



Full wwPDB EM Validation Report ⓘ

Nov 11, 2025 – 09:36 PM JST

PDB ID : 9J6W / pdb_00009j6w
EMDB ID : EMD-61186
Title : Complex I from respirasome closed state 1 bound by metformin and CoQ10 (SC-MetC1-v)
Authors : Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.
Deposited on : 2024-08-17
Resolution : 2.99 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

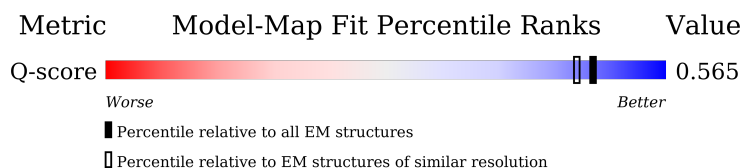
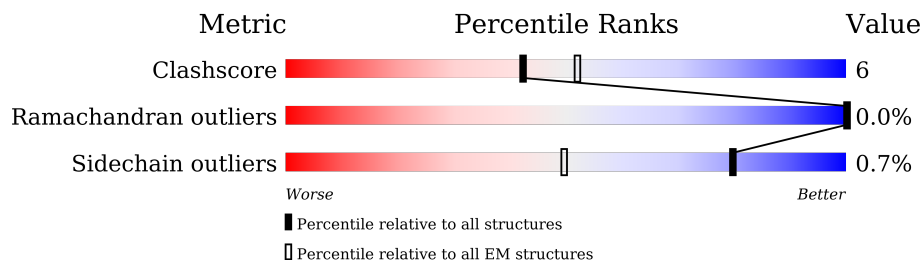
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.99 Å.

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



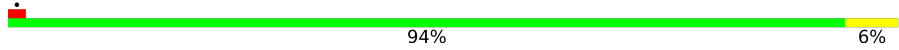




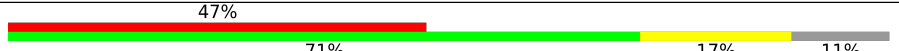
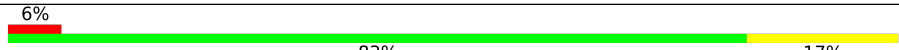

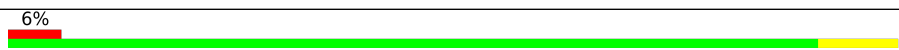
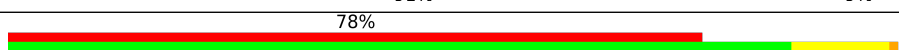
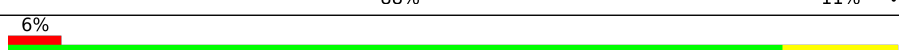
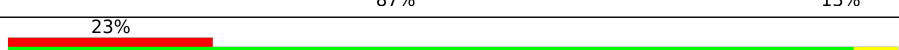
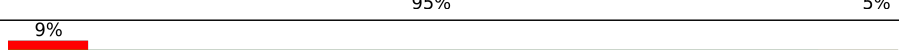
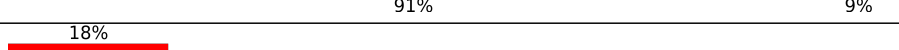
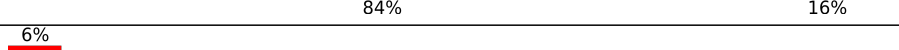
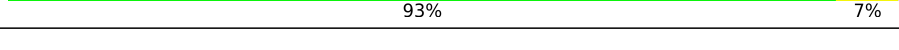
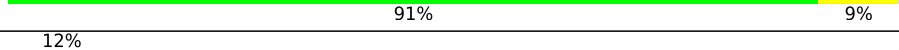


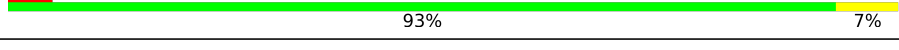

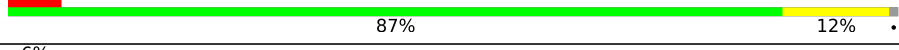
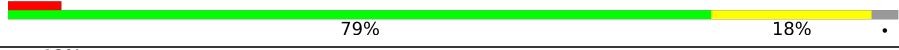
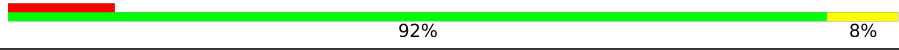

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13287 (2.49 - 3.49)

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	



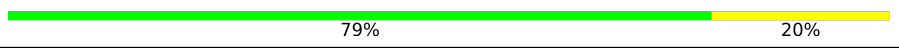




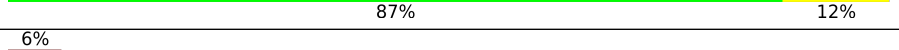
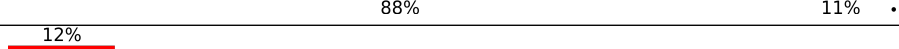
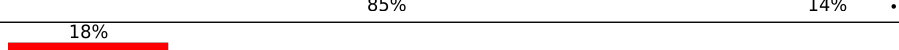
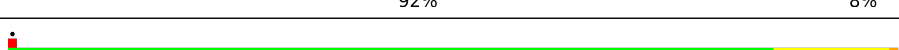
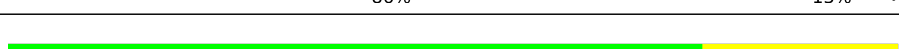


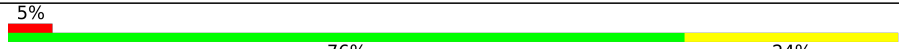

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Mol	Chain	Length	Quality of chain
5	A5	112	
6	A6	114	
7	A7	112	
8	A8	171	
9	A9	341	
10	AB	87	
10	AC	87	
11	AK	321	
12	AL	140	
13	AM	144	
14	AN	142	
15	B1	56	
16	B2	67	
17	B3	80	
18	B4	128	
19	B5	138	
20	B6	126	
21	B7	125	
22	B8	156	
23	B9	178	
24	BK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

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

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 68554 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 10 is a protein called Acyl carrier protein.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	321	Total	C	N	O	S	0	0
			2601	1655	444	492	10		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

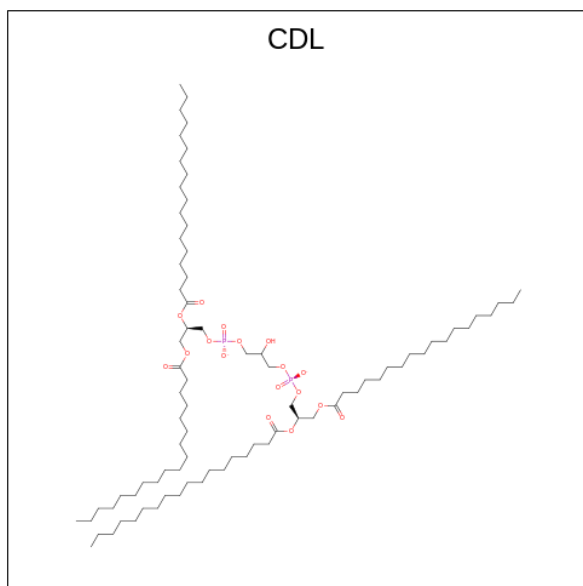
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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

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

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

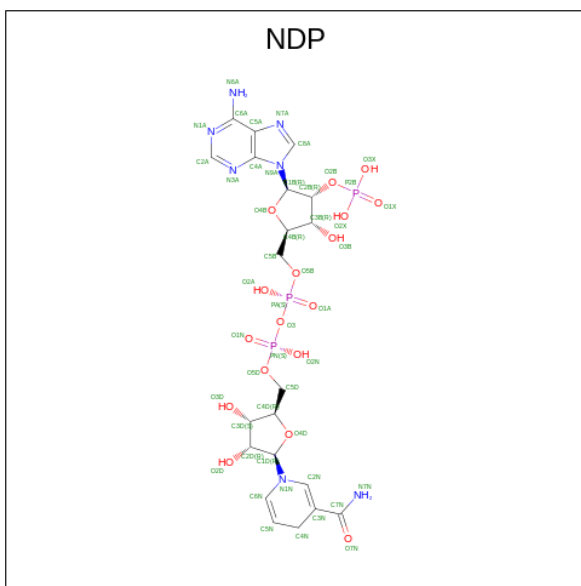
- Molecule 45 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
45	4L	1	Total	C	O	P	0
			92	73	17	2	
45	A7	1	Total	C	O	P	0
			51	32	17	2	
45	A8	1	Total	C	O	P	0
			83	64	17	2	
45	AK	1	Total	C	O	P	0
			68	49	17	2	
45	AL	1	Total	C	O	P	0
			94	75	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	N4	1	Total	C	O	P	0
			100	81	17	2	
45	N4	1	Total	C	O	P	0
			62	43	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	

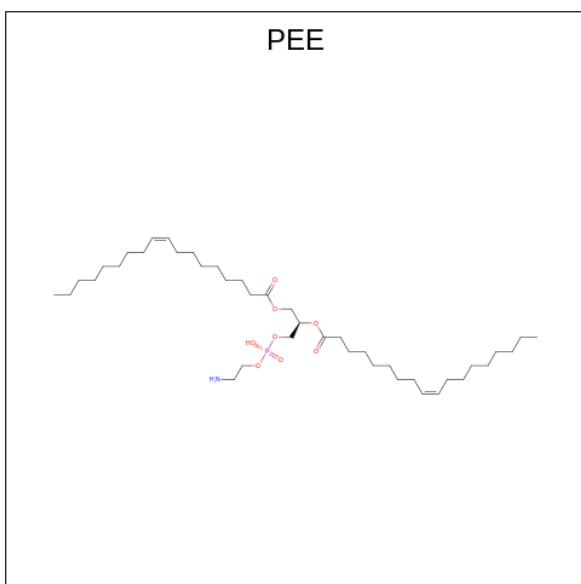
- Molecule 46 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



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

- Molecule 47 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



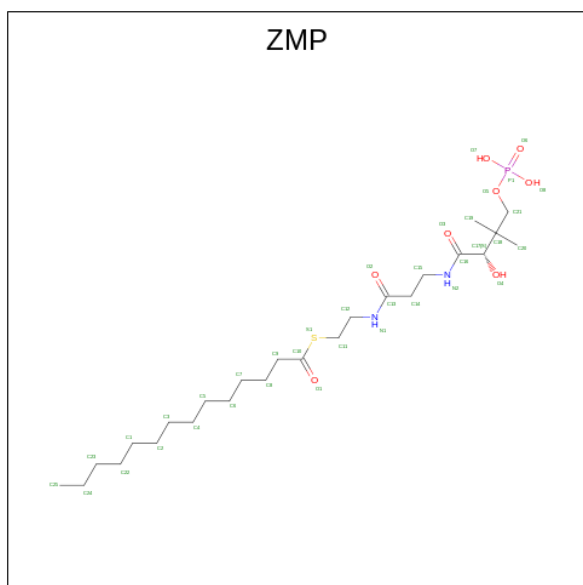
Mol	Chain	Residues	Atoms					AltConf
47	A9	1	Total 39	C 29	N 1	O 8	P 1	0

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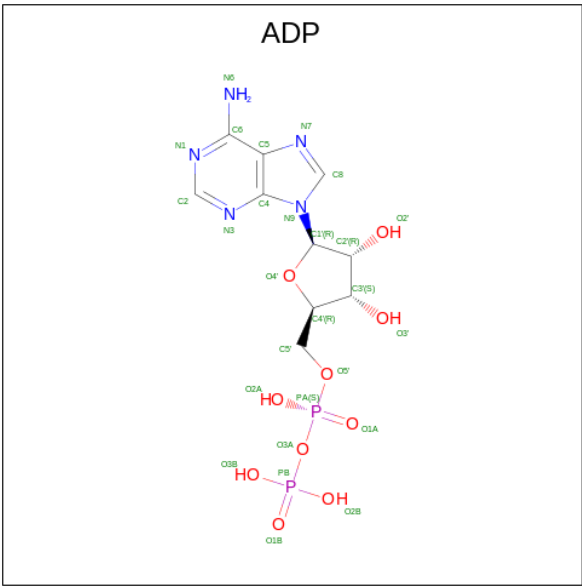
Mol	Chain	Residues	Atoms					AltConf
47	AL	1	Total	C	N	O	P	0
			49	39	1	8	1	
47	N1	1	Total	C	N	O	P	0
			31	21	1	8	1	
47	N3	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
47	N5	1	Total	C	N	O	P	0
			40	30	1	8	1	
47	N5	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	S2	1	Total	C	N	O	P	0
			48	38	1	8	1	
47	S8	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 48 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).



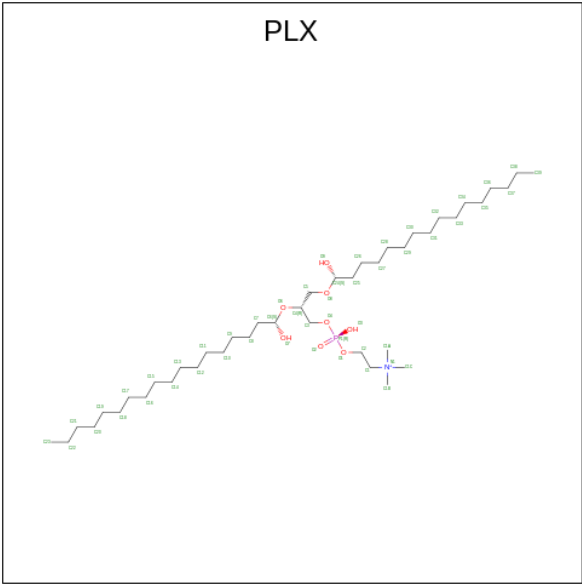
Mol	Chain	Residues	Atoms						AltConf
48	AB	1	Total 36	C 25	N 2	O 7	P 1	S 1	0
48	AC	1	Total 36	C 25	N 2	O 7	P 1	S 1	0

- Molecule 49 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 50 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P).



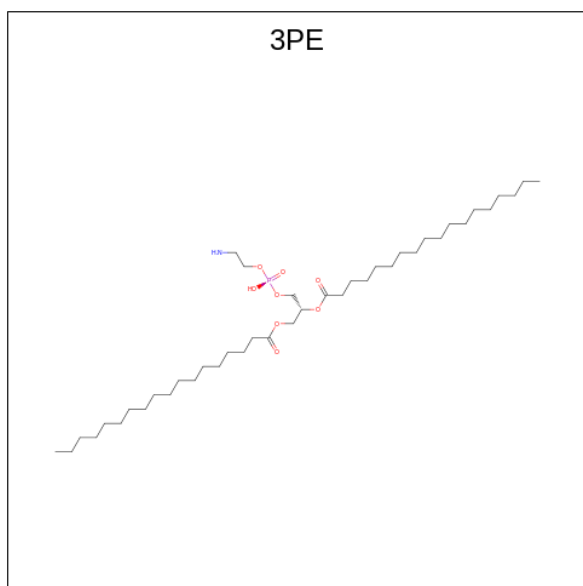
Mol	Chain	Residues	Atoms					AltConf
50	AL	1	Total	C	N	O	P	0
			47	37	1	8	1	

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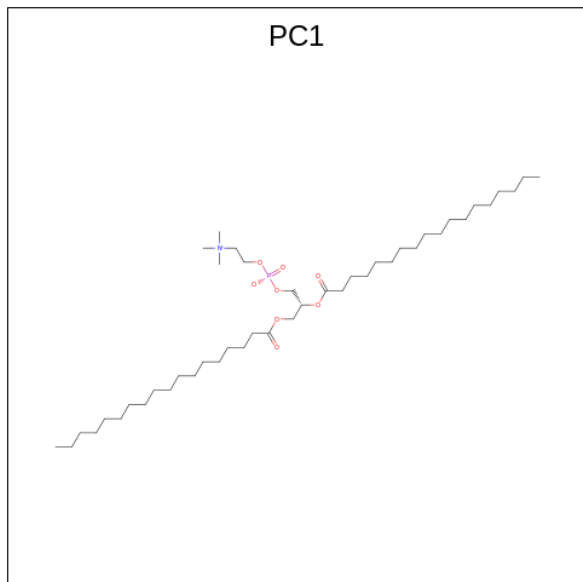
Mol	Chain	Residues	Atoms					AltConf
50	AM	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	B1	1	Total	C	N	O	P	0
			52	42	1	8	1	
50	CB	1	Total	C	N	O	P	0
			52	42	1	8	1	
50	N3	1	Total	C	N	O	P	0
			52	42	1	8	1	
50	N4	1	Total	C	N	O	P	0
			49	39	1	8	1	
50	S7	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 51 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



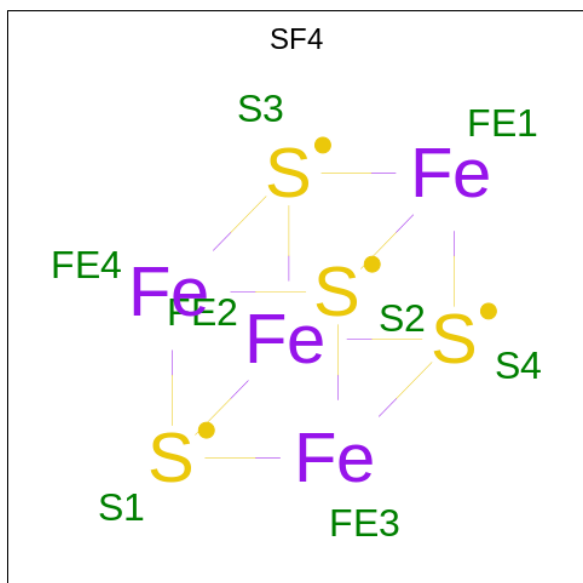
Mol	Chain	Residues	Atoms					AltConf
51	B8	1	Total	C	N	O	P	0
			32	22	1	8	1	
51	CA	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	CB	1	Total	C	N	O	P	0
			46	36	1	8	1	
51	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
51	S7	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 52 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



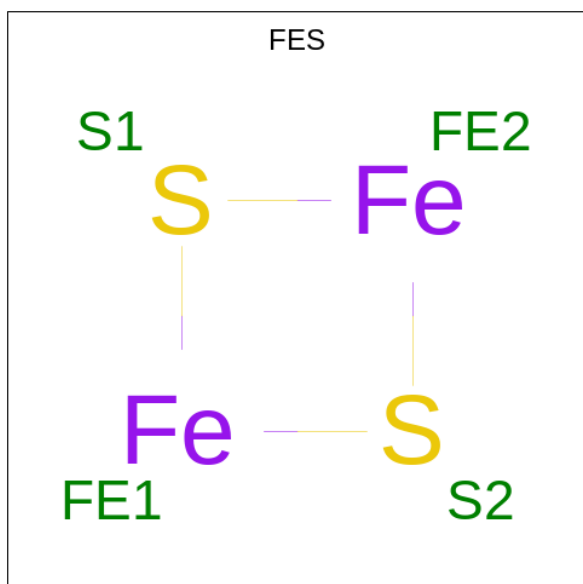
Mol	Chain	Residues	Atoms					AltConf
52	N1	1	Total	C	N	O	P	0
			48	38	1	8	1	
52	N3	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 53 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

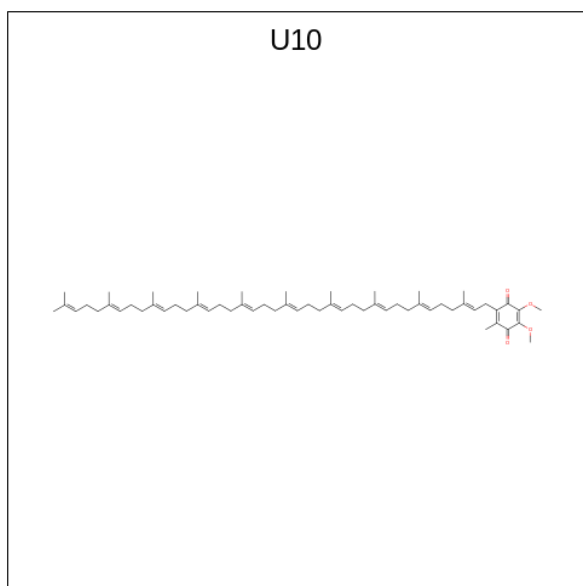
- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

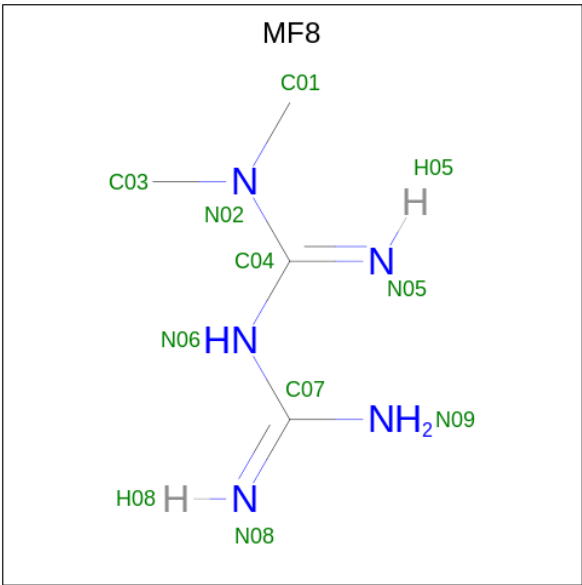
Mol	Chain	Residues	Atoms		AltConf
56	S6	1	Total	Zn	0
			1	1	

- Molecule 57 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



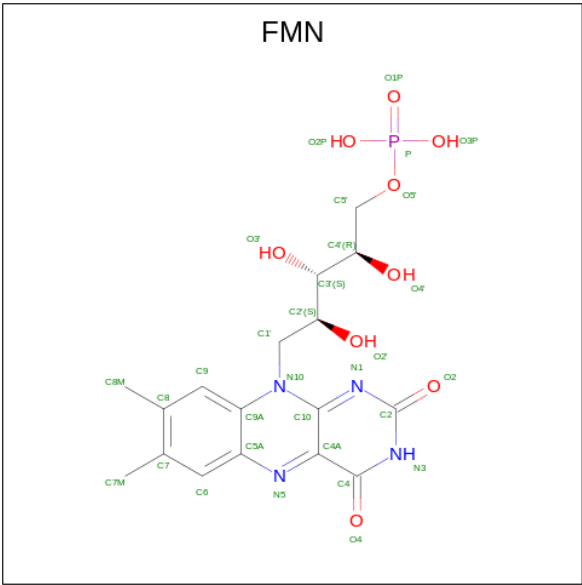
Mol	Chain	Residues	Atoms			AltConf
57	S7	1	Total	C	O	0
			63	59	4	

- Molecule 58 is Metformin (CCD ID: MF8) (formula: C₄H₁₁N₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
58	S7	1	Total	C	N	0
			9	4	5	

- Molecule 59 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

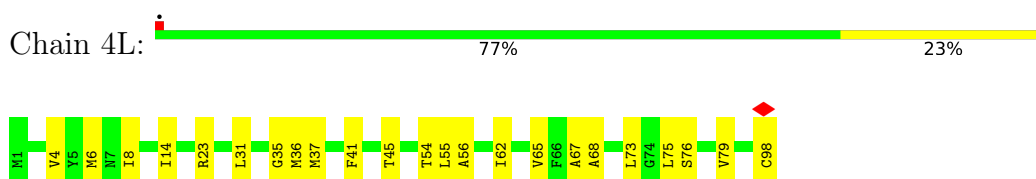


Mol	Chain	Residues	Atoms					AltConf
59	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

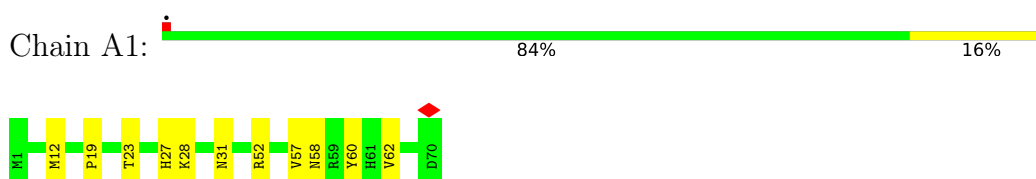
3 Residue-property plots [i](#)

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

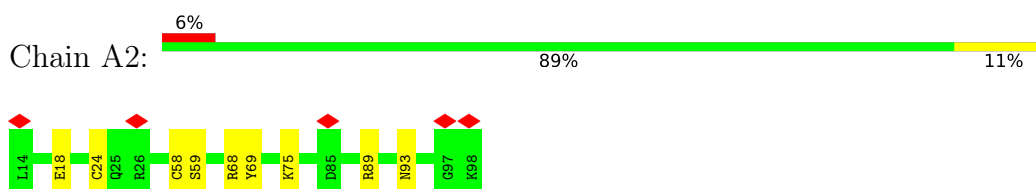
- Molecule 1: NADH-ubiquinone oxidoreductase chain 4L



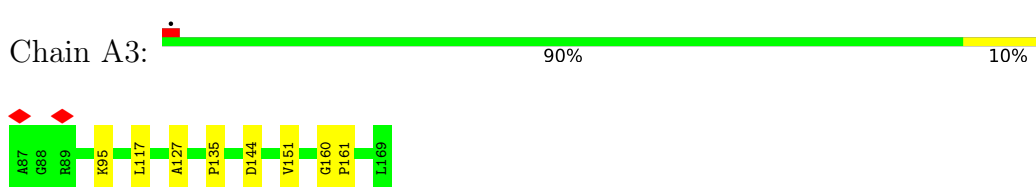
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



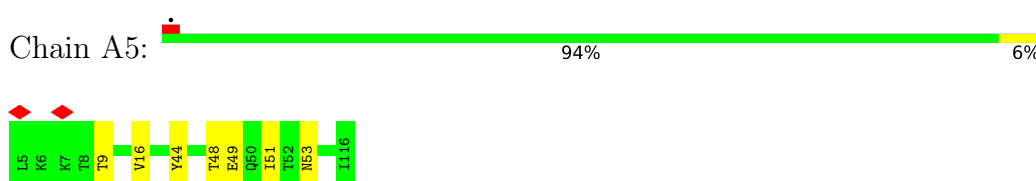
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



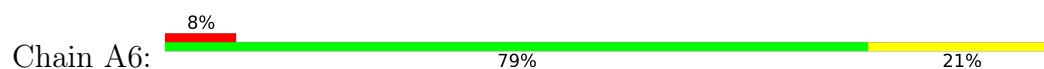
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



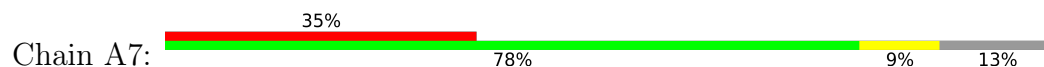
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



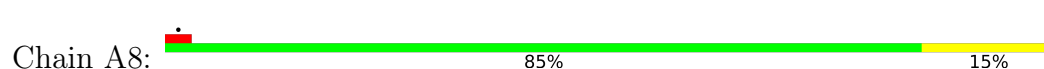
- Molecule 6: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



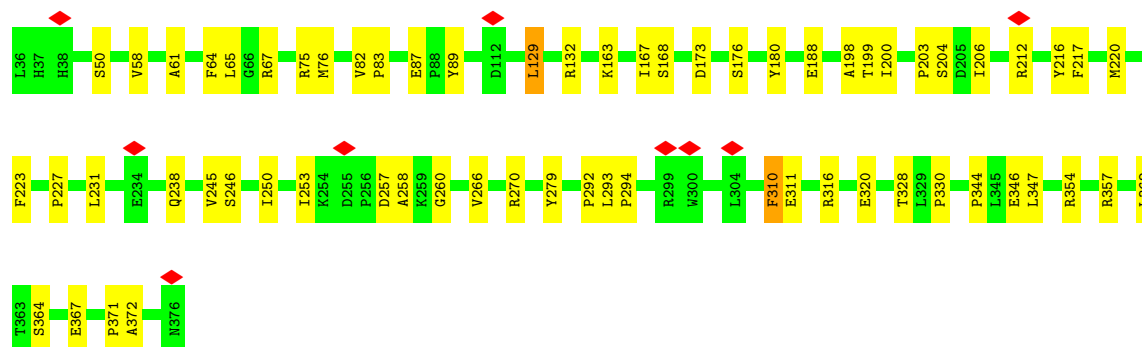
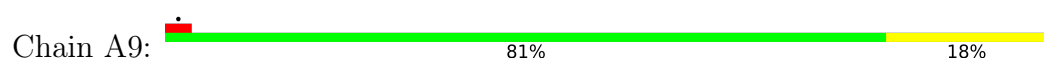
- Molecule 7: Complex I-B14.5a



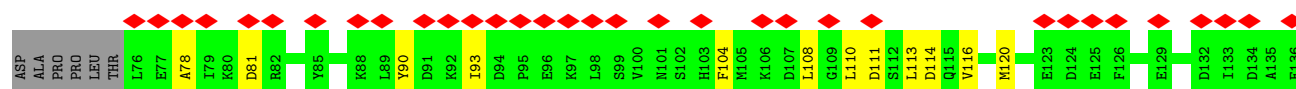
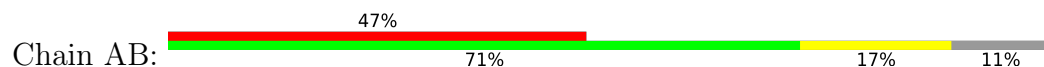
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

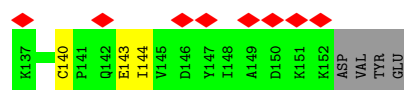


- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

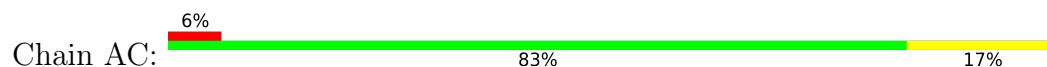


- Molecule 10: Acyl carrier protein

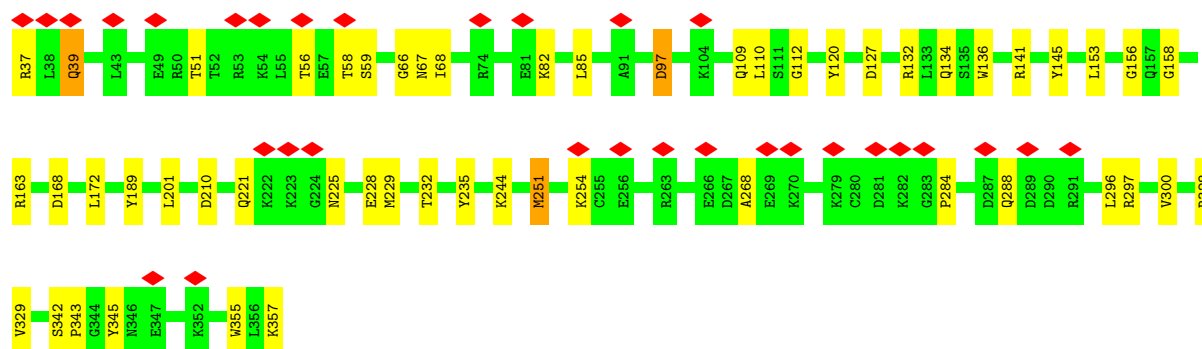
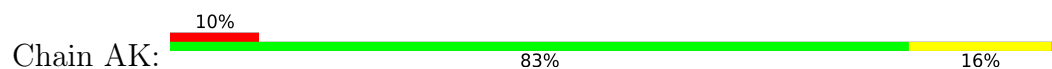




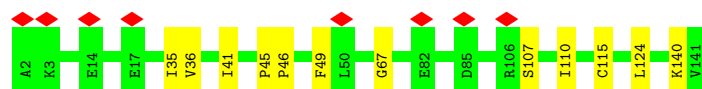
- Molecule 10: Acyl carrier protein



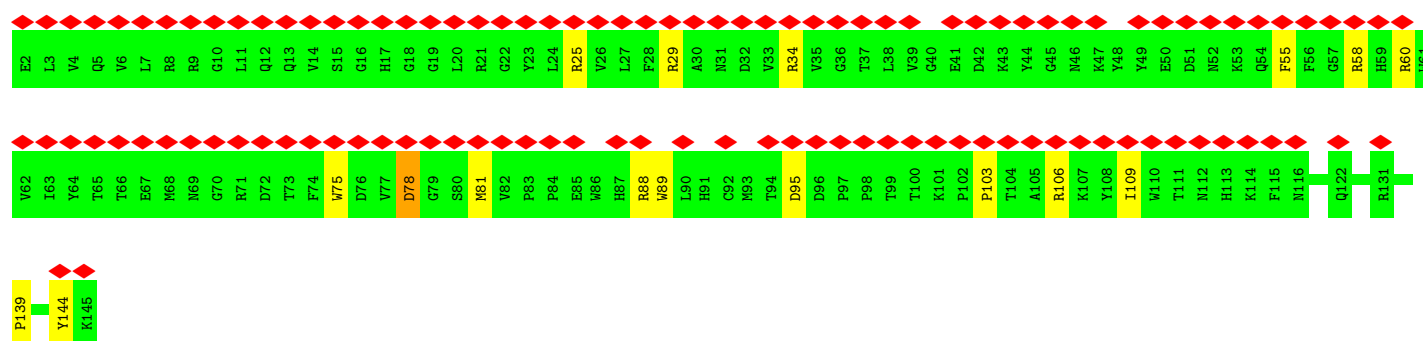
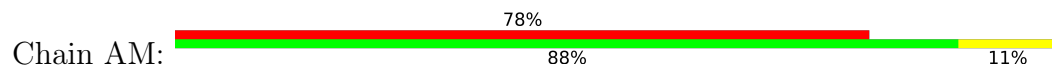
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



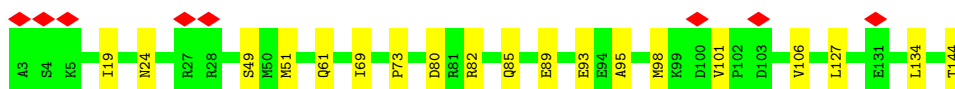
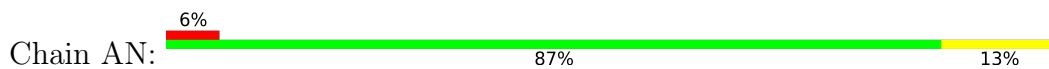
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



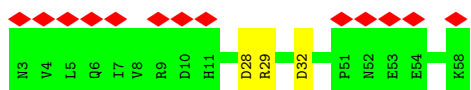
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



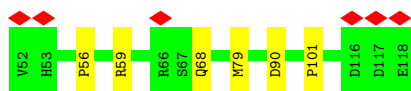
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



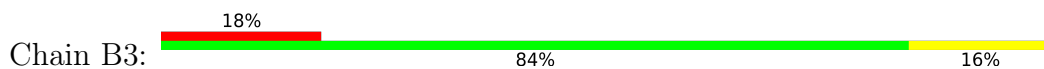
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



- 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

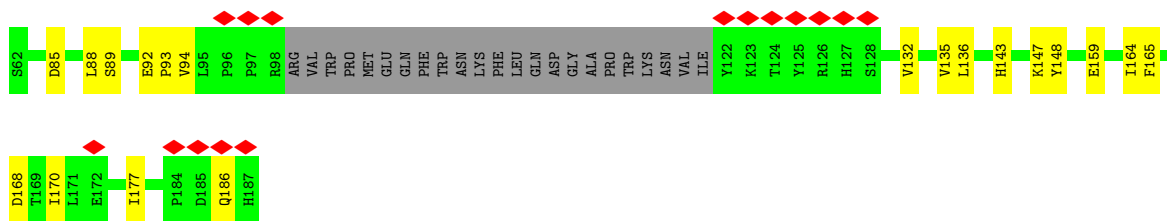


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

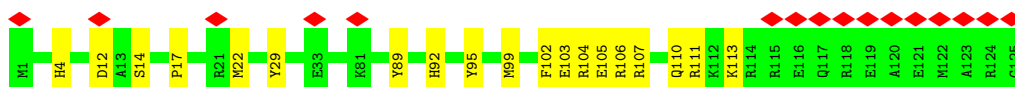
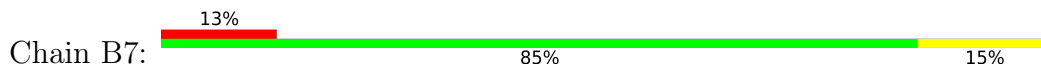


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

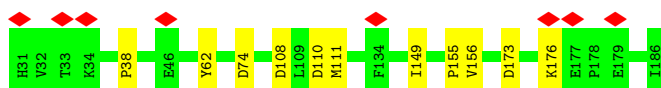




- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



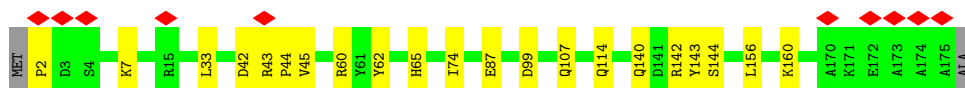
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



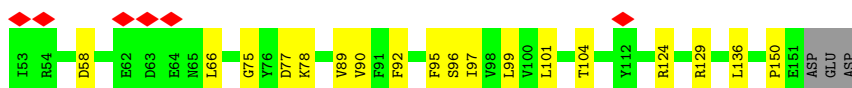
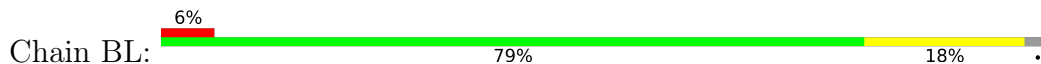
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



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

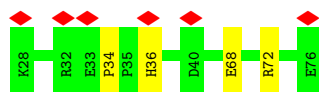


- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

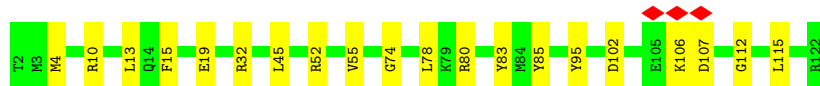
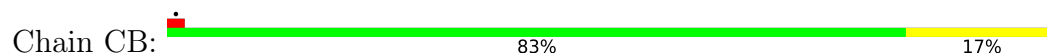


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

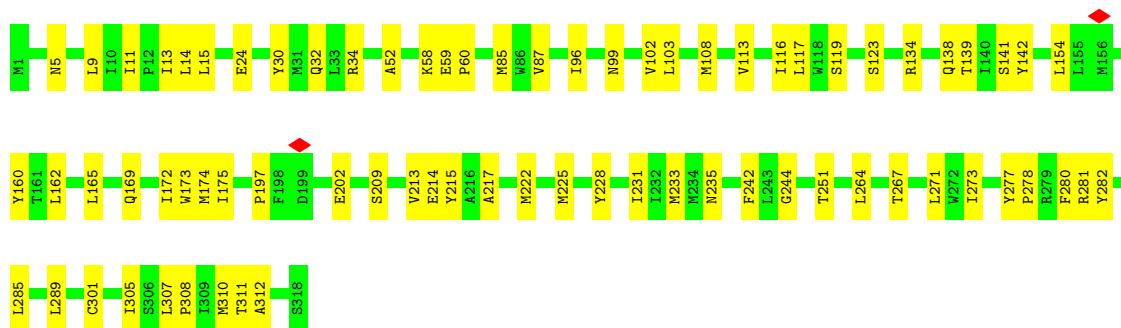
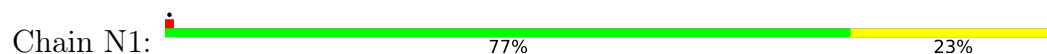




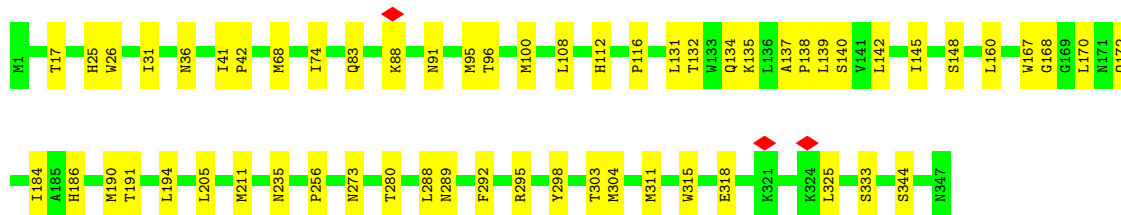
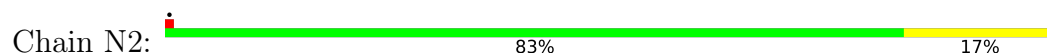
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C2



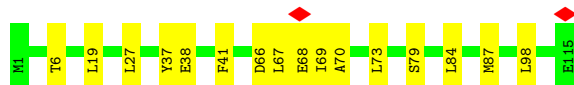
- Molecule 28: NADH-ubiquinone oxidoreductase chain 1



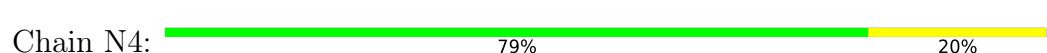
- Molecule 29: NADH-ubiquinone oxidoreductase chain 2



- Molecule 30: NADH-ubiquinone oxidoreductase chain 3



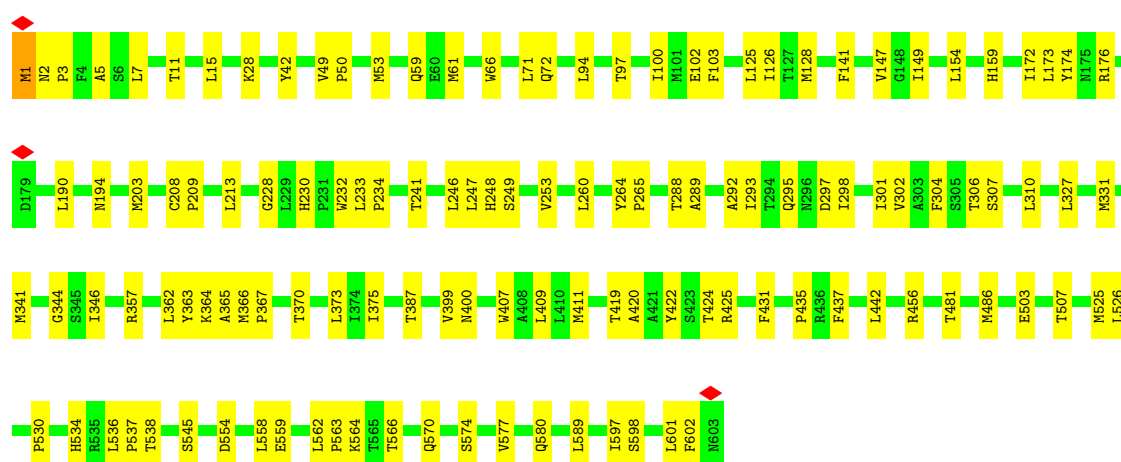
- Molecule 31: NADH-ubiquinone oxidoreductase chain 4





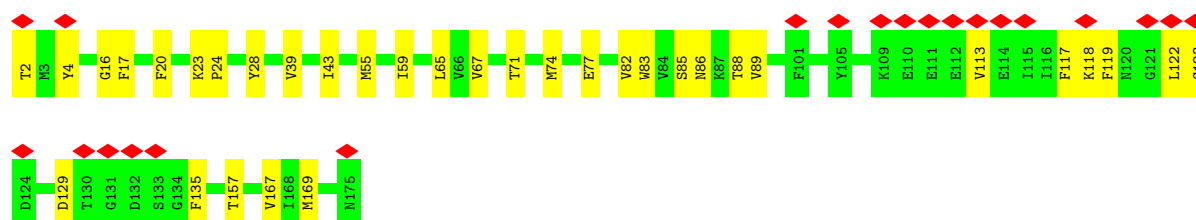
• Molecule 32: NADH-ubiquinone oxidoreductase chain 5

Chain N5: 79% 21%



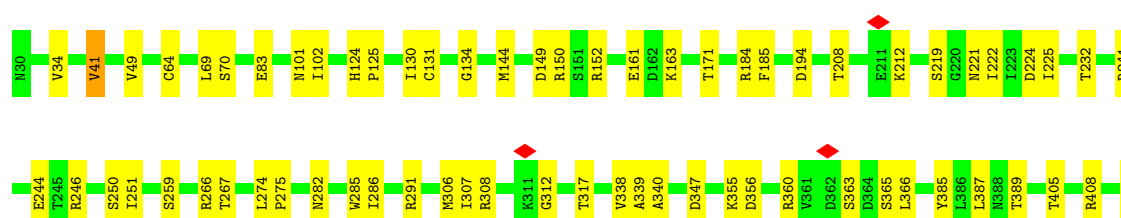
• Molecule 33: NADH-ubiquinone oxidoreductase chain 6

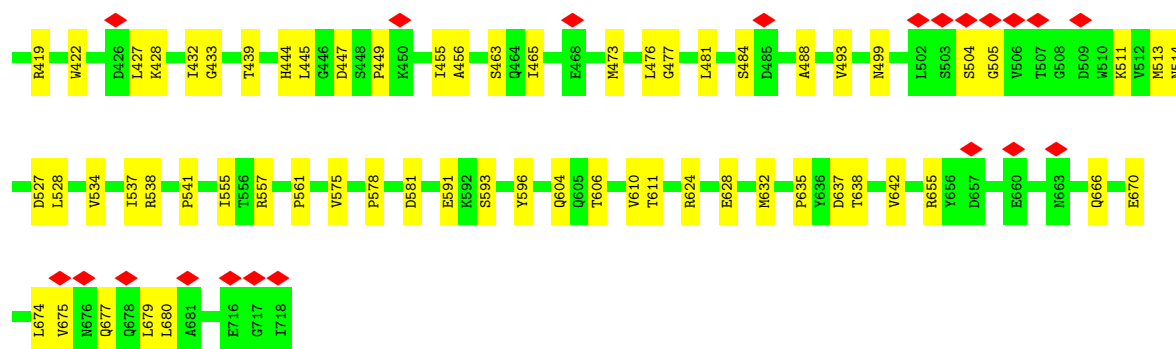
Chain N6: 12% 80% 20%



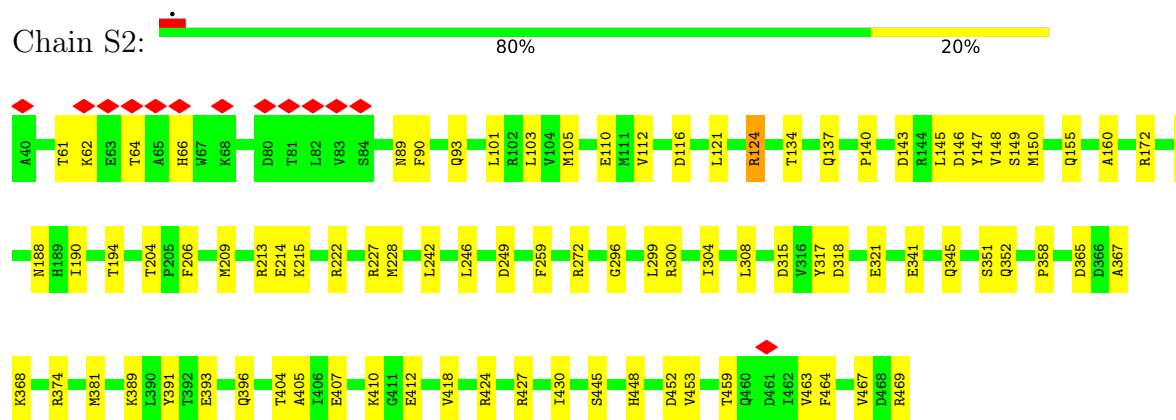
• Molecule 34: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain S1: 81% 19%

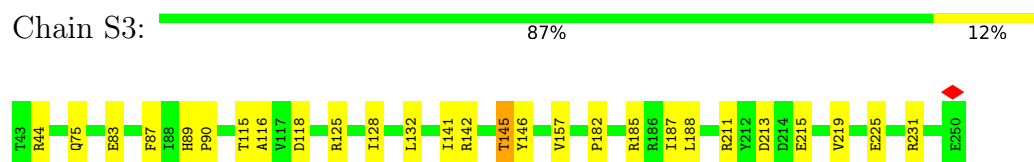




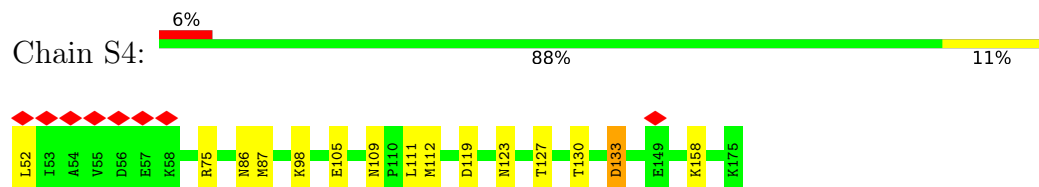
- Molecule 35: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



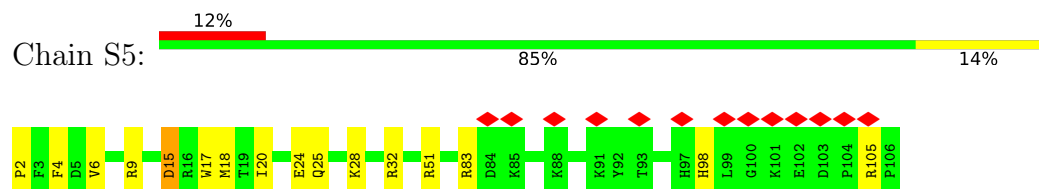
- Molecule 36: Complex I-30kD



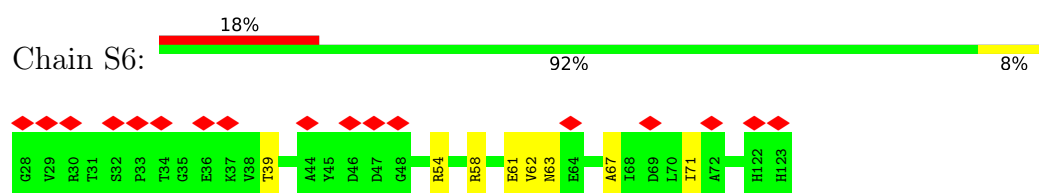
- Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



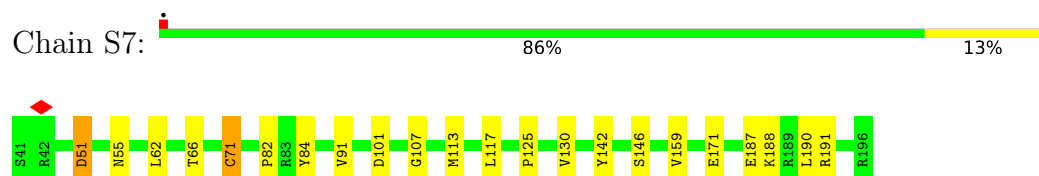
- Molecule 38: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



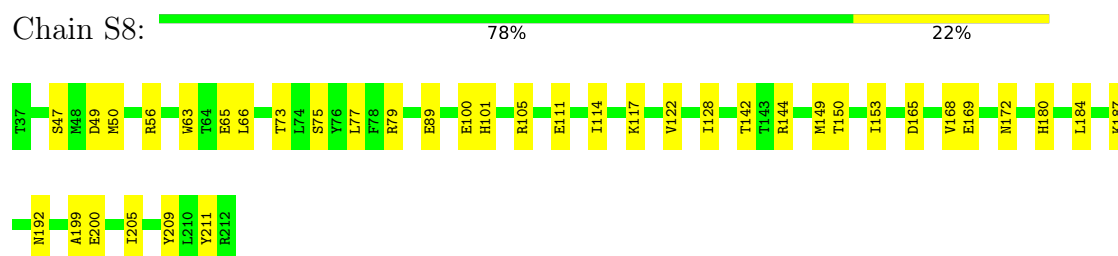
- Molecule 39: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



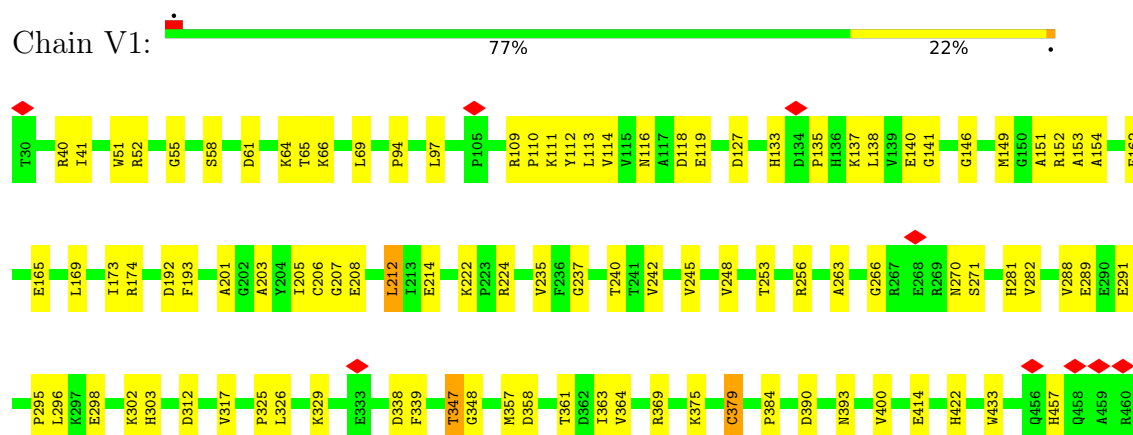
- Molecule 40: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



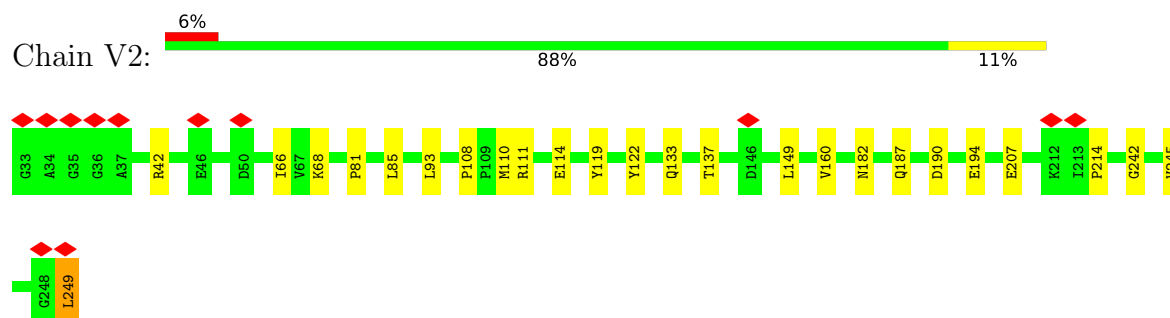
- Molecule 41: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



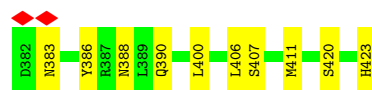
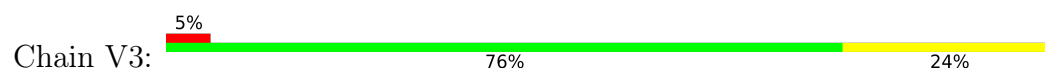
- Molecule 42: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



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



- Molecule 44: NADH:ubiquinone oxidoreductase subunit V3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94033	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	51.105	Depositor
Minimum map value	-27.104	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.993	Depositor
Recommended contour level	5.07	Depositor
Map size (\AA)	576.0, 576.0, 576.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.21	0/759	0.33	0/1029
2	A1	0.18	0/577	0.28	0/777
3	A2	0.14	0/697	0.27	0/938
4	A3	0.14	0/664	0.25	0/912
5	A5	0.17	0/929	0.23	0/1258
6	A6	0.18	0/991	0.29	0/1335
7	A7	0.15	0/798	0.26	0/1079
8	A8	0.16	0/1436	0.27	0/1938
9	A9	0.19	0/2820	0.29	0/3823
10	AB	0.11	0/633	0.22	0/851
10	AC	0.17	0/714	0.25	0/965
11	AK	0.16	0/2661	0.29	0/3602
12	AL	0.15	0/1042	0.24	0/1411
13	AM	0.11	0/1245	0.23	0/1694
14	AN	0.18	0/1204	0.27	0/1624
15	B1	0.14	0/491	0.24	0/663
16	B2	0.16	0/610	0.26	0/836
17	B3	0.15	0/660	0.27	0/892
18	B4	0.17	0/1092	0.27	0/1481
19	B5	0.19	0/1184	0.29	0/1603
20	B6	0.18	0/910	0.33	0/1237
21	B7	0.15	0/1092	0.26	0/1459
22	B8	0.17	0/1371	0.27	0/1875
23	B9	0.19	0/1590	0.29	0/2155
24	BK	0.17	0/1489	0.26	0/2008
25	BL	0.18	0/851	0.30	0/1155
26	CA	0.14	0/430	0.21	0/581
27	CB	0.19	0/1031	0.28	0/1394
28	N1	0.24	0/2581	0.39	0/3529
29	N2	0.23	0/2773	0.36	0/3768
30	N3	0.20	0/938	0.29	0/1281
31	N4	0.22	0/3723	0.34	0/5078

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	N5	0.21	0/4914	0.36	0/6683
33	N6	0.19	0/1364	0.30	0/1850
34	S1	0.21	0/5378	0.33	0/7287
35	S2	0.24	0/3538	0.33	0/4796
36	S3	0.22	0/1789	0.31	0/2436
37	S4	0.20	0/1030	0.31	0/1391
38	S5	0.16	0/889	0.24	0/1190
39	S6	0.15	0/755	0.29	0/1018
40	S7	0.24	0/1279	0.32	0/1730
41	S8	0.23	0/1443	0.29	0/1952
42	V1	0.19	0/3391	0.32	0/4583
43	V2	0.17	0/1711	0.31	0/2328
44	V3	0.13	0/365	0.28	0/493
All	All	0.19	0/67832	0.31	0/91968

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	8	0
3	A2	686	0	699	6	0
4	A3	643	0	642	8	0
5	A5	910	0	950	4	0
6	A6	967	0	972	19	0
7	A7	780	0	808	10	0
8	A8	1398	0	1372	20	0
9	A9	2743	0	2762	39	0
10	AB	624	0	625	11	0
10	AC	702	0	694	9	0
11	AK	2601	0	2566	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	AL	1021	0	1025	12	0
13	AM	1204	0	1162	12	0
14	AN	1173	0	1166	17	0
15	B1	479	0	486	3	0
16	B2	584	0	529	6	0
17	B3	641	0	620	9	0
18	B4	1062	0	1072	6	0
19	B5	1151	0	1164	10	0
20	B6	882	0	899	19	0
21	B7	1068	0	1043	15	0
22	B8	1315	0	1208	9	0
23	B9	1534	0	1470	18	0
24	BK	1456	0	1426	18	0
25	BL	828	0	788	12	0
26	CA	417	0	422	3	0
27	CB	1000	0	994	16	0
28	N1	2508	0	2607	60	0
29	N2	2710	0	2874	45	0
30	N3	914	0	951	14	0
31	N4	3631	0	3839	70	0
32	N5	4785	0	4933	89	0
33	N6	1329	0	1326	32	0
34	S1	5290	0	5321	86	0
35	S2	3459	0	3396	66	0
36	S3	1738	0	1693	18	0
37	S4	1007	0	1008	13	0
38	S5	867	0	871	17	0
39	S6	741	0	701	6	0
40	S7	1248	0	1254	18	0
41	S8	1412	0	1363	31	0
42	V1	3316	0	3272	60	0
43	V2	1671	0	1673	17	0
44	V3	355	0	329	9	0
45	4L	92	0	137	11	0
45	A7	51	0	46	1	0
45	A8	83	0	113	8	0
45	AK	68	0	80	1	0
45	AL	94	0	138	6	0
45	B4	80	0	107	4	0
45	B5	100	0	156	3	0
45	N1	78	0	103	5	0
45	N4	162	0	224	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	N5	189	0	284	10	0
46	A9	48	0	26	1	0
47	A9	39	0	52	4	0
47	AL	49	0	75	4	0
47	N1	31	0	36	3	0
47	N3	51	0	82	1	0
47	N5	137	0	205	10	0
47	S2	48	0	73	4	0
47	S8	51	0	82	6	0
48	AB	36	0	47	4	0
48	AC	36	0	47	3	0
49	AK	27	0	12	4	0
50	AL	47	0	75	3	0
50	AM	51	0	83	4	0
50	B1	52	0	88	2	0
50	CB	52	0	88	3	0
50	N3	52	0	88	3	0
50	N4	49	0	79	3	0
50	S7	52	0	88	1	0
51	B8	32	0	38	1	0
51	CA	51	0	82	2	0
51	CB	46	0	69	1	0
51	N5	46	0	69	1	0
51	S7	51	0	82	0	0
52	N1	48	0	73	3	0
52	N3	54	0	88	2	0
53	S1	16	0	0	0	0
53	S7	8	0	0	1	0
53	S8	16	0	0	1	0
53	V1	8	0	0	0	0
54	S1	4	0	0	0	0
54	V2	4	0	0	0	0
55	S1	1	0	0	0	0
56	S6	1	0	0	0	0
57	S7	63	0	90	14	0
58	S7	9	0	0	0	0
59	V1	31	0	19	1	0
All	All	68554	0	69655	899	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (899) 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	1.63	0.99
41:S8:63:TRP:HE1	47:S8:303:PEE:H13	1.38	0.86
20:B6:88:LEU:HD22	20:B6:92:GLU:HG2	1.61	0.83
1:4L:37:MET:HG2	1:4L:67:ALA:HB2	1.61	0.82
1:4L:68:ALA:HB3	30:N3:67:LEU:HD11	1.62	0.80
12:AL:140:LYS:H	29:N2:273:ASN:HD22	1.32	0.77
13:AM:34:ARG:NH2	41:S8:89:GLU:OE2	2.20	0.75
34:S1:64:CYS:O	34:S1:184:ARG:NH2	2.16	0.75
29:N2:88:LYS:HG3	29:N2:148:SER:HB3	1.68	0.74
9:A9:212:ARG:NH1	9:A9:311:GLU:OE2	2.21	0.73
42:V1:110:PRO:HB3	42:V1:152:ARG:HD3	1.69	0.73
12:AL:140:LYS:O	29:N2:273:ASN:ND2	2.22	0.73
34:S1:433:GLY:HA2	34:S1:447:ASP:HA	1.72	0.72
45:4L:201:CDL:H521	33:N6:88:THR:HG23	1.71	0.72
6:A6:66:TYR:O	6:A6:86:ARG:NH1	2.22	0.71
37:S4:109:ASN:ND2	37:S4:111:LEU:O	2.24	0.71
11:AK:141:ARG:NH2	49:AK:401:ADP:N7	2.38	0.71
17:B3:27:THR:HG22	17:B3:29:LEU:H	1.55	0.71
34:S1:149:ASP:HB2	35:S2:367:ALA:HB3	1.71	0.71
28:N1:102:VAL:HG11	28:N1:154:LEU:HD11	1.72	0.70
28:N1:141:SER:HB2	28:N1:289:LEU:HD12	1.73	0.70
31:N4:369:LEU:HD21	32:N5:149:ILE:HD13	1.73	0.70
42:V1:235:VAL:HG12	42:V1:240:THR:HG21	1.73	0.70
11:AK:109:GLN:OE1	11:AK:328:ARG:NH1	2.25	0.70
39:S6:61:GLU:OE2	41:S8:192:ASN:ND2	2.25	0.70
4:A3:95:LYS:NZ	41:S8:50:MET:SD	2.63	0.69
29:N2:108:LEU:HD11	29:N2:191:THR:HG21	1.74	0.69
35:S2:222:ARG:NH1	35:S2:249:ASP:OD2	2.17	0.69
30:N3:37:TYR:OH	35:S2:93:GLN:NE2	2.25	0.69
21:B7:29:TYR:OH	21:B7:111:ARG:NH2	2.26	0.69
25:BL:129:ARG:NH1	25:BL:136:LEU:O	2.25	0.69
28:N1:58:LYS:HE2	40:S7:125:PRO:HG2	1.75	0.69
3:A2:24:CYS:N	3:A2:58:CYS:SG	2.66	0.68
28:N1:99:ASN:N	52:N1:402:PC1:O12	2.25	0.68
40:S7:188:LYS:HB2	40:S7:191:ARG:HB2	1.73	0.68
31:N4:371:PRO:HD2	45:N5:703:CDL:H391	1.73	0.68
8:A8:219:TYR:OH	19:B5:189:ASN:ND2	2.23	0.68
42:V1:111:LYS:HB2	42:V1:151:ALA:HA	1.73	0.68
13:AM:88:ARG:HD3	41:S8:200:GLU:HG3	1.75	0.68
47:AL:202:PEE:H46	47:S2:501:PEE:H37	1.76	0.68
45:B4:201:CDL:H852	32:N5:558:LEU:HD21	1.76	0.67
31:N4:211:GLY:H	31:N4:213:HIS:HD2	1.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:S1:246:ARG:HH22	37:S4:123:ASN:HD21	1.41	0.67
42:V1:214:GLU:OE2	42:V1:224:ARG:NE	2.23	0.67
35:S2:90:PHE:HB3	35:S2:103:LEU:HB3	1.76	0.67
40:S7:55:ASN:ND2	40:S7:187:GLU:O	2.28	0.66
10:AC:114:ASP:OD1	23:B9:87:ARG:NH2	2.28	0.66
21:B7:29:TYR:O	21:B7:104:ARG:NH2	2.29	0.66
9:A9:346:GLU:HG2	9:A9:371:PRO:HB3	1.78	0.66
9:A9:87:GLU:HG3	9:A9:89:TYR:H	1.61	0.65
25:BL:95:PHE:O	25:BL:99:LEU:HB2	1.96	0.65
31:N4:391:ILE:HG23	31:N4:394:ILE:HD12	1.79	0.65
32:N5:2:ASN:ND2	32:N5:59:GLN:OE1	2.30	0.65
1:4L:31:LEU:HD21	33:N6:67:VAL:HG11	1.77	0.65
35:S2:188:ASN:OD1	35:S2:410:LYS:NZ	2.30	0.65
35:S2:374:ARG:NH2	41:S8:165:ASP:OD1	2.30	0.65
34:S1:419:ARG:NH1	34:S1:439:THR:O	2.30	0.64
42:V1:40:ARG:NH1	42:V1:289:GLU:O	2.31	0.64
43:V2:111:ARG:NH1	43:V2:114:GLU:OE2	2.31	0.64
52:N1:402:PC1:H112	52:N1:402:PC1:H32	1.79	0.64
43:V2:182:ASN:HB3	43:V2:194:GLU:HB3	1.78	0.64
41:S8:142:THR:O	41:S8:187:LYS:NZ	2.31	0.64
11:AK:120:TYR:OH	49:AK:401:ADP:O2'	2.14	0.64
37:S4:75:ARG:NH1	37:S4:119:ASP:OD1	2.31	0.64
16:B2:101:PRO:HD2	21:B7:99:MET:HE1	1.79	0.64
34:S1:266:ARG:HD2	34:S1:267:THR:HG23	1.79	0.63
32:N5:5:ALA:HB2	32:N5:61:MET:HE1	1.80	0.63
9:A9:188:GLU:HG3	9:A9:200:ILE:HD13	1.79	0.63
11:AK:120:TYR:HH	49:AK:401:ADP:HO2'	1.43	0.63
35:S2:124:2MR:O	40:S7:146:SER:OG	2.14	0.63
35:S2:272:ARG:HH11	47:S8:303:PEE:H2	1.64	0.63
23:B9:119:PRO:HB3	32:N5:525:MET:HE2	1.80	0.63
28:N1:87:VAL:HG11	30:N3:6:THR:HG21	1.80	0.63
28:N1:231:ILE:O	28:N1:235:ASN:ND2	2.29	0.63
6:A6:92:MET:HB2	48:AB:201:ZMP:H4A	1.80	0.62
34:S1:250:SER:HB2	34:S1:606:THR:HG23	1.80	0.62
34:S1:124:HIS:HD2	35:S2:381:MET:HE2	1.63	0.62
29:N2:142:LEU:HB3	29:N2:194:LEU:HD21	1.80	0.62
50:N3:202:PLX:H162	50:N3:202:PLX:H392	1.81	0.62
11:AK:145:TYR:OH	11:AK:201:LEU:O	2.12	0.62
43:V2:187:GLN:HE21	43:V2:190:ASP:HA	1.64	0.62
9:A9:61:ALA:HB3	9:A9:82:VAL:HG13	1.81	0.62
35:S2:308:LEU:HB2	35:S2:407:GLU:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A3:161:PRO:HD2	8:A8:204:LYS:HG2	1.80	0.62
21:B7:92:HIS:ND1	32:N5:481:THR:OG1	2.25	0.62
28:N1:160:TYR:OH	30:N3:73:LEU:O	2.18	0.62
34:S1:282:ASN:ND2	34:S1:285:TRP:O	2.32	0.62
31:N4:369:LEU:HD23	45:N5:703:CDL:H362	1.81	0.62
3:A2:89:ARG:O	3:A2:93:ASN:ND2	2.33	0.62
34:S1:338:VAL:O	34:S1:365:SER:HB2	2.00	0.62
34:S1:666:GLN:NE2	34:S1:670:GLU:OE2	2.33	0.62
25:BL:150:PRO:HG3	27:CB:115:LEU:HD22	1.81	0.61
45:A8:301:CDL:H572	45:A8:301:CDL:H532	1.81	0.61
31:N4:445:LEU:HB3	45:N5:703:CDL:H452	1.81	0.61
32:N5:362:LEU:HA	32:N5:365:ALA:HB3	1.82	0.61
6:A6:42:SER:HB3	37:S4:52:LEU:HB3	1.82	0.61
8:A8:201:GLU:HA	8:A8:204:LYS:HD3	1.82	0.61
20:B6:132:VAL:O	20:B6:136:LEU:HB3	1.99	0.61
34:S1:433:GLY:O	34:S1:444:HIS:NE2	2.30	0.61
30:N3:70:ALA:HB2	33:N6:59:ILE:HD11	1.82	0.61
1:4L:98:CYS:HB3	32:N5:580:GLN:HB2	1.82	0.61
29:N2:289:ASN:HA	29:N2:292:PHE:CE2	2.35	0.61
24:BK:2:PRO:O	24:BK:7:LYS:NZ	2.34	0.60
41:S8:47:SER:O	41:S8:56:ARG:NH2	2.34	0.60
24:BK:107:GLN:HE22	32:N5:194:ASN:HD22	1.49	0.60
41:S8:205:ILE:O	41:S8:209:TYR:HB3	2.01	0.60
42:V1:52:ARG:HH21	44:V3:390:GLN:HG2	1.66	0.60
42:V1:364:VAL:HG12	42:V1:400:VAL:HG12	1.84	0.60
32:N5:102:GLU:OE1	32:N5:456:ARG:NH2	2.25	0.60
34:S1:387:LEU:HD12	34:S1:514:ASN:HB3	1.84	0.60
29:N2:170:LEU:O	29:N2:295:ARG:NH2	2.33	0.60
34:S1:149:ASP:OD2	34:S1:150:ARG:NH2	2.35	0.60
42:V1:118:ASP:HB3	42:V1:207:GLY:HA2	1.84	0.60
43:V2:108:PRO:HB2	43:V2:111:ARG:HG2	1.82	0.60
35:S2:62:LYS:O	35:S2:66:HIS:ND1	2.35	0.60
45:A8:301:CDL:H112	27:CB:32:ARG:HG2	1.82	0.60
3:A2:59:SER:HB2	34:S1:655:ARG:HD3	1.84	0.59
8:A8:124:ARG:NE	14:AN:80:ASP:OD2	2.33	0.59
45:N4:502:CDL:H851	45:N4:502:CDL:H242	1.84	0.59
20:B6:85:ASP:O	23:B9:163:LYS:NZ	2.33	0.59
34:S1:488:ALA:HB2	34:S1:677:GLN:HG3	1.84	0.59
27:CB:19:GLU:OE2	27:CB:83:TYR:OH	2.18	0.59
10:AB:116:VAL:HG12	10:AB:120:MET:HE2	1.85	0.59
22:B8:62:TYR:OH	22:B8:74:ASP:O	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:N4:392:THR:O	31:N4:396:MET:HG2	2.03	0.59
15:B1:29:ARG:NH2	50:B1:101:PLX:O2	2.36	0.59
34:S1:347:ASP:OD1	34:S1:347:ASP:N	2.36	0.59
20:B6:143:HIS:CD2	24:BK:45:VAL:HG21	2.38	0.58
43:V2:85:LEU:HD13	44:V3:400:LEU:HD22	1.85	0.58
28:N1:169:GLN:HB3	28:N1:244:GLY:HA3	1.84	0.58
41:S8:100:GLU:OE1	41:S8:172:ASN:ND2	2.35	0.58
8:A8:246:PHE:HE1	45:A8:301:CDL:H341	1.68	0.58
32:N5:419:THR:HA	32:N5:422:TYR:CE2	2.39	0.58
2:A1:23:THR:HG23	28:N1:5:ASN:HD21	1.69	0.58
31:N4:403:THR:HA	31:N4:406:TYR:CE2	2.39	0.58
36:S3:132:LEU:HB2	36:S3:141:ILE:HG22	1.86	0.58
28:N1:173:TRP:HB3	28:N1:175:ILE:HG22	1.86	0.58
32:N5:97:THR:HG21	32:N5:125:LEU:HD22	1.86	0.58
35:S2:299:LEU:HD22	35:S2:304:ILE:HD12	1.85	0.58
35:S2:300:ARG:NH2	35:S2:407:GLU:OE2	2.36	0.58
32:N5:126:ILE:HG21	45:N5:703:CDL:H621	1.84	0.58
36:S3:187:ILE:HG23	36:S3:188:LEU:HG	1.84	0.58
42:V1:112:TYR:HB2	42:V1:240:THR:HG22	1.85	0.58
42:V1:281:HIS:ND1	42:V1:358:ASP:OD1	2.37	0.58
42:V1:205:ILE:HG12	42:V1:379:CYS:HB3	1.86	0.57
6:A6:78:LEU:HD22	6:A6:130:MET:HE3	1.86	0.57
21:B7:103:GLU:OE2	21:B7:106:ARG:NH2	2.33	0.57
42:V1:338:ASP:OD1	42:V1:339:PHE:N	2.37	0.57
9:A9:173:ASP:HB3	9:A9:176:SER:HB2	1.86	0.57
28:N1:58:LYS:NZ	40:S7:101:ASP:OD1	2.31	0.57
45:4L:201:CDL:H181	32:N5:589:LEU:HD11	1.85	0.57
7:A7:52:ASN:OD1	7:A7:57:ARG:NE	2.36	0.57
29:N2:298:TYR:O	29:N2:303:THR:OG1	2.22	0.57
6:A6:88:LYS:NZ	6:A6:132:PHE:O	2.29	0.57
48:AC:201:ZMP:H14	23:B9:102:ALA:HB1	1.87	0.57
24:BK:114:GLN:HG3	32:N5:203:MET:HG2	1.86	0.57
1:4L:55:LEU:H	38:S5:25:GLN:HE22	1.53	0.57
9:A9:129:LEU:HD23	9:A9:167:ILE:HG13	1.87	0.57
34:S1:161:GLU:OE2	43:V2:42:ARG:NH1	2.38	0.57
6:A6:78:LEU:HD23	6:A6:126:ARG:HD3	1.87	0.56
19:B5:133:TYR:OH	24:BK:87:GLU:OE1	2.12	0.56
36:S3:83:GLU:OE1	36:S3:142:ARG:NH2	2.33	0.56
12:AL:140:LYS:H	29:N2:273:ASN:ND2	2.03	0.56
29:N2:131:LEU:O	29:N2:135:LYS:HG2	2.05	0.56
19:B5:163:ARG:NH1	27:CB:102:ASP:OD2	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B6:89:SER:HB2	20:B6:92:GLU:HB2	1.86	0.56
31:N4:211:GLY:H	31:N4:213:HIS:CD2	2.23	0.56
47:N5:701:PEE:H36	45:N5:703:CDL:H231	1.86	0.56
34:S1:624:ARG:NH2	34:S1:637:ASP:OD1	2.34	0.56
11:AK:82:LYS:HZ2	11:AK:268:ALA:HB3	1.71	0.56
45:AL:201:CDL:H532	32:N5:577:VAL:HG22	1.88	0.56
8:A8:107:HIS:HB3	8:A8:197:PRO:HD2	1.88	0.56
34:S1:69:LEU:O	37:S4:158:LYS:NZ	2.36	0.56
34:S1:405:THR:HB	34:S1:477:GLY:HA3	1.87	0.56
21:B7:107:ARG:HA	21:B7:110:GLN:HG2	1.87	0.56
31:N4:282:LEU:HD13	31:N4:342:MET:HG3	1.88	0.56
6:A6:81:SER:OG	9:A9:367:GLU:OE2	2.22	0.56
11:AK:134:GLN:HE22	49:AK:401:ADP:HN62	1.54	0.56
14:AN:144:THR:HB	28:N1:96:ILE:HG23	1.88	0.56
35:S2:393:GLU:OE2	35:S2:396:GLN:NE2	2.39	0.56
42:V1:109:ARG:NH1	42:V1:237:GLY:O	2.39	0.56
29:N2:83:GLN:HE22	38:S5:20:ILE:HG22	1.71	0.56
42:V1:288:VAL:HG21	42:V1:303:HIS:CD2	2.41	0.56
2:A1:52:ARG:NH1	2:A1:58:ASN:OD1	2.39	0.55
28:N1:32:GLN:OE1	28:N1:34:ARG:NH2	2.34	0.55
28:N1:174:MET:HB2	28:N1:242:PHE:HA	1.88	0.55
34:S1:340:ALA:HB3	34:S1:366:LEU:HD23	1.89	0.55
34:S1:163:LYS:O	34:S1:171:THR:OG1	2.25	0.55
36:S3:128:ILE:HB	36:S3:145:THR:HG23	1.89	0.55
9:A9:357:ARG:NH1	9:A9:364:SER:OG	2.40	0.55
27:CB:15:PHE:O	27:CB:80:ARG:NH1	2.37	0.55
34:S1:308:ARG:NH1	34:S1:312:GLY:O	2.40	0.55
42:V1:235:VAL:H	42:V1:240:THR:HG21	1.72	0.55
34:S1:484:SER:HB2	34:S1:680:LEU:HD11	1.89	0.55
42:V1:112:TYR:O	42:V1:240:THR:HA	2.06	0.55
32:N5:530:PRO:O	32:N5:534:HIS:HB2	2.07	0.55
29:N2:42:PRO:HG3	33:N6:167:VAL:HG13	1.88	0.55
32:N5:103:PHE:HB2	32:N5:341:MET:HE3	1.89	0.54
35:S2:146:ASP:OD2	35:S2:149:SER:OG	2.25	0.54
29:N2:42:PRO:HG2	33:N6:167:VAL:HG22	1.89	0.54
34:S1:593:SER:HA	34:S1:606:THR:O	2.08	0.54
2:A1:28:LYS:NZ	8:A8:168:TYR:OH	2.32	0.54
28:N1:139:THR:HA	28:N1:142:TYR:CE2	2.42	0.54
41:S8:63:TRP:HB3	41:S8:66:LEU:HD12	1.88	0.54
24:BK:65:HIS:CD2	25:BL:124:ARG:HH12	2.25	0.54
31:N4:366:ASN:ND2	31:N4:407:SER:OG	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:N1:197:PRO:HB2	28:N1:280:PHE:HD1	1.72	0.54
18:B4:15:PRO:HG2	18:B4:18:LEU:HB2	1.89	0.54
45:N5:703:CDL:H591	45:N5:703:CDL:H642	1.89	0.54
40:S7:62:LEU:O	40:S7:91:VAL:HA	2.08	0.54
45:4L:201:CDL:H262	45:4L:201:CDL:H371	1.89	0.54
7:A7:62:GLU:OE2	36:S3:44:ARG:NH1	2.39	0.54
50:AM:201:PLX:H51	50:S7:204:PLX:H91	1.88	0.54
42:V1:192:ASP:HB3	44:V3:411:MET:SD	2.48	0.54
2:A1:12:MET:HE3	28:N1:264:LEU:HD22	1.89	0.54
14:AN:51:MET:HE2	28:N1:311:THR:HB	1.88	0.54
14:AN:98:MET:HE3	14:AN:101:VAL:HG21	1.90	0.54
29:N2:96:THR:HG22	29:N2:100:MET:HE2	1.89	0.54
30:N3:79:SER:HA	30:N3:87:MET:HE2	1.90	0.54
37:S4:112:MET:HG3	41:S8:184:LEU:HD23	1.89	0.54
34:S1:274:LEU:HD21	37:S4:87:MET:HE2	1.89	0.53
17:B3:33:GLN:NE2	17:B3:43:ASP:OD1	2.41	0.53
1:4L:37:MET:HG2	1:4L:67:ALA:CB	2.36	0.53
22:B8:173:ASP:OD2	22:B8:176:LYS:NZ	2.36	0.53
15:B1:28:ASP:OD2	31:N4:3:LYS:NZ	2.37	0.53
28:N1:113:VAL:HG13	28:N1:139:THR:HG21	1.91	0.53
31:N4:408:LEU:HD12	32:N5:172:ILE:HG21	1.90	0.53
5:A5:44:TYR:O	5:A5:48:THR:HG22	2.09	0.53
23:B9:218:GLU:HG2	23:B9:219:ARG:HG2	1.91	0.53
32:N5:295:GLN:O	32:N5:425:ARG:NH1	2.42	0.53
42:V1:138:LEU:HD13	42:V1:245:VAL:HG13	1.90	0.53
4:A3:160:GLY:HA3	8:A8:204:LYS:HE3	1.91	0.53
9:A9:293:LEU:HD12	9:A9:294:PRO:HD2	1.90	0.53
6:A6:89:VAL:HG22	48:AB:201:ZMP:H2A	1.90	0.53
45:N1:401:CDL:HB31	33:N6:82:VAL:HG21	1.89	0.53
42:V1:203:ALA:HB3	42:V1:206:CYS:HB2	1.89	0.53
4:A3:151:VAL:O	8:A8:207:LYS:NZ	2.29	0.52
50:AL:203:PLX:H111	50:AL:203:PLX:H301	1.91	0.52
34:S1:408:ARG:HD2	34:S1:439:THR:HG23	1.91	0.52
35:S2:182:GLU:OE2	35:S2:317:TYR:OH	2.14	0.52
1:4L:54:THR:HB	38:S5:25:GLN:HE21	1.74	0.52
8:A8:95:VAL:HG12	8:A8:97:VAL:HG22	1.90	0.52
32:N5:100:ILE:HG21	32:N5:246:LEU:HB2	1.90	0.52
32:N5:559:GLU:O	32:N5:564:LYS:HB2	2.09	0.52
34:S1:34:VAL:HG23	34:S1:41:VAL:HG13	1.91	0.52
35:S2:430:ILE:HB	35:S2:469:ARG:HD2	1.91	0.52
1:4L:56:ALA:HA	38:S5:18:MET:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BL:90:VAL:HG22	31:N4:28:THR:HG21	1.91	0.52
24:BK:142:ARG:NH1	24:BK:143:TYR:OH	2.42	0.52
42:V1:61:ASP:OD1	42:V1:137:LYS:NZ	2.42	0.52
20:B6:143:HIS:HD2	24:BK:45:VAL:HG21	1.72	0.52
45:N4:502:CDL:H342	45:N4:502:CDL:H191	1.91	0.52
28:N1:123:SER:HB3	28:N1:214:GLU:HG3	1.92	0.52
45:A7:201:CDL:HA61	45:A7:201:CDL:H521	1.91	0.52
30:N3:66:ASP:O	30:N3:69:ILE:HG13	2.10	0.52
33:N6:17:PHE:HA	33:N6:20:PHE:CE2	2.45	0.52
35:S2:90:PHE:HB2	35:S2:105:MET:HE2	1.91	0.52
42:V1:162:PHE:HB3	42:V1:165:GLU:HB2	1.92	0.52
10:AC:128:PHE:HZ	10:AC:148:ILE:HG12	1.73	0.52
28:N1:281:ARG:NH1	35:S2:452:ASP:OD1	2.43	0.52
34:S1:275:PRO:HG3	34:S1:286:ILE:HG12	1.91	0.52
34:S1:534:VAL:HG22	34:S1:537:ILE:HB	1.91	0.52
31:N4:41:LEU:O	31:N4:44:GLN:NE2	2.41	0.52
35:S2:140:PRO:HB2	40:S7:142:TYR:CE2	2.45	0.52
5:A5:48:THR:HA	5:A5:51:ILE:HG12	1.92	0.52
9:A9:198:ALA:O	9:A9:260:GLY:HA2	2.09	0.51
32:N5:562:LEU:HB3	32:N5:563:PRO:HD3	1.91	0.51
9:A9:354:ARG:NH1	9:A9:362:LEU:O	2.43	0.51
14:AN:49:SER:HB2	28:N1:172:ILE:HD13	1.93	0.51
31:N4:168:GLN:HB2	31:N4:174:LEU:HG	1.91	0.51
32:N5:400:ASN:HB3	32:N5:486:MET:HE3	1.93	0.51
28:N1:117:LEU:HD11	33:N6:65:LEU:HD12	1.92	0.51
32:N5:566:THR:O	32:N5:570:GLN:HG2	2.10	0.51
34:S1:83:GLU:HB2	34:S1:101:ASN:HB3	1.91	0.51
34:S1:389:THR:HG21	34:S1:473:MET:HE2	1.92	0.51
42:V1:326:LEU:HD22	42:V1:363:ILE:HD11	1.91	0.51
11:AK:66:GLY:O	11:AK:163:ARG:NH2	2.38	0.51
24:BK:60:ARG:NH1	24:BK:62:TYR:OH	2.43	0.51
34:S1:449:PRO:HB2	34:S1:679:LEU:HD13	1.92	0.51
18:B4:71:ALA:HB2	22:B8:38:PRO:HG2	1.90	0.51
25:BL:89:VAL:HG21	31:N4:25:ILE:HG23	1.91	0.51
29:N2:140:SER:HB3	38:S5:2:PRO:HA	1.93	0.51
42:V1:112:TYR:CD1	42:V1:153:ALA:HB3	2.46	0.51
1:4L:55:LEU:HD13	38:S5:17:TRP:HE3	1.76	0.51
1:4L:79:VAL:HG12	33:N6:74:MET:HE3	1.93	0.51
28:N1:52:ALA:HB2	57:S7:201:U10:H38	1.91	0.51
10:AB:111:ASP:OD1	10:AB:111:ASP:N	2.44	0.51
27:CB:13:LEU:HD21	38:S5:4:PHE:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:S1:389:THR:OG1	34:S1:511:LYS:O	2.29	0.51
44:V3:383:ASN:O	44:V3:383:ASN:ND2	2.44	0.51
7:A7:25:GLN:NE2	41:S8:79:ARG:HH11	2.09	0.51
15:B1:32:ASP:OD1	19:B5:135:LYS:NZ	2.38	0.51
23:B9:143:GLU:O	23:B9:164:ARG:NH2	2.44	0.51
33:N6:86:ASN:HD22	33:N6:89:VAL:HG23	1.75	0.51
33:N6:113:VAL:HG13	33:N6:118:LYS:HG2	1.93	0.51
32:N5:597:ILE:HG23	32:N5:601:LEU:HD22	1.93	0.50
7:A7:23:LYS:HG3	35:S2:259:PHE:CD1	2.46	0.50
50:N3:202:PLX:H151	50:N3:202:PLX:H332	1.92	0.50
31:N4:196:TRP:CD1	31:N4:250:LEU:HB3	2.47	0.50
42:V1:375:LYS:NZ	42:V1:390:ASP:OD1	2.44	0.50
35:S2:464:PHE:HA	35:S2:467:VAL:HB	1.92	0.50
13:AM:106:ARG:HB2	13:AM:109:ILE:HG13	1.94	0.50
27:CB:106:LYS:NZ	27:CB:107:ASP:OD1	2.31	0.50
33:N6:82:VAL:HG22	33:N6:83:TRP:H	1.76	0.50
35:S2:101:LEU:HB2	35:S2:464:PHE:CZ	2.45	0.50
42:V1:296:LEU:HD21	42:V1:317:VAL:HG11	1.94	0.50
28:N1:103:LEU:HD13	33:N6:55:MET:HE3	1.94	0.50
31:N4:122:PHE:HE2	31:N4:206:LYS:HG3	1.77	0.50
31:N4:216:LEU:HB3	31:N4:217:PRO:HD3	1.93	0.50
28:N1:24:GLU:OE1	28:N1:228:TYR:OH	2.23	0.50
9:A9:75:ARG:NH2	36:S3:213:ASP:OD2	2.45	0.50
34:S1:208:THR:HG21	34:S1:212:LYS:HB3	1.93	0.50
34:S1:538:ARG:HG2	34:S1:555:ILE:HD11	1.94	0.50
19:B5:53:ARG:NH2	20:B6:89:SER:O	2.42	0.50
31:N4:445:LEU:HD22	45:N5:703:CDL:H401	1.94	0.50
34:S1:624:ARG:NH1	34:S1:628:GLU:OE1	2.41	0.50
45:4L:201:CDL:HA61	12:AL:49:PHE:HA	1.93	0.49
20:B6:147:LYS:NZ	24:BK:42:ASP:OD1	2.43	0.49
31:N4:324:SER:HG	31:N4:440:HIS:CD2	2.26	0.49
31:N4:398:MET:HG2	47:N5:705:PEE:H79	1.93	0.49
32:N5:536:LEU:HB3	32:N5:537:PRO:HD3	1.95	0.49
20:B6:164:ILE:HD12	20:B6:170:ILE:HD11	1.94	0.49
31:N4:383:THR:HG21	32:N5:190:LEU:HD22	1.94	0.49
45:4L:201:CDL:H231	12:AL:41:ILE:HD12	1.93	0.49
47:AL:202:PEE:H8	47:AL:202:PEE:H15	1.95	0.49
31:N4:243:MET:HB3	31:N4:301:ILE:HG21	1.93	0.49
35:S2:194:THR:HG21	35:S2:209:MET:HB2	1.93	0.49
42:V1:55:GLY:O	42:V1:58:SER:OG	2.20	0.49
1:4L:4:VAL:O	1:4L:8:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A8:115:LYS:HB3	8:A8:116:PRO:HD3	1.95	0.49
12:AL:36:VAL:HG22	45:AL:201:CDL:H742	1.94	0.49
13:AM:139:PRO:HG3	34:S1:306:MET:HE1	1.94	0.49
29:N2:36:ASN:OD1	29:N2:134:GLN:NE2	2.33	0.49
33:N6:82:VAL:HG12	33:N6:85:SER:HB2	1.94	0.49
36:S3:231:ARG:NH2	41:S8:128:ILE:O	2.45	0.49
1:4L:14:ILE:HG12	45:4L:201:CDL:H781	1.93	0.49
31:N4:296:LEU:HD21	31:N4:378:GLU:HG3	1.94	0.49
32:N5:15:LEU:HD11	32:N5:94:LEU:HD21	1.95	0.49
32:N5:248:HIS:O	32:N5:253:VAL:HG22	2.12	0.49
42:V1:208:GLU:O	42:V1:212:LEU:HB2	2.11	0.49
10:AC:105:MET:HE3	10:AC:139:MET:HE1	1.94	0.49
45:B5:201:CDL:HB62	50:N4:501:PLX:H21	1.94	0.49
35:S2:214:GLU:OE2	35:S2:227:ARG:NH2	2.43	0.49
1:4L:75:LEU:O	1:4L:79:VAL:HG13	2.13	0.49
6:A6:88:LYS:NZ	6:A6:133:PHE:HA	2.28	0.49
11:AK:210:ASP:OD1	11:AK:244:LYS:NZ	2.33	0.49
31:N4:375:LEU:HD11	32:N5:141:PHE:HE2	1.78	0.49
32:N5:241:THR:HG21	32:N5:344:GLY:HA3	1.94	0.49
29:N2:26:TRP:HB3	29:N2:74:ILE:HD13	1.94	0.49
29:N2:112:HIS:O	29:N2:116:PRO:HD2	2.12	0.49
29:N2:186:HIS:O	29:N2:190:MET:HG3	2.13	0.49
29:N2:235:ASN:O	29:N2:315:TRP:NE1	2.46	0.49
47:N1:403:PEE:H57	52:N3:203:PC1:H3I2	1.94	0.49
32:N5:66:TRP:HZ3	47:N5:701:PEE:H34	1.77	0.49
36:S3:145:THR:OG1	36:S3:146:TYR:N	2.44	0.49
5:A5:9:THR:HG23	5:A5:16:VAL:HG22	1.94	0.49
5:A5:49:GLU:O	5:A5:53:ASN:ND2	2.46	0.49
14:AN:127:LEU:HD22	38:S5:83:ARG:HD3	1.95	0.49
20:B6:85:ASP:OD2	23:B9:167:TRP:NE1	2.37	0.49
40:S7:66:THR:HG22	57:S7:201:U10:H3M3	1.94	0.49
40:S7:130:VAL:HB	40:S7:159:VAL:HA	1.94	0.49
42:V1:113:LEU:O	42:V1:154:ALA:HA	2.12	0.49
31:N4:151:PHE:HB2	47:S2:501:PEE:H25	1.95	0.48
37:S4:112:MET:O	41:S8:144:ARG:NH1	2.36	0.48
2:A1:19:PRO:HB3	28:N1:9:LEU:HD12	1.94	0.48
45:AK:402:CDL:H372	29:N2:132:THR:HG21	1.95	0.48
44:V3:386:TYR:CZ	44:V3:388:ASN:HB3	2.48	0.48
10:AB:90:TYR:HD2	10:AB:93:ILE:HG12	1.77	0.48
28:N1:11:ILE:HG23	57:S7:201:U10:H462	1.94	0.48
47:S2:501:PEE:H27	47:S2:501:PEE:H34	1.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AN:93:GLU:HG3	38:S5:98:HIS:CD2	2.48	0.48
31:N4:5:ILE:HG23	31:N4:104:LEU:HD11	1.94	0.48
32:N5:253:VAL:HG23	32:N5:310:LEU:HD21	1.95	0.48
34:S1:224:ASP:OD2	34:S1:291:ARG:NH2	2.43	0.48
35:S2:61:THR:H	35:S2:64:THR:HG1	1.56	0.48
42:V1:263:ALA:HA	42:V1:271:SER:HB3	1.94	0.48
45:A8:301:CDL:H381	29:N2:256:PRO:HB2	1.96	0.48
12:AL:35:ILE:HD12	45:AL:201:CDL:H811	1.94	0.48
28:N1:213:VAL:HG13	28:N1:214:GLU:HG2	1.96	0.48
34:S1:493:VAL:HG23	34:S1:513:MET:HE1	1.95	0.48
35:S2:410:LYS:HE2	35:S2:463:VAL:HG23	1.94	0.48
37:S4:133:ASP:N	37:S4:133:ASP:OD1	2.44	0.48
4:A3:127:ALA:HB2	28:N1:312:ALA:HA	1.96	0.48
25:BL:77:ASP:OD1	25:BL:78:LYS:N	2.46	0.48
29:N2:304:MET:HE3	31:N4:135:ARG:HH22	1.79	0.48
34:S1:476:LEU:HD21	34:S1:481:LEU:HD21	1.96	0.48
35:S2:112:VAL:HG21	35:S2:453:VAL:HG21	1.95	0.48
17:B3:47:ARG:HA	17:B3:50:ALA:HB3	1.94	0.48
29:N2:167:TRP:HB3	32:N5:574:SER:HA	1.95	0.48
34:S1:251:ILE:HD11	34:S1:596:TYR:HB2	1.95	0.48
7:A7:28:TYR:CZ	13:AM:55:PHE:HB3	2.48	0.48
35:S2:145:LEU:HD13	35:S2:430:ILE:HG21	1.96	0.48
9:A9:206:ILE:HG12	9:A9:245:VAL:HG21	1.95	0.48
31:N4:94:LEU:HD21	45:N4:502:CDL:H312	1.96	0.48
32:N5:292:ALA:HB2	32:N5:304:PHE:HB3	1.96	0.48
23:B9:150:HIS:CD2	23:B9:151:PRO:HD2	2.49	0.48
39:S6:39:THR:HG22	39:S6:62:VAL:HG22	1.96	0.48
42:V1:64:LYS:HD3	43:V2:249:LEU:HD21	1.96	0.48
12:AL:124:LEU:HD11	47:AL:202:PEE:H70	1.96	0.47
34:S1:456:ALA:O	34:S1:499:ASN:ND2	2.47	0.47
8:A8:228:ASN:OD1	38:S5:51:ARG:NH1	2.44	0.47
9:A9:163:LYS:NZ	9:A9:253:ILE:O	2.39	0.47
9:A9:212:ARG:O	9:A9:216:TYR:N	2.36	0.47
23:B9:147:ASP:HB3	23:B9:164:ARG:HH12	1.79	0.47
32:N5:373:LEU:HD22	32:N5:431:PHE:HE2	1.78	0.47
42:V1:302:LYS:HE3	42:V1:303:HIS:CE1	2.49	0.47
4:A3:117:LEU:HD13	28:N1:310:MET:HE1	1.96	0.47
6:A6:127:THR:HG23	36:S3:219:VAL:O	2.15	0.47
10:AC:119:ILE:HG21	10:AC:135:ALA:HB1	1.96	0.47
11:AK:97:ASP:N	11:AK:97:ASP:OD1	2.47	0.47
21:B7:4:HIS:NE2	22:B8:155:PRO:HD3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B7:22:MET:HE1	21:B7:102:PHE:HD2	1.79	0.47
34:S1:49:VAL:HG13	34:S1:102:ILE:HD13	1.94	0.47
9:A9:344:PRO:HG2	9:A9:347:LEU:HD13	1.96	0.47
11:AK:328:ARG:HH21	25:BL:58:ASP:CG	2.23	0.47
23:B9:181:GLN:NE2	23:B9:198:PRO:O	2.45	0.47
31:N4:76:MET:SD	31:N4:230:VAL:HB	2.54	0.47
6:A6:94:MET:HE2	10:AB:113:LEU:HD12	1.95	0.47
31:N4:106:LEU:HD13	31:N4:234:VAL:HG11	1.96	0.47
11:AK:127:ASP:O	11:AK:132:ARG:NH1	2.45	0.47
28:N1:24:GLU:HA	28:N1:271:LEU:HD13	1.97	0.47
28:N1:225:MET:SD	57:S7:201:U10:H403	2.54	0.47
29:N2:139:LEU:HD13	29:N2:190:MET:HE1	1.96	0.47
31:N4:266:MET:HB3	31:N4:395:LEU:HD13	1.95	0.47
31:N4:361:VAL:HG22	45:N5:703:CDL:H311	1.96	0.47
33:N6:2:THR:HG22	33:N6:4:TYR:H	1.79	0.47
1:4L:41:PHE:O	1:4L:45:THR:HG22	2.14	0.47
8:A8:174:PHE:HB3	8:A8:178:ARG:HH12	1.79	0.47
9:A9:246:SER:O	9:A9:250:ILE:HG12	2.15	0.47
9:A9:310:PHE:CE2	52:N3:203:PC1:H11	2.49	0.47
48:AC:201:ZMP:H5A	23:B9:109:ALA:HB1	1.96	0.47
16:B2:90:ASP:N	16:B2:90:ASP:OD1	2.47	0.47
24:BK:107:GLN:HE22	32:N5:194:ASN:ND2	2.11	0.47
29:N2:211:MET:HG2	29:N2:333:SER:HB2	1.96	0.47
31:N4:201:MET:HE1	31:N4:212:LEU:HD11	1.95	0.47
31:N4:324:SER:OG	31:N4:440:HIS:NE2	2.34	0.47
32:N5:327:LEU:HG	32:N5:331:MET:HE2	1.97	0.47
32:N5:327:LEU:O	32:N5:331:MET:HG2	2.14	0.47
35:S2:190:ILE:HG23	35:S2:209:MET:HB3	1.97	0.47
42:V1:94:PRO:HB2	42:V1:97:LEU:HB2	1.96	0.47
10:AB:78:ALA:HA	10:AB:81:ASP:OD2	2.15	0.47
13:AM:78:ASP:HB2	13:AM:81:MET:HG3	1.97	0.47
29:N2:91:ASN:HD21	33:N6:117:PHE:HE1	1.62	0.47
1:4L:62:ILE:HG21	29:N2:31:ILE:HD11	1.97	0.47
4:A3:135:PRO:HB2	14:AN:69:ILE:HD11	1.97	0.47
24:BK:74:ILE:HG23	24:BK:156:LEU:HD22	1.97	0.47
35:S2:160:ALA:HA	35:S2:404:THR:HG21	1.96	0.47
42:V1:51:TRP:CD1	44:V3:388:ASN:HD22	2.33	0.47
1:4L:73:LEU:HD21	29:N2:41:ILE:HG13	1.97	0.47
31:N4:207:MET:HE1	31:N4:294:MET:HE3	1.96	0.47
32:N5:174:TYR:CD2	32:N5:232:TRP:HB3	2.50	0.47
9:A9:204:SER:HB2	9:A9:266:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:60:ARG:NH1	13:AM:89:TRP:O	2.47	0.46
29:N2:137:ALA:HB3	29:N2:138:PRO:HD3	1.97	0.46
33:N6:24:PRO:HG2	33:N6:28:TYR:HB2	1.97	0.46
33:N6:129:ASP:HB2	38:S5:32:ARG:NH1	2.30	0.46
34:S1:222:ILE:HA	34:S1:225:ILE:HG12	1.96	0.46
35:S2:93:GLN:NE2	35:S2:93:GLN:O	2.47	0.46
7:A7:39:PRO:HG3	41:S8:211:TYR:CZ	2.50	0.46
21:B7:103:GLU:O	21:B7:107:ARG:HG2	2.15	0.46
50:CB:201:PLX:H171	38:S5:9:ARG:HH22	1.80	0.46
28:N1:233:MET:HB3	28:N1:233:MET:HE3	1.85	0.46
29:N2:168:GLY:O	29:N2:172:GLN:HG2	2.15	0.46
32:N5:3:PRO:HB2	32:N5:53:MET:HE1	1.97	0.46
6:A6:92:MET:CB	48:AB:201:ZMP:H4A	2.44	0.46
11:AK:221:GLN:HE22	11:AK:229:MET:HE3	1.81	0.46
32:N5:249:SER:HA	32:N5:306:THR:HG21	1.97	0.46
34:S1:611:THR:HG21	37:S4:105:GLU:HA	1.96	0.46
39:S6:67:ALA:HB2	41:S8:111:GLU:HG3	1.97	0.46
6:A6:66:TYR:CE2	6:A6:86:ARG:HD3	2.50	0.46
9:A9:180:TYR:OH	46:A9:401:NDP:O2D	2.30	0.46
10:AB:140:CYS:HB2	10:AB:143:GLU:HG3	1.98	0.46
34:S1:70:SER:O	34:S1:184:ARG:NH1	2.46	0.46
35:S2:194:THR:HB	35:S2:206:PHE:HA	1.98	0.46
36:S3:157:VAL:HG21	36:S3:182:PRO:HD3	1.97	0.46
41:S8:150:THR:HG21	41:S8:180:HIS:CD2	2.50	0.46
3:A2:18:GLU:HG2	3:A2:68:ARG:HB3	1.96	0.46
17:B3:52:ARG:HD3	32:N5:435:PRO:O	2.16	0.46
24:BK:160:LYS:NZ	27:CB:112:GLY:O	2.45	0.46
51:CA:101:3PE:H261	51:CA:101:3PE:H2A2	1.97	0.46
28:N1:202:GLU:HG2	28:N1:209:SER:O	2.16	0.46
29:N2:170:LEU:HD11	29:N2:288:LEU:HD22	1.97	0.46
42:V1:141:GLY:HA3	42:V1:248:VAL:O	2.16	0.46
9:A9:64:PHE:O	9:A9:67:ARG:HG2	2.15	0.46
13:AM:75:TRP:HE1	50:AM:201:PLX:H11	1.81	0.46
45:N1:401:CDL:H791	33:N6:16:GLY:HA2	1.98	0.46
9:A9:65:LEU:HG	9:A9:129:LEU:HD22	1.97	0.46
11:AK:225:ASN:HB3	11:AK:228:GLU:HG2	1.98	0.46
11:AK:342:SER:HB2	11:AK:345:TYR:HD2	1.80	0.46
31:N4:211:GLY:N	31:N4:213:HIS:HD2	2.12	0.46
32:N5:49:VAL:HB	32:N5:50:PRO:HD3	1.98	0.46
35:S2:190:ILE:HG21	35:S2:213:ARG:HG3	1.98	0.46
36:S3:89:HIS:CG	36:S3:90:PRO:HD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:V1:112:TYR:HD1	42:V1:153:ALA:HB3	1.80	0.46
43:V2:93:LEU:HD12	43:V2:122:TYR:HB3	1.97	0.46
50:N4:501:PLX:H192	45:N5:703:CDL:H611	1.97	0.46
41:S8:49:ASP:OD1	41:S8:49:ASP:N	2.49	0.46
43:V2:133:GLN:NE2	43:V2:187:GLN:OE1	2.49	0.46
43:V2:149:LEU:HD11	43:V2:160:VAL:HG23	1.98	0.46
1:4L:76:SER:O	1:4L:79:VAL:HG22	2.16	0.45
14:AN:82:ARG:HA	38:S5:105:ARG:HD3	1.98	0.45
20:B6:92:GLU:O	20:B6:94:VAL:N	2.49	0.45
27:CB:107:ASP:OD1	27:CB:107:ASP:N	2.49	0.45
28:N1:9:LEU:O	28:N1:13:ILE:HG12	2.15	0.45
33:N6:169:MET:HB3	33:N6:169:MET:HE2	1.83	0.45
34:S1:385:TYR:OH	34:S1:527:ASP:OD1	2.28	0.45
42:V1:375:LYS:HD2	42:V1:393:ASN:ND2	2.31	0.45
45:4L:201:CDL:H172	45:4L:201:CDL:H211	1.98	0.45
9:A9:328:THR:HG22	9:A9:330:PRO:HD3	1.99	0.45
50:AM:201:PLX:H1A2	50:AM:201:PLX:H22	1.73	0.45
28:N1:34:ARG:HG2	40:S7:82:PRO:HA	1.98	0.45
32:N5:7:LEU:O	32:N5:11:THR:HG23	2.16	0.45
33:N6:24:PRO:HG3	33:N6:83:TRP:CE2	2.52	0.45
34:S1:575:VAL:C	34:S1:578:PRO:HD2	2.41	0.45
45:4L:201:CDL:H191	45:4L:201:CDL:H152	1.97	0.45
45:4L:201:CDL:H261	45:4L:201:CDL:H221	1.98	0.45
13:AM:60:ARG:HH22	13:AM:95:ASP:HA	1.80	0.45
21:B7:12:ASP:OD1	21:B7:14:SER:OG	2.29	0.45
34:S1:259:SER:HB3	34:S1:282:ASN:HD22	1.82	0.45
10:AB:104:PHE:HD1	10:AB:108:LEU:HD12	1.82	0.45
11:AK:112:GLY:HA2	11:AK:136:TRP:CD2	2.52	0.45
19:B5:71:MET:HE3	31:N4:442:LEU:HD11	1.99	0.45
50:CB:201:PLX:H271	50:CB:201:PLX:H302	1.66	0.45
28:N1:119:SER:HB2	28:N1:215:TYR:CE2	2.52	0.45
30:N3:68:GLU:HG3	30:N3:98:LEU:HD13	1.99	0.45
40:S7:51:ASP:HB3	40:S7:190:LEU:HB2	1.98	0.45
42:V1:146:GLY:HA3	42:V1:193:PHE:CE1	2.50	0.45
19:B5:139:ILE:HG23	31:N4:54:LEU:HD23	1.98	0.45
20:B6:165:PHE:O	20:B6:168:ASP:HB2	2.17	0.45
28:N1:277:TYR:CE2	47:S8:303:PEE:H57	2.52	0.45
47:N5:705:PEE:H53	47:N5:705:PEE:H58	1.74	0.45
34:S1:541:PRO:HB3	34:S1:561:PRO:HD3	1.98	0.45
39:S6:71:ILE:HD12	39:S6:71:ILE:HA	1.86	0.45
43:V2:207:GLU:HB3	43:V2:214:PRO:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A7:54:TYR:CZ	35:S2:368:LYS:HD2	2.52	0.45
50:AL:203:PLX:H21	50:AL:203:PLX:H1A2	1.58	0.45
21:B7:14:SER:HB2	21:B7:113:LYS:HE3	1.99	0.45
21:B7:17:PRO:HB3	21:B7:105:GLU:HG2	1.98	0.45
22:B8:110:ASP:HB3	31:N4:278:ARG:NH1	2.32	0.45
32:N5:304:PHE:CZ	32:N5:526:LEU:HD22	2.52	0.45
32:N5:526:LEU:HD12	32:N5:530:PRO:HG3	1.98	0.45
34:S1:455:ILE:O	34:S1:463:SER:OG	2.30	0.45
35:S2:147:TYR:CB	40:S7:71:CYS:HB3	2.47	0.45
35:S2:155:GLN:NE2	35:S2:315:ASP:OD2	2.42	0.45
35:S2:272:ARG:NE	41:S8:65:GLU:OE2	2.41	0.45
9:A9:257:ASP:OD1	9:A9:257:ASP:N	2.42	0.45
50:AL:203:PLX:H321	50:AL:203:PLX:H351	1.70	0.45
14:AN:19:ILE:HD12	35:S2:351:SER:HB2	1.99	0.45
29:N2:25:HIS:HB2	38:S5:15:ASP:HB2	1.99	0.45
32:N5:288:THR:HG21	32:N5:307:SER:HB3	1.99	0.45
34:S1:152:ARG:NH1	42:V1:414:GLU:OE1	2.50	0.45
34:S1:219:SER:O	34:S1:222:ILE:HG12	2.16	0.45
34:S1:251:ILE:HD13	34:S1:604:GLN:HB2	1.99	0.45
34:S1:339:ALA:HA	34:S1:365:SER:HB2	1.99	0.45
39:S6:54:ARG:O	39:S6:58:ARG:NH2	2.50	0.45
9:A9:238:GLN:OE1	9:A9:270:ARG:NH1	2.50	0.45
11:AK:357:LYS:HD3	26:CA:36:HIS:O	2.16	0.45
18:B4:26:SER:OG	18:B4:28:GLU:OE1	2.34	0.45
32:N5:435:PRO:HB3	32:N5:437:PHE:CZ	2.52	0.45
35:S2:137:GLN:O	40:S7:142:TYR:OH	2.35	0.45
42:V1:174:ARG:HA	44:V3:406:LEU:HD21	1.98	0.45
42:V1:295:PRO:HG2	42:V1:298:GLU:HB2	1.99	0.45
45:A8:301:CDL:H522	45:A8:301:CDL:H181	1.99	0.45
11:AK:85:LEU:HD22	11:AK:158:GLY:HA3	1.99	0.45
28:N1:85:MET:SD	28:N1:108:MET:HB2	2.57	0.45
42:V1:266:GLY:N	42:V1:291:GLU:OE2	2.49	0.45
2:A1:52:ARG:HG3	2:A1:60:TYR:HB3	1.99	0.45
10:AC:103:HIS:N	10:AC:107:ASP:OD1	2.50	0.45
20:B6:170:ILE:HD13	20:B6:177:ILE:HG12	1.98	0.45
28:N1:30:TYR:HB3	41:S8:77:LEU:HD12	1.99	0.45
28:N1:113:VAL:O	28:N1:116:ILE:HG12	2.17	0.45
30:N3:38:GLU:HG3	35:S2:89:ASN:HB2	1.98	0.45
45:N4:502:CDL:H832	45:N4:502:CDL:H231	1.98	0.45
34:S1:185:PHE:CZ	34:S1:221:ASN:HB2	2.51	0.45
51:CA:101:3PE:H3C1	29:N2:325:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:N1:401:CDL:H331	45:N1:401:CDL:H181	1.99	0.44
31:N4:82:SER:HB2	31:N4:432:ARG:NH1	2.32	0.44
31:N4:347:GLY:O	31:N4:350:THR:HG22	2.17	0.44
34:S1:131:CYS:O	34:S1:241:ARG:NH1	2.43	0.44
57:S7:201:U10:H48	57:S7:201:U10:H521	1.71	0.44
32:N5:503:GLU:O	32:N5:507:THR:HG23	2.18	0.44
34:S1:144:MET:HG3	35:S2:389:LYS:HG3	1.98	0.44
34:S1:246:ARG:HH12	37:S4:123:ASN:HD22	1.65	0.44
35:S2:418:VAL:HB	35:S2:427:ARG:HB3	1.98	0.44
11:AK:232:THR:HG23	11:AK:235:TYR:H	1.82	0.44
16:B2:56:PRO:HB3	32:N5:442:LEU:HD23	2.00	0.44
45:B5:201:CDL:HB21	47:N5:701:PEE:H49	1.99	0.44
31:N4:416:ARG:HG2	32:N5:159:HIS:HB3	1.99	0.44
39:S6:63:ASN:OD1	41:S8:105:ARG:NH2	2.50	0.44
1:4L:23:ARG:HG3	33:N6:23:LYS:NZ	2.33	0.44
1:4L:65:VAL:HG11	33:N6:157:THR:HG23	1.99	0.44
48:AC:201:ZMP:H11A	23:B9:58:VAL:HG23	1.98	0.44
45:AL:201:CDL:H612	29:N2:160:LEU:HD11	2.00	0.44
28:N1:15:LEU:HD23	57:S7:201:U10:H43	2.00	0.44
29:N2:112:HIS:HB2	29:N2:184:ILE:HD13	2.00	0.44
31:N4:449:LEU:HG	45:N5:703:CDL:H441	2.00	0.44
35:S2:134:THR:HA	35:S2:424:ARG:HG2	1.99	0.44
35:S2:272:ARG:NH1	47:S8:303:PEE:H2	2.30	0.44
42:V1:347:THR:HG22	42:V1:348:GLY:H	1.83	0.44
17:B3:18:ASP:O	17:B3:21:GLN:HG2	2.18	0.44
28:N1:222:MET:HA	28:N1:225:MET:HE3	2.00	0.44
34:S1:124:HIS:CG	34:S1:125:PRO:HD2	2.53	0.44
34:S1:557:ARG:NH2	34:S1:581:ASP:OD1	2.49	0.44
35:S2:116:ASP:OD1	36:S3:185:ARG:NH2	2.50	0.44
38:S5:24:GLU:OE2	38:S5:28:LYS:NZ	2.46	0.44
42:V1:113:LEU:HD13	42:V1:149:MET:HE1	1.99	0.44
11:AK:67:ASN:ND2	11:AK:68:ILE:H	2.16	0.44
12:AL:67:GLY:HA2	45:AL:201:CDL:H221	2.00	0.44
47:AL:202:PEE:H19	29:N2:280:THR:HG21	1.99	0.44
16:B2:79:MET:SD	32:N5:375:ILE:HG12	2.58	0.44
17:B3:24:ILE:O	17:B3:30:GLU:HB3	2.17	0.44
28:N1:138:GLN:HG3	28:N1:285:LEU:HD21	2.00	0.44
28:N1:301:CYS:O	28:N1:305:ILE:HG13	2.18	0.44
19:B5:110:TRP:O	19:B5:119:ARG:HG2	2.18	0.44
28:N1:99:ASN:HB2	52:N1:402:PC1:H133	2.00	0.44
31:N4:131:ILE:O	31:N4:135:ARG:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:N5:233:LEU:HB3	32:N5:234:PRO:HD3	1.98	0.44
33:N6:122:LEU:HG	33:N6:123:GLY:H	1.83	0.44
36:S3:118:ASP:OD2	36:S3:125:ARG:NH2	2.48	0.44
27:CB:45:LEU:HD22	27:CB:55:VAL:HG12	2.00	0.44
47:N1:403:PEE:H55	30:N3:19:LEU:HD11	2.00	0.44
33:N6:39:VAL:O	33:N6:43:ILE:HG13	2.18	0.44
42:V1:357:MET:HB3	42:V1:361:THR:HG21	1.99	0.44
9:A9:168:SER:O	9:A9:203:PRO:HD2	2.18	0.44
11:AK:172:LEU:HD22	11:AK:189:TYR:CD1	2.53	0.44
22:B8:149:ILE:HD12	51:B8:201:3PE:H12	2.00	0.44
45:N1:401:CDL:H112	47:N1:403:PEE:H7	2.00	0.44
34:S1:251:ILE:HG21	34:S1:604:GLN:HB3	1.99	0.44
44:V3:420:SER:HB3	44:V3:423:HIS:ND1	2.33	0.44
45:4L:201:CDL:H241	45:4L:201:CDL:H351	2.00	0.43
8:A8:248:THR:OG1	45:A8:301:CDL:HA31	2.18	0.43
28:N1:162:LEU:O	28:N1:165:LEU:HB2	2.17	0.43
1:4L:65:VAL:HA	30:N3:67:LEU:HD22	2.00	0.43
10:AC:120:MET:HE1	23:B9:66:LEU:HB3	2.00	0.43
11:AK:297:ARG:HA	11:AK:300:VAL:HG22	2.00	0.43
14:AN:95:ALA:HA	14:AN:106:VAL:HG11	2.00	0.43
18:B4:82:PRO:HB2	45:B4:201:CDL:HB4	2.00	0.43
28:N1:197:PRO:HB3	28:N1:278:PRO:O	2.18	0.43
31:N4:12:LEU:HB2	31:N4:13:PRO:HD3	1.99	0.43
32:N5:260:LEU:HD23	32:N5:260:LEU:HA	1.83	0.43
1:4L:6:MET:HB2	33:N6:119:PHE:CD1	2.53	0.43
1:4L:36:MET:HE3	29:N2:68:MET:HG3	1.99	0.43
32:N5:298:ILE:O	32:N5:302:VAL:HG23	2.17	0.43
32:N5:598:SER:HA	32:N5:602:PHE:HD2	1.83	0.43
34:S1:194:ASP:O	34:S1:208:THR:HG23	2.18	0.43
34:S1:360:ARG:HH21	34:S1:635:PRO:HD3	1.83	0.43
35:S2:143:ASP:OD1	35:S2:150:MET:HB3	2.19	0.43
35:S2:341:GLU:O	35:S2:345:GLN:HG2	2.19	0.43
57:S7:201:U10:H1M1	57:S7:201:U10:H103	2.00	0.43
42:V1:214:GLU:HG3	42:V1:222:LYS:O	2.19	0.43
2:A1:57:VAL:HG11	2:A1:62:VAL:HG21	2.00	0.43
7:A7:31:ILE:H	7:A7:31:ILE:HG13	1.65	0.43
9:A9:227:PRO:HG3	47:A9:402:PEE:H25	2.01	0.43
11:AK:59:SER:OG	11:AK:156:GLY:O	2.19	0.43
47:N3:201:PEE:H30	47:N3:201:PEE:H36	1.74	0.43
31:N4:87:GLU:O	31:N4:92:LYS:NZ	2.38	0.43
32:N5:420:ALA:O	32:N5:424:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B6:147:LYS:HE3	20:B6:148:TYR:CZ	2.53	0.43
32:N5:173:LEU:HD13	47:N5:705:PEE:H15	1.99	0.43
32:N5:297:ASP:O	32:N5:301:ILE:HG13	2.19	0.43
42:V1:114:VAL:O	42:V1:242:VAL:HA	2.18	0.43
11:AK:51:THR:HG21	11:AK:153:LEU:HD22	2.00	0.43
11:AK:355:TRP:H	11:AK:355:TRP:CD1	2.36	0.43
50:B1:101:PLX:H192	25:BL:104:THR:HG23	2.01	0.43
27:CB:4:MET:O	27:CB:10:ARG:NH1	2.51	0.43
28:N1:15:LEU:HD21	57:S7:201:U10:H461	2.00	0.43
32:N5:407:TRP:O	32:N5:411:MET:HG2	2.19	0.43
34:S1:674:LEU:HD12	34:S1:675:VAL:HG23	2.00	0.43
35:S2:391:TYR:HD1	41:S8:122:VAL:HG21	1.83	0.43
41:S8:153:ILE:HG12	53:S8:302:SF4:S1	2.58	0.43
43:V2:242:GLY:HA2	43:V2:245:VAL:HG23	2.01	0.43
3:A2:69:TYR:HE2	3:A2:75:LYS:HD3	1.83	0.43
11:AK:37:ARG:C	11:AK:39:GLN:H	2.26	0.43
27:CB:13:LEU:HD11	38:S5:6:VAL:HG12	1.99	0.43
28:N1:142:TYR:CD1	28:N1:142:TYR:C	2.96	0.43
35:S2:140:PRO:HA	35:S2:143:ASP:HB2	2.01	0.43
8:A8:157:GLU:HB2	8:A8:158:PRO:HD3	2.01	0.43
45:A8:301:CDL:H211	45:A8:301:CDL:H581	2.00	0.43
10:AB:140:CYS:O	10:AB:144:ILE:HG12	2.18	0.43
23:B9:178:GLU:OE2	23:B9:209:TRP:NE1	2.51	0.43
31:N4:127:VAL:HB	31:N4:128:PRO:HD3	2.00	0.43
31:N4:328:CYS:O	31:N4:332:THR:HG23	2.19	0.43
35:S2:140:PRO:HB2	40:S7:142:TYR:HE2	1.83	0.43
42:V1:384:PRO:HG2	42:V1:422:HIS:O	2.19	0.43
43:V2:66:ILE:HG21	43:V2:81:PRO:HB2	2.00	0.43
47:A9:402:PEE:H54	47:A9:402:PEE:H49	1.86	0.43
10:AC:90:TYR:HE1	17:B3:44:PRO:HB2	1.83	0.43
11:AK:56:THR:C	11:AK:58:THR:H	2.27	0.43
50:CB:201:PLX:H1C3	50:CB:201:PLX:H22	1.65	0.43
29:N2:95:MET:HE1	29:N2:145:ILE:HD12	2.00	0.43
47:S2:501:PEE:H71	47:S2:501:PEE:H76	1.80	0.43
6:A6:81:SER:HB3	6:A6:84:GLN:HG3	2.01	0.43
24:BK:43:ARG:HB2	24:BK:44:PRO:HD3	2.01	0.43
34:S1:282:ASN:HA	34:S1:413:LEU:HD13	2.00	0.43
35:S2:296:GLY:HA2	35:S2:300:ARG:HH21	1.83	0.43
57:S7:201:U10:H321	57:S7:201:U10:H301	1.61	0.43
42:V1:369:ARG:HA	42:V1:369:ARG:HD2	1.87	0.43
6:A6:115:GLU:OE2	48:AB:201:ZMP:H5	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A7:54:TYR:CE2	35:S2:368:LYS:HD2	2.53	0.42
14:AN:89:GLU:O	14:AN:93:GLU:HG2	2.19	0.42
21:B7:22:MET:HE1	21:B7:102:PHE:CD2	2.54	0.42
25:BL:66:LEU:HD12	25:BL:75:GLY:HA2	2.00	0.42
32:N5:331:MET:HB3	32:N5:387:THR:HG22	2.01	0.42
35:S2:318:ASP:OD1	35:S2:318:ASP:N	2.48	0.42
42:V1:119:GLU:OE2	42:V1:127:ASP:N	2.45	0.42
42:V1:133:HIS:C	42:V1:135:PRO:HD3	2.43	0.42
42:V1:201:ALA:HB3	43:V2:119:TYR:CD1	2.54	0.42
8:A8:111:ALA:HB2	8:A8:197:PRO:HG3	2.02	0.42
31:N4:231:LEU:HD23	31:N4:235:LEU:HD12	2.01	0.42
31:N4:306:PRO:HB2	32:N5:72:GLN:HE22	1.84	0.42
32:N5:176:ARG:HD2	32:N5:176:ARG:HA	1.83	0.42
35:S2:445:SER:HB2	35:S2:453:VAL:HG22	2.01	0.42
35:S2:448:HIS:HB3	35:S2:452:ASP:HB2	2.01	0.42
6:A6:48:SER:O	6:A6:50:ASP:N	2.52	0.42
45:A8:301:CDL:H782	51:CB:202:3PE:H281	2.01	0.42
9:A9:50:SER:OG	36:S3:225:GLU:OE2	2.36	0.42
11:AK:153:LEU:HD11	11:AK:296:LEU:HD23	2.00	0.42
12:AL:110:ILE:HG12	47:N5:702:PEE:H14	2.02	0.42
18:B4:48:LEU:HB3	23:B9:208:LEU:HD13	2.01	0.42
28:N1:59:GLU:HG3	30:N3:27:LEU:HD13	2.01	0.42
31:N4:318:ALA:HB2	31:N4:373:ILE:HG13	2.00	0.42
37:S4:98:LYS:NZ	37:S4:127:THR:OG1	2.43	0.42
42:V1:169:LEU:O	42:V1:173:ILE:HG13	2.19	0.42
9:A9:316:ARG:O	9:A9:320:GLU:HG2	2.19	0.42
11:AK:343:PRO:HB2	26:CA:34:PRO:HB3	2.02	0.42
31:N4:210:TYR:CG	31:N4:268:GLY:HA3	2.55	0.42
31:N4:221:VAL:HA	31:N4:283:LYS:HD3	2.01	0.42
31:N4:382:ILE:HG12	31:N4:396:MET:HG3	2.02	0.42
34:S1:307:ILE:HG23	34:S1:317:THR:HG21	2.01	0.42
57:S7:201:U10:H8	57:S7:201:U10:H121	1.69	0.42
6:A6:88:LYS:HD2	6:A6:88:LYS:HA	1.68	0.42
8:A8:117:ASN:HB3	14:AN:73:PRO:HG2	2.01	0.42
9:A9:217:PHE:HA	9:A9:220:MET:HE2	2.02	0.42
9:A9:220:MET:HG2	47:A9:402:PEE:H17	2.01	0.42
19:B5:160:MET:HE2	27:CB:95:TYR:CD1	2.54	0.42
45:B5:201:CDL:H362	24:BK:45:VAL:HG12	2.01	0.42
27:CB:85:TYR:CZ	29:N2:344:SER:HB3	2.55	0.42
45:N4:502:CDL:H712	45:N4:502:CDL:OA9	2.18	0.42
32:N5:213:LEU:HD23	32:N5:213:LEU:HA	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A8:124:ARG:HA	8:A8:124:ARG:HD2	1.93	0.42
9:A9:76:MET:HE2	9:A9:76:MET:HB3	1.84	0.42
9:A9:223:PHE:HE2	47:A9:402:PEE:H13	1.85	0.42
14:AN:85:GLN:OE1	38:S5:105:ARG:NH1	2.40	0.42
30:N3:38:GLU:HB3	30:N3:41:PHE:O	2.20	0.42
34:S1:528:LEU:HD23	34:S1:528:LEU:HA	1.92	0.42
35:S2:242:LEU:HD22	35:S2:246:LEU:HD22	2.01	0.42
35:S2:321:GLU:O	35:S2:352:GLN:NE2	2.52	0.42
26:CA:68:GLU:OE2	26:CA:72:ARG:NE	2.47	0.42
32:N5:366:MET:O	32:N5:370:THR:OG1	2.29	0.42
33:N6:67:VAL:O	33:N6:71:THR:HG22	2.18	0.42
35:S2:61:THR:N	35:S2:64:THR:OG1	2.32	0.42
35:S2:172:ARG:NH1	35:S2:358:PRO:O	2.50	0.42
1:4L:35:GLY:HA3	33:N6:20:PHE:CZ	2.55	0.42
20:B6:132:VAL:O	20:B6:136:LEU:CB	2.67	0.42
22:B8:110:ASP:HB3	31:N4:278:ARG:HH11	1.83	0.42
32:N5:208:CYS:HA	32:N5:209:PRO:HD3	1.77	0.42
41:S8:101:HIS:ND1	41:S8:149:MET:HE1	2.35	0.42
42:V1:65:THR:O	42:V1:69:LEU:HG	2.20	0.42
12:AL:107:SER:HB3	12:AL:110:ILE:HB	2.01	0.42
23:B9:74:VAL:HG22	32:N5:357:ARG:HG2	2.02	0.42
27:CB:74:GLY:O	27:CB:78:LEU:HG	2.20	0.42
28:N1:134:ARG:NH2	35:S2:110:GLU:OE2	2.50	0.42
34:S1:356:ASP:O	34:S1:360:ARG:HG2	2.20	0.42
42:V1:325:PRO:HG3	42:V1:433:TRP:HB3	2.01	0.42
10:AB:110:LEU:HB3	10:AB:114:ASP:HB2	2.02	0.42
13:AM:55:PHE:CZ	13:AM:58:ARG:HG3	2.55	0.42
14:AN:24:ASN:ND2	14:AN:24:ASN:O	2.53	0.42
14:AN:134:LEU:HD23	14:AN:134:LEU:HA	1.87	0.42
20:B6:186:GLN:HG3	21:B7:89:TYR:HE2	1.85	0.42
25:BL:92:PHE:O	25:BL:96:SER:HB2	2.20	0.42
27:CB:52:ARG:NH1	29:N2:318:GLU:OE1	2.52	0.42
28:N1:273:ILE:HD13	47:S8:303:PEE:H59	2.02	0.42
29:N2:17:THR:HG23	29:N2:137:ALA:HB2	2.01	0.42
31:N4:259:TYR:O	31:N4:263:MET:HG2	2.19	0.42
32:N5:289:ALA:O	32:N5:293:ILE:HG23	2.20	0.42
34:S1:130:ILE:HG23	41:S8:114:ILE:HD12	2.00	0.42
42:V1:41:ILE:HG12	42:V1:253:THR:HG21	2.02	0.42
11:AK:168:ASP:OD2	11:AK:189:TYR:OH	2.33	0.41
31:N4:282:LEU:HD11	31:N4:410:MET:HG3	2.02	0.41
32:N5:172:ILE:O	32:N5:176:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:S7:201:U10:H18	57:S7:201:U10:H221	1.70	0.41
8:A8:179:LYS:HG2	8:A8:183:LYS:HE2	2.01	0.41
11:AK:251:MET:HE3	11:AK:254:LYS:HD2	2.01	0.41
32:N5:399:VAL:HG12	32:N5:409:LEU:HD13	2.01	0.41
34:S1:338:VAL:HB	34:S1:363:SER:CB	2.51	0.41
34:S1:355:LYS:HA	34:S1:366:LEU:HD11	2.01	0.41
13:AM:103:PRO:HB2	41:S8:199:ALA:HB1	2.03	0.41
19:B5:146:LYS:O	19:B5:150:ARG:HG3	2.20	0.41
30:N3:84:LEU:HD23	30:N3:84:LEU:HA	1.85	0.41
32:N5:128:MET:HE2	32:N5:147:VAL:HG11	2.03	0.41
32:N5:228:GLY:H	32:N5:230:HIS:HD2	1.68	0.41
32:N5:538:THR:HG21	47:N5:705:PEE:H14	2.01	0.41
34:S1:246:ARG:HH22	37:S4:123:ASN:ND2	2.12	0.41
35:S2:145:LEU:HD11	35:S2:430:ILE:HD13	2.02	0.41
42:V1:270:ASN:ND2	42:V1:339:PHE:HB2	2.35	0.41
31:N4:257:MET:HE3	31:N4:257:MET:HB3	1.89	0.41
34:S1:259:SER:HB3	34:S1:282:ASN:ND2	2.35	0.41
42:V1:119:GLU:HA	59:V1:502:FMN:HM71	2.02	0.41
42:V1:140:GLU:OE2	42:V1:256:ARG:NH1	2.53	0.41
43:V2:111:ARG:HA	43:V2:111:ARG:HD3	1.90	0.41
6:A6:107:LEU:O	6:A6:111:LYS:HG3	2.20	0.41
20:B6:159:GLU:HA	32:N5:61:MET:HG2	2.02	0.41
25:BL:97:ILE:O	25:BL:101:LEU:HB2	2.21	0.41
45:N1:401:CDL:H752	45:N1:401:CDL:H782	1.77	0.41
50:N4:501:PLX:H1A3	50:N4:501:PLX:H22	1.68	0.41
32:N5:364:LYS:HE2	32:N5:364:LYS:HB3	1.90	0.41
47:N5:705:PEE:H54	47:N5:705:PEE:H48	1.88	0.41
40:S7:84:TYR:CE1	40:S7:171:GLU:HG3	2.56	0.41
10:AB:93:ILE:HD12	10:AB:108:LEU:HD13	2.01	0.41
45:B4:201:CDL:H782	45:B4:201:CDL:H752	1.88	0.41
23:B9:77:ASP:OD1	23:B9:77:ASP:N	2.53	0.41
32:N5:264:TYR:CG	32:N5:265:PRO:HD3	2.55	0.41
35:S2:121:LEU:HD23	40:S7:113:MET:SD	2.61	0.41
36:S3:75:GLN:HB3	36:S3:87:PHE:CD1	2.55	0.41
41:S8:75:SER:O	41:S8:79:ARG:HG3	2.20	0.41
4:A3:144:ASP:HB3	8:A8:209:LYS:HD2	2.01	0.41
9:A9:199:THR:OG1	9:A9:258:ALA:O	2.38	0.41
10:AC:90:TYR:CE1	17:B3:44:PRO:HB2	2.56	0.41
31:N4:233:ALA:HA	31:N4:320:GLY:HA2	2.02	0.41
34:S1:134:GLY:HA3	34:S1:241:ARG:NH1	2.35	0.41
34:S1:591:GLU:HG2	34:S1:610:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:V1:312:ASP:HA	42:V1:329:LYS:NZ	2.35	0.41
7:A7:25:GLN:O	35:S2:215:LYS:NZ	2.33	0.41
50:AM:201:PLX:H372	50:AM:201:PLX:H341	1.76	0.41
28:N1:307:LEU:HB3	28:N1:308:PRO:HD3	2.03	0.41
32:N5:154:LEU:HD12	32:N5:247:LEU:HD21	2.03	0.41
33:N6:77:GLU:OE1	33:N6:77:GLU:N	2.54	0.41
34:S1:428:LYS:HE2	34:S1:465:ILE:HD13	2.03	0.41
34:S1:504:SER:OG	34:S1:505:GLY:N	2.54	0.41
41:S8:168:VAL:HG11	41:S8:205:ILE:HD11	2.03	0.41
45:4L:201:CDL:H351	45:4L:201:CDL:H222	2.03	0.41
3:A2:69:TYR:CE2	3:A2:75:LYS:HD3	2.56	0.41
6:A6:90:ARG:NH2	10:AB:114:ASP:OD1	2.53	0.41
9:A9:58:VAL:O	9:A9:83:PRO:HD2	2.21	0.41
16:B2:68:GLN:NE2	32:N5:367:PRO:HD2	2.36	0.41
20:B6:92:GLU:HB3	20:B6:93:PRO:HD3	2.02	0.41
29:N2:190:MET:HE1	29:N2:205:LEU:HB2	2.03	0.41
31:N4:267:TRP:O	31:N4:271:MET:HG2	2.21	0.41
31:N4:398:MET:O	31:N4:402:ILE:HG13	2.21	0.41
33:N6:2:THR:C	33:N6:4:TYR:H	2.27	0.41
33:N6:135:PHE:HD1	33:N6:135:PHE:HA	1.73	0.41
34:S1:632:MET:H	34:S1:632:MET:HG2	1.77	0.41
36:S3:211:ARG:NH2	36:S3:213:ASP:OD1	2.54	0.41
42:V1:116:ASN:O	42:V1:245:VAL:HG23	2.20	0.41
23:B9:52:LEU:O	23:B9:57:LYS:NZ	2.51	0.41
28:N1:228:TYR:HA	28:N1:231:ILE:HD12	2.02	0.41
45:N4:502:CDL:H801	45:N4:502:CDL:H372	2.03	0.41
32:N5:363:TYR:CD2	32:N5:370:THR:HG21	2.56	0.41
34:S1:150:ARG:NH1	35:S2:365:ASP:OD1	2.53	0.41
34:S1:244:GLU:OE2	41:S8:117:LYS:HD3	2.20	0.41
34:S1:432:ILE:HG12	34:S1:445:LEU:HB2	2.02	0.41
40:S7:66:THR:CG2	57:S7:201:U10:H3M3	2.51	0.41
13:AM:25:ARG:O	13:AM:29:ARG:HG2	2.21	0.40
22:B8:108:ASP:HB3	22:B8:111:MET:HG2	2.03	0.40
28:N1:267:THR:O	28:N1:271:LEU:HG	2.22	0.40
31:N4:274:SER:O	32:N5:545:SER:HB3	2.21	0.40
47:N5:705:PEE:H76	47:N5:705:PEE:H71	1.62	0.40
10:AC:93:ILE:HG21	10:AC:98:LEU:HD13	2.04	0.40
12:AL:45:PRO:HA	12:AL:46:PRO:HD3	1.90	0.40
16:B2:59:ARG:HD3	17:B3:51:TRP:CG	2.56	0.40
24:BK:33:LEU:HD13	32:N5:49:VAL:HG13	2.02	0.40
28:N1:60:PRO:HB3	28:N1:217:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:N4:302:MET:HE2	31:N4:302:MET:HA	2.02	0.40
31:N4:449:LEU:HD23	31:N4:449:LEU:HA	1.87	0.40
32:N5:28:LYS:HD3	32:N5:28:LYS:HA	1.91	0.40
57:S7:201:U10:H162	57:S7:201:U10:H122	1.86	0.40
9:A9:75:ARG:NH2	36:S3:215:GLU:OE1	2.38	0.40
9:A9:231:LEU:HD13	9:A9:292:PRO:HG3	2.03	0.40
11:AK:110:LEU:HD23	11:AK:329:VAL:HG13	2.03	0.40
14:AN:61:GLN:HE21	14:AN:61:GLN:HB3	1.65	0.40
20:B6:135:VAL:HG21	32:N5:42:TYR:HD2	1.86	0.40
24:BK:99:ASP:OD2	24:BK:143:TYR:OH	2.27	0.40
28:N1:14:LEU:HB3	57:S7:201:U10:H401	2.02	0.40
28:N1:113:VAL:CG1	28:N1:139:THR:HG21	2.52	0.40
29:N2:311:MET:HG3	29:N2:315:TRP:NE1	2.37	0.40
50:N3:202:PLX:H22	50:N3:202:PLX:H1C2	1.68	0.40
31:N4:21:ASN:OD1	31:N4:21:ASN:N	2.54	0.40
32:N5:346:ILE:HD11	32:N5:431:PHE:CZ	2.57	0.40
51:N5:706:3PE:H3D1	51:N5:706:3PE:H391	2.02	0.40
41:S8:63:TRP:HZ3	47:S8:303:PEE:H69	1.86	0.40
43:V2:68:LYS:NZ	44:V3:407:SER:OG	2.30	0.40
2:A1:27:HIS:O	2:A1:31:ASN:ND2	2.36	0.40
9:A9:279:TYR:HB2	9:A9:372:ALA:HB2	2.03	0.40
45:AL:201:CDL:H552	29:N2:112:HIS:HE1	1.86	0.40
18:B4:51:TYR:OH	31:N4:421:HIS:HB3	2.21	0.40
21:B7:95:TYR:CZ	22:B8:156:VAL:HG11	2.57	0.40
32:N5:230:HIS:CD2	32:N5:230:HIS:H	2.38	0.40
35:S2:405:ALA:HB1	35:S2:412:GLU:HG3	2.04	0.40
36:S3:115:THR:OG1	36:S3:116:ALA:N	2.55	0.40
40:S7:107:GLY:HA2	53:S7:203:SF4:S4	2.61	0.40
43:V2:110:MET:O	43:V2:114:GLU:HG3	2.21	0.40
1:4L:55:LEU:HD23	1:4L:55:LEU:HA	1.87	0.40
11:AK:284:PRO:O	11:AK:288:GLN:HG2	2.22	0.40
45:B4:201:CDL:H521	45:B4:201:CDL:HA62	2.04	0.40
31:N4:278:ARG:HG3	32:N5:545:SER:HB2	2.02	0.40
32:N5:1:MET:HE3	32:N5:1:MET:HB3	1.93	0.40
33:N6:28:TYR:HB3	33:N6:83:TRP:CH2	2.57	0.40
34:S1:422:TRP:HA	34:S1:427:LEU:HB3	2.03	0.40
34:S1:638:THR:O	34:S1:642:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4L	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
2	A1	68/70 (97%)	68 (100%)	0	0	100	100
3	A2	83/85 (98%)	79 (95%)	4 (5%)	0	100	100
4	A3	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
5	A5	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
6	A6	112/114 (98%)	108 (96%)	3 (3%)	1 (1%)	14	49
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%)	326 (96%)	13 (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	319/321 (99%)	306 (96%)	13 (4%)	0	100	100
12	AL	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
13	AM	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	AN	140/142 (99%)	130 (93%)	10 (7%)	0	100	100
15	B1	54/56 (96%)	54 (100%)	0	0	100	100
16	B2	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
17	B3	78/80 (98%)	77 (99%)	1 (1%)	0	100	100
18	B4	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
19	B5	136/138 (99%)	135 (99%)	1 (1%)	0	100	100
20	B6	99/126 (79%)	94 (95%)	5 (5%)	0	100	100
21	B7	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
22	B8	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
23	B9	176/178 (99%)	174 (99%)	2 (1%)	0	100	100
24	BK	172/176 (98%)	171 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	BL	97/102 (95%)	89 (92%)	8 (8%)	0	100	100
26	CA	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
27	CB	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
28	N1	316/318 (99%)	302 (96%)	14 (4%)	0	100	100
29	N2	345/347 (99%)	335 (97%)	10 (3%)	0	100	100
30	N3	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
31	N4	457/459 (100%)	452 (99%)	5 (1%)	0	100	100
32	N5	601/603 (100%)	573 (95%)	28 (5%)	0	100	100
33	N6	172/174 (99%)	163 (95%)	9 (5%)	0	100	100
34	S1	687/689 (100%)	658 (96%)	29 (4%)	0	100	100
35	S2	427/430 (99%)	411 (96%)	16 (4%)	0	100	100
36	S3	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
37	S4	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
38	S5	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
39	S6	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
40	S7	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
41	S8	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
42	V1	429/431 (100%)	410 (96%)	19 (4%)	0	100	100
43	V2	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
44	V3	40/42 (95%)	36 (90%)	4 (10%)	0	100	100
All	All	8151/8299 (98%)	7882 (97%)	268 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A6	49	ARG

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%)	76 (100%)	0	100	100
4	A3	69/69 (100%)	69 (100%)	0	100	100
5	A5	99/99 (100%)	99 (100%)	0	100	100
6	A6	107/107 (100%)	105 (98%)	2 (2%)	52	79
7	A7	87/97 (90%)	86 (99%)	1 (1%)	70	87
8	A8	153/153 (100%)	152 (99%)	1 (1%)	81	91
9	A9	295/295 (100%)	292 (99%)	3 (1%)	73	88
10	AB	71/80 (89%)	71 (100%)	0	100	100
10	AC	80/80 (100%)	78 (98%)	2 (2%)	42	73
11	AK	284/284 (100%)	281 (99%)	3 (1%)	70	87
12	AL	101/101 (100%)	100 (99%)	1 (1%)	73	88
13	AM	130/130 (100%)	128 (98%)	2 (2%)	60	83
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%)	112 (99%)	1 (1%)	75	89
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%)	141 (100%)	0	100	100
23	B9	159/159 (100%)	159 (100%)	0	100	100
24	BK	155/156 (99%)	155 (100%)	0	100	100
25	BL	91/94 (97%)	91 (100%)	0	100	100
26	CA	45/45 (100%)	45 (100%)	0	100	100
27	CB	108/108 (100%)	108 (100%)	0	100	100
28	N1	275/275 (100%)	273 (99%)	2 (1%)	81	91
29	N2	311/311 (100%)	311 (100%)	0	100	100
30	N3	100/100 (100%)	100 (100%)	0	100	100
31	N4	410/410 (100%)	408 (100%)	2 (0%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	N5	537/537 (100%)	534 (99%)	3 (1%)	84	93
33	N6	140/140 (100%)	140 (100%)	0	100	100
34	S1	579/579 (100%)	577 (100%)	2 (0%)	91	96
35	S2	370/370 (100%)	366 (99%)	4 (1%)	70	87
36	S3	190/190 (100%)	189 (100%)	1 (0%)	86	94
37	S4	112/112 (100%)	109 (97%)	3 (3%)	40	71
38	S5	93/93 (100%)	92 (99%)	1 (1%)	70	87
39	S6	79/79 (100%)	79 (100%)	0	100	100
40	S7	132/132 (100%)	129 (98%)	3 (2%)	45	75
41	S8	151/151 (100%)	149 (99%)	2 (1%)	65	85
42	V1	344/344 (100%)	338 (98%)	6 (2%)	56	81
43	V2	183/183 (100%)	181 (99%)	2 (1%)	70	87
44	V3	41/41 (100%)	41 (100%)	0	100	100
All	All	7185/7229 (99%)	7138 (99%)	47 (1%)	80	91

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	A6	122	VAL
6	A6	137	GLU
7	A7	43	VAL
8	A8	151	ILE
9	A9	129	LEU
9	A9	132	ARG
9	A9	310	PHE
10	AC	100	VAL
10	AC	112	SER
11	AK	39	GLN
11	AK	97	ASP
11	AK	251	MET
12	AL	115	CYS
13	AM	78	ASP
13	AM	144	TYR
18	B4	123	GLN
28	N1	251	THR
28	N1	282	TYR
31	N4	122	PHE

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Mol	Chain	Res	Type
31	N4	375	LEU
32	N5	1	MET
32	N5	71	LEU
32	N5	554	ASP
34	S1	41	VAL
34	S1	232	THR
35	S2	148	VAL
35	S2	204	THR
35	S2	228	MET
35	S2	459	THR
36	S3	145	THR
37	S4	86	ASN
37	S4	130	THR
37	S4	133	ASP
38	S5	15	ASP
40	S7	51	ASP
40	S7	71	CYS
40	S7	117	LEU
41	S8	73	THR
41	S8	169	GLU
42	V1	66	LYS
42	V1	212	LEU
42	V1	282	VAL
42	V1	347	THR
42	V1	379	CYS
42	V1	457	HIS
43	V2	137	THR
43	V2	249	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	4L	7	ASN
1	4L	52	HIS
2	A1	61	HIS
2	A1	68	ASN
3	A2	25	GLN
5	A5	71	GLN
5	A5	86	ASN
6	A6	84	GLN
7	A7	9	GLN
7	A7	21	GLN

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Mol	Chain	Res	Type
7	A7	25	GLN
8	A8	107	HIS
8	A8	112	GLN
8	A8	141	ASN
8	A8	142	GLN
9	A9	38	HIS
9	A9	72	HIS
9	A9	122	HIS
9	A9	138	ASN
9	A9	154	GLN
10	AB	142	GLN
11	AK	39	GLN
11	AK	67	ASN
11	AK	134	GLN
11	AK	221	GLN
11	AK	331	GLN
12	AL	79	GLN
13	AM	113	HIS
14	AN	61	GLN
14	AN	90	ASN
15	B1	3	ASN
15	B1	6	GLN
16	B2	63	GLN
16	B2	68	GLN
16	B2	71	GLN
17	B3	33	GLN
17	B3	91	GLN
18	B4	50	GLN
18	B4	123	GLN
19	B5	170	GLN
19	B5	189	ASN
20	B6	127	HIS
20	B6	143	HIS
21	B7	76	ASN
21	B7	85	HIS
21	B7	110	GLN
22	B8	56	ASN
22	B8	115	ASN
22	B8	154	GLN
22	B8	164	ASN
23	B9	104	GLN
23	B9	117	GLN

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Mol	Chain	Res	Type
24	BK	107	GLN
28	N1	5	ASN
28	N1	138	GLN
28	N1	169	GLN
28	N1	194	ASN
28	N1	317	GLN
29	N2	49	ASN
29	N2	83	GLN
29	N2	112	HIS
29	N2	171	ASN
29	N2	186	HIS
29	N2	273	ASN
29	N2	316	GLN
29	N2	322	GLN
30	N3	10	ASN
30	N3	26	GLN
31	N4	51	ASN
31	N4	213	HIS
31	N4	338	HIS
31	N4	366	ASN
31	N4	399	ASN
32	N5	2	ASN
32	N5	59	GLN
32	N5	136	ASN
32	N5	159	HIS
32	N5	170	GLN
32	N5	230	HIS
32	N5	248	HIS
32	N5	348	HIS
32	N5	470	ASN
32	N5	524	ASN
32	N5	540	HIS
32	N5	580	GLN
33	N6	86	ASN
33	N6	175	ASN
34	S1	39	GLN
34	S1	278	HIS
34	S1	282	ASN
34	S1	331	GLN
34	S1	336	ASN
34	S1	425	ASN
34	S1	453	GLN

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Mol	Chain	Res	Type
34	S1	498	GLN
34	S1	604	GLN
34	S1	652	ASN
34	S1	688	GLN
35	S2	93	GLN
35	S2	166	ASN
35	S2	189	HIS
35	S2	239	HIS
36	S3	123	GLN
36	S3	131	ASN
36	S3	196	HIS
36	S3	228	GLN
37	S4	123	ASN
37	S4	163	ASN
38	S5	25	GLN
38	S5	34	HIS
38	S5	45	HIS
38	S5	70	GLN
39	S6	74	GLN
39	S6	117	GLN
42	V1	270	ASN
42	V1	277	ASN
42	V1	284	HIS
42	V1	303	HIS
42	V1	344	GLN
42	V1	381	GLN
42	V1	393	ASN
42	V1	422	HIS
42	V1	456	GLN
43	V2	74	HIS
43	V2	90	ASN
43	V2	131	HIS
43	V2	133	GLN
43	V2	153	GLN
43	V2	246	GLN
44	V3	419	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	2MR	S2	124	35	10,12,13	2.42	3 (30%)	5,13,15	0.93	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	2MR	S2	124	35	-	3/10/13/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S2	124	2MR	CZ-NE	5.04	1.45	1.34
35	S2	124	2MR	CZ-NH2	4.98	1.44	1.33
35	S2	124	2MR	CQ1-NH1	-2.10	1.42	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 2 are monoatomic - leaving 50 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	$\# Z > 2$
53	SF4	S1	801	34	0,12,12	-	-	-		
59	FMN	V1	502	-	33,33,33	0.29	0	48,50,50	0.42	0
49	ADP	AK	401	-	24,29,29	0.97	1 (4%)	29,45,45	1.37	4 (13%)
50	PLX	AL	203	-	46,46,51	1.17	5 (10%)	50,54,59	0.85	1 (2%)
47	PEE	S8	303	-	50,50,50	1.31	5 (10%)	53,55,55	1.24	3 (5%)
57	U10	S7	201	-	63,63,63	2.12	22 (34%)	76,79,79	1.65	19 (25%)
47	PEE	S2	501	-	47,47,50	1.34	5 (10%)	50,52,55	1.22	4 (8%)
50	PLX	N4	501	-	48,48,51	1.14	4 (8%)	52,56,59	0.95	2 (3%)
47	PEE	AL	202	-	48,48,50	1.33	5 (10%)	51,53,55	1.20	2 (3%)
45	CDL	B5	201	-	99,99,99	0.30	0	105,111,111	0.37	0
45	CDL	AL	201	-	93,93,99	0.31	0	99,105,111	0.34	0
47	PEE	N3	201	-	50,50,50	1.31	5 (10%)	53,55,55	1.17	5 (9%)
50	PLX	AM	201	-	50,50,51	1.12	3 (6%)	54,58,59	0.87	1 (1%)
45	CDL	4L	201	-	91,91,99	0.32	0	97,103,111	0.37	0
45	CDL	A8	301	-	82,82,99	0.33	0	88,94,111	0.34	0
51	3PE	CA	101	-	50,50,50	0.31	0	53,55,55	0.28	0
53	SF4	S1	802	34	0,12,12	-	-	-		
50	PLX	CB	201	-	51,51,51	1.11	4 (7%)	55,59,59	0.92	1 (1%)
47	PEE	N5	701	-	45,45,50	1.39	5 (11%)	48,50,55	1.17	4 (8%)
46	NDP	A9	401	-	45,52,52	0.55	0	53,80,80	0.54	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CDL	N5	703	-	88,88,99	0.31	0	94,100,111	0.33	0
45	CDL	N4	503	-	61,61,99	0.37	0	67,73,111	0.36	0
47	PEE	N5	702	-	39,39,50	1.48	5 (12%)	41,44,55	1.22	3 (7%)
47	PEE	N5	705	-	50,50,50	1.31	5 (10%)	53,55,55	1.16	3 (5%)
48	ZMP	AB	201	10	29,35,36	0.71	1 (3%)	34,42,45	0.80	1 (2%)
53	SF4	V1	501	42	0,12,12	-	-	-	-	-
48	ZMP	AC	201	10	29,35,36	0.73	1 (3%)	34,42,45	0.79	1 (2%)
58	MF8	S7	202	-	7,8,8	0.91	0	7,10,10	1.49	1 (14%)
50	PLX	B1	101	-	51,51,51	1.11	4 (7%)	55,59,59	0.88	1 (1%)
51	3PE	S7	205	-	50,50,50	0.31	0	53,55,55	0.41	0
53	SF4	S8	302	41	0,12,12	-	-	-	-	-
45	CDL	A7	201	-	50,50,99	0.40	0	56,62,111	0.35	0
45	CDL	N4	502	-	99,99,99	0.30	0	105,111,111	0.30	0
51	3PE	CB	202	-	45,45,50	0.32	0	48,50,55	0.29	0
53	SF4	S7	203	40	0,12,12	-	-	-	-	-
47	PEE	N1	403	-	30,30,50	1.27	3 (10%)	33,35,55	1.18	2 (6%)
45	CDL	AK	402	-	67,67,99	0.36	0	73,79,111	0.38	0
52	PC1	N3	203	-	53,53,53	0.30	0	59,61,61	0.32	0
54	FES	S1	803	34	0,4,4	-	-	-	-	-
45	CDL	N5	704	-	99,99,99	0.30	0	105,111,111	0.28	0
54	FES	V2	301	43	0,4,4	-	-	-	-	-
53	SF4	S8	301	41	0,12,12	-	-	-	-	-
47	PEE	A9	402	-	38,38,50	1.47	5 (13%)	41,43,55	1.25	5 (12%)
50	PLX	N3	202	-	51,51,51	1.11	3 (5%)	55,59,59	0.86	1 (1%)
51	3PE	N5	706	-	45,45,50	0.33	0	48,50,55	0.29	0
45	CDL	B4	201	-	79,79,99	0.33	0	85,91,111	0.30	0
45	CDL	N1	401	-	77,77,99	0.34	0	83,89,111	0.30	0
50	PLX	S7	204	-	51,51,51	1.10	4 (7%)	55,59,59	0.92	2 (3%)
51	3PE	B8	201	-	31,31,50	0.37	0	34,36,55	0.34	0
52	PC1	N1	402	-	47,47,53	0.31	0	53,55,61	0.30	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
53	SF4	S1	801	34	-	-	0/6/5/5
59	FMN	V1	502	-	-	1/18/18/18	0/3/3/3
49	ADP	AK	401	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	PLX	AL	203	-	-	21/50/50/55	-
47	PEE	S8	303	-	-	22/54/54/54	-
57	U10	S7	201	-	-	19/63/87/87	0/1/1/1
47	PEE	S2	501	-	-	31/51/51/54	-
50	PLX	N4	501	-	-	15/52/52/55	-
47	PEE	AL	202	-	-	34/52/52/54	-
45	CDL	B5	201	-	-	17/110/110/110	-
45	CDL	AL	201	-	-	26/104/104/110	-
47	PEE	N3	201	-	-	23/54/54/54	-
50	PLX	AM	201	-	-	17/54/54/55	-
45	CDL	4L	201	-	-	20/102/102/110	-
45	CDL	A8	301	-	-	25/93/93/110	-
51	3PE	CA	101	-	-	14/54/54/54	-
53	SF4	S1	802	34	-	-	0/6/5/5
50	PLX	CB	201	-	-	24/55/55/55	-
47	PEE	N5	701	-	-	26/49/49/54	-
46	NDP	A9	401	-	-	7/30/77/77	0/5/5/5
45	CDL	N5	703	-	-	25/99/99/110	-
45	CDL	N4	503	-	-	24/72/72/110	-
47	PEE	N5	702	-	-	22/43/43/54	-
47	PEE	N5	705	-	-	23/54/54/54	-
48	ZMP	AB	201	10	-	12/40/42/43	-
53	SF4	V1	501	42	-	-	0/6/5/5
48	ZMP	AC	201	10	-	20/40/42/43	-
58	MF8	S7	202	-	-	5/8/8/8	-
50	PLX	B1	101	-	-	18/55/55/55	-
51	3PE	S7	205	-	-	10/54/54/54	-
53	SF4	S8	302	41	-	-	0/6/5/5
45	CDL	A7	201	-	-	10/61/61/110	-
45	CDL	N4	502	-	-	26/110/110/110	-
51	3PE	CB	202	-	-	11/49/49/54	-
53	SF4	S7	203	40	-	-	0/6/5/5
47	PEE	N1	403	-	-	18/34/34/54	-
45	CDL	AK	402	-	-	19/78/78/110	-
52	PC1	N3	203	-	-	15/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	FES	S1	803	34	-	-	0/1/1/1
45	CDL	N5	704	-	-	16/110/110/110	-
54	FES	V2	301	43	-	-	0/1/1/1
53	SF4	S8	301	41	-	-	0/6/5/5
47	PEE	A9	402	-	-	23/42/42/54	-
50	PLX	N3	202	-	-	22/55/55/55	-
51	3PE	N5	706	-	-	12/49/49/54	-
45	CDL	B4	201	-	-	22/90/90/110	-
45	CDL	N1	401	-	-	16/88/88/110	-
50	PLX	S7	204	-	-	24/55/55/55	-
51	3PE	B8	201	-	-	5/35/35/54	-
52	PC1	N1	402	-	-	13/51/51/57	-

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	S7	201	U10	C6-C1	10.01	1.53	1.35
57	S7	201	U10	C4-C3	4.29	1.53	1.36
47	N5	701	PEE	C18-C19	4.06	1.55	1.31
47	AL	202	PEE	C18-C19	4.05	1.55	1.31
47	N5	702	PEE	C18-C19	4.04	1.55	1.31
47	N5	705	PEE	C18-C19	4.04	1.55	1.31
47	S8	303	PEE	C18-C19	4.03	1.55	1.31
47	A9	402	PEE	C18-C19	4.03	1.55	1.31
47	N3	201	PEE	C18-C19	4.02	1.55	1.31
47	S2	501	PEE	C18-C19	4.01	1.55	1.31
47	AL	202	PEE	C39-C38	3.96	1.54	1.31
47	N5	702	PEE	C39-C38	3.95	1.54	1.31
47	S8	303	PEE	C39-C38	3.93	1.54	1.31
47	N5	701	PEE	C39-C38	3.92	1.54	1.31
47	S2	501	PEE	C39-C38	3.91	1.54	1.31
47	N5	705	PEE	C39-C38	3.91	1.54	1.31
47	N3	201	PEE	C39-C38	3.89	1.54	1.31
47	A9	402	PEE	C39-C38	3.88	1.54	1.28
47	N3	201	PEE	O3-C30	3.25	1.42	1.33
47	N1	403	PEE	O3-C30	3.25	1.42	1.33
47	N5	701	PEE	O3-C30	3.24	1.42	1.33
47	N5	702	PEE	O3-C30	3.21	1.42	1.33
47	A9	402	PEE	O3-C30	3.19	1.42	1.33
50	N4	501	PLX	O6-C4	-3.16	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S2	501	PEE	O3-C30	3.15	1.42	1.33
47	N5	705	PEE	O3-C30	3.14	1.42	1.33
50	CB	201	PLX	O6-C4	-3.08	1.40	1.44
47	S8	303	PEE	O3-C30	3.07	1.42	1.33
47	AL	202	PEE	O3-C30	3.06	1.42	1.33
50	S7	204	PLX	O6-C4	-3.05	1.40	1.44
57	S7	201	U10	C41-C39	2.98	1.57	1.51
50	B1	101	PLX	O6-C4	-2.96	1.40	1.44
50	AM	201	PLX	O6-C4	-2.93	1.40	1.44
50	AL	203	PLX	O6-C4	-2.90	1.40	1.44
50	N3	202	PLX	O6-C4	-2.87	1.40	1.44
48	AC	201	ZMP	C9-C10	-2.84	1.48	1.50
47	S8	303	PEE	O2-C10	2.71	1.42	1.34
57	S7	201	U10	C7-C8	2.70	1.54	1.50
47	AL	202	PEE	O2-C2	-2.70	1.39	1.46
48	AB	201	ZMP	C9-C10	-2.65	1.48	1.50
47	N5	701	PEE	O2-C10	2.65	1.41	1.34
47	N3	201	PEE	O2-C10	2.62	1.41	1.34
47	N5	702	PEE	O2-C10	2.62	1.41	1.34
57	S7	201	U10	C26-C24	2.59	1.56	1.51
47	N5	705	PEE	O2-C2	-2.59	1.40	1.46
47	S2	501	PEE	O2-C10	2.57	1.41	1.34
57	S7	201	U10	C31-C29	2.57	1.56	1.51
57	S7	201	U10	O5-C5	-2.57	1.17	1.23
47	N5	705	PEE	O2-C10	2.55	1.41	1.34
57	S7	201	U10	C7-C6	2.55	1.55	1.51
47	S2	501	PEE	O2-C2	-2.54	1.40	1.46
47	N1	403	PEE	O2-C2	-2.54	1.40	1.46
47	N1	403	PEE	O2-C10	2.53	1.41	1.34
47	A9	402	PEE	O2-C2	-2.52	1.40	1.46
47	S8	303	PEE	O2-C2	-2.52	1.40	1.46
47	A9	402	PEE	O2-C10	2.50	1.41	1.34
47	N5	702	PEE	O2-C2	-2.50	1.40	1.46
47	N3	201	PEE	O2-C2	-2.47	1.40	1.46
57	S7	201	U10	C21-C19	2.46	1.56	1.51
57	S7	201	U10	O2-C2	-2.45	1.18	1.23
47	N5	701	PEE	O2-C2	-2.45	1.40	1.46
47	AL	202	PEE	O2-C10	2.44	1.41	1.34
57	S7	201	U10	C36-C34	2.41	1.56	1.51
49	AK	401	ADP	C5-C4	2.39	1.47	1.40
57	S7	201	U10	C46-C44	2.34	1.56	1.51
57	S7	201	U10	C51-C49	2.25	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	N4	501	PLX	C1B-N1	-2.23	1.43	1.50
50	AL	203	PLX	C1B-N1	-2.22	1.43	1.50
50	N3	202	PLX	C1B-N1	-2.21	1.43	1.50
57	S7	201	U10	O3-C3M	-2.20	1.40	1.45
57	S7	201	U10	C6-C5	2.20	1.52	1.46
57	S7	201	U10	O4-C4M	-2.20	1.40	1.45
50	B1	101	PLX	C1B-N1	-2.19	1.43	1.50
50	CB	201	PLX	C1B-N1	-2.18	1.43	1.50
57	S7	201	U10	C16-C14	2.15	1.55	1.51
50	CB	201	PLX	C1A-N1	-2.14	1.43	1.50
57	S7	201	U10	C27-C28	2.14	1.57	1.50
57	S7	201	U10	C42-C43	2.14	1.57	1.50
57	S7	201	U10	C11-C9	2.13	1.55	1.51
50	AM	201	PLX	C1B-N1	-2.11	1.43	1.50
50	S7	204	PLX	C1B-N1	-2.10	1.43	1.50
50	AL	203	PLX	C1A-N1	-2.09	1.43	1.50
50	N3	202	PLX	C1A-N1	-2.08	1.43	1.50
57	S7	201	U10	C22-C23	2.08	1.57	1.50
50	N4	501	PLX	C1A-N1	-2.07	1.44	1.50
50	AM	201	PLX	P1-O4	2.07	1.67	1.59
50	AL	203	PLX	C7-C6	2.06	1.55	1.50
50	AL	203	PLX	P1-O4	2.04	1.67	1.59
50	B1	101	PLX	C1A-N1	-2.03	1.44	1.50
50	CB	201	PLX	P1-O3	-2.03	1.45	1.55
57	S7	201	U10	C32-C33	2.02	1.57	1.50
50	N4	501	PLX	P1-O3	-2.01	1.45	1.55
50	B1	101	PLX	P1-O4	2.01	1.67	1.59
50	S7	204	PLX	C1A-N1	-2.01	1.44	1.50
50	S7	204	PLX	P1-O4	2.00	1.67	1.59

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S8	303	PEE	O2-C10-C11	4.79	121.82	111.50
47	N1	403	PEE	O2-C10-C11	4.10	120.33	111.50
47	S2	501	PEE	O2-C10-C11	4.07	120.28	111.50
57	S7	201	U10	C7-C8-C9	-4.06	120.03	126.79
47	N3	201	PEE	O2-C10-C11	4.04	120.20	111.50
47	N5	701	PEE	O2-C10-C11	3.96	120.04	111.50
47	A9	402	PEE	O2-C10-C11	3.95	120.02	111.50
47	N5	702	PEE	O2-C10-C11	3.95	120.01	111.50
47	N5	705	PEE	O2-C10-C11	3.91	119.93	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	AL	202	PEE	O2-C10-C11	3.86	119.82	111.50
57	S7	201	U10	C17-C18-C19	-3.56	119.10	127.66
49	AK	401	ADP	PA-O3A-PB	-3.50	120.80	132.83
58	S7	202	MF8	C07-N06-C04	3.27	131.70	124.55
49	AK	401	ADP	N3-C2-N1	-3.12	123.80	128.68
57	S7	201	U10	C42-C43-C44	-3.12	120.15	127.66
57	S7	201	U10	C12-C13-C14	-3.03	120.35	127.66
57	S7	201	U10	C30-C29-C31	2.97	120.26	115.27
57	S7	201	U10	C22-C23-C24	-2.92	120.62	127.66
57	S7	201	U10	C27-C28-C29	-2.89	120.70	127.66
57	S7	201	U10	C32-C33-C34	-2.87	120.74	127.66
57	S7	201	U10	C20-C19-C21	2.83	120.03	115.27
57	S7	201	U10	C25-C24-C26	2.83	120.03	115.27
57	S7	201	U10	C10-C9-C11	2.71	119.83	115.27
47	N5	705	PEE	O3-C30-C31	2.66	120.26	111.91
47	AL	202	PEE	O3-C30-C31	2.65	120.22	111.91
47	N1	403	PEE	O3-C30-C31	2.60	120.06	111.91
47	S2	501	PEE	O3-C30-C31	2.59	120.03	111.91
57	S7	201	U10	C15-C14-C16	2.59	119.62	115.27
57	S7	201	U10	C37-C38-C39	-2.57	121.46	127.66
49	AK	401	ADP	C4-C5-N7	-2.57	106.72	109.40
47	N5	701	PEE	O3-C30-C31	2.56	119.94	111.91
57	S7	201	U10	C45-C44-C46	2.55	119.57	115.27
47	N5	702	PEE	O3-C30-C31	2.55	119.91	111.91
47	A9	402	PEE	C37-C38-C39	-2.52	109.69	126.84
57	S7	201	U10	C47-C48-C49	-2.52	121.59	127.66
47	S8	303	PEE	O3-C30-C31	2.48	119.69	111.91
47	N3	201	PEE	O3-C30-C31	2.46	119.62	111.91
47	A9	402	PEE	O3-C30-C31	2.43	119.53	111.91
57	S7	201	U10	C56-C54-C55	2.41	119.93	114.60
57	S7	201	U10	C50-C49-C51	2.38	119.27	115.27
50	N4	501	PLX	C26-C25-C24	-2.35	107.94	113.38
50	B1	101	PLX	O3-P1-O2	-2.31	100.84	112.24
50	N4	501	PLX	O3-P1-O2	-2.28	100.97	112.24
49	AK	401	ADP	C3'-C2'-C1'	2.27	104.40	100.98
50	N3	202	PLX	O3-P1-O2	-2.26	101.05	112.24
48	AB	201	ZMP	C15-C14-C13	-2.26	108.59	112.36
57	S7	201	U10	C40-C39-C41	2.26	119.08	115.27
50	AM	201	PLX	O3-P1-O2	-2.24	101.15	112.24
50	CB	201	PLX	O3-P1-O2	-2.24	101.17	112.24
50	S7	204	PLX	O3-P1-O2	-2.23	101.21	112.24
50	AL	203	PLX	O3-P1-O2	-2.19	101.43	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A9	401	NDP	C5A-C6A-N6A	2.16	123.64	120.35
50	S7	204	PLX	C8-C7-C6	-2.16	108.38	113.38
57	S7	201	U10	C35-C34-C36	2.10	118.80	115.27
47	S8	303	PEE	C17-C18-C19	-2.09	108.70	124.73
47	N3	201	PEE	C37-C38-C39	-2.05	108.96	124.73
47	N5	705	PEE	C37-C38-C39	-2.05	108.97	124.73
48	AC	201	ZMP	O1-C10-C9	-2.05	121.57	123.99
47	N3	201	PEE	C20-C19-C18	-2.03	109.18	124.73
47	S2	501	PEE	C17-C18-C19	-2.03	109.18	124.73
47	N5	701	PEE	C37-C38-C39	-2.02	109.19	124.73
47	A9	402	PEE	C17-C18-C19	-2.02	109.21	124.73
47	N3	201	PEE	C40-C39-C38	-2.02	109.22	124.73
47	N5	702	PEE	C37-C38-C39	-2.01	109.33	124.73
47	A9	402	PEE	C20-C19-C18	-2.00	109.35	124.73
47	N5	701	PEE	C40-C39-C38	-2.00	109.36	124.73
47	S2	501	PEE	C37-C38-C39	-2.00	109.37	124.73

There are no chirality outliers.

All (757) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	4L	201	CDL	CA2-OA2-PA1-OA3
45	4L	201	CDL	CA2-OA2-PA1-OA4
45	4L	201	CDL	CA2-OA2-PA1-OA5
45	4L	201	CDL	CB2-OB2-PB2-OB3
45	4L	201	CDL	CB2-OB2-PB2-OB4
45	4L	201	CDL	CB2-OB2-PB2-OB5
45	A7	201	CDL	O1-C1-CA2-OA2
45	A7	201	CDL	CA2-OA2-PA1-OA3
45	A7	201	CDL	CB2-OB2-PB2-OB3
45	A8	301	CDL	CA2-OA2-PA1-OA3
45	A8	301	CDL	CA2-OA2-PA1-OA4
45	A8	301	CDL	CA3-OA5-PA1-OA3
45	A8	301	CDL	CA3-OA5-PA1-OA4
45	A8	301	CDL	CB2-OB2-PB2-OB3
45	A8	301	CDL	CB2-OB2-PB2-OB5
45	A8	301	CDL	CB3-OB5-PB2-OB2
45	A8	301	CDL	CB3-OB5-PB2-OB3
45	A8	301	CDL	CB3-OB5-PB2-OB4
45	AK	402	CDL	CA2-OA2-PA1-OA3
45	AK	402	CDL	CA2-OA2-PA1-OA4
45	AK	402	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
45	AK	402	CDL	CA3-OA5-PA1-OA4
45	AK	402	CDL	CB2-OB2-PB2-OB3
45	AK	402	CDL	CB2-OB2-PB2-OB4
45	AK	402	CDL	CB2-OB2-PB2-OB5
45	AL	201	CDL	CA2-OA2-PA1-OA3
45	AL	201	CDL	CB2-OB2-PB2-OB5
45	AL	201	CDL	CB3-OB5-PB2-OB3
45	AL	201	CDL	CB3-OB5-PB2-OB4
45	B4	201	CDL	CA2-OA2-PA1-OA3
45	B4	201	CDL	CA2-OA2-PA1-OA5
45	B4	201	CDL	CA3-OA5-PA1-OA3
45	B4	201	CDL	CB2-OB2-PB2-OB3
45	B5	201	CDL	CA2-OA2-PA1-OA3
45	N1	401	CDL	CA2-C1-CB2-OB2
45	N1	401	CDL	CA2-OA2-PA1-OA5
45	N1	401	CDL	CB2-OB2-PB2-OB3
45	N1	401	CDL	CB2-OB2-PB2-OB4
45	N1	401	CDL	CB2-OB2-PB2-OB5
45	N4	502	CDL	CA2-OA2-PA1-OA3
45	N4	503	CDL	CA2-OA2-PA1-OA3
45	N4	503	CDL	CA3-OA5-PA1-OA3
45	N4	503	CDL	CA3-OA5-PA1-OA4
45	N5	703	CDL	CA2-OA2-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	CB3-OB5-PB2-OB3
45	N5	703	CDL	CB3-OB5-PB2-OB4
47	A9	402	PEE	C11-C10-O2-C2
47	A9	402	PEE	C1-O3P-P-O1P
47	A9	402	PEE	C4-O4P-P-O3P
47	A9	402	PEE	C4-O4P-P-O2P
47	AL	202	PEE	C1-O3P-P-O2P
47	AL	202	PEE	C1-O3P-P-O1P
47	AL	202	PEE	C4-O4P-P-O2P
47	AL	202	PEE	C4-O4P-P-O1P
47	AL	202	PEE	O4P-C4-C5-N
47	AL	202	PEE	C37-C38-C39-C40
47	N1	403	PEE	C1-O3P-P-O2P
47	N1	403	PEE	C1-O3P-P-O1P
47	N1	403	PEE	C4-O4P-P-O3P
47	N1	403	PEE	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
47	N1	403	PEE	C4-O4P-P-O1P
47	N3	201	PEE	C17-C18-C19-C20
47	N3	201	PEE	C1-O3P-P-O2P
47	N3	201	PEE	C4-O4P-P-O3P
47	N3	201	PEE	C31-C30-O3-C3
47	N5	701	PEE	C4-O4P-P-O2P
47	N5	702	PEE	C11-C10-O2-C2
47	N5	702	PEE	C1-O3P-P-O2P
47	N5	702	PEE	C1-O3P-P-O1P
47	N5	702	PEE	C1-O3P-P-O4P
47	N5	702	PEE	C37-C38-C39-C40
47	N5	705	PEE	C1-O3P-P-O2P
47	S2	501	PEE	C11-C10-O2-C2
47	S2	501	PEE	O4-C10-O2-C2
47	S2	501	PEE	C1-O3P-P-O2P
47	S2	501	PEE	C1-O3P-P-O1P
47	S2	501	PEE	C4-O4P-P-O3P
47	S2	501	PEE	C4-O4P-P-O2P
47	S2	501	PEE	C4-O4P-P-O1P
47	S8	303	PEE	O4-C10-O2-C2
48	AC	201	ZMP	C17-C18-C21-O5
48	AC	201	ZMP	S1-C11-C12-N1
48	AC	201	ZMP	C12-C11-S1-C10
48	AC	201	ZMP	O1-C10-S1-C11
48	AC	201	ZMP	C9-C10-S1-C11
48	AC	201	ZMP	C7-C8-C9-C10
49	AK	401	ADP	C5'-O5'-PA-O2A
49	AK	401	ADP	C5'-O5'-PA-O3A
50	AL	203	PLX	O7-C6-C7-C8
50	AL	203	PLX	O7-C6-O6-C4
50	AL	203	PLX	C3-O4-P1-O2
50	AL	203	PLX	C3-O4-P1-O3
50	AL	203	PLX	C25-C24-O8-C5
50	AL	203	PLX	O9-C24-C25-C26
50	AM	201	PLX	O7-C6-O6-C4
50	AM	201	PLX	C2-O1-P1-O4
50	AM	201	PLX	C2-O1-P1-O2
50	AM	201	PLX	N1-C1-C2-O1
50	B1	101	PLX	O7-C6-C7-C8
50	B1	101	PLX	O7-C6-O6-C4
50	B1	101	PLX	C3-O4-P1-O1
50	B1	101	PLX	C3-O4-P1-O2

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Mol	Chain	Res	Type	Atoms
50	B1	101	PLX	N1-C1-C2-O1
50	CB	201	PLX	O7-C6-C7-C8
50	CB	201	PLX	C3-C4-O6-C6
50	CB	201	PLX	C2-O1-P1-O2
50	CB	201	PLX	O9-C24-O8-C5
50	N3	202	PLX	O7-C6-O6-C4
50	N3	202	PLX	N1-C1-C2-O1
50	N4	501	PLX	O7-C6-O6-C4
50	N4	501	PLX	C3-O4-P1-O2
50	N4	501	PLX	C3-O4-P1-O3
50	S7	204	PLX	O7-C6-C7-C8
50	S7	204	PLX	C2-O1-P1-O3
51	B8	201	3PE	C1-O11-P-O12
51	B8	201	3PE	O13-C11-C12-N
51	CA	101	3PE	O13-C11-C12-N
51	CB	202	3PE	C1-O11-P-O12
51	CB	202	3PE	C11-O13-P-O12
51	N5	706	3PE	C1-O11-P-O12
51	N5	706	3PE	O13-C11-C12-N
51	S7	205	3PE	O21-C2-C3-O31
52	N1	402	PC1	C11-O13-P-O12
52	N1	402	PC1	C1-O11-P-O12
52	N3	203	PC1	C11-O13-P-O12
52	N3	203	PC1	C11-O13-P-O14
52	N3	203	PC1	C11-O13-P-O11
52	N3	203	PC1	C1-O11-P-O12
52	N3	203	PC1	C1-O11-P-O14
52	N3	203	PC1	C1-O11-P-O13
57	S7	201	U10	C19-C21-C22-C23
57	S7	201	U10	C30-C29-C31-C32
57	S7	201	U10	C29-C31-C32-C33
47	AL	202	PEE	O5-C30-O3-C3
47	N3	201	PEE	O5-C30-O3-C3
47	AL	202	PEE	C31-C30-O3-C3
47	N5	702	PEE	O5-C30-O3-C3
47	A9	402	PEE	O4-C10-O2-C2
47	N5	702	PEE	O4-C10-O2-C2
47	S8	303	PEE	C11-C10-O2-C2
47	N1	403	PEE	O5-C30-O3-C3
57	S7	201	U10	C28-C29-C31-C32
47	N5	702	PEE	C31-C30-O3-C3
47	N5	701	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
47	N5	705	PEE	C37-C38-C39-C40
47	S8	303	PEE	C37-C38-C39-C40
47	N1	403	PEE	C31-C30-O3-C3
47	N5	705	PEE	C11-C10-O2-C2
57	S7	201	U10	C9-C11-C12-C13
57	S7	201	U10	C24-C26-C27-C28
57	S7	201	U10	C39-C41-C42-C43
45	A7	201	CDL	CB2-C1-CA2-OA2
45	N1	401	CDL	O1-C1-CB2-OB2
47	N5	702	PEE	C30-C31-C32-C33
47	N3	201	PEE	C10-C11-C12-C13
47	A9	402	PEE	C17-C18-C19-C20
47	A9	402	PEE	C10-C11-C12-C13
47	N5	705	PEE	O4-C10-O2-C2
47	N1	403	PEE	C33-C34-C35-C36
52	N1	402	PC1	C11-C12-N-C15
45	N4	503	CDL	CA7-C31-C32-C33
45	N4	503	CDL	C13-C14-C15-C16
47	N5	705	PEE	C33-C34-C35-C36
57	S7	201	U10	C34-C36-C37-C38
51	CB	202	3PE	C21-C22-C23-C24
45	A8	301	CDL	O1-C1-CB2-OB2
45	B4	201	CDL	O1-C1-CA2-OA2
45	4L	201	CDL	CA3-OA5-PA1-OA2
45	A8	301	CDL	CA2-OA2-PA1-OA5
45	A8	301	CDL	CA3-OA5-PA1-OA2
45	AK	402	CDL	CA2-OA2-PA1-OA5
45	AK	402	CDL	CA3-OA5-PA1-OA2
45	AL	201	CDL	CA2-OA2-PA1-OA5
45	AL	201	CDL	CB3-OB5-PB2-OB2
45	B5	201	CDL	CA3-OA5-PA1-OA2
45	B5	201	CDL	CB3-OB5-PB2-OB2
45	N1	401	CDL	CB3-OB5-PB2-OB2
45	N4	502	CDL	CA2-OA2-PA1-OA5
45	N4	502	CDL	CB3-OB5-PB2-OB2
45	N4	503	CDL	CA2-OA2-PA1-OA5
45	N4	503	CDL	CA3-OA5-PA1-OA2
45	N4	503	CDL	CB2-OB2-PB2-OB5
45	N5	703	CDL	CA2-OA2-PA1-OA5
45	N5	703	CDL	CA3-OA5-PA1-OA2
45	N5	703	CDL	CB2-OB2-PB2-OB5
45	N5	703	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
47	AL	202	PEE	C1-O3P-P-O4P
47	AL	202	PEE	C4-O4P-P-O3P
47	N1	403	PEE	C1-O3P-P-O4P
47	N3	201	PEE	C1-O3P-P-O4P
47	N5	701	PEE	C4-O4P-P-O3P
47	S2	501	PEE	C1-O3P-P-O4P
47	S8	303	PEE	C1-O3P-P-O4P
50	AL	203	PLX	C3-O4-P1-O1
50	B1	101	PLX	C2-O1-P1-O4
50	CB	201	PLX	C2-O1-P1-O4
50	N3	202	PLX	C3-O4-P1-O1
50	N4	501	PLX	C3-O4-P1-O1
50	S7	204	PLX	C2-O1-P1-O4
51	B8	201	3PE	C1-O11-P-O13
51	CA	101	3PE	C11-O13-P-O11
51	CB	202	3PE	C1-O11-P-O13
51	N5	706	3PE	C1-O11-P-O13
51	S7	205	3PE	C1-O11-P-O13
52	N1	402	PC1	C11-O13-P-O11
52	N1	402	PC1	C1-O11-P-O13
45	A8	301	CDL	CA2-C1-CB2-OB2
45	B4	201	CDL	CB2-C1-CA2-OA2
47	A9	402	PEE	C31-C30-O3-C3
50	CB	201	PLX	O8-C24-C25-C26
50	N3	202	PLX	O8-C24-C25-C26
50	S7	204	PLX	O6-C6-C7-C8
45	N1	401	CDL	C76-C77-C78-C79
47	A9	402	PEE	C12-C13-C14-C15
47	N1	403	PEE	C12-C13-C14-C15
47	S8	303	PEE	C13-C14-C15-C16
50	AL	203	PLX	C33-C34-C35-C36
50	N3	202	PLX	C34-C35-C36-C37
50	AL	203	PLX	C29-C30-C31-C32
47	N3	201	PEE	C33-C34-C35-C36
47	N5	702	PEE	C14-C15-C16-C17
47	N5	702	PEE	C12-C13-C14-C15
47	S2	501	PEE	C11-C12-C13-C14
47	N5	701	PEE	C37-C38-C39-C40
52	N3	203	PC1	C23-C24-C25-C26
50	AL	203	PLX	C12-C13-C14-C15
48	AB	201	ZMP	C2-C3-C4-C5
47	A9	402	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
47	N5	701	PEE	C21-C22-C23-C24
47	N5	702	PEE	C11-C12-C13-C14
50	B1	101	PLX	C25-C26-C27-C28
47	AL	202	PEE	C22-C23-C24-C25
47	N3	201	PEE	C22-C23-C24-C25
48	AC	201	ZMP	C3-C4-C5-C6
50	CB	201	PLX	C31-C32-C33-C34
47	N5	701	PEE	C15-C16-C17-C18
47	S2	501	PEE	C15-C16-C17-C18
45	4L	201	CDL	C39-C40-C41-C42
45	AL	201	CDL	C52-C53-C54-C55
47	AL	202	PEE	C21-C22-C23-C24
50	AM	201	PLX	C12-C13-C14-C15
52	N1	402	PC1	C11-C12-N-C13
47	N5	701	PEE	C32-C33-C34-C35
45	AL	201	CDL	C33-C34-C35-C36
47	N3	201	PEE	C30-C31-C32-C33
47	N3	201	PEE	C40-C41-C42-C43
47	N5	701	PEE	C12-C13-C14-C15
47	N5	701	PEE	C31-C32-C33-C34
47	S8	303	PEE	C33-C34-C35-C36
51	N5	706	3PE	C35-C36-C37-C38
51	CA	101	3PE	C2A-C2B-C2C-C2D
50	N4	501	PLX	C29-C30-C31-C32
57	S7	201	U10	C50-C49-C51-C52
57	S7	201	U10	C12-C11-C9-C8
57	S7	201	U10	C18-C19-C21-C22
47	S2	501	PEE	C14-C15-C16-C17
50	AM	201	PLX	O9-C24-C25-C26
50	CB	201	PLX	O9-C24-C25-C26
50	N3	202	PLX	O9-C24-C25-C26
50	S7	204	PLX	O9-C24-C25-C26
45	N4	502	CDL	C38-C39-C40-C41
50	S7	204	PLX	C13-C14-C15-C16
47	S8	303	PEE	C35-C36-C37-C38
45	N1	401	CDL	C31-C32-C33-C34
45	N4	502	CDL	C78-C79-C80-C81
47	N5	702	PEE	C10-C11-C12-C13
47	AL	202	PEE	C23-C24-C25-C26
47	S2	501	PEE	C20-C21-C22-C23
50	B1	101	PLX	C14-C15-C16-C17
50	CB	201	PLX	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
47	N3	201	PEE	C21-C22-C23-C24
47	N5	701	PEE	C14-C15-C16-C17
47	AL	202	PEE	C11-C10-O2-C2
47	N1	403	PEE	C30-C31-C32-C33
47	N5	702	PEE	C18-C19-C20-C21
57	S7	201	U10	C48-C49-C51-C52
45	N4	502	CDL	C32-C33-C34-C35
47	AL	202	PEE	C39-C40-C41-C42
47	N3	201	PEE	C35-C36-C37-C38
47	N5	705	PEE	C35-C36-C37-C38
47	AL	202	PEE	O4-C10-O2-C2
51	S7	205	3PE	C21-C22-C23-C24
50	S7	204	PLX	C7-C8-C9-C10
45	N4	502	CDL	C22-C23-C24-C25
47	S8	303	PEE	C22-C23-C24-C25
47	S8	303	PEE	C14-C15-C16-C17
48	AC	201	ZMP	C6-C7-C8-C9
45	4L	201	CDL	CA5-C11-C12-C13
47	N5	701	PEE	C11-C10-O2-C2
47	S8	303	PEE	O3P-C1-C2-O2
47	S2	501	PEE	C38-C39-C40-C41
45	N4	502	CDL	C61-C62-C63-C64
48	AC	201	ZMP	C22-C23-C24-C25
47	N5	701	PEE	O4-C10-O2-C2
48	AB	201	ZMP	C6-C7-C8-C9
47	N5	705	PEE	C21-C22-C23-C24
52	N1	402	PC1	C11-C12-N-C14
45	N4	502	CDL	C81-C82-C83-C84
47	A9	402	PEE	C35-C36-C37-C38
47	AL	202	PEE	C19-C20-C21-C22
47	N5	705	PEE	C19-C20-C21-C22
57	S7	201	U10	C12-C11-C9-C10
57	S7	201	U10	C20-C19-C21-C22
45	N5	704	CDL	C51-C52-C53-C54
47	S2	501	PEE	C40-C41-C42-C43
50	AM	201	PLX	C31-C32-C33-C34
45	B4	201	CDL	CB2-OB2-PB2-OB5
47	A9	402	PEE	C1-O3P-P-O4P
50	CB	201	PLX	C3-O4-P1-O1
51	CA	101	3PE	C1-O11-P-O13
50	N4	501	PLX	C9-C10-C11-C12
45	AL	201	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
45	A8	301	CDL	OA5-CA3-CA4-CA6
45	B5	201	CDL	OB5-CB3-CB4-CB6
47	N5	705	PEE	C11-C12-C13-C14
50	AL	203	PLX	C7-C8-C9-C10
47	N1	403	PEE	C11-C12-C13-C14
45	N5	703	CDL	C61-C62-C63-C64
47	N5	701	PEE	C11-C12-C13-C14
47	N5	701	PEE	C35-C36-C37-C38
47	N3	201	PEE	C32-C33-C34-C35
50	S7	204	PLX	C35-C36-C37-C38
45	N4	503	CDL	CA3-CA4-CA6-OA8
47	N1	403	PEE	C1-C2-C3-O3
47	N5	701	PEE	C1-C2-C3-O3
47	N5	702	PEE	C32-C33-C34-C35
47	S8	303	PEE	C21-C22-C23-C24
50	AL	203	PLX	C3-C4-C5-O8
50	N4	501	PLX	C3-C4-C5-O8
51	S7	205	3PE	C1-C2-C3-O31
47	S2	501	PEE	C21-C22-C23-C24
50	CB	201	PLX	C9-C10-C11-C12
50	S7	204	PLX	C25-C26-C27-C28
45	N5	703	CDL	CA7-C31-C32-C33
50	S7	204	PLX	O8-C24-C25-C26
48	AB	201	ZMP	O3-C16-C17-O4
47	AL	202	PEE	C35-C36-C37-C38
45	N4	502	CDL	C63-C64-C65-C66
47	AL	202	PEE	C10-C11-C12-C13
47	S2	501	PEE	C31-C30-O3-C3
47	AL	202	PEE	C11-C12-C13-C14
47	S2	501	PEE	C42-C43-C44-C45
50	S7	204	PLX	C11-C10-C9-C8
48	AB	201	ZMP	C3-C4-C5-C6
50	AM	201	PLX	O4-C3-C4-O6
50	S7	204	PLX	C33-C34-C35-C36
47	A9	402	PEE	C30-C31-C32-C33
45	A8	301	CDL	OB6-CB4-CB6-OB8
50	AL	203	PLX	O6-C4-C5-O8
45	B4	201	CDL	C80-C81-C82-C83
47	S2	501	PEE	C18-C19-C20-C21
45	B4	201	CDL	C74-C75-C76-C77
47	A9	402	PEE	C33-C34-C35-C36
50	B1	101	PLX	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
45	AK	402	CDL	C53-C54-C55-C56
47	AL	202	PEE	C17-C18-C19-C20
50	AL	203	PLX	C32-C33-C34-C35
51	CA	101	3PE	C35-C36-C37-C38
47	S8	303	PEE	O3P-C1-C2-C3
51	S7	205	3PE	O11-C1-C2-C3
45	A8	301	CDL	C11-C12-C13-C14
47	N5	701	PEE	C30-C31-C32-C33
47	S2	501	PEE	O5-C30-O3-C3
51	CB	202	3PE	C39-C3A-C3B-C3C
52	N1	402	PC1	C2-C1-O11-P
47	S2	501	PEE	C16-C17-C18-C19
50	N3	202	PLX	C30-C31-C32-C33
52	N3	203	PC1	C32-C33-C34-C35
45	N5	704	CDL	C22-C23-C24-C25
47	A9	402	PEE	C11-C12-C13-C14
50	CB	201	PLX	C11-C12-C13-C14
50	B1	101	PLX	C31-C32-C33-C34
45	A8	301	CDL	CB3-CB4-CB6-OB8
47	AL	202	PEE	C1-C2-C3-O3
47	N5	705	PEE	C1-C2-C3-O3
47	S8	303	PEE	C1-C2-C3-O3
50	CB	201	PLX	C3-C4-C5-O8
45	B5	201	CDL	C21-C22-C23-C24
47	N1	403	PEE	C10-C11-C12-C13
48	AB	201	ZMP	N2-C16-C17-C18
48	AC	201	ZMP	N2-C16-C17-C18
45	N1	401	CDL	C75-C76-C77-C78
45	N1	401	CDL	C13-C14-C15-C16
50	B1	101	PLX	C5-C4-O6-C6
50	N3	202	PLX	C5-C4-O6-C6
50	N4	501	PLX	C5-C4-O6-C6
50	B1	101	PLX	O9-C24-C25-C26
51	N5	706	3PE	C3A-C3B-C3C-C3D
45	A8	301	CDL	OB5-CB3-CB4-OB6
45	B4	201	CDL	OB5-CB3-CB4-OB6
47	N5	705	PEE	O3P-C1-C2-O2
50	CB	201	PLX	O4-C3-C4-O6
50	N3	202	PLX	O4-C3-C4-O6
47	S8	303	PEE	C10-C11-C12-C13
45	A8	301	CDL	C38-C39-C40-C41
50	AL	203	PLX	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
47	AL	202	PEE	O2-C2-C3-O3
47	N1	403	PEE	O2-C2-C3-O3
47	N5	701	PEE	O2-C2-C3-O3
50	CB	201	PLX	O6-C4-C5-O8
45	N5	703	CDL	C59-C60-C61-C62
45	B5	201	CDL	CB2-C1-CA2-OA2
57	S7	201	U10	C49-C51-C52-C53
48	AC	201	ZMP	C2-C3-C4-C5
45	N4	503	CDL	CB4-CB3-OB5-PB2
50	N4	501	PLX	C4-C3-O4-P1
45	N5	704	CDL	C17-C18-C19-C20
50	N4	501	PLX	C34-C35-C36-C37
48	AC	201	ZMP	S1-C10-C9-C8
48	AC	201	ZMP	O1-C10-C9-C8
45	4L	201	CDL	C15-C16-C17-C18
47	AL	202	PEE	C24-C25-C26-C27
50	AL	203	PLX	O6-C6-C7-C8
50	AL	203	PLX	O8-C24-C25-C26
45	A8	301	CDL	OB5-CB3-CB4-CB6
45	N4	503	CDL	OB5-CB3-CB4-CB6
47	A9	402	PEE	O3P-C1-C2-C3
47	AL	202	PEE	O3P-C1-C2-C3
45	A8	301	CDL	C17-C18-C19-C20
47	S8	303	PEE	C11-C12-C13-C14
48	AB	201	ZMP	N2-C16-C17-O4
45	N5	704	CDL	CB5-C51-C52-C53
50	S7	204	PLX	C12-C13-C14-C15
47	N5	702	PEE	C31-C32-C33-C34
47	N5	705	PEE	C14-C15-C16-C17
45	N5	704	CDL	C59-C60-C61-C62
45	AK	402	CDL	C1-CA2-OA2-PA1
45	N4	502	CDL	CB3-CB4-CB6-OB8
45	N5	703	CDL	C1-CB2-OB2-PB2
50	AM	201	PLX	C3-C4-C5-O8
45	AK	402	CDL	OA5-CA3-CA4-OA6
45	B5	201	CDL	OB5-CB3-CB4-OB6
45	N4	503	CDL	OB5-CB3-CB4-OB6
58	S7	202	MF8	N06-C04-N02-C01
47	S2	501	PEE	C43-C44-C45-C46
47	N5	705	PEE	O2-C2-C3-O3
47	S8	303	PEE	O2-C2-C3-O3
50	AM	201	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
50	N4	501	PLX	O6-C4-C5-O8
50	S7	204	PLX	O6-C4-C5-O8
47	S2	501	PEE	C44-C45-C46-C47
48	AC	201	ZMP	C14-C15-N2-C16
47	S2	501	PEE	C35-C36-C37-C38
46	A9	401	NDP	PN-O3-PA-O2A
52	N3	203	PC1	C22-C23-C24-C25
45	N4	503	CDL	CA5-C11-C12-C13
50	B1	101	PLX	C11-C12-C13-C14
47	N5	702	PEE	C33-C34-C35-C36
45	A7	201	CDL	CA2-OA2-PA1-OA5
45	A7	201	CDL	CB2-OB2-PB2-OB5
45	B4	201	CDL	CA3-OA5-PA1-OA2
45	B5	201	CDL	CA2-OA2-PA1-OA5
47	N5	702	PEE	C4-O4P-P-O3P
47	N5	705	PEE	C1-O3P-P-O4P
51	CB	202	3PE	C11-O13-P-O11
50	N4	501	PLX	C26-C27-C28-C29
45	N4	503	CDL	CA4-CA3-OA5-PA1
45	N5	704	CDL	CA4-CA3-OA5-PA1
47	S2	501	PEE	C2-C1-O3P-P
51	S7	205	3PE	C2-C1-O11-P
47	AL	202	PEE	C40-C41-C42-C43
45	4L	201	CDL	CA3-OA5-PA1-OA3
45	4L	201	CDL	CA3-OA5-PA1-OA4
45	AL	201	CDL	CA2-OA2-PA1-OA4
45	B4	201	CDL	CB2-OB2-PB2-OB4
45	B5	201	CDL	CA2-OA2-PA1-OA4
45	B5	201	CDL	CA3-OA5-PA1-OA3
45	B5	201	CDL	CA3-OA5-PA1-OA4
45	B5	201	CDL	CB3-OB5-PB2-OB3
45	N1	401	CDL	CA2-OA2-PA1-OA4
45	N1	401	CDL	CB3-OB5-PB2-OB3
45	N4	502	CDL	CA2-OA2-PA1-OA4
45	N4	502	CDL	CB3-OB5-PB2-OB3
45	N4	503	CDL	CA2-OA2-PA1-OA4
45	N4	503	CDL	CB2-OB2-PB2-OB3
45	N5	703	CDL	CA2-OA2-PA1-OA4
47	A9	402	PEE	C4-O4P-P-O1P
47	N3	201	PEE	C1-O3P-P-O1P
47	N5	701	PEE	C4-O4P-P-O1P
47	N5	705	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
47	S8	303	PEE	C1-O3P-P-O1P
50	AM	201	PLX	C3-O4-P1-O2
50	B1	101	PLX	C3-O4-P1-O3
50	B1	101	PLX	C2-O1-P1-O3
50	CB	201	PLX	C3-O4-P1-O3
50	N3	202	PLX	C3-O4-P1-O2
50	N3	202	PLX	C3-O4-P1-O3
50	S7	204	PLX	C2-O1-P1-O2
51	CA	101	3PE	C1-O11-P-O12
51	CA	101	3PE	C1-O11-P-O14
51	CA	101	3PE	C11-O13-P-O14
51	CB	202	3PE	C1-O11-P-O14
51	CB	202	3PE	C11-O13-P-O14
51	S7	205	3PE	C1-O11-P-O14
52	N1	402	PC1	C11-O13-P-O14
45	N4	502	CDL	C33-C34-C35-C36
47	N5	701	PEE	O3P-C1-C2-C3
50	AM	201	PLX	O4-C3-C4-C5
50	N3	202	PLX	O4-C3-C4-C5
45	4L	201	CDL	C76-C77-C78-C79
47	AL	202	PEE	C12-C13-C14-C15
57	S7	201	U10	C5-C4-O4-C4M
45	AL	201	CDL	C36-C37-C38-C39
47	N3	201	PEE	C5-C4-O4P-P
50	B1	101	PLX	C1-C2-O1-P1
50	N3	202	PLX	C25-C24-O8-C5
50	N4	501	PLX	C25-C24-O8-C5
50	S7	204	PLX	C25-C24-O8-C5
51	CA	101	3PE	C12-C11-O13-P
50	CB	201	PLX	C7-C8-C9-C10
47	AL	202	PEE	C34-C35-C36-C37
47	S2	501	PEE	C34-C35-C36-C37
50	AM	201	PLX	C7-C8-C9-C10
45	A8	301	CDL	OA5-CA3-CA4-OA6
47	A9	402	PEE	O3P-C1-C2-O2
47	AL	202	PEE	O3P-C1-C2-O2
47	N5	701	PEE	O3P-C1-C2-O2
50	CB	201	PLX	C11-C10-C9-C8
51	CA	101	3PE	C27-C28-C29-C2A
46	A9	401	NDP	C2D-C1D-N1N-C6N
50	N3	202	PLX	C3-C4-C5-O8
50	S7	204	PLX	N1-C1-C2-O1

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Mol	Chain	Res	Type	Atoms
52	N3	203	PC1	O13-C11-C12-N
45	N4	503	CDL	OA6-CA4-CA6-OA8
47	A9	402	PEE	O2-C2-C3-O3
50	N3	202	PLX	O6-C4-C5-O8
51	N5	706	3PE	O21-C2-C3-O31
45	N1	401	CDL	C73-C74-C75-C76
50	N4	501	PLX	C36-C37-C38-C39
50	AL	203	PLX	C13-C14-C15-C16
45	N1	401	CDL	C1-CB2-OB2-PB2
45	N4	503	CDL	C1-CA2-OA2-PA1
49	AK	401	ADP	C4'-C5'-O5'-PA
45	N4	502	CDL	C12-C13-C14-C15
50	N3	202	PLX	C26-C27-C28-C29
48	AC	201	ZMP	O3-C16-C17-O4
47	N5	701	PEE	C33-C34-C35-C36
50	N3	202	PLX	C27-C28-C29-C30
47	N5	705	PEE	C24-C25-C26-C27
45	N4	503	CDL	O1-C1-CB2-OB2
48	AC	201	ZMP	C20-C18-C21-O5
47	N3	201	PEE	C41-C42-C43-C44
45	N5	704	CDL	C72-C73-C74-C75
45	N5	703	CDL	OB5-CB3-CB4-CB6
50	S7	204	PLX	C14-C15-C16-C17
47	N1	403	PEE	C14-C15-C16-C17
45	AL	201	CDL	OB5-CB3-CB4-OB6
46	A9	401	NDP	O4D-C1D-N1N-C6N
52	N3	203	PC1	C26-C27-C28-C29
45	N4	502	CDL	C72-C71-CB7-OB8
45	B4	201	CDL	C78-C79-C80-C81
45	AL	201	CDL	OB6-CB4-CB6-OB8
45	N4	502	CDL	OB6-CB4-CB6-OB8
45	A7	201	CDL	CB3-OB5-PB2-OB2
45	AL	201	CDL	CA3-OA5-PA1-OA2
45	N4	502	CDL	CA3-OA5-PA1-OA2
45	N4	502	CDL	CB2-OB2-PB2-OB5
45	N5	704	CDL	CA3-OA5-PA1-OA2
50	N3	202	PLX	C2-O1-P1-O4
50	N4	501	PLX	C2-O1-P1-O4
50	S7	204	PLX	C3-O4-P1-O1
50	AM	201	PLX	C27-C28-C29-C30
50	S7	204	PLX	C6-C7-C8-C9
45	B4	201	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
57	S7	201	U10	C2-C3-O3-C3M
45	4L	201	CDL	C79-C80-C81-C82
45	B5	201	CDL	C1-CA2-OA2-PA1
45	B5	201	CDL	CB4-CB3-OB5-PB2
45	B5	201	CDL	C17-C18-C19-C20
58	S7	202	MF8	N08-C07-N06-C04
45	AL	201	CDL	C34-C35-C36-C37
47	N5	705	PEE	C18-C19-C20-C21
50	S7	204	PLX	C32-C33-C34-C35
52	N1	402	PC1	C2A-C2B-C2C-C2D
45	N1	401	CDL	C12-C13-C14-C15
50	N3	202	PLX	C10-C11-C12-C13
58	S7	202	MF8	N06-C04-N02-C03
45	N4	502	CDL	C77-C78-C79-C80
50	CB	201	PLX	C28-C29-C30-C31
48	AB	201	ZMP	O3-C16-C17-C18
50	CB	201	PLX	C17-C18-C19-C20
45	A8	301	CDL	C1-CB2-OB2-PB2
45	N4	502	CDL	CB4-CB3-OB5-PB2
48	AB	201	ZMP	S1-C11-C12-N1
47	S8	303	PEE	C15-C16-C17-C18
45	N5	703	CDL	C36-C37-C38-C39
47	S8	303	PEE	C31-C32-C33-C34
48	AB	201	ZMP	C19-C18-C21-O5
48	AC	201	ZMP	C19-C18-C21-O5
50	N3	202	PLX	C7-C8-C9-C10
45	4L	201	CDL	CA6-CA4-OA6-CA5
47	S8	303	PEE	C3-C2-O2-C10
51	S7	205	3PE	C1-C2-O21-C21
57	S7	201	U10	C4-C3-O3-C3M
58	S7	202	MF8	N05-C04-N02-C01
45	4L	201	CDL	OB5-CB3-CB4-CB6
45	AL	201	CDL	OB5-CB3-CB4-CB6
45	N5	704	CDL	OB5-CB3-CB4-CB6
45	AK	402	CDL	C72-C73-C74-C75
47	AL	202	PEE	C33-C34-C35-C36
48	AB	201	ZMP	C12-C11-S1-C10
45	B4	201	CDL	C52-C53-C54-C55
46	A9	401	NDP	C2D-C1D-N1N-C2N
52	N3	203	PC1	C38-C39-C3A-C3B
45	N5	703	CDL	C60-C61-C62-C63
45	N5	704	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
52	N3	203	PC1	C3B-C3C-C3D-C3E
45	A8	301	CDL	C22-C23-C24-C25
47	N5	701	PEE	C22-C23-C24-C25
45	N4	503	CDL	C34-C35-C36-C37
47	N5	705	PEE	C42-C43-C44-C45
45	4L	201	CDL	OB5-CB3-CB4-OB6
45	N4	502	CDL	OA5-CA3-CA4-OA6
45	4L	201	CDL	C23-C24-C25-C26
50	CB	201	PLX	C15-C16-C17-C18
50	AM	201	PLX	O6-C6-C7-C8
50	AM	201	PLX	O8-C24-C25-C26
50	N3	202	PLX	O6-C6-C7-C8
47	N5	705	PEE	O3P-C1-C2-C3
50	CB	201	PLX	O4-C3-C4-C5
45	N5	704	CDL	OA6-CA4-CA6-OA8
45	AL	201	CDL	C52-C51-CB5-OB6
47	N5	705	PEE	O3-C30-C31-C32
50	AL	203	PLX	C11-C10-C9-C8
50	N3	202	PLX	C35-C36-C37-C38
49	AK	401	ADP	O4'-C4'-C5'-O5'
48	AC	201	ZMP	N2-C16-C17-O4
45	A7	201	CDL	C72-C71-CB7-OB8
47	N1	403	PEE	O2-C10-C11-C12
47	N3	201	PEE	O2-C10-C11-C12
51	N5	706	3PE	C22-C23-C24-C25
45	N5	703	CDL	C57-C58-C59-C60
47	S2	501	PEE	C19-C20-C21-C22
45	B4	201	CDL	C84-C85-C86-C87
52	N1	402	PC1	C2F-C2G-C2H-C2I
47	N5	705	PEE	C31-C32-C33-C34
47	A9	402	PEE	O2-C10-C11-C12
45	AK	402	CDL	CA6-CA4-OA6-CA5
45	AL	201	CDL	CA3-CA4-OA6-CA5
45	AL	201	CDL	CA6-CA4-OA6-CA5
45	B5	201	CDL	CB3-CB4-OB6-CB5
45	N4	503	CDL	CB6-CB4-OB6-CB5
46	A9	401	NDP	O4D-C1D-N1N-C2N
45	AL	201	CDL	C12-C11-CA5-OA6
50	CB	201	PLX	C32-C33-C34-C35
45	N5	703	CDL	C12-C11-CA5-OA6
50	AL	203	PLX	C7-C6-O6-C4
51	N5	706	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
50	B1	101	PLX	C30-C31-C32-C33
45	N4	502	CDL	OB5-CB3-CB4-OB6
45	N5	704	CDL	OB5-CB3-CB4-OB6
47	N5	702	PEE	O3P-C1-C2-O2
45	AL	201	CDL	C32-C31-CA7-OA8
45	N5	703	CDL	C72-C71-CB7-OB8
47	S2	501	PEE	O2-C10-C11-C12
46	A9	401	NDP	O4B-C4B-C5B-O5B
45	AK	402	CDL	C12-C11-CA5-OA6
45	B4	201	CDL	C12-C11-CA5-OA6
47	AL	202	PEE	O2-C10-C11-C12
47	AL	202	PEE	C16-C17-C18-C19
45	N4	502	CDL	CB5-C51-C52-C53
47	S2	501	PEE	C31-C32-C33-C34
47	N5	701	PEE	O2-C10-C11-C12
45	N5	704	CDL	C11-C12-C13-C14
45	AK	402	CDL	OA5-CA3-CA4-CA6
45	B4	201	CDL	OB5-CB3-CB4-CB6
47	S2	501	PEE	C13-C14-C15-C16
50	S7	204	PLX	C27-C28-C29-C30
45	AL	201	CDL	C59-C60-C61-C62
47	N5	701	PEE	C16-C17-C18-C19
50	AL	203	PLX	C14-C15-C16-C17
45	AL	201	CDL	CB4-CB3-OB5-PB2
45	N5	704	CDL	C71-C72-C73-C74
48	AB	201	ZMP	C1-C2-C3-C4
45	N4	503	CDL	C72-C71-CB7-OB8
45	B5	201	CDL	O1-C1-CA2-OA2
57	S7	201	U10	C3-C4-O4-C4M
45	B4	201	CDL	C12-C13-C14-C15
46	A9	401	NDP	PN-O3-PA-O1A
45	A8	301	CDL	C33-C34-C35-C36
47	A9	402	PEE	C18-C19-C20-C21
47	N5	702	PEE	C36-C37-C38-C39
47	N3	201	PEE	C15-C16-C17-C18
45	A7	201	CDL	C72-C71-CB7-OB9
47	N1	403	PEE	O4-C10-C11-C12
47	N5	705	PEE	O5-C30-C31-C32
45	N4	503	CDL	C31-C32-C33-C34
47	AL	202	PEE	C32-C33-C34-C35
47	N3	201	PEE	C11-C12-C13-C14
45	N5	703	CDL	C72-C71-CB7-OB9

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Mol	Chain	Res	Type	Atoms
45	AL	201	CDL	C12-C11-CA5-OA7
47	N5	702	PEE	C13-C14-C15-C16
51	CA	101	3PE	C36-C37-C38-C39
47	N3	201	PEE	O4-C10-C11-C12
47	N5	701	PEE	O4-C10-C11-C12
47	A9	402	PEE	C1-C2-C3-O3
50	S7	204	PLX	C3-C4-C5-O8
50	S7	204	PLX	C29-C30-C31-C32
48	AB	201	ZMP	C22-C23-C24-C25
45	N5	703	CDL	C12-C11-CA5-OA7
45	N5	703	CDL	C71-C72-C73-C74
45	A7	201	CDL	C1-CA2-OA2-PA1
47	N3	201	PEE	C2-C1-O3P-P
47	S2	501	PEE	C33-C34-C35-C36
45	AL	201	CDL	C32-C31-CA7-OA9
47	A9	402	PEE	O4-C10-C11-C12
45	AL	201	CDL	CB2-OB2-PB2-OB4
45	N4	502	CDL	CB2-OB2-PB2-OB3
47	N5	705	PEE	C4-O4P-P-O1P
51	N5	706	3PE	C1-O11-P-O14
51	N5	706	3PE	C11-O13-P-O14
51	S7	205	3PE	C1-O11-P-O12
51	S7	205	3PE	C11-O13-P-O14
51	B8	201	3PE	O21-C21-C22-C23
51	CB	202	3PE	O31-C31-C32-C33
47	N5	702	PEE	O4P-C4-C5-N
52	N3	203	PC1	C29-C2A-C2B-C2C
58	S7	202	MF8	N09-C07-N06-C04
45	N5	704	CDL	C42-C43-C44-C45
45	N4	502	CDL	CA5-C11-C12-C13
47	S2	501	PEE	O4-C10-C11-C12
45	B4	201	CDL	C31-C32-C33-C34
45	N4	503	CDL	CB3-CB4-OB6-CB5
47	N5	701	PEE	C5-C4-O4P-P
47	S8	303	PEE	C1-C2-O2-C10
48	AC	201	ZMP	O3-C16-C17-C18
50	AM	201	PLX	C1-C2-O1-P1
51	CB	202	3PE	C12-C11-O13-P
45	B4	201	CDL	C12-C11-CA5-OA7
47	AL	202	PEE	O4-C10-C11-C12
50	CB	201	PLX	C27-C28-C29-C30
47	N3	201	PEE	O3-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
51	N5	706	3PE	O21-C21-C22-C23
52	N1	402	PC1	O21-C21-C22-C23
45	N5	703	CDL	OB5-CB3-CB4-OB6
59	V1	502	FMN	N10-C1'-C2'-O2'
45	4L	201	CDL	C12-C11-CA5-OA6
45	AK	402	CDL	C32-C31-CA7-OA8
51	CA	101	3PE	O21-C21-C22-C23
51	CA	101	3PE	C26-C27-C28-C29
52	N1	402	PC1	O22-C21-C22-C23
45	B4	201	CDL	C75-C76-C77-C78
48	AC	201	ZMP	C1-C22-C23-C24
50	B1	101	PLX	C17-C18-C19-C20
51	CA	101	3PE	O22-C21-C22-C23
51	CB	202	3PE	O32-C31-C32-C33
51	N5	706	3PE	O22-C21-C22-C23
52	N3	203	PC1	C28-C29-C2A-C2B
45	AK	402	CDL	C72-C71-CB7-OB8
45	N5	704	CDL	C12-C11-CA5-OA6
45	4L	201	CDL	C12-C11-CA5-OA7
45	AK	402	CDL	C32-C31-CA7-OA9
51	B8	201	3PE	O22-C21-C22-C23
47	S8	303	PEE	C34-C35-C36-C37

There are no ring outliers.

40 monomers are involved in 136 short contacts:

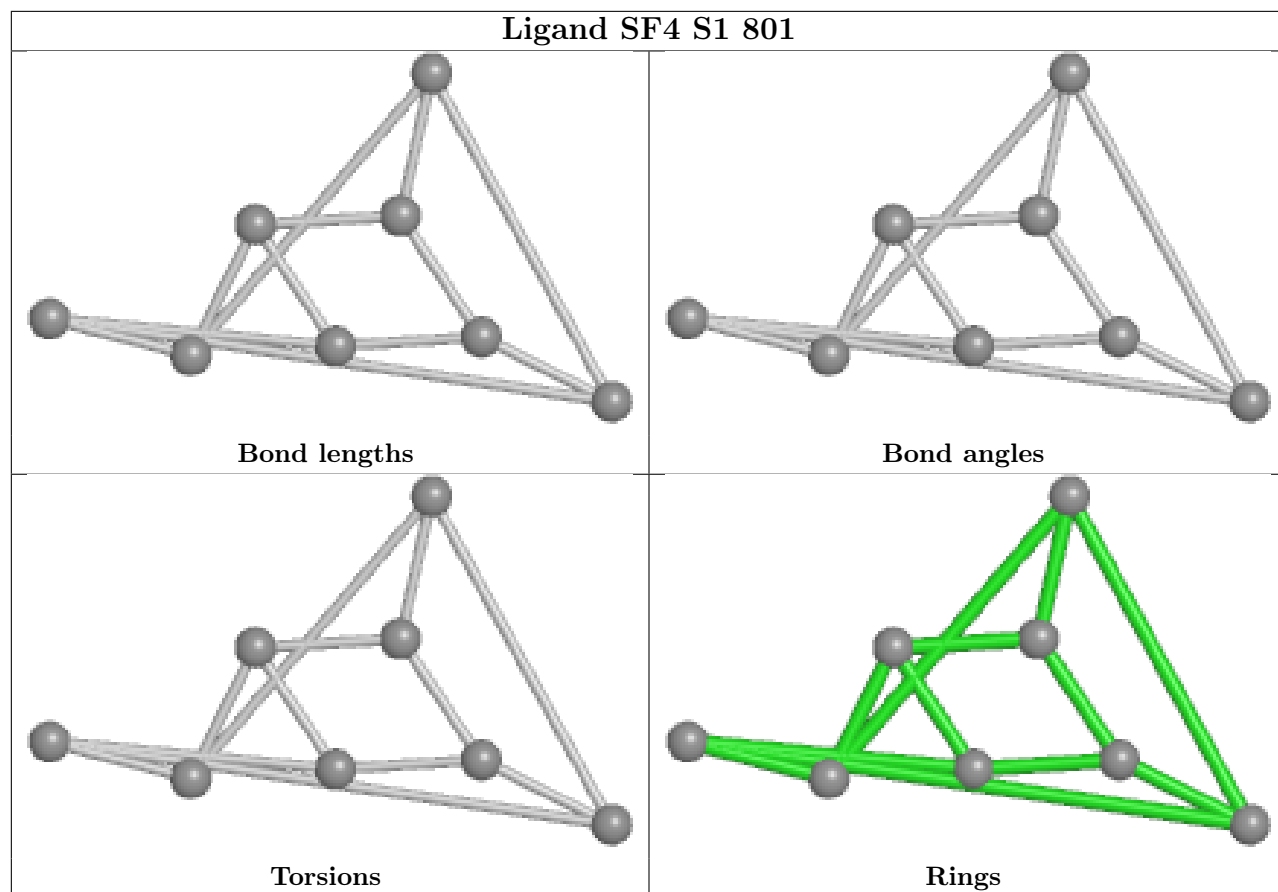
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	V1	502	FMN	1	0
49	AK	401	ADP	4	0
50	AL	203	PLX	3	0
47	S8	303	PEE	6	0
57	S7	201	U10	14	0
47	S2	501	PEE	4	0
50	N4	501	PLX	3	0
47	AL	202	PEE	4	0
45	B5	201	CDL	3	0
45	AL	201	CDL	6	0
47	N3	201	PEE	1	0
50	AM	201	PLX	4	0
45	4L	201	CDL	11	0
45	A8	301	CDL	8	0
51	CA	101	3PE	2	0

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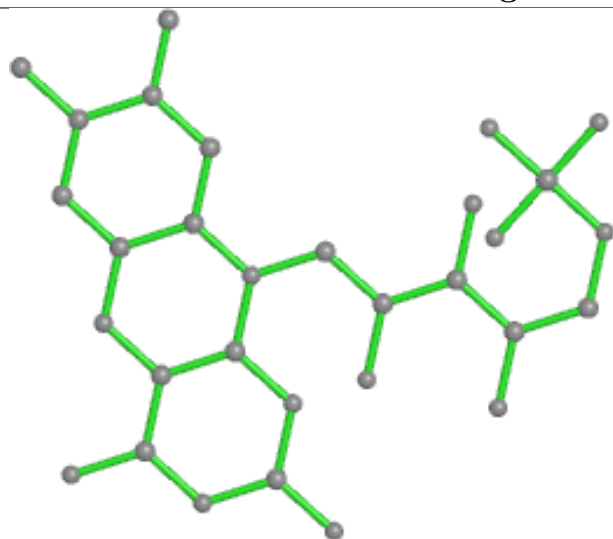
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	CB	201	PLX	3	0
47	N5	701	PEE	3	0
46	A9	401	NDP	1	0
45	N5	703	CDL	10	0
47	N5	702	PEE	1	0
47	N5	705	PEE	6	0
48	AB	201	ZMP	4	0
48	AC	201	ZMP	3	0
50	B1	101	PLX	2	0
53	S8	302	SF4	1	0
45	A7	201	CDL	1	0
45	N4	502	CDL	6	0
51	CB	202	3PE	1	0
53	S7	203	SF4	1	0
47	N1	403	PEE	3	0
45	AK	402	CDL	1	0
52	N3	203	PC1	2	0
47	A9	402	PEE	4	0
50	N3	202	PLX	3	0
51	N5	706	3PE	1	0
45	B4	201	CDL	4	0
45	N1	401	CDL	5	0
50	S7	204	PLX	1	0
51	B8	201	3PE	1	0
52	N1	402	PC1	3	0

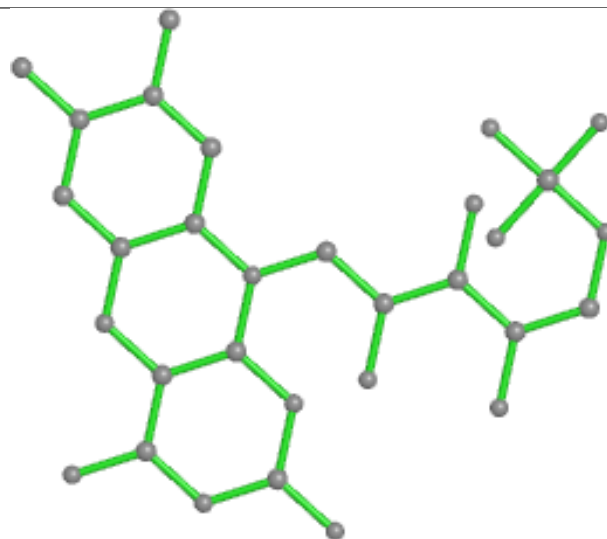
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



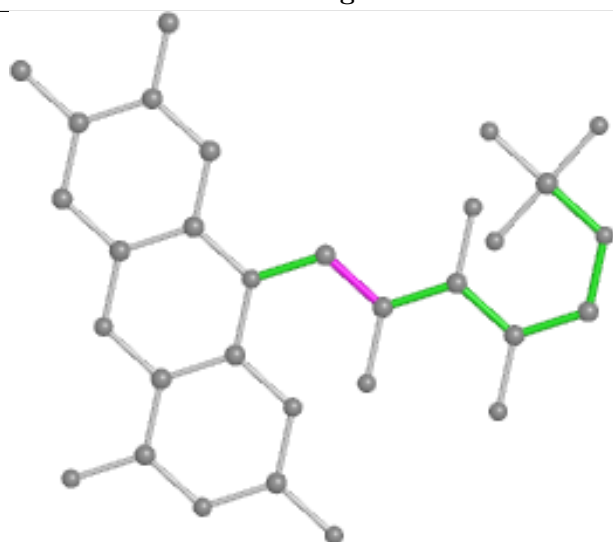
Ligand FMN V1 502



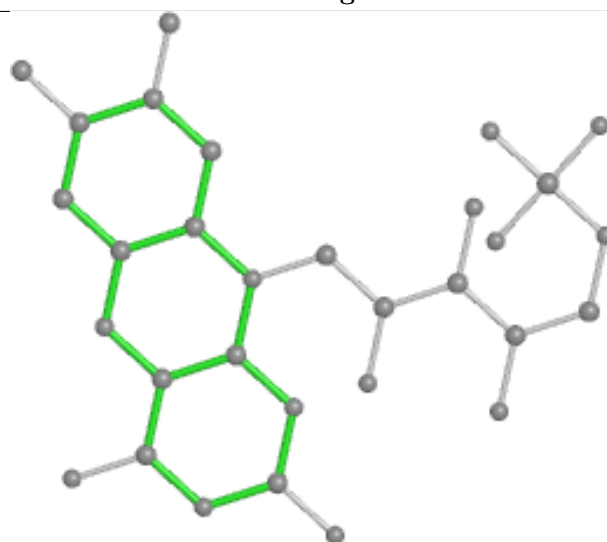
Bond lengths



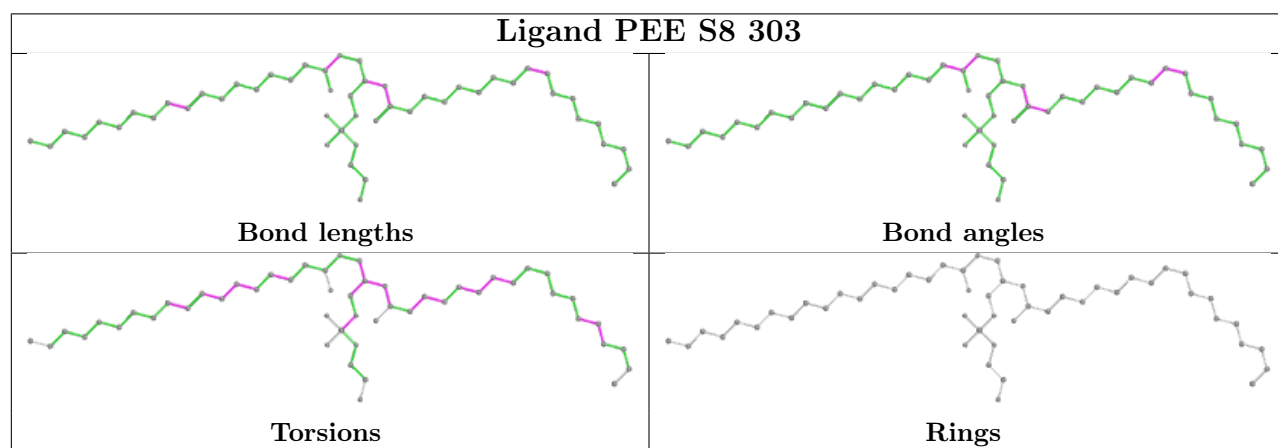
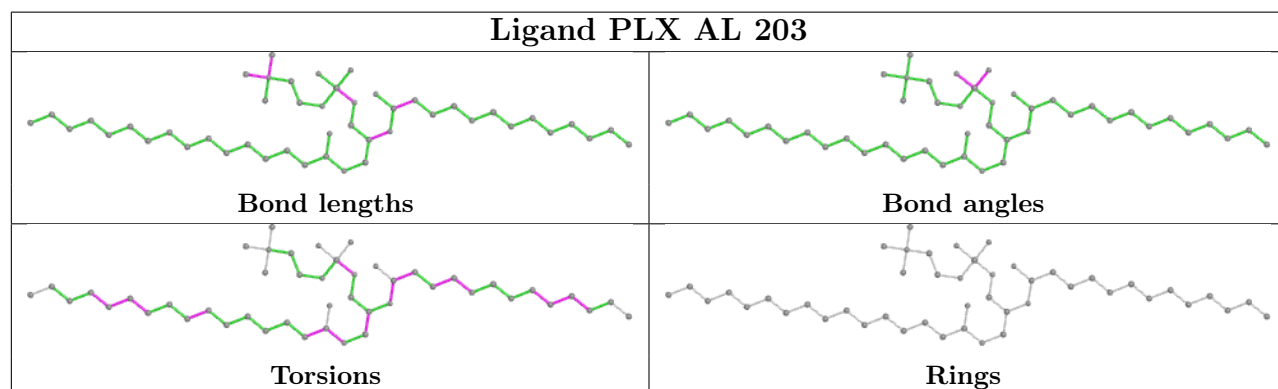
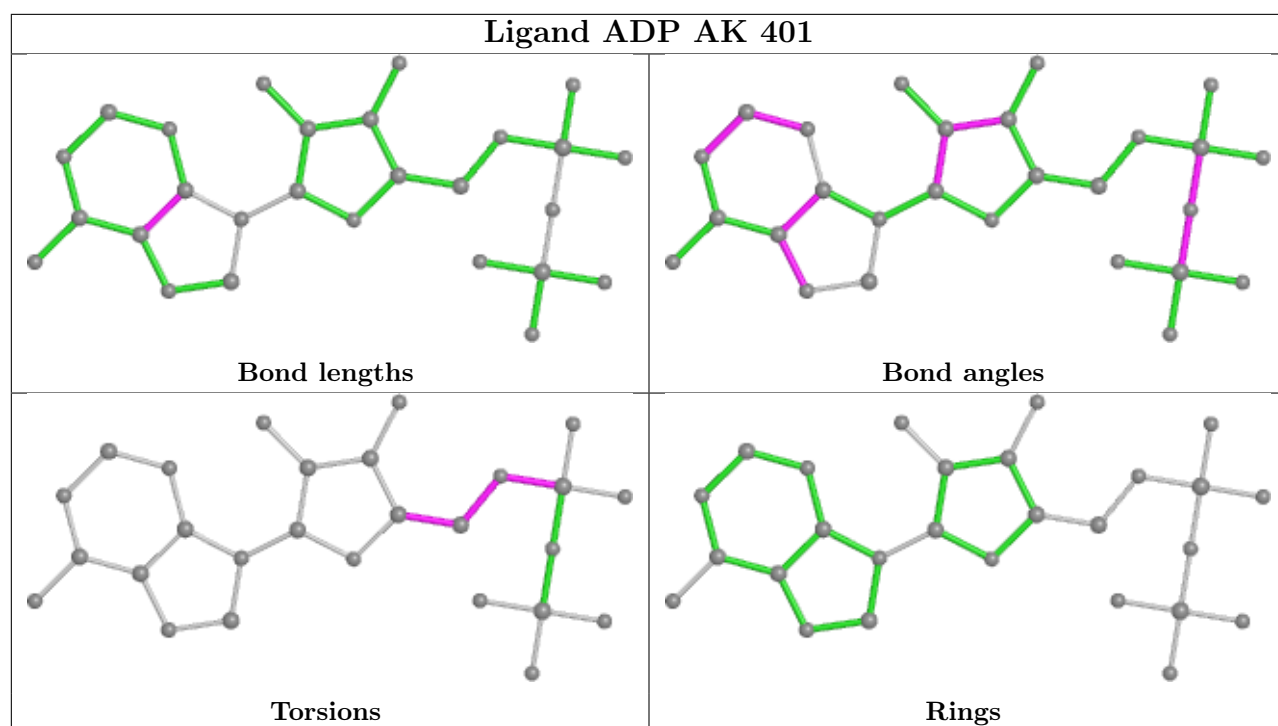
Bond angles

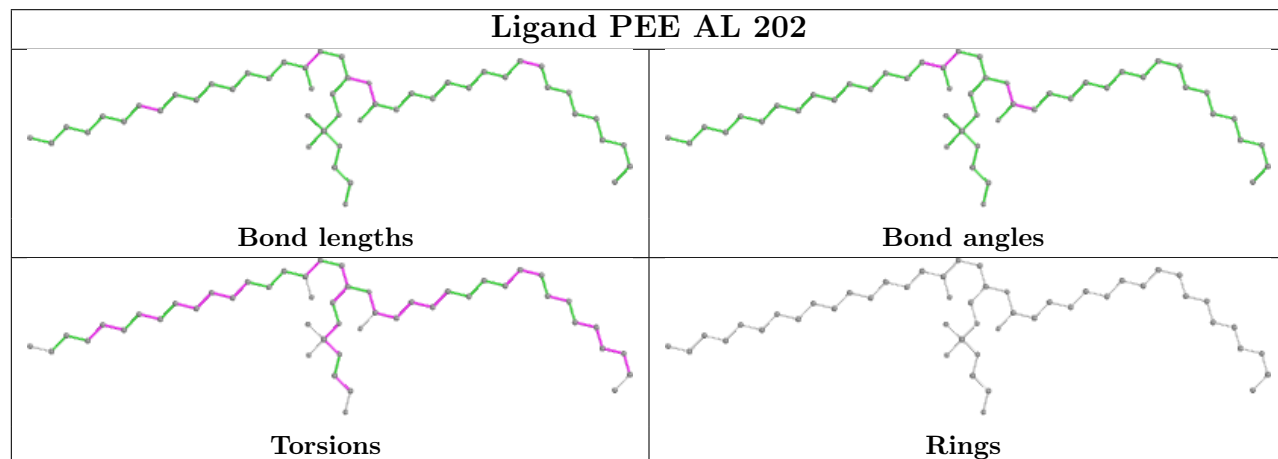
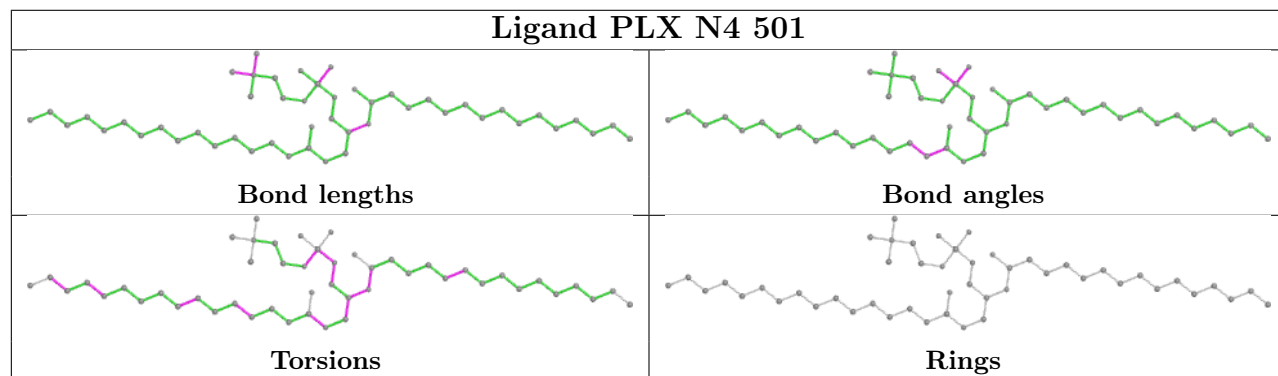
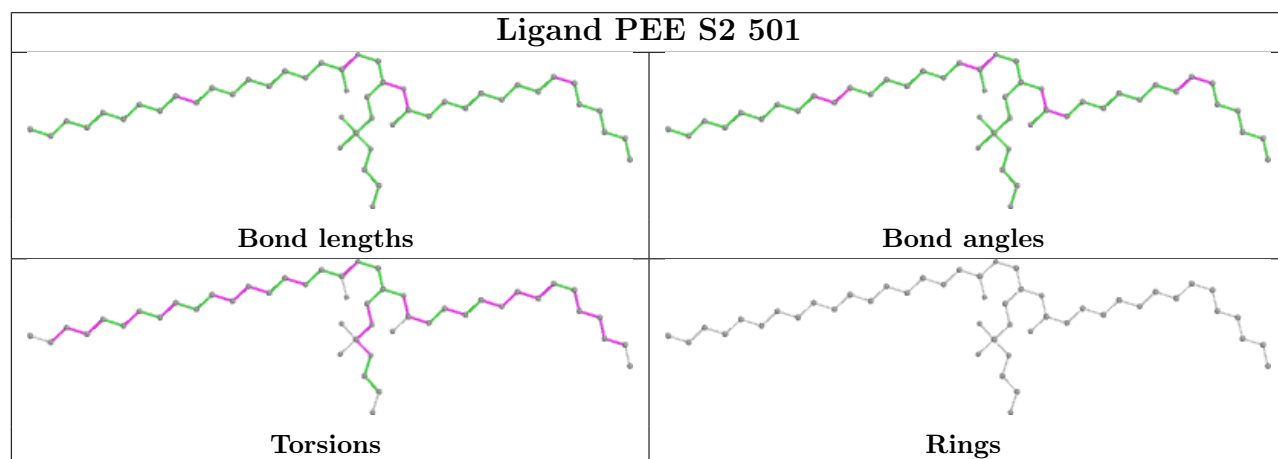
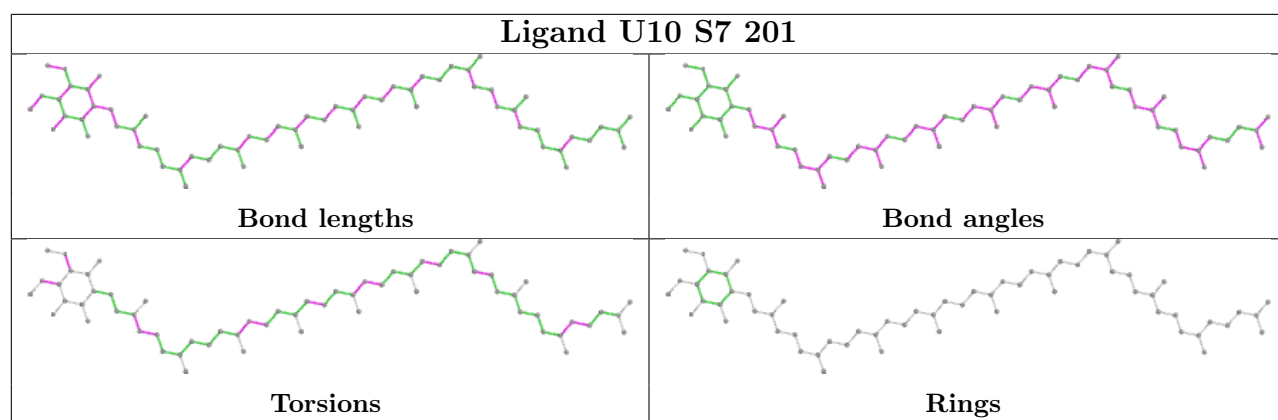


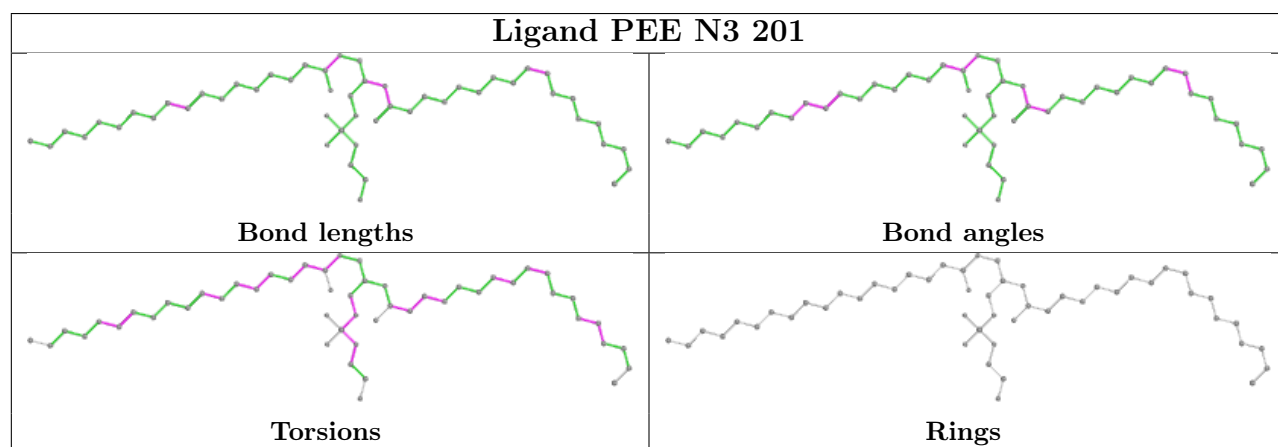
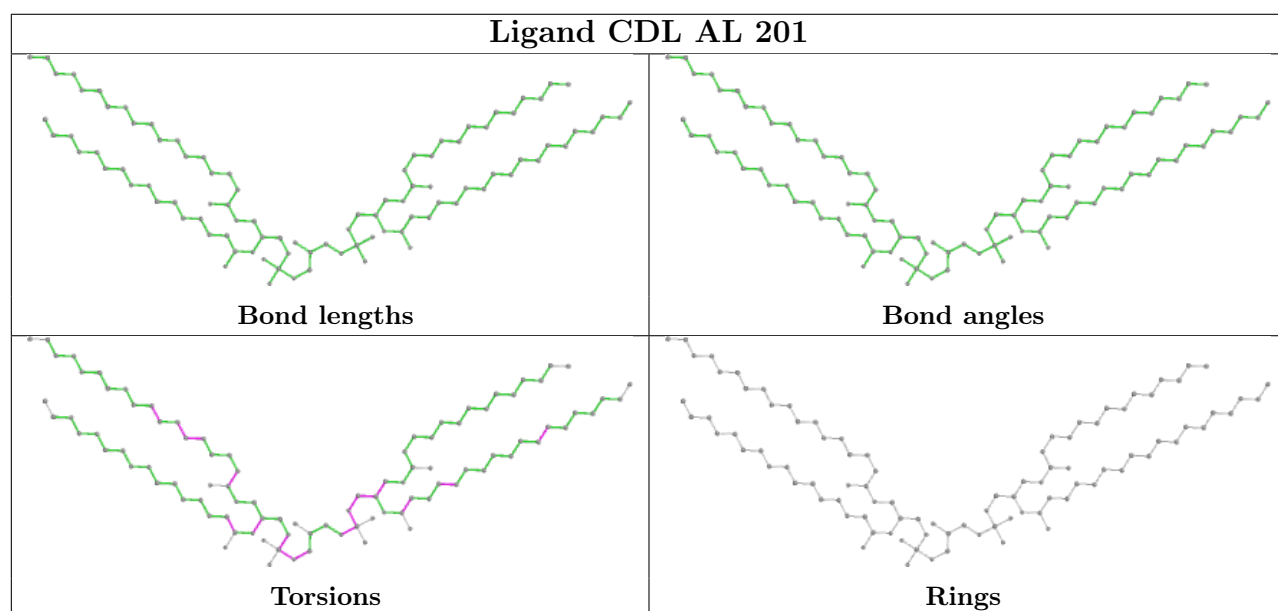
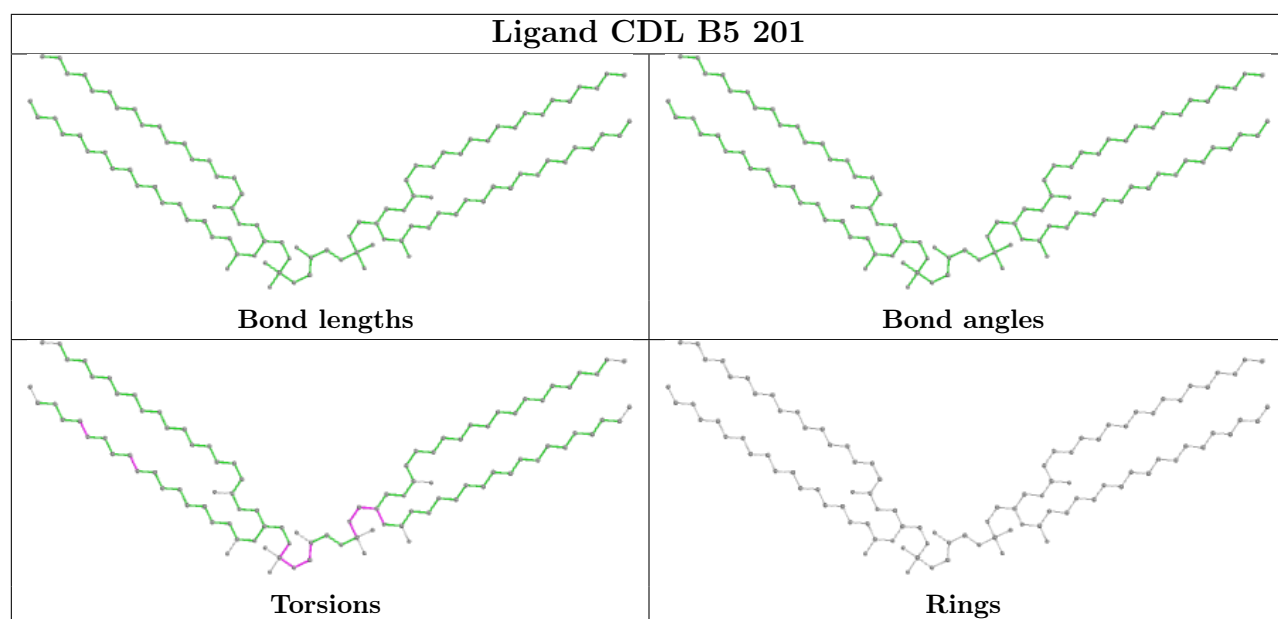
Torsions

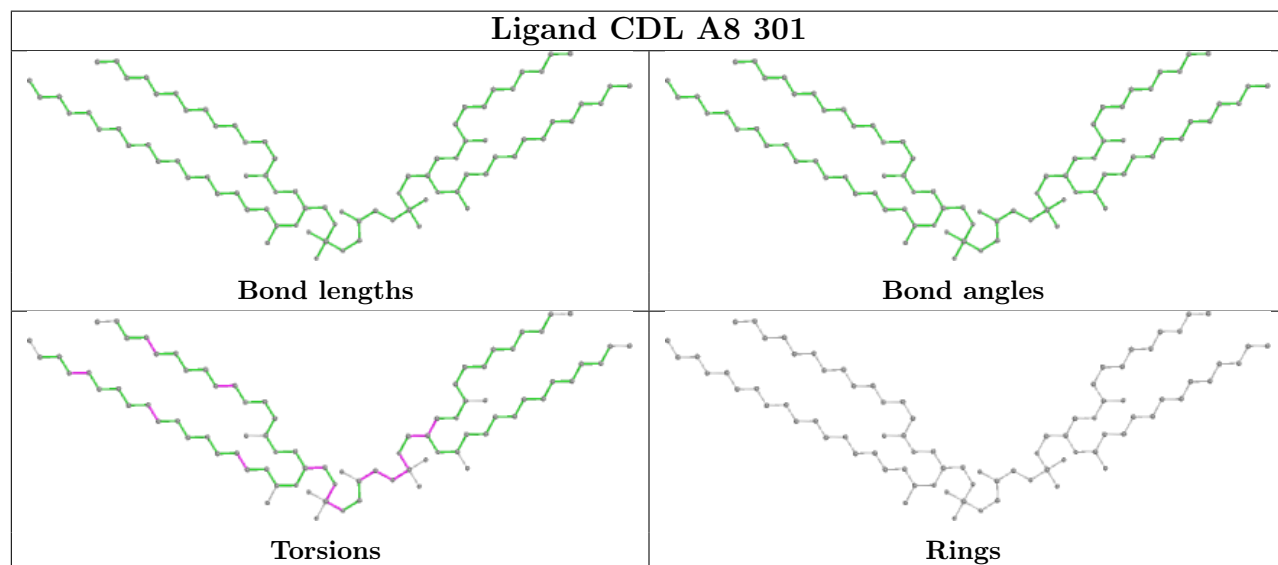
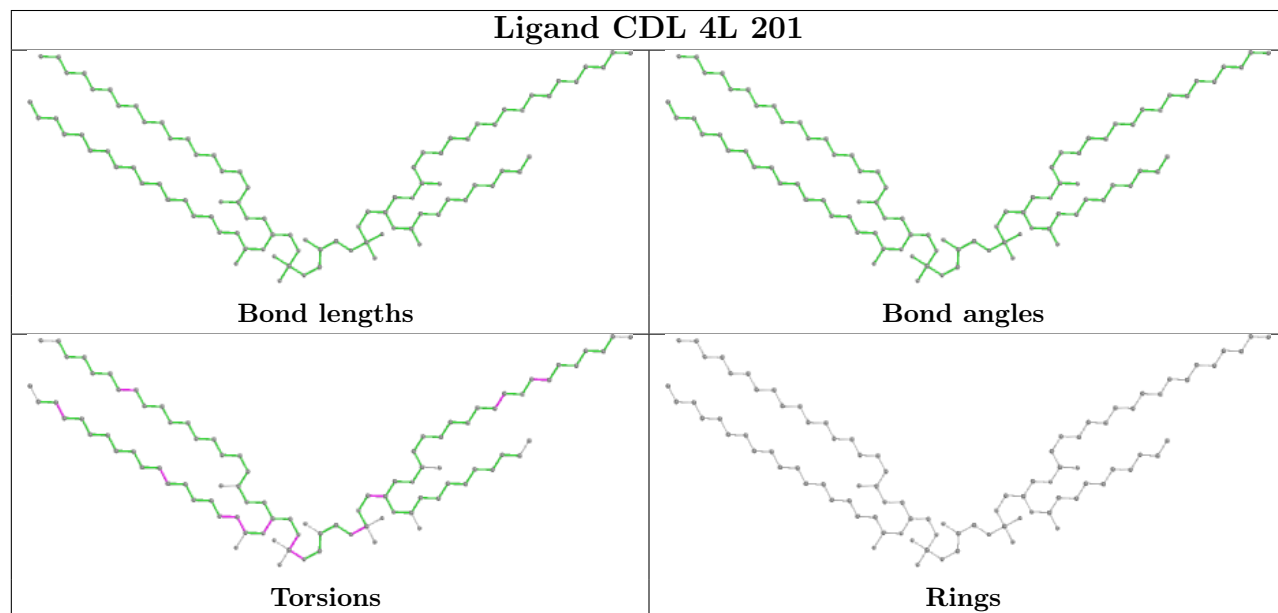
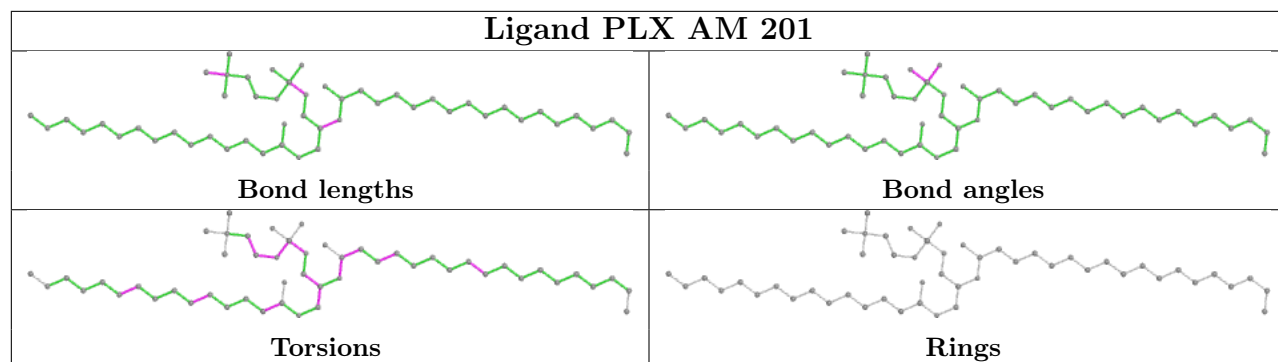


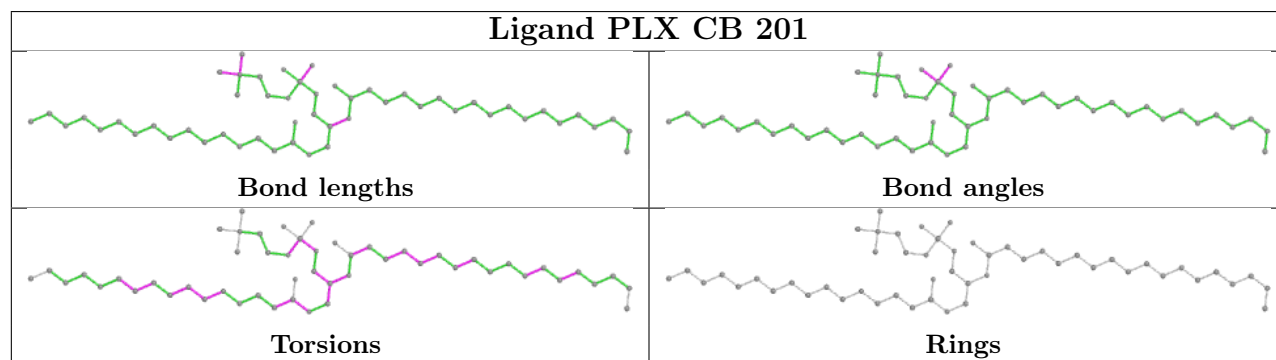
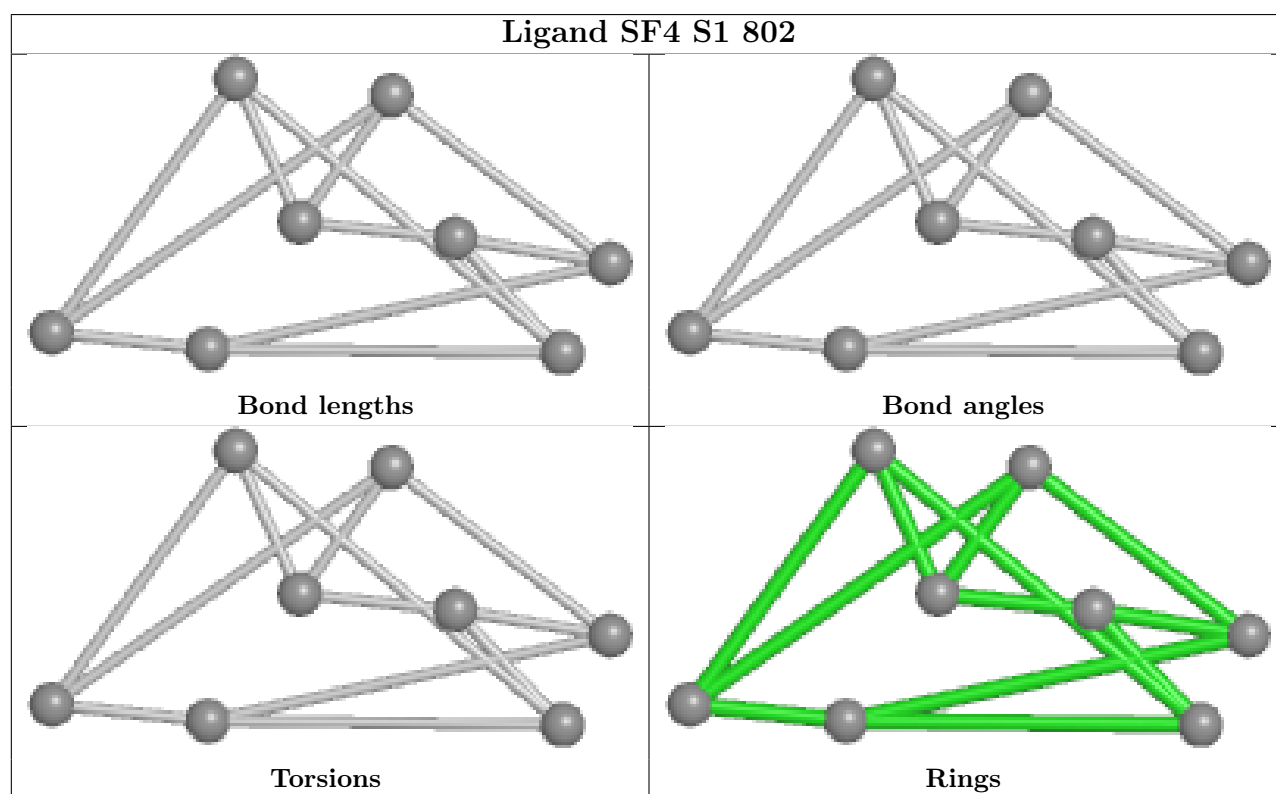
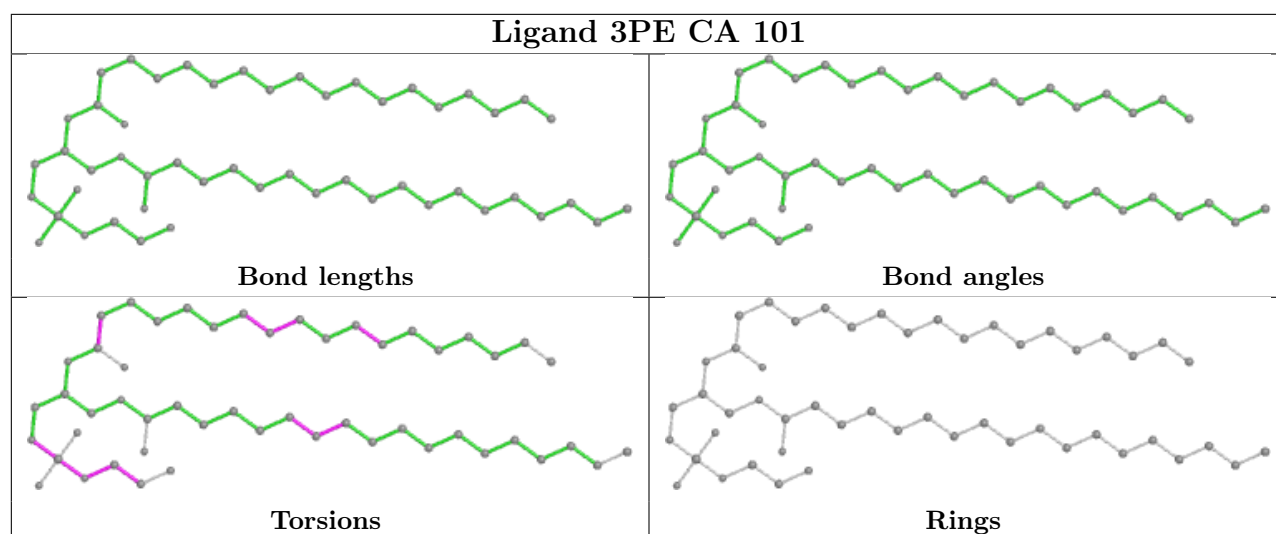
Rings

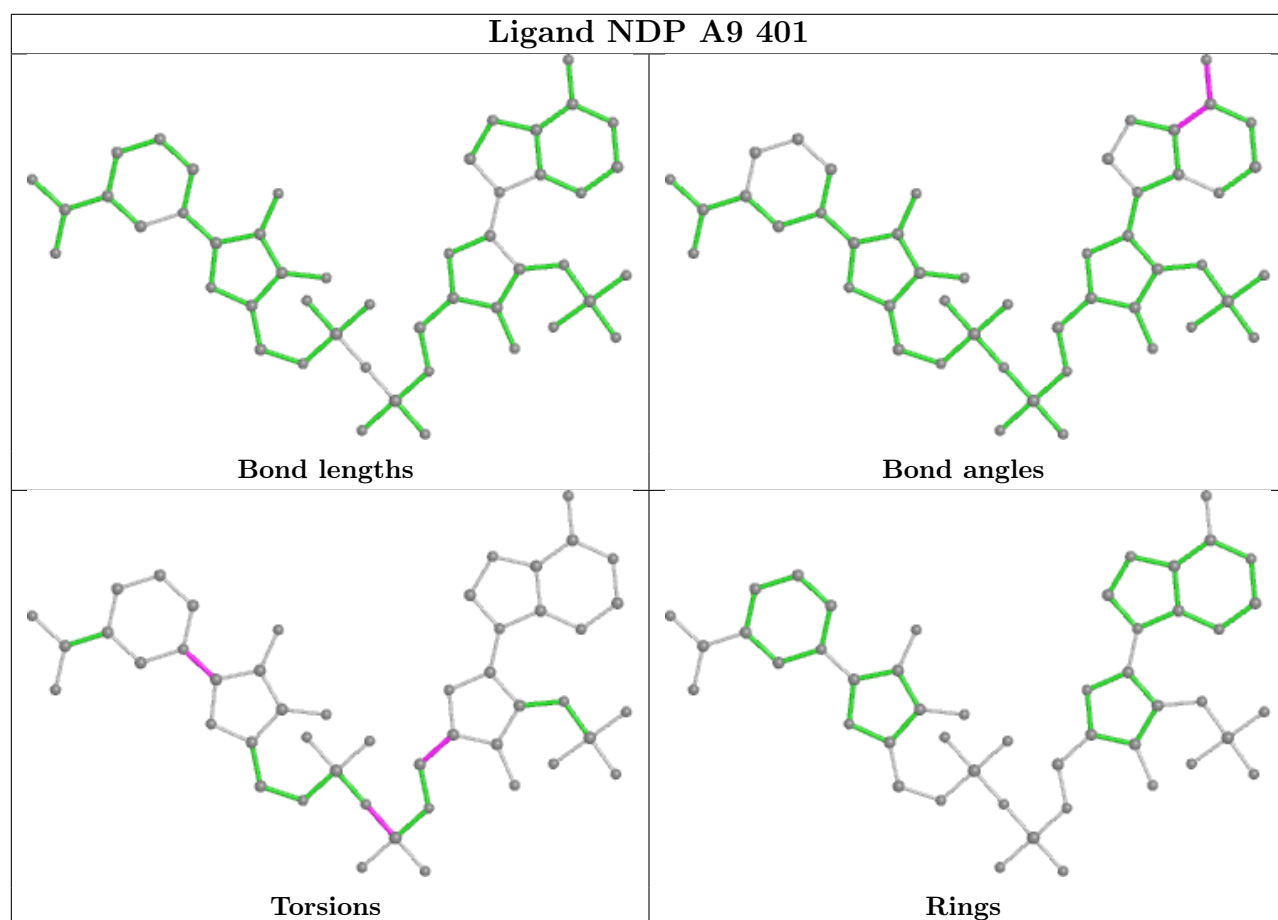
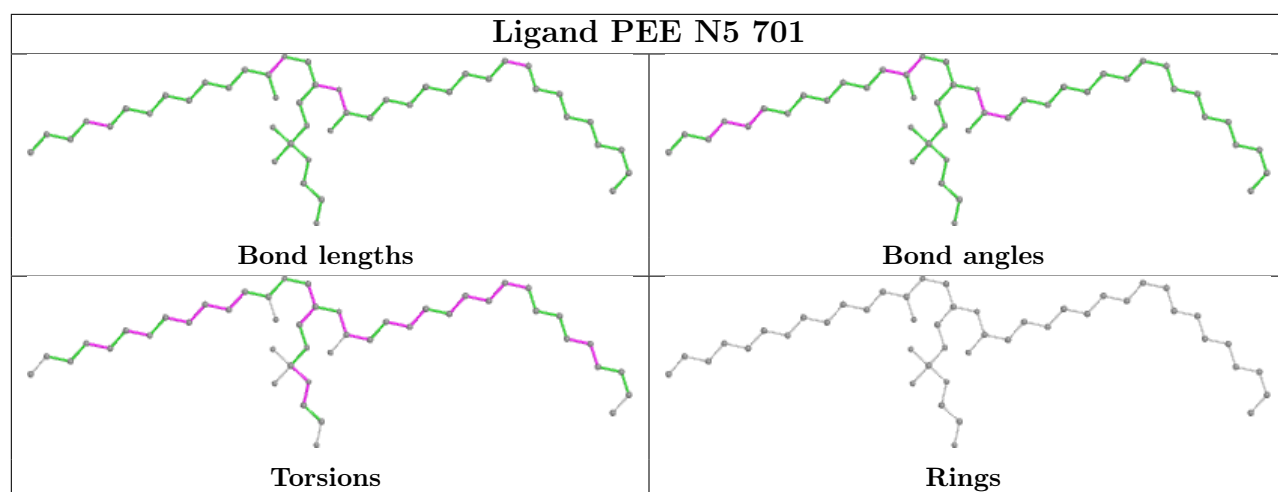


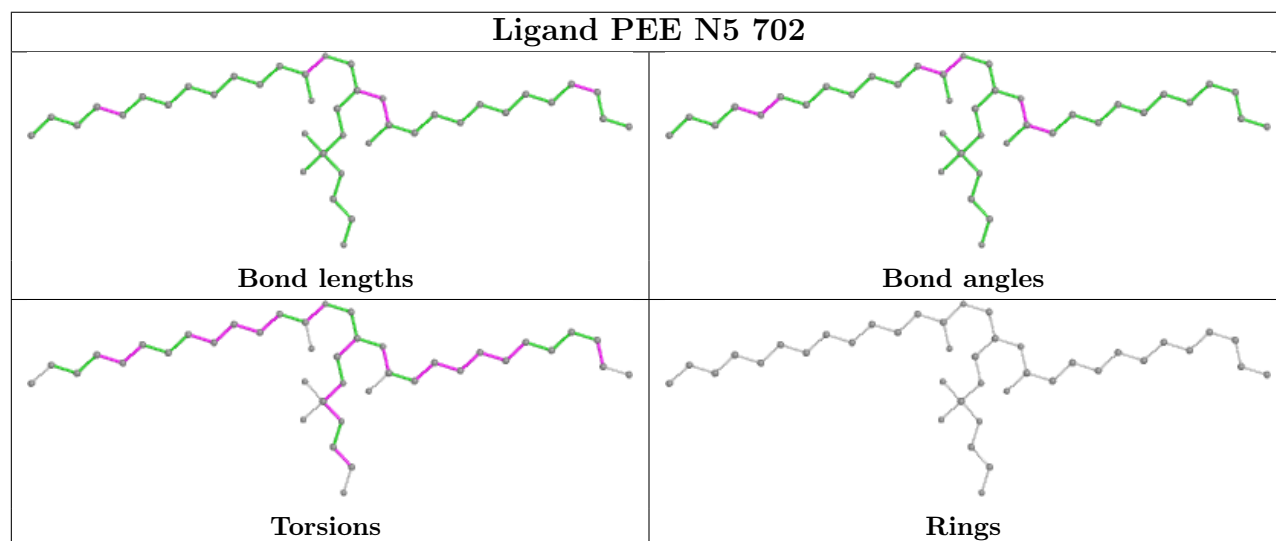
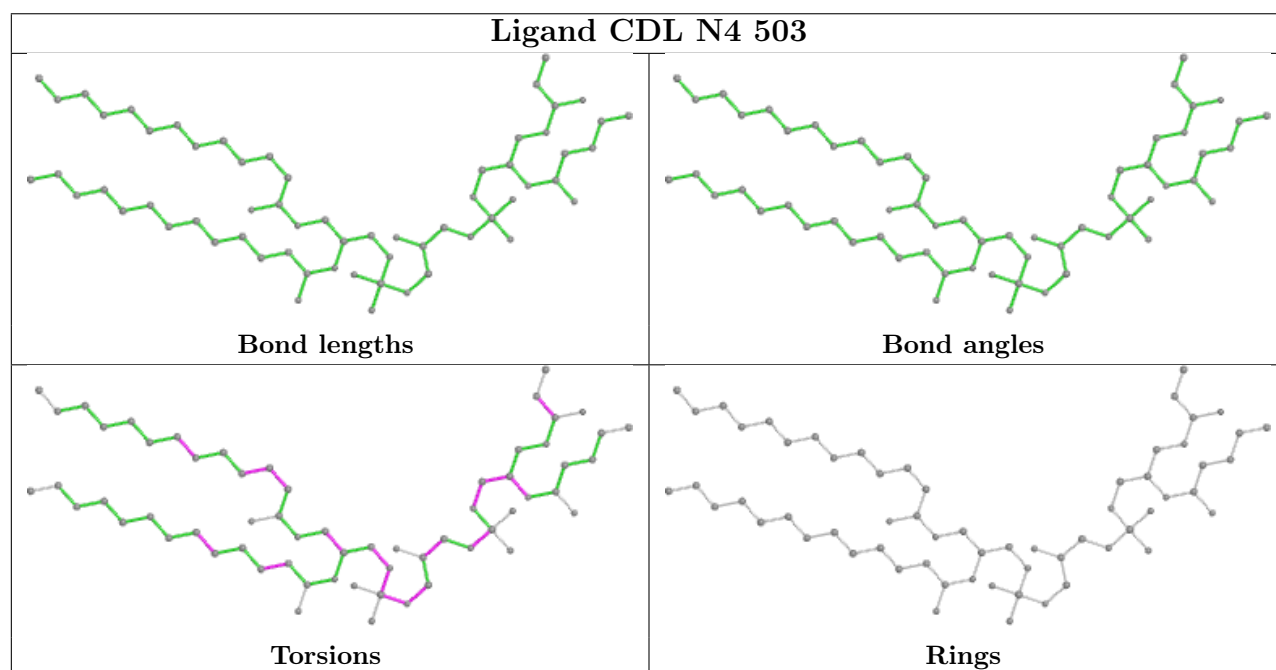
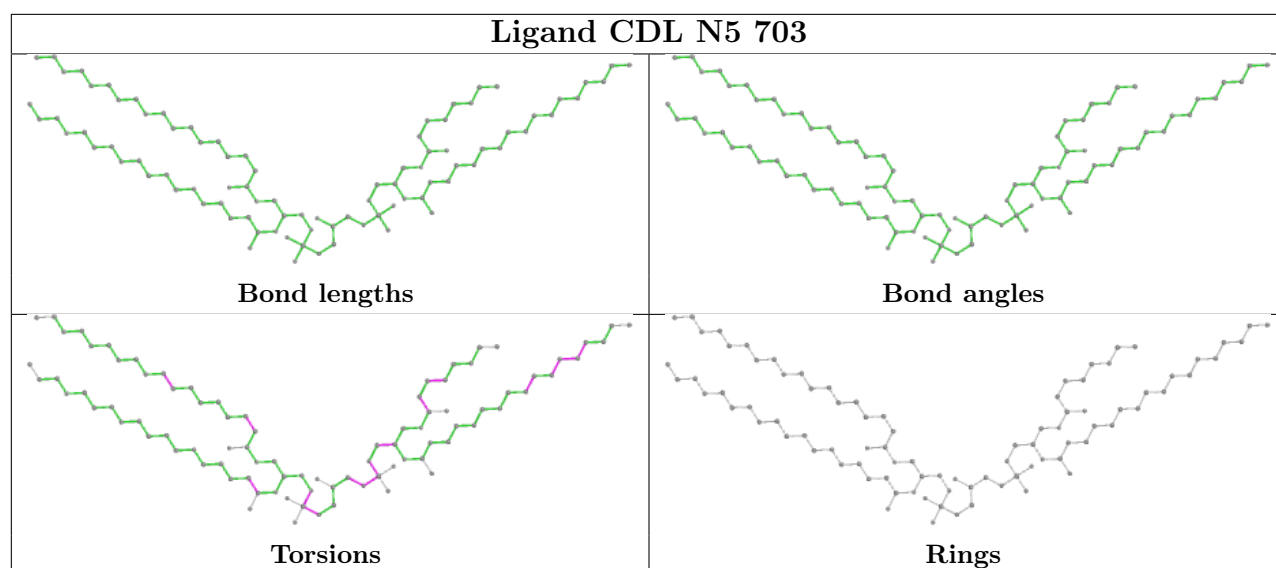


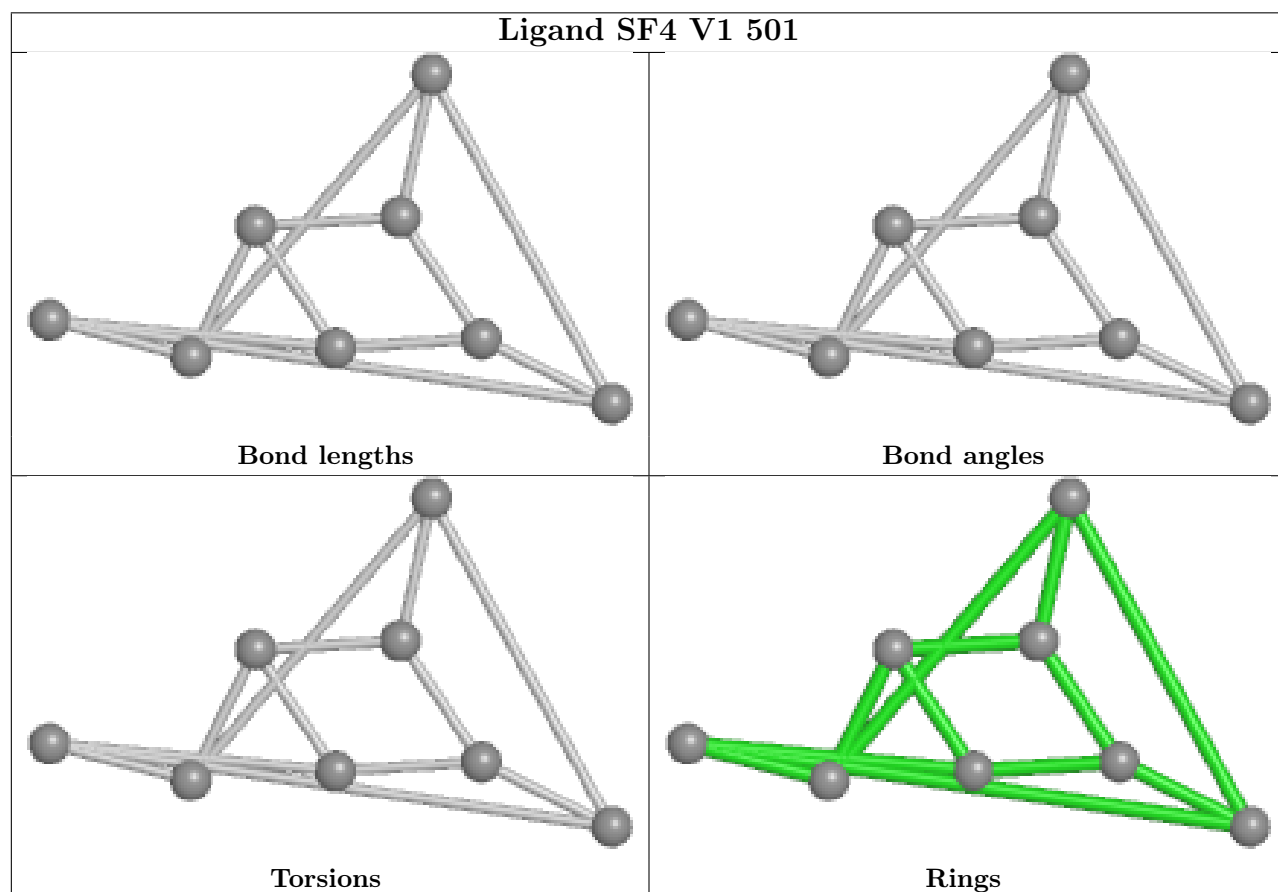
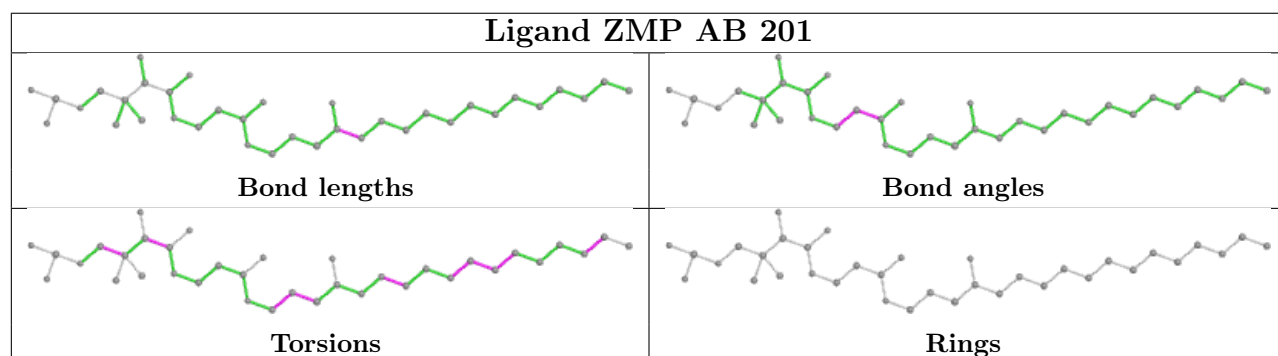
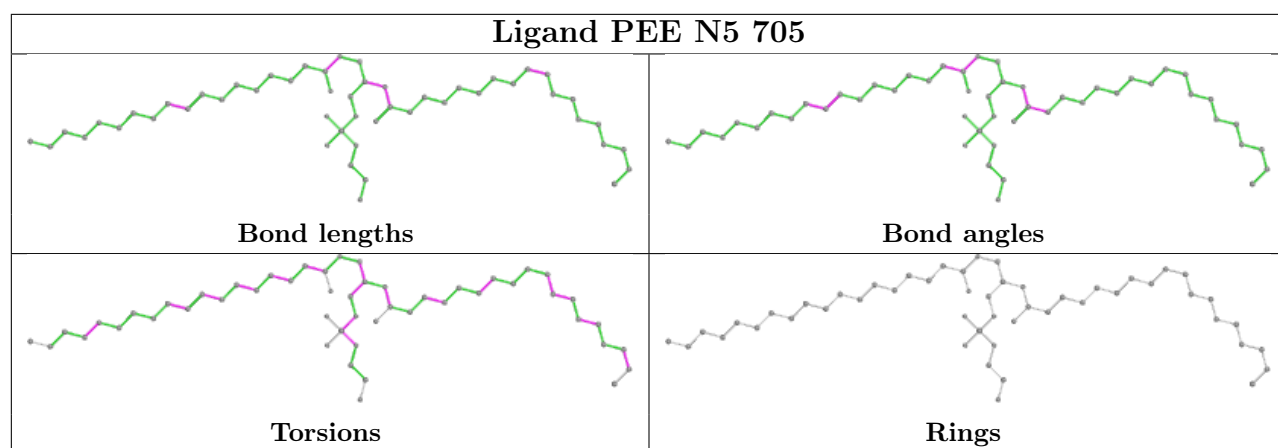


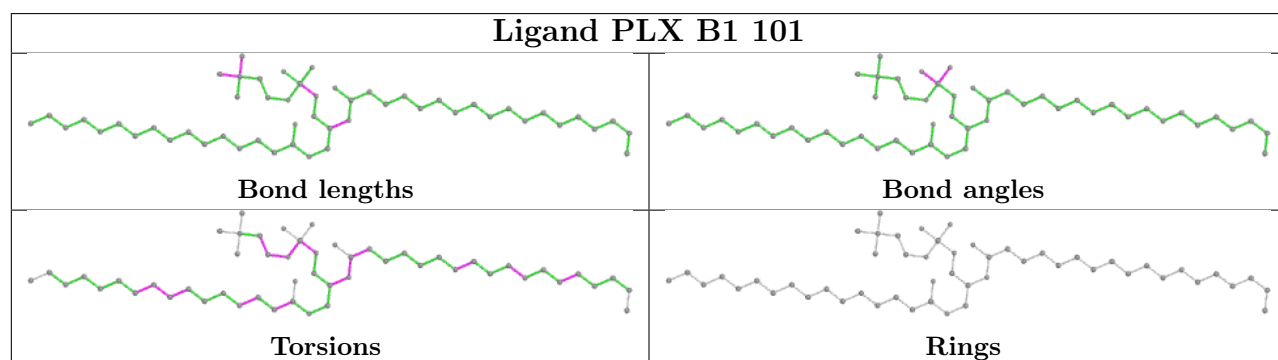
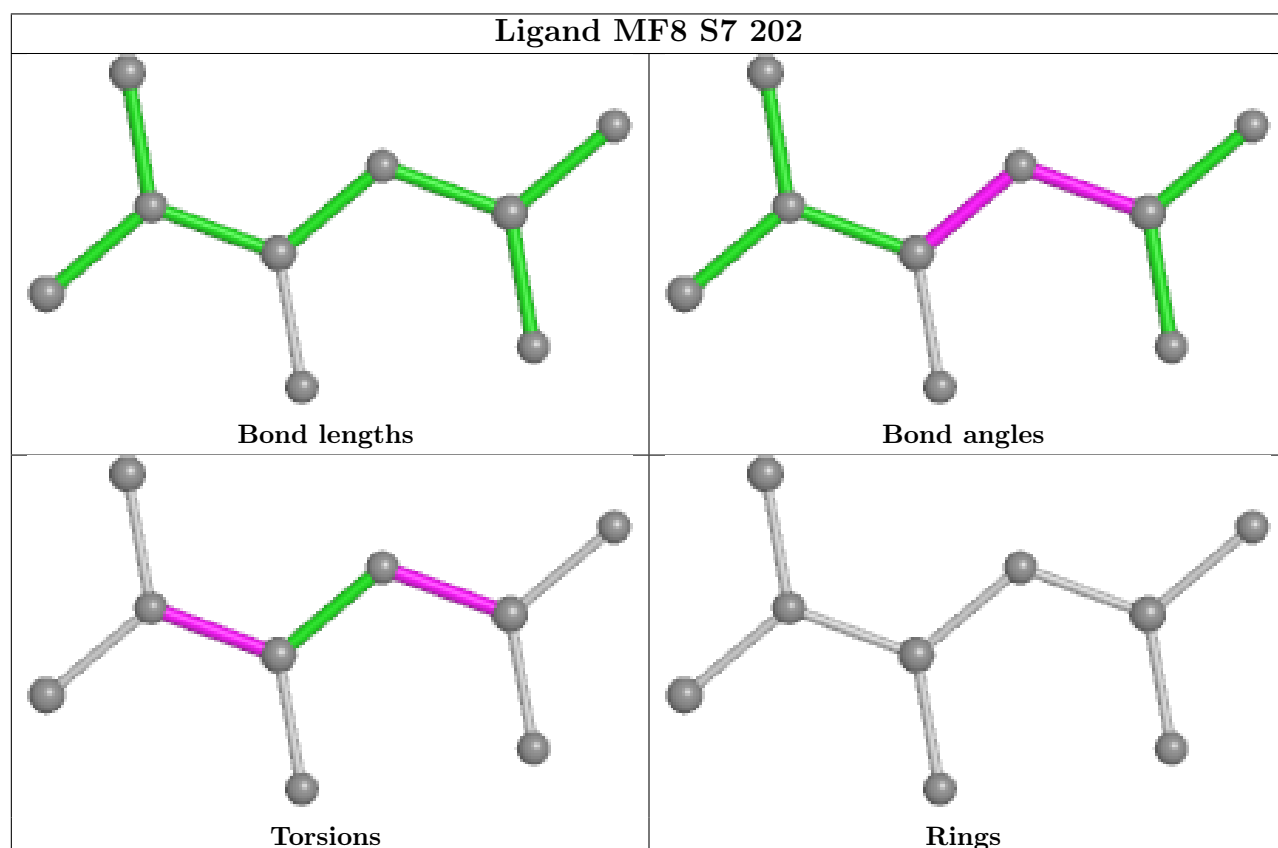
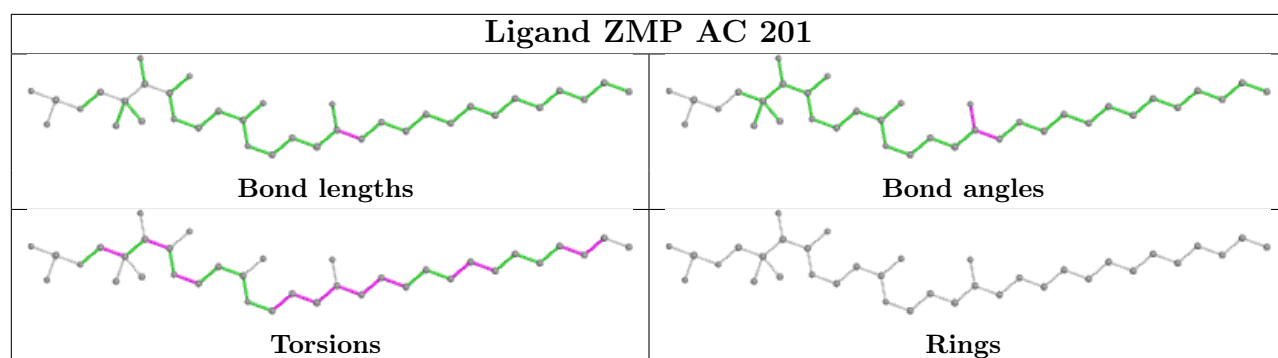


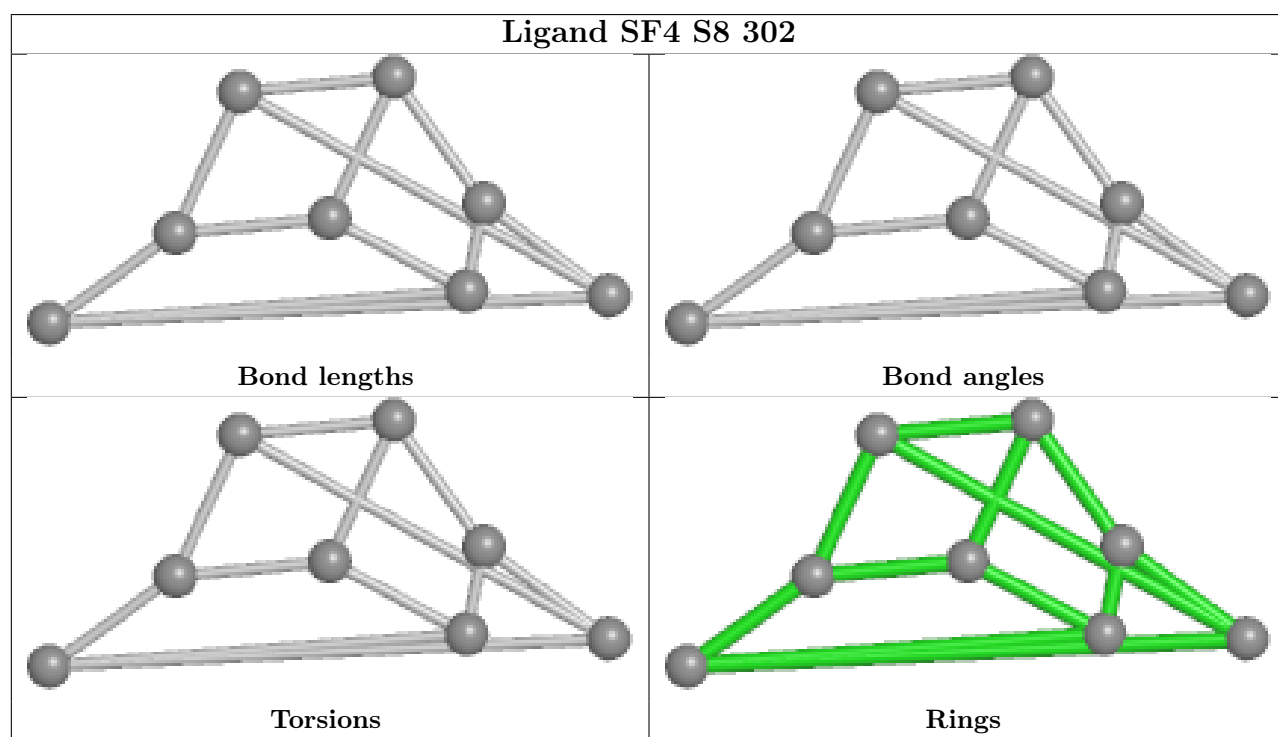
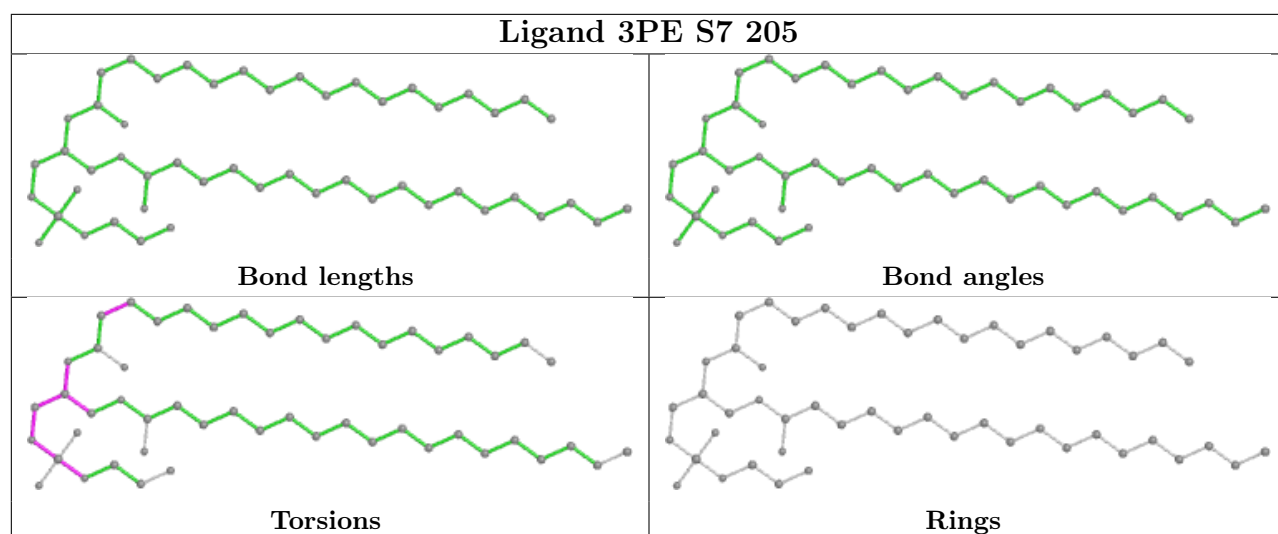


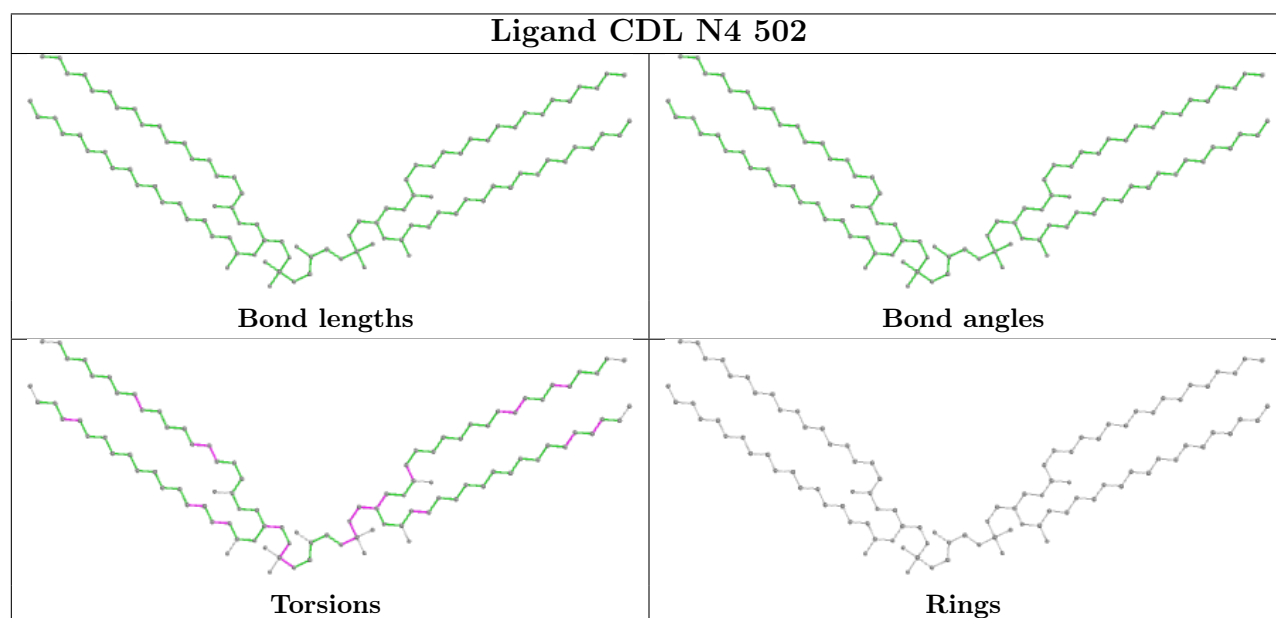
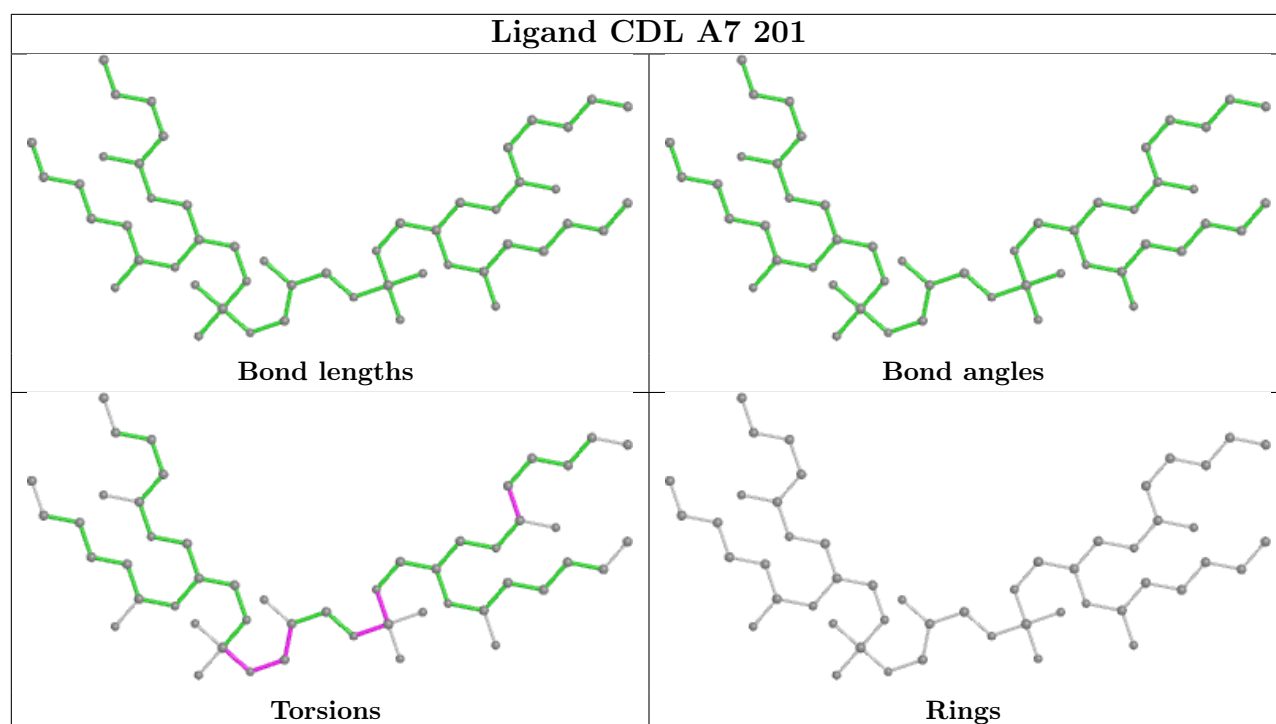


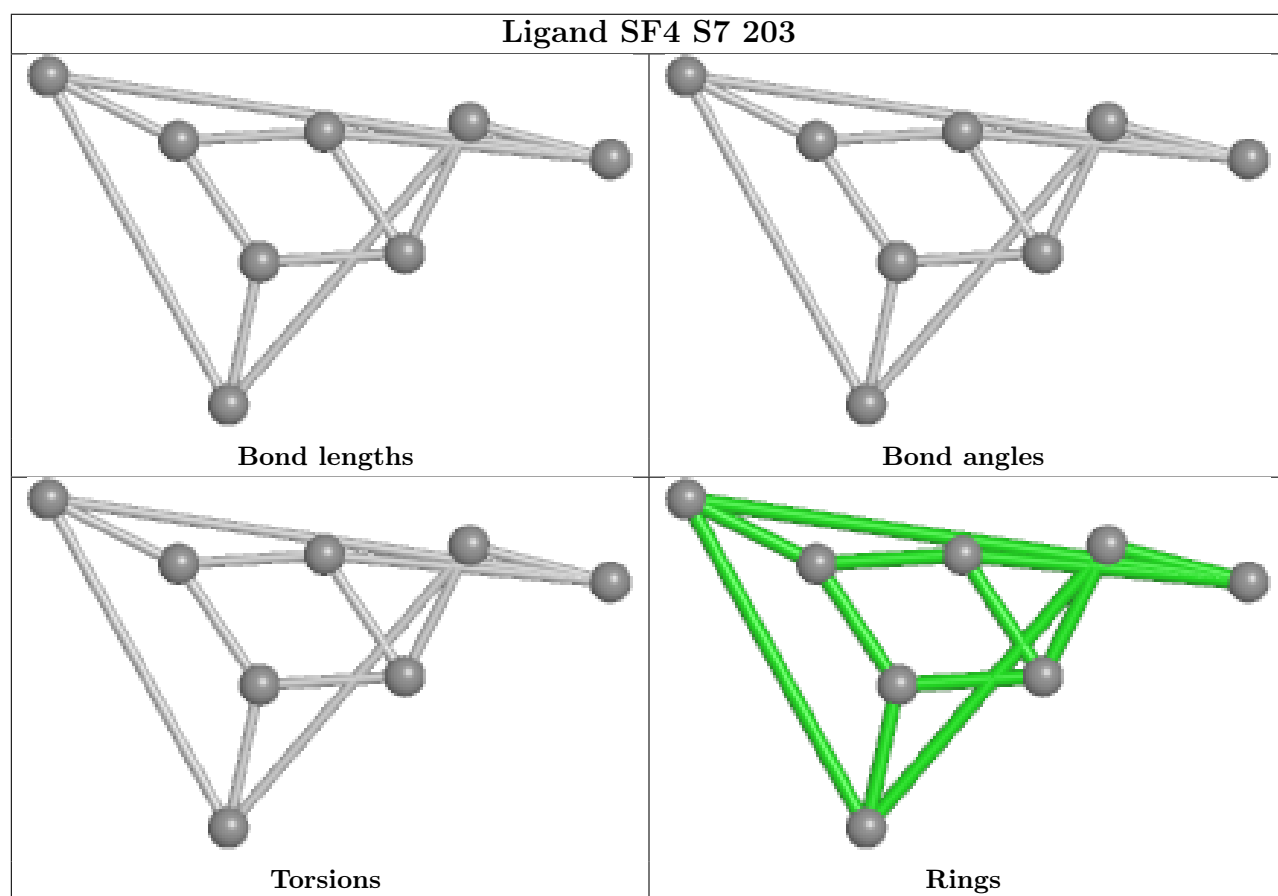
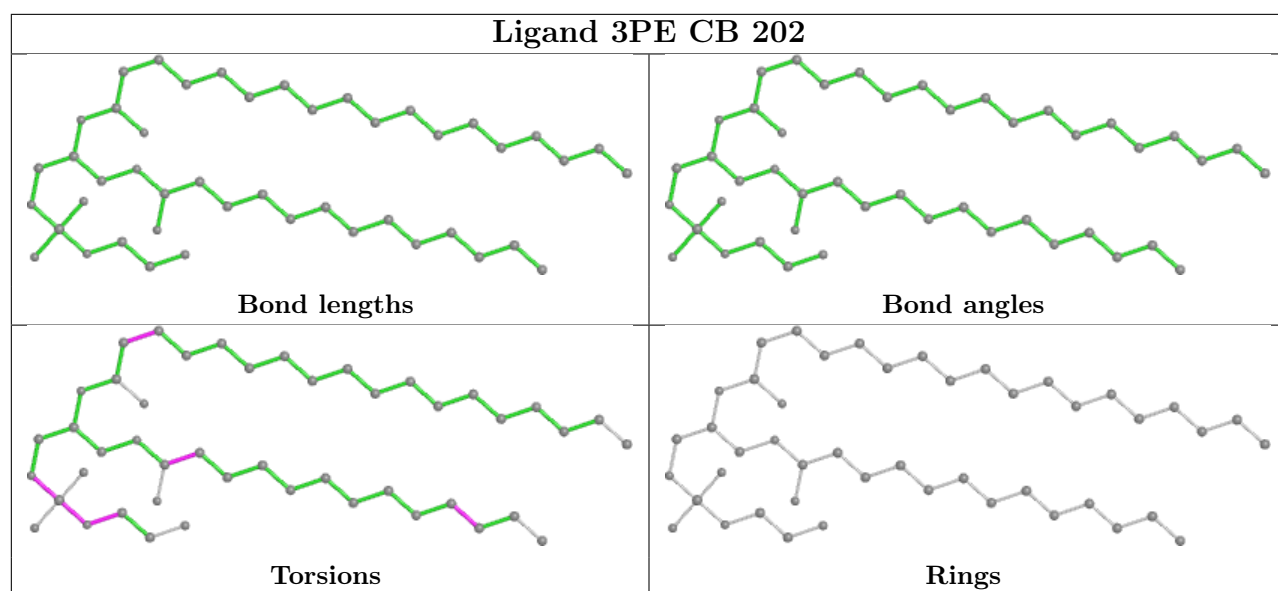


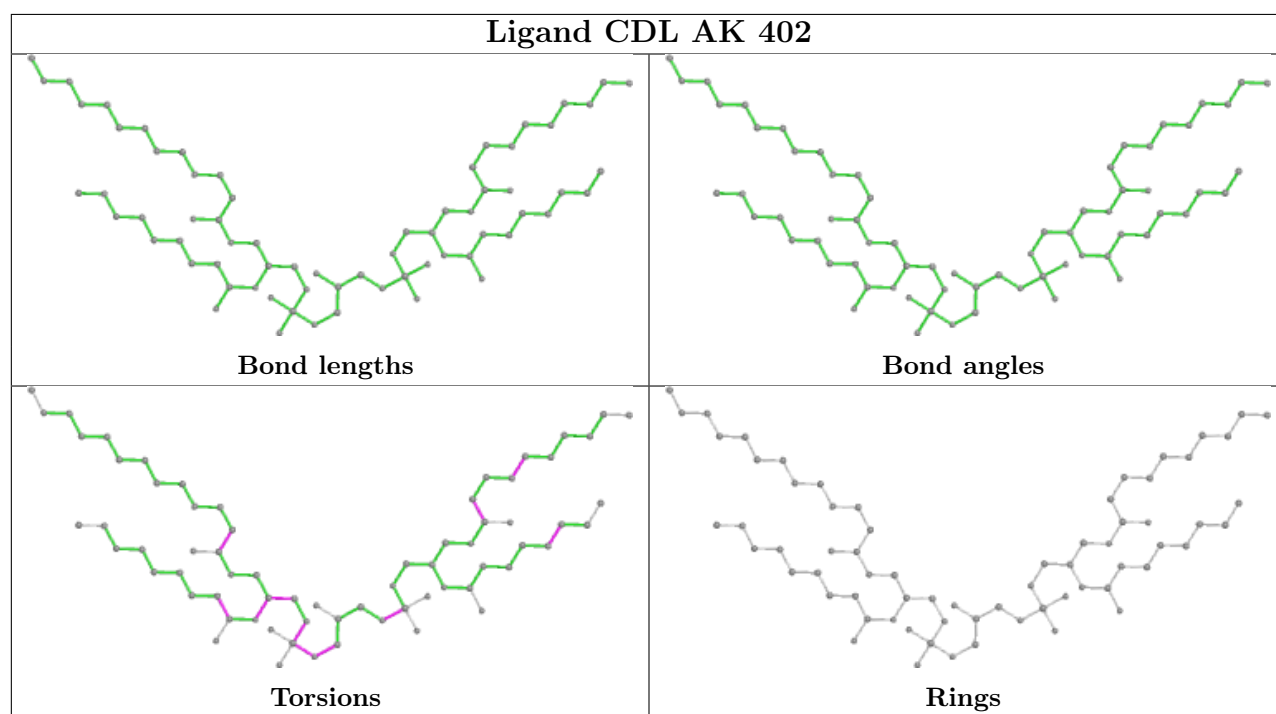
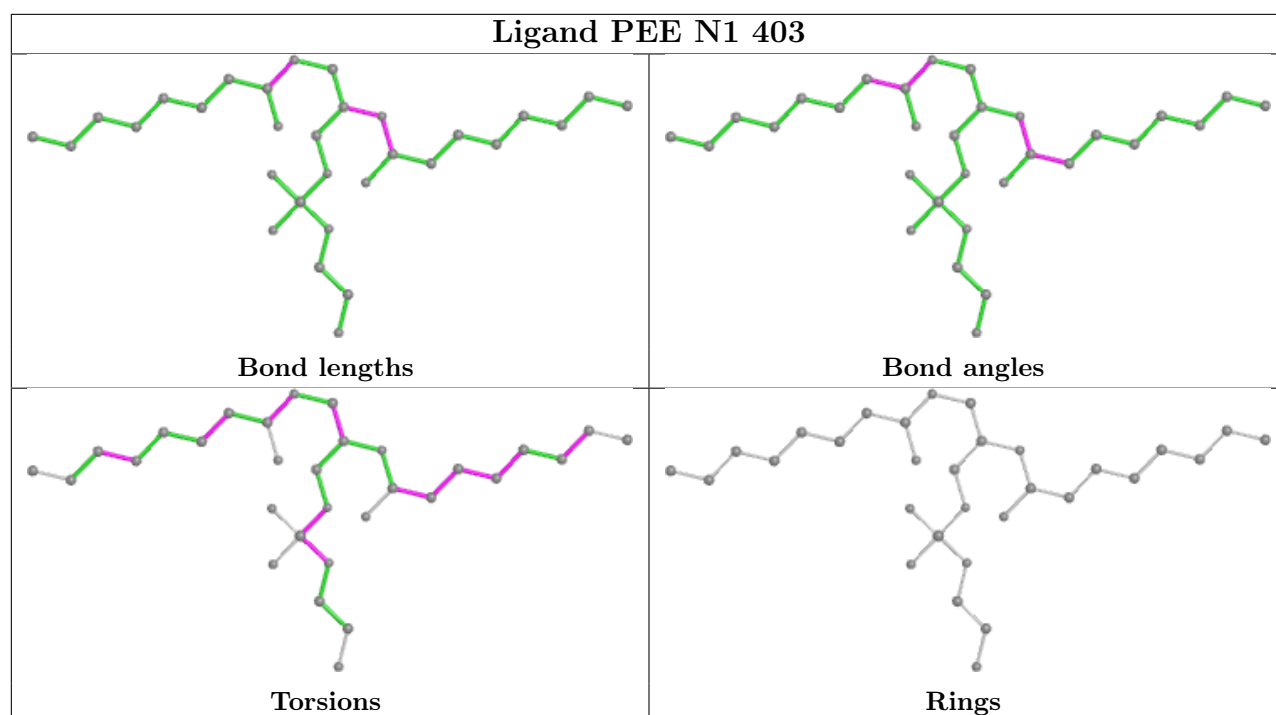


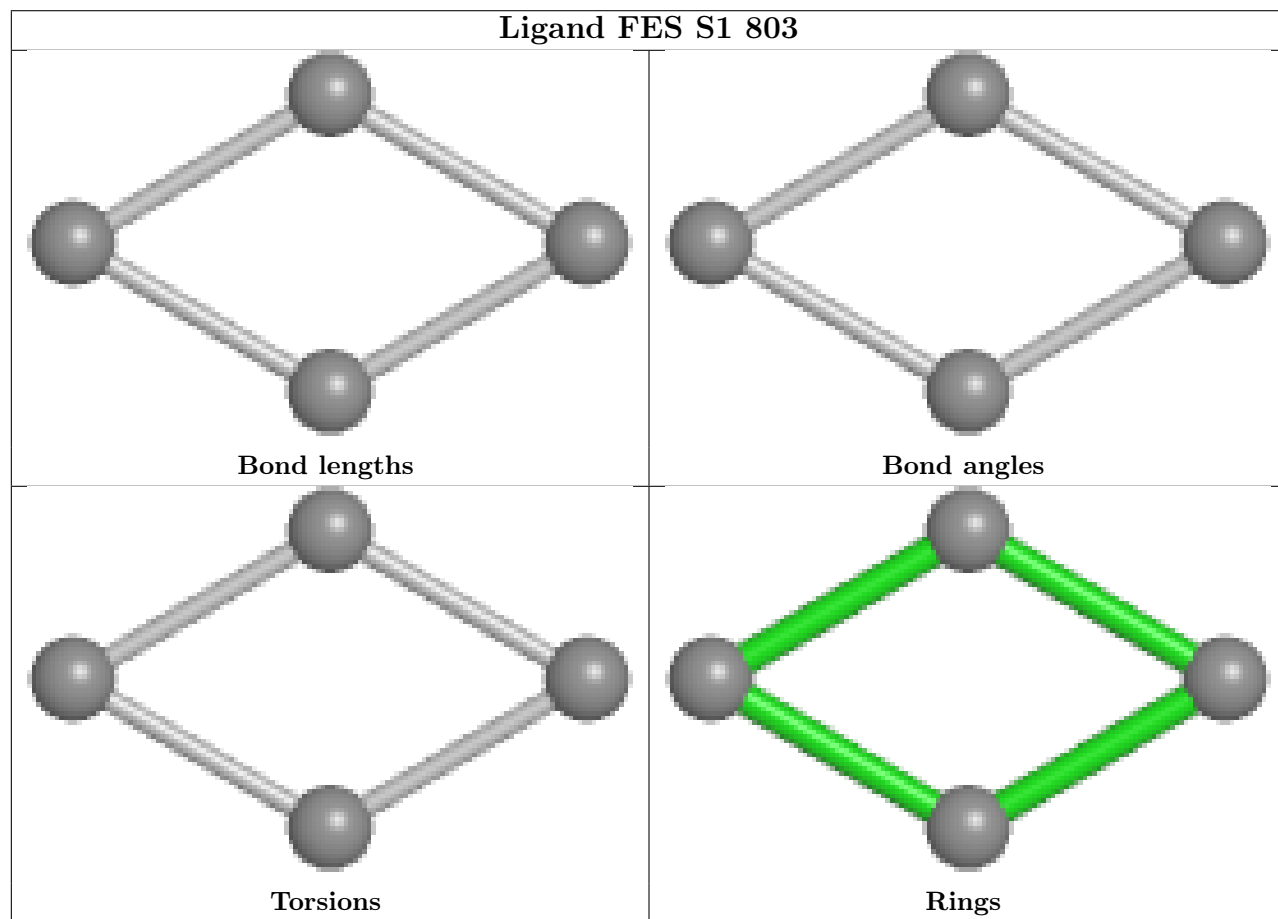
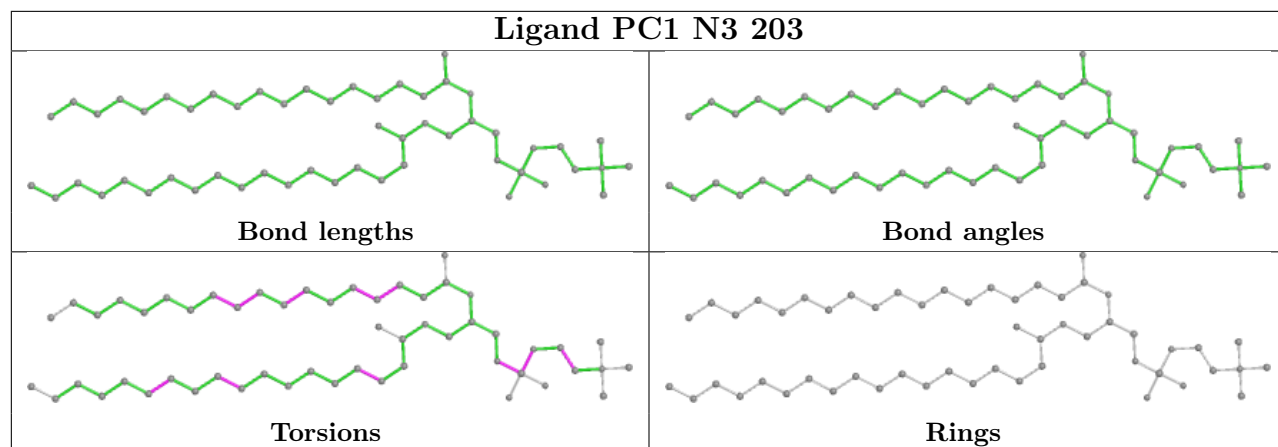


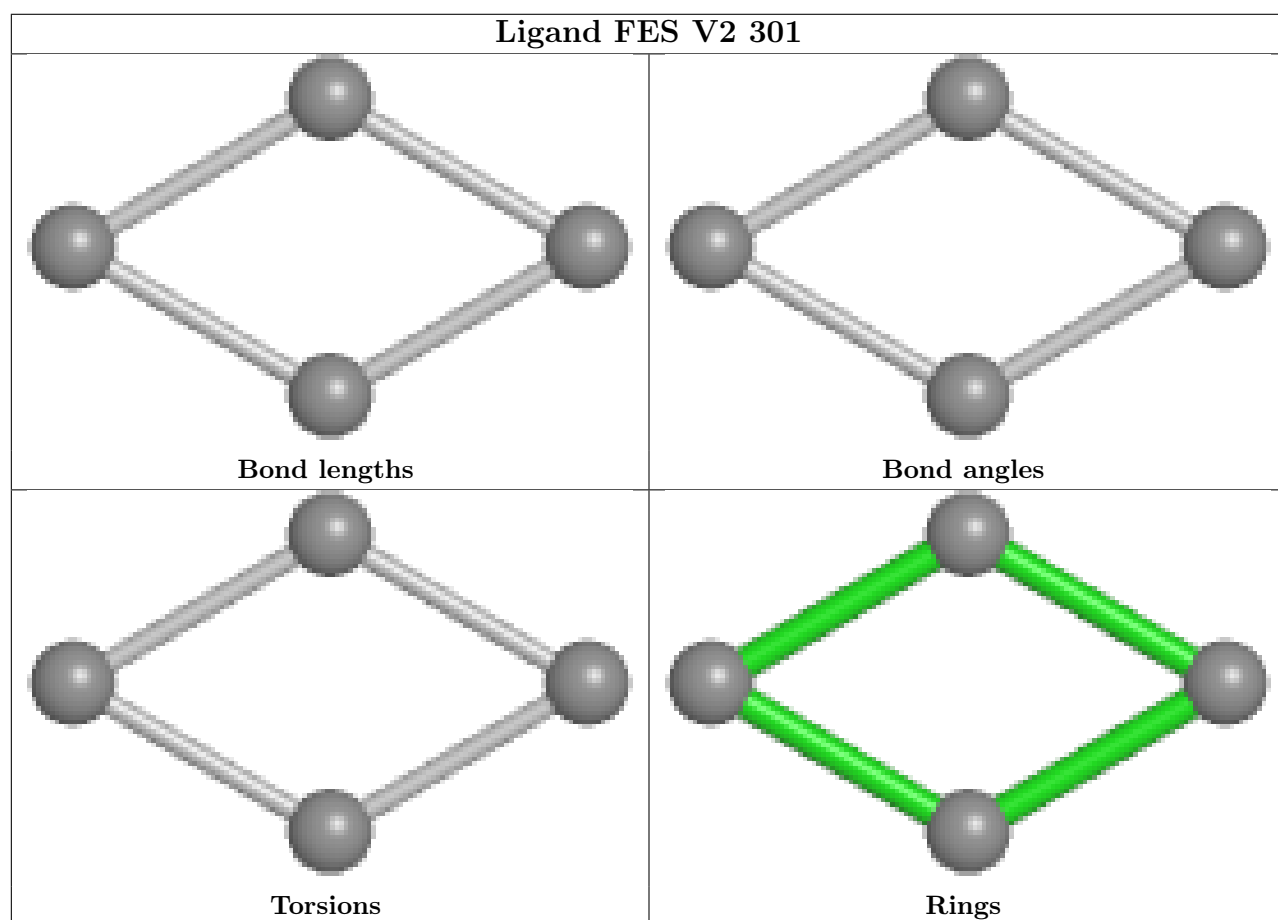
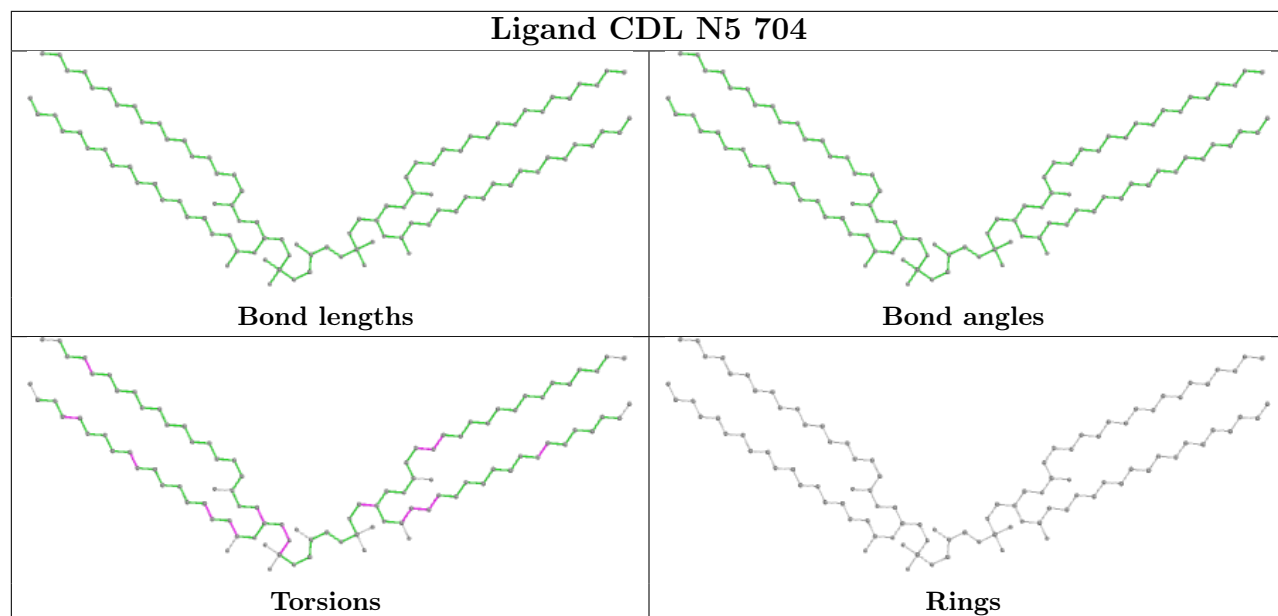


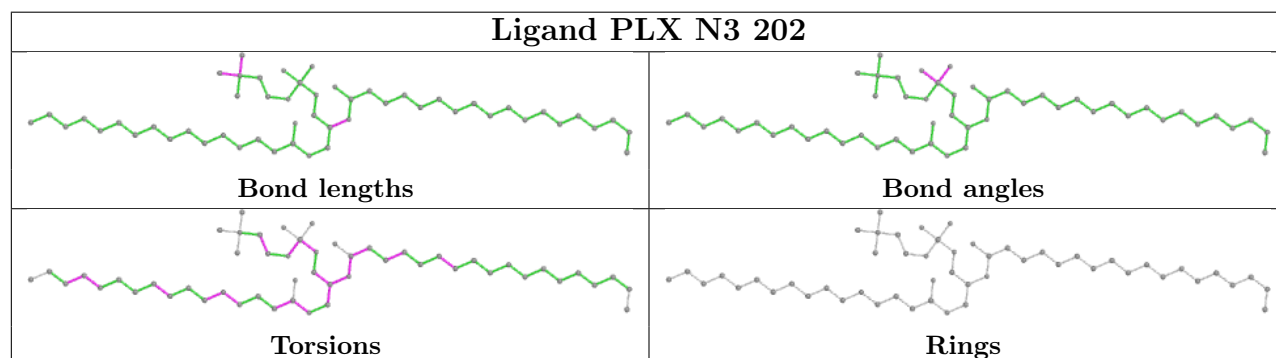
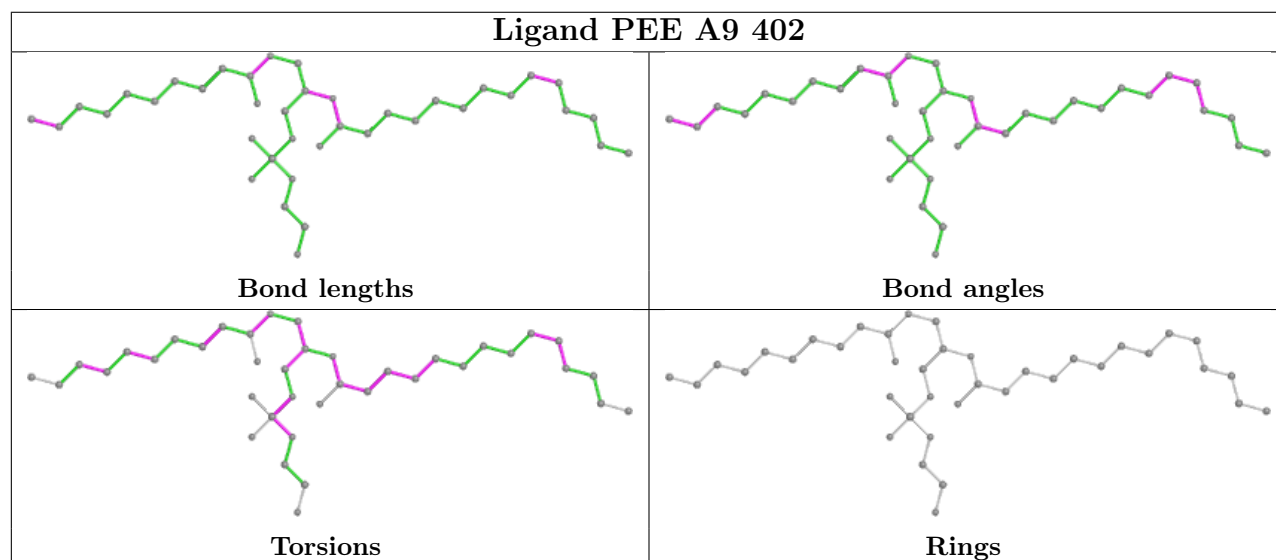
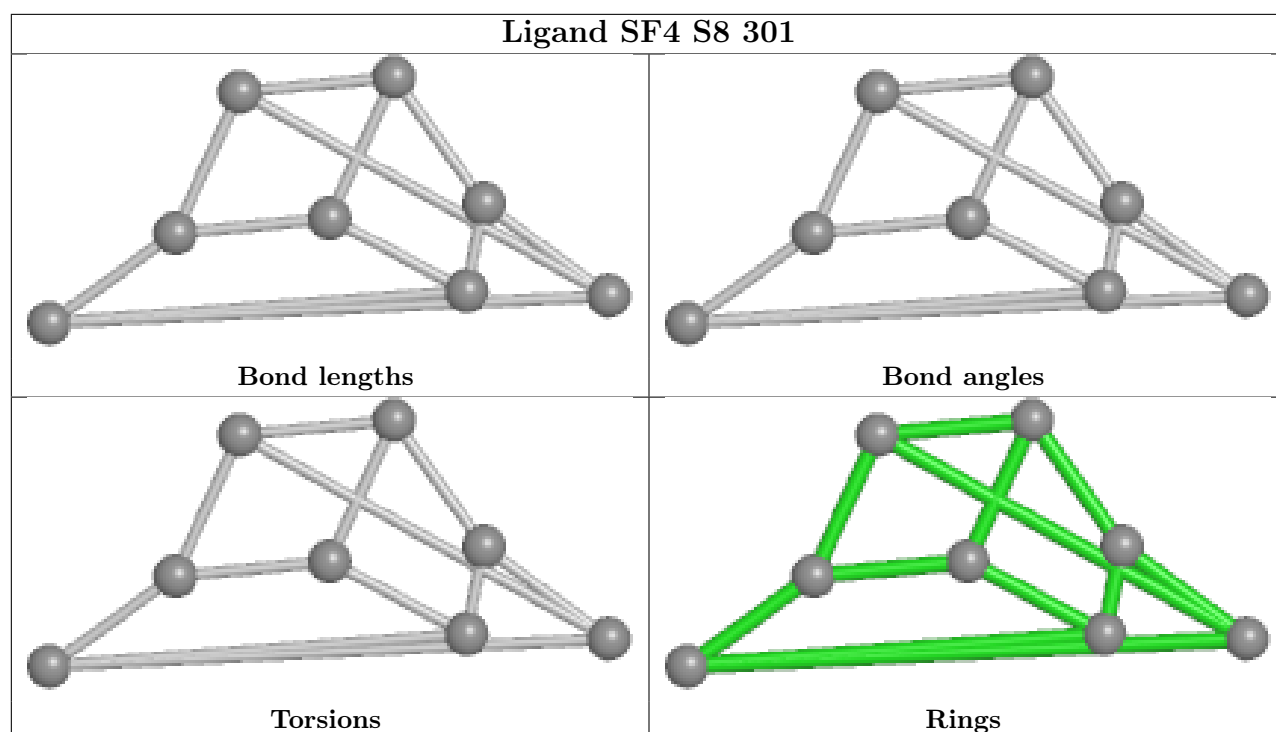


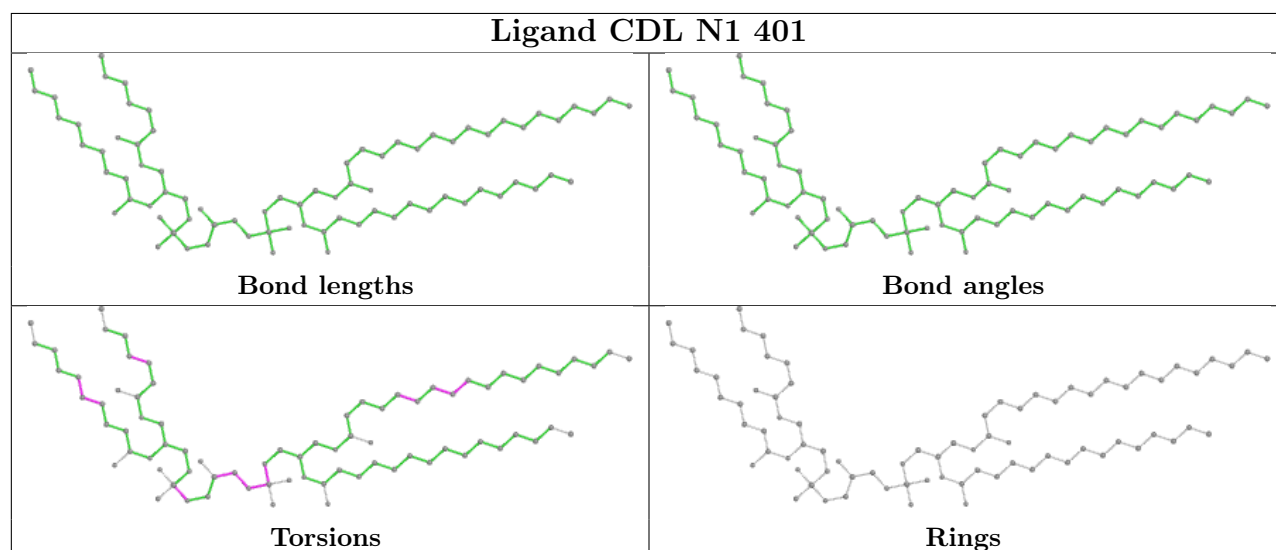
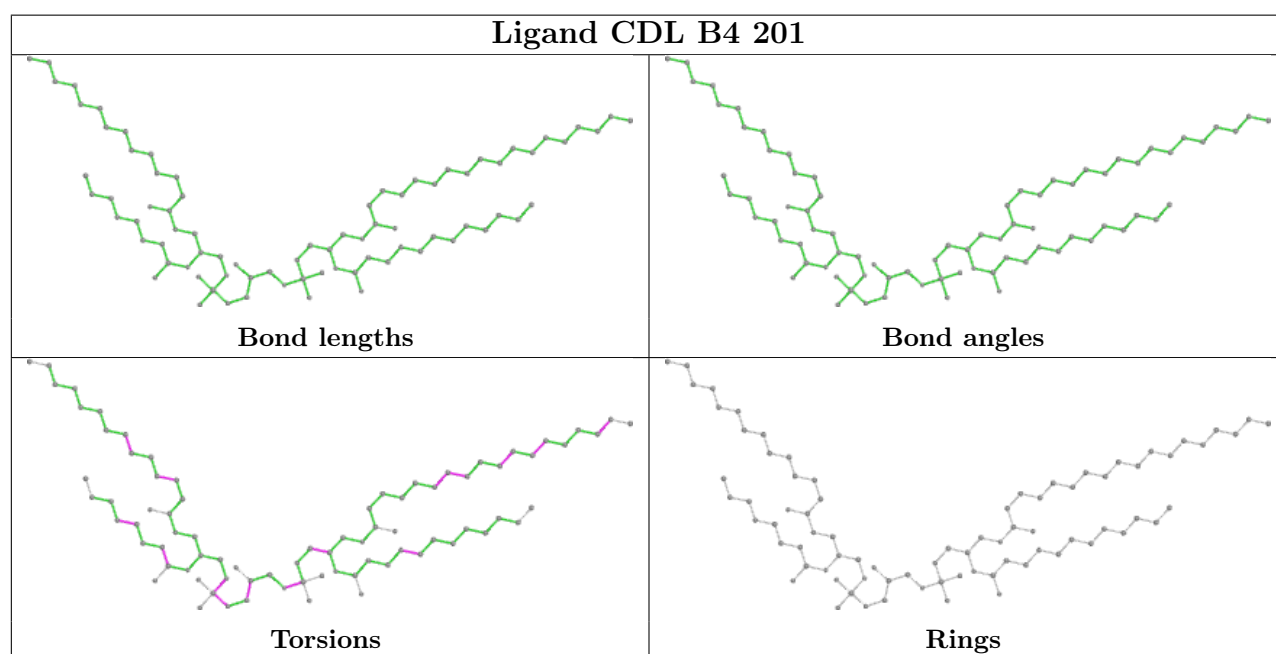
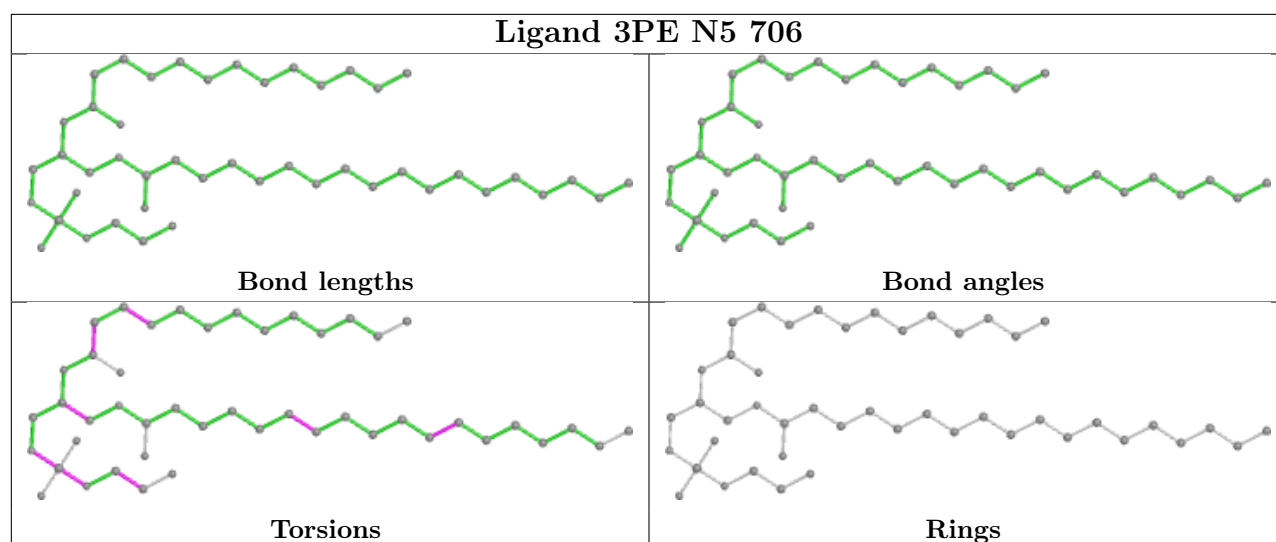


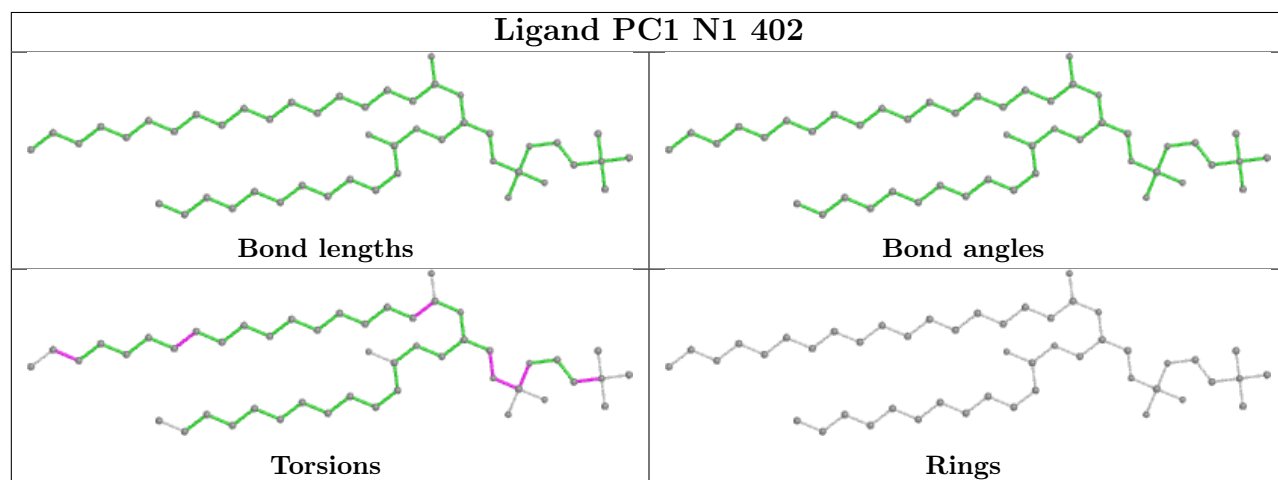
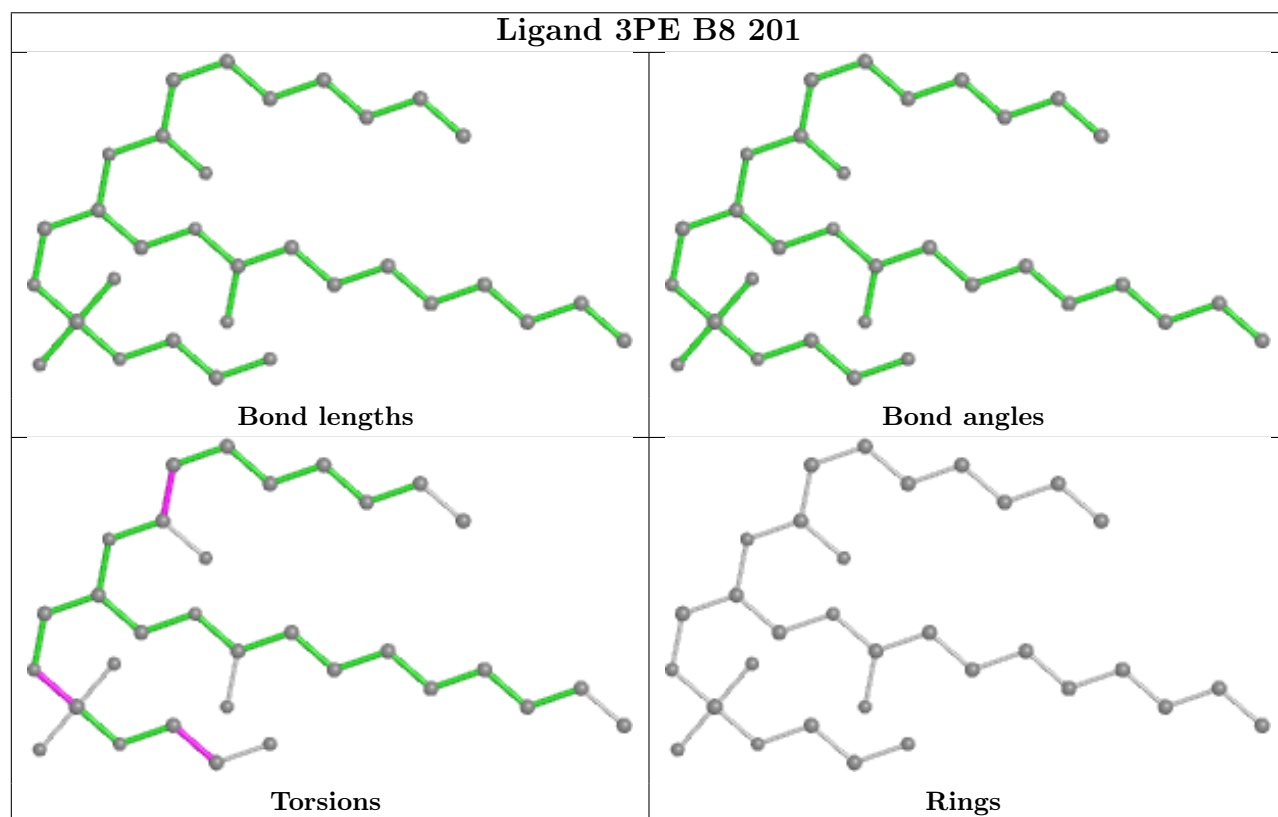
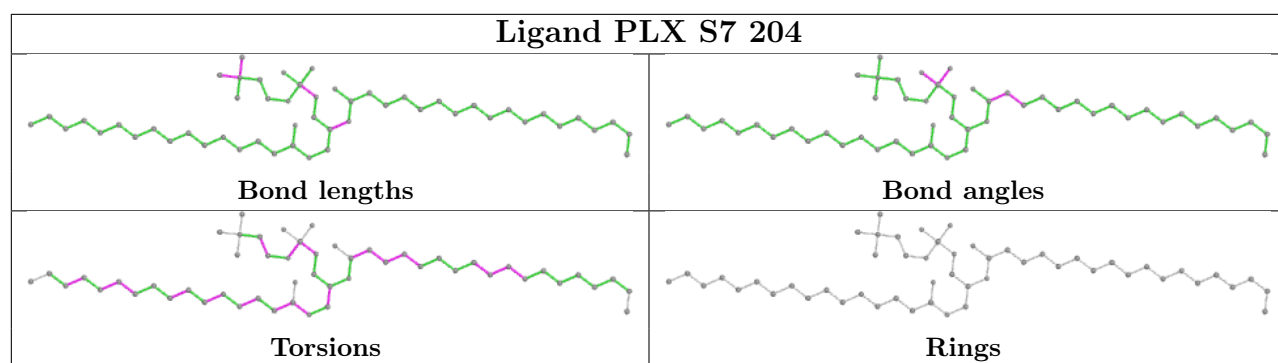












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

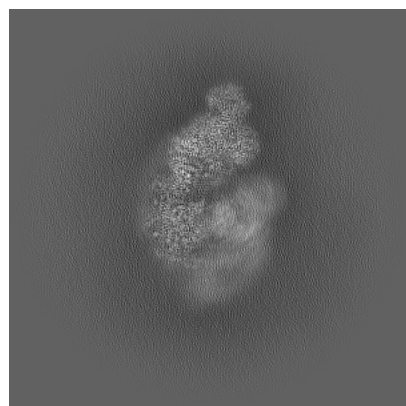
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61186. These allow visual inspection of the internal detail of the map and identification of artifacts.

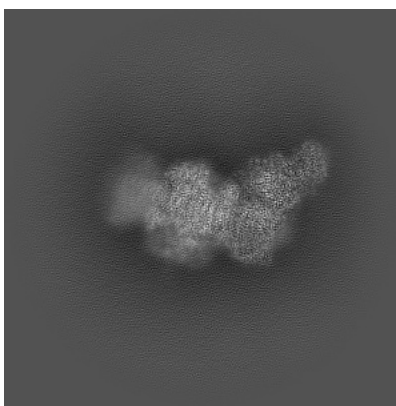
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

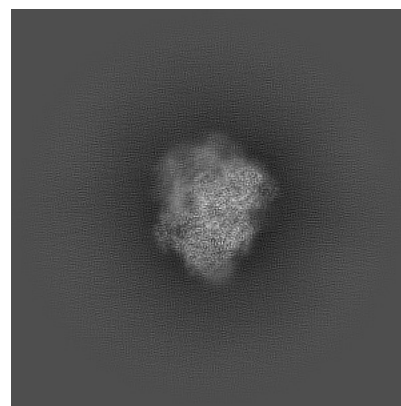
6.1.1 Primary map



X

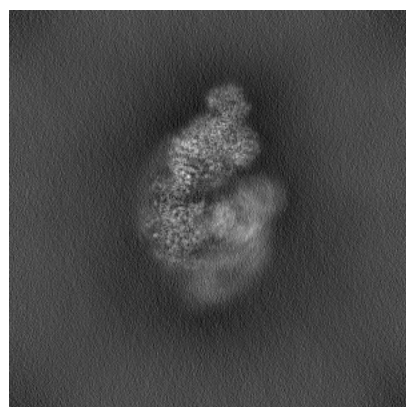


Y

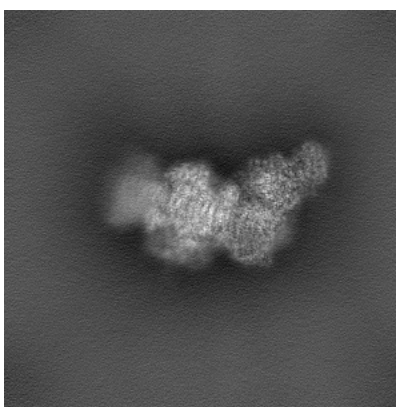


Z

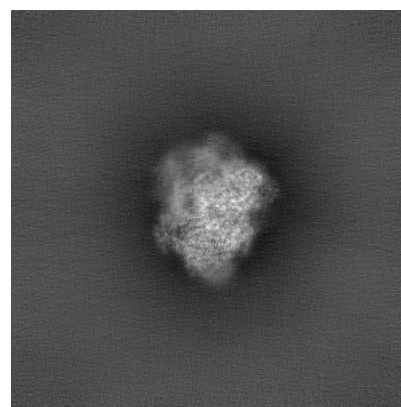
6.1.2 Raw map



X



Y

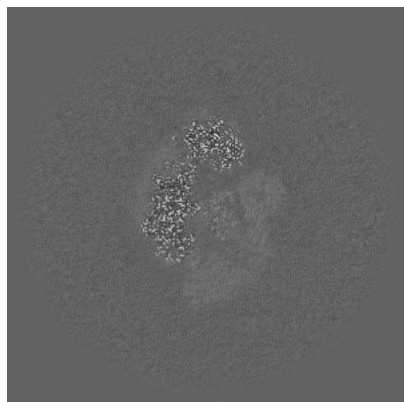


Z

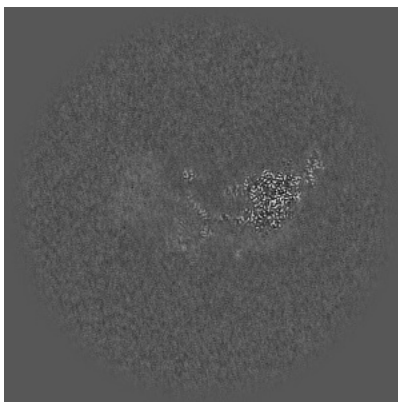
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

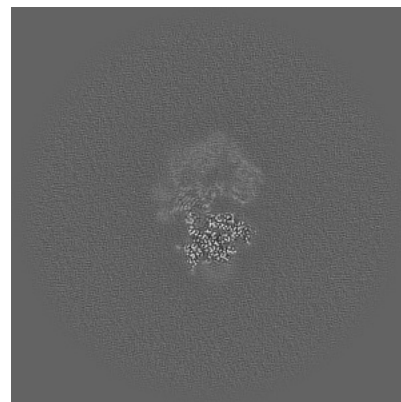
6.2.1 Primary map



X Index: 240

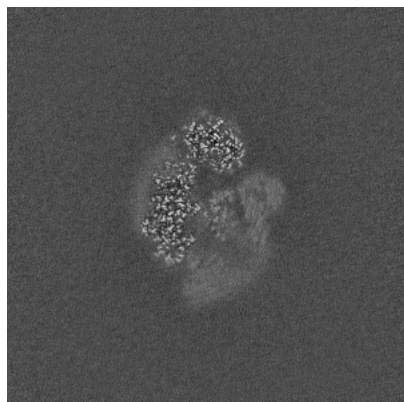


Y Index: 240

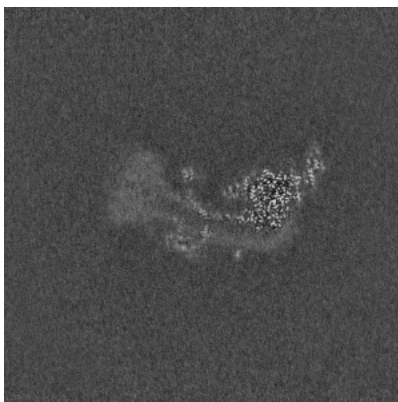


Z Index: 240

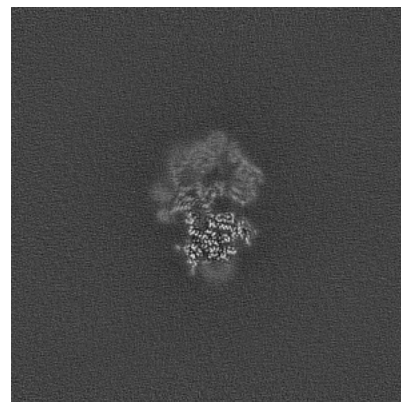
6.2.2 Raw map



X Index: 240



Y Index: 240

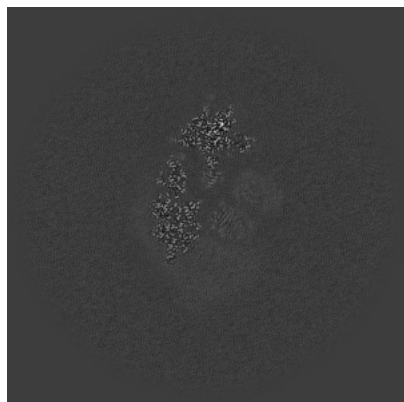


Z Index: 240

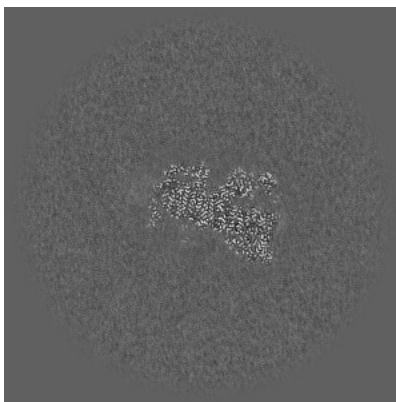
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

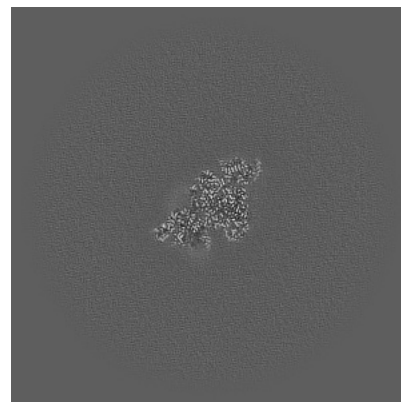
6.3.1 Primary map



X Index: 256

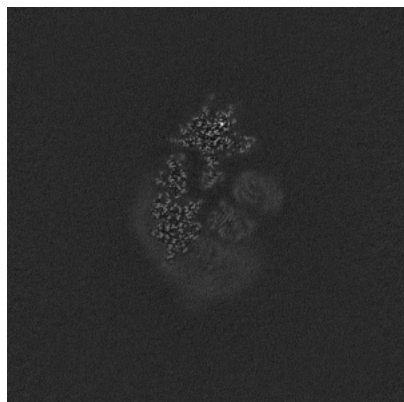


Y Index: 206

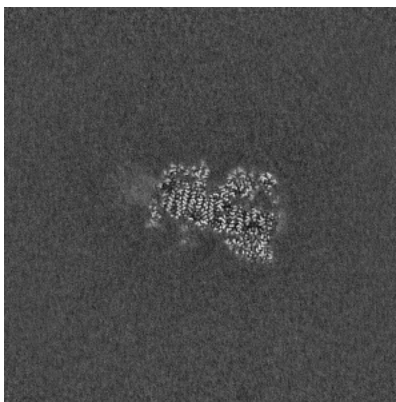


Z Index: 314

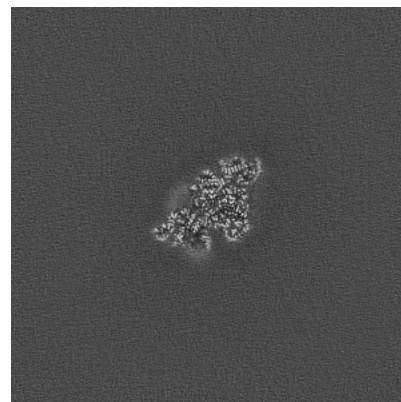
6.3.2 Raw map



X Index: 256



Y Index: 206

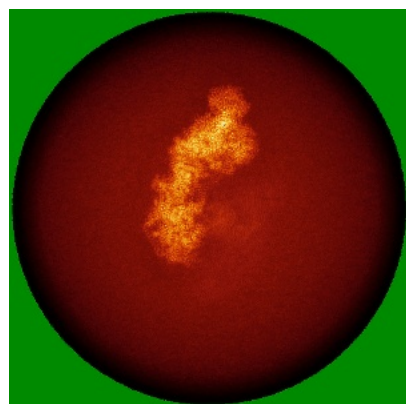


Z Index: 314

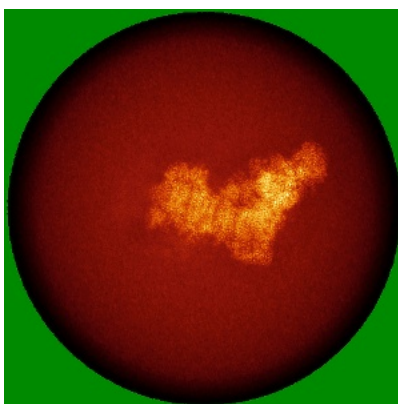
The images above show the largest variance slices of the map in three orthogonal directions.

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

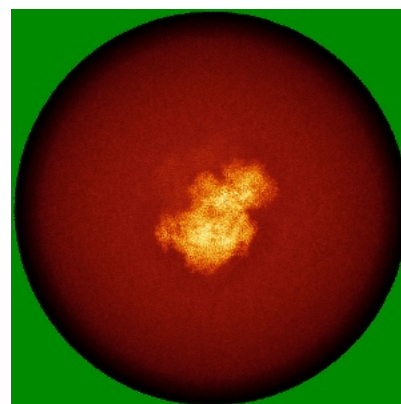
6.4.1 Primary map



X

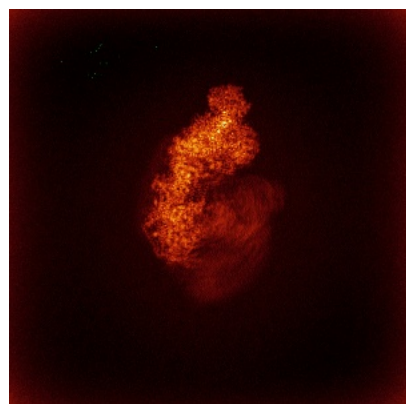


Y

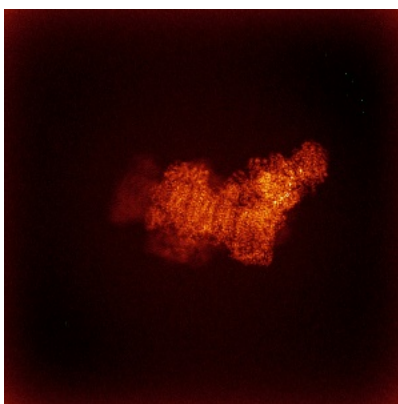


Z

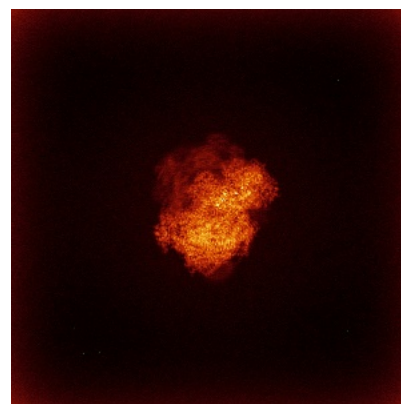
6.4.2 Raw map



X



Y

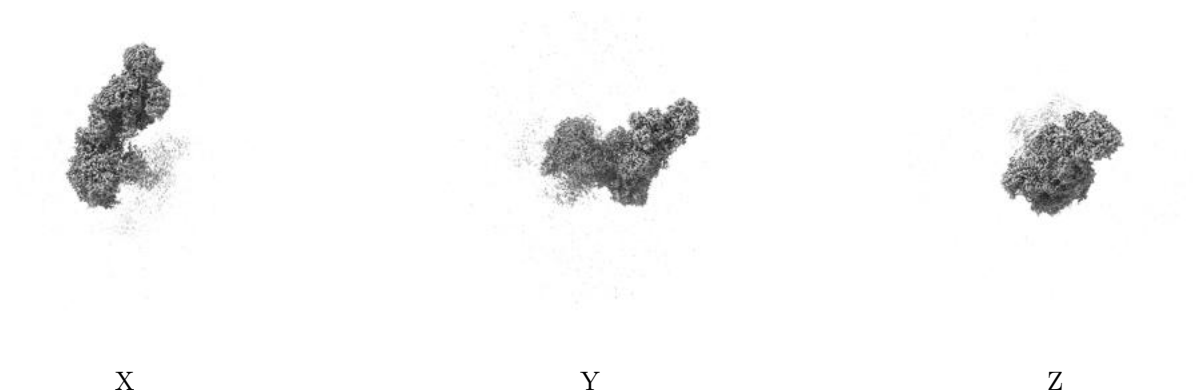


Z

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.

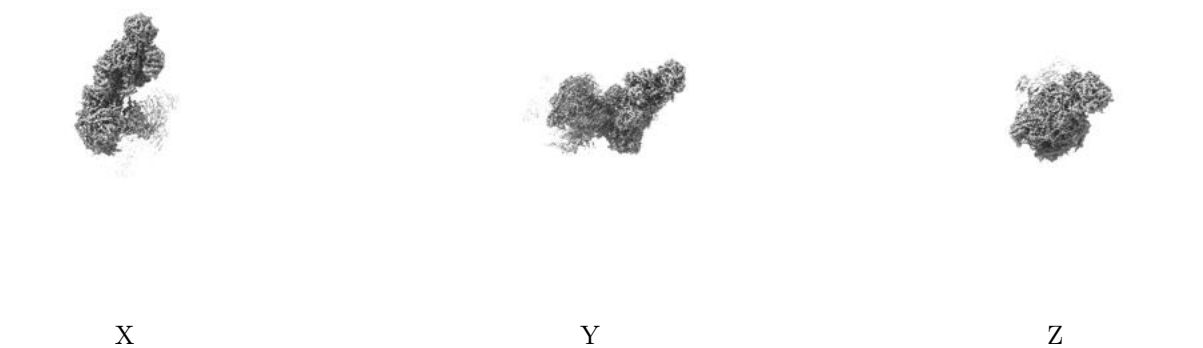
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.07. 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.

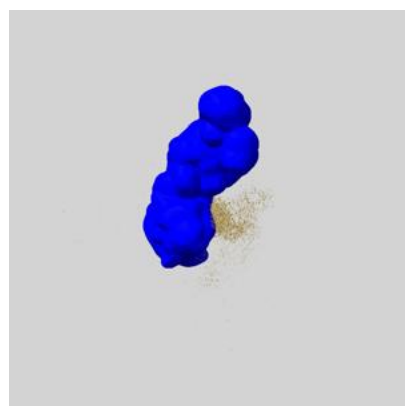
6.6 Mask visualisation [i](#)

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

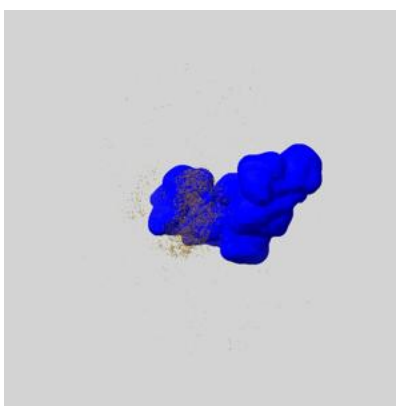
A mask typically either:

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

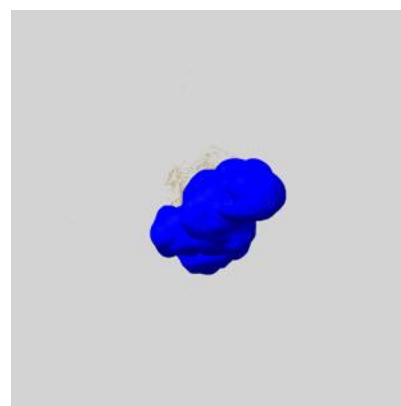
6.6.1 emd_61186_msk_1.map [i](#)



X



Y

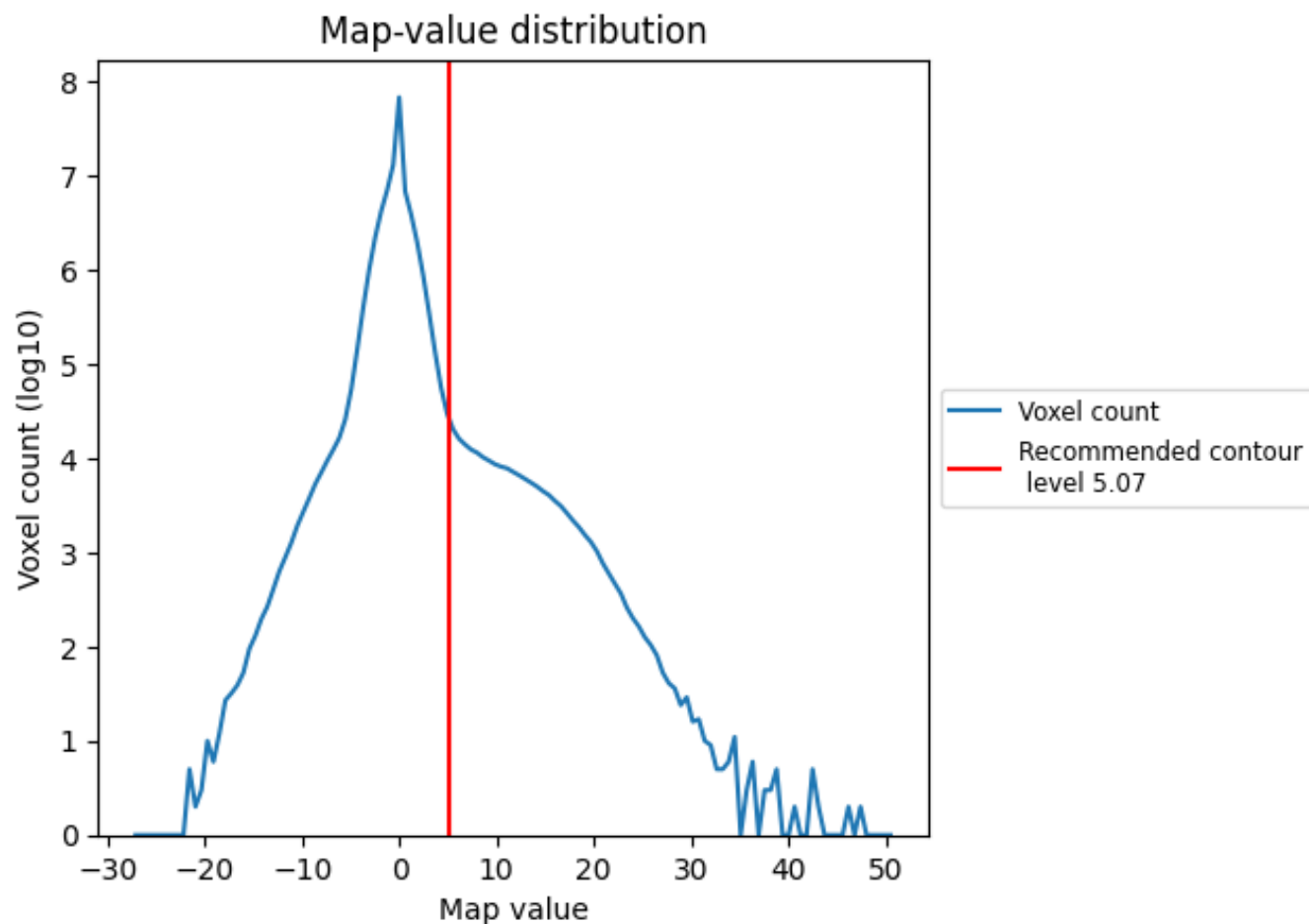


Z

7 Map analysis [i](#)

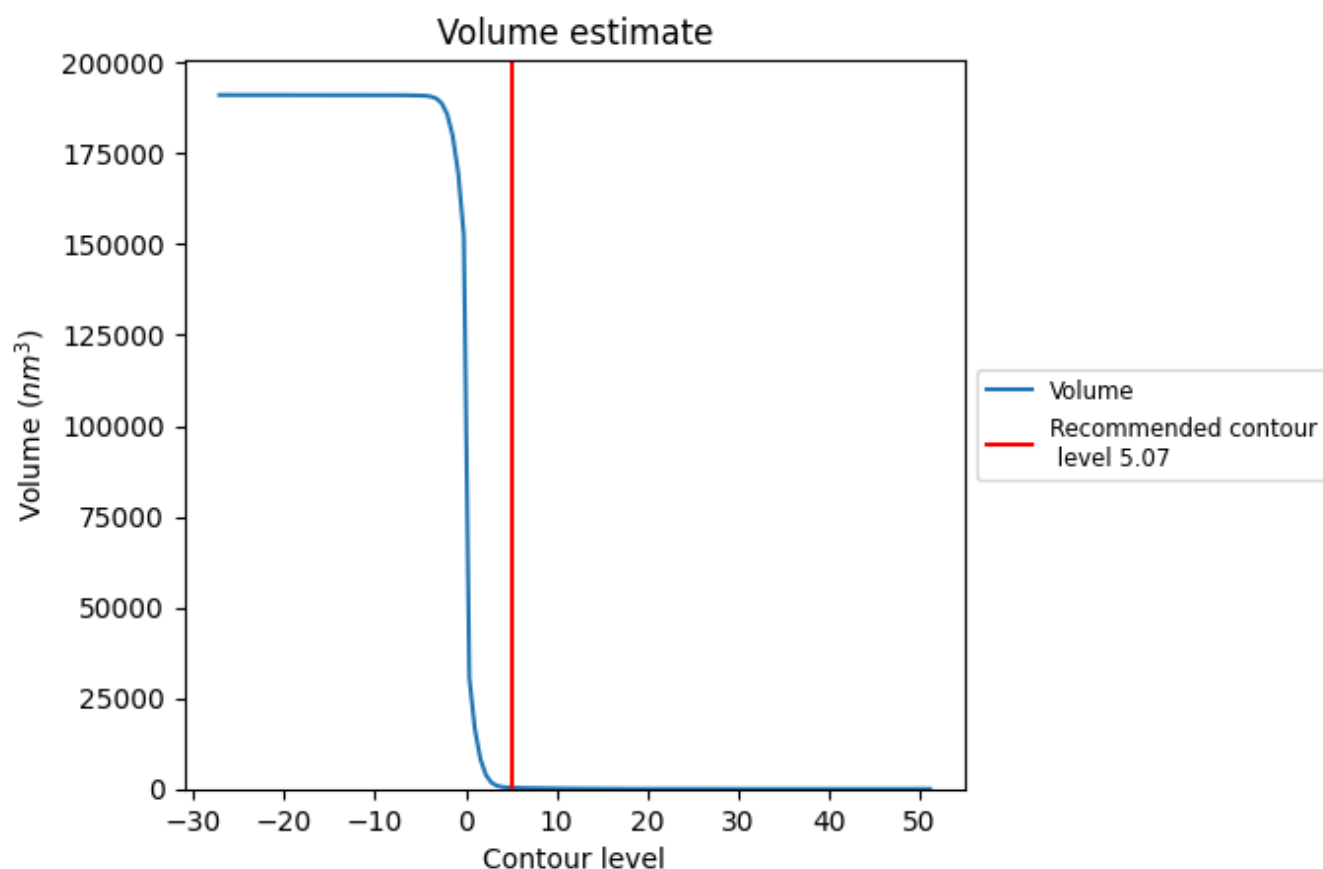
This section contains the results of statistical analysis of the map.

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.

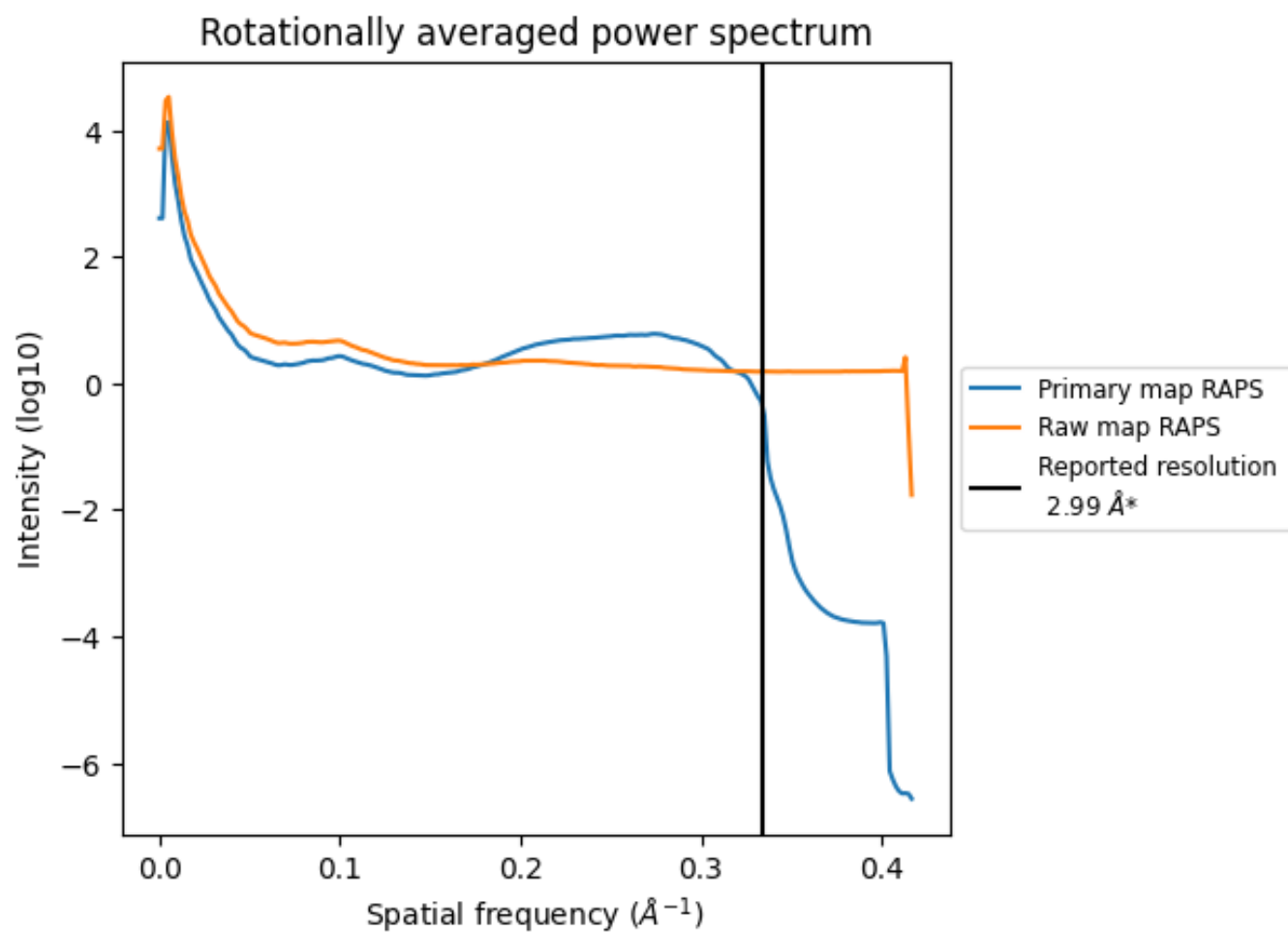
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 348 nm^3 ; this corresponds to an approximate mass of 315 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 ⓘ

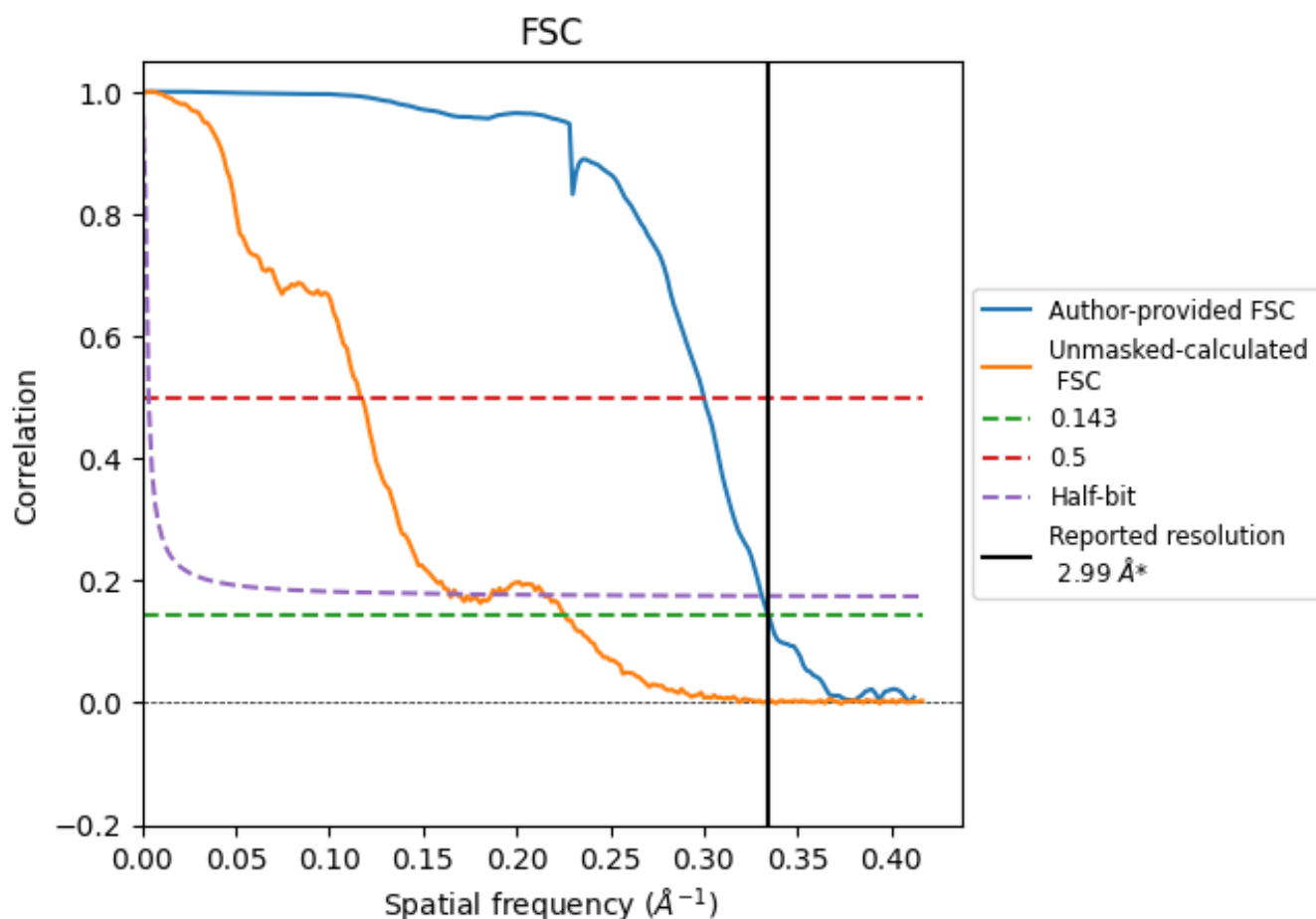


*Reported resolution corresponds to spatial frequency of 0.334 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.334 \AA^{-1}

8.2 Resolution estimates [i](#)

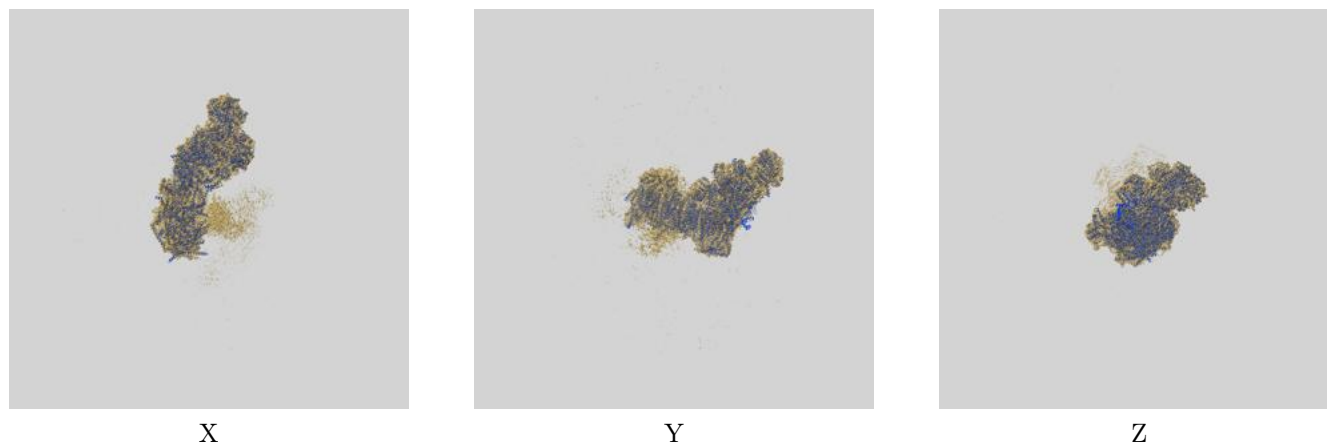
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.99	-	-
Author-provided FSC curve	2.99	3.33	3.02
Unmasked-calculated*	4.43	8.55	6.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.43 differs from the reported value 2.99 by more than 10 %

9 Map-model fit [i](#)

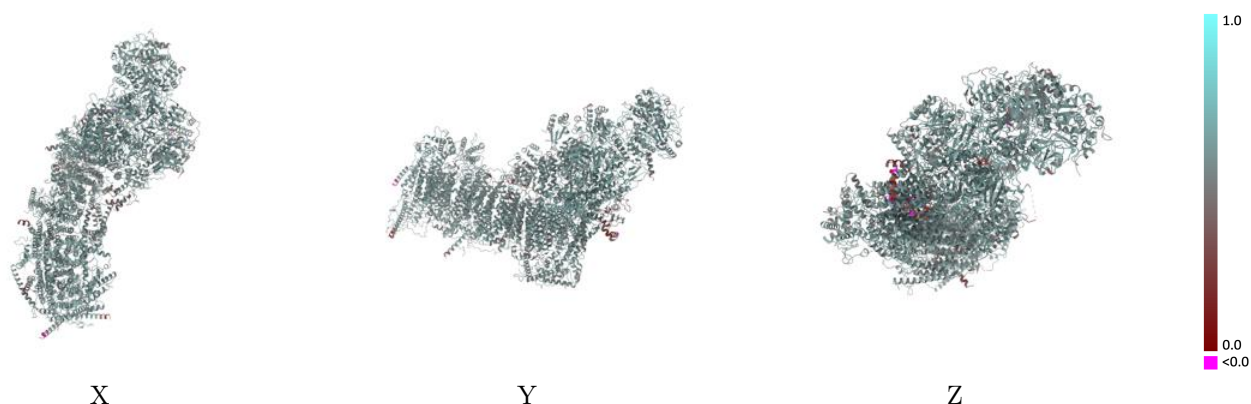
This section contains information regarding the fit between EMDB map EMD-61186 and PDB model 9J6W. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



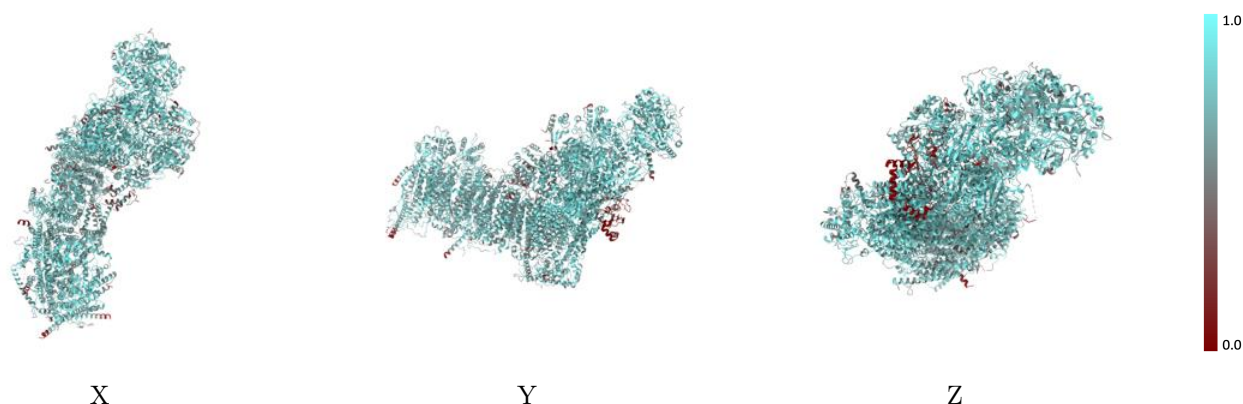
The images above show the 3D surface view of the map at the recommended contour level 5.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



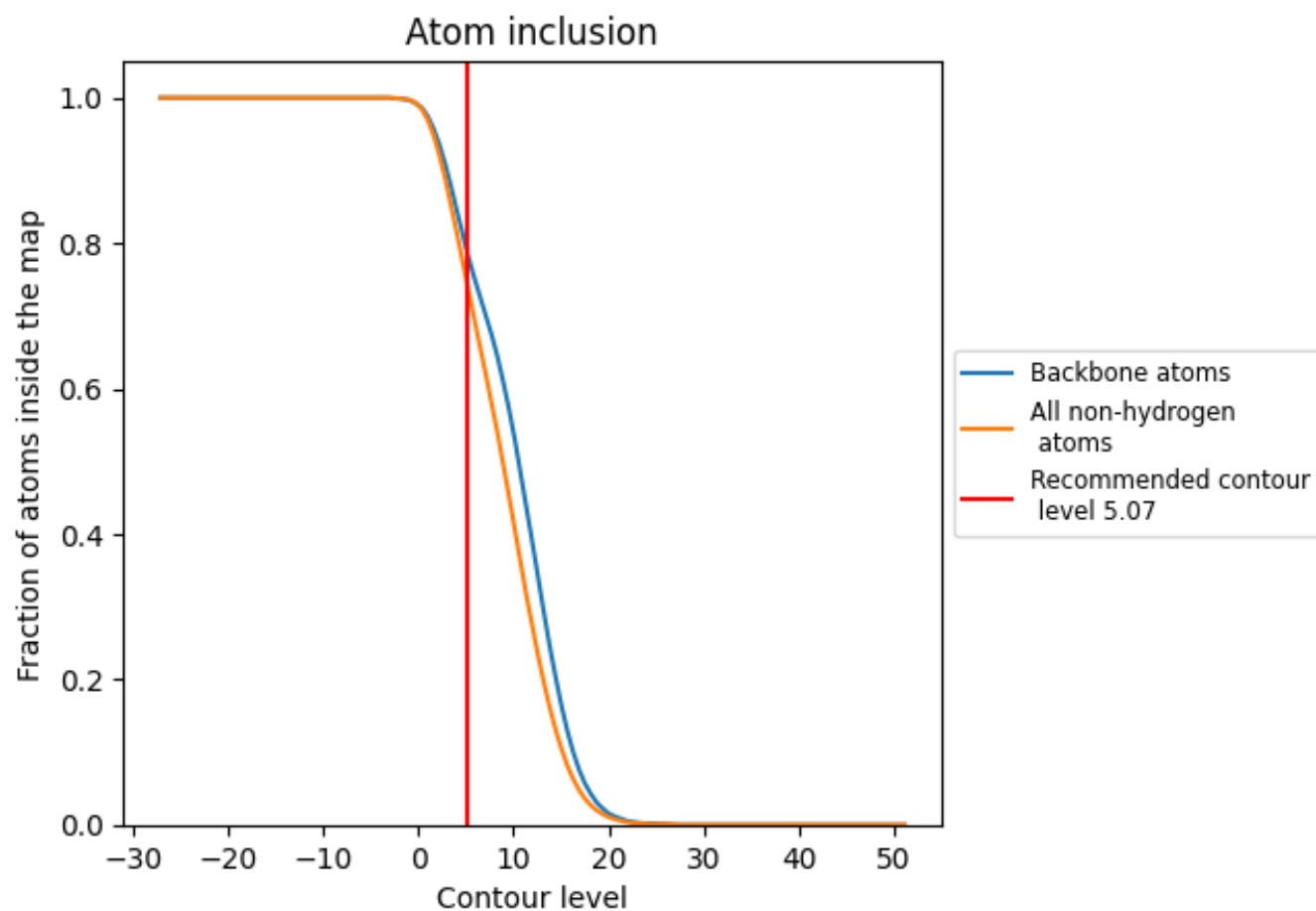
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.07).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary























The table lists the average atom inclusion at the recommended contour level (5.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7470	 0.5650
4L	 0.7710	 0.5820
A1	 0.7930	 0.5600
A2	 0.6750	 0.5420
A3	 0.7460	 0.5530
A5	 0.7400	 0.5670
A6	 0.7450	 0.5650
A7	 0.4560	 0.4360
A8	 0.7580	 0.5630
A9	 0.7870	 0.5820
AB	 0.4720	 0.4690
AC	 0.7530	 0.5650
AK	 0.6970	 0.5440
AL	 0.6580	 0.5500
AM	 0.1980	 0.4300
AN	 0.7380	 0.5530
B1	 0.6110	 0.5200
B2	 0.7190	 0.5680
B3	 0.6450	 0.5180
B4	 0.6760	 0.5630
B5	 0.7910	 0.5790
B6	 0.6680	 0.5210
B7	 0.6870	 0.5430
B8	 0.7550	 0.5720
B9	 0.7900	 0.5750
BK	 0.7380	 0.5520
BL	 0.7390	 0.5570
CA	 0.6440	 0.5440
CB	 0.7800	 0.5790
N1	 0.7990	 0.5790
N2	 0.8220	 0.5870
N3	 0.7190	 0.5720
N4	 0.8100	 0.5840
N5	 0.7740	 0.5790
N6	 0.7040	 0.5410



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Chain	Atom inclusion	Q-score
S1	 0.7830	 0.5720
S2	 0.8290	 0.5920
S3	 0.8710	 0.6080
S4	 0.7710	 0.5880
S5	 0.6930	 0.5510
S6	 0.6470	 0.5630
S7	 0.7950	 0.5850
S8	 0.8590	 0.5990
V1	 0.7750	 0.5670
V2	 0.7220	 0.5550
V3	 0.7040	 0.5620