.03	0.41
27:CB:74:GLY:O	27:CB:78:LEU:HG	2.21	0.41
28:N1:84:THR:O	28:N1:87:VAL:HG22	2.21	0.41
31:N4:16:TRP:NE1	31:N4:97:THR:OG1	2.53	0.41
31:N4:299:VAL:O	31:N4:303:ILE:HG23	2.21	0.41
31:N4:427:LYS:HA	31:N4:427:LYS:HD3	1.94	0.41
45:N4:503:CDL:H341	45:N4:503:CDL:H182	2.02	0.41
32:N5:327:LEU:HG	32:N5:331:MET:HE2	2.03	0.41
40:S7:49:LYS:HE3	51:S7:302:PLX:H301	2.03	0.41
42:V1:312:ASP:HA	42:V1:329:LYS:NZ	2.36	0.41
1:4L:37:MET:HE2	29:N2:68:MET:HE1	2.03	0.40
7:A7:52:ASN:OD1	7:A7:57:ARG:NE	2.54	0.40
12:AL:134:GLN:HA	45:AL:203:CDL:H531	2.03	0.40
26:CA:70:LYS:HD3	26:CA:75:LEU:HD12	2.03	0.40
54:N1:403:U10:H371	54:N1:403:U10:H351	1.94	0.40
29:N2:197:ASN:HD22	29:N2:200:MET:HG2	1.87	0.40
31:N4:449:LEU:HG	45:N5:703:CDL:H441	2.02	0.40
32:N5:350:LEU:HD12	32:N5:359:MET:HG2	2.03	0.40
33:N6:35:VAL:O	33:N6:39:VAL:HG23	2.21	0.40
35:S2:272:ARG:HH11	48:S8:303:PEE:H1	1.85	0.40
42:V1:129:GLU:OE2	42:V1:132:ARG:NH2	2.54	0.40
42:V1:217:GLU:OE2	42:V1:224:ARG:NH2	2.54	0.40
1:4L:5:TYR:HB3	1:4L:43:MET:HE1	2.04	0.40
1:4L:41:PHE:O	1:4L:45:THR:HG22	2.20	0.40
5:A5:38:ILE:O	5:A5:45:ARG:NH1	2.54	0.40
11:AK:307:LEU:HD13	29:N2:313:MET:HG2	2.03	0.40
25:BL:85:TRP:CZ2	48:BL:201:PEE:H16	2.56	0.40
28:N1:11:ILE:HB	28:N1:12:PRO:HD3	2.04	0.40
54:N1:403:U10:H122	54:N1:403:U10:H161	1.92	0.40
31:N4:59:ASP:OD1	31:N4:60:SER:N	2.49	0.40
31:N4:398:MET:O	31:N4:402:ILE:HG13	2.21	0.40
35:S2:184:THR:OG1	35:S2:220:TYR:OH	2.29	0.40
36:S3:168:ARG:HG3	36:S3:181:HIS:CE1	2.57	0.40
40:S7:171:GLU:HB3	41:S8:173:PHE:CE2	2.56	0.40
9:A9:175:LYS:HE2	9:A9:175:LYS:HB2	1.93	0.40
21:B7:53:LEU:HD23	22:B8:170:ARG:HG2	2.03	0.40
21:B7:92:HIS:O	21:B7:96:VAL:HG13	2.22	0.40
48:N4:501:PEE:H51	48:N4:501:PEE:H22	2.03	0.40
36:S3:87:PHE:CE1	36:S3:144:LYS:HD3	2.56	0.40
41:S8:63:TRP:HB3	41:S8:66:LEU:HD12	2.03	0.40
42:V1:110:PRO:HB2	42:V1:112:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:V1:396:MET:HE2	42:V1:396:MET:HB2	1.89	0.40
19:B5:72:ARG:HG3	45:B5:201:CDL:H873	2.03	0.40
28:N1:32:GLN:HG2	35:S2:204:THR:HG22	2.04	0.40
34:S1:281:ILE:HD11	34:S1:602:ARG:NE	2.36	0.40
34:S1:382:ARG:C	34:S1:384:ASN:H	2.29	0.40
37:S4:168:LYS:HA	37:S4:168:LYS:HD3	1.92	0.40
60:V1:502:FMN:HM83	60:V1:502:FMN:HM71	1.93	0.40
6:A6:89:VAL:CG2	49:AB:201:ZMP:H22A	2.51	0.40
10:AC:90:TYR:CE1	17:B3:44:PRO:HB2	2.57	0.40
20:B6:177:ILE:HA	20:B6:178:PRO:HD3	1.88	0.40
27:CB:85:TYR:CZ	29:N2:344:SER:HB3	2.56	0.40
48:N1:404:PEE:H36	48:N1:404:PEE:H30	1.72	0.40
29:N2:342:ALA:O	29:N2:345:SER:OG	2.23	0.40
31:N4:78:MET:O	31:N4:81:GLN:HG2	2.21	0.40
31:N4:401:MET:HE1	48:N5:705:PEE:H71	2.03	0.40
32:N5:14:ILE:HD11	32:N5:43:ALA:HA	2.02	0.40
34:S1:53:CYS:O	34:S1:56:VAL:HG12	2.22	0.40
35:S2:142:PHE:HA	35:S2:145:LEU:HD22	2.04	0.40
40:S7:45:TYR:O	40:S7:49:LYS:HG2	2.21	0.40
40:S7:118:ARG:HA	40:S7:118:ARG:HD2	1.96	0.40
51:S7:302:PLX:H141	51:S7:302:PLX:H111	1.83	0.40
42:V1:63:TYR:H	42:V1:256:ARG:NH1	2.20	0.40
43:V2:237:PRO:HA	43:V2:238:PRO:HD3	1.95	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A2	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
4	A3	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
5	A5	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
6	A6	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
7	A7	93/112 (83%)	90 (97%)	3 (3%)	0	100	100
8	A8	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
9	A9	339/341 (99%)	327 (96%)	12 (4%)	0	100	100
10	AB	75/87 (86%)	74 (99%)	1 (1%)	0	100	100
10	AC	85/87 (98%)	85 (100%)	0	0	100	100
11	AK	318/321 (99%)	308 (97%)	10 (3%)	0	100	100
12	AL	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
13	AM	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
14	AN	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
15	B1	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
16	B2	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
17	B3	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
18	B4	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
19	B5	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
20	B6	99/126 (79%)	93 (94%)	6 (6%)	0	100	100
21	B7	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
22	B8	154/156 (99%)	151 (98%)	3 (2%)	0	100	100
23	B9	176/178 (99%)	173 (98%)	3 (2%)	0	100	100
24	BK	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
25	BL	97/102 (95%)	87 (90%)	10 (10%)	0	100	100
26	CA	47/49 (96%)	47 (100%)	0	0	100	100
27	CB	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
28	N1	316/318 (99%)	306 (97%)	10 (3%)	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%)	453 (99%)	4 (1%)	0	100	100
32	N5	601/603 (100%)	572 (95%)	29 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	N6	172/174 (99%)	163 (95%)	9 (5%)	0	100	100
34	S1	687/689 (100%)	659 (96%)	28 (4%)	0	100	100
35	S2	427/430 (99%)	412 (96%)	15 (4%)	0	100	100
36	S3	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
37	S4	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
38	S5	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
39	S6	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
40	S7	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
41	S8	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
42	V1	429/431 (100%)	409 (95%)	20 (5%)	0	100	100
43	V2	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
44	V3	40/42 (95%)	37 (92%)	3 (8%)	0	100	100
All	All	8152/8301 (98%)	7896 (97%)	256 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4L	85/85 (100%)	85 (100%)	0	100	100
2	A1	58/58 (100%)	58 (100%)	0	100	100
3	A2	76/76 (100%)	74 (97%)	2 (3%)	40	68
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%)	70	80
7	A7	87/97 (90%)	87 (100%)	0	100	100
8	A8	153/153 (100%)	152 (99%)	1 (1%)	76	82
9	A9	295/295 (100%)	294 (100%)	1 (0%)	86	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AB	71/80 (89%)	71 (100%)	0	100	100
10	AC	80/80 (100%)	79 (99%)	1 (1%)	61	77
11	AK	283/284 (100%)	280 (99%)	3 (1%)	65	78
12	AL	101/101 (100%)	100 (99%)	1 (1%)	68	79
13	AM	130/130 (100%)	128 (98%)	2 (2%)	57	75
14	AN	123/123 (100%)	123 (100%)	0	100	100
15	B1	53/53 (100%)	53 (100%)	0	100	100
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%)	98 (100%)	0	100	100
21	B7	112/112 (100%)	112 (100%)	0	100	100
22	B8	141/141 (100%)	140 (99%)	1 (1%)	76	82
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%)	45 (100%)	0	100	100
27	CB	108/108 (100%)	108 (100%)	0	100	100
28	N1	275/275 (100%)	273 (99%)	2 (1%)	76	82
29	N2	311/311 (100%)	308 (99%)	3 (1%)	68	79
30	N3	100/100 (100%)	98 (98%)	2 (2%)	48	72
31	N4	410/410 (100%)	406 (99%)	4 (1%)	68	79
32	N5	537/537 (100%)	536 (100%)	1 (0%)	87	89
33	N6	140/140 (100%)	139 (99%)	1 (1%)	76	82
34	S1	579/579 (100%)	575 (99%)	4 (1%)	76	82
35	S2	370/370 (100%)	367 (99%)	3 (1%)	73	81
36	S3	190/190 (100%)	189 (100%)	1 (0%)	81	85
37	S4	113/113 (100%)	112 (99%)	1 (1%)	70	80
38	S5	93/93 (100%)	92 (99%)	1 (1%)	65	78
39	S6	79/79 (100%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	S7	132/132 (100%)	130 (98%)	2 (2%)	57	75
41	S8	151/151 (100%)	151 (100%)	0	100	100
42	V1	344/344 (100%)	340 (99%)	4 (1%)	63	78
43	V2	183/183 (100%)	181 (99%)	2 (1%)	65	78
44	V3	41/41 (100%)	41 (100%)	0	100	100
All	All	7185/7230 (99%)	7141 (99%)	44 (1%)	76	83

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A2	23	LEU
3	A2	91	LEU
6	A6	41	THR
8	A8	235	LEU
9	A9	129	LEU
10	AC	112	SER
11	AK	38	LEU
11	AK	58	THR
11	AK	97	ASP
12	AL	115	CYS
13	AM	6	VAL
13	AM	78	ASP
22	B8	33	THR
28	N1	251	THR
28	N1	282	TYR
29	N2	139	LEU
29	N2	313	MET
29	N2	347	ASN
30	N3	63	LEU
30	N3	69	ILE
31	N4	8	THR
31	N4	122	PHE
31	N4	256	TYR
31	N4	303	ILE
32	N5	340	PHE
33	N6	126	VAL
34	S1	56	VAL
34	S1	379	THR
34	S1	555	ILE
34	S1	690	THR

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Mol	Chain	Res	Type
35	S2	145	LEU
35	S2	148	VAL
35	S2	415	VAL
36	S3	68	ILE
37	S4	51	GLN
38	S5	15	ASP
40	S7	66	THR
40	S7	71	CYS
42	V1	241	THR
42	V1	347	THR
42	V1	379	CYS
42	V1	385	CYS
43	V2	137	THR
43	V2	249	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	4L	52	HIS
1	4L	57	ASN
4	A3	156	GLN
5	A5	86	ASN
6	A6	152	HIS
8	A8	112	GLN
9	A9	37	HIS
9	A9	138	ASN
9	A9	154	GLN
9	A9	278	GLN
9	A9	295	HIS
10	AC	103	HIS
11	AK	67	ASN
11	AK	134	GLN
11	AK	346	ASN
12	AL	79	GLN
13	AM	12	GLN
13	AM	31	ASN
13	AM	54	GLN
14	AN	24	ASN
15	B1	6	GLN
15	B1	14	HIS
16	B2	60	GLN
17	B3	91	GLN

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Mol	Chain	Res	Type
18	B4	117	GLN
18	B4	123	GLN
19	B5	189	ASN
21	B7	50	GLN
21	B7	76	ASN
21	B7	85	HIS
23	B9	56	GLN
23	B9	104	GLN
23	B9	117	GLN
24	BK	134	GLN
24	BK	149	HIS
25	BL	86	ASN
25	BL	145	ASN
26	CA	73	ASN
27	CB	63	GLN
28	N1	99	ASN
29	N2	112	HIS
29	N2	273	ASN
29	N2	310	ASN
31	N4	81	GLN
31	N4	83	HIS
31	N4	251	ASN
31	N4	304	GLN
31	N4	333	ASN
31	N4	366	ASN
31	N4	415	GLN
31	N4	434	ASN
32	N5	23	ASN
32	N5	34	ASN
32	N5	136	ASN
32	N5	323	HIS
33	N6	46	ASN
34	S1	278	HIS
34	S1	282	ASN
34	S1	424	HIS
34	S1	604	GLN
35	S2	85	ASN
35	S2	93	GLN
35	S2	137	GLN
35	S2	239	HIS
35	S2	256	ASN
35	S2	460	GLN

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Mol	Chain	Res	Type
36	S3	75	GLN
36	S3	77	GLN
36	S3	247	GLN
37	S4	51	GLN
37	S4	92	ASN
37	S4	141	ASN
38	S5	98	HIS
40	S7	144	HIS
42	V1	168	ASN
42	V1	303	HIS
42	V1	381	GLN
42	V1	418	GLN
42	V1	441	HIS
43	V2	41	HIS
43	V2	182	ASN
43	V2	187	GLN
43	V2	246	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
35	2MR	S2	124	35	10,12,13	2.51	2 (20%)	5,13,15	0.94	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S2	124	2MR	CZ-NH2	5.34	1.44	1.33
35	S2	124	2MR	CZ-NE	5.22	1.45	1.34

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	C-CA-CB-CG
35	S2	124	2MR	CA-CB-CG-CD

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 62 ligands modelled in this entry, 2 are monoatomic - leaving 60 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
46	PC1	A3	201	-	49,49,53	0.30	0	55,57,61	0.47	0
48	PEE	S8	303	-	50,50,50	1.33	5 (10%)	53,55,55	1.18	6 (11%)
55	SF4	S7	301	40	0,12,12	-	-	-	-	-
48	PEE	N3	202	-	50,50,50	1.35	5 (10%)	53,55,55	1.20	6 (11%)
52	3PE	N5	706	-	45,45,50	0.32	0	48,50,55	0.31	0
55	SF4	V1	501	42	0,12,12	-	-	-	-	-
56	FES	V2	301	43	0,4,4	-	-	-	-	-
45	CDL	N5	703	-	88,88,99	0.31	0	94,100,111	0.33	0
48	PEE	A9	402	-	38,38,50	1.52	5 (13%)	41,43,55	1.24	5 (12%)
45	CDL	AL	201	-	93,93,99	0.31	0	99,105,111	0.36	0
51	PLX	N4	502	-	46,46,51	1.21	4 (8%)	48,54,59	0.88	1 (2%)
51	PLX	B1	101	-	51,51,51	1.15	4 (7%)	53,59,59	0.90	1 (1%)
48	PEE	B6	201	-	45,45,50	1.41	5 (11%)	48,50,55	1.18	5 (10%)
46	PC1	A3	202	-	53,53,53	0.29	0	59,61,61	0.28	0
48	PEE	N5	701	-	34,34,50	1.43	4 (11%)	37,39,55	1.18	3 (8%)
56	FES	S1	803	34	0,4,4	-	-	-	-	-
55	SF4	S1	802	34	0,12,12	-	-	-	-	-
45	CDL	AN	201	-	99,99,99	0.30	0	105,111,111	0.34	0
45	CDL	AL	203	-	70,70,99	0.36	0	76,82,111	0.49	0
49	ZMP	AC	201	10	30,35,36	0.71	1 (3%)	34,42,45	0.75	0
54	U10	N1	403	-	63,63,63	2.21	23 (36%)	78,79,79	1.68	22 (28%)
45	CDL	4L	201	-	91,91,99	0.32	0	97,103,111	0.38	0
51	PLX	N1	402	-	46,46,51	1.18	5 (10%)	48,54,59	0.89	1 (2%)
60	FMN	V1	502	-	33,33,33	0.24	0	48,50,50	0.37	0
51	PLX	N2	402	-	51,51,51	1.14	4 (7%)	53,59,59	0.91	1 (1%)
45	CDL	B4	201	-	79,79,99	0.32	0	85,91,111	0.32	0
45	CDL	B1	102	-	75,75,99	0.34	0	81,87,111	0.33	0
48	PEE	N5	702	-	39,39,50	1.50	5 (12%)	42,44,55	1.25	6 (14%)
51	PLX	CB	201	-	51,51,51	1.14	4 (7%)	53,59,59	0.91	1 (1%)
45	CDL	N2	401	-	67,67,99	0.36	0	73,79,111	0.39	0
46	PC1	N1	406	-	53,53,53	0.28	0	59,61,61	0.31	0
50	ADP	AK	401	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	10 (23%)
46	PC1	B5	202	-	53,53,53	0.28	0	59,61,61	0.29	0
45	CDL	N5	704	-	99,99,99	0.30	0	105,111,111	0.29	0
51	PLX	BL	202	-	51,51,51	1.14	4 (7%)	53,59,59	0.91	1 (1%)
52	3PE	CB	202	-	45,45,50	0.32	0	48,50,55	0.35	0
53	PX2	CA	101	-	35,35,35	0.98	4 (11%)	38,40,40	0.98	2 (5%)
48	PEE	N1	405	-	30,30,50	1.29	3 (10%)	33,35,55	1.17	2 (6%)
48	PEE	N5	705	-	50,50,50	1.34	5 (10%)	53,55,55	1.22	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CDL	B5	201	-	99,99,99	0.30	0	105,111,111	0.28	0
47	NDP	A9	401	-	51,52,52	0.33	0	71,80,80	0.34	0
55	SF4	S1	801	34	0,12,12	-	-	-		
46	PC1	B4	202	-	51,51,53	0.29	0	57,59,61	0.31	0
55	SF4	S8	301	41	0,12,12	-	-	-		
48	PEE	N1	404	-	50,50,50	1.34	5 (10%)	53,55,55	1.19	5 (9%)
45	CDL	N4	503	-	99,99,99	0.29	0	105,111,111	0.27	0
49	ZMP	AB	201	10	30,35,36	0.69	1 (3%)	34,42,45	0.72	0
46	PC1	N3	201	-	53,53,53	0.29	0	59,61,61	0.31	0
45	CDL	N1	401	-	77,77,99	0.33	0	83,89,111	0.38	0
48	PEE	N4	501	-	48,48,50	1.37	5 (10%)	51,53,55	1.21	4 (7%)
48	PEE	S2	501	-	47,47,50	1.37	5 (10%)	50,52,55	1.22	6 (12%)
48	PEE	AL	202	-	35,35,50	1.38	4 (11%)	38,40,55	1.12	4 (10%)
58	MF8	S2	502	-	7,8,8	1.00	0	8,10,10	1.46	1 (12%)
48	PEE	BL	201	-	50,50,50	1.36	5 (10%)	53,55,55	1.15	3 (5%)
46	PC1	N3	203	-	53,53,53	0.29	0	59,61,61	0.33	0
51	PLX	S7	302	-	51,51,51	1.14	4 (7%)	53,59,59	0.93	1 (1%)
46	PC1	B5	203	-	53,53,53	0.29	0	59,61,61	0.29	0
52	3PE	B8	201	-	31,31,50	0.38	0	34,36,55	0.40	0
55	SF4	S8	302	41	0,12,12	-	-	-		
45	CDL	AM	201	-	87,87,99	0.31	0	93,99,111	0.29	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
46	PC1	A3	201	-	-	13/53/53/57	-
48	PEE	S8	303	-	-	21/54/54/54	-
55	SF4	S7	301	40	-	-	0/6/5/5
48	PEE	N3	202	-	-	22/54/54/54	-
52	3PE	N5	706	-	-	8/49/49/54	-
55	SF4	V1	501	42	-	-	0/6/5/5
56	FES	V2	301	43	-	-	0/1/1/1
45	CDL	N5	703	-	-	27/99/99/110	-
48	PEE	A9	402	-	-	21/42/42/54	-
45	CDL	AL	201	-	-	27/104/104/110	-
51	PLX	N4	502	-	-	20/50/50/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	PLX	B1	101	-	-	20/55/55/55	-
48	PEE	B6	201	-	-	22/49/49/54	-
46	PC1	A3	202	-	-	16/57/57/57	-
48	PEE	N5	701	-	-	16/38/38/54	-
56	FES	S1	803	34	-	-	0/1/1/1
55	SF4	S1	802	34	-	-	0/6/5/5
45	CDL	AN	201	-	-	24/110/110/110	-
45	CDL	AL	203	-	-	19/81/81/110	-
49	ZMP	AC	201	10	-	16/40/42/43	-
54	U10	N1	403	-	-	15/63/87/87	0/1/1/1
45	CDL	4L	201	-	-	22/102/102/110	-
51	PLX	N1	402	-	-	19/50/50/55	-
60	FMN	V1	502	-	-	5/18/18/18	0/3/3/3
51	PLX	N2	402	-	-	19/55/55/55	-
45	CDL	B4	201	-	-	13/90/90/110	-
45	CDL	B1	102	-	-	18/86/86/110	-
48	PEE	N5	702	-	-	23/43/43/54	-
51	PLX	CB	201	-	-	23/55/55/55	-
45	CDL	N2	401	-	-	12/78/78/110	-
46	PC1	N1	406	-	-	9/57/57/57	-
50	ADP	AK	401	-	-	1/16/32/32	0/3/3/3
46	PC1	B5	202	-	-	13/57/57/57	-
45	CDL	N5	704	-	-	21/110/110/110	-
51	PLX	BL	202	-	-	13/55/55/55	-
52	3PE	CB	202	-	-	10/49/49/54	-
53	PX2	CA	101	-	-	21/37/37/37	-
48	PEE	N1	405	-	-	18/34/34/54	-
48	PEE	N5	705	-	-	20/54/54/54	-
45	CDL	B5	201	-	-	23/110/110/110	-
47	NDP	A9	401	-	-	8/34/77/77	0/5/5/5
55	SF4	S1	801	34	-	-	0/6/5/5
46	PC1	B4	202	-	-	7/55/55/57	-
55	SF4	S8	301	41	-	-	0/6/5/5
48	PEE	N1	404	-	-	25/54/54/54	-
45	CDL	N4	503	-	-	21/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	ZMP	AB	201	10	-	13/40/42/43	-
46	PC1	N3	201	-	-	15/57/57/57	-
45	CDL	N1	401	-	-	18/88/88/110	-
48	PEE	N4	501	-	-	32/52/52/54	-
48	PEE	S2	501	-	-	29/51/51/54	-
48	PEE	AL	202	-	-	20/39/39/54	-
58	MF8	S2	502	-	-	5/8/8/8	-
48	PEE	BL	201	-	-	21/54/54/54	-
46	PC1	N3	203	-	-	9/57/57/57	-
51	PLX	S7	302	-	-	25/55/55/55	-
46	PC1	B5	203	-	-	13/57/57/57	-
52	3PE	B8	201	-	-	15/35/35/54	-
55	SF4	S8	302	41	-	-	0/6/5/5
45	CDL	AM	201	-	-	18/98/98/110	-

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	N1	403	U10	C6-C1	10.43	1.53	1.35
54	N1	403	U10	C4-C3	4.87	1.53	1.36
50	AK	401	ADP	C5-C4	4.58	1.47	1.39
48	BL	201	PEE	C18-C19	4.17	1.55	1.31
48	N5	705	PEE	C18-C19	4.16	1.55	1.31
48	N3	202	PEE	C18-C19	4.15	1.55	1.31
48	N5	702	PEE	C18-C19	4.14	1.55	1.31
48	N5	701	PEE	C18-C19	4.14	1.55	1.31
48	A9	402	PEE	C18-C19	4.14	1.55	1.31
48	S8	303	PEE	C18-C19	4.13	1.55	1.31
48	N4	501	PEE	C18-C19	4.12	1.55	1.31
48	B6	201	PEE	C18-C19	4.12	1.55	1.31
48	N1	404	PEE	C18-C19	4.12	1.55	1.31
48	S2	501	PEE	C18-C19	4.11	1.55	1.31
48	N4	501	PEE	C39-C38	4.06	1.54	1.31
48	N1	404	PEE	C39-C38	4.05	1.54	1.31
48	N5	702	PEE	C39-C38	4.04	1.54	1.31
48	BL	201	PEE	C39-C38	4.04	1.54	1.31
48	B6	201	PEE	C39-C38	4.03	1.54	1.31
48	AL	202	PEE	C39-C38	4.03	1.54	1.31
48	N3	202	PEE	C39-C38	4.02	1.54	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	501	PEE	C39-C38	4.01	1.54	1.31
48	S8	303	PEE	C39-C38	4.00	1.54	1.31
48	N5	705	PEE	C39-C38	4.00	1.54	1.31
48	A9	402	PEE	C39-C38	3.95	1.54	1.29
48	BL	201	PEE	O3-C30	3.28	1.42	1.33
48	A9	402	PEE	O3-C30	3.28	1.42	1.33
48	B6	201	PEE	O3-C30	3.28	1.42	1.33
48	N1	404	PEE	O3-C30	3.28	1.42	1.33
48	S8	303	PEE	O3-C30	3.27	1.42	1.33
48	N3	202	PEE	O3-C30	3.24	1.42	1.33
48	N1	405	PEE	O3-C30	3.22	1.42	1.33
48	S2	501	PEE	O3-C30	3.21	1.42	1.33
48	AL	202	PEE	O3-C30	3.19	1.42	1.33
48	N5	701	PEE	O3-C30	3.19	1.42	1.33
51	N4	502	PLX	O6-C4	-3.17	1.40	1.44
48	N5	702	PEE	O3-C30	3.15	1.42	1.33
51	B1	101	PLX	O6-C4	-3.15	1.40	1.44
48	N4	501	PEE	O3-C30	3.14	1.42	1.33
51	S7	302	PLX	O6-C4	-3.14	1.40	1.44
51	CB	201	PLX	O6-C4	-3.13	1.40	1.44
48	N5	705	PEE	O3-C30	3.12	1.42	1.33
51	BL	202	PLX	O6-C4	-3.06	1.40	1.44
51	N2	402	PLX	O6-C4	-3.03	1.40	1.44
51	N1	402	PLX	O6-C4	-3.02	1.40	1.44
54	N1	403	U10	C41-C39	2.97	1.57	1.51
48	N5	702	PEE	O2-C10	2.84	1.42	1.34
54	N1	403	U10	C31-C29	2.80	1.57	1.51
48	N4	501	PEE	O2-C2	-2.77	1.40	1.46
54	N1	403	U10	C7-C8	2.75	1.54	1.50
48	N3	202	PEE	O2-C10	2.73	1.42	1.34
48	S8	303	PEE	O2-C10	2.72	1.42	1.34
48	N5	705	PEE	O2-C2	-2.72	1.40	1.46
50	AK	401	ADP	C5-C6	2.70	1.48	1.41
49	AC	201	ZMP	C9-C10	-2.69	1.48	1.50
48	AL	202	PEE	O2-C2	-2.69	1.40	1.46
48	A9	402	PEE	O2-C10	2.69	1.41	1.34
48	S2	501	PEE	O2-C2	-2.68	1.40	1.46
48	BL	201	PEE	O2-C10	2.68	1.41	1.34
48	N1	405	PEE	O2-C2	-2.68	1.40	1.46
48	B6	201	PEE	O2-C2	-2.66	1.40	1.46
48	N5	701	PEE	O2-C10	2.65	1.41	1.34
48	N1	404	PEE	O2-C2	-2.65	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	N1	403	U10	C26-C24	2.65	1.56	1.51
48	N5	705	PEE	O2-C10	2.63	1.41	1.34
48	N1	404	PEE	O2-C10	2.63	1.41	1.34
48	B6	201	PEE	O2-C10	2.63	1.41	1.34
48	N5	701	PEE	O2-C2	-2.62	1.40	1.46
48	N4	501	PEE	O2-C10	2.61	1.41	1.34
48	AL	202	PEE	O2-C10	2.60	1.41	1.34
48	N1	405	PEE	O2-C10	2.58	1.41	1.34
48	S2	501	PEE	O2-C10	2.58	1.41	1.34
48	BL	201	PEE	O2-C2	-2.57	1.40	1.46
54	N1	403	U10	C21-C19	2.56	1.56	1.51
48	A9	402	PEE	O2-C2	-2.55	1.40	1.46
48	N3	202	PEE	O2-C2	-2.55	1.40	1.46
49	AB	201	ZMP	C9-C10	-2.54	1.48	1.50
54	N1	403	U10	C36-C34	2.44	1.56	1.51
53	CA	101	PX2	O7-C2	-2.42	1.40	1.46
54	N1	403	U10	C46-C44	2.42	1.56	1.51
54	N1	403	U10	C11-C9	2.41	1.56	1.51
48	S8	303	PEE	O2-C2	-2.41	1.40	1.46
54	N1	403	U10	C6-C5	2.39	1.53	1.46
53	CA	101	PX2	O5-C4	2.38	1.40	1.33
54	N1	403	U10	C51-C49	2.37	1.56	1.51
54	N1	403	U10	O5-C5	-2.36	1.18	1.23
54	N1	403	U10	C7-C6	2.33	1.55	1.51
54	N1	403	U10	O3-C3M	-2.32	1.40	1.45
48	N5	702	PEE	O2-C2	-2.29	1.41	1.46
50	AK	401	ADP	C8-N7	2.29	1.36	1.31
50	AK	401	ADP	C5-N7	-2.28	1.34	1.39
54	N1	403	U10	C22-C23	2.27	1.57	1.50
54	N1	403	U10	C27-C28	2.26	1.57	1.50
54	N1	403	U10	O2-C2	-2.25	1.18	1.23
53	CA	101	PX2	O7-C16	2.22	1.40	1.34
51	BL	202	PLX	C1B-N1	-2.20	1.43	1.50
54	N1	403	U10	C42-C43	2.19	1.57	1.50
51	N4	502	PLX	C1B-N1	-2.18	1.43	1.50
51	B1	101	PLX	C1B-N1	-2.17	1.43	1.50
54	N1	403	U10	C32-C33	2.16	1.57	1.50
54	N1	403	U10	C12-C13	2.15	1.57	1.50
51	CB	201	PLX	C1B-N1	-2.15	1.43	1.50
51	N2	402	PLX	C1B-N1	-2.14	1.43	1.50
51	S7	302	PLX	C1B-N1	-2.14	1.43	1.50
51	N4	502	PLX	P1-O4	2.13	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	N1	402	PLX	C1B-N1	-2.13	1.43	1.50
54	N1	403	U10	C16-C14	2.10	1.55	1.51
51	N2	402	PLX	P1-O4	2.09	1.67	1.59
53	CA	101	PX2	O5-C3	-2.09	1.40	1.45
54	N1	403	U10	O4-C4M	-2.09	1.40	1.45
51	B1	101	PLX	P1-O4	2.09	1.67	1.59
51	BL	202	PLX	C1A-N1	-2.08	1.44	1.50
51	N1	402	PLX	P1-O4	2.08	1.67	1.59
51	N2	402	PLX	C1A-N1	-2.07	1.44	1.50
51	B1	101	PLX	C1A-N1	-2.06	1.44	1.50
51	N4	502	PLX	C1A-N1	-2.06	1.44	1.50
51	CB	201	PLX	P1-O4	2.06	1.67	1.59
51	S7	302	PLX	C1A-N1	-2.05	1.44	1.50
51	S7	302	PLX	P1-O4	2.05	1.67	1.59
51	CB	201	PLX	C1A-N1	-2.04	1.44	1.50
51	N1	402	PLX	C1A-N1	-2.03	1.44	1.50
51	N1	402	PLX	C7-C6	2.03	1.55	1.50
51	BL	202	PLX	P1-O4	2.00	1.67	1.59

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	AK	401	ADP	C5-C4-N3	-5.73	118.82	126.72
50	AK	401	ADP	N3-C4-N9	4.61	135.00	127.17
48	N3	202	PEE	O2-C10-C11	4.26	120.69	111.48
48	N5	705	PEE	O2-C10-C11	4.17	120.49	111.48
48	A9	402	PEE	O2-C10-C11	4.09	120.34	111.48
48	N1	404	PEE	O2-C10-C11	4.06	120.27	111.48
48	S8	303	PEE	O2-C10-C11	4.02	120.17	111.48
48	BL	201	PEE	O2-C10-C11	3.99	120.12	111.48
48	S2	501	PEE	O2-C10-C11	3.95	120.03	111.48
48	N4	501	PEE	O2-C10-C11	3.95	120.02	111.48
48	N1	405	PEE	O2-C10-C11	3.91	119.93	111.48
54	N1	403	U10	C7-C8-C9	-3.82	120.26	126.83
48	B6	201	PEE	O2-C10-C11	3.81	119.72	111.48
48	N5	701	PEE	O2-C10-C11	3.76	119.61	111.48
50	AK	401	ADP	C2-N3-C4	3.73	120.93	111.83
48	N5	702	PEE	O2-C10-C11	3.71	119.51	111.48
53	CA	101	PX2	O7-C16-C17	3.69	119.47	111.48
54	N1	403	U10	C37-C38-C39	-3.47	119.69	127.62
50	AK	401	ADP	C4-C5-N7	-3.40	106.70	110.58
50	AK	401	ADP	N3-C2-N1	-3.32	123.55	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	N1	403	U10	C20-C19-C21	3.23	120.83	115.23
58	S2	502	MF8	N06-C04-N02	-3.22	112.58	117.44
54	N1	403	U10	C30-C29-C31	3.18	120.75	115.23
54	N1	403	U10	C10-C9-C11	3.09	120.59	115.23
54	N1	403	U10	C42-C43-C44	-3.08	120.58	127.62
54	N1	403	U10	C47-C48-C49	-2.99	120.78	127.62
54	N1	403	U10	C35-C34-C36	2.94	120.34	115.23
54	N1	403	U10	C32-C33-C34	-2.94	120.89	127.62
53	CA	101	PX2	O5-C4-C5	2.87	120.57	111.83
48	S8	303	PEE	O3-C30-C31	2.84	120.50	111.83
48	N5	702	PEE	C20-C19-C18	-2.84	109.35	126.42
50	AK	401	ADP	C4-N9-C8	2.82	108.70	105.74
48	A9	402	PEE	O3-C30-C31	2.80	120.37	111.83
54	N1	403	U10	C45-C44-C46	2.78	120.06	115.23
54	N1	403	U10	C40-C39-C41	2.78	120.05	115.23
54	N1	403	U10	C17-C18-C19	-2.70	121.44	127.62
48	N5	701	PEE	O3-C30-C31	2.70	120.06	111.83
48	S2	501	PEE	O3-C30-C31	2.68	120.01	111.83
48	BL	201	PEE	O3-C30-C31	2.68	120.00	111.83
48	N1	405	PEE	O3-C30-C31	2.67	119.99	111.83
48	B6	201	PEE	O3-C30-C31	2.67	119.96	111.83
48	N3	202	PEE	O3-C30-C31	2.65	119.93	111.83
48	N1	404	PEE	O3-C30-C31	2.64	119.89	111.83
54	N1	403	U10	C50-C49-C51	2.64	119.81	115.23
54	N1	403	U10	C7-C6-C1	-2.61	120.41	124.89
48	N4	501	PEE	O3-C30-C31	2.60	119.78	111.83
48	N5	705	PEE	O3-C30-C31	2.57	119.67	111.83
48	N5	702	PEE	O3-C30-C31	2.57	119.67	111.83
54	N1	403	U10	C12-C13-C14	-2.57	121.75	127.62
54	N1	403	U10	C1M-C1-C6	-2.57	120.23	124.45
48	AL	202	PEE	O3-C30-C31	2.54	119.59	111.83
50	AK	401	ADP	C5-N7-C8	2.52	107.41	103.45
48	AL	202	PEE	O2-C10-C11	2.52	120.17	110.93
51	N4	502	PLX	O3-P1-O2	-2.47	100.97	112.44
51	CB	201	PLX	O3-P1-O2	-2.43	101.16	112.44
51	N2	402	PLX	O3-P1-O2	-2.42	101.19	112.44
54	N1	403	U10	C15-C14-C16	2.42	119.43	115.23
54	N1	403	U10	C22-C23-C24	-2.40	122.14	127.62
51	N1	402	PLX	O3-P1-O2	-2.39	101.31	112.44
51	S7	302	PLX	O3-P1-O2	-2.39	101.33	112.44
51	BL	202	PLX	O3-P1-O2	-2.37	101.44	112.44
51	B1	101	PLX	O3-P1-O2	-2.36	101.45	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	N1	403	U10	C25-C24-C26	2.35	119.31	115.23
48	A9	402	PEE	C37-C38-C39	-2.35	109.52	126.65
54	N1	403	U10	C56-C54-C55	2.30	119.87	114.59
54	N1	403	U10	C30-C29-C28	-2.29	117.73	123.63
54	N1	403	U10	C52-C53-C54	-2.21	120.28	127.64
50	AK	401	ADP	C6-C5-N7	2.12	136.18	132.09
48	B6	201	PEE	C40-C39-C38	-2.12	108.94	124.83
48	S8	303	PEE	C37-C38-C39	-2.12	108.94	124.83
48	S2	501	PEE	C17-C18-C19	-2.12	108.98	124.83
48	N4	501	PEE	C17-C18-C19	-2.12	108.98	124.83
48	N5	705	PEE	C40-C39-C38	-2.12	108.99	124.83
48	N5	705	PEE	C37-C38-C39	-2.11	109.04	124.83
48	N1	404	PEE	C20-C19-C18	-2.10	109.09	124.83
48	S8	303	PEE	C17-C18-C19	-2.10	109.09	124.83
48	S8	303	PEE	C40-C39-C38	-2.10	109.13	124.83
48	N5	701	PEE	C20-C19-C18	-2.09	109.14	124.83
48	BL	201	PEE	C37-C38-C39	-2.09	109.20	124.83
48	N3	202	PEE	C37-C38-C39	-2.09	109.21	124.83
48	S2	501	PEE	C37-C38-C39	-2.07	109.33	124.83
48	N5	702	PEE	C40-C39-C38	-2.07	109.33	124.83
48	B6	201	PEE	C20-C19-C18	-2.06	109.37	124.83
50	AK	401	ADP	N9-C8-N7	-2.06	111.02	113.94
48	AL	202	PEE	C37-C38-C39	-2.06	109.43	124.83
48	N3	202	PEE	C17-C18-C19	-2.05	109.47	124.83
48	N3	202	PEE	C40-C39-C38	-2.05	109.50	124.83
48	N5	702	PEE	C17-C18-C19	-2.04	109.56	124.83
48	N4	501	PEE	C37-C38-C39	-2.04	109.57	124.83
48	S8	303	PEE	C20-C19-C18	-2.03	109.59	124.83
48	N1	404	PEE	C17-C18-C19	-2.03	109.61	124.83
48	AL	202	PEE	C40-C39-C38	-2.03	109.64	124.83
48	N5	702	PEE	C37-C38-C39	-2.03	109.64	124.83
48	S2	501	PEE	C40-C39-C38	-2.03	109.64	124.83
48	S2	501	PEE	C20-C19-C18	-2.02	109.67	124.83
48	N1	404	PEE	C40-C39-C38	-2.02	109.70	124.83
48	A9	402	PEE	C20-C19-C18	-2.02	109.71	124.83
48	N3	202	PEE	C20-C19-C18	-2.02	109.73	124.83
50	AK	401	ADP	C3'-C2'-C1'	2.01	105.27	101.46
48	B6	201	PEE	C17-C18-C19	-2.01	109.81	124.83
48	N5	705	PEE	C17-C18-C19	-2.00	109.84	124.83
48	A9	402	PEE	C17-C18-C19	-2.00	109.85	124.83

There are no chirality outliers.

All (904) 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-OA5
45	4L	201	CDL	CA3-OA5-PA1-OA3
45	4L	201	CDL	CB2-OB2-PB2-OB3
45	4L	201	CDL	CB2-OB2-PB2-OB4
45	4L	201	CDL	CB2-OB2-PB2-OB5
45	AL	201	CDL	CA2-OA2-PA1-OA3
45	AL	201	CDL	CA2-OA2-PA1-OA5
45	AL	201	CDL	CB2-OB2-PB2-OB3
45	AL	201	CDL	CB2-OB2-PB2-OB5
45	AL	203	CDL	CB2-C1-CA2-OA2
45	AM	201	CDL	CA3-OA5-PA1-OA2
45	AM	201	CDL	CA3-OA5-PA1-OA3
45	AM	201	CDL	CB3-OB5-PB2-OB2
45	AM	201	CDL	CB3-OB5-PB2-OB3
45	AN	201	CDL	CA2-OA2-PA1-OA4
45	AN	201	CDL	CA2-OA2-PA1-OA5
45	AN	201	CDL	CA3-OA5-PA1-OA2
45	AN	201	CDL	CA3-OA5-PA1-OA4
45	AN	201	CDL	CB3-OB5-PB2-OB2
45	AN	201	CDL	CB3-OB5-PB2-OB3
45	AN	201	CDL	CB3-OB5-PB2-OB4
45	B1	102	CDL	CA3-OA5-PA1-OA2
45	B1	102	CDL	CA3-OA5-PA1-OA3
45	B1	102	CDL	CA3-OA5-PA1-OA4
45	B1	102	CDL	CB3-OB5-PB2-OB2
45	B1	102	CDL	CB3-OB5-PB2-OB4
45	B4	201	CDL	CA2-OA2-PA1-OA4
45	B4	201	CDL	CA2-OA2-PA1-OA5
45	B4	201	CDL	CB3-OB5-PB2-OB2
45	B4	201	CDL	CB3-OB5-PB2-OB3
45	B4	201	CDL	CB3-OB5-PB2-OB4
45	B5	201	CDL	CA2-OA2-PA1-OA3
45	B5	201	CDL	CA2-OA2-PA1-OA4
45	B5	201	CDL	CA2-OA2-PA1-OA5
45	B5	201	CDL	CA3-OA5-PA1-OA2
45	B5	201	CDL	CB2-OB2-PB2-OB3
45	B5	201	CDL	CB2-OB2-PB2-OB5
45	B5	201	CDL	CB3-OB5-PB2-OB2
45	B5	201	CDL	CB3-OB5-PB2-OB3
45	B5	201	CDL	CB3-OB5-PB2-OB4
45	N1	401	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
45	N1	401	CDL	CA3-OA5-PA1-OA2
45	N1	401	CDL	CA3-OA5-PA1-OA3
45	N1	401	CDL	CB2-OB2-PB2-OB3
45	N2	401	CDL	CA3-OA5-PA1-OA2
45	N2	401	CDL	CA3-OA5-PA1-OA4
45	N4	503	CDL	CA2-OA2-PA1-OA4
45	N4	503	CDL	CA2-OA2-PA1-OA5
45	N4	503	CDL	CB2-OB2-PB2-OB4
45	N4	503	CDL	CB2-OB2-PB2-OB5
45	N4	503	CDL	CB3-OB5-PB2-OB2
45	N4	503	CDL	CB3-OB5-PB2-OB4
45	N5	703	CDL	CA2-OA2-PA1-OA3
45	N5	703	CDL	CA2-OA2-PA1-OA5
45	N5	703	CDL	CA3-OA5-PA1-OA2
45	N5	703	CDL	CA3-OA5-PA1-OA3
45	N5	703	CDL	CA3-OA5-PA1-OA4
45	N5	703	CDL	CB2-OB2-PB2-OB3
45	N5	703	CDL	CB2-OB2-PB2-OB4
45	N5	703	CDL	CB2-OB2-PB2-OB5
45	N5	703	CDL	CB3-OB5-PB2-OB2
45	N5	703	CDL	CB3-OB5-PB2-OB3
45	N5	704	CDL	CA3-OA5-PA1-OA2
45	N5	704	CDL	CA3-OA5-PA1-OA4
45	N5	704	CDL	CB3-OB5-PB2-OB2
45	N5	704	CDL	CB3-OB5-PB2-OB3
45	N5	704	CDL	CB3-OB5-PB2-OB4
46	A3	201	PC1	C1-O11-P-O12
46	A3	201	PC1	C1-O11-P-O14
46	A3	201	PC1	C1-O11-P-O13
46	A3	201	PC1	O21-C2-C3-O31
46	A3	202	PC1	C11-O13-P-O12
46	A3	202	PC1	C11-O13-P-O14
46	A3	202	PC1	C11-O13-P-O11
46	A3	202	PC1	C1-O11-P-O12
46	B4	202	PC1	C1-O11-P-O12
46	B4	202	PC1	C1-O11-P-O14
46	B4	202	PC1	C1-O11-P-O13
46	B5	202	PC1	C11-O13-P-O12
46	B5	202	PC1	C11-O13-P-O14
46	B5	202	PC1	C11-O13-P-O11
46	B5	203	PC1	C11-O13-P-O14
46	B5	203	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
46	B5	203	PC1	C1-O11-P-O14
46	B5	203	PC1	C1-O11-P-O13
46	N1	406	PC1	C11-O13-P-O14
46	N1	406	PC1	C11-O13-P-O11
46	N3	201	PC1	C11-O13-P-O11
46	N3	201	PC1	C1-O11-P-O12
46	N3	201	PC1	C1-O11-P-O14
46	N3	203	PC1	C11-O13-P-O14
46	N3	203	PC1	C11-O13-P-O11
46	N3	203	PC1	C1-O11-P-O12
47	A9	401	NDP	C5D-O5D-PN-O3
47	A9	401	NDP	C5D-O5D-PN-O1N
48	A9	402	PEE	C11-C10-O2-C2
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	C4-O4P-P-O3P
48	AL	202	PEE	C4-O4P-P-O2P
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	BL	201	PEE	O4-C10-O2-C2
48	BL	201	PEE	C1-O3P-P-O4P
48	BL	201	PEE	C4-O4P-P-O3P
48	BL	201	PEE	C4-O4P-P-O2P
48	BL	201	PEE	C4-O4P-P-O1P
48	N1	404	PEE	C1-O3P-P-O2P
48	N1	405	PEE	C1-O3P-P-O2P
48	N1	405	PEE	C1-O3P-P-O1P
48	N1	405	PEE	C1-O3P-P-O4P
48	N3	202	PEE	C11-C10-O2-C2
48	N3	202	PEE	O4-C10-O2-C2
48	N3	202	PEE	C1-O3P-P-O2P
48	N3	202	PEE	C1-O3P-P-O1P
48	N3	202	PEE	C1-O3P-P-O4P
48	N3	202	PEE	C31-C30-O3-C3
48	N5	701	PEE	C11-C10-O2-C2
48	N5	701	PEE	O4-C10-O2-C2
48	N5	701	PEE	C4-O4P-P-O3P
48	N5	701	PEE	C4-O4P-P-O2P
48	N5	702	PEE	C1-O3P-P-O2P
48	N5	705	PEE	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
48	N5	705	PEE	C37-C38-C39-C40
48	S2	501	PEE	C1-O3P-P-O2P
48	S2	501	PEE	C1-O3P-P-O1P
48	S2	501	PEE	C4-O4P-P-O3P
48	S2	501	PEE	C4-O4P-P-O2P
48	S2	501	PEE	C4-O4P-P-O1P
48	S8	303	PEE	C4-O4P-P-O3P
48	S8	303	PEE	C4-O4P-P-O2P
48	S8	303	PEE	C4-O4P-P-O1P
49	AB	201	ZMP	C12-C11-S1-C10
49	AC	201	ZMP	C20-C18-C21-O5
49	AC	201	ZMP	C17-C18-C21-O5
49	AC	201	ZMP	S1-C11-C12-N1
49	AC	201	ZMP	C7-C8-C9-C10
51	B1	101	PLX	O7-C6-O6-C4
51	B1	101	PLX	C3-C4-O6-C6
51	B1	101	PLX	C2-O1-P1-O2
51	BL	202	PLX	C2-O1-P1-O4
51	BL	202	PLX	C2-O1-P1-O2
51	CB	201	PLX	O7-C6-C7-C8
51	CB	201	PLX	O7-C6-O6-C4
51	CB	201	PLX	C2-O1-P1-O4
51	CB	201	PLX	C2-O1-P1-O2
51	CB	201	PLX	C2-O1-P1-O3
51	CB	201	PLX	N1-C1-C2-O1
51	CB	201	PLX	C25-C24-O8-C5
51	N1	402	PLX	O7-C6-O6-C4
51	N1	402	PLX	C3-O4-P1-O1
51	N1	402	PLX	C3-O4-P1-O2
51	N1	402	PLX	C3-O4-P1-O3
51	N1	402	PLX	C2-O1-P1-O4
51	N1	402	PLX	C2-O1-P1-O2
51	N1	402	PLX	N1-C1-C2-O1
51	N1	402	PLX	O9-C24-O8-C5
51	N2	402	PLX	O9-C24-O8-C5
51	N4	502	PLX	O6-C4-C5-O8
51	N4	502	PLX	N1-C1-C2-O1
51	S7	302	PLX	O4-C3-C4-O6
51	S7	302	PLX	C3-O4-P1-O1
51	S7	302	PLX	C3-O4-P1-O3
51	S7	302	PLX	C2-O1-P1-O4
51	S7	302	PLX	C2-O1-P1-O3

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Mol	Chain	Res	Type	Atoms
51	S7	302	PLX	O9-C24-C25-C26
52	B8	201	3PE	C1-O11-P-O12
52	B8	201	3PE	C1-O11-P-O14
52	B8	201	3PE	C11-O13-P-O11
52	B8	201	3PE	C11-O13-P-O12
52	B8	201	3PE	C11-O13-P-O14
52	B8	201	3PE	O13-C11-C12-N
52	CB	202	3PE	C1-O11-P-O12
52	CB	202	3PE	C1-O11-P-O13
52	CB	202	3PE	C11-O13-P-O11
52	N5	706	3PE	O13-C11-C12-N
53	CA	101	PX2	C1-O4-P1-O1
53	CA	101	PX2	C1-O4-P1-O3
54	N1	403	U10	C19-C21-C22-C23
60	V1	502	FMN	N10-C1'-C2'-O2'
60	V1	502	FMN	C5'-O5'-P-O2P
60	V1	502	FMN	C5'-O5'-P-O3P
48	N1	405	PEE	O5-C30-O3-C3
48	N3	202	PEE	O5-C30-O3-C3
48	N4	501	PEE	O5-C30-O3-C3
53	CA	101	PX2	O6-C4-O5-C3
48	N1	405	PEE	C31-C30-O3-C3
48	N4	501	PEE	C31-C30-O3-C3
53	CA	101	PX2	C5-C4-O5-C3
48	A9	402	PEE	O5-C30-O3-C3
48	AL	202	PEE	O5-C30-O3-C3
48	N5	701	PEE	O5-C30-O3-C3
48	N5	702	PEE	O5-C30-O3-C3
48	S2	501	PEE	O5-C30-O3-C3
48	A9	402	PEE	O4-C10-O2-C2
48	A9	402	PEE	C31-C30-O3-C3
48	AL	202	PEE	C31-C30-O3-C3
48	N5	701	PEE	C31-C30-O3-C3
48	N5	702	PEE	C31-C30-O3-C3
48	BL	201	PEE	C11-C10-O2-C2
54	N1	403	U10	C20-C19-C21-C22
54	N1	403	U10	C35-C34-C36-C37
54	N1	403	U10	C33-C34-C36-C37
48	S2	501	PEE	C31-C30-O3-C3
48	A9	402	PEE	C17-C18-C19-C20
48	N5	705	PEE	C17-C18-C19-C20
48	S2	501	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
48	S8	303	PEE	O4-C10-O2-C2
45	AL	203	CDL	O1-C1-CA2-OA2
48	S8	303	PEE	C11-C10-O2-C2
54	N1	403	U10	C18-C19-C21-C22
48	BL	201	PEE	C31-C30-O3-C3
48	B6	201	PEE	C17-C18-C19-C20
48	BL	201	PEE	C17-C18-C19-C20
48	N1	404	PEE	C17-C18-C19-C20
48	N4	501	PEE	C17-C18-C19-C20
46	B5	203	PC1	C11-C12-N-C15
45	B4	201	CDL	CA7-C31-C32-C33
48	N5	701	PEE	C10-C11-C12-C13
45	N1	401	CDL	OB5-CB3-CB4-OB6
53	CA	101	PX2	C17-C16-O7-C2
48	N1	404	PEE	O2-C2-C3-O3
52	N5	706	3PE	O21-C2-C3-O31
48	N4	501	PEE	C10-C11-C12-C13
48	B6	201	PEE	C30-C31-C32-C33
54	N1	403	U10	C49-C51-C52-C53
46	B5	202	PC1	C11-C12-N-C15
46	B5	203	PC1	C11-C12-N-C13
48	N4	501	PEE	C14-C15-C16-C17
45	AL	203	CDL	CB7-C71-C72-C73
48	A9	402	PEE	C10-C11-C12-C13
48	N3	202	PEE	C10-C11-C12-C13
48	AL	202	PEE	C11-C10-O2-C2
48	BL	201	PEE	C2-C1-O3P-P
48	BL	201	PEE	C30-C31-C32-C33
48	N3	202	PEE	C30-C31-C32-C33
48	BL	201	PEE	O5-C30-O3-C3
48	N1	405	PEE	C10-C11-C12-C13
48	S8	303	PEE	C31-C30-O3-C3
48	N3	202	PEE	C12-C13-C14-C15
48	AL	202	PEE	O4-C10-O2-C2
53	CA	101	PX2	O8-C16-O7-C2
48	N5	705	PEE	C31-C30-O3-C3
51	CB	201	PLX	O6-C6-C7-C8
48	N5	702	PEE	C11-C10-O2-C2
48	N5	702	PEE	O4-C10-O2-C2
52	CB	202	3PE	C21-C22-C23-C24
48	B6	201	PEE	C33-C34-C35-C36
49	AC	201	ZMP	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
48	N4	501	PEE	O3P-C1-C2-O2
48	S8	303	PEE	C22-C23-C24-C25
46	N1	406	PC1	C11-C12-N-C14
48	N5	702	PEE	C10-C11-C12-C13
48	S8	303	PEE	O5-C30-O3-C3
48	BL	201	PEE	C12-C13-C14-C15
45	AL	203	CDL	C34-C35-C36-C37
46	A3	201	PC1	C28-C29-C2A-C2B
51	N4	502	PLX	C30-C31-C32-C33
51	N4	502	PLX	C32-C33-C34-C35
46	N3	201	PC1	C32-C33-C34-C35
48	B6	201	PEE	C21-C22-C23-C24
51	B1	101	PLX	O9-C24-C25-C26
51	CB	201	PLX	O9-C24-C25-C26
51	N4	502	PLX	O7-C6-C7-C8
51	N4	502	PLX	O9-C24-C25-C26
48	N4	501	PEE	C23-C24-C25-C26
51	CB	201	PLX	C31-C32-C33-C34
48	N5	702	PEE	C12-C13-C14-C15
51	BL	202	PLX	C33-C34-C35-C36
48	S8	303	PEE	C10-C11-C12-C13
48	N1	404	PEE	C32-C33-C34-C35
48	N5	701	PEE	C11-C12-C13-C14
51	B1	101	PLX	C34-C35-C36-C37
48	S2	501	PEE	C11-C10-O2-C2
48	N1	405	PEE	C11-C12-C13-C14
51	N2	402	PLX	C13-C14-C15-C16
51	N1	402	PLX	C11-C10-C9-C8
48	BL	201	PEE	C11-C12-C13-C14
48	S2	501	PEE	C33-C34-C35-C36
49	AC	201	ZMP	C1-C22-C23-C24
51	CB	201	PLX	C33-C34-C35-C36
48	S8	303	PEE	C21-C22-C23-C24
48	N1	405	PEE	C33-C34-C35-C36
48	N1	404	PEE	C33-C34-C35-C36
48	N1	405	PEE	C31-C32-C33-C34
48	S8	303	PEE	C14-C15-C16-C17
48	N5	702	PEE	C30-C31-C32-C33
51	N1	402	PLX	C29-C30-C31-C32
48	N5	705	PEE	O5-C30-O3-C3
46	B5	202	PC1	C11-C12-N-C14
46	B5	203	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
48	AL	202	PEE	C31-C32-C33-C34
48	S2	501	PEE	C12-C13-C14-C15
48	B6	201	PEE	C11-C10-O2-C2
48	N5	705	PEE	C35-C36-C37-C38
51	CB	201	PLX	C18-C19-C20-C21
48	N1	404	PEE	C30-C31-C32-C33
48	S2	501	PEE	C30-C31-C32-C33
48	N3	202	PEE	C21-C22-C23-C24
51	N1	402	PLX	C15-C16-C17-C18
48	S8	303	PEE	C33-C34-C35-C36
49	AC	201	ZMP	C2-C3-C4-C5
45	B1	102	CDL	C11-C12-C13-C14
48	S8	303	PEE	C12-C13-C14-C15
45	N5	703	CDL	C42-C43-C44-C45
48	N3	202	PEE	C33-C34-C35-C36
49	AB	201	ZMP	C4-C5-C6-C7
51	N4	502	PLX	C29-C30-C31-C32
48	AL	202	PEE	C43-C44-C45-C46
48	N5	702	PEE	C18-C19-C20-C21
51	BL	202	PLX	C9-C10-C11-C12
51	N4	502	PLX	C27-C28-C29-C30
51	S7	302	PLX	C34-C35-C36-C37
48	B6	201	PEE	C31-C30-O3-C3
49	AC	201	ZMP	C22-C23-C24-C25
48	N4	501	PEE	C11-C10-O2-C2
45	N2	401	CDL	CA5-C11-C12-C13
48	S2	501	PEE	O4-C10-O2-C2
48	BL	201	PEE	C21-C22-C23-C24
48	N4	501	PEE	C15-C16-C17-C18
48	N4	501	PEE	C35-C36-C37-C38
48	N5	702	PEE	C35-C36-C37-C38
48	N5	702	PEE	C33-C34-C35-C36
51	B1	101	PLX	C29-C30-C31-C32
51	CB	201	PLX	C14-C15-C16-C17
51	BL	202	PLX	C32-C33-C34-C35
46	B5	202	PC1	C11-C12-N-C13
46	N1	406	PC1	C11-C12-N-C13
46	N1	406	PC1	C11-C12-N-C15
45	B1	102	CDL	C52-C53-C54-C55
48	N1	404	PEE	C41-C42-C43-C44
51	S7	302	PLX	C12-C13-C14-C15
45	N5	703	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
48	S8	303	PEE	C34-C35-C36-C37
46	B4	202	PC1	C25-C26-C27-C28
49	AB	201	ZMP	C6-C7-C8-C9
48	N5	702	PEE	C32-C33-C34-C35
53	CA	101	PX2	C6-C7-C8-C9
54	N1	403	U10	C9-C11-C12-C13
49	AC	201	ZMP	C14-C15-N2-C16
49	AC	201	ZMP	C22-C1-C2-C3
48	B6	201	PEE	C15-C16-C17-C18
51	N1	402	PLX	O6-C4-C5-O8
48	BL	201	PEE	C20-C21-C22-C23
46	A3	202	PC1	C2C-C2D-C2E-C2F
49	AB	201	ZMP	C5-C6-C7-C8
45	N5	703	CDL	C21-C22-C23-C24
48	B6	201	PEE	C32-C33-C34-C35
48	BL	201	PEE	C33-C34-C35-C36
48	S2	501	PEE	C38-C39-C40-C41
51	N1	402	PLX	C25-C26-C27-C28
45	B5	201	CDL	C19-C20-C21-C22
48	A9	402	PEE	C34-C35-C36-C37
48	N5	705	PEE	C33-C34-C35-C36
45	N5	704	CDL	C59-C60-C61-C62
45	N5	703	CDL	CB5-C51-C52-C53
48	A9	402	PEE	C30-C31-C32-C33
48	N4	501	PEE	O4-C10-O2-C2
52	CB	202	3PE	C29-C2A-C2B-C2C
48	AL	202	PEE	C40-C41-C42-C43
48	N1	404	PEE	C21-C22-C23-C24
45	AN	201	CDL	C79-C80-C81-C82
45	N1	401	CDL	C52-C53-C54-C55
45	N5	704	CDL	C33-C34-C35-C36
48	AL	202	PEE	C41-C42-C43-C44
45	B5	201	CDL	C51-C52-C53-C54
49	AB	201	ZMP	O3-C16-C17-O4
48	A9	402	PEE	C33-C34-C35-C36
48	A9	402	PEE	C35-C36-C37-C38
48	BL	201	PEE	C35-C36-C37-C38
48	N3	202	PEE	C35-C36-C37-C38
48	N5	701	PEE	C15-C16-C17-C18
48	N5	705	PEE	C15-C16-C17-C18
45	AL	201	CDL	OB5-CB3-CB4-CB6
45	AL	203	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
45	AM	201	CDL	OB5-CB3-CB4-CB6
46	B5	202	PC1	O11-C1-C2-C3
48	N4	501	PEE	O3P-C1-C2-C3
51	BL	202	PLX	O4-C3-C4-C5
48	A9	402	PEE	C31-C32-C33-C34
48	N3	202	PEE	C31-C32-C33-C34
51	N2	402	PLX	C34-C35-C36-C37
53	CA	101	PX2	C17-C18-C19-C20
53	CA	101	PX2	C4-C5-C6-C7
49	AC	201	ZMP	C3-C4-C5-C6
49	AC	201	ZMP	C1-C2-C3-C4
51	B1	101	PLX	O8-C24-C25-C26
51	N2	402	PLX	O6-C6-C7-C8
45	N5	703	CDL	C60-C61-C62-C63
48	N5	705	PEE	C11-C10-O2-C2
48	A9	402	PEE	C32-C33-C34-C35
48	B6	201	PEE	O4-C10-O2-C2
48	N1	404	PEE	C37-C38-C39-C40
45	AM	201	CDL	CB3-CB4-CB6-OB8
46	A3	201	PC1	C1-C2-C3-O31
46	B5	203	PC1	C1-C2-C3-O31
48	B6	201	PEE	C1-C2-C3-O3
51	B1	101	PLX	C3-C4-C5-O8
53	CA	101	PX2	C5-C6-C7-C8
48	A9	402	PEE	C19-C20-C21-C22
48	AL	202	PEE	C35-C36-C37-C38
48	N4	501	PEE	C22-C23-C24-C25
51	S7	302	PLX	C16-C17-C18-C19
48	B6	201	PEE	O5-C30-O3-C3
48	N5	701	PEE	C14-C15-C16-C17
53	CA	101	PX2	C1-O4-P1-O2
60	V1	502	FMN	C5'-O5'-P-O1P
45	AL	203	CDL	C51-C52-C53-C54
48	A9	402	PEE	C12-C13-C14-C15
48	S2	501	PEE	C35-C36-C37-C38
48	N4	501	PEE	C37-C38-C39-C40
48	N5	702	PEE	C11-C12-C13-C14
51	N2	402	PLX	C15-C16-C17-C18
48	N4	501	PEE	C11-C12-C13-C14
45	N4	503	CDL	OB5-CB3-CB4-OB6
53	CA	101	PX2	O4-C1-C2-O7
51	CB	201	PLX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
51	N4	502	PLX	C9-C10-C11-C12
48	N5	705	PEE	C22-C23-C24-C25
48	S8	303	PEE	C44-C45-C46-C47
51	S7	302	PLX	O6-C4-C5-O8
45	N5	704	CDL	C52-C53-C54-C55
48	N1	404	PEE	C40-C41-C42-C43
53	CA	101	PX2	C12-C13-C14-C15
45	N5	704	CDL	C39-C40-C41-C42
48	B6	201	PEE	C35-C36-C37-C38
48	BL	201	PEE	C19-C20-C21-C22
45	4L	201	CDL	C38-C39-C40-C41
48	N3	202	PEE	C14-C15-C16-C17
45	AL	203	CDL	C33-C34-C35-C36
48	A9	402	PEE	C11-C12-C13-C14
51	CB	201	PLX	C11-C12-C13-C14
48	B6	201	PEE	C31-C32-C33-C34
51	N2	402	PLX	O7-C6-C7-C8
46	B4	202	PC1	C33-C34-C35-C36
48	N5	705	PEE	C42-C43-C44-C45
45	N2	401	CDL	CB4-CB3-OB5-PB2
45	N4	503	CDL	CB4-CB3-OB5-PB2
46	N1	406	PC1	C2-C1-O11-P
46	A3	202	PC1	C37-C38-C39-C3A
48	N1	404	PEE	C12-C13-C14-C15
51	N2	402	PLX	C14-C15-C16-C17
45	4L	201	CDL	C35-C36-C37-C38
45	AM	201	CDL	C15-C16-C17-C18
48	N5	705	PEE	C19-C20-C21-C22
51	BL	202	PLX	C29-C30-C31-C32
46	B5	203	PC1	C31-C32-C33-C34
45	AN	201	CDL	OA5-CA3-CA4-CA6
45	N1	401	CDL	OB5-CB3-CB4-CB6
48	N5	705	PEE	O3P-C1-C2-C3
52	B8	201	3PE	O11-C1-C2-C3
51	N4	502	PLX	C7-C8-C9-C10
45	AN	201	CDL	C31-C32-C33-C34
46	N3	201	PC1	C37-C38-C39-C3A
48	N4	501	PEE	C30-C31-C32-C33
49	AB	201	ZMP	N2-C16-C17-C18
46	A3	202	PC1	C23-C24-C25-C26
49	AB	201	ZMP	C1-C22-C23-C24
45	B1	102	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
48	S8	303	PEE	C13-C14-C15-C16
51	N1	402	PLX	C28-C29-C30-C31
45	AN	201	CDL	CB3-CB4-CB6-OB8
48	N1	404	PEE	C1-C2-C3-O3
48	N5	702	PEE	C1-C2-C3-O3
48	S2	501	PEE	C1-C2-C3-O3
51	N1	402	PLX	C3-C4-C5-O8
51	N4	502	PLX	C3-C4-C5-O8
52	N5	706	3PE	C1-C2-C3-O31
48	N5	701	PEE	C12-C13-C14-C15
45	4L	201	CDL	C24-C25-C26-C27
48	N3	202	PEE	C22-C23-C24-C25
48	N5	705	PEE	C30-C31-C32-C33
45	AL	203	CDL	OB5-CB3-CB4-OB6
45	AM	201	CDL	OB5-CB3-CB4-OB6
46	B5	202	PC1	O11-C1-C2-O21
48	N1	405	PEE	O3P-C1-C2-O2
48	N5	702	PEE	O3P-C1-C2-O2
51	BL	202	PLX	O4-C3-C4-O6
51	S7	302	PLX	C19-C20-C21-C22
48	N5	705	PEE	C14-C15-C16-C17
48	N5	701	PEE	C2-C1-O3P-P
45	4L	201	CDL	C20-C21-C22-C23
45	AL	201	CDL	C52-C51-CB5-OB6
45	AL	201	CDL	OB6-CB4-CB6-OB8
45	AM	201	CDL	OB6-CB4-CB6-OB8
45	B4	201	CDL	OA6-CA4-CA6-OA8
46	B5	203	PC1	O21-C2-C3-O31
48	AL	202	PEE	O2-C2-C3-O3
48	N5	702	PEE	O2-C2-C3-O3
51	B1	101	PLX	O6-C4-C5-O8
45	B5	201	CDL	C63-C64-C65-C66
45	N5	704	CDL	C35-C36-C37-C38
51	CB	201	PLX	O8-C24-C25-C26
51	N4	502	PLX	O6-C6-C7-C8
48	N5	705	PEE	C41-C42-C43-C44
51	N4	502	PLX	C33-C34-C35-C36
45	AN	201	CDL	C33-C34-C35-C36
45	N5	703	CDL	C55-C56-C57-C58
48	N1	404	PEE	C14-C15-C16-C17
51	B1	101	PLX	C17-C18-C19-C20
45	N4	503	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
46	A3	201	PC1	C34-C35-C36-C37
53	CA	101	PX2	C7-C8-C9-C10
49	AC	201	ZMP	C9-C10-S1-C11
46	A3	202	PC1	C21-C22-C23-C24
51	BL	202	PLX	C28-C29-C30-C31
45	N2	401	CDL	CB2-C1-CA2-OA2
48	N4	501	PEE	C13-C14-C15-C16
51	B1	101	PLX	C13-C14-C15-C16
48	S2	501	PEE	C21-C22-C23-C24
48	S2	501	PEE	C10-C11-C12-C13
45	N4	503	CDL	OB5-CB3-CB4-CB6
51	S7	302	PLX	O4-C3-C4-C5
48	AL	202	PEE	C36-C37-C38-C39
45	AN	201	CDL	C81-C82-C83-C84
45	N4	503	CDL	C81-C82-C83-C84
45	N2	401	CDL	C72-C73-C74-C75
45	AL	201	CDL	CB7-C71-C72-C73
48	N1	404	PEE	C22-C23-C24-C25
48	N5	705	PEE	O4-C10-O2-C2
45	N4	503	CDL	C79-C80-C81-C82
45	N5	703	CDL	C72-C73-C74-C75
48	N4	501	PEE	C42-C43-C44-C45
48	S8	303	PEE	C3-C2-O2-C10
45	AL	201	CDL	C55-C56-C57-C58
51	N1	402	PLX	C26-C27-C28-C29
51	N4	502	PLX	C25-C26-C27-C28
45	AL	203	CDL	C40-C41-C42-C43
48	S2	501	PEE	C41-C42-C43-C44
45	AL	201	CDL	OA5-CA3-CA4-OA6
45	AN	201	CDL	OA5-CA3-CA4-OA6
48	S2	501	PEE	O3P-C1-C2-O2
52	B8	201	3PE	O11-C1-C2-O21
52	CB	202	3PE	O11-C1-C2-O21
48	AL	202	PEE	C1-C2-C3-O3
54	N1	403	U10	C39-C41-C42-C43
48	A9	402	PEE	C20-C21-C22-C23
45	AL	201	CDL	C52-C53-C54-C55
51	N1	402	PLX	C1-C2-O1-P1
52	N5	706	3PE	C12-C11-O13-P
48	S2	501	PEE	O2-C2-C3-O3
53	CA	101	PX2	O7-C2-C3-O5
46	N1	406	PC1	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
46	A3	201	PC1	C31-C32-C33-C34
46	B5	202	PC1	C2-C1-O11-P
51	N2	402	PLX	C4-C3-O4-P1
45	4L	201	CDL	C33-C34-C35-C36
46	A3	201	PC1	O13-C11-C12-N
46	B5	202	PC1	O13-C11-C12-N
46	N3	201	PC1	O13-C11-C12-N
46	N3	203	PC1	O13-C11-C12-N
51	N2	402	PLX	N1-C1-C2-O1
48	N1	404	PEE	C31-C32-C33-C34
48	BL	201	PEE	C39-C40-C41-C42
48	N1	404	PEE	C35-C36-C37-C38
46	A3	202	PC1	C26-C27-C28-C29
49	AC	201	ZMP	O3-C16-C17-O4
51	BL	202	PLX	C25-C24-O8-C5
51	N4	502	PLX	C25-C24-O8-C5
51	S7	302	PLX	C25-C24-O8-C5
45	N5	704	CDL	C51-C52-C53-C54
51	B1	101	PLX	C25-C26-C27-C28
51	S7	302	PLX	C28-C29-C30-C31
51	N1	402	PLX	C31-C32-C33-C34
48	AL	202	PEE	C33-C34-C35-C36
45	AL	201	CDL	OA5-CA3-CA4-CA6
45	B5	201	CDL	OB5-CB3-CB4-CB6
45	N4	503	CDL	OA5-CA3-CA4-CA6
48	N1	405	PEE	O3P-C1-C2-C3
52	CB	202	3PE	O11-C1-C2-C3
49	AB	201	ZMP	C19-C18-C21-O5
49	AC	201	ZMP	C19-C18-C21-O5
60	V1	502	FMN	N10-C1'-C2'-C3'
45	B5	201	CDL	C37-C38-C39-C40
48	N5	701	PEE	C21-C22-C23-C24
48	N5	702	PEE	C17-C18-C19-C20
48	S2	501	PEE	C37-C38-C39-C40
45	AL	203	CDL	CA4-CA3-OA5-PA1
46	A3	201	PC1	C2-C1-O11-P
48	N5	702	PEE	C2-C1-O3P-P
47	A9	401	NDP	C2B-O2B-P2B-O1X
51	N4	502	PLX	C10-C11-C12-C13
51	S7	302	PLX	O8-C24-C25-C26
45	AL	201	CDL	OB5-CB3-CB4-OB6
45	B5	201	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
45	N4	503	CDL	OA5-CA3-CA4-OA6
51	B1	101	PLX	O4-C3-C4-O6
51	N2	402	PLX	C32-C33-C34-C35
58	S2	502	MF8	N06-C04-N02-C01
46	B5	203	PC1	C21-C22-C23-C24
48	B6	201	PEE	O2-C2-C3-O3
48	N4	501	PEE	O2-C2-C3-O3
52	B8	201	3PE	O21-C2-C3-O31
45	N5	704	CDL	C17-C18-C19-C20
45	B4	201	CDL	C82-C83-C84-C85
45	N5	704	CDL	CB3-CB4-CB6-OB8
51	N2	402	PLX	C3-C4-C5-O8
52	B8	201	3PE	C1-C2-C3-O31
58	S2	502	MF8	N02-C04-N06-C07
45	B1	102	CDL	C33-C34-C35-C36
46	N3	201	PC1	C3B-C3C-C3D-C3E
54	N1	403	U10	C5-C4-O4-C4M
46	A3	201	PC1	C24-C25-C26-C27
48	B6	201	PEE	C23-C24-C25-C26
48	N1	405	PEE	C12-C13-C14-C15
45	4L	201	CDL	CA2-OA2-PA1-OA4
45	4L	201	CDL	CA3-OA5-PA1-OA2
45	AL	201	CDL	CA2-OA2-PA1-OA4
45	AL	201	CDL	CB2-OB2-PB2-OB4
45	AL	203	CDL	CA3-OA5-PA1-OA3
45	B4	201	CDL	CA3-OA5-PA1-OA3
45	B5	201	CDL	CB2-OB2-PB2-OB4
45	N1	401	CDL	CA2-OA2-PA1-OA5
45	N1	401	CDL	CA3-OA5-PA1-OA4
45	N1	401	CDL	CB2-OB2-PB2-OB4
45	N1	401	CDL	CB2-OB2-PB2-OB5
45	N2	401	CDL	CA3-OA5-PA1-OA3
45	N4	503	CDL	CB3-OB5-PB2-OB3
45	N5	703	CDL	CA2-OA2-PA1-OA4
45	N5	703	CDL	CB3-OB5-PB2-OB4
46	A3	202	PC1	C1-O11-P-O14
46	A3	202	PC1	C1-O11-P-O13
46	B5	203	PC1	C11-O13-P-O12
46	B5	203	PC1	C11-O13-P-O11
46	N1	406	PC1	C11-O13-P-O12
46	N3	201	PC1	C11-O13-P-O14
46	N3	201	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
46	N3	203	PC1	C1-O11-P-O14
46	N3	203	PC1	C1-O11-P-O13
47	A9	401	NDP	C5D-O5D-PN-O2N
48	AL	202	PEE	O4P-C4-C5-N
48	N1	404	PEE	C1-O3P-P-O1P
48	N1	404	PEE	C1-O3P-P-O4P
48	N1	404	PEE	C4-O4P-P-O1P
48	N1	405	PEE	C4-O4P-P-O3P
48	N1	405	PEE	C4-O4P-P-O2P
48	N1	405	PEE	C4-O4P-P-O1P
48	N3	202	PEE	C4-O4P-P-O1P
48	N4	501	PEE	C1-O3P-P-O2P
48	N4	501	PEE	C1-O3P-P-O1P
48	N4	501	PEE	C1-O3P-P-O4P
48	N4	501	PEE	C4-O4P-P-O1P
48	N5	701	PEE	C4-O4P-P-O1P
48	N5	702	PEE	C1-O3P-P-O4P
48	N5	705	PEE	C4-O4P-P-O1P
48	S2	501	PEE	C1-O3P-P-O4P
51	B1	101	PLX	C5-C4-O6-C6
51	CB	201	PLX	C3-C4-O6-C6
51	CB	201	PLX	C5-C4-O6-C6
51	CB	201	PLX	C3-O4-P1-O1
51	CB	201	PLX	C3-O4-P1-O3
51	N2	402	PLX	C3-O4-P1-O1
51	N2	402	PLX	C3-O4-P1-O2
51	N2	402	PLX	C3-O4-P1-O3
51	S7	302	PLX	C3-O4-P1-O2
51	S7	302	PLX	C2-O1-P1-O2
52	B8	201	3PE	C1-O11-P-O13
52	CB	202	3PE	C11-O13-P-O14
52	N5	706	3PE	C1-O11-P-O14
45	N5	704	CDL	CA4-CA3-OA5-PA1
48	N5	702	PEE	C34-C35-C36-C37
51	S7	302	PLX	C25-C26-C27-C28
45	4L	201	CDL	CA6-CA4-OA6-CA5
45	AL	203	CDL	CB3-CB4-OB6-CB5
45	N1	401	CDL	CB6-CB4-OB6-CB5
46	A3	201	PC1	C1-C2-O21-C21
48	N3	202	PEE	C3-C2-O2-C10
48	N5	702	PEE	C1-C2-O2-C10
53	CA	101	PX2	C3-C2-O7-C16

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Mol	Chain	Res	Type	Atoms
48	BL	201	PEE	C31-C32-C33-C34
48	N3	202	PEE	C41-C42-C43-C44
46	A3	202	PC1	C11-C12-N-C14
45	B1	102	CDL	OB5-CB3-CB4-CB6
48	N5	702	PEE	O3P-C1-C2-C3
48	S2	501	PEE	O3P-C1-C2-C3
53	CA	101	PX2	O4-C1-C2-C3
51	N4	502	PLX	C14-C15-C16-C17
45	AN	201	CDL	OB5-CB3-CB4-OB6
45	B1	102	CDL	OB5-CB3-CB4-OB6
45	N2	401	CDL	OA5-CA3-CA4-OA6
51	S7	302	PLX	C11-C12-C13-C14
49	AB	201	ZMP	C22-C23-C24-C25
49	AB	201	ZMP	C3-C4-C5-C6
45	AM	201	CDL	C1-CB2-OB2-PB2
45	AN	201	CDL	C73-C74-C75-C76
45	N5	704	CDL	OB6-CB4-CB6-OB8
45	AM	201	CDL	C32-C33-C34-C35
48	S8	303	PEE	C17-C18-C19-C20
45	N5	704	CDL	CA5-C11-C12-C13
51	BL	202	PLX	C24-C25-C26-C27
45	B1	102	CDL	C52-C51-CB5-OB6
48	N4	501	PEE	C24-C25-C26-C27
51	S7	302	PLX	C3-C4-C5-O8
51	BL	202	PLX	C31-C32-C33-C34
51	N2	402	PLX	C7-C8-C9-C10
48	N3	202	PEE	C32-C33-C34-C35
51	S7	302	PLX	C6-C7-C8-C9
49	AB	201	ZMP	O3-C16-C17-C18
45	AN	201	CDL	C53-C54-C55-C56
48	AL	202	PEE	C30-C31-C32-C33
52	B8	201	3PE	C21-C22-C23-C24
48	A9	402	PEE	C36-C37-C38-C39
48	S8	303	PEE	C40-C41-C42-C43
48	B6	201	PEE	C22-C23-C24-C25
48	BL	201	PEE	C40-C41-C42-C43
46	N1	406	PC1	C28-C29-C2A-C2B
51	S7	302	PLX	C14-C15-C16-C17
45	AM	201	CDL	C37-C38-C39-C40
45	B5	201	CDL	C52-C53-C54-C55
48	N4	501	PEE	C20-C21-C22-C23
45	N5	704	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
48	N1	404	PEE	C2-C1-O3P-P
45	AL	201	CDL	C41-C42-C43-C44
49	AC	201	ZMP	N2-C16-C17-O4
54	N1	403	U10	C24-C26-C27-C28
48	N1	404	PEE	C43-C44-C45-C46
48	S2	501	PEE	C11-C12-C13-C14
45	AM	201	CDL	C12-C11-CA5-OA6
45	AL	201	CDL	CA6-CA4-OA6-CA5
45	AN	201	CDL	CB6-CB4-OB6-CB5
45	AL	201	CDL	C73-C74-C75-C76
51	B1	101	PLX	C32-C33-C34-C35
47	A9	401	NDP	O4D-C1D-N1N-C6N
45	N2	401	CDL	C12-C11-CA5-OA6
58	S2	502	MF8	N06-C04-N02-C03
45	N5	704	CDL	C19-C20-C21-C22
53	CA	101	PX2	C23-C24-C25-C26
54	N1	403	U10	C15-C14-C16-C17
54	N1	403	U10	C30-C29-C31-C32
51	CB	201	PLX	C11-C10-C9-C8
48	N1	405	PEE	O2-C2-C3-O3
45	N5	704	CDL	C37-C38-C39-C40
48	S8	303	PEE	C42-C43-C44-C45
45	4L	201	CDL	C75-C76-C77-C78
45	N5	703	CDL	C15-C16-C17-C18
46	N3	201	PC1	C2C-C2D-C2E-C2F
48	N1	404	PEE	C42-C43-C44-C45
45	4L	201	CDL	C13-C14-C15-C16
45	AM	201	CDL	C21-C22-C23-C24
46	B5	202	PC1	C36-C37-C38-C39
48	N4	501	PEE	C33-C34-C35-C36
45	4L	201	CDL	CB5-C51-C52-C53
45	AL	203	CDL	C1-CA2-OA2-PA1
45	N4	503	CDL	C1-CA2-OA2-PA1
45	N5	703	CDL	C1-CB2-OB2-PB2
51	N4	502	PLX	C4-C3-O4-P1
45	4L	201	CDL	C74-C75-C76-C77
45	AL	201	CDL	CB3-CB4-CB6-OB8
45	B4	201	CDL	CA3-CA4-CA6-OA8
48	N4	501	PEE	C1-C2-C3-O3
48	S8	303	PEE	C1-C2-C3-O3
54	N1	403	U10	C29-C31-C32-C33
45	AN	201	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
51	S7	302	PLX	O7-C6-C7-C8
45	4L	201	CDL	C55-C56-C57-C58
45	AN	201	CDL	C12-C11-CA5-OA6
48	N4	501	PEE	C12-C13-C14-C15
45	N1	401	CDL	C76-C77-C78-C79
51	B1	101	PLX	C31-C32-C33-C34
46	A3	202	PC1	C11-C12-N-C13
46	B4	202	PC1	C24-C25-C26-C27
51	N4	502	PLX	C24-C25-C26-C27
45	B1	102	CDL	OA5-CA3-CA4-CA6
45	AL	201	CDL	C11-C12-C13-C14
48	AL	202	PEE	O2-C10-C11-C12
46	B5	202	PC1	C2A-C2B-C2C-C2D
45	AM	201	CDL	C60-C61-C62-C63
48	A9	402	PEE	C14-C15-C16-C17
53	CA	101	PX2	C22-C23-C24-C25
48	N5	705	PEE	C11-C12-C13-C14
45	B4	201	CDL	C37-C38-C39-C40
51	S7	302	PLX	C4-C5-O8-C24
52	N5	706	3PE	C37-C38-C39-C3A
45	AL	203	CDL	CA6-CA4-OA6-CA5
45	N2	401	CDL	CA6-CA4-OA6-CA5
46	N3	201	PC1	C28-C29-C2A-C2B
47	A9	401	NDP	C2D-C1D-N1N-C6N
45	B1	102	CDL	OA5-CA3-CA4-OA6
45	AL	201	CDL	C40-C41-C42-C43
53	CA	101	PX2	C1-C2-C3-O5
58	S2	502	MF8	N09-C07-N06-C04
48	S2	501	PEE	C44-C45-C46-C47
45	AL	203	CDL	C71-C72-C73-C74
51	N1	402	PLX	C9-C10-C11-C12
45	B4	201	CDL	C12-C11-CA5-OA6
46	A3	202	PC1	O31-C31-C32-C33
45	AM	201	CDL	C61-C62-C63-C64
45	B1	102	CDL	OB6-CB4-CB6-OB8
45	B5	201	CDL	C21-C22-C23-C24
48	N1	404	PEE	C16-C17-C18-C19
45	B1	102	CDL	C32-C31-CA7-OA8
51	B1	101	PLX	O4-C3-C4-C5
48	N5	701	PEE	C30-C31-C32-C33
46	A3	202	PC1	C11-C12-N-C15
51	CB	201	PLX	C7-C6-O6-C4

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Mol	Chain	Res	Type	Atoms
45	AL	201	CDL	C52-C51-CB5-OB7
48	B6	201	PEE	C34-C35-C36-C37
48	N5	705	PEE	C24-C25-C26-C27
51	B1	101	PLX	C14-C15-C16-C17
58	S2	502	MF8	N08-C07-N06-C04
45	AL	203	CDL	C12-C11-CA5-OA6
52	N5	706	3PE	O21-C21-C22-C23
51	N4	502	PLX	C11-C10-C9-C8
46	N3	203	PC1	O21-C21-C22-C23
46	B4	202	PC1	C27-C28-C29-C2A
52	CB	202	3PE	C38-C39-C3A-C3B
45	N4	503	CDL	C32-C31-CA7-OA8
45	N5	703	CDL	C12-C11-CA5-OA6
52	B8	201	3PE	O21-C21-C22-C23
52	CB	202	3PE	C27-C28-C29-C2A
45	N5	703	CDL	C52-C51-CB5-OB6
45	AL	201	CDL	C32-C31-CA7-OA8
47	A9	401	NDP	O4B-C4B-C5B-O5B
45	4L	201	CDL	C36-C37-C38-C39
45	4L	201	CDL	C11-C12-C13-C14
45	AN	201	CDL	C12-C13-C14-C15
45	AL	201	CDL	C12-C11-CA5-OA6
48	N1	405	PEE	O2-C10-C11-C12
51	B1	101	PLX	C25-C24-O8-C5
51	N2	402	PLX	C20-C21-C22-C23
45	N1	401	CDL	OB6-CB4-CB6-OB8
45	N5	704	CDL	C22-C23-C24-C25
45	N1	401	CDL	C32-C31-CA7-OA8
46	N3	203	PC1	C37-C38-C39-C3A
51	B1	101	PLX	C33-C34-C35-C36
45	AN	201	CDL	C15-C16-C17-C18
46	N3	201	PC1	C3C-C3D-C3E-C3F
49	AB	201	ZMP	C20-C18-C21-O5
45	AM	201	CDL	C36-C37-C38-C39
45	B5	201	CDL	C77-C78-C79-C80
45	AL	203	CDL	CA3-CA4-OA6-CA5
48	N4	501	PEE	C1-C2-O2-C10
48	N4	501	PEE	C3-C2-O2-C10
48	N1	404	PEE	O2-C10-C11-C12
48	AL	202	PEE	C44-C45-C46-C47
45	N4	503	CDL	C78-C79-C80-C81
45	B1	102	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
45	N5	704	CDL	C15-C16-C17-C18
45	AL	201	CDL	CA4-CA3-OA5-PA1
45	N2	401	CDL	C1-CA2-OA2-PA1
45	B1	102	CDL	C32-C31-CA7-OA9
54	N1	403	U10	C28-C29-C31-C32
46	N3	203	PC1	O22-C21-C22-C23
48	N1	404	PEE	O4-C10-C11-C12
45	B5	201	CDL	C20-C21-C22-C23
45	AN	201	CDL	C62-C63-C64-C65
46	A3	201	PC1	C32-C33-C34-C35
48	N4	501	PEE	C36-C37-C38-C39
48	S2	501	PEE	C36-C37-C38-C39
45	AL	201	CDL	C32-C31-CA7-OA9
46	A3	202	PC1	O32-C31-C32-C33
51	N2	402	PLX	C28-C29-C30-C31
48	B6	201	PEE	O2-C10-C11-C12
45	N4	503	CDL	C32-C31-CA7-OA9
45	AL	203	CDL	C12-C13-C14-C15
45	N2	401	CDL	O1-C1-CA2-OA2
45	B4	201	CDL	C12-C11-CA5-OA7
45	N5	703	CDL	C12-C11-CA5-OA7
48	S2	501	PEE	O2-C10-C11-C12
51	BL	202	PLX	O9-C24-O8-C5
51	S7	302	PLX	O9-C24-O8-C5
45	B5	201	CDL	C62-C63-C64-C65
45	AL	203	CDL	C12-C11-CA5-OA7
48	N1	405	PEE	O4-C10-C11-C12
52	N5	706	3PE	O22-C21-C22-C23
45	4L	201	CDL	C42-C43-C44-C45
45	N4	503	CDL	C74-C75-C76-C77
50	AK	401	ADP	O4'-C4'-C5'-O5'
48	N3	202	PEE	O2-C2-C3-O3
51	N2	402	PLX	O6-C4-C5-O8
46	N3	201	PC1	C26-C27-C28-C29
45	N1	401	CDL	C53-C54-C55-C56
48	N3	202	PEE	C38-C39-C40-C41
49	AB	201	ZMP	N2-C16-C17-O4
45	N5	703	CDL	C52-C51-CB5-OB7
53	CA	101	PX2	C21-C22-C23-C24
52	B8	201	3PE	C2-C1-O11-P
45	N1	401	CDL	C72-C71-CB7-OB8
54	N1	403	U10	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
45	N1	401	CDL	C32-C31-CA7-OA9
45	AM	201	CDL	C72-C73-C74-C75
45	AL	201	CDL	C12-C11-CA5-OA7
52	B8	201	3PE	O22-C21-C22-C23
48	N4	501	PEE	C40-C41-C42-C43
48	N5	701	PEE	O3P-C1-C2-C3
46	N3	201	PC1	O31-C31-C32-C33
45	B5	201	CDL	C18-C19-C20-C21
51	CB	201	PLX	C12-C13-C14-C15
45	N5	703	CDL	C31-C32-C33-C34
46	B5	202	PC1	O31-C31-C32-C33
48	AL	202	PEE	O3-C30-C31-C32
45	AN	201	CDL	C36-C37-C38-C39
45	B5	201	CDL	C60-C61-C62-C63
47	A9	401	NDP	PA-O3-PN-O2N
48	B6	201	PEE	O4-C10-C11-C12
48	S2	501	PEE	O4-C10-C11-C12
45	N4	503	CDL	C20-C21-C22-C23
45	N5	703	CDL	C37-C38-C39-C40
48	N5	702	PEE	C36-C37-C38-C39
46	N3	201	PC1	O32-C31-C32-C33
51	N2	402	PLX	C11-C12-C13-C14

There are no ring outliers.

49 monomers are involved in 178 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	A3	201	PC1	3	0
48	S8	303	PEE	9	0
48	N3	202	PEE	6	0
52	N5	706	3PE	3	0
45	N5	703	CDL	10	0
48	A9	402	PEE	2	0
45	AL	201	CDL	5	0
51	N4	502	PLX	4	0
51	B1	101	PLX	3	0
48	B6	201	PEE	2	0
46	A3	202	PC1	3	0
48	N5	701	PEE	1	0
55	S1	802	SF4	1	0
45	AN	201	CDL	6	0
45	AL	203	CDL	5	0

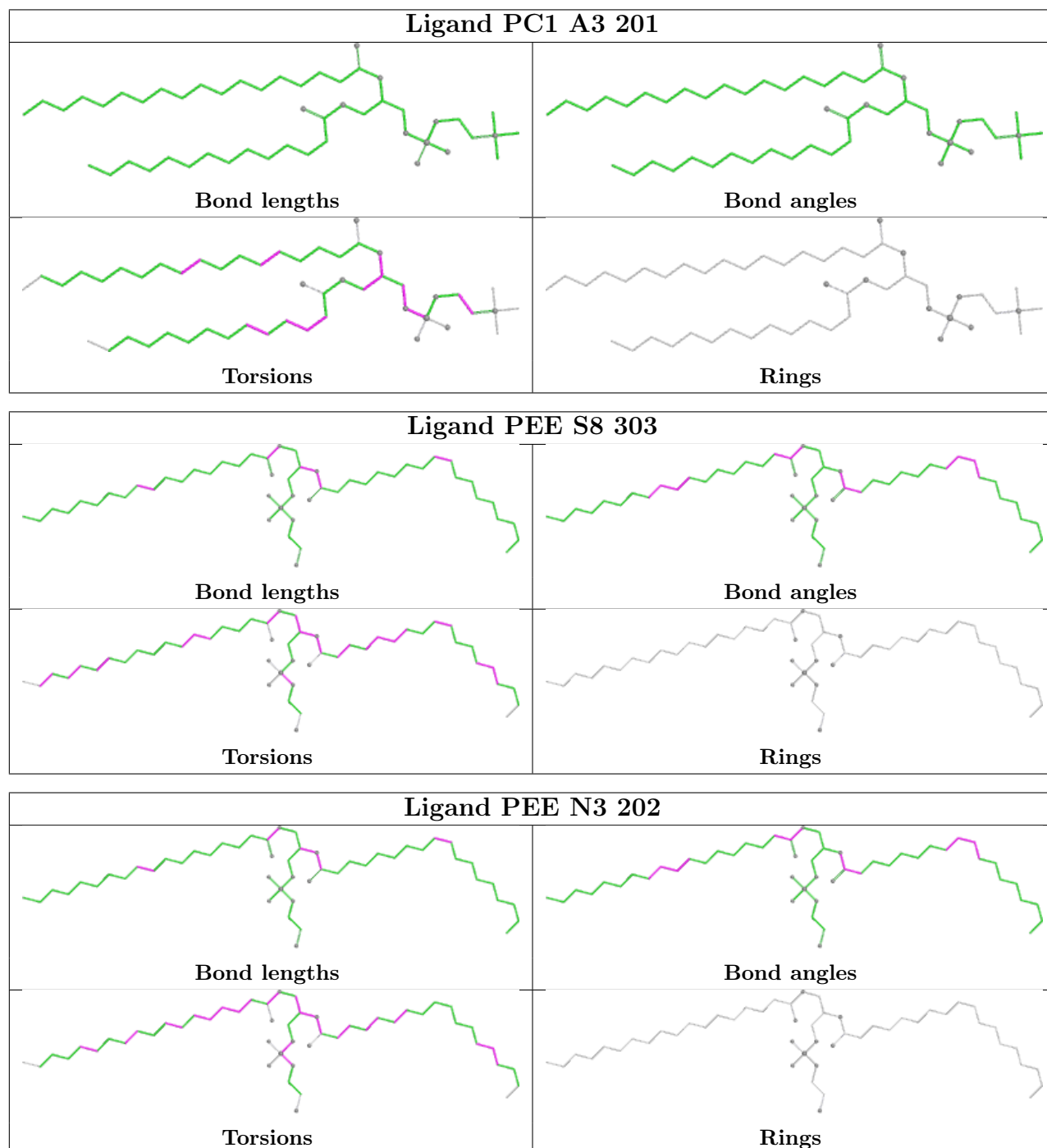
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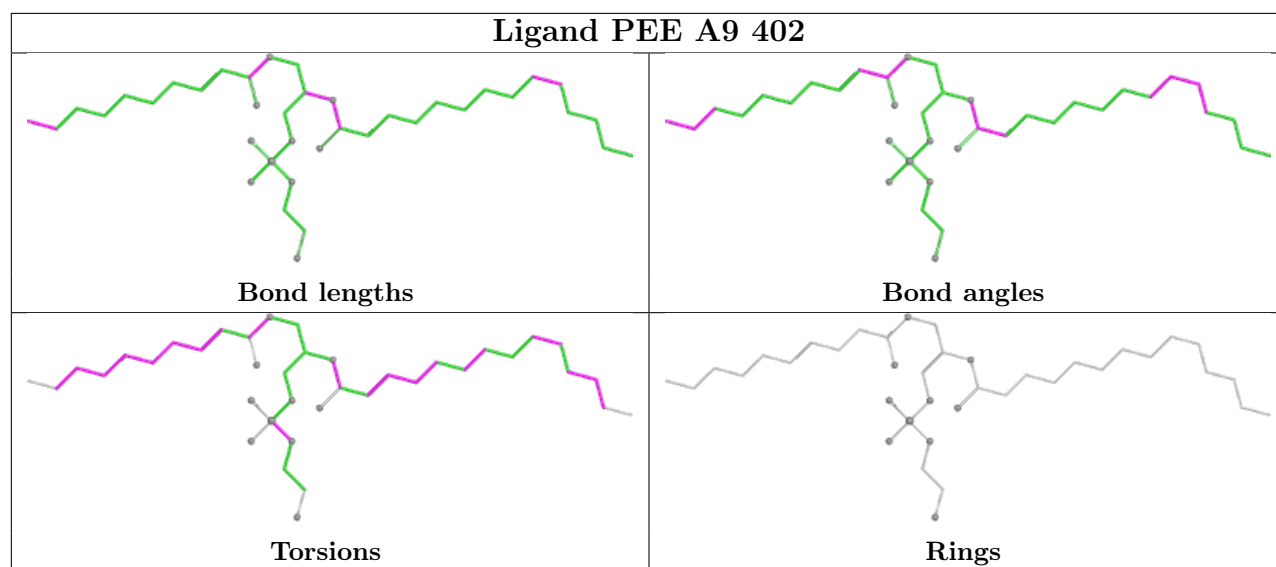
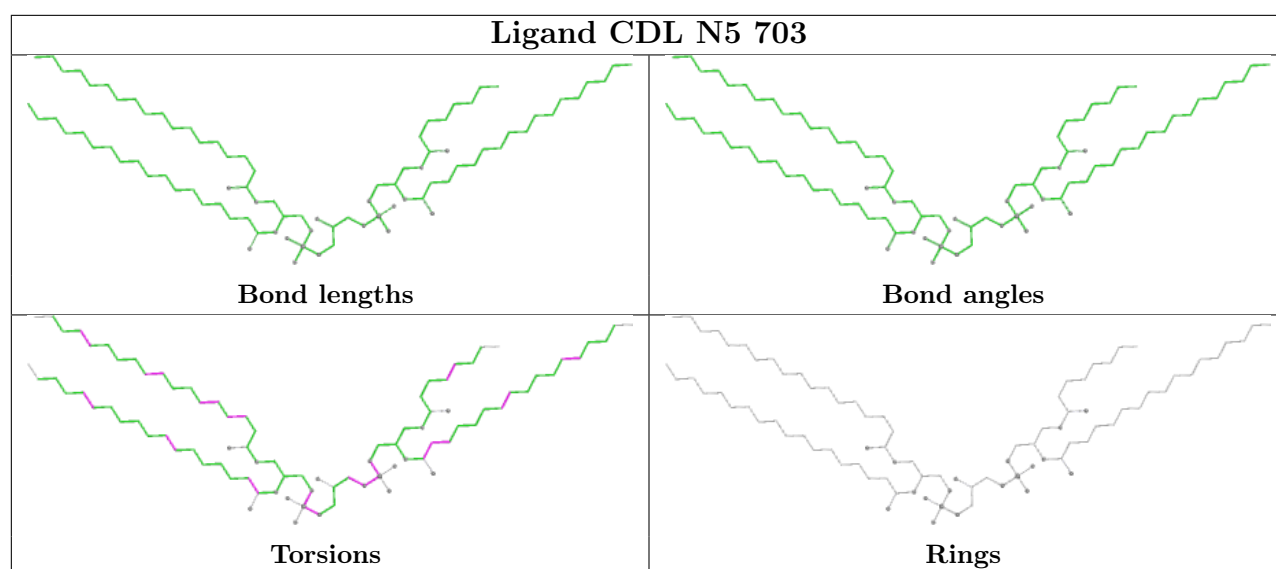
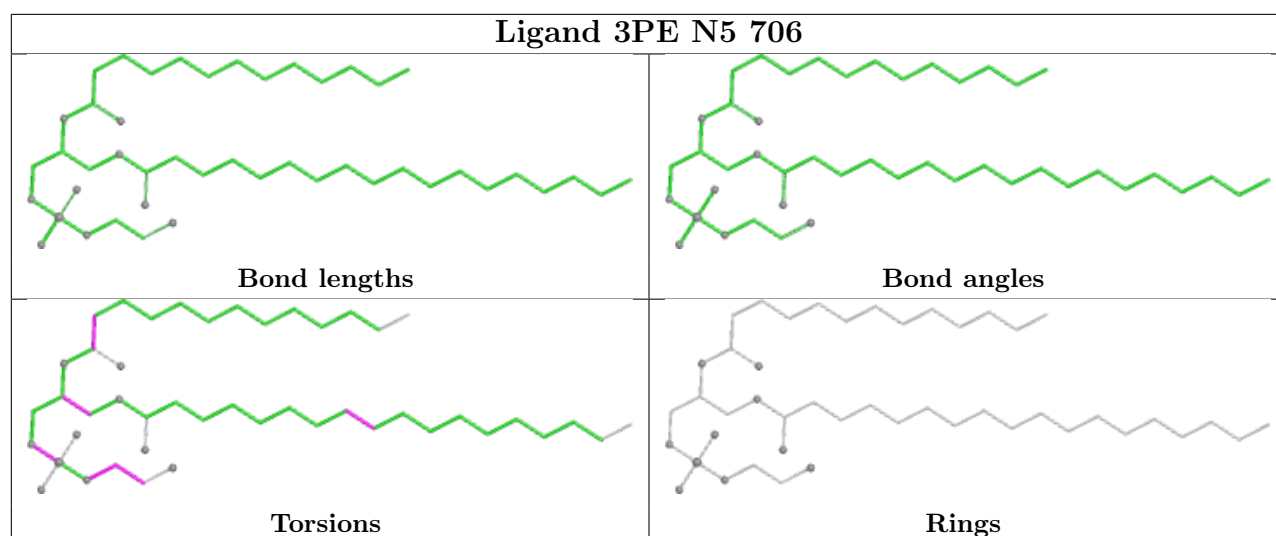
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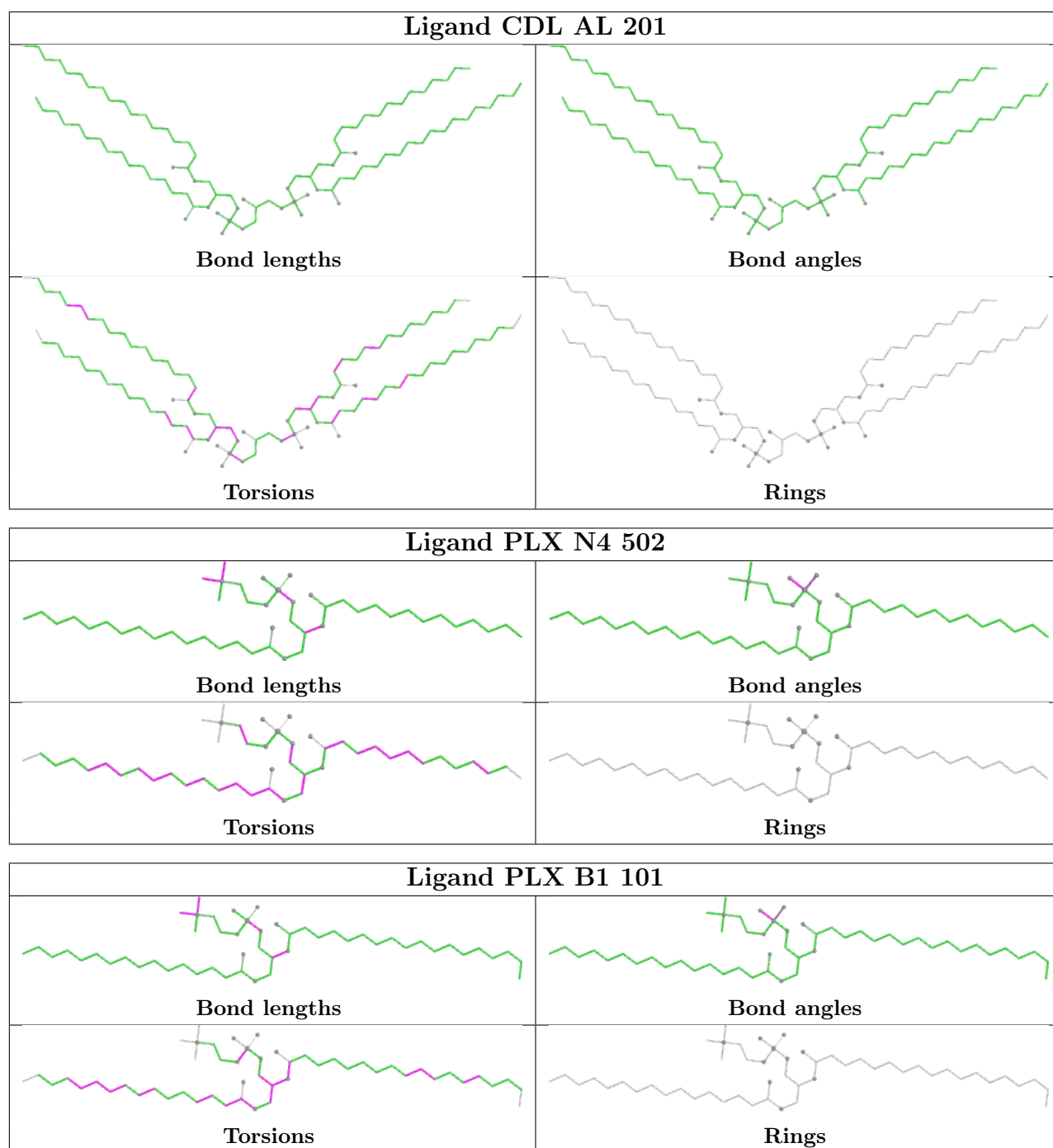
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	AC	201	ZMP	5	0
54	N1	403	U10	9	0
45	4L	201	CDL	6	0
51	N1	402	PLX	2	0
60	V1	502	FMN	2	0
51	N2	402	PLX	2	0
45	B4	201	CDL	4	0
45	B1	102	CDL	2	0
48	N5	702	PEE	1	0
45	N2	401	CDL	3	0
46	N1	406	PC1	7	0
50	AK	401	ADP	4	0
46	B5	202	PC1	1	0
45	N5	704	CDL	4	0
51	BL	202	PLX	4	0
48	N1	405	PEE	2	0
48	N5	705	PEE	3	0
45	B5	201	CDL	5	0
46	B4	202	PC1	4	0
55	S8	301	SF4	1	0
48	N1	404	PEE	6	0
45	N4	503	CDL	10	0
49	AB	201	ZMP	2	0
46	N3	201	PC1	4	0
45	N1	401	CDL	5	0
48	N4	501	PEE	5	0
48	S2	501	PEE	3	0
58	S2	502	MF8	1	0
48	BL	201	PEE	1	0
46	N3	203	PC1	6	0
51	S7	302	PLX	11	0
46	B5	203	PC1	1	0
55	S8	302	SF4	1	0
45	AM	201	CDL	7	0

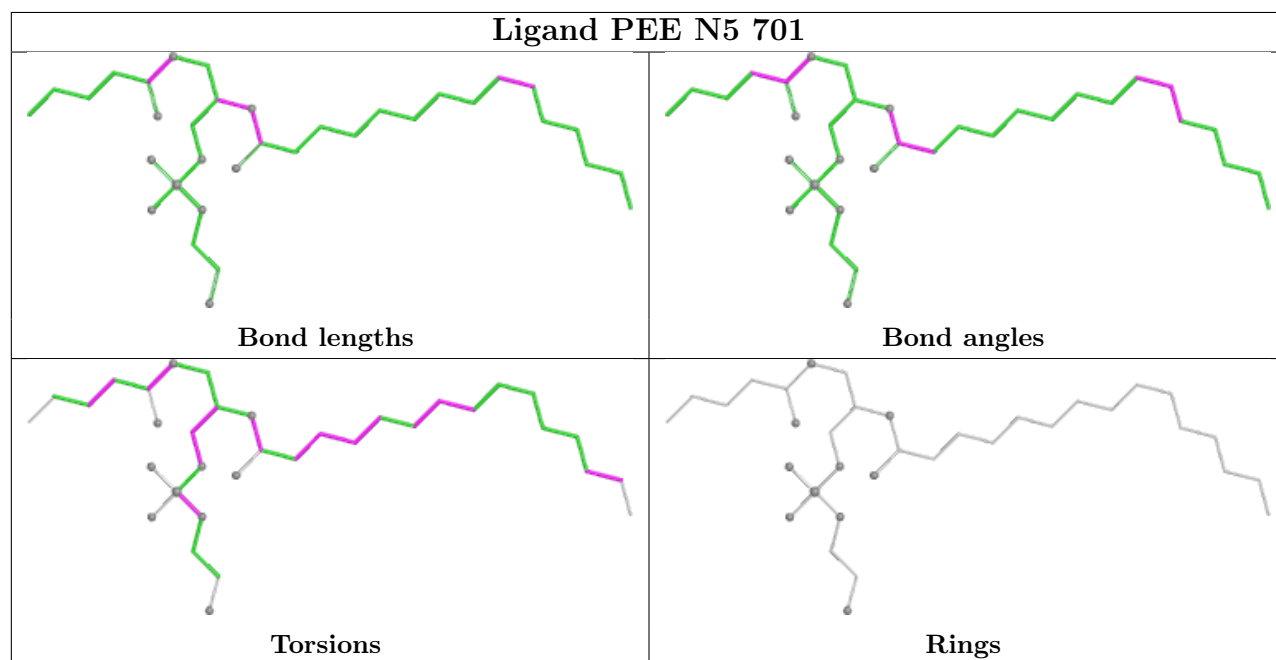
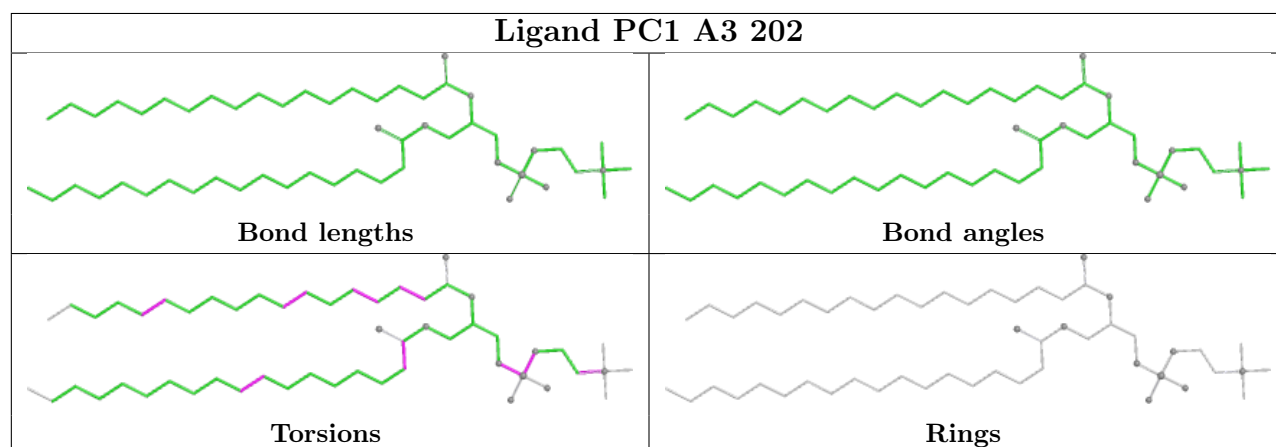
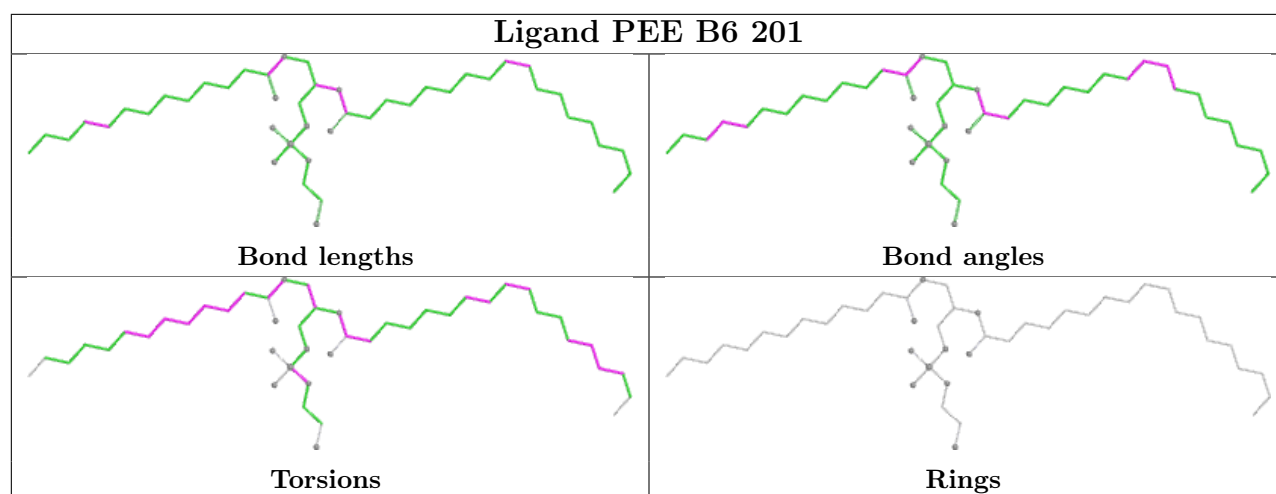
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

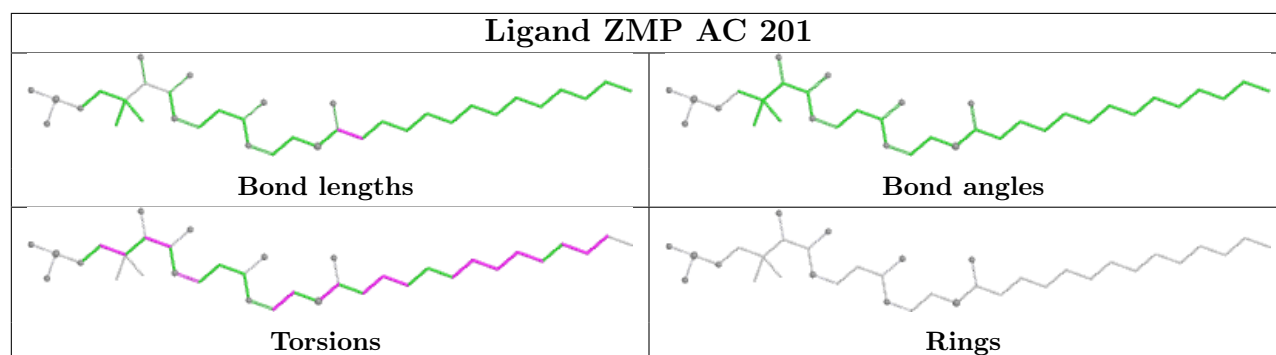
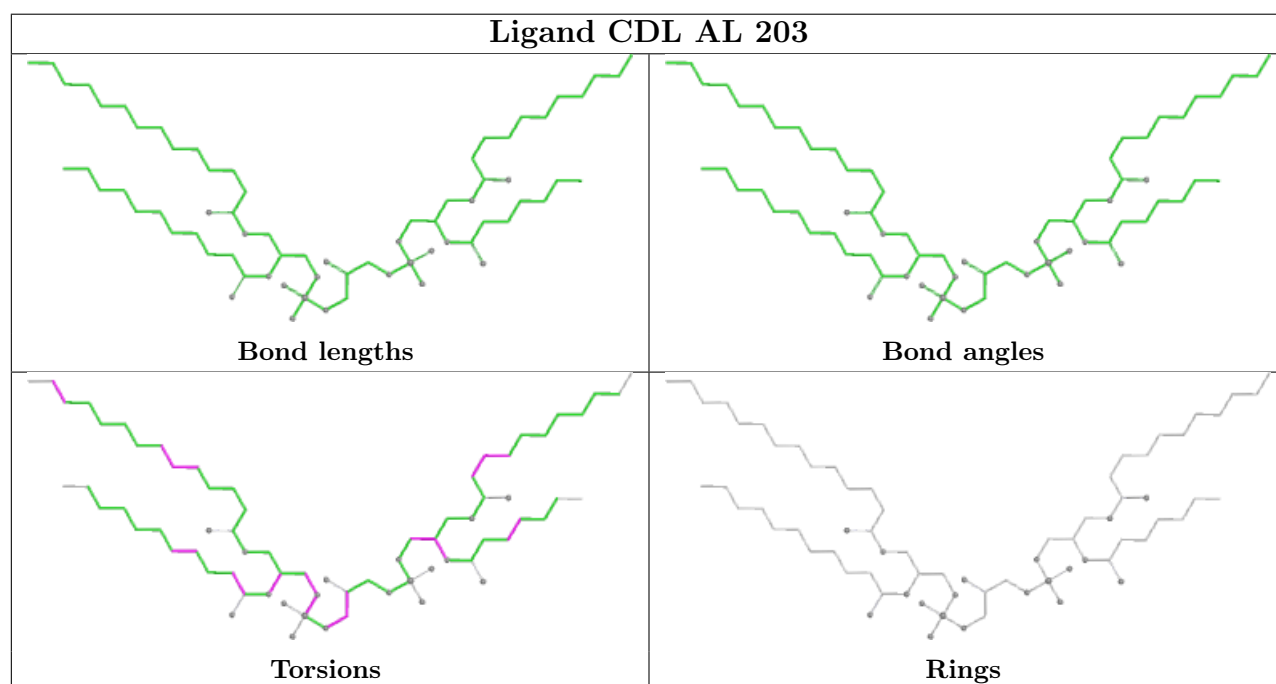
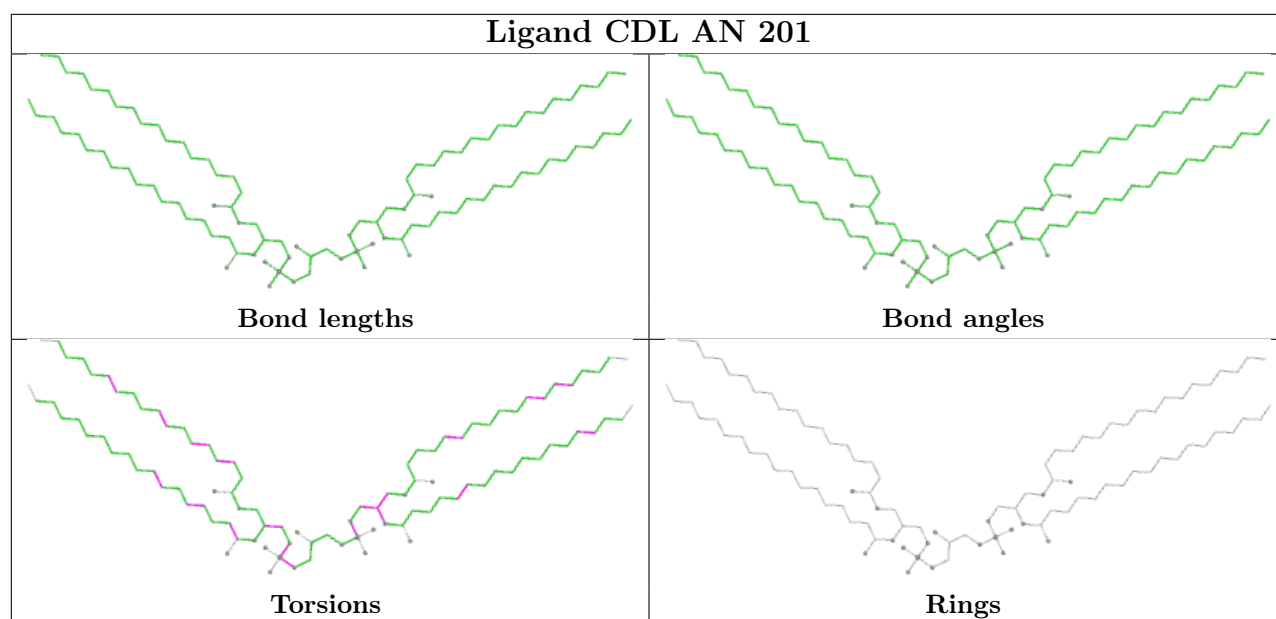
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

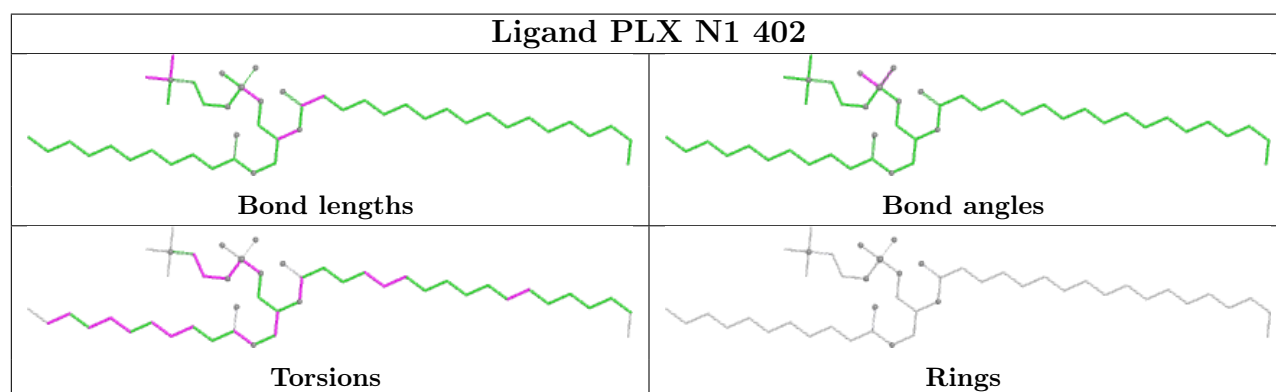
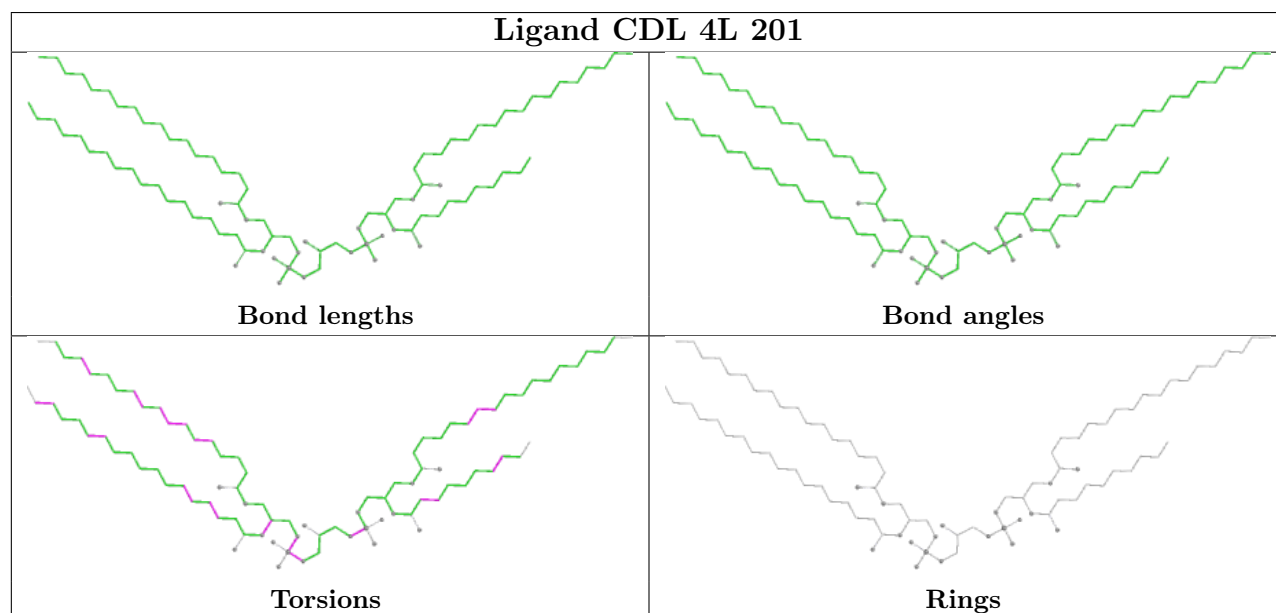
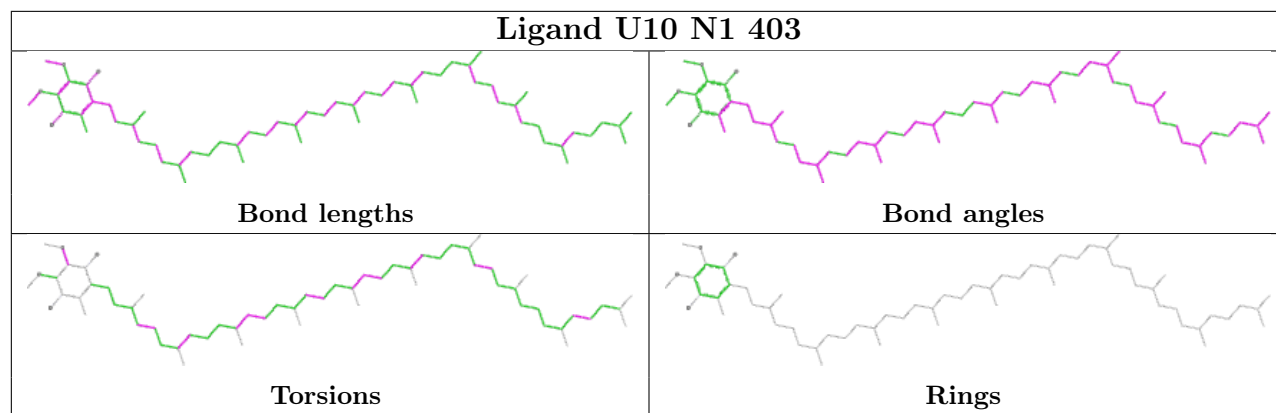


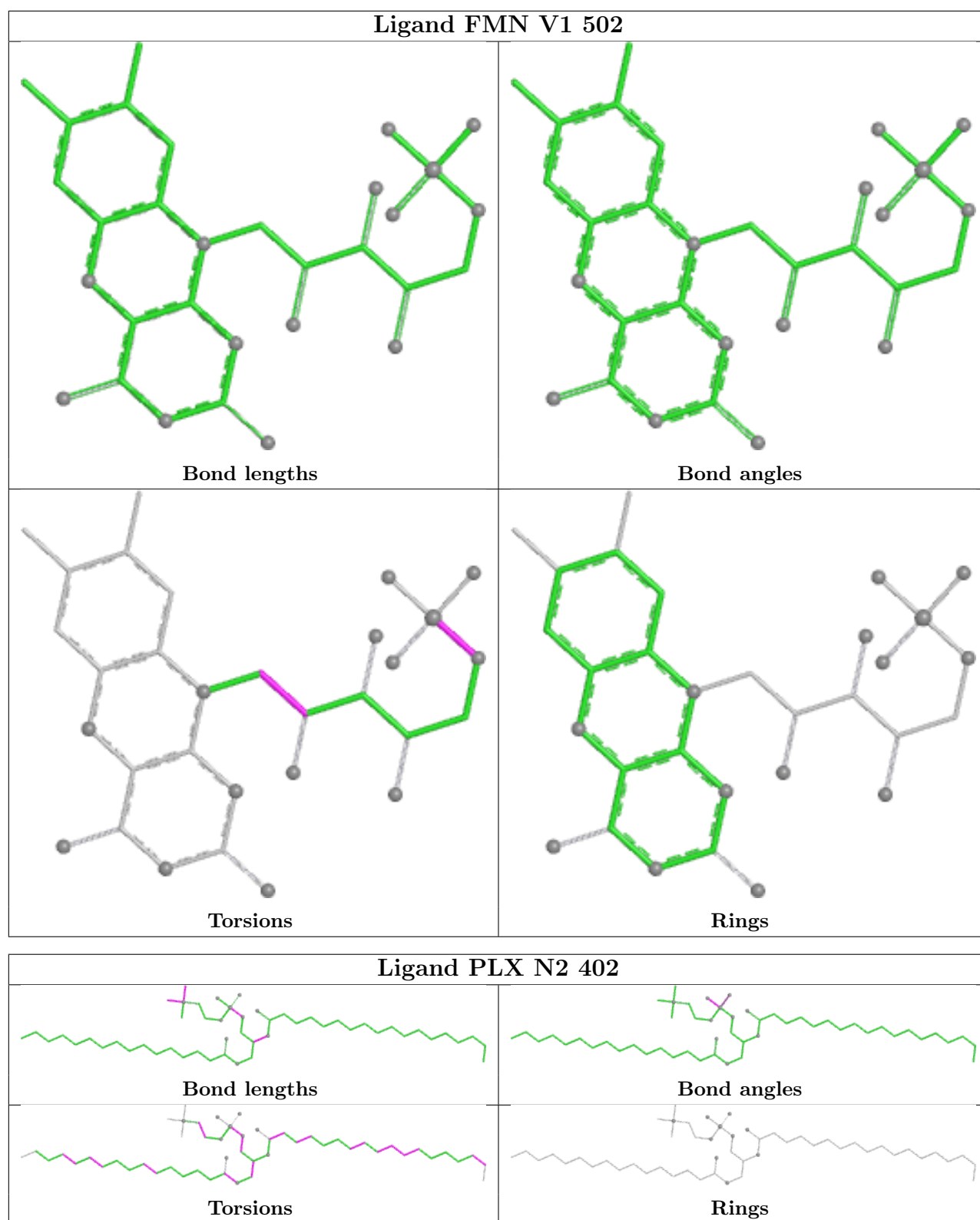


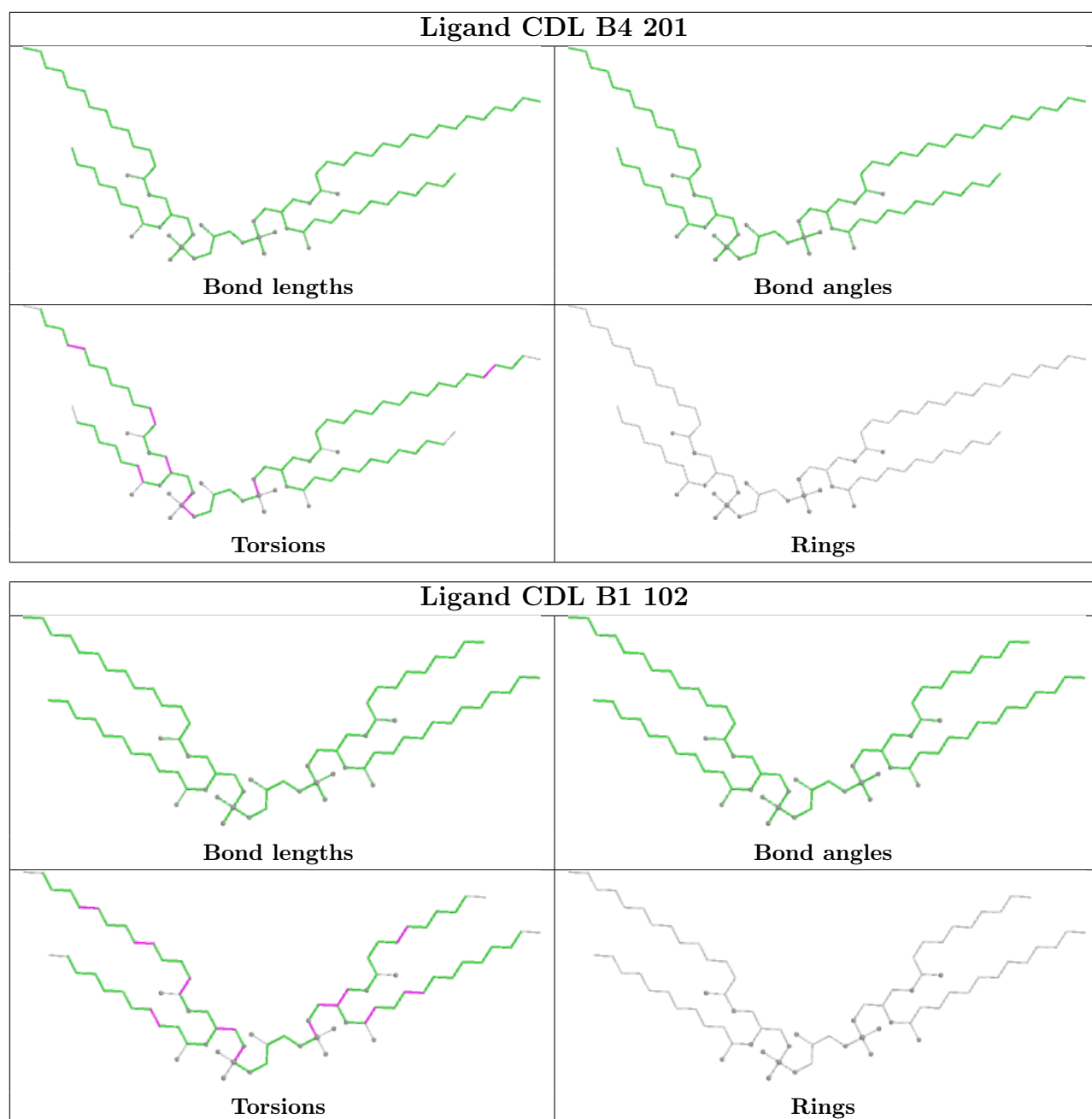


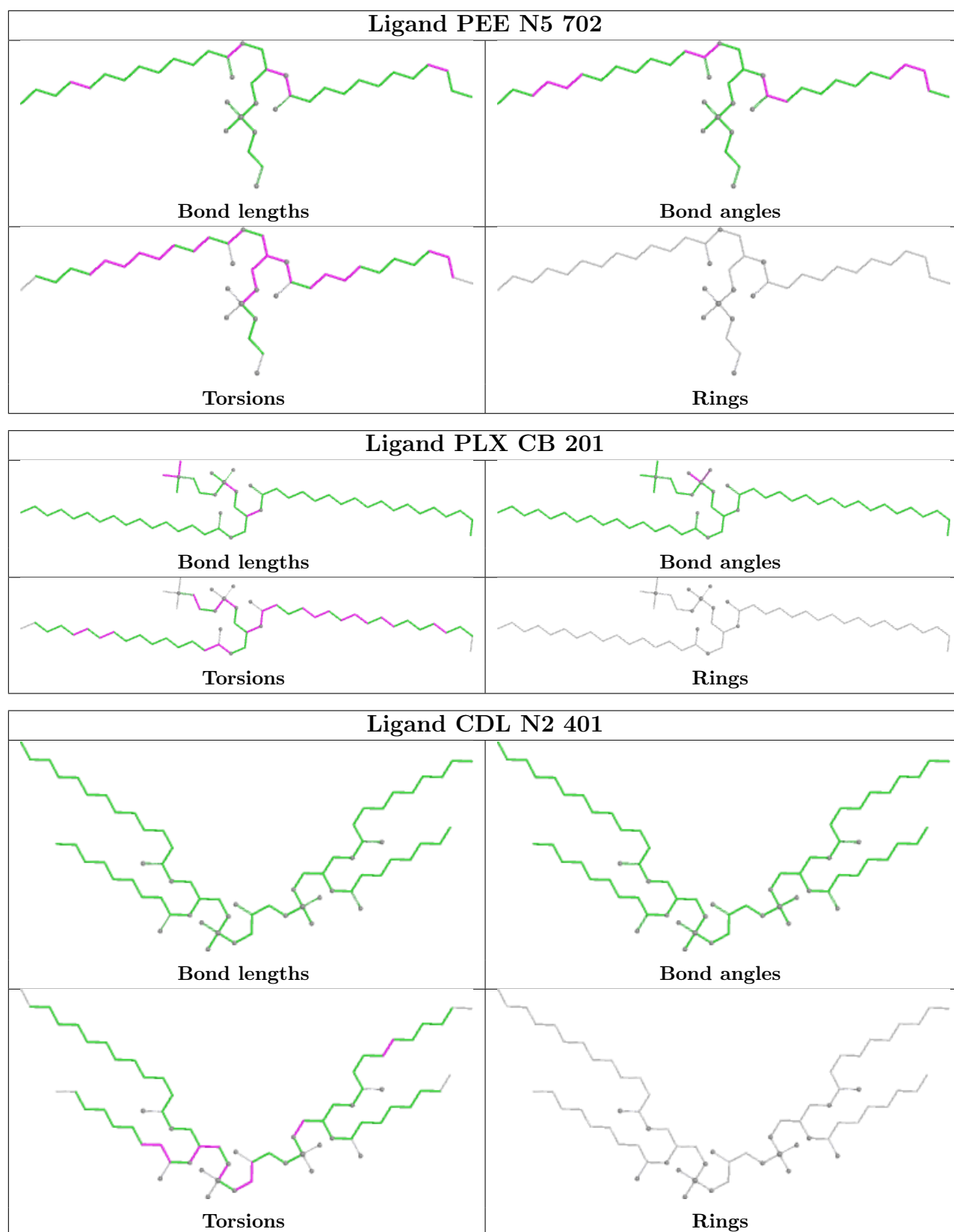


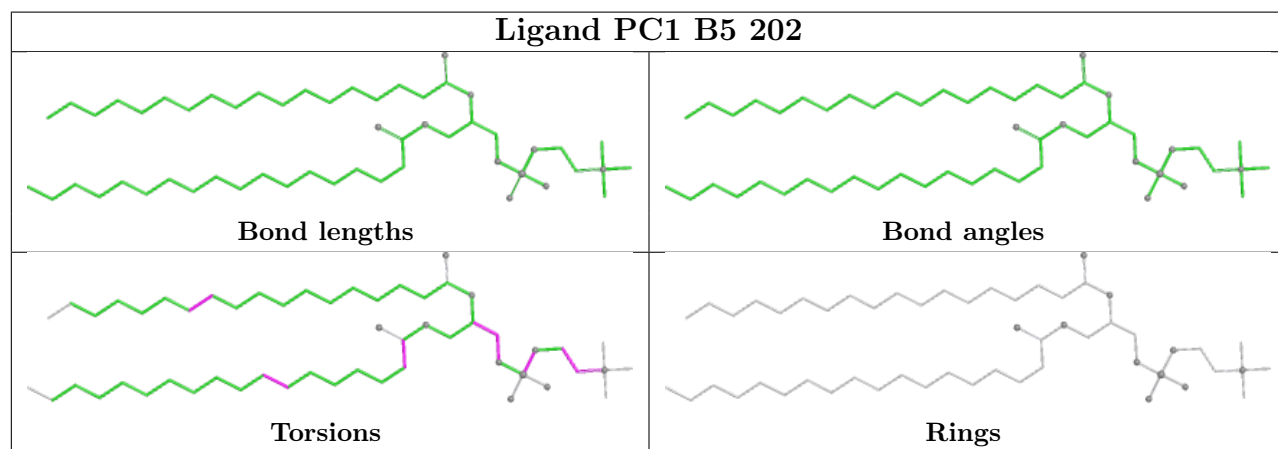
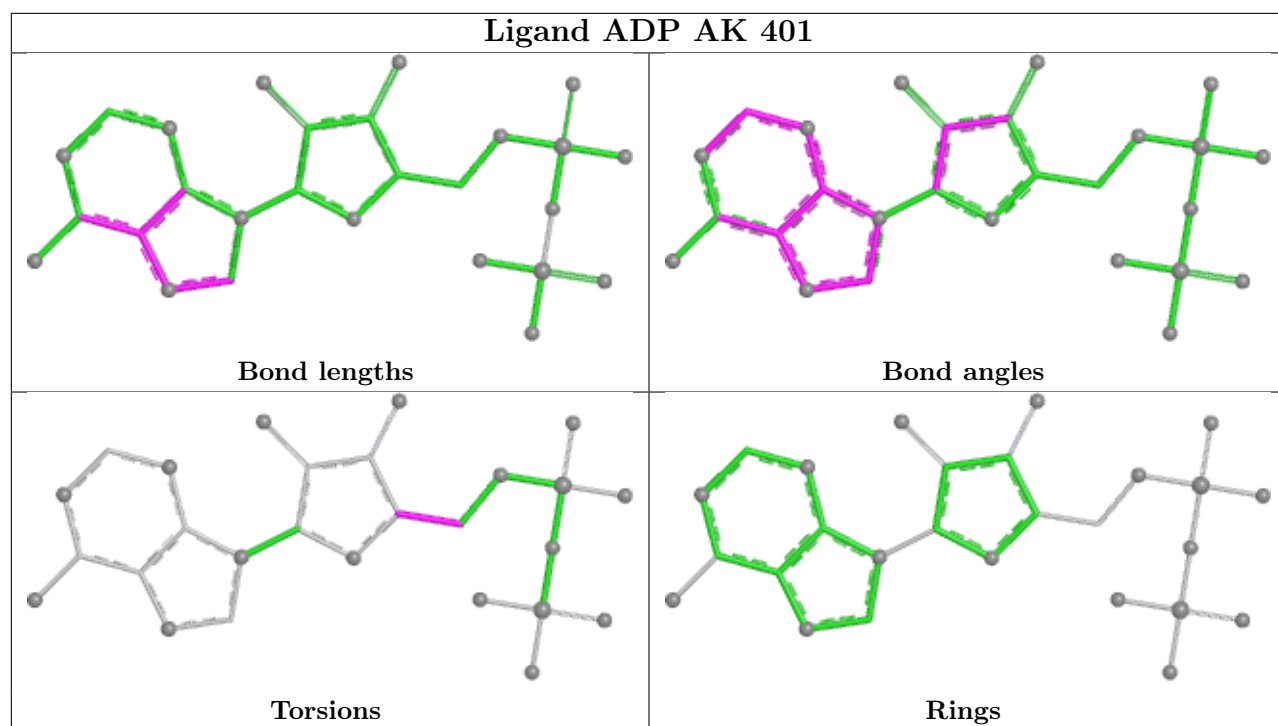
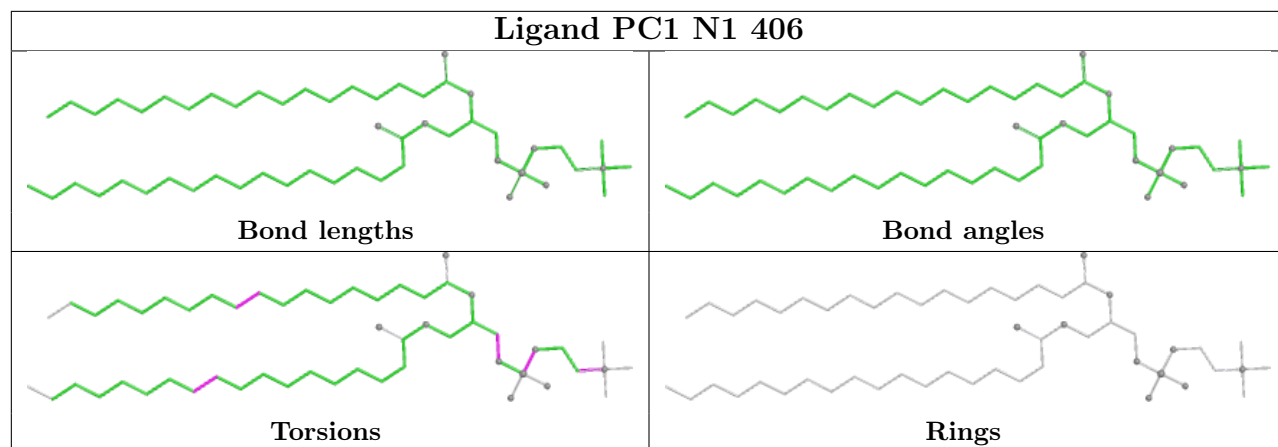


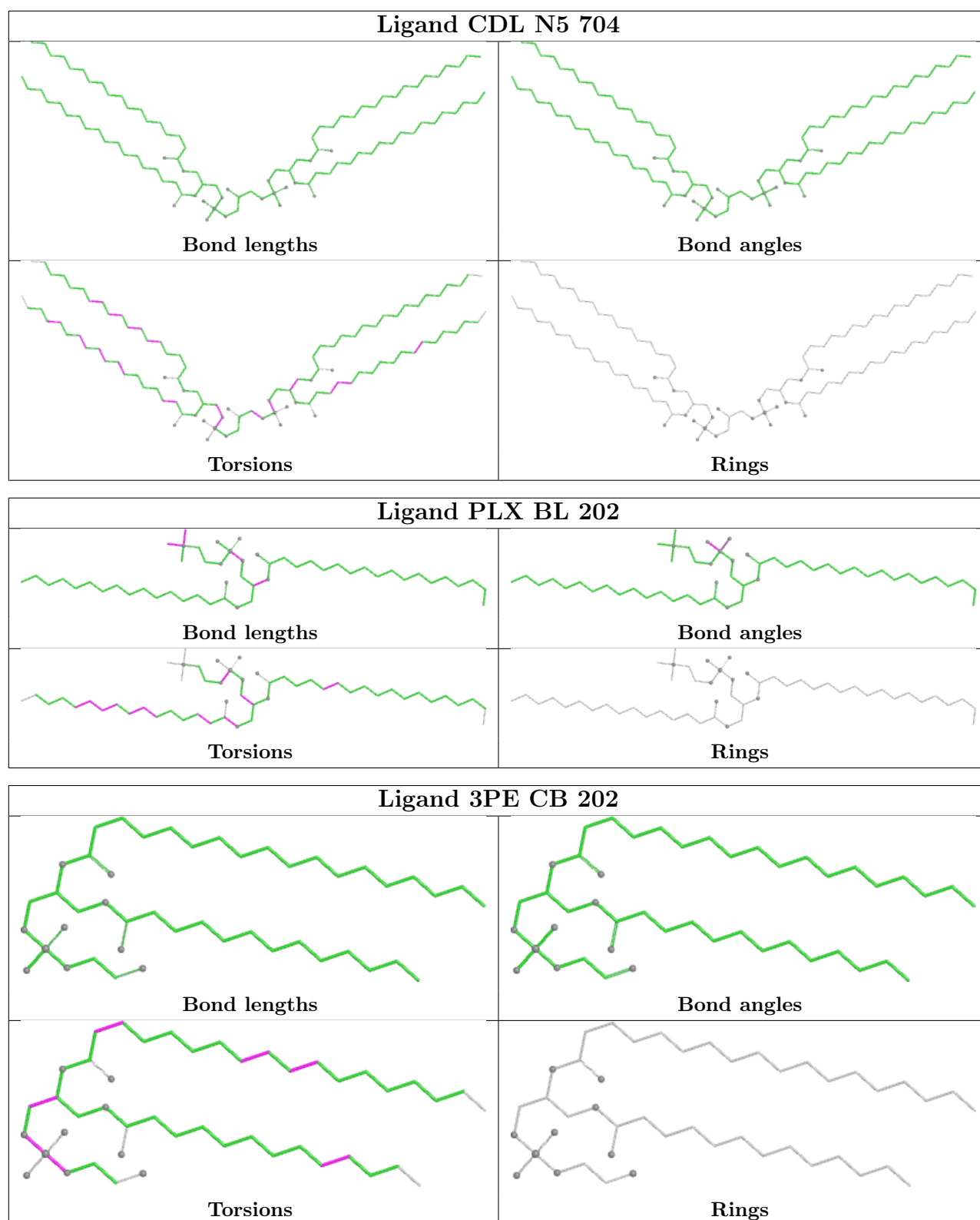


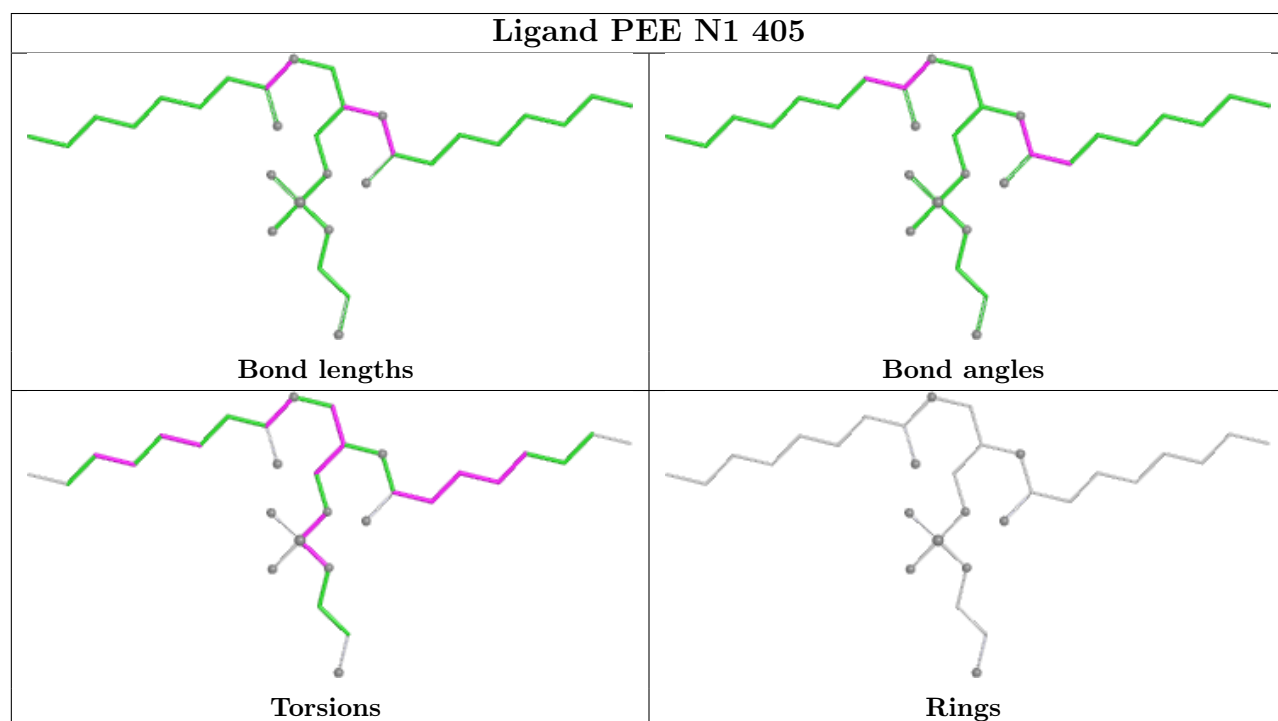
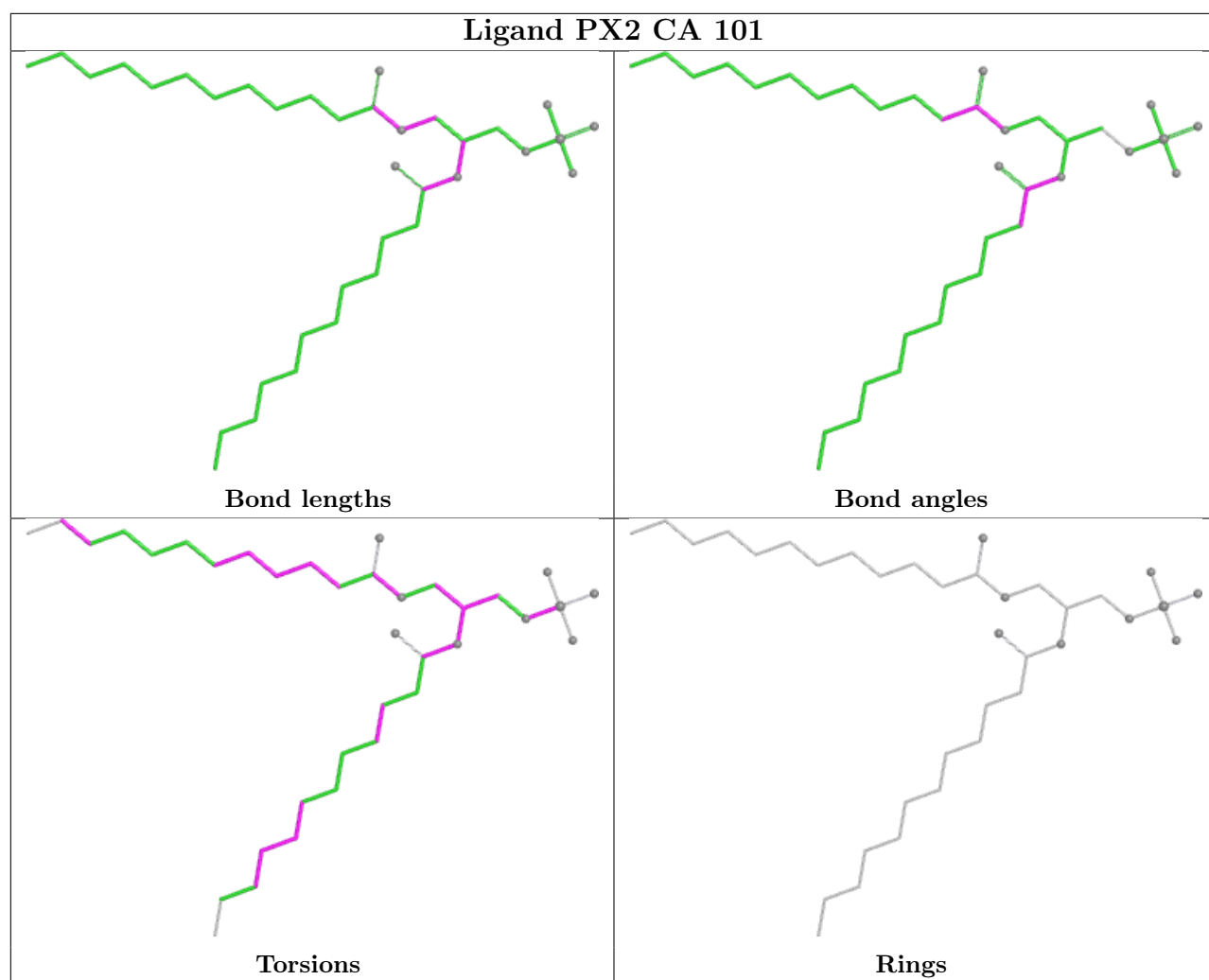


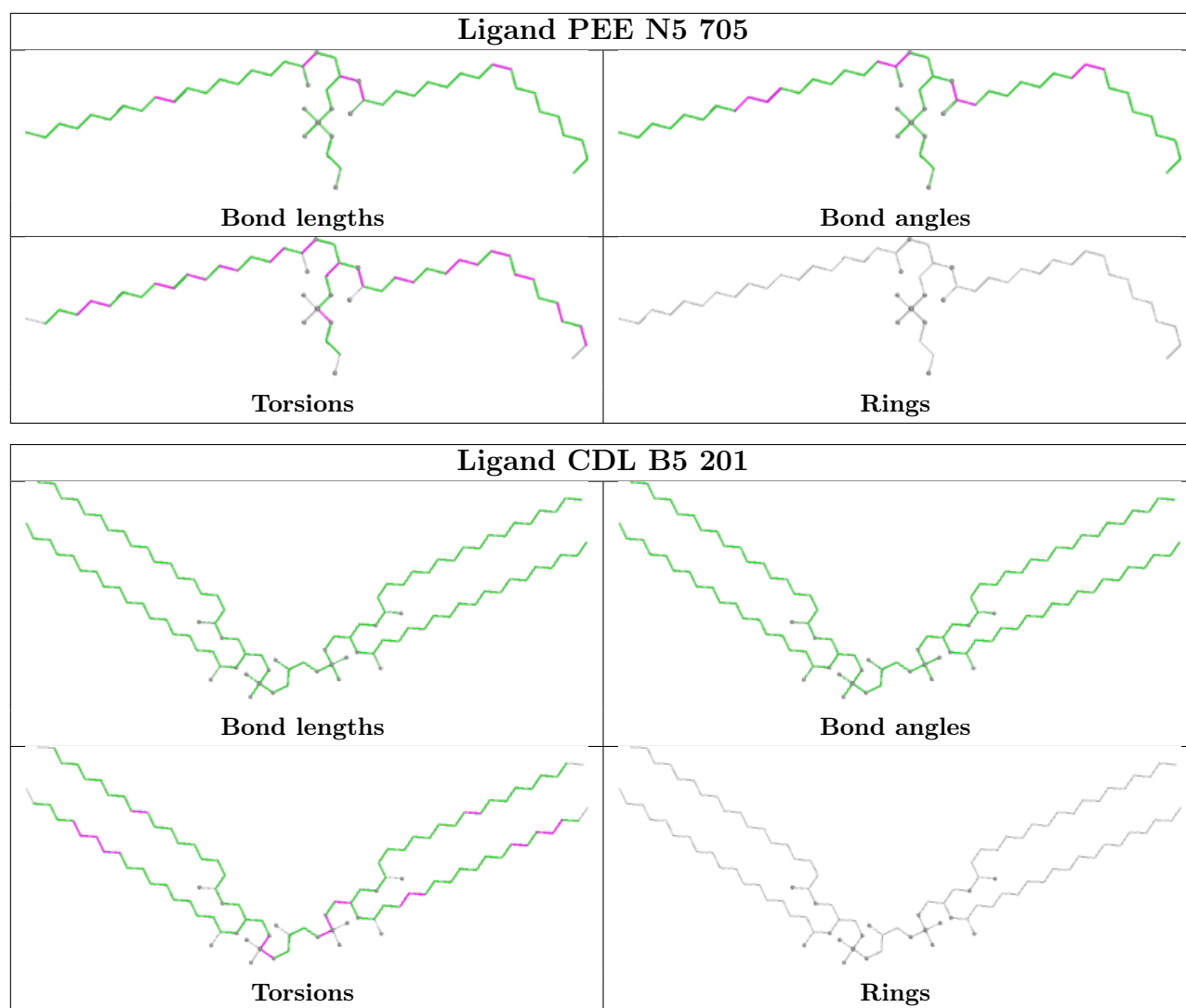


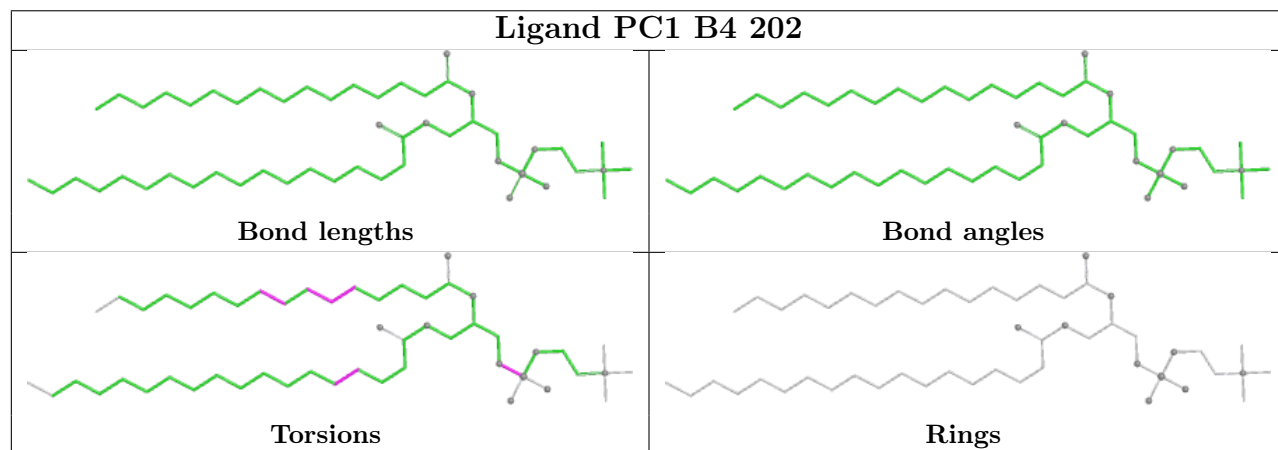
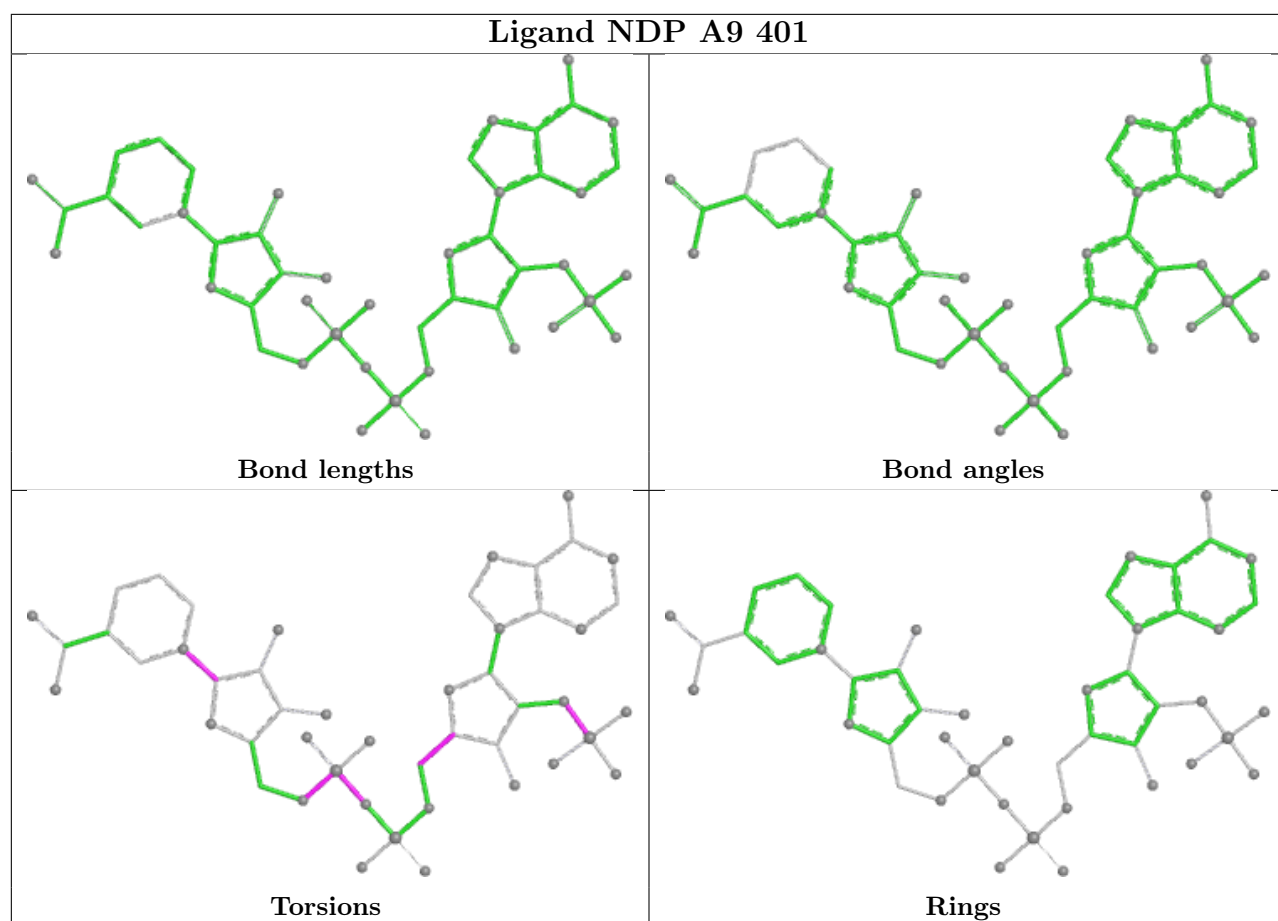


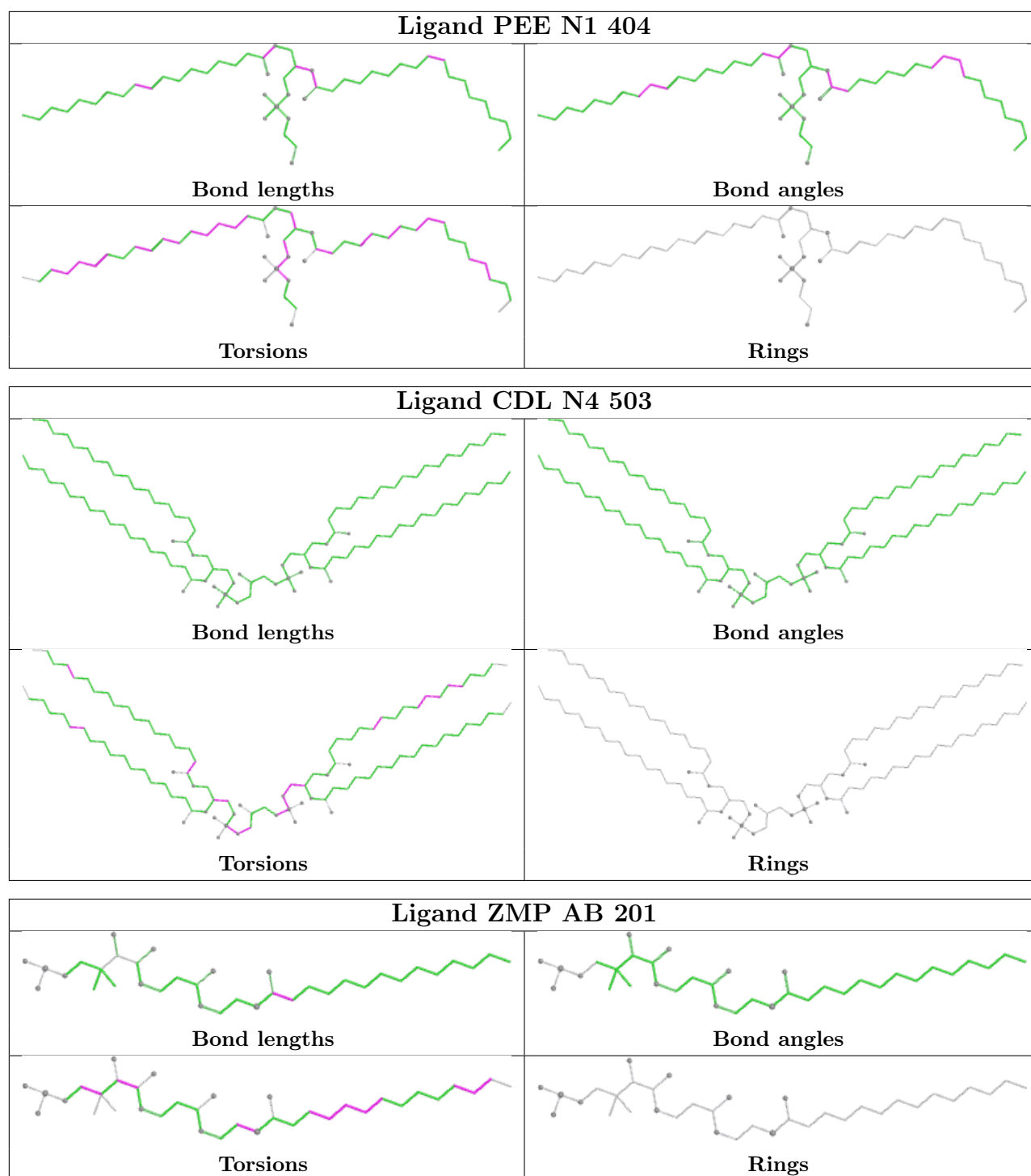


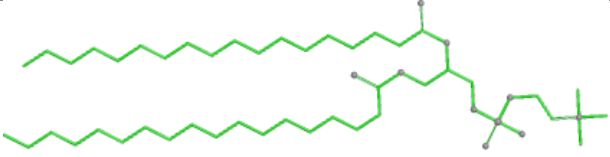
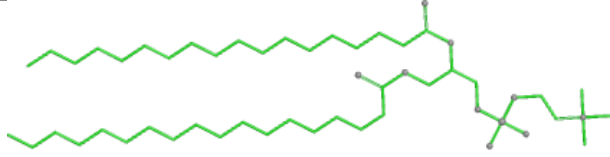
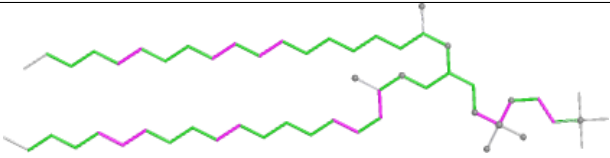
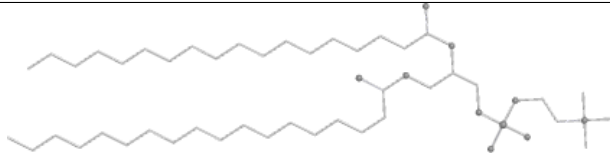
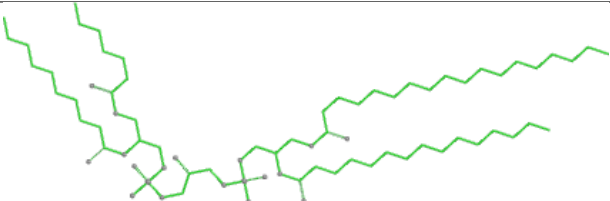
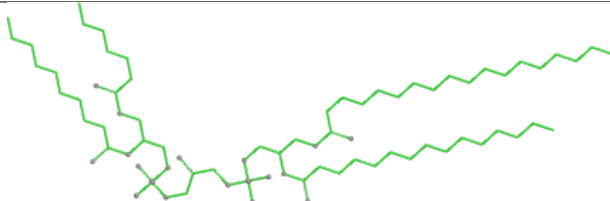
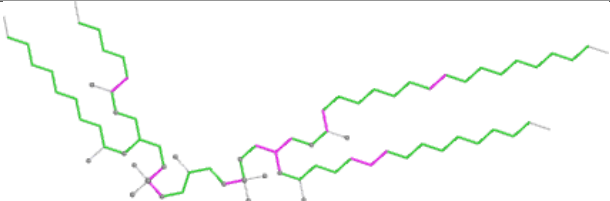
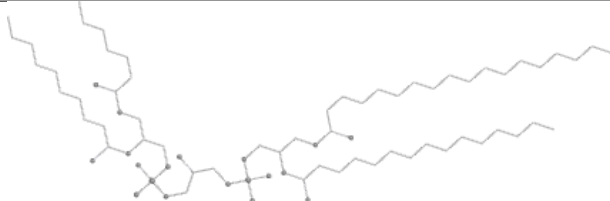
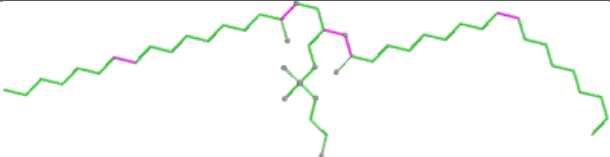
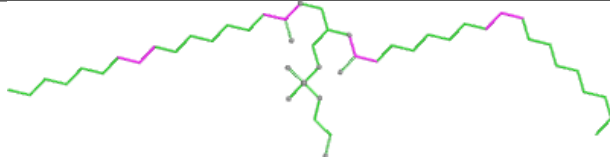
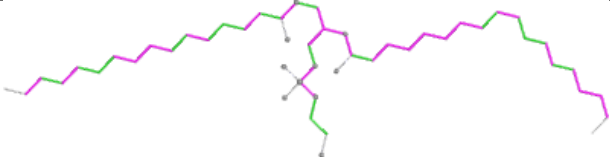
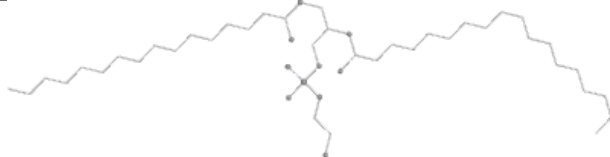


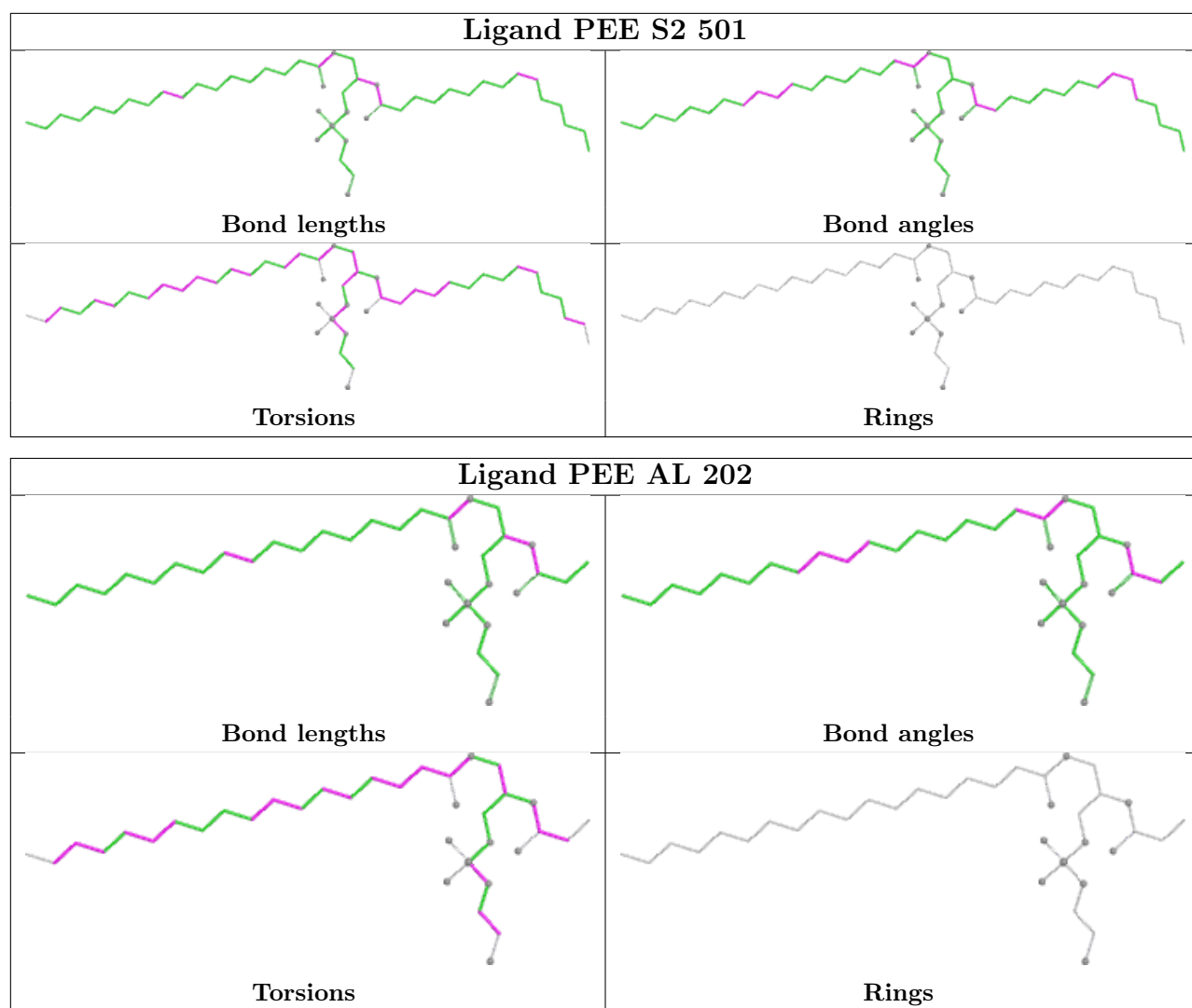


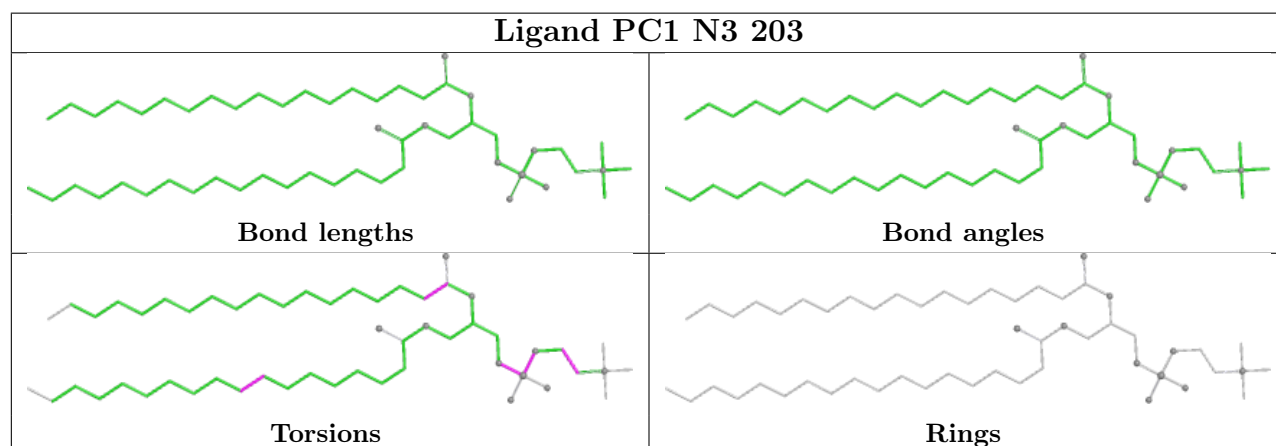
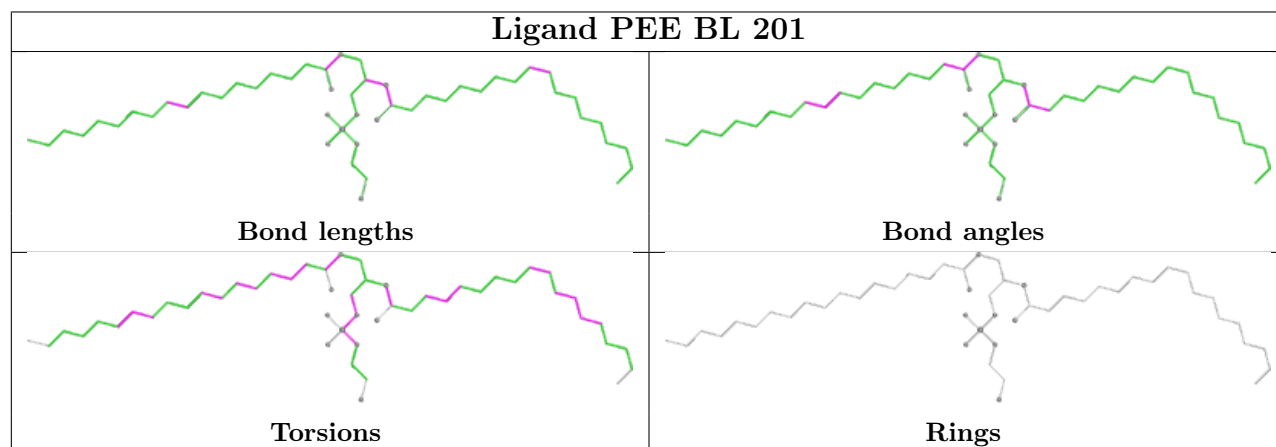
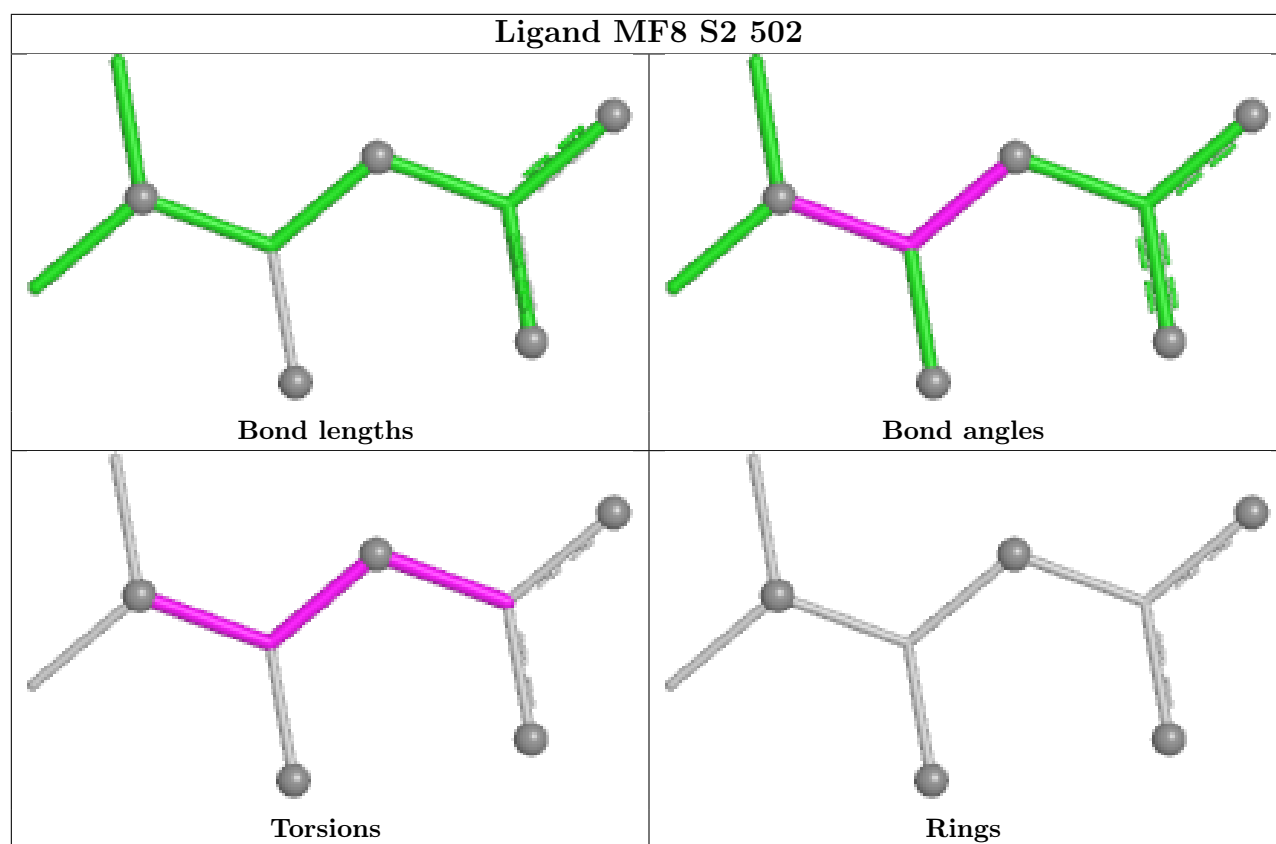


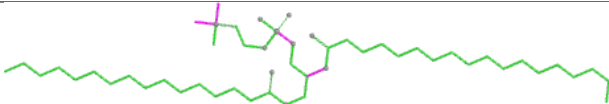
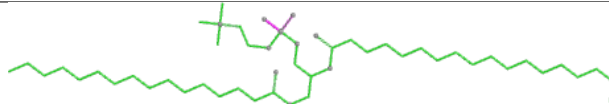
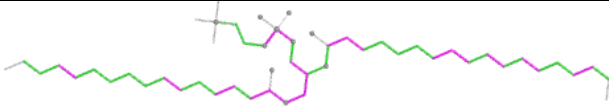
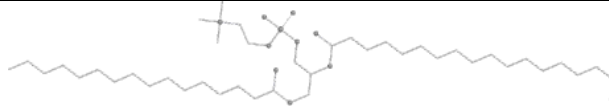


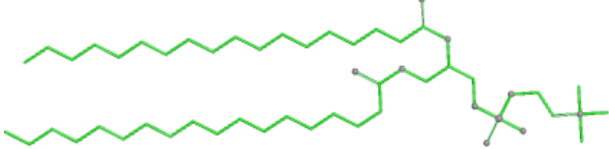
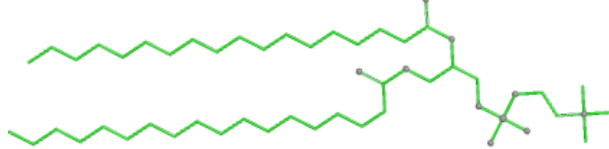
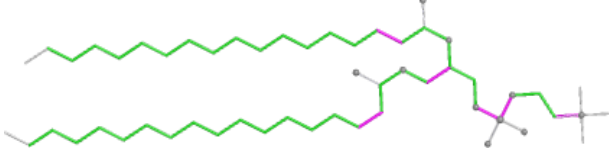
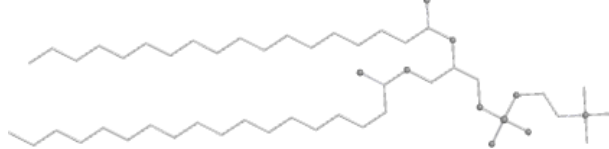


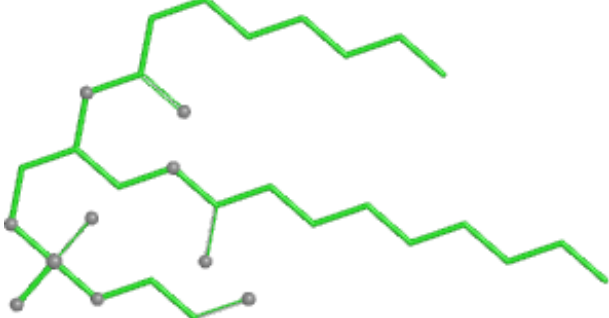
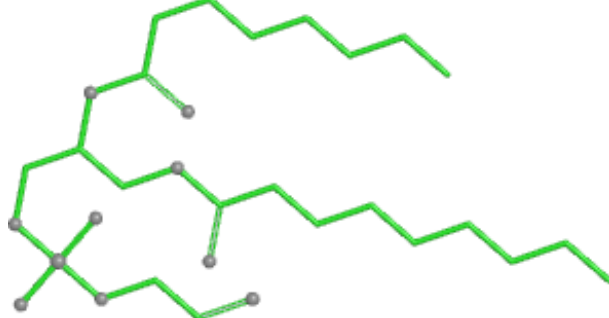
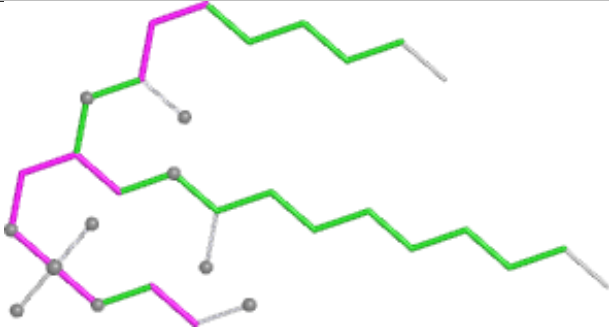
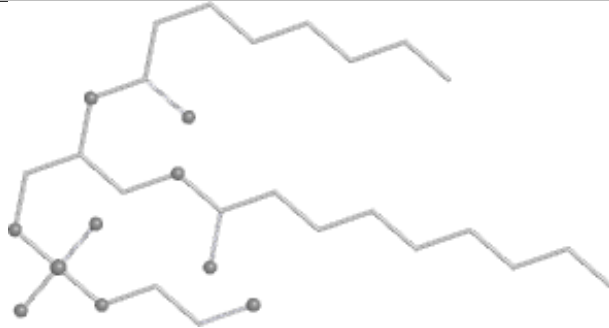
Ligand PC1 N3 201	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CDL N1 401	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEE N4 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

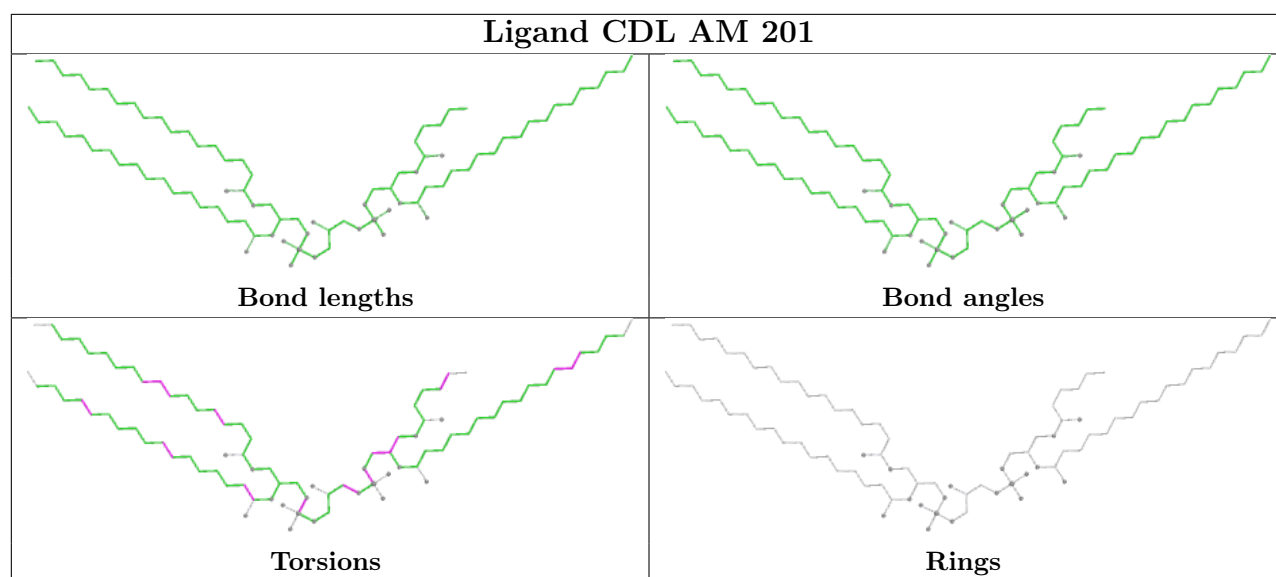




Ligand PLX S7 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PC1 B5 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 3PE B8 201	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

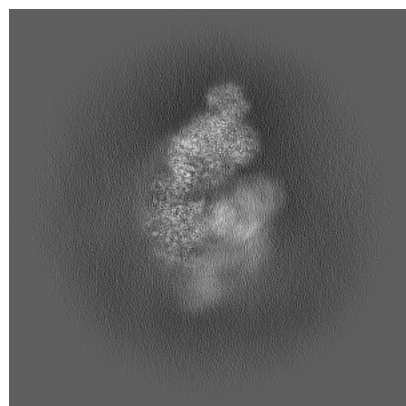
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60418. These allow visual inspection of the internal detail of the map and identification of artifacts.

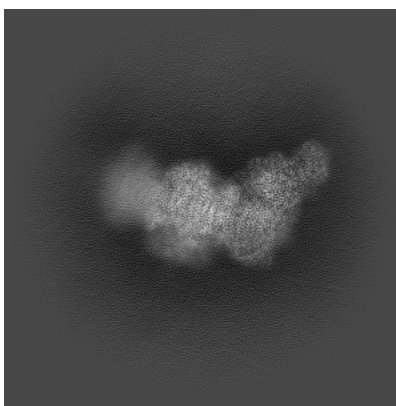
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

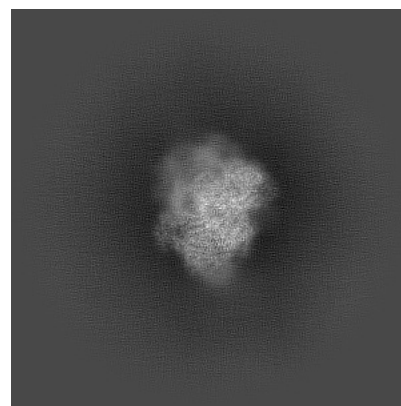
6.1.1 Primary map



X

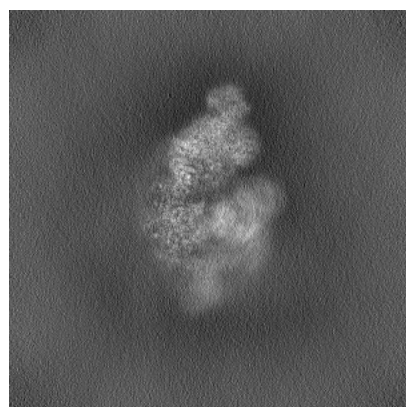


Y

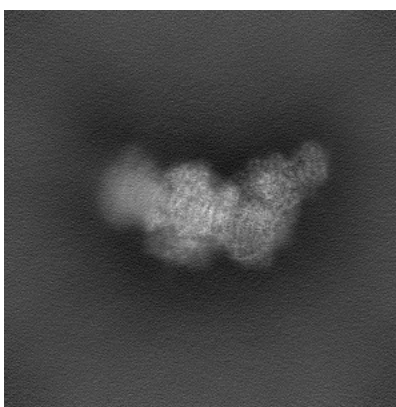


Z

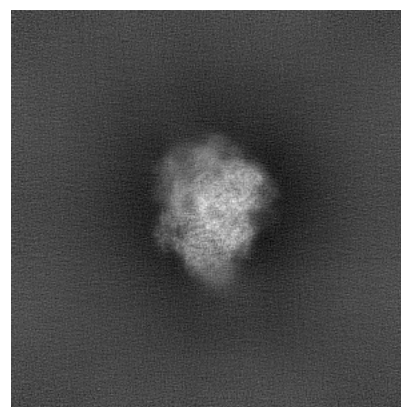
6.1.2 Raw map



X



Y

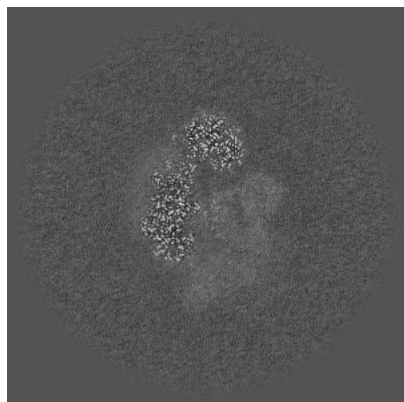


Z

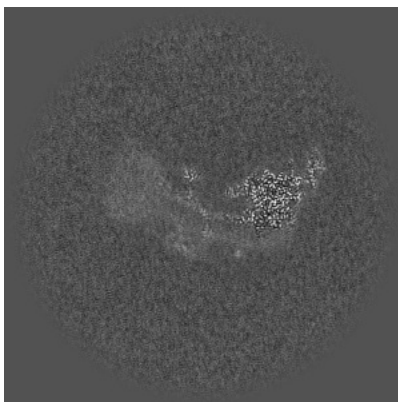
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

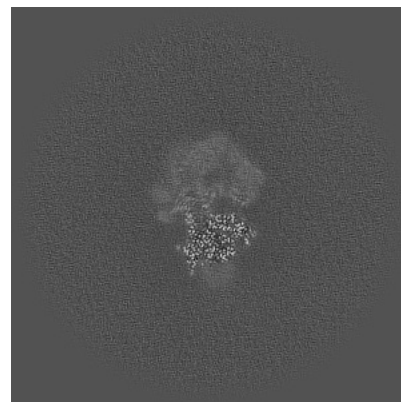
6.2.1 Primary map



X Index: 240

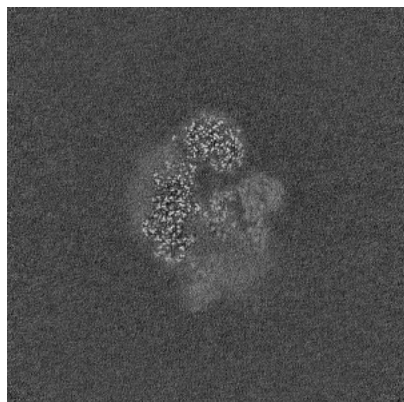


Y Index: 240

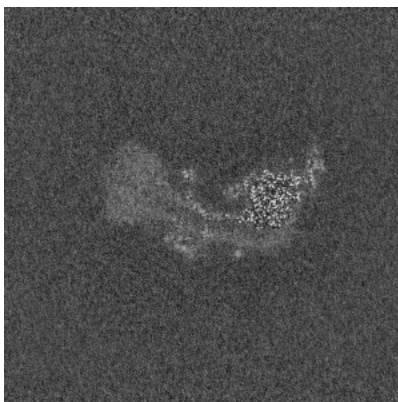


Z Index: 240

6.2.2 Raw map



X Index: 240



Y Index: 240

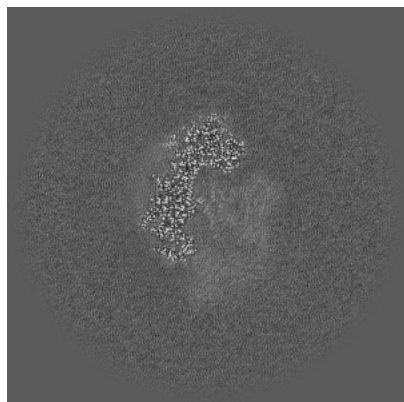


Z Index: 240

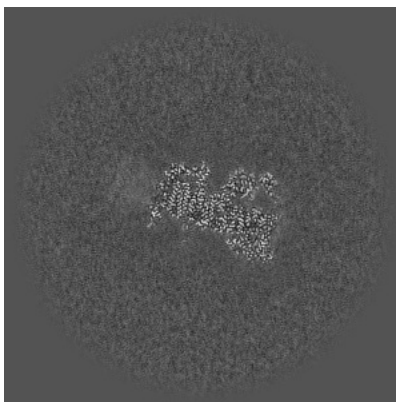
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

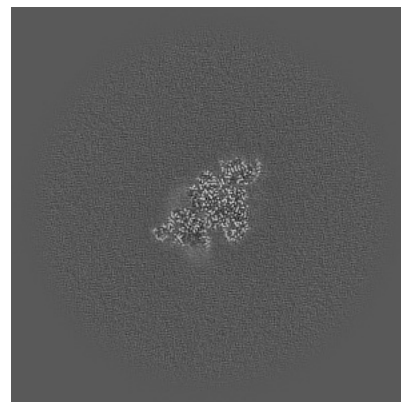
6.3.1 Primary map



X Index: 235

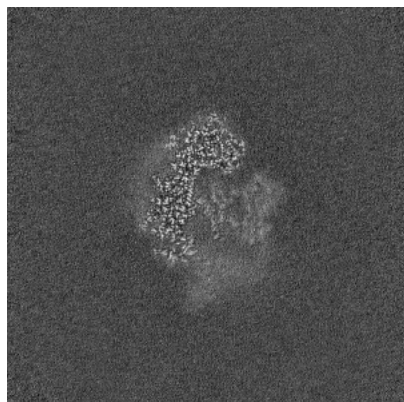


Y Index: 206

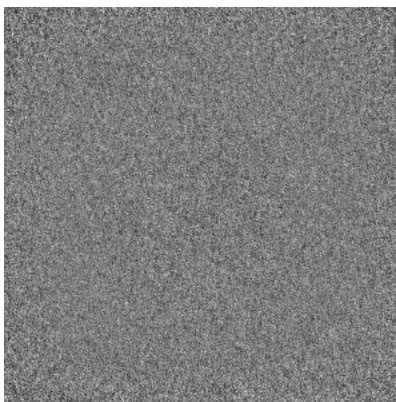


Z Index: 315

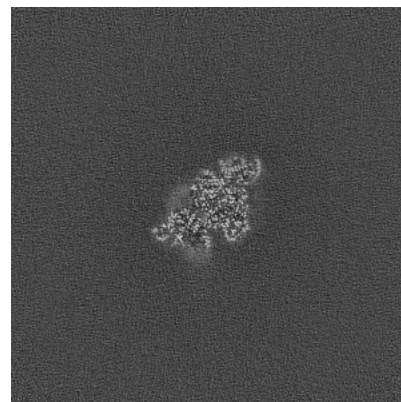
6.3.2 Raw map



X Index: 235



Y Index: 0

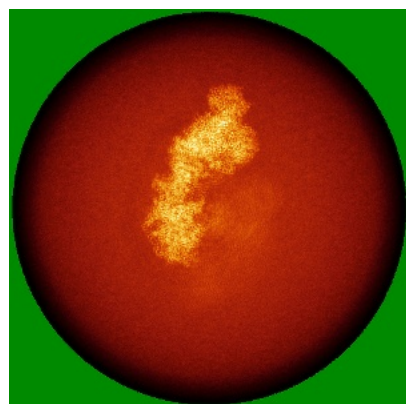


Z Index: 314

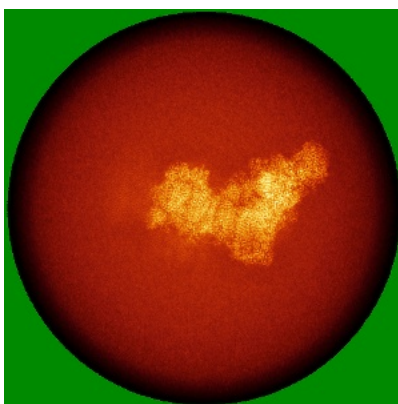
The images above show the largest variance slices of the map in three orthogonal directions.

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

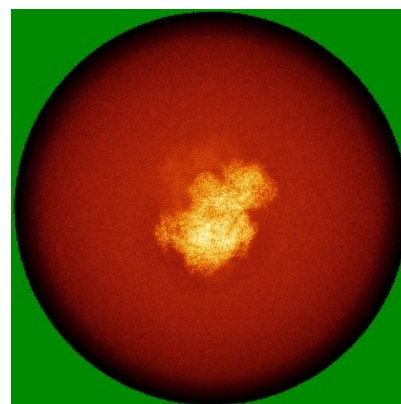
6.4.1 Primary map



X

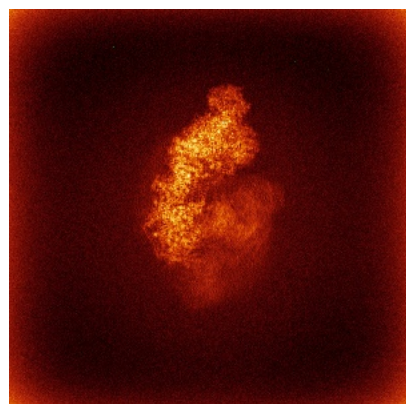


Y

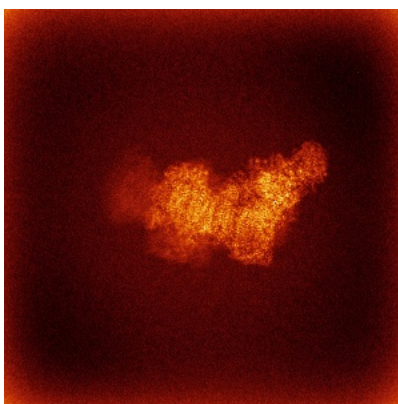


Z

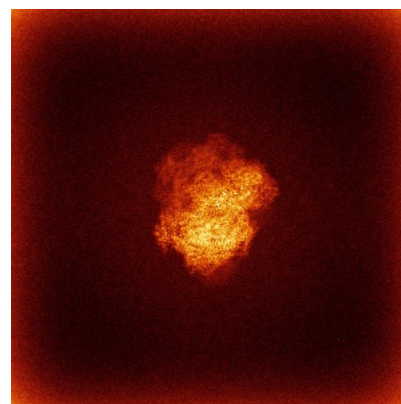
6.4.2 Raw map



X



Y

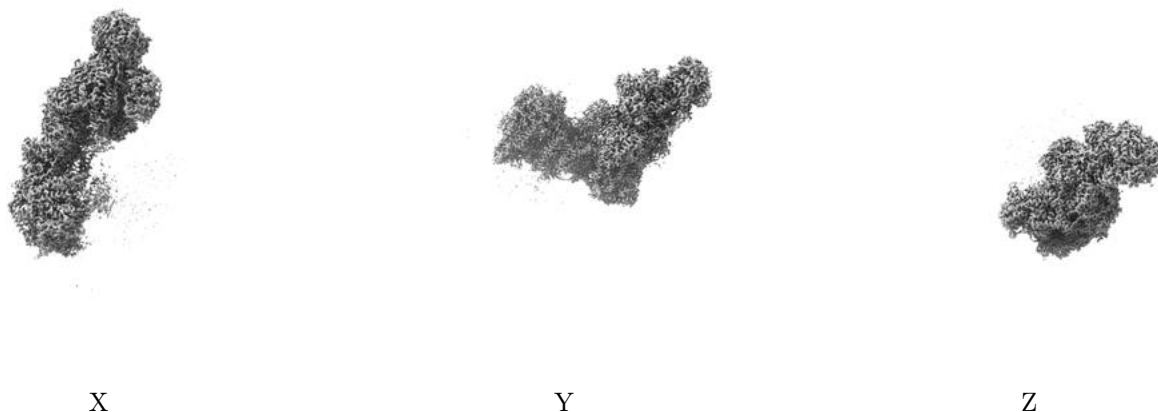


Z

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.

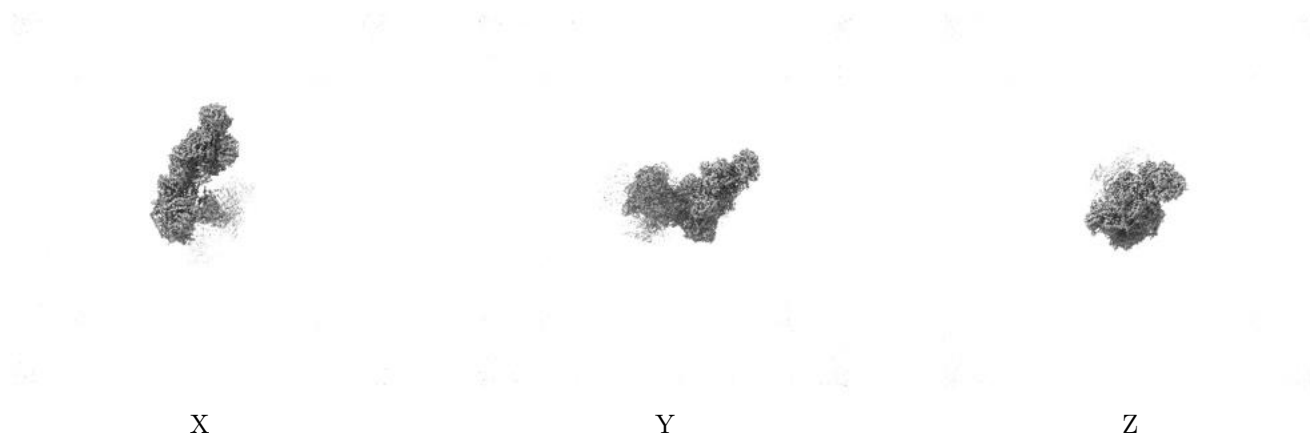
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

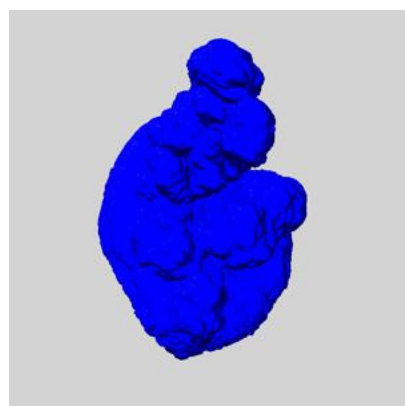
6.6 Mask visualisation [i](#)

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

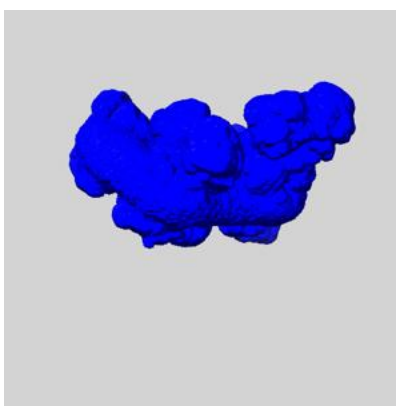
A mask typically either:

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

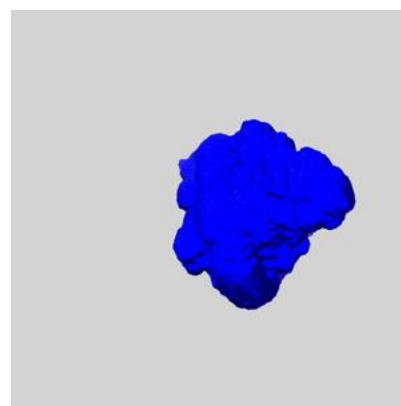
6.6.1 emd_60418_msk_1.map [i](#)



X



Y

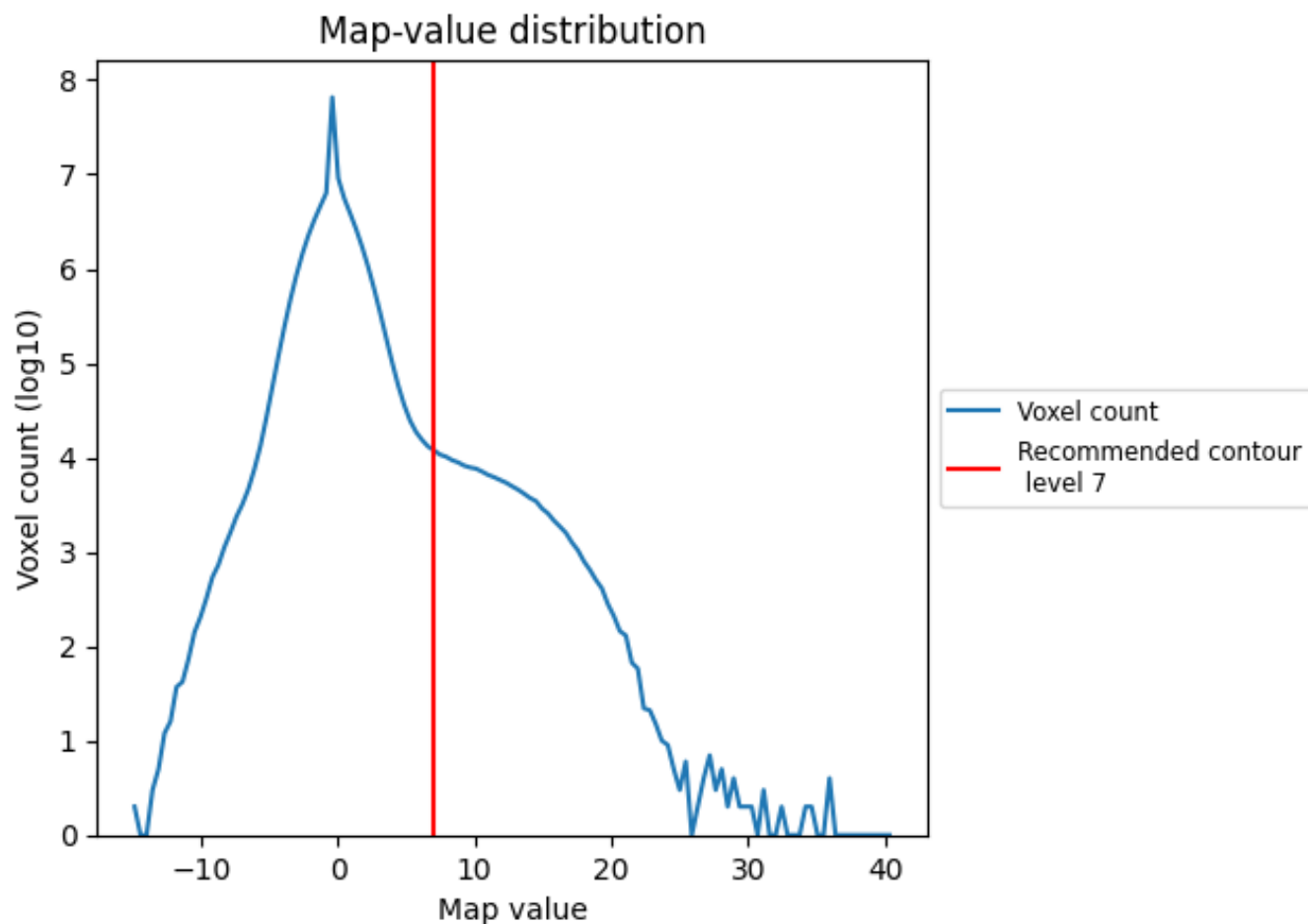


Z

7 Map analysis [i](#)

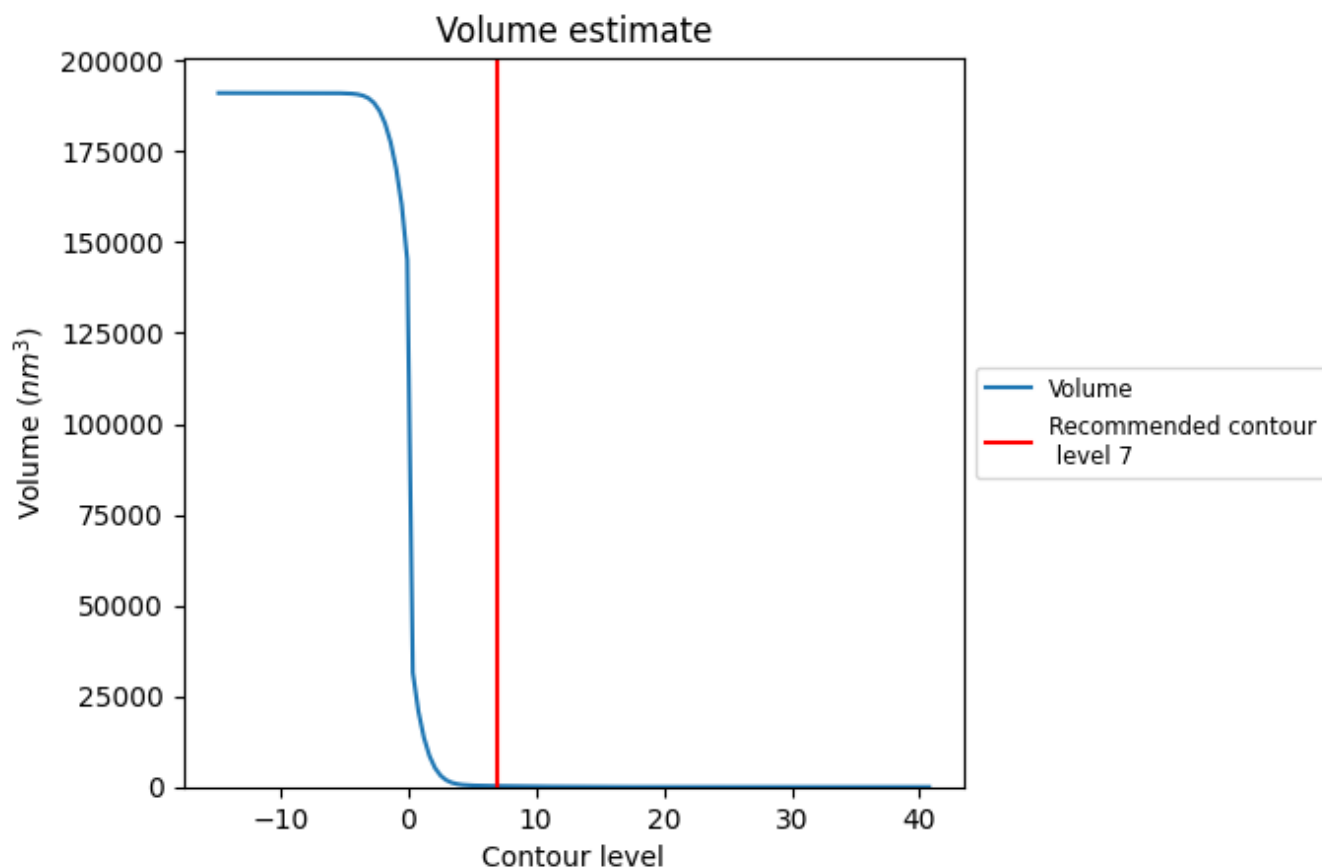
This section contains the results of statistical analysis of the map.

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.

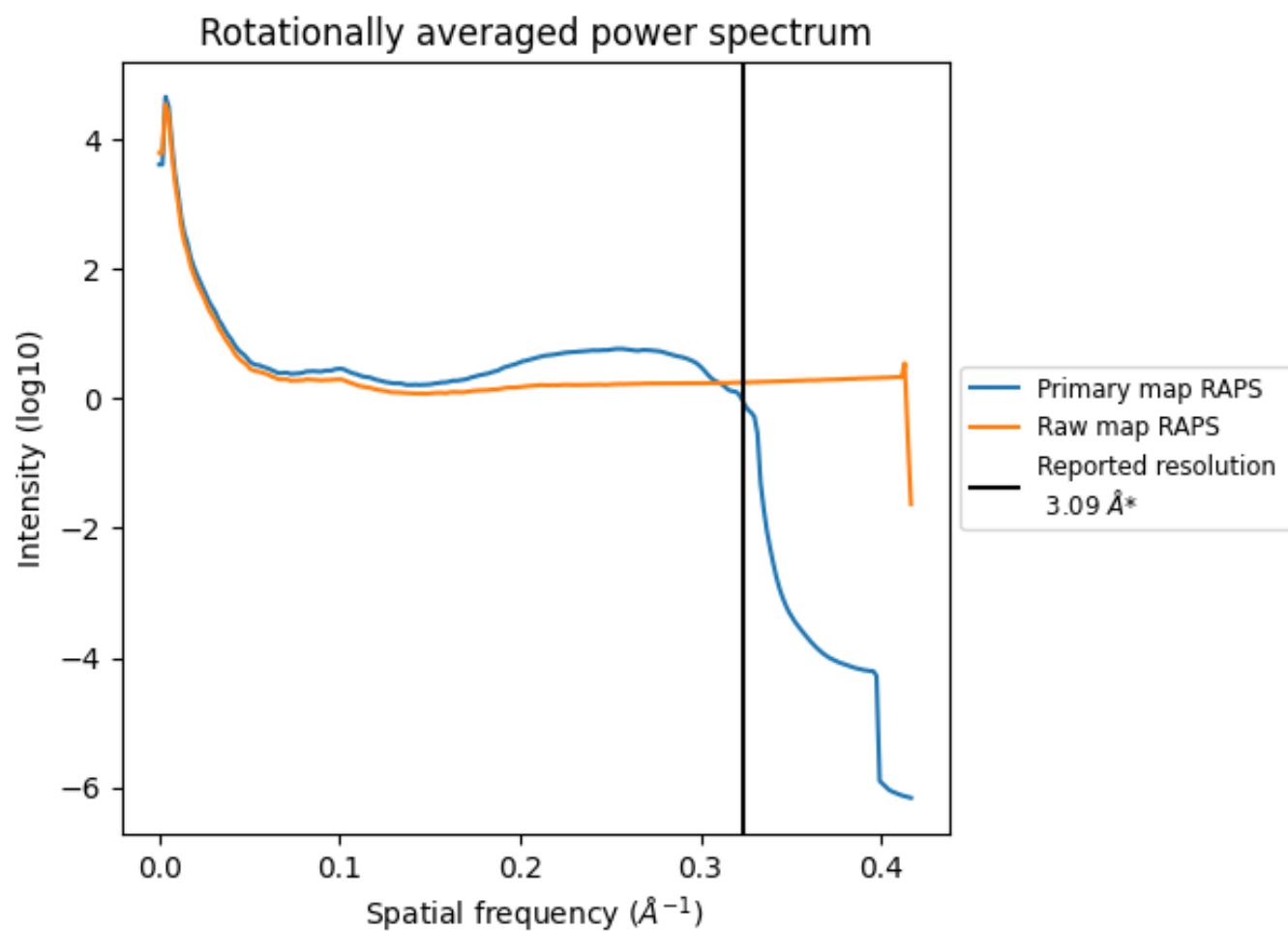
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 251 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 ⓘ

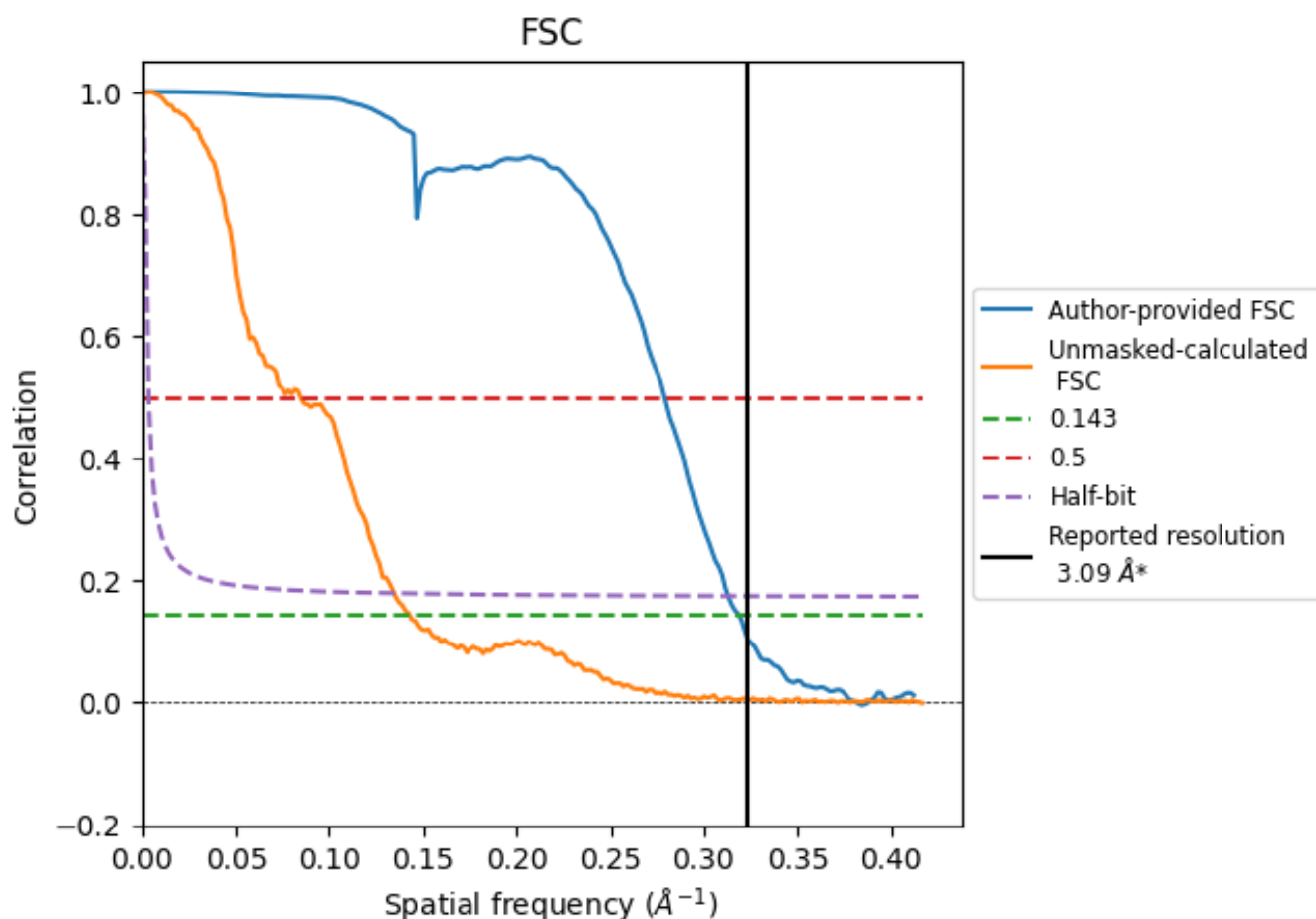


*Reported resolution corresponds to spatial frequency of 0.324 Å⁻¹

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 0.324 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

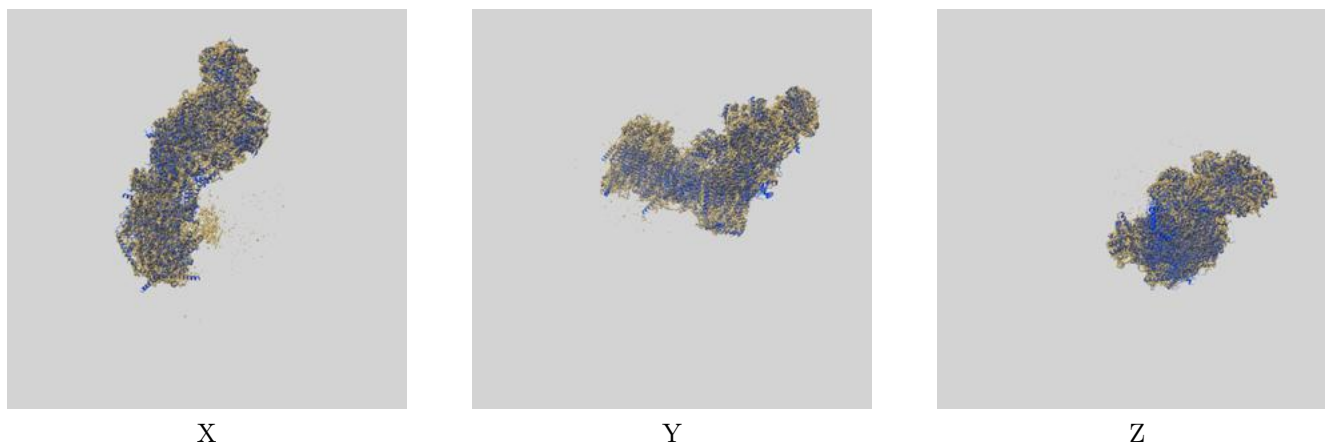
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.14	3.58	3.19
Unmasked-calculated*	7.00	11.79	7.43

*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 7.00 differs from the reported value 3.09 by more than 10 %

9 Map-model fit [i](#)

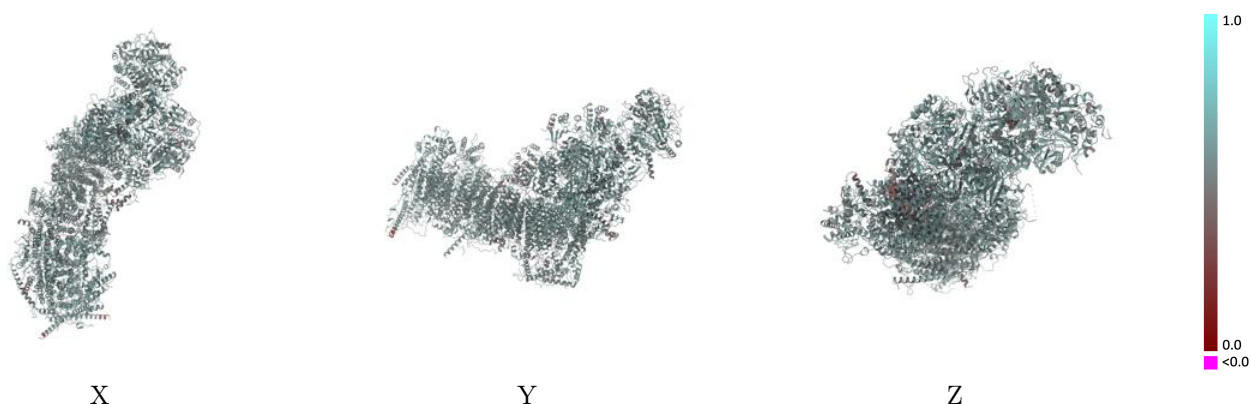
This section contains information regarding the fit between EMDB map EMD-60418 and PDB model 8ZSK. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



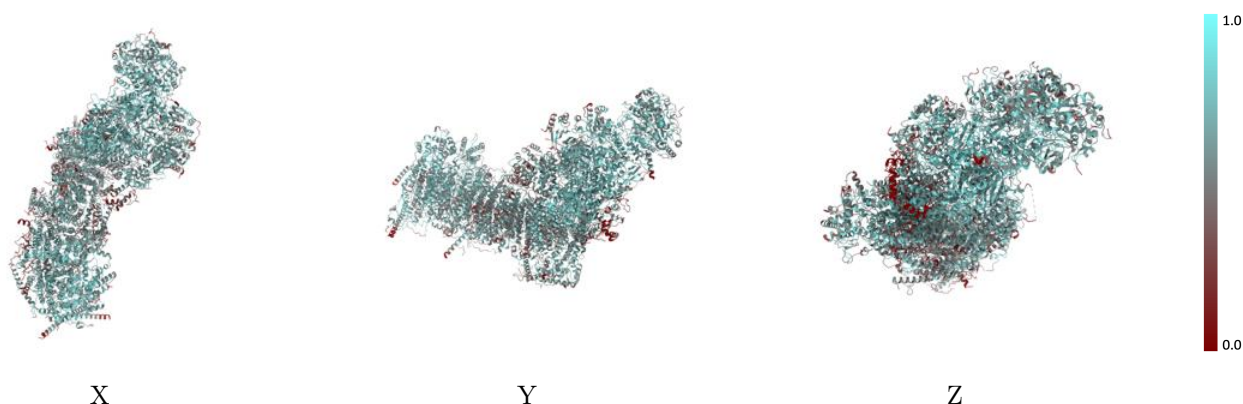
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



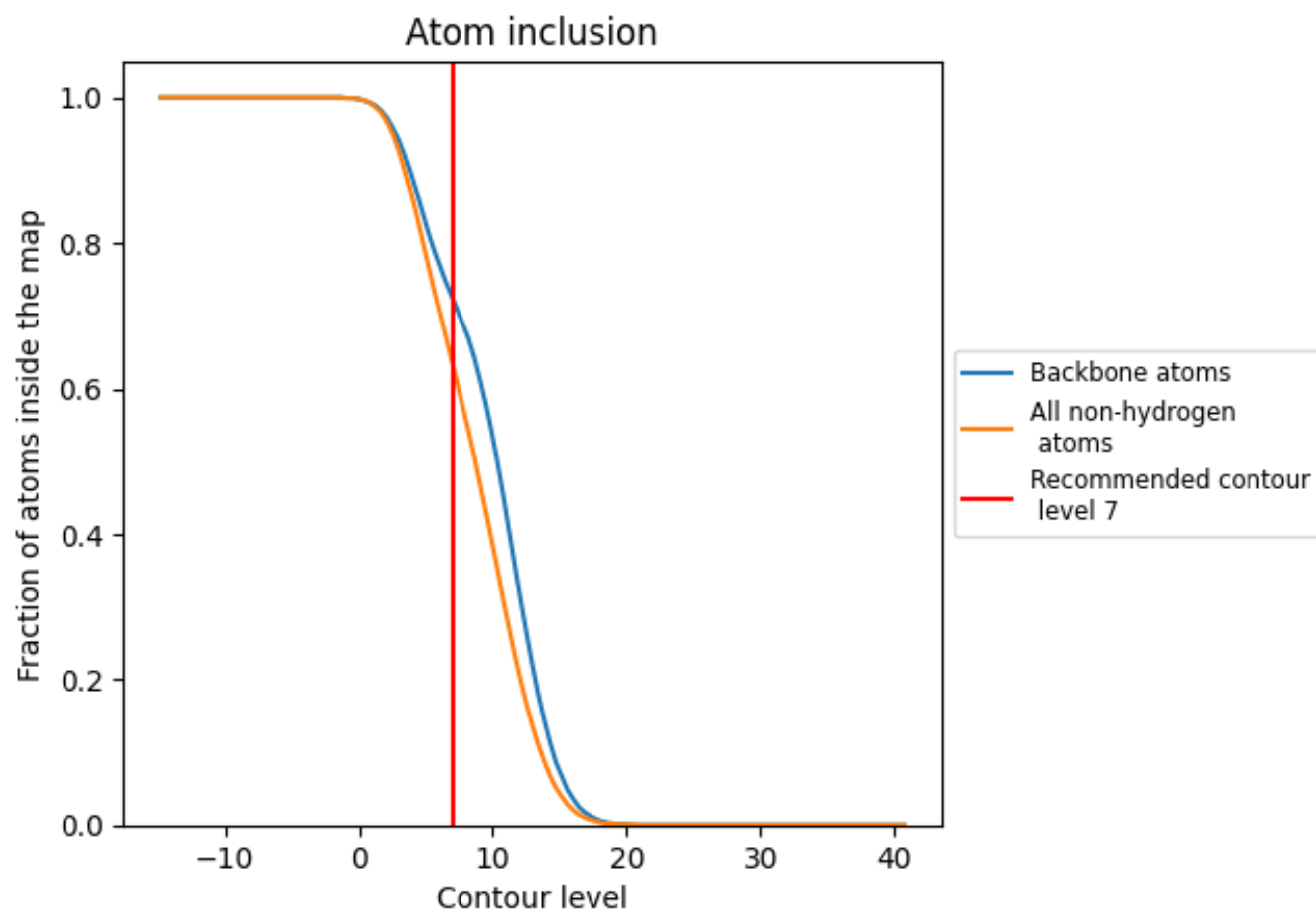
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 63% 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	 0.6320	 0.5570
4L	 0.6400	 0.5670
A1	 0.6440	 0.5530
A2	 0.5310	 0.5370
A3	 0.5110	 0.5470
A5	 0.6320	 0.5610
A6	 0.6460	 0.5590
A7	 0.4000	 0.5110
A8	 0.6170	 0.5580
A9	 0.6880	 0.5710
AB	 0.3500	 0.4720
AC	 0.6630	 0.5670
AK	 0.5510	 0.5320
AL	 0.4890	 0.5370
AM	 0.3100	 0.5220
AN	 0.5650	 0.5430
B1	 0.4710	 0.5340
B2	 0.6410	 0.5530
B3	 0.5630	 0.5320
B4	 0.5460	 0.5570
B5	 0.6160	 0.5670
B6	 0.5590	 0.5270
B7	 0.6390	 0.5420
B8	 0.6800	 0.5700
B9	 0.7040	 0.5670
BK	 0.6300	 0.5520
BL	 0.5820	 0.5550
CA	 0.4640	 0.5410
CB	 0.6120	 0.5620
N1	 0.6500	 0.5610
N2	 0.6750	 0.5650
N3	 0.5970	 0.5600
N4	 0.6960	 0.5690
N5	 0.6830	 0.5710
N6	 0.5700	 0.5230



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
S1	 0.6700	 0.5600
S2	 0.7310	 0.5760
S3	 0.7470	 0.5890
S4	 0.6690	 0.5720
S5	 0.5720	 0.5370
S6	 0.5730	 0.5490
S7	 0.7450	 0.5790
S8	 0.7510	 0.5850
V1	 0.6510	 0.5520
V2	 0.5990	 0.5460
V3	 0.5260	 0.5430