wwPDB EM Validation Summary Report

Aug 12, 2026 – 10:47 PM JST

PDB ID	:	9J6H / pdb_00009j6h
EMDB ID	:	EMD-61173
Title	:	Complex I from respirasome closed state 1 bound by metformin and CoQ10 (SC-MetC1-iv)
Authors	:	Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.
Deposited on	:	2024-08-16
Resolution	:	2.92 Å(reported)

This is a wwPDB EM Validation Summary 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:

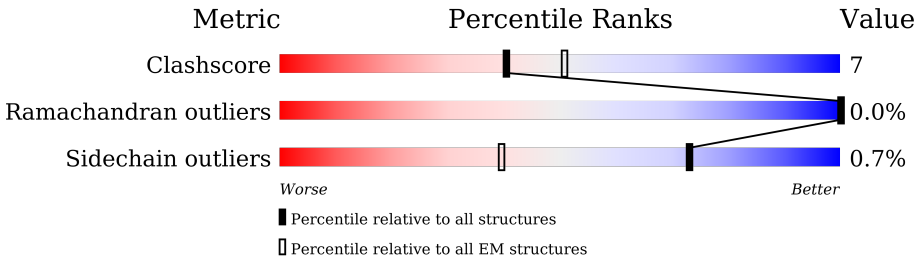
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

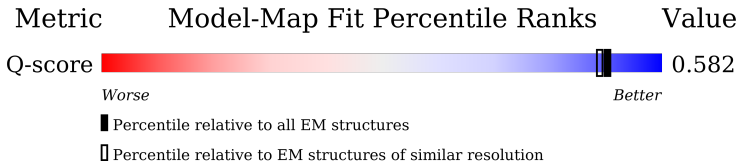
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.92 Å.

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





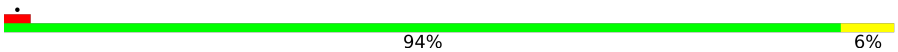
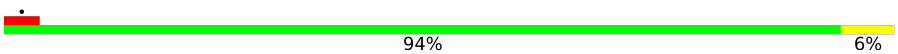
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13007 (2.42 - 3.42)

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 <=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	77% 23%
2	A1	70	87% 13%
3	A2	85	5% 87% 13%
4	A3	83	90% 10%

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	N2	347	79% 21%
30	N3	115	83% 17%
31	N4	459	77% 22%
32	N5	603	78% 22%
33	N6	174	9% 80% 18%
34	S1	689	78% 22%
35	S2	430	76% 23%
36	S3	208	88% 12%
37	S4	124	6% 87% 13%
38	S5	105	90% 10%
39	S6	96	5% 88% 12%
40	S7	156	77% 22%
41	S8	176	77% 23%
42	V1	431	77% 22%
43	V2	217	84% 15%
44	V3	42	74% 26%

2 Entry composition (i)

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
			Total	C	N	O	S		
1	4L	98	748	493	113	128	14	0	0

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

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

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

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

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

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

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

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

- 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		

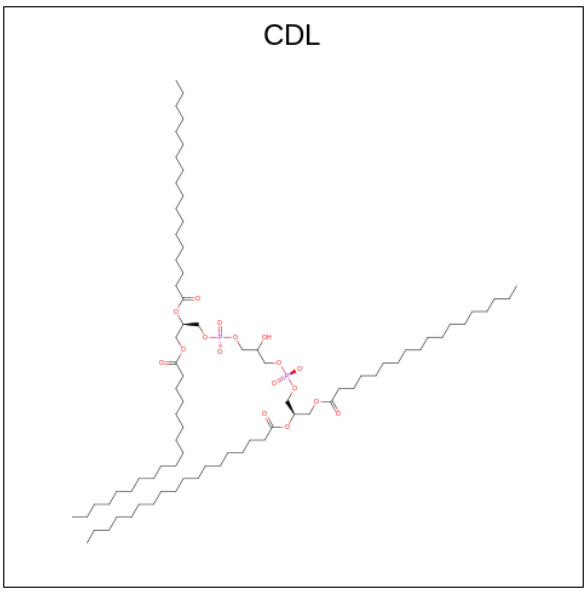
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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		

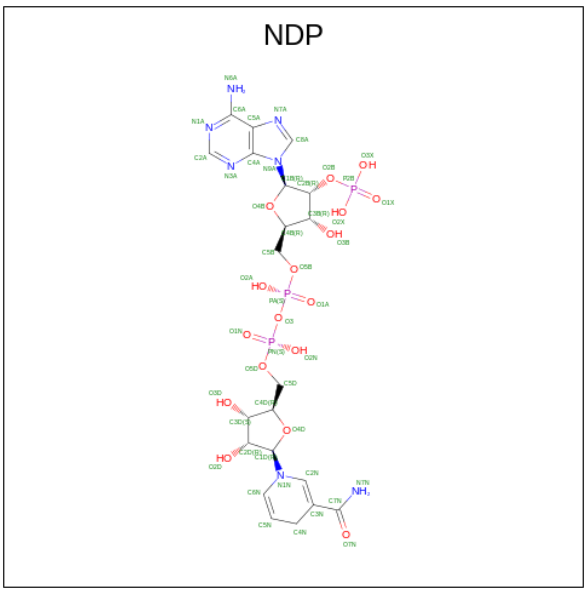
- Molecule 45 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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	

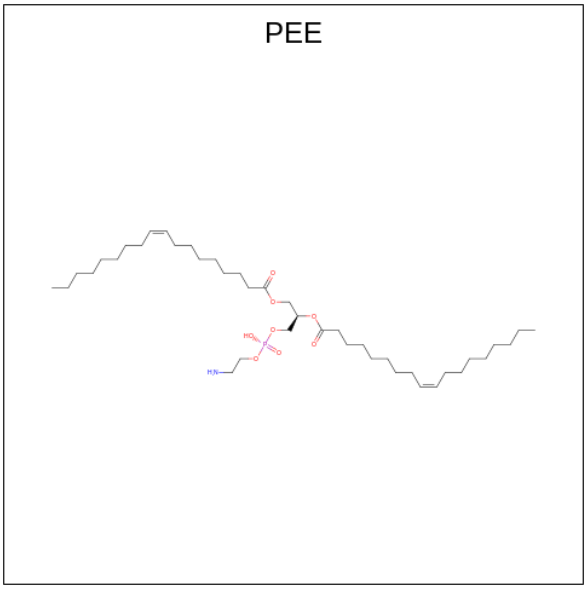
- Molecule 46 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

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



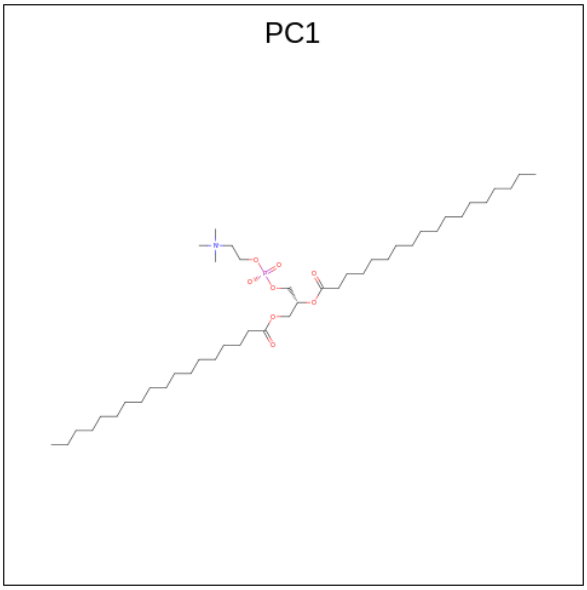
Mol	Chain	Residues	Atoms					AltConf
47	A9	1	Total	C	N	O	P	0
			39	29	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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	N4	1	Total	C	N	O	P	0
			49	39	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	

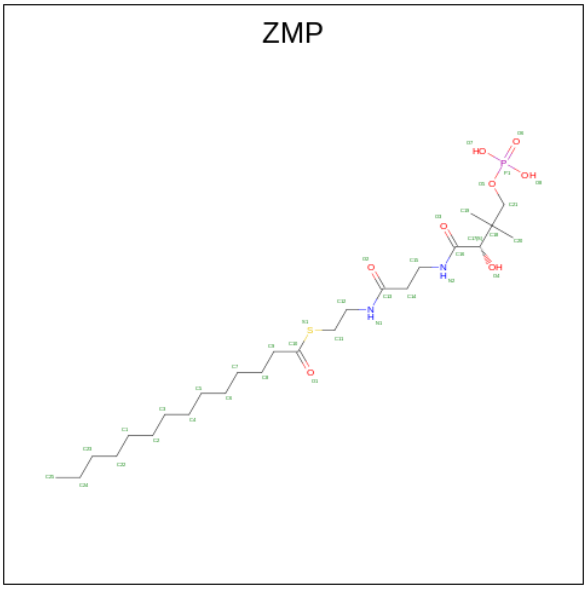
- Molecule 48 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
48	A9	1	Total	C	N	O	P	0
			54	44	1	8	1	
48	N1	1	Total	C	N	O	P	0
			48	38	1	8	1	

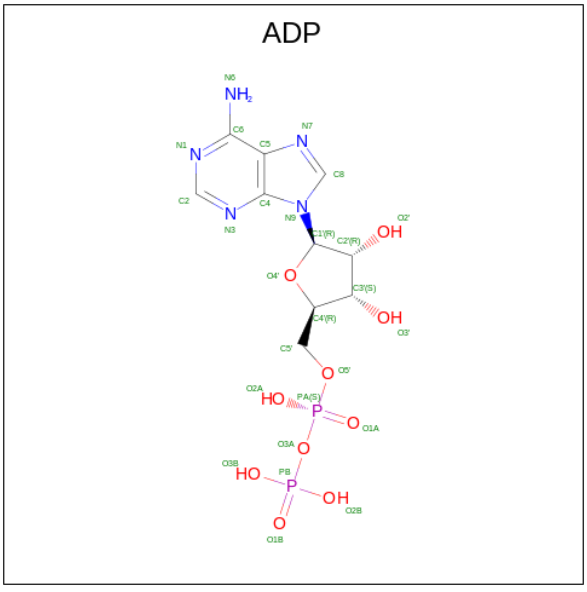
- Molecule 49 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alan

yl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



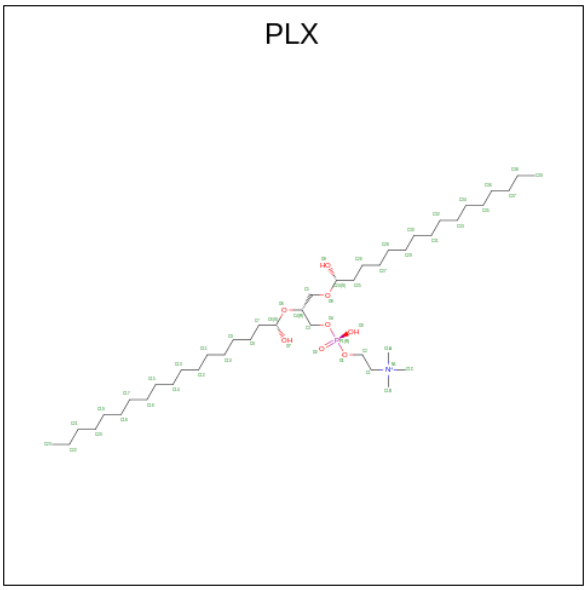
Mol	Chain	Residues	Atoms						AltConf
49	AB	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	
49	AC	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 50 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



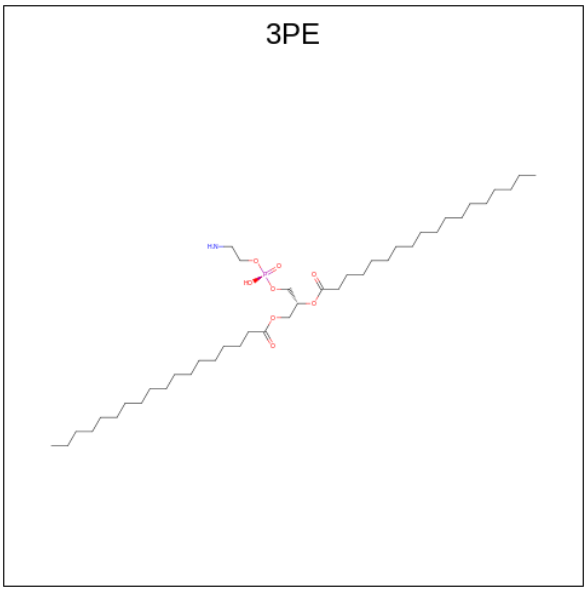
Mol	Chain	Residues	Atoms					AltConf
50	AK	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 51 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$).



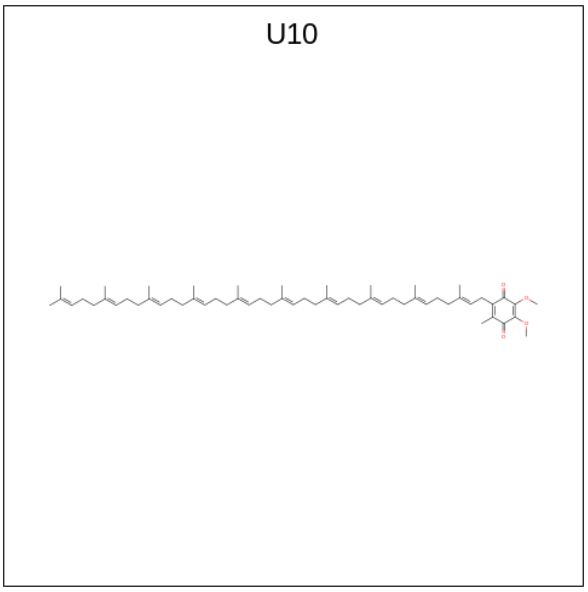
Mol	Chain	Residues	Atoms					AltConf
51	AL	1	Total	C	N	O	P	0
			47	37	1	8	1	
51	AM	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	B1	1	Total	C	N	O	P	0
			52	42	1	8	1	
51	CB	1	Total	C	N	O	P	0
			52	42	1	8	1	
51	N4	1	Total	C	N	O	P	0
			49	39	1	8	1	
51	N6	1	Total	C	N	O	P	0
			52	42	1	8	1	
51	S7	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 52 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



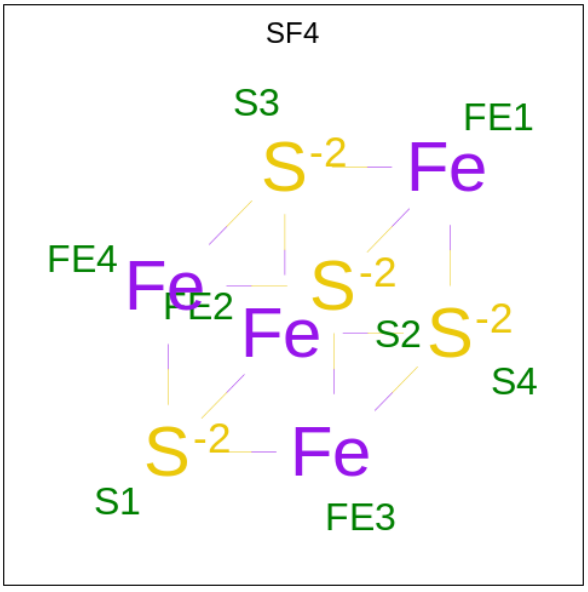
Mol	Chain	Residues	Atoms					AltConf
52	B8	1	Total	C	N	O	P	0
			32	22	1	8	1	
52	CA	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	CB	1	Total	C	N	O	P	0
			46	36	1	8	1	
52	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
52	S7	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



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

- Molecule 54 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



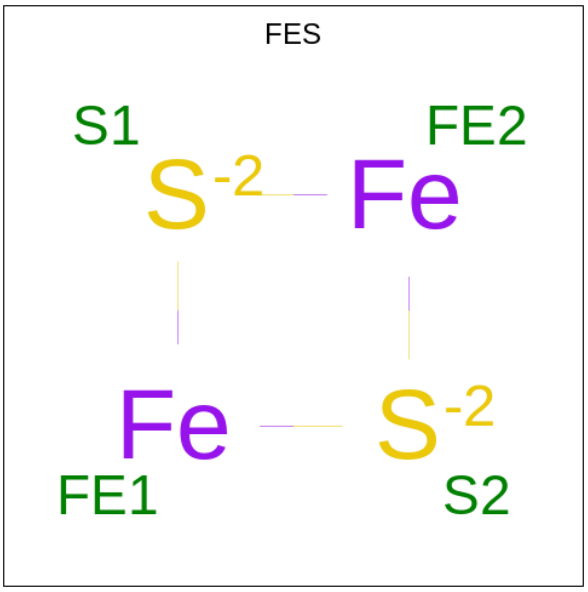
Mol	Chain	Residues	Atoms			AltConf
54	S1	1	Total	Fe	S	0
			8	4	4	
54	S1	1	Total	Fe	S	0
			8	4	4	
54	S7	1	Total	Fe	S	0
			8	4	4	

Continued on next page...

Continued from previous page...

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

- Molecule 55 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

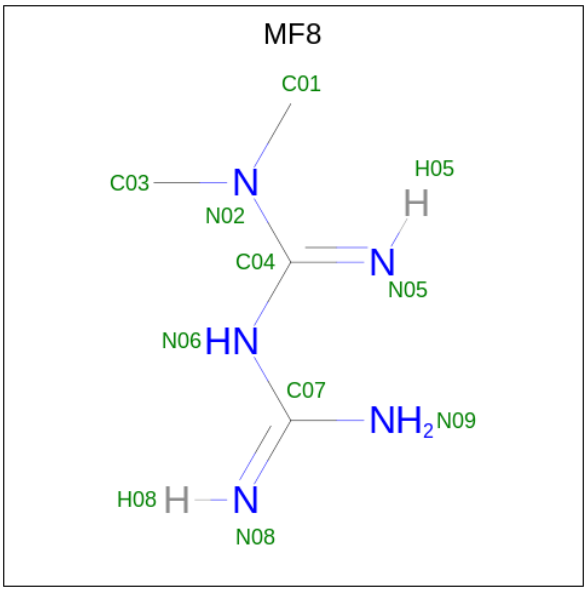


Mol	Chain	Residues	Atoms	AltConf
55	S1	1	Total Fe S 4 2 2	0
55	V2	1	Total Fe S 4 2 2	0

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

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

- Molecule 57 is Metformin (CCD ID: MF8) (formula: $C_4H_{11}N_5$) (labeled as "Ligand of Interest" by depositor).

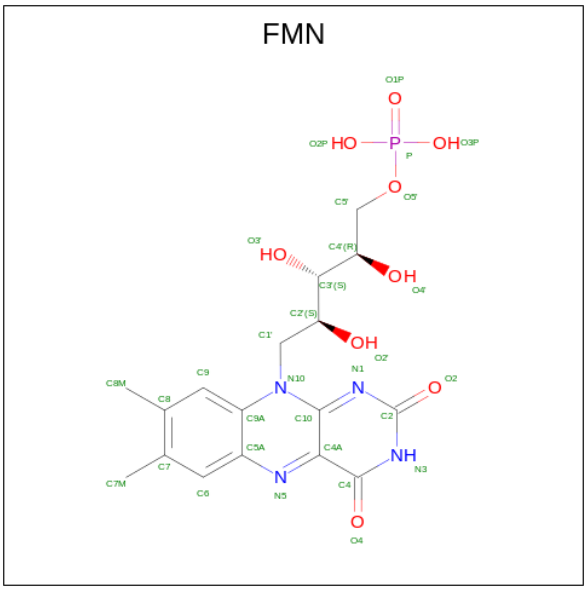


Mol	Chain	Residues	Atoms	AltConf
57	S2	1	Total C N 9 4 5	0

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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



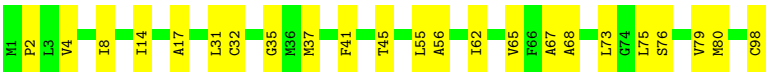
Mol	Chain	Residues	Atoms					AltConf
59	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

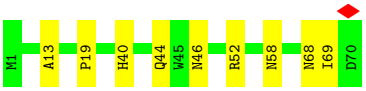
Chain 4L:



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

Chain A1:

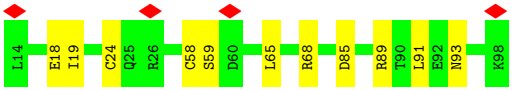




• Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain A2:





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

Chain A3:

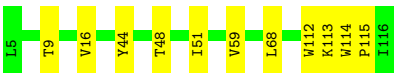




• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain A5:

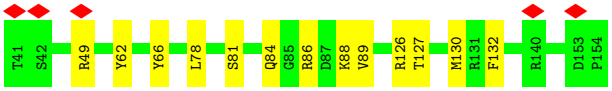




• Molecule 6: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain A6:

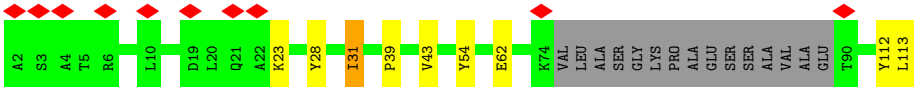




• Molecule 7: Complex I-B14.5a

Chain A7:

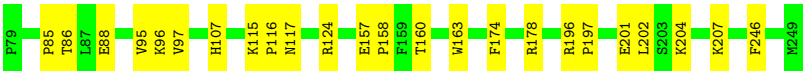




• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8:



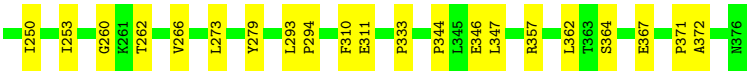


• Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain A9:







• Molecule 10: Acyl carrier protein

Chain AB:

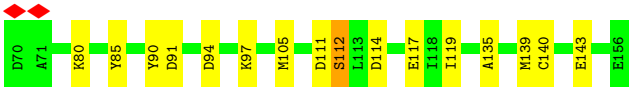




• Molecule 10: Acyl carrier protein

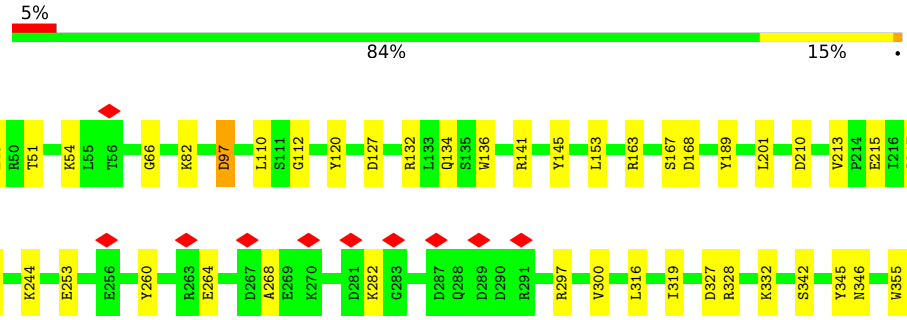
Chain AC:





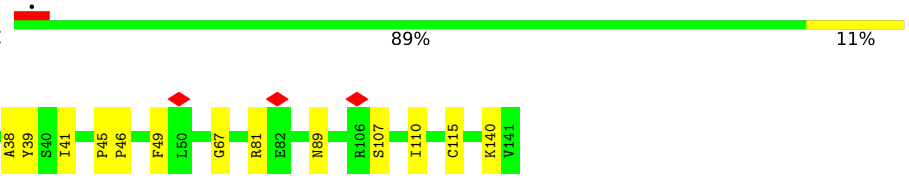
• Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain AK:



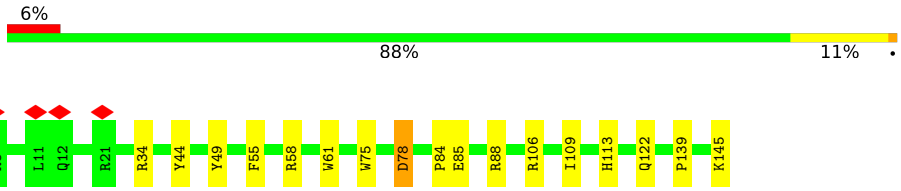
• Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain AL:



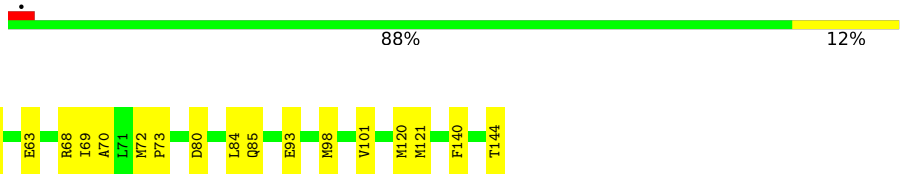
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AM:



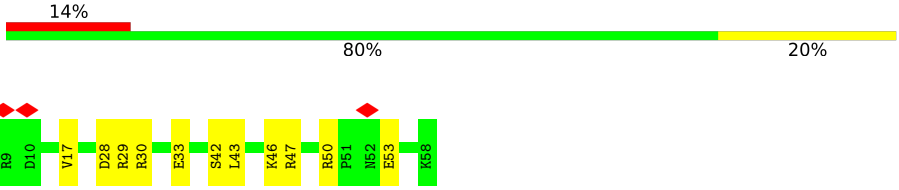
• Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain AN:



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

Chain B1:



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

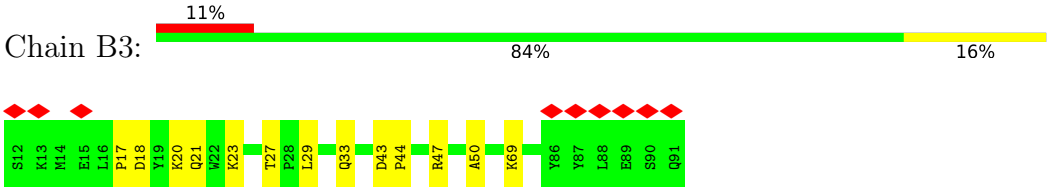
Chain B2:





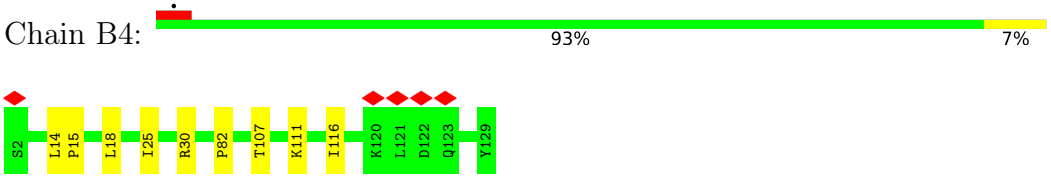
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain B3:



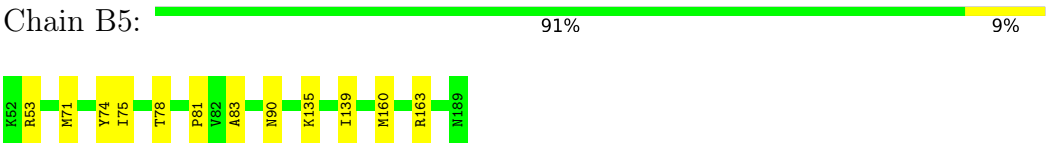
• Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain B4:



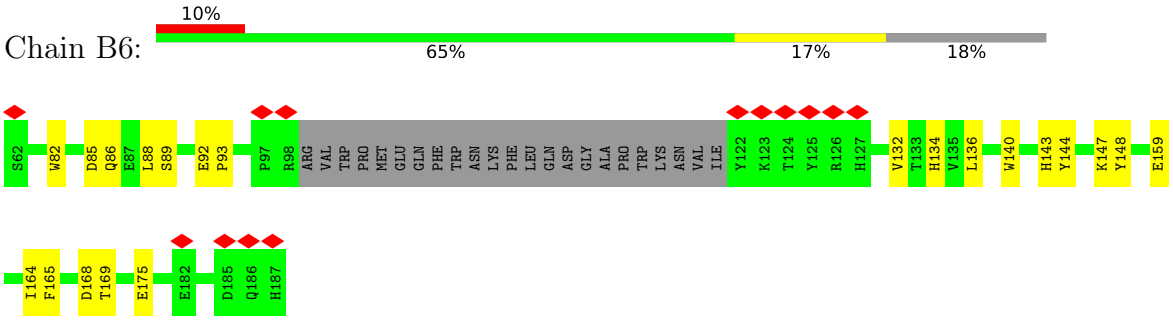
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain B5:



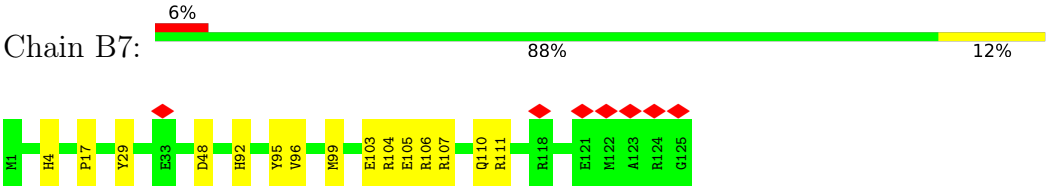
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain B6:



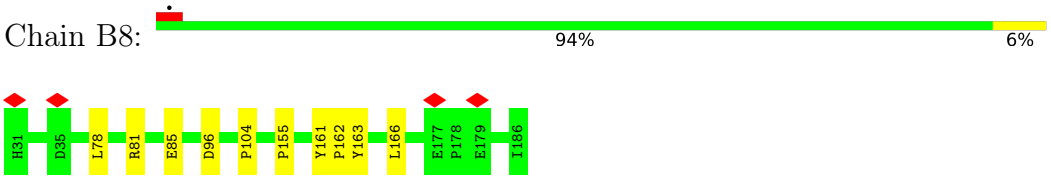
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain B7:



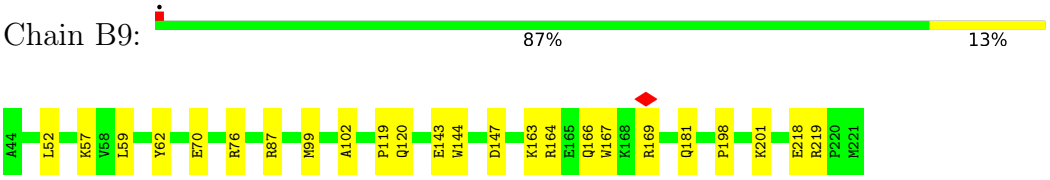
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain B8:



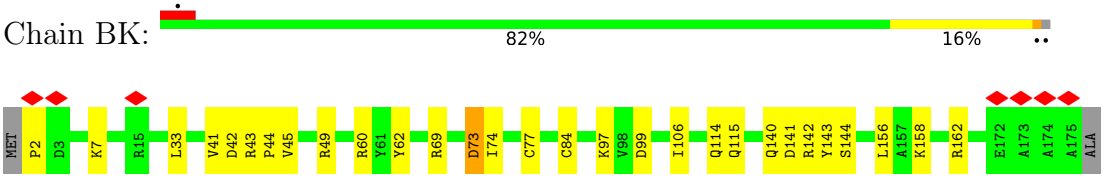
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain B9:



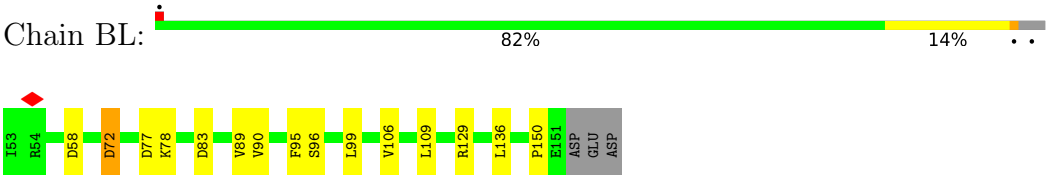
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain BK:



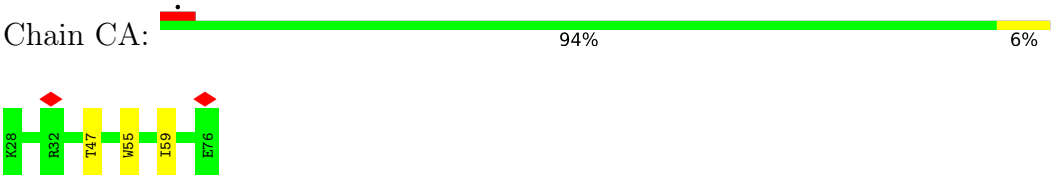
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain BL:



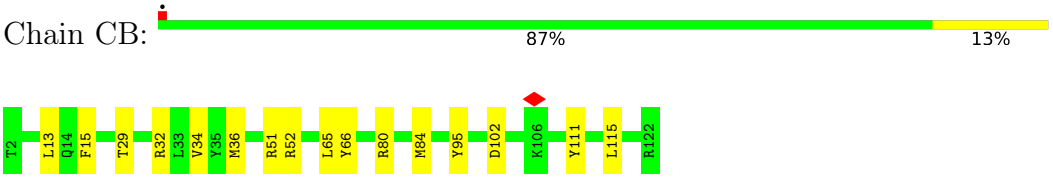
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain CA:



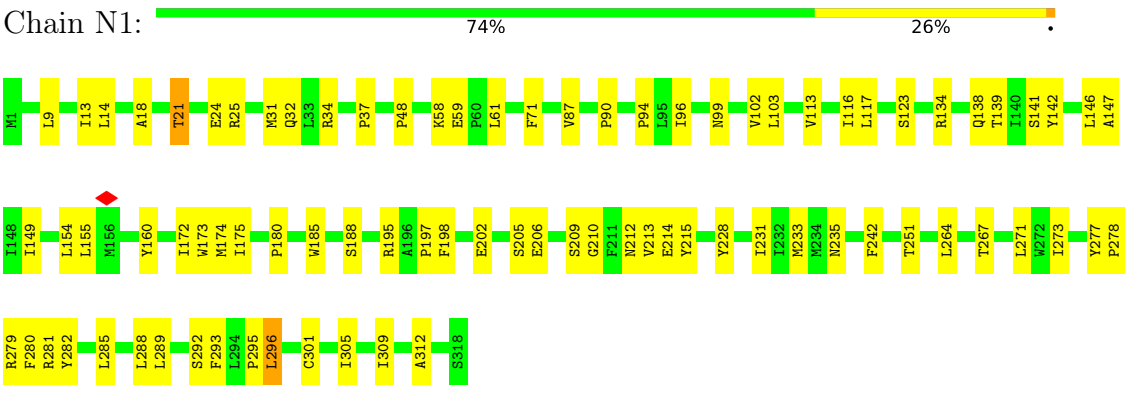
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain CB:



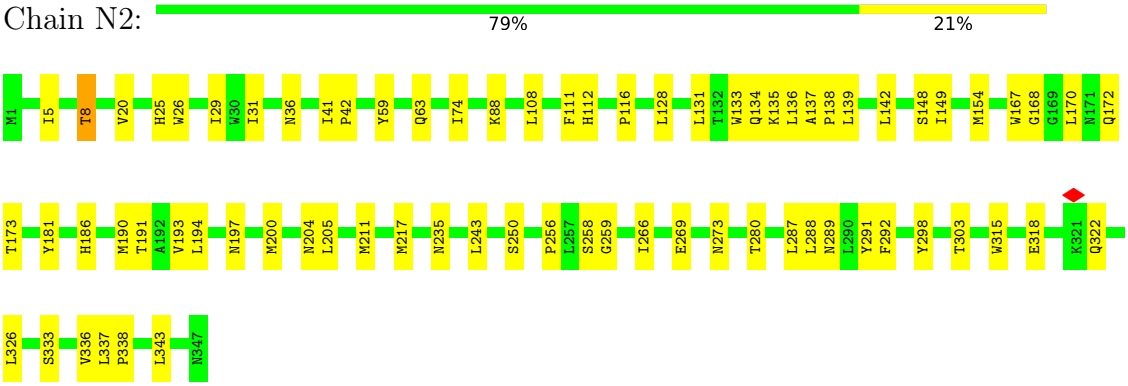
• Molecule 28: NADH-ubiquinone oxidoreductase chain 1

Chain N1:



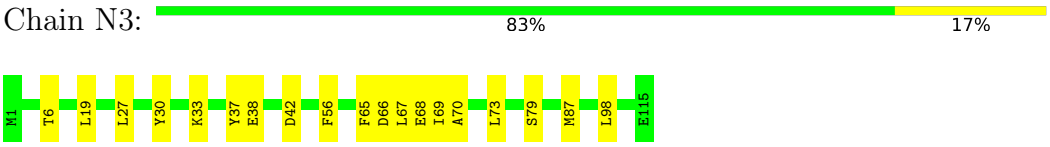
• Molecule 29: NADH-ubiquinone oxidoreductase chain 2

Chain N2:



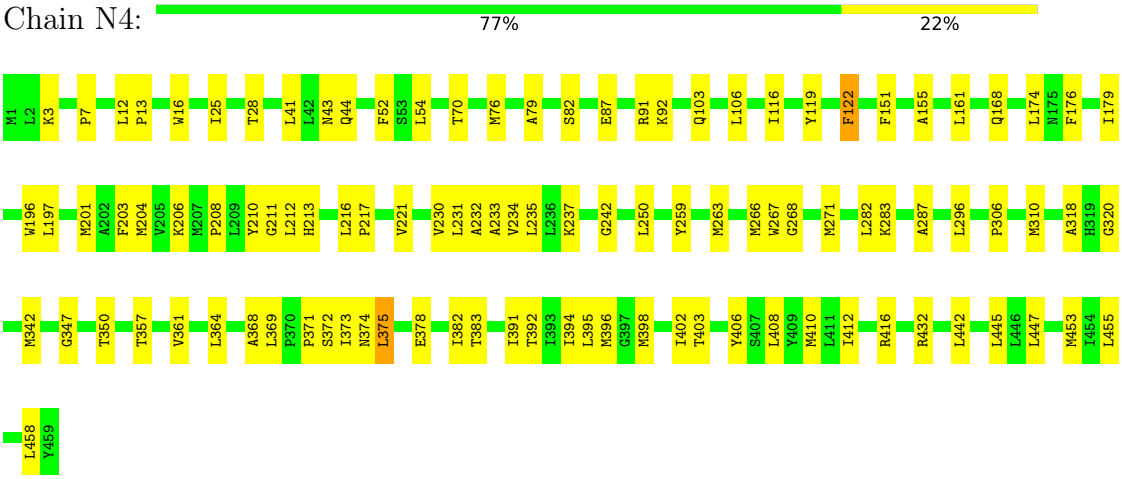
• Molecule 30: NADH-ubiquinone oxidoreductase chain 3

Chain N3:



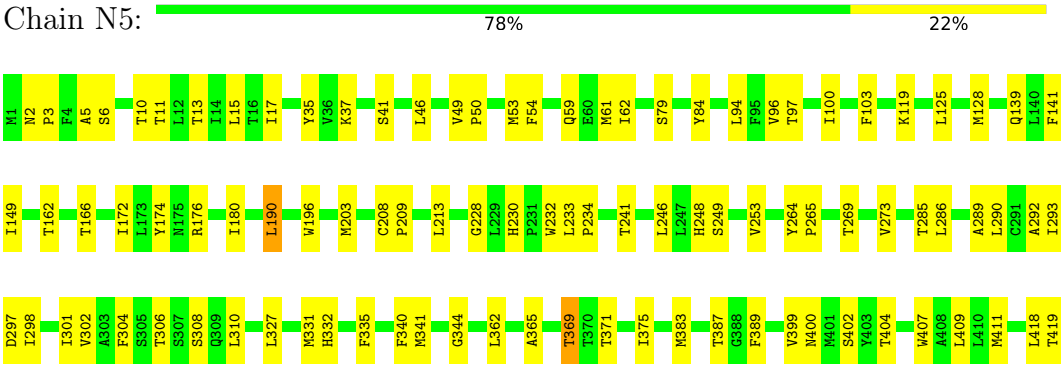
• Molecule 31: NADH-ubiquinone oxidoreductase chain 4

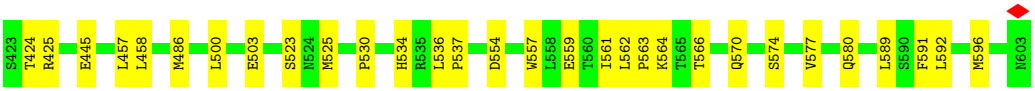
Chain N4:



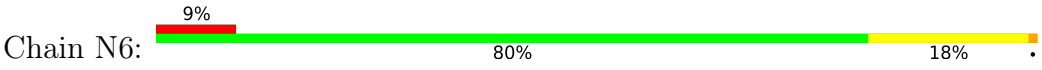
• Molecule 32: NADH-ubiquinone oxidoreductase chain 5

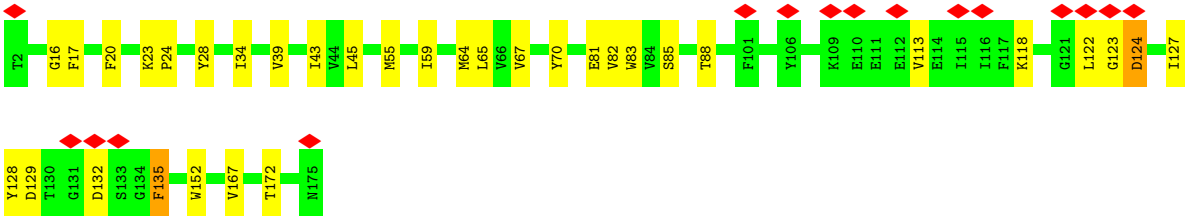
Chain N5:



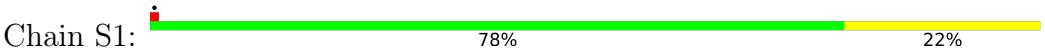


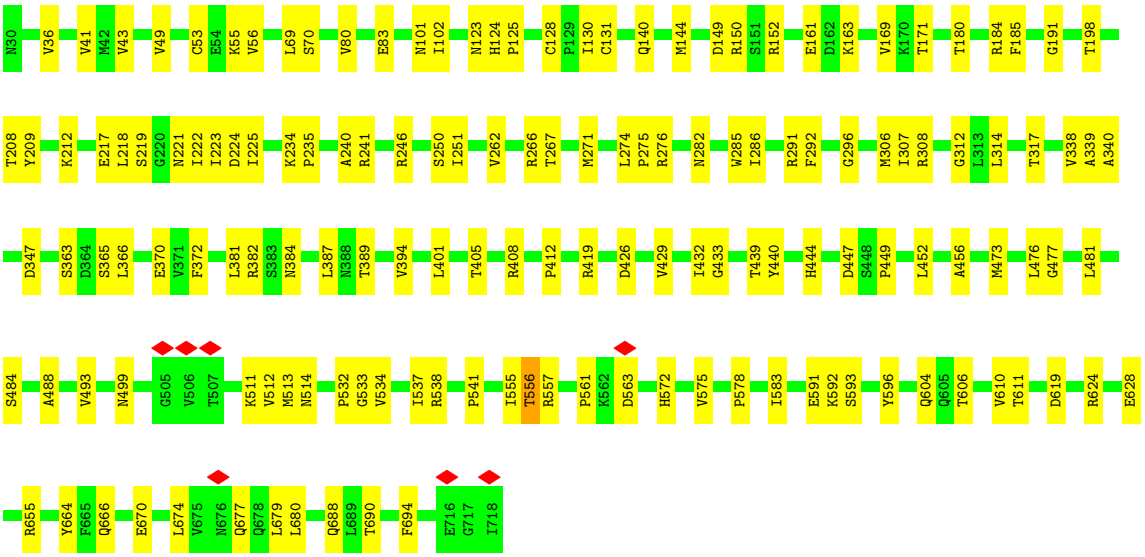
• Molecule 33: NADH-ubiquinone oxidoreductase chain 6



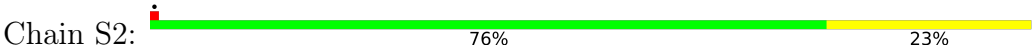


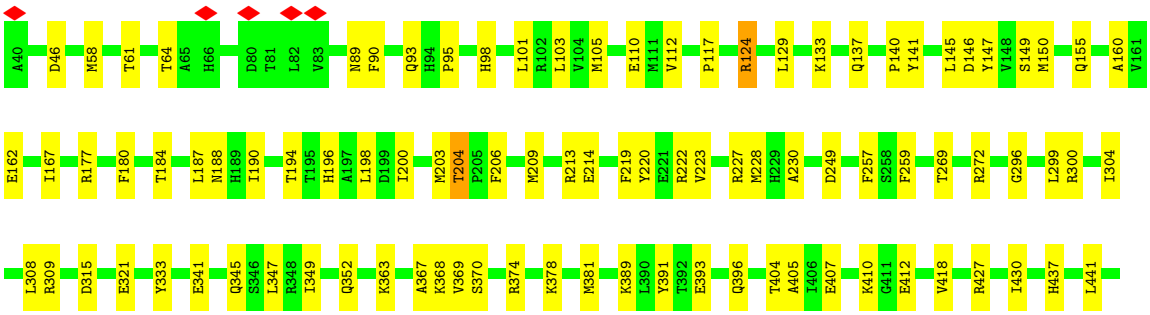
• Molecule 34: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial





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







• Molecule 36: Complex I-30kD

Chain S3:

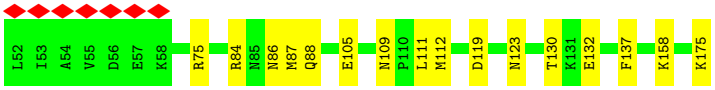




• Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain S4:





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

Chain S5:

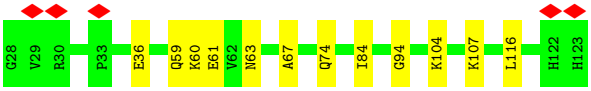




• Molecule 39: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain S6:

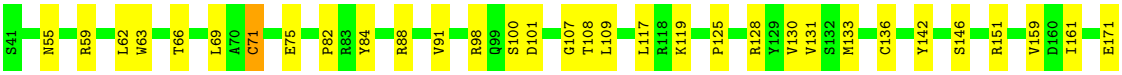


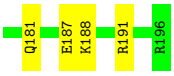


• Molecule 40: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain S7:



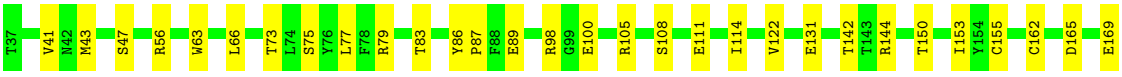


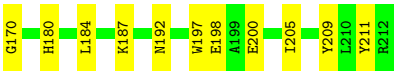


• Molecule 41: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain S8:





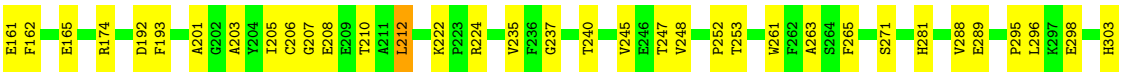


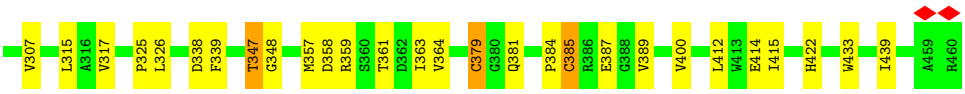
• Molecule 42: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain V1:





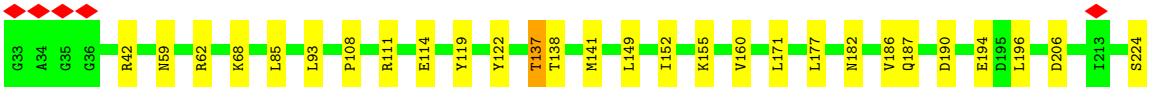




• Molecule 43: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain V2:







• Molecule 44: NADH:ubiquinone oxidoreductase subunit V3

Chain V3:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	269763	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 ($e^-/Å^2$)	51.9	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	47.538	Depositor
Minimum map value	-25.261	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	1.019	Depositor
Recommended contour level	4.62	Depositor
Map size (Å)	576.0, 576.0, 576.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	4L	0.14	0/759	0.30	0/1029
2	A1	0.14	0/577	0.34	0/777
3	A2	0.10	0/697	0.26	0/938
4	A3	0.10	0/664	0.23	0/912
5	A5	0.11	0/929	0.22	0/1258
6	A6	0.13	0/991	0.27	0/1335
7	A7	0.11	0/798	0.25	0/1079
8	A8	0.11	0/1436	0.25	0/1938
9	A9	0.12	0/2820	0.26	0/3823
10	AB	0.08	0/633	0.21	0/851
10	AC	0.12	0/714	0.22	0/965
11	AK	0.11	0/2661	0.27	0/3602
12	AL	0.12	0/1042	0.22	0/1411
13	AM	0.09	0/1245	0.23	0/1694
14	AN	0.13	0/1204	0.26	0/1624
15	B1	0.11	0/491	0.23	0/663
16	B2	0.11	0/610	0.23	0/836
17	B3	0.12	0/660	0.24	0/892
18	B4	0.12	0/1092	0.25	0/1481
19	B5	0.13	0/1184	0.29	0/1603
20	B6	0.14	0/910	0.32	0/1237
21	B7	0.11	0/1092	0.24	0/1459
22	B8	0.12	0/1371	0.25	0/1875
23	B9	0.12	0/1590	0.27	0/2155
24	BK	0.12	0/1489	0.24	0/2008
25	BL	0.13	0/851	0.27	0/1155
26	CA	0.12	0/430	0.23	0/581
27	CB	0.13	0/1031	0.25	0/1394
28	N1	0.17	0/2581	0.34	0/3529
29	N2	0.17	0/2773	0.33	0/3768
30	N3	0.15	0/938	0.27	0/1281
31	N4	0.16	0/3723	0.30	0/5078

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
32	N5	0.15	0/4914	0.33	0/6683
33	N6	0.14	0/1364	0.30	0/1850
34	S1	0.14	0/5378	0.30	0/7287
35	S2	0.16	0/3538	0.29	0/4796
36	S3	0.13	0/1789	0.27	0/2436
37	S4	0.12	0/1030	0.26	0/1391
38	S5	0.11	0/889	0.23	0/1190
39	S6	0.12	0/755	0.27	0/1018
40	S7	0.14	0/1279	0.28	0/1730
41	S8	0.14	0/1443	0.27	0/1952
42	V1	0.14	0/3391	0.30	0/4583
43	V2	0.12	0/1711	0.29	0/2328
44	V3	0.09	0/365	0.25	0/493
All	All	0.14	0/67832	0.28	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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4L	748	0	799	23	0
2	A1	562	0	557	7	0
3	A2	686	0	699	7	0
4	A3	643	0	642	7	0
5	A5	910	0	950	7	0
6	A6	967	0	972	11	0
7	A7	780	0	808	8	0
8	A8	1398	0	1372	20	0
9	A9	2743	0	2762	31	0
10	AB	624	0	625	8	0
10	AC	702	0	694	12	0
11	AK	2601	0	2566	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	AL	1021	0	1025	13	0
13	AM	1204	0	1162	18	0
14	AN	1173	0	1166	15	0
15	B1	479	0	486	8	0
16	B2	584	0	529	7	0
17	B3	641	0	620	9	0
18	B4	1062	0	1072	6	0
19	B5	1151	0	1164	11	0
20	B6	882	0	899	22	0
21	B7	1068	0	1043	13	0
22	B8	1315	0	1208	6	0
23	B9	1534	0	1470	17	0
24	BK	1456	0	1426	24	0
25	BL	828	0	788	12	0
26	CA	417	0	422	2	0
27	CB	1000	0	994	16	0
28	N1	2508	0	2607	70	0
29	N2	2710	0	2874	50	0
30	N3	914	0	951	21	0
31	N4	3631	0	3839	73	0
32	N5	4785	0	4933	86	0
33	N6	1329	0	1326	33	0
34	S1	5290	0	5321	99	0
35	S2	3459	0	3396	76	0
36	S3	1738	0	1693	18	0
37	S4	1007	0	1008	15	0
38	S5	867	0	871	11	0
39	S6	741	0	701	10	0
40	S7	1248	0	1254	31	0
41	S8	1412	0	1363	34	0
42	V1	3316	0	3272	62	0
43	V2	1671	0	1673	21	0
44	V3	355	0	329	11	0
45	4L	92	0	137	9	0
45	A7	51	0	46	1	0
45	A8	83	0	113	9	0
45	AK	68	0	80	3	0
45	AL	94	0	138	7	0
45	B4	80	0	107	3	0
45	B5	100	0	156	9	0
45	N1	78	0	103	5	0
45	N4	162	0	224	8	0

Continued on next page...

Continued from previous page...

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	N1	31	0	36	3	0
47	N3	51	0	82	4	0
47	N4	49	0	75	6	0
47	N5	137	0	205	9	0
47	S2	48	0	73	6	0
47	S8	51	0	82	8	0
48	A9	54	0	88	2	0
48	N1	48	0	73	2	0
49	AB	36	0	47	2	0
49	AC	36	0	47	2	0
50	AK	27	0	12	4	0
51	AL	47	0	75	1	0
51	AM	51	0	83	4	0
51	B1	52	0	88	2	0
51	CB	52	0	88	5	0
51	N4	49	0	79	6	0
51	N6	52	0	88	3	0
51	S7	52	0	88	5	0
52	B8	32	0	38	0	0
52	CA	51	0	82	2	0
52	CB	46	0	69	1	0
52	N5	46	0	69	1	0
52	S7	51	0	82	1	0
53	N1	63	0	90	10	0
54	S1	16	0	0	1	0
54	S7	8	0	0	0	0
54	S8	16	0	0	1	0
54	V1	8	0	0	0	0
55	S1	4	0	0	0	0
55	V2	4	0	0	0	0
56	S1	1	0	0	0	0
57	S2	9	0	0	0	0
58	S6	1	0	0	0	0
59	V1	31	0	19	1	0
All	All	68554	0	69655	965	0

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

The worst 5 of 965 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	1.73	0.88
49:AC:201:ZMP:H14	23:B9:102:ALA:HB1	1.65	0.78
34:S1:149:ASP:HB2	35:S2:367:ALA:HB3	1.64	0.77
35:S2:222:ARG:NH1	35:S2:249:ASP:OD2	2.19	0.76
20:B6:88:LEU:HD22	20:B6:92:GLU:HG2	1.68	0.76

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4L	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
2	A1	68/70 (97%)	68 (100%)	0	0	100	100
3	A2	83/85 (98%)	78 (94%)	5 (6%)	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	40
7	A7	93/112 (83%)	91 (98%)	2 (2%)	0	100	100
8	A8	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
9	A9	339/341 (99%)	330 (97%)	9 (3%)	0	100	100
10	AB	75/87 (86%)	75 (100%)	0	0	100	100
10	AC	85/87 (98%)	85 (100%)	0	0	100	100
11	AK	319/321 (99%)	309 (97%)	10 (3%)	0	100	100
12	AL	138/140 (99%)	138 (100%)	0	0	100	100
13	AM	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
14	AN	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
15	B1	54/56 (96%)	54 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	B2	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
17	B3	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
18	B4	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
19	B5	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
20	B6	99/126 (79%)	95 (96%)	4 (4%)	0	100	100
21	B7	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
22	B8	154/156 (99%)	151 (98%)	3 (2%)	0	100	100
23	B9	176/178 (99%)	173 (98%)	3 (2%)	0	100	100
24	BK	172/176 (98%)	169 (98%)	3 (2%)	0	100	100
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%)	117 (98%)	2 (2%)	0	100	100
28	N1	316/318 (99%)	307 (97%)	9 (3%)	0	100	100
29	N2	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
30	N3	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
31	N4	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
32	N5	601/603 (100%)	577 (96%)	24 (4%)	0	100	100
33	N6	172/174 (99%)	161 (94%)	11 (6%)	0	100	100
34	S1	687/689 (100%)	660 (96%)	27 (4%)	0	100	100
35	S2	427/430 (99%)	412 (96%)	15 (4%)	0	100	100
36	S3	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
37	S4	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
38	S5	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
39	S6	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
40	S7	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
41	S8	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
42	V1	429/431 (100%)	413 (96%)	16 (4%)	0	100	100
43	V2	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
44	V3	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
All	All	8151/8299 (98%)	7911 (97%)	239 (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 (i)

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%)	107 (100%)	0	100	100
7	A7	87/97 (90%)	85 (98%)	2 (2%)	44	74
8	A8	153/153 (100%)	153 (100%)	0	100	100
9	A9	295/295 (100%)	293 (99%)	2 (1%)	76	91
10	AB	71/80 (89%)	71 (100%)	0	100	100
10	AC	80/80 (100%)	79 (99%)	1 (1%)	61	84
11	AK	284/284 (100%)	281 (99%)	3 (1%)	65	86
12	AL	101/101 (100%)	100 (99%)	1 (1%)	68	87
13	AM	130/130 (100%)	129 (99%)	1 (1%)	73	89
14	AN	123/123 (100%)	123 (100%)	0	100	100
15	B1	53/53 (100%)	53 (100%)	0	100	100
16	B2	62/62 (100%)	62 (100%)	0	100	100
17	B3	62/62 (100%)	62 (100%)	0	100	100
18	B4	113/113 (100%)	113 (100%)	0	100	100
19	B5	121/121 (100%)	121 (100%)	0	100	100
20	B6	98/119 (82%)	98 (100%)	0	100	100
21	B7	112/112 (100%)	112 (100%)	0	100	100
22	B8	141/141 (100%)	141 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	B9	159/159 (100%)	159 (100%)	0	100 100
24	BK	155/156 (99%)	154 (99%)	1 (1%)	78 92
25	BL	91/94 (97%)	89 (98%)	2 (2%)	45 75
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%)	271 (98%)	4 (2%)	57 82
29	N2	311/311 (100%)	308 (99%)	3 (1%)	68 87
30	N3	100/100 (100%)	100 (100%)	0	100 100
31	N4	410/410 (100%)	408 (100%)	2 (0%)	81 93
32	N5	537/537 (100%)	530 (99%)	7 (1%)	61 84
33	N6	140/140 (100%)	137 (98%)	3 (2%)	47 76
34	S1	579/579 (100%)	575 (99%)	4 (1%)	76 91
35	S2	370/370 (100%)	369 (100%)	1 (0%)	86 95
36	S3	190/190 (100%)	189 (100%)	1 (0%)	81 93
37	S4	112/112 (100%)	111 (99%)	1 (1%)	70 88
38	S5	93/93 (100%)	93 (100%)	0	100 100
39	S6	79/79 (100%)	79 (100%)	0	100 100
40	S7	132/132 (100%)	131 (99%)	1 (1%)	73 89
41	S8	151/151 (100%)	149 (99%)	2 (1%)	61 84
42	V1	344/344 (100%)	339 (98%)	5 (2%)	57 82
43	V2	183/183 (100%)	181 (99%)	2 (1%)	65 86
44	V3	41/41 (100%)	41 (100%)	0	100 100
All	All	7185/7229 (99%)	7136 (99%)	49 (1%)	73 91

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	N5	554	ASP
34	S1	690	THR
33	N6	45	LEU
34	S1	41	VAL
36	S3	145	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
42	V1	277	ASN
42	V1	456	GLN
24	BK	107	GLN
24	BK	55	GLN
43	V2	87	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	2.43	2 (20%)	5,13,15	0.95	0

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S2	124	2MR	CZ-NE	5.14	1.45	1.34
35	S2	124	2MR	CZ-NH2	5.07	1.44	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	$\#\|Z\| > 2$
54	SF4	S1	801	34	0,12,12	-	-	-		
48	PC1	N1	402	-	47,47,53	0.30	0	53,55,61	0.31	0
54	SF4	S1	802	34	0,12,12	-	-	-		
47	PEE	N5	705	-	50,50,50	1.32	5 (10%)	53,55,55	1.16	4 (7%)
57	MF8	S2	502	-	7,8,8	0.87	0	7,10,10	1.44	1 (14%)
55	FES	S1	803	34	0,4,4	-	-	-		
52	3PE	B8	201	-	31,31,50	0.37	0	34,36,55	0.35	0
53	U10	N1	403	-	63,63,63	2.16	21 (33%)	76,79,79	1.68	21 (27%)
50	ADP	AK	401	-	27,29,29	1.35	4 (14%)	42,45,45	1.94	10 (23%)
47	PEE	N5	702	-	39,39,50	1.49	5 (12%)	41,44,55	1.23	3 (7%)
45	CDL	N5	703	-	88,88,99	0.31	0	94,100,111	0.31	0
54	SF4	V1	501	42	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	PEE	A9	402	-	38,38,50	1.49	5 (13%)	41,43,55	1.24	3 (7%)
51	PLX	AL	202	-	46,46,51	1.15	4 (8%)	50,54,59	0.87	1 (2%)
52	3PE	S7	303	-	50,50,50	0.31	0	53,55,55	0.46	0
45	CDL	N1	401	-	77,77,99	0.34	0	83,89,111	0.30	0
47	PEE	N5	701	-	45,45,50	1.39	5 (11%)	48,50,55	1.18	4 (8%)
52	3PE	N5	706	-	45,45,50	0.32	0	48,50,55	0.28	0
51	PLX	B1	101	-	51,51,51	1.11	4 (7%)	55,59,59	0.89	1 (1%)
52	3PE	CA	101	-	50,50,50	0.31	0	53,55,55	0.29	0
55	FES	V2	301	43	0,4,4	-	-	-		
59	FMN	V1	502	-	33,33,33	0.23	0	48,50,50	0.40	0
46	NDP	A9	401	-	49,52,52	0.33	0	66,80,80	0.33	0
47	PEE	S8	303	-	50,50,50	1.32	5 (10%)	53,55,55	1.22	3 (5%)
49	ZMP	AC	201	10	29,35,36	0.64	1 (3%)	34,42,45	0.70	0
49	ZMP	AB	201	10	29,35,36	0.65	1 (3%)	34,42,45	0.74	0
45	CDL	N4	503	-	99,99,99	0.29	0	105,111,111	0.28	0
51	PLX	N6	201	-	51,51,51	1.11	4 (7%)	55,59,59	0.86	1 (1%)
52	3PE	CB	202	-	45,45,50	0.32	0	48,50,55	0.30	0
45	CDL	B5	201	-	99,99,99	0.30	0	105,111,111	0.31	0
54	SF4	S8	301	41	0,12,12	-	-	-		
45	CDL	A7	201	-	50,50,99	0.40	0	56,62,111	0.33	0
47	PEE	N1	404	-	30,30,50	1.28	3 (10%)	33,35,55	1.18	2 (6%)
48	PC1	A9	403	-	53,53,53	0.30	0	59,61,61	0.31	0
47	PEE	N4	501	-	48,48,50	1.34	5 (10%)	51,53,55	1.21	4 (7%)
51	PLX	CB	201	-	51,51,51	1.10	3 (5%)	55,59,59	0.89	1 (1%)
45	CDL	N4	504	-	61,61,99	0.37	0	67,73,111	0.35	0
51	PLX	S7	302	-	51,51,51	1.10	3 (5%)	55,59,59	0.88	1 (1%)
45	CDL	AK	402	-	67,67,99	0.36	0	73,79,111	0.38	0
54	SF4	S8	302	41	0,12,12	-	-	-		
47	PEE	S2	501	-	47,47,50	1.35	5 (10%)	50,52,55	1.19	3 (6%)
45	CDL	AL	201	-	93,93,99	0.31	0	99,105,111	0.31	0
51	PLX	N4	502	-	48,48,51	1.13	4 (8%)	52,56,59	0.88	1 (1%)
45	CDL	N5	704	-	99,99,99	0.30	0	105,111,111	0.28	0
51	PLX	AM	201	-	50,50,51	1.11	4 (8%)	54,58,59	0.86	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	0.32	0	88,94,111	0.33	0
45	CDL	B4	201	-	79,79,99	0.33	0	85,91,111	0.29	0
54	SF4	S7	301	40	0,12,12	-	-	-		
47	PEE	N3	201	-	50,50,50	1.32	5 (10%)	53,55,55	1.15	4 (7%)

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
54	SF4	S1	801	34	-	-	0/6/5/5
48	PC1	N1	402	-	-	14/51/51/57	-
54	SF4	S1	802	34	-	-	0/6/5/5
47	PEE	N5	705	-	-	20/54/54/54	-
57	MF8	S2	502	-	-	5/8/8/8	-
55	FES	S1	803	34	-	-	0/1/1/1
52	3PE	B8	201	-	-	8/35/35/54	-
53	U10	N1	403	-	-	18/63/87/87	0/1/1/1
50	ADP	AK	401	-	-	5/16/32/32	0/3/3/3
47	PEE	N5	702	-	-	22/43/43/54	-
45	CDL	N5	703	-	-	28/99/99/110	-
54	SF4	V1	501	42	-	-	0/6/5/5
47	PEE	A9	402	-	-	27/42/42/54	-
51	PLX	AL	202	-	-	21/50/50/55	-
52	3PE	S7	303	-	-	11/54/54/54	-
45	CDL	N1	401	-	-	16/88/88/110	-
47	PEE	N5	701	-	-	26/49/49/54	-
52	3PE	N5	706	-	-	8/49/49/54	-
51	PLX	B1	101	-	-	17/55/55/55	-
52	3PE	CA	101	-	-	11/54/54/54	-
55	FES	V2	301	43	-	-	0/1/1/1
59	FMN	V1	502	-	-	0/18/18/18	0/3/3/3
46	NDP	A9	401	-	-	5/34/77/77	0/5/5/5
47	PEE	S8	303	-	-	27/54/54/54	-
49	ZMP	AC	201	10	-	20/40/42/43	-
49	ZMP	AB	201	10	-	11/40/42/43	-
45	CDL	N4	503	-	-	26/110/110/110	-
51	PLX	N6	201	-	-	23/55/55/55	-
52	3PE	CB	202	-	-	10/49/49/54	-
45	CDL	B5	201	-	-	24/110/110/110	-
54	SF4	S8	301	41	-	-	0/6/5/5
45	CDL	A7	201	-	-	8/61/61/110	-
47	PEE	N1	404	-	-	20/34/34/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PC1	A9	403	-	-	15/57/57/57	-
47	PEE	N4	501	-	-	32/52/52/54	-
51	PLX	CB	201	-	-	26/55/55/55	-
45	CDL	N4	504	-	-	21/72/72/110	-
51	PLX	S7	302	-	-	24/55/55/55	-
45	CDL	AK	402	-	-	14/78/78/110	-
54	SF4	S8	302	41	-	-	0/6/5/5
47	PEE	S2	501	-	-	33/51/51/54	-
45	CDL	AL	201	-	-	25/104/104/110	-
51	PLX	N4	502	-	-	19/52/52/55	-
45	CDL	N5	704	-	-	20/110/110/110	-
51	PLX	AM	201	-	-	24/54/54/55	-
45	CDL	4L	201	-	-	19/102/102/110	-
45	CDL	A8	301	-	-	25/93/93/110	-
45	CDL	B4	201	-	-	20/90/90/110	-
54	SF4	S7	301	40	-	-	0/6/5/5
47	PEE	N3	201	-	-	25/54/54/54	-

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	N1	403	U10	C6-C1	10.28	1.54	1.35
50	AK	401	ADP	C5-C4	4.44	1.47	1.39
53	N1	403	U10	C4-C3	4.26	1.53	1.36
47	N5	705	PEE	C18-C19	4.05	1.55	1.31
47	N3	201	PEE	C18-C19	4.05	1.55	1.31

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	AK	401	ADP	C5-C4-N3	-6.19	118.67	126.75
50	AK	401	ADP	N3-C4-N9	4.88	135.12	127.08
47	S8	303	PEE	O2-C10-C11	4.62	121.46	111.50
53	N1	403	U10	C7-C8-C9	-4.32	119.60	126.79
47	N5	702	PEE	O2-C10-C11	4.14	120.42	111.50

There are no chirality outliers.

5 of 773 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	CA3-OA5-PA1-OA3
45	4L	201	CDL	CB2-OB2-PB2-OB4
45	A7	201	CDL	CB3-OB5-PB2-OB4

There are no ring outliers.

42 monomers are involved in 148 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	N1	402	PC1	2	0
54	S1	802	SF4	1	0
47	N5	705	PEE	3	0
53	N1	403	U10	10	0
50	AK	401	ADP	4	0
47	N5	702	PEE	1	0
45	N5	703	CDL	8	0
47	A9	402	PEE	4	0
51	AL	202	PLX	1	0
52	S7	303	3PE	1	0
45	N1	401	CDL	5	0
47	N5	701	PEE	5	0
52	N5	706	3PE	1	0
51	B1	101	PLX	2	0
52	CA	101	3PE	2	0
59	V1	502	FMN	1	0
46	A9	401	NDP	1	0
47	S8	303	PEE	8	0
49	AC	201	ZMP	2	0
49	AB	201	ZMP	2	0
45	N4	503	CDL	6	0
51	N6	201	PLX	3	0
52	CB	202	3PE	1	0
45	B5	201	CDL	9	0
45	A7	201	CDL	1	0
47	N1	404	PEE	3	0
48	A9	403	PC1	2	0
47	N4	501	PEE	6	0
51	CB	201	PLX	5	0
45	N4	504	CDL	2	0
51	S7	302	PLX	5	0
45	AK	402	CDL	3	0
54	S8	302	SF4	1	0

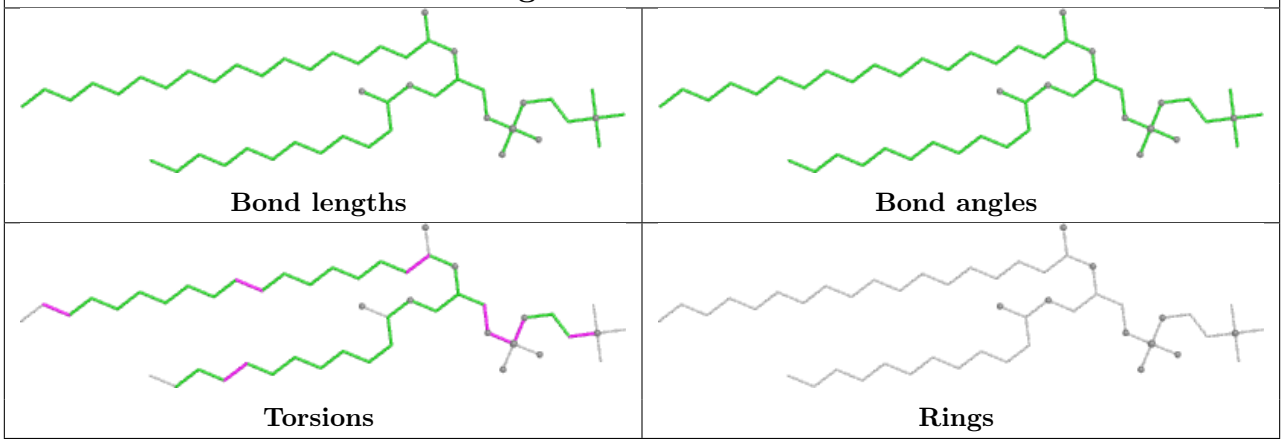
Continued on next page...

Continued from previous page...

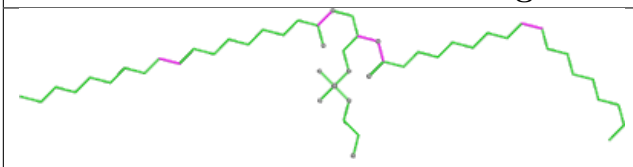
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	S2	501	PEE	6	0
45	AL	201	CDL	7	0
51	N4	502	PLX	6	0
45	N5	704	CDL	2	0
51	AM	201	PLX	4	0
45	4L	201	CDL	9	0
45	A8	301	CDL	9	0
45	B4	201	CDL	3	0
47	N3	201	PEE	4	0

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

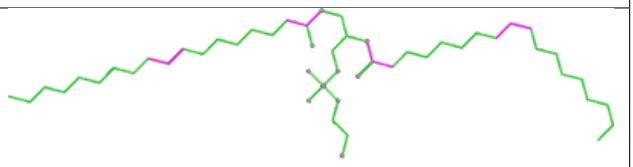
Ligand PC1 N1 402



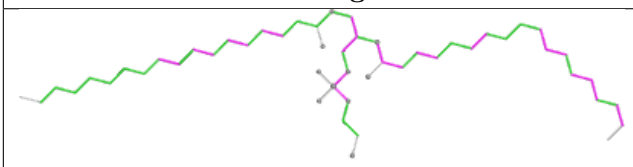
Ligand PEE N5 705



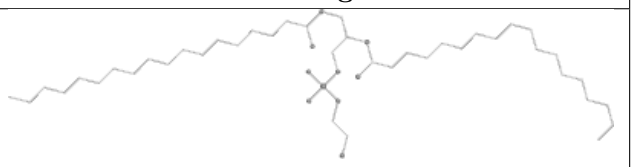
Bond lengths



Bond angles

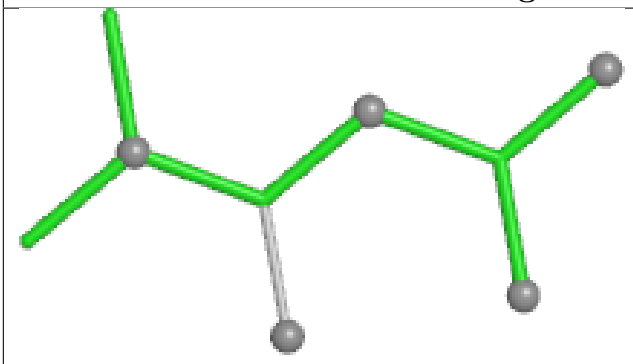


Torsions

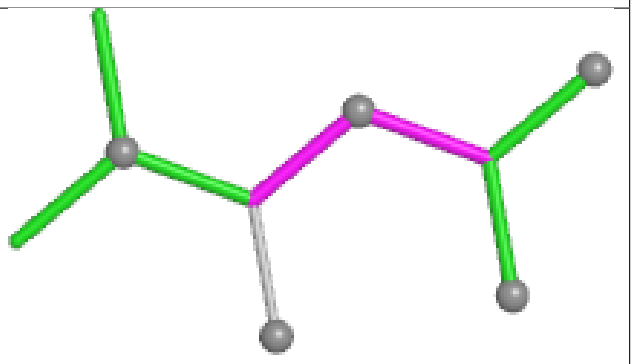


Rings

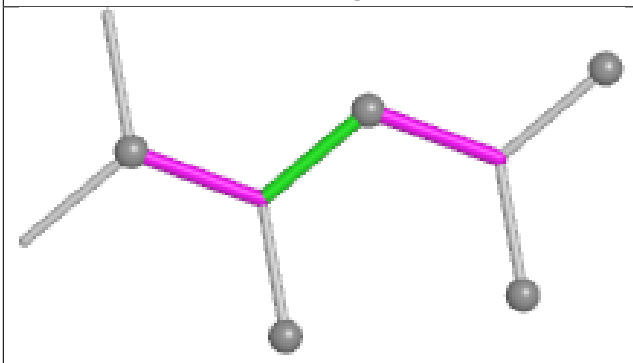
Ligand MF8 S2 502



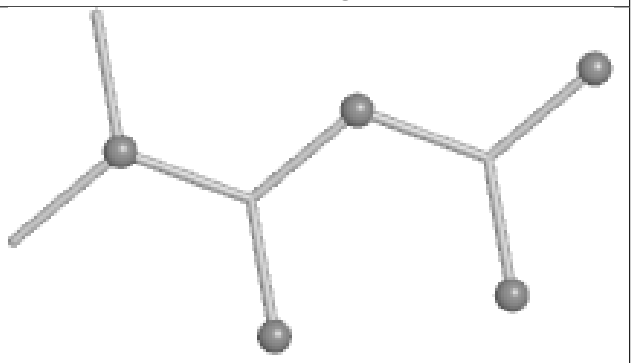
Bond lengths



Bond angles

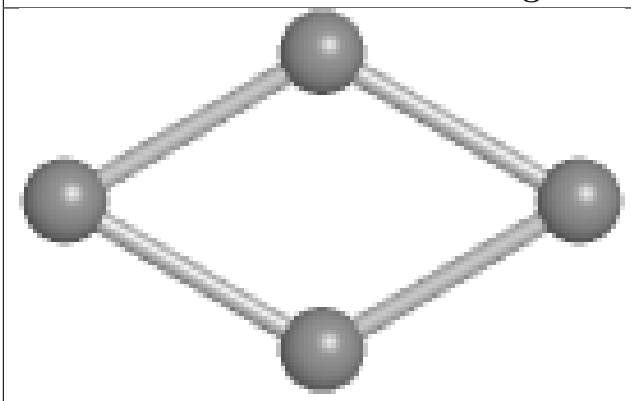


Torsions

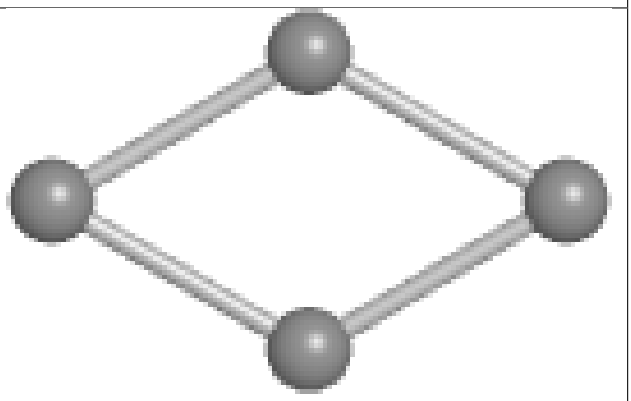


Rings

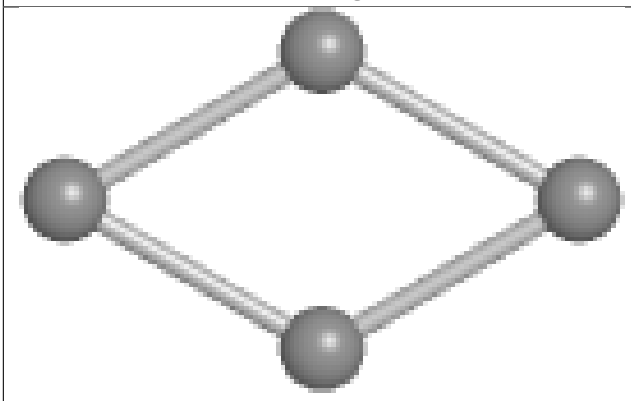
Ligand FES S1 803



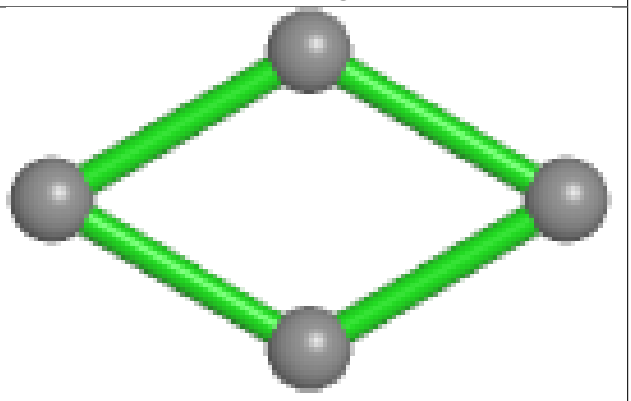
Bond lengths



Bond angles

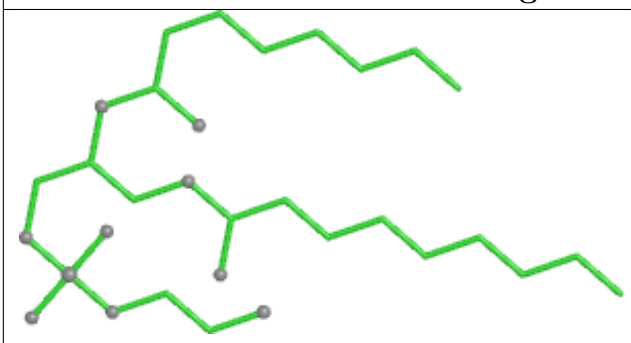


Torsions

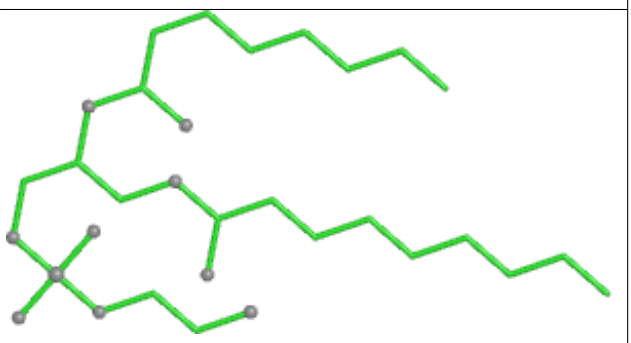


Rings

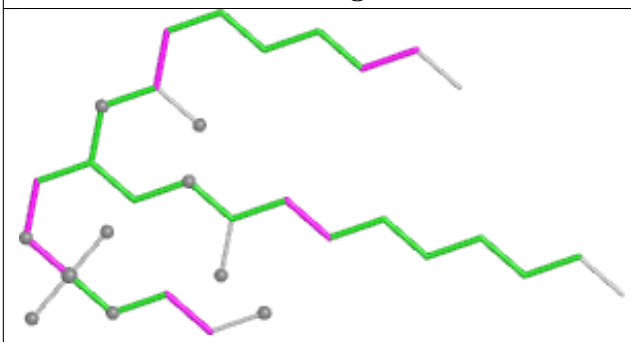
Ligand 3PE B8 201



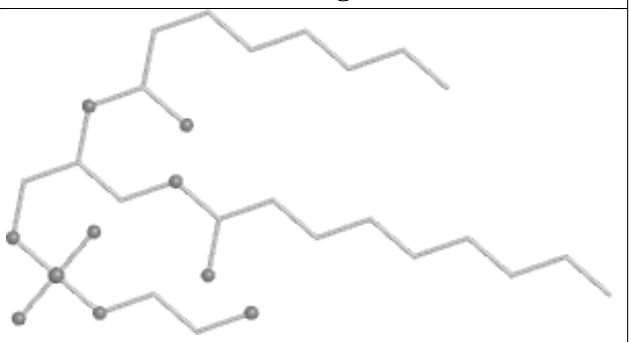
Bond lengths



Bond angles

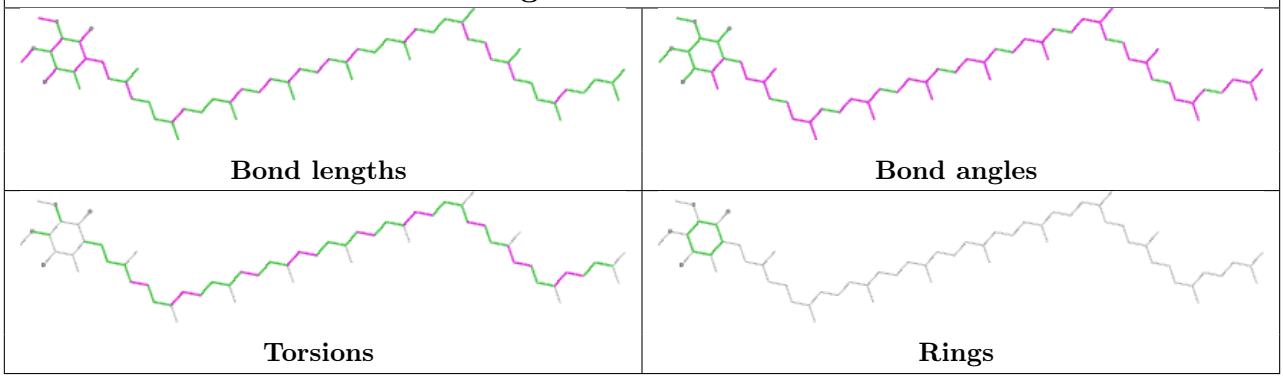


Torsions

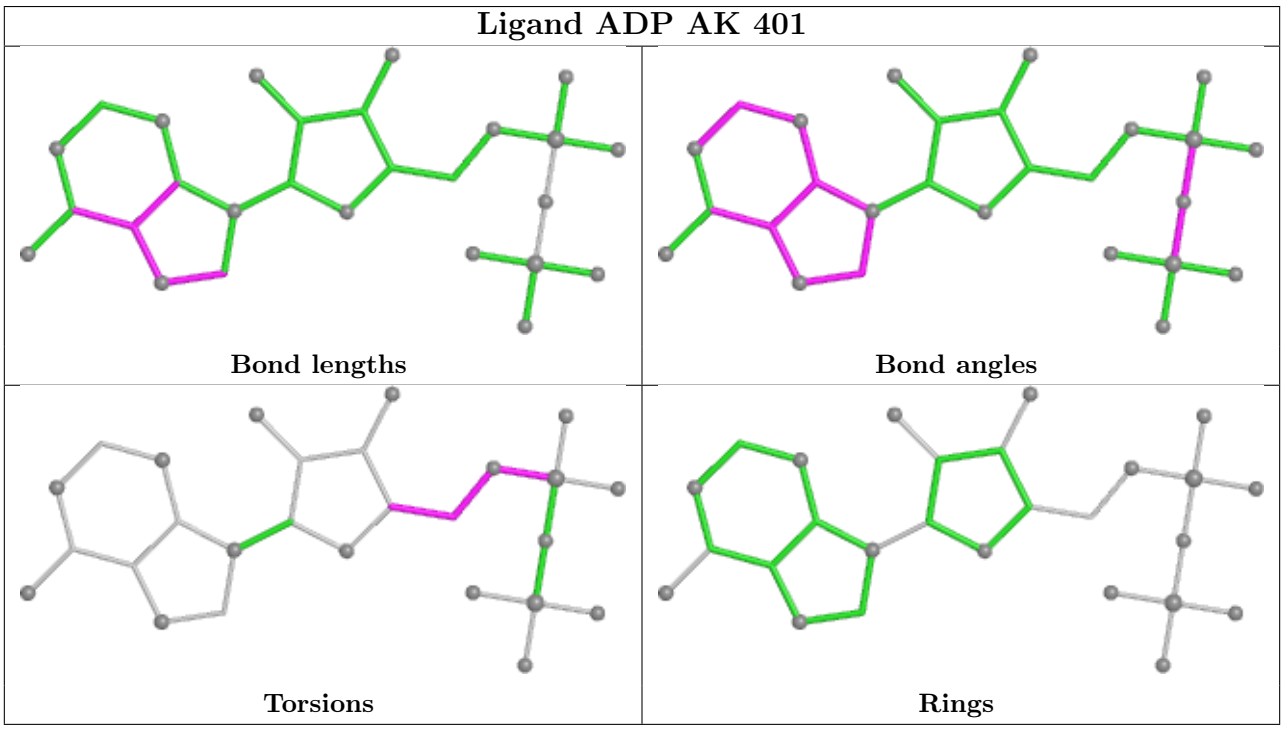


Rings

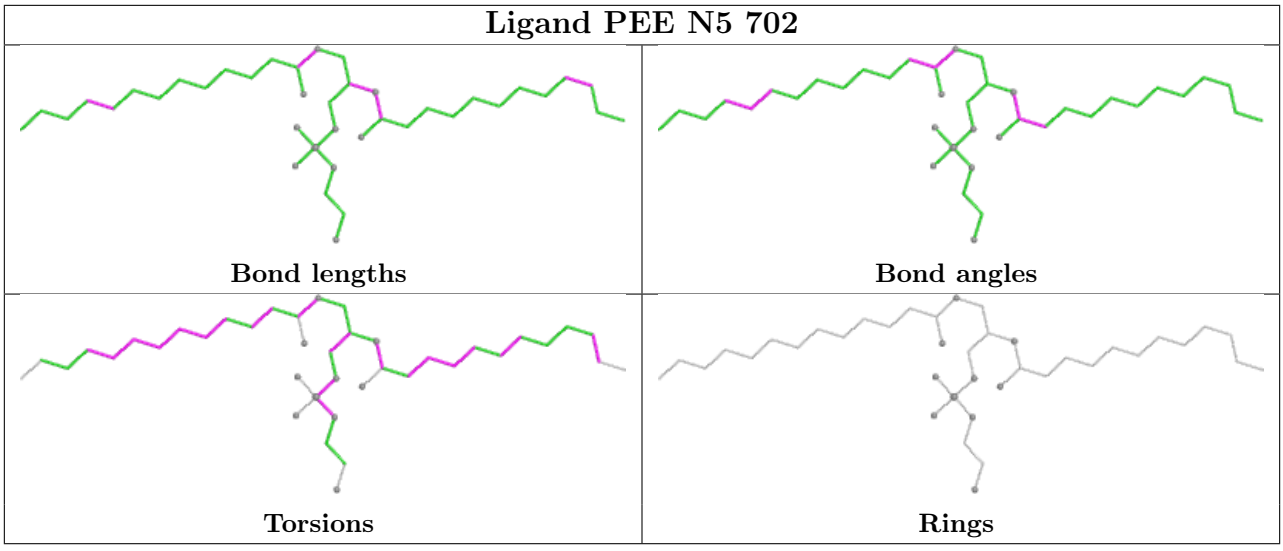
Ligand U10 N1 403



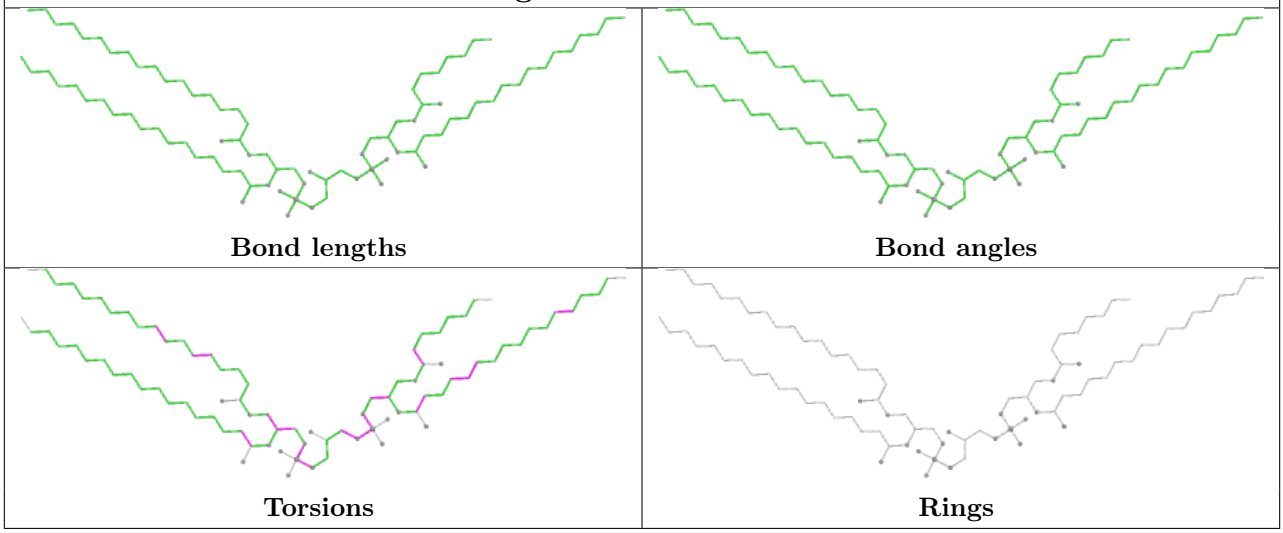
Ligand ADP AK 401



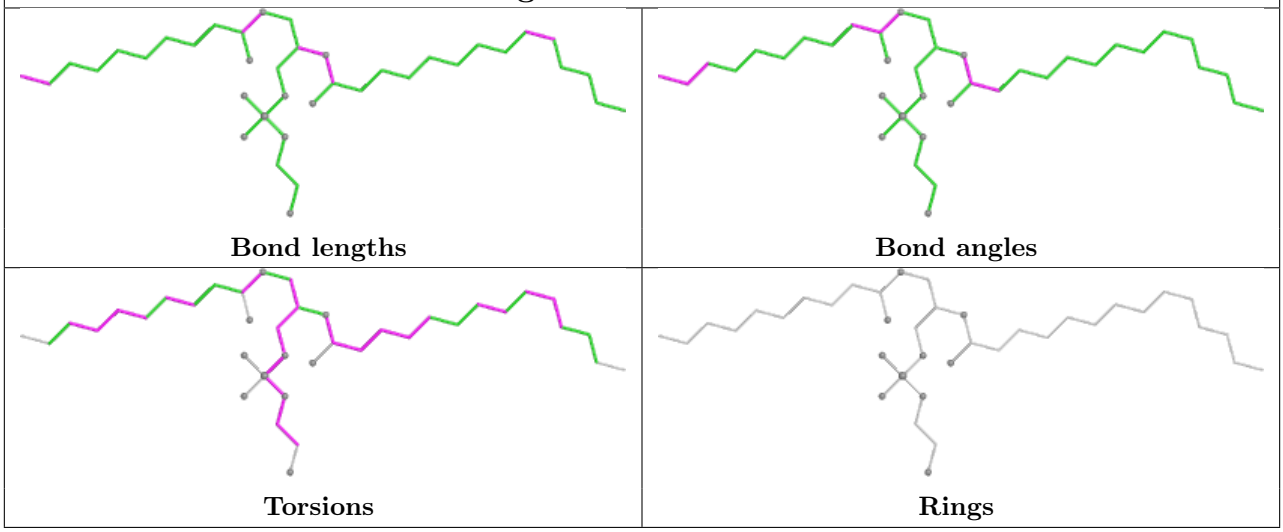
Ligand PEE N5 702



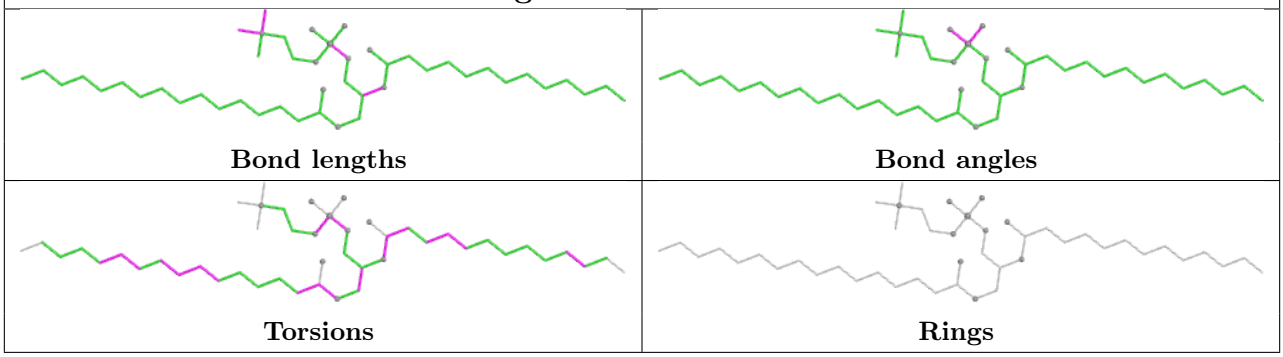
Ligand CDL N5 703



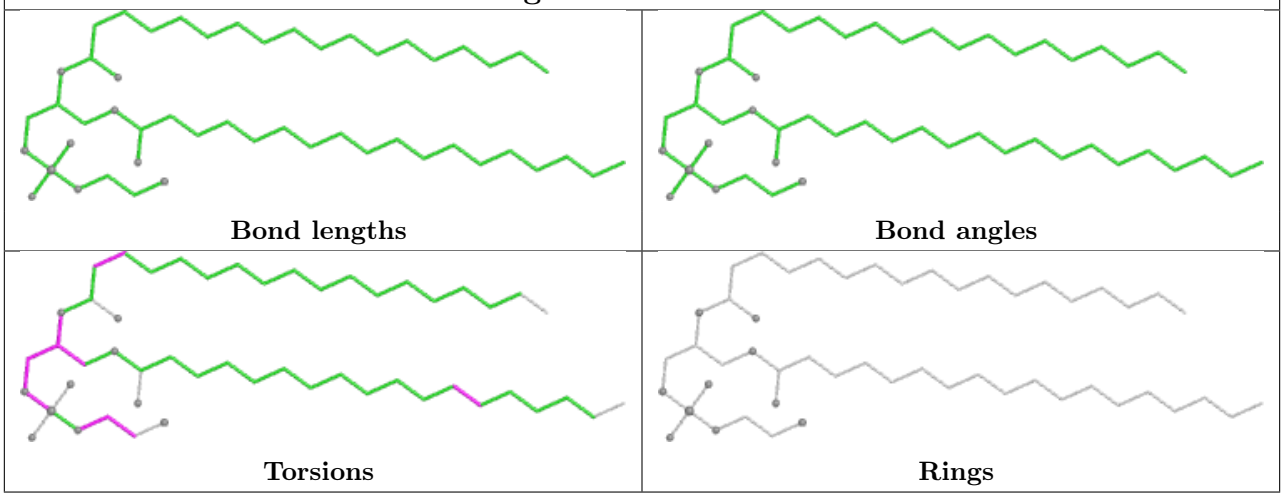
Ligand PEE A9 402



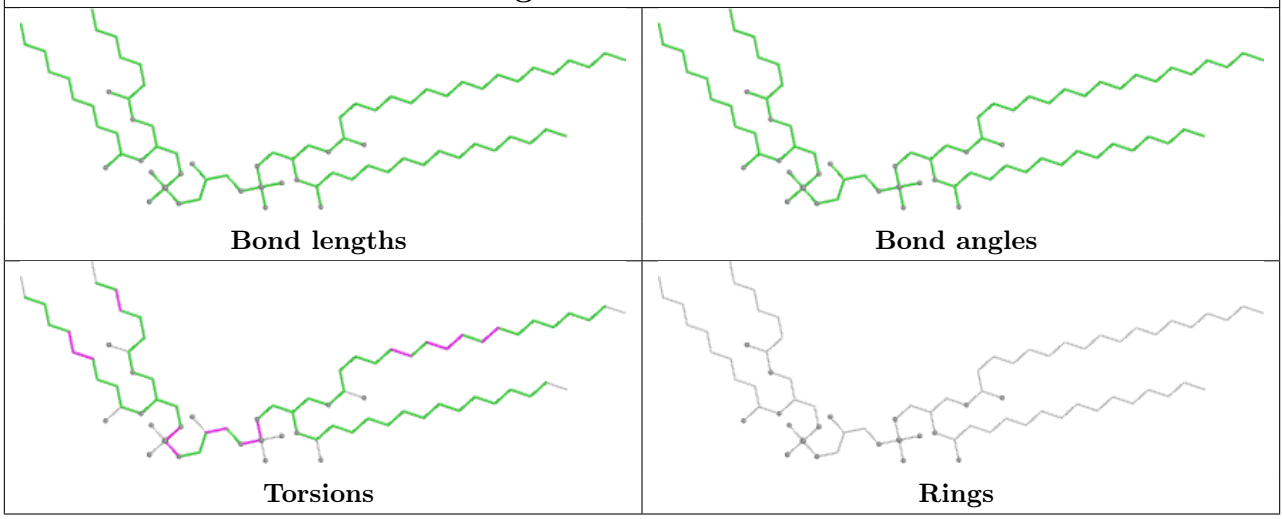
Ligand PLX AL 202



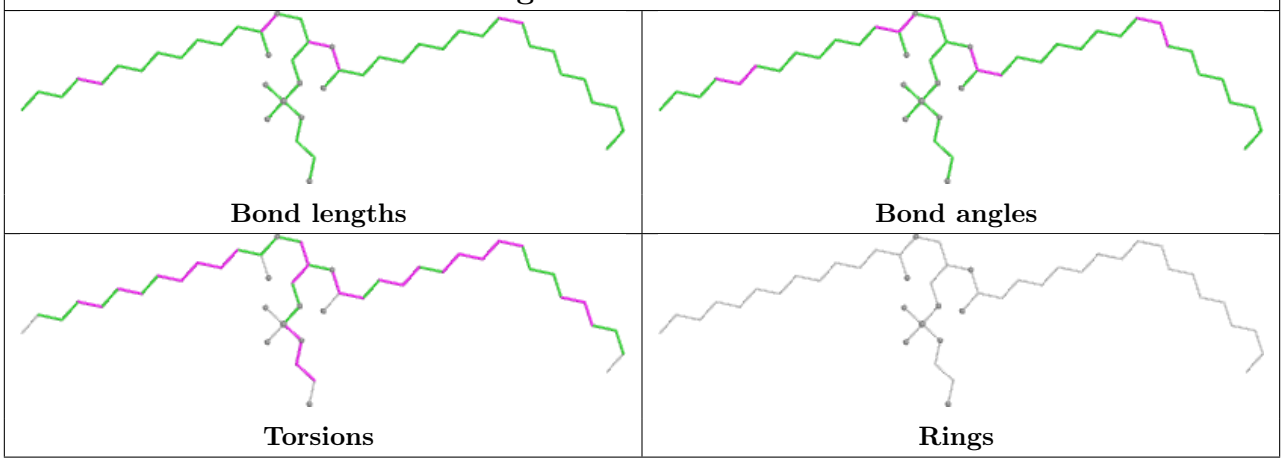
Ligand 3PE S7 303



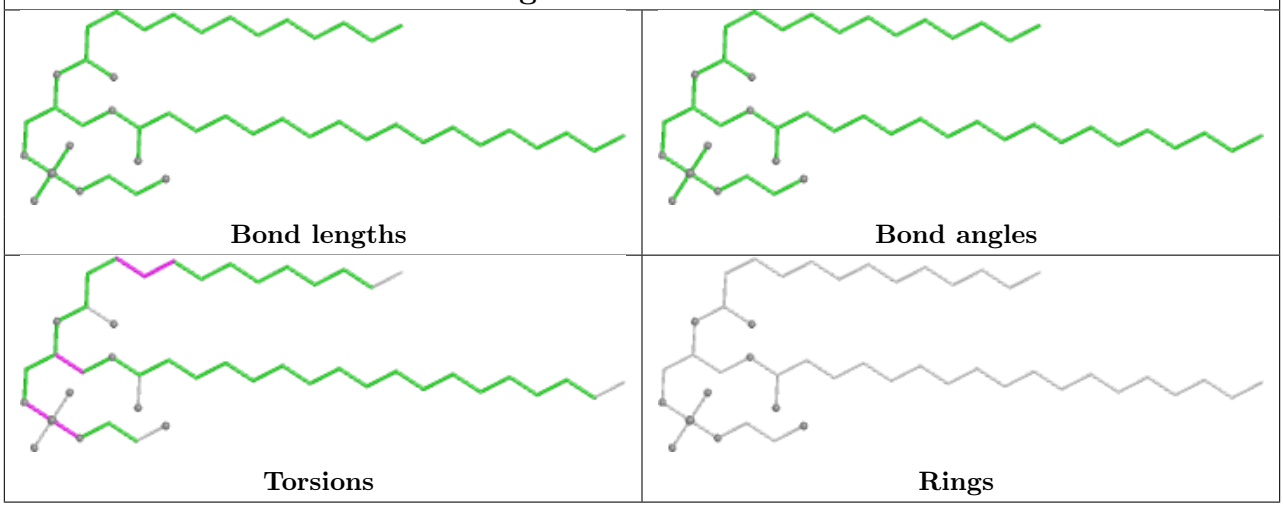
Ligand CDL N1 401



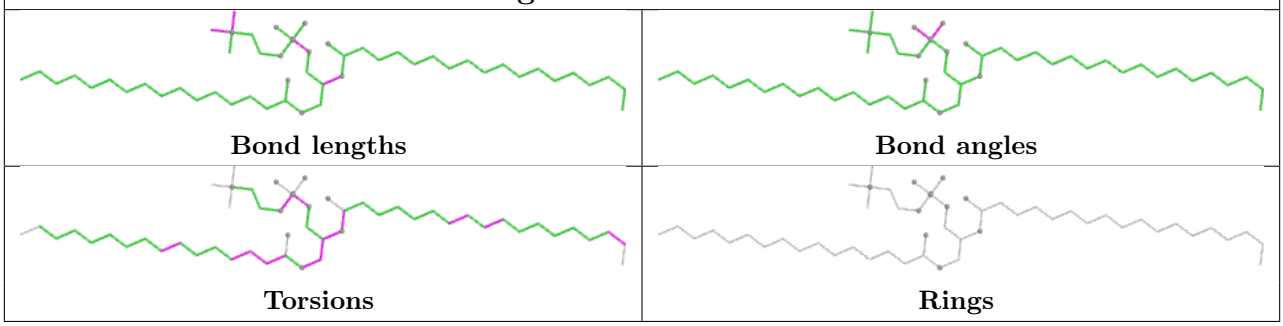
Ligand PEE N5 701



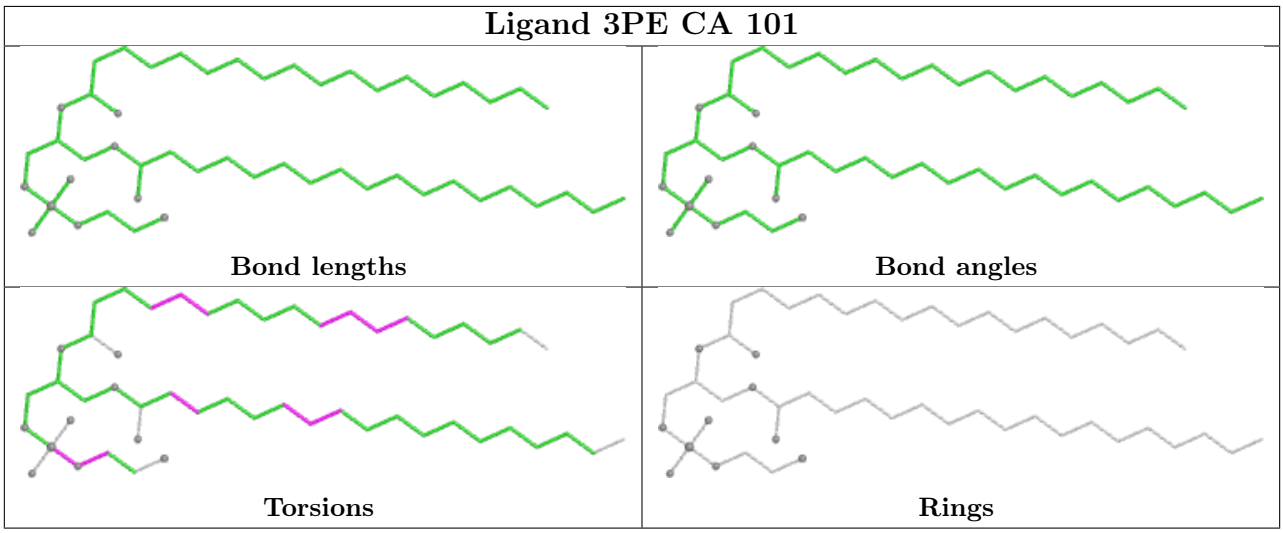
Ligand 3PE N5 706



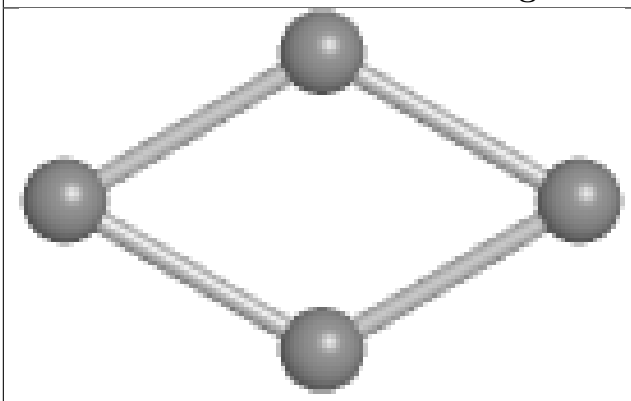
Ligand PLX B1 101



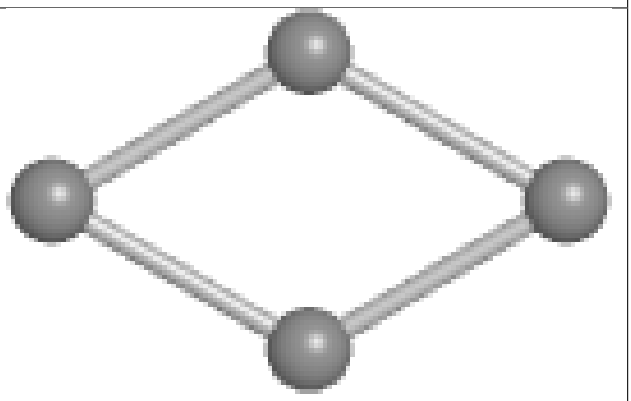
Ligand 3PE CA 101



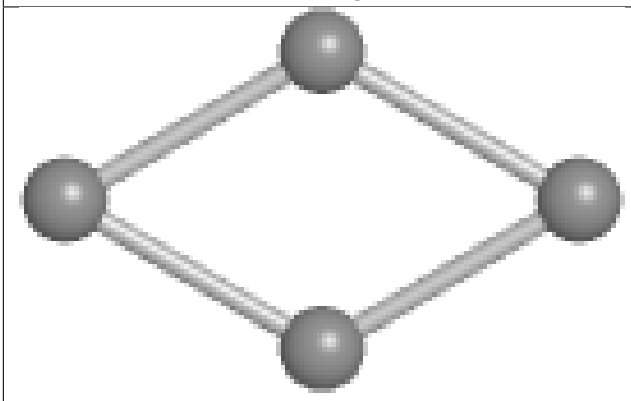
Ligand FES V2 301



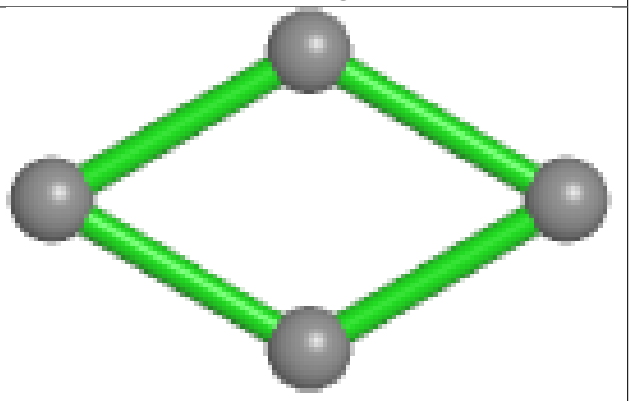
Bond lengths



Bond angles

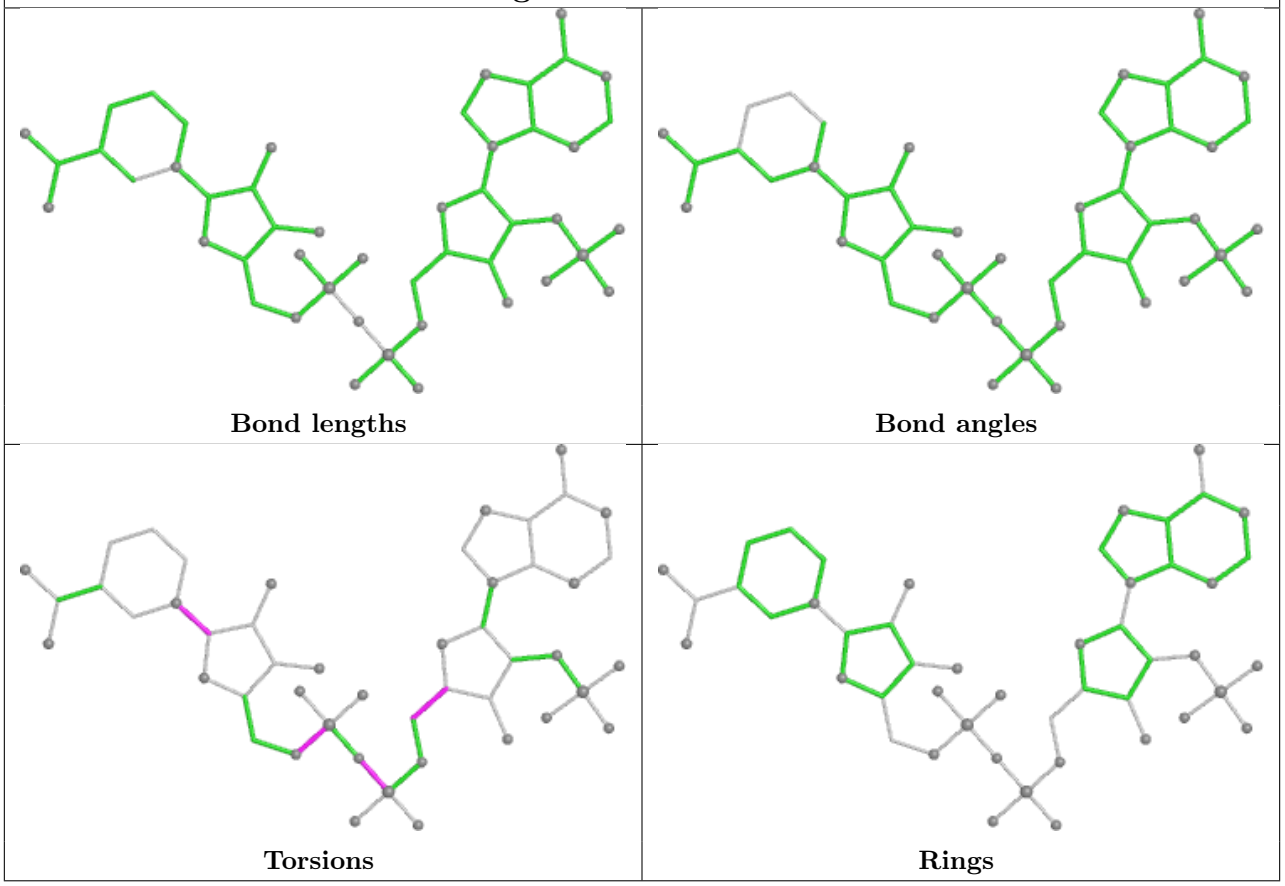


Torsions

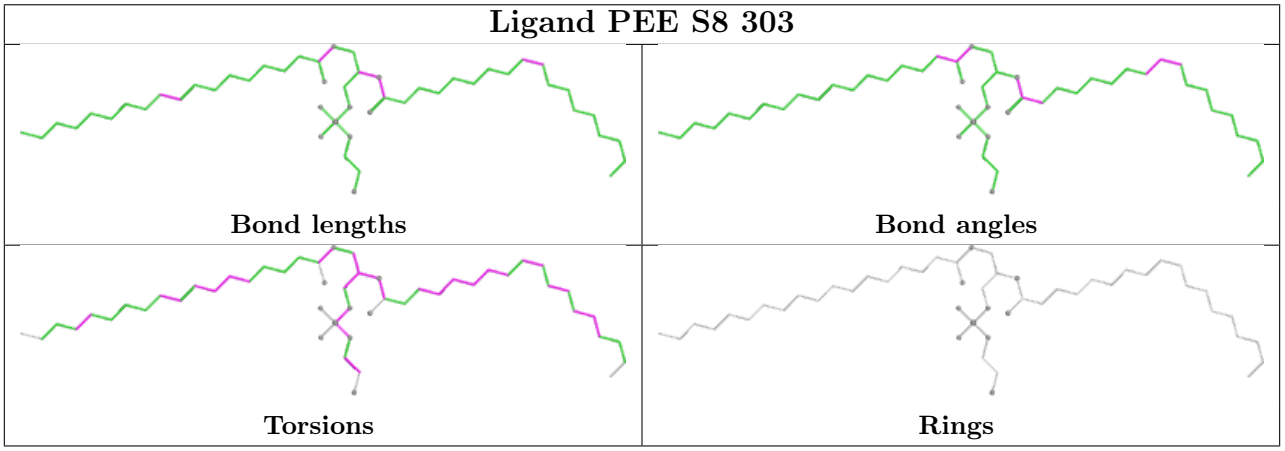


Rings

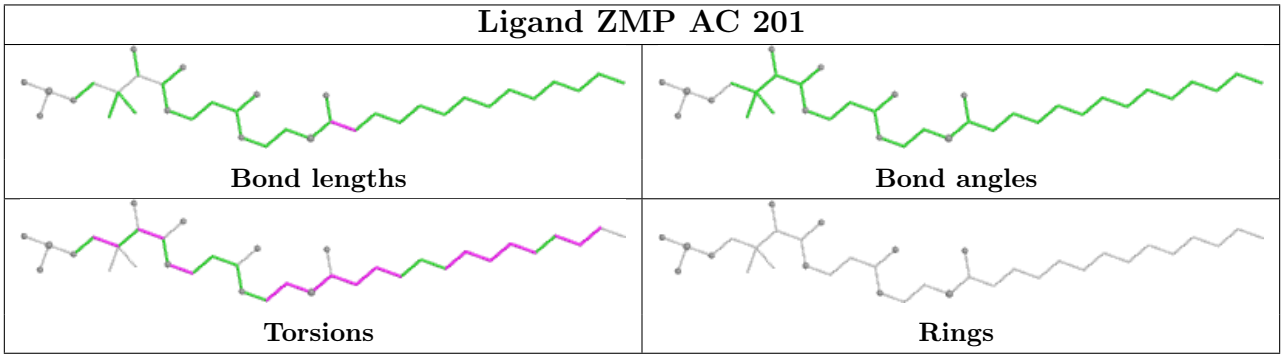
Ligand NDP A9 401



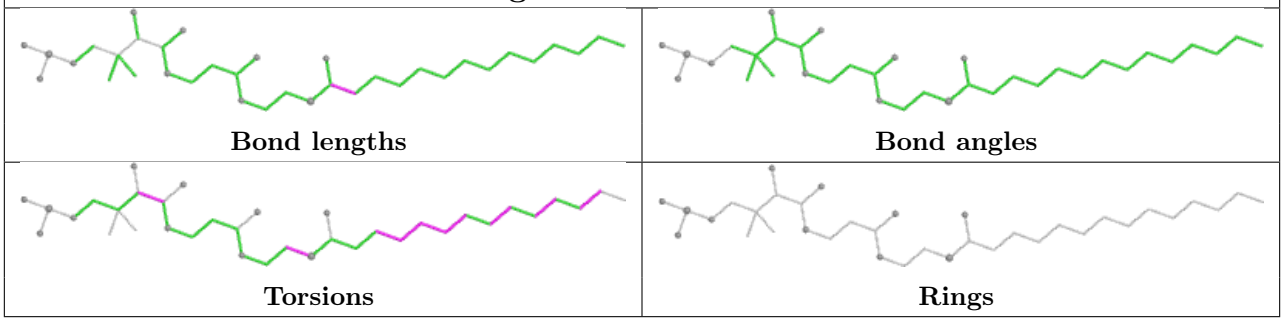
Ligand PEE S8 303



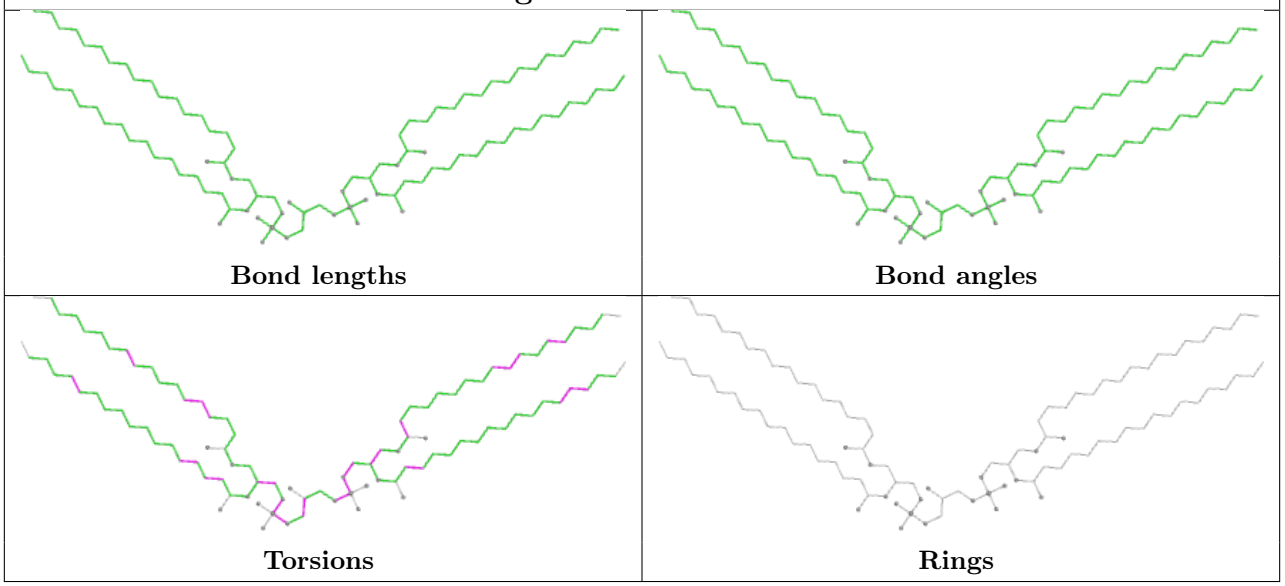
Ligand ZMP AC 201



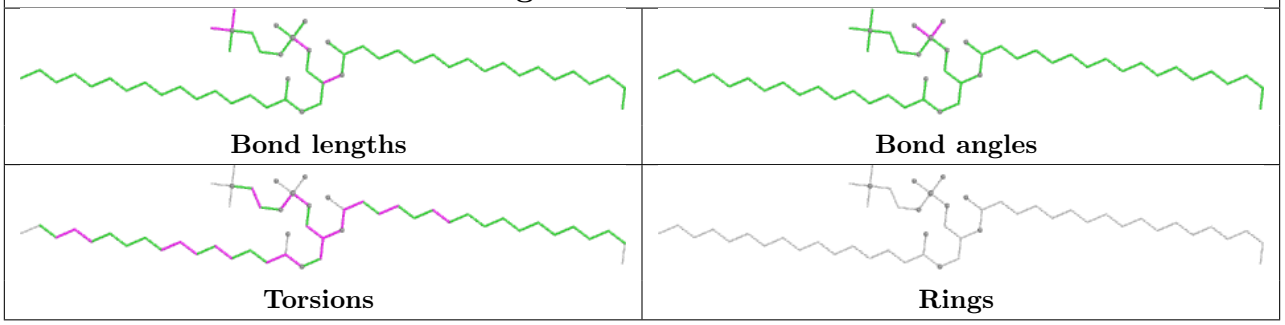
Ligand ZMP AB 201



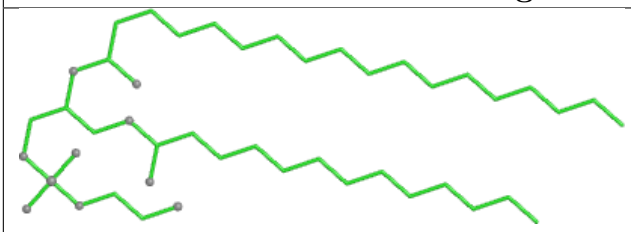
Ligand CDL N4 503



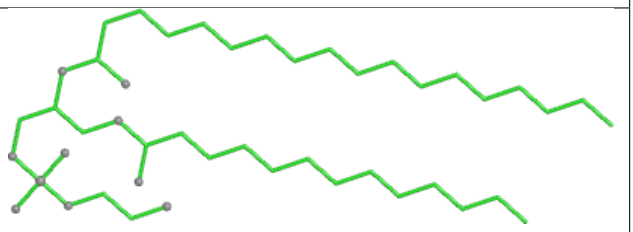
Ligand PLX N6 201



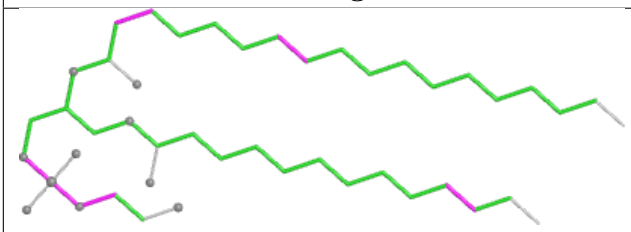
Ligand 3PE CB 202



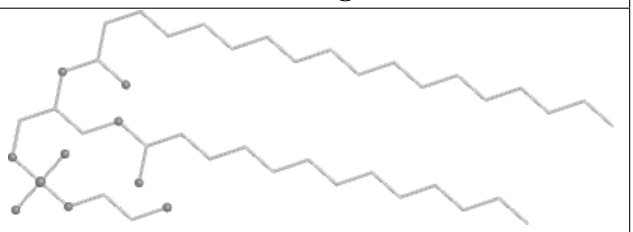
Bond lengths



Bond angles

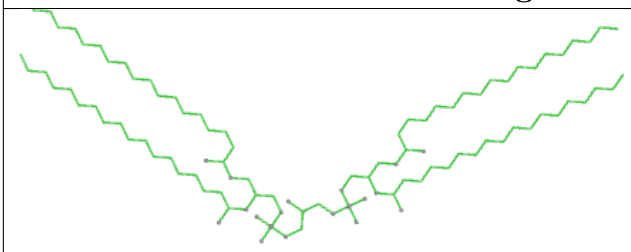


Torsions

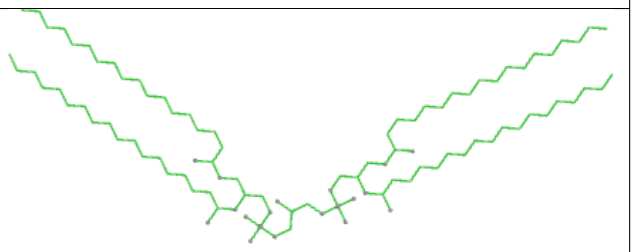


Rings

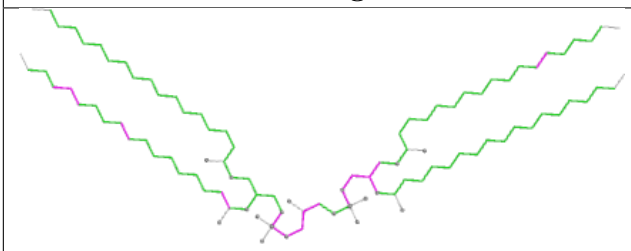
Ligand CDL B5 201



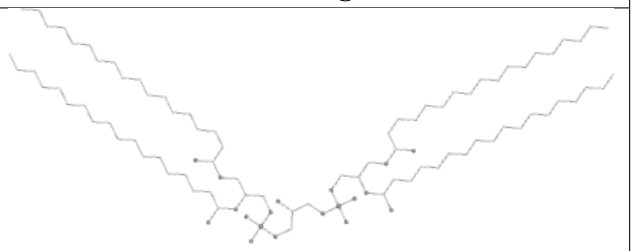
Bond lengths



Bond angles

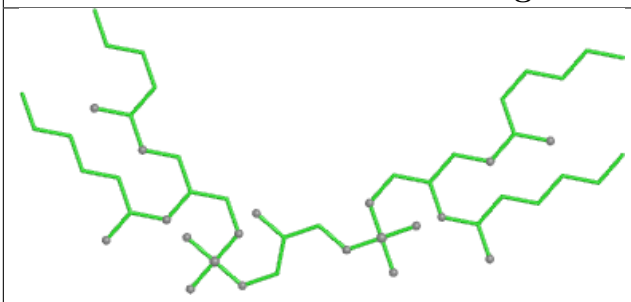


Torsions

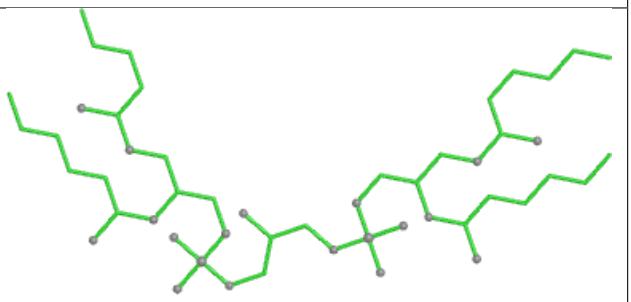


Rings

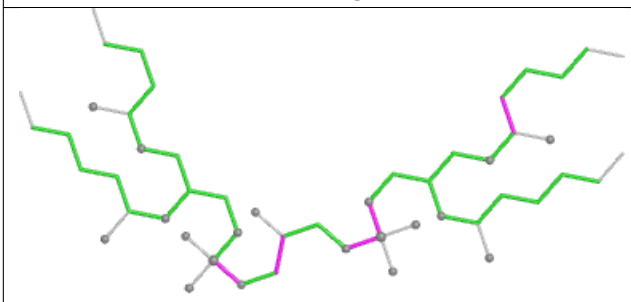
Ligand CDL A7 201



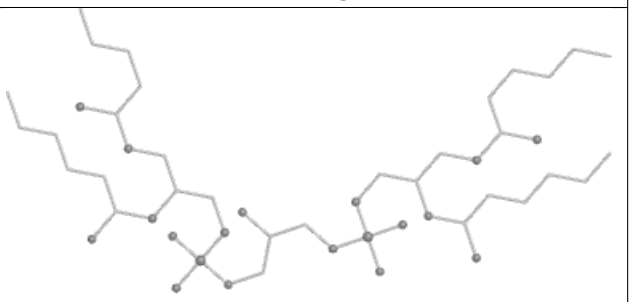
Bond lengths



Bond angles

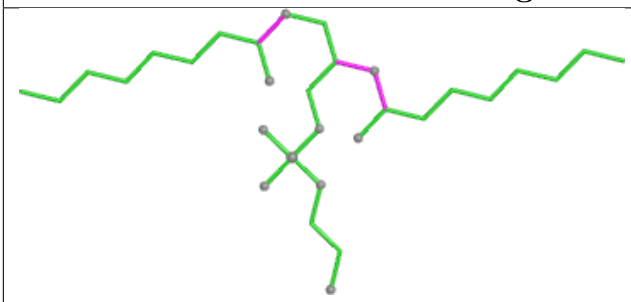


Torsions

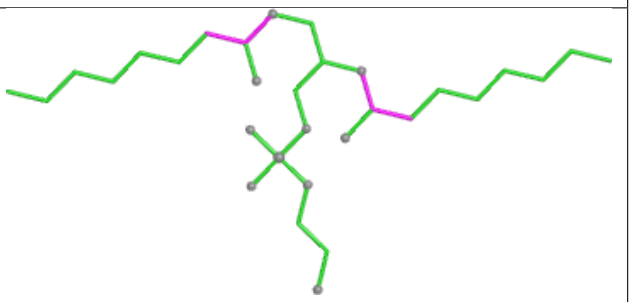


Rings

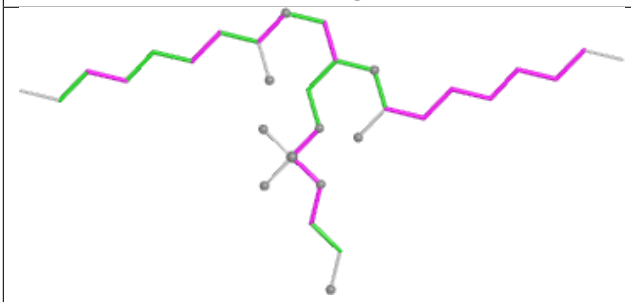
Ligand PEE N1 404



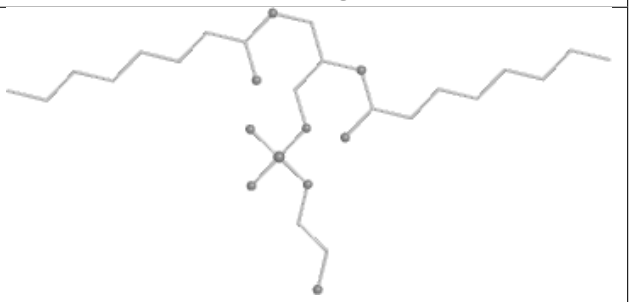
Bond lengths



Bond angles

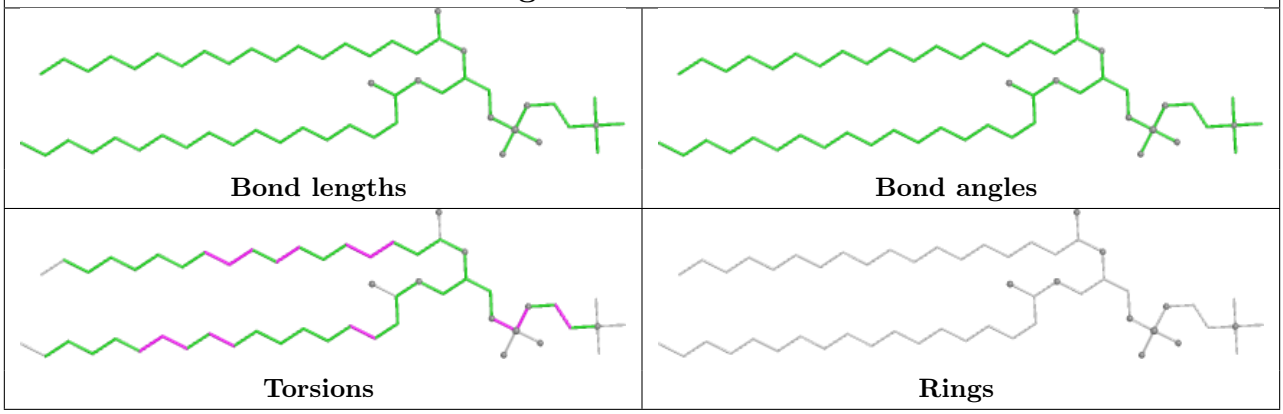


Torsions

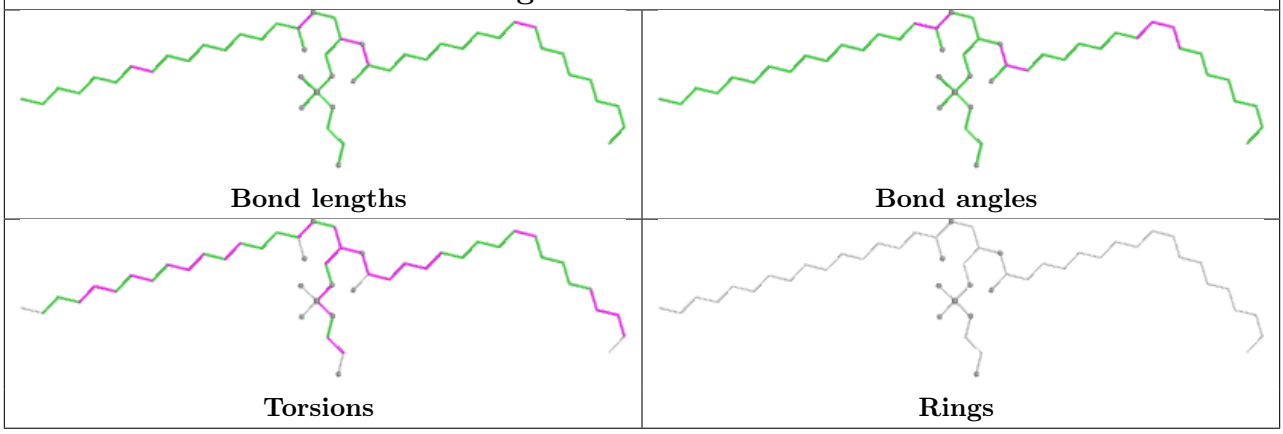


Rings

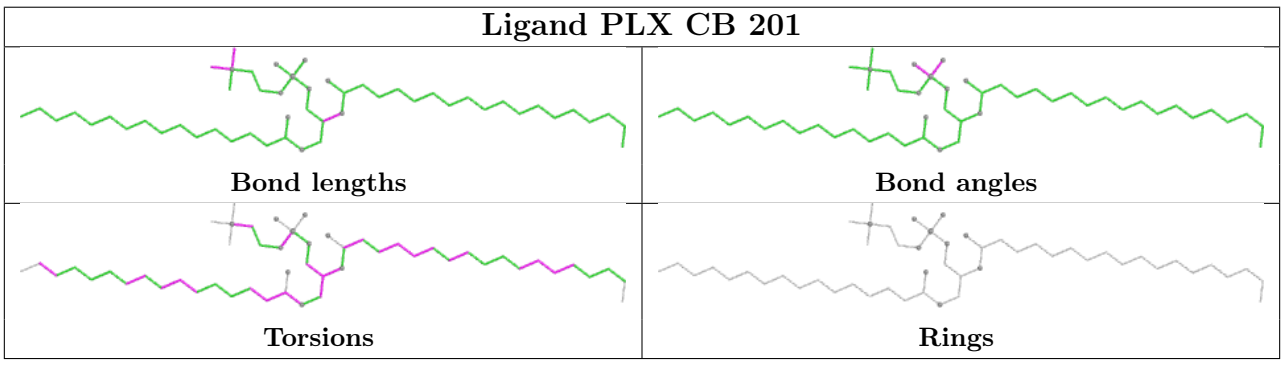
Ligand PC1 A9 403



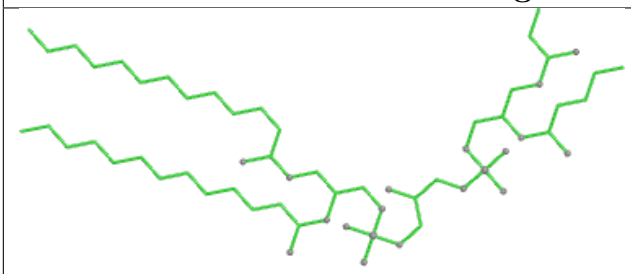
Ligand PEE N4 501



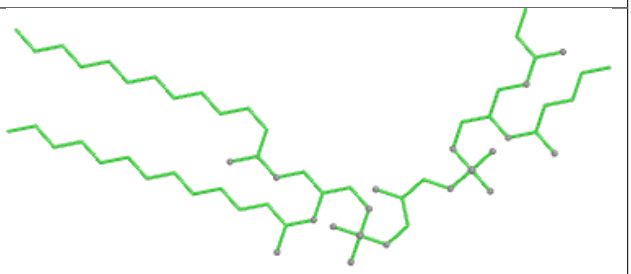
Ligand PLX CB 201



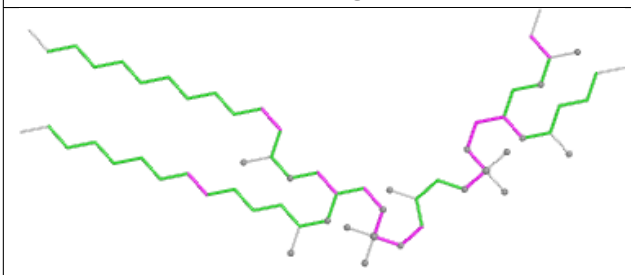
Ligand CDL N4 504



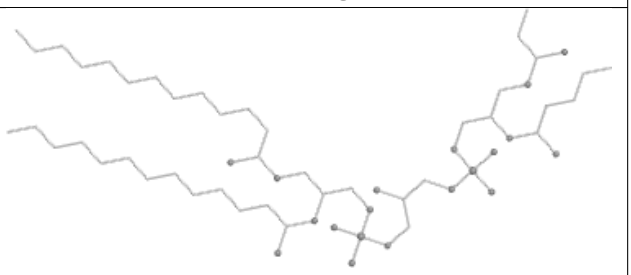
Bond lengths



Bond angles

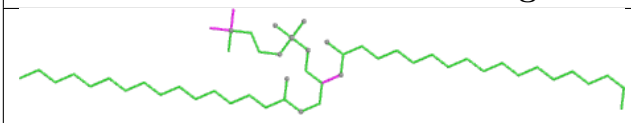


Torsions

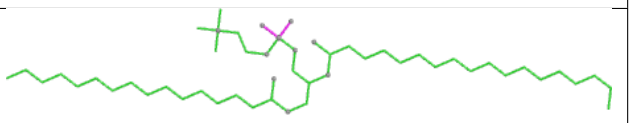


Rings

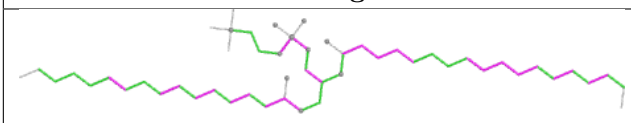
Ligand PLX S7 302



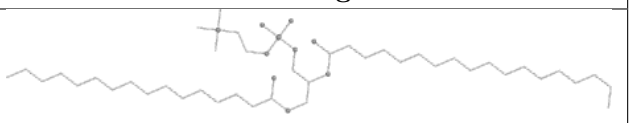
Bond lengths



Bond angles

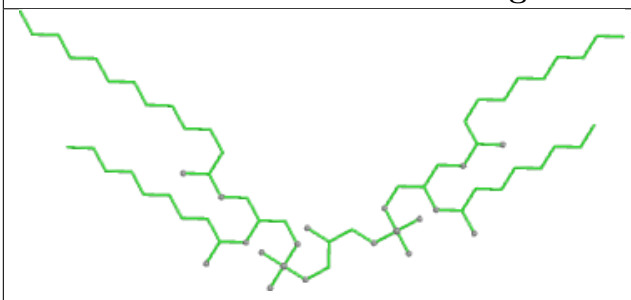


Torsions

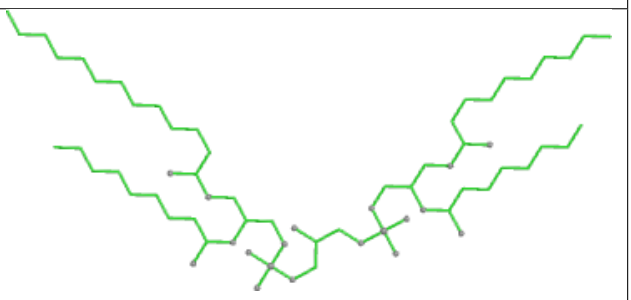


Rings

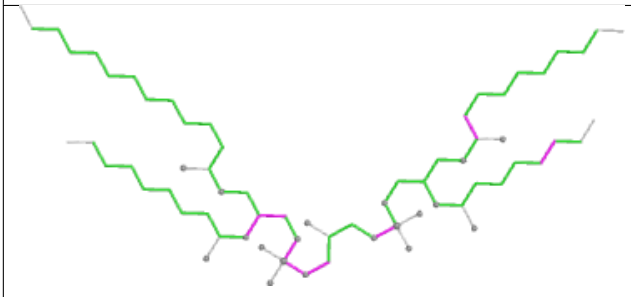
Ligand CDL AK 402



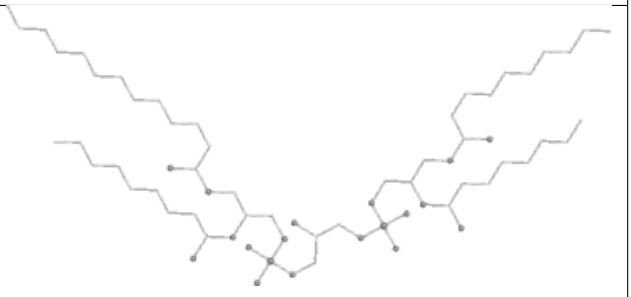
Bond lengths



Bond angles

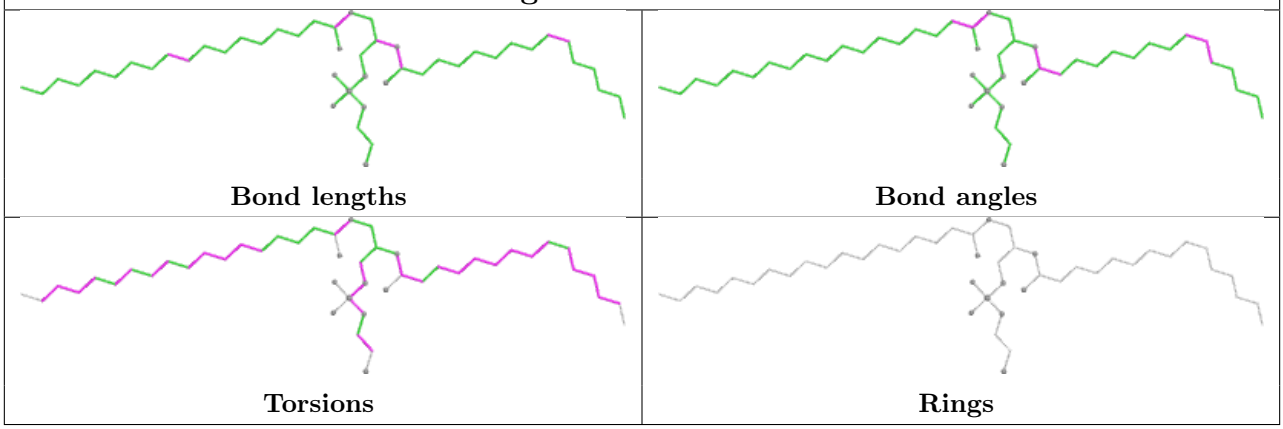


Torsions

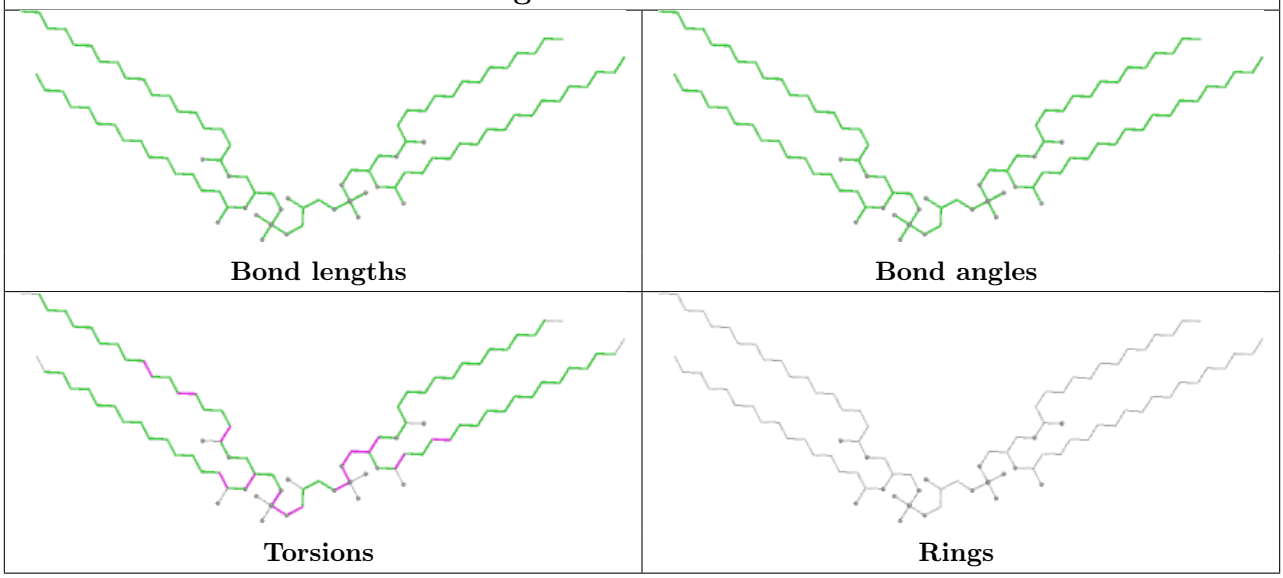


Rings

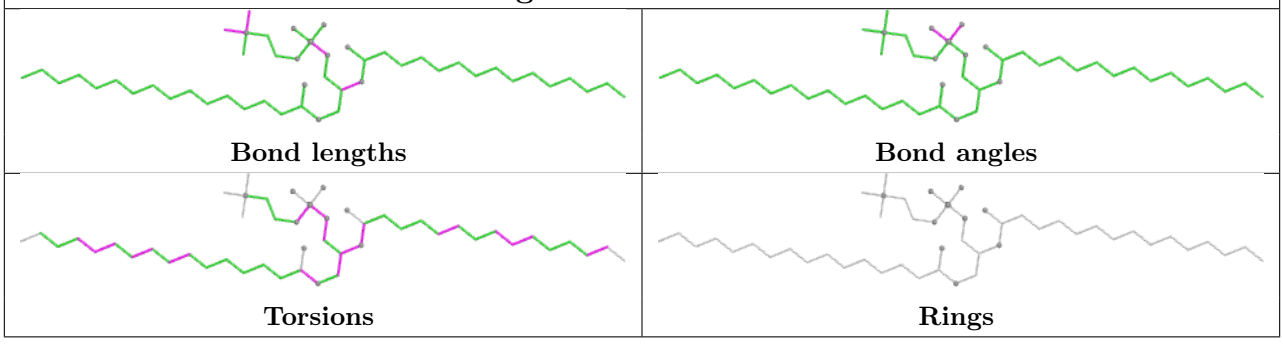
Ligand PEE S2 501



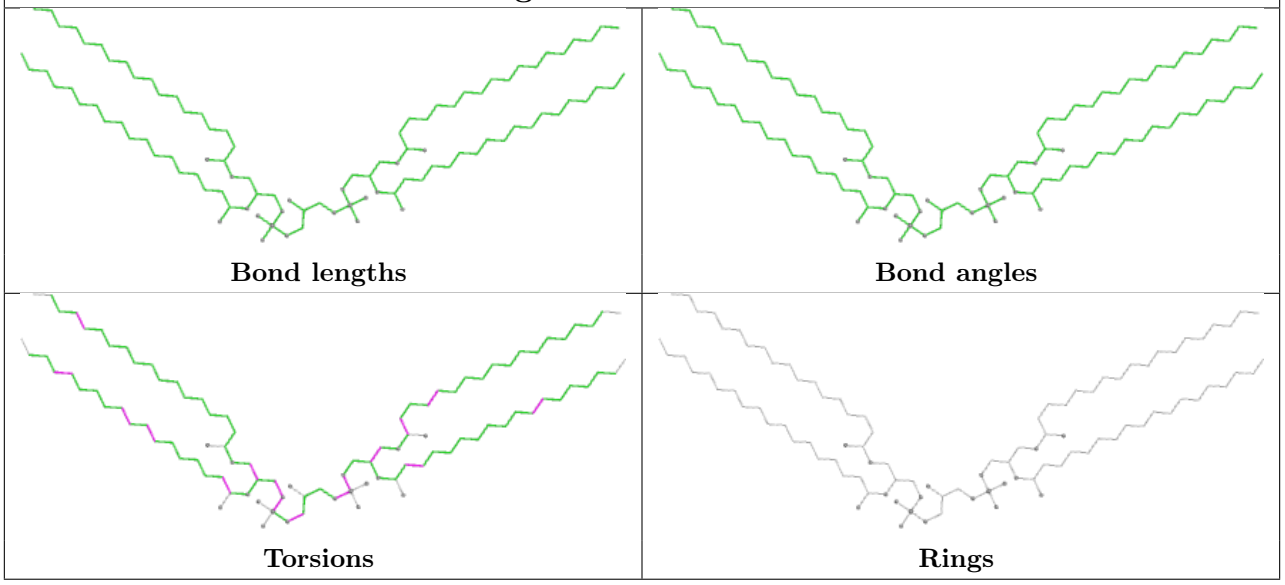
Ligand CDL AL 201



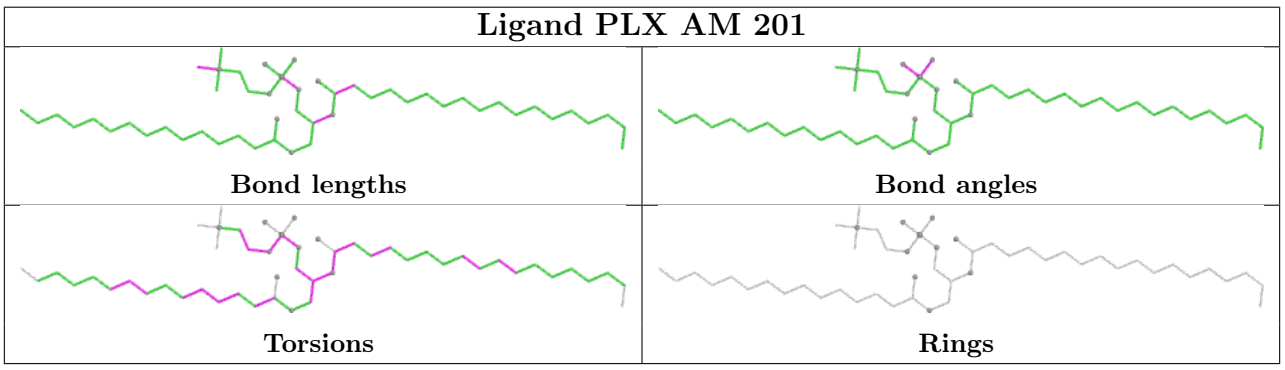
Ligand PLX N4 502



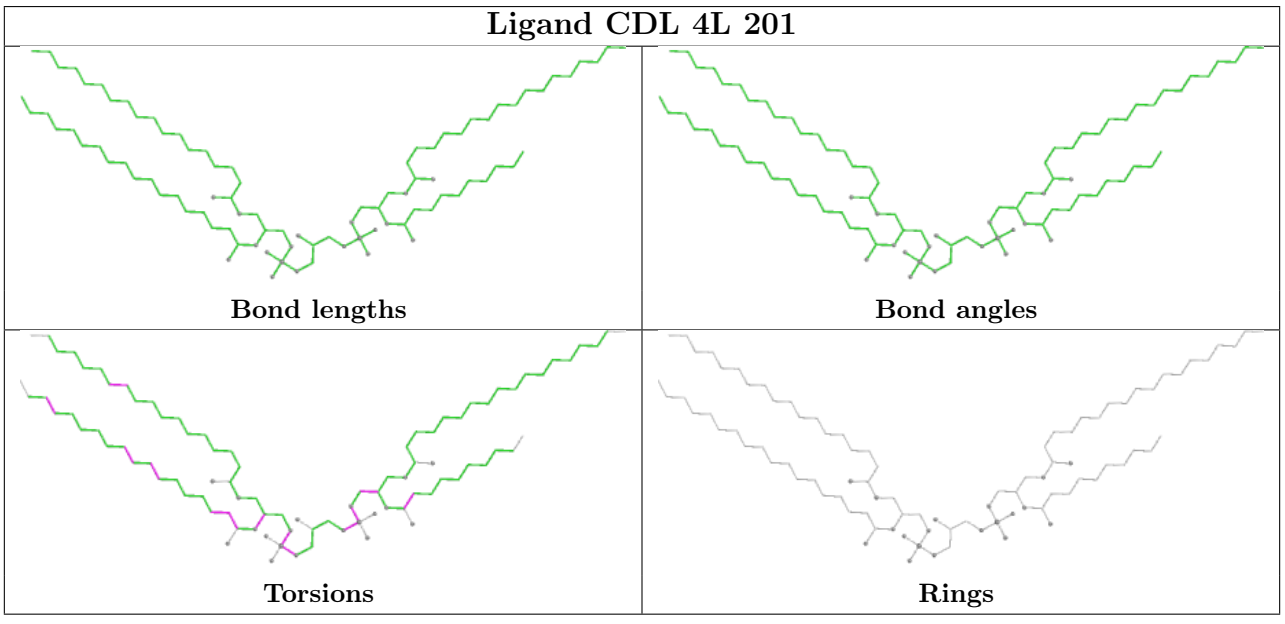
Ligand CDL N5 704



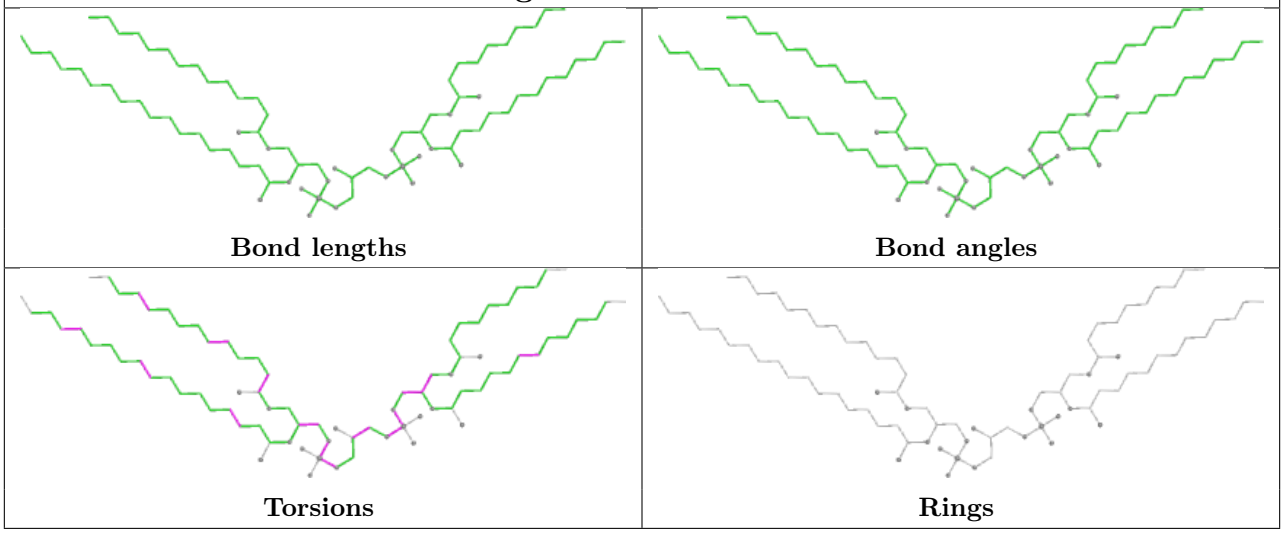
Ligand PLX AM 201



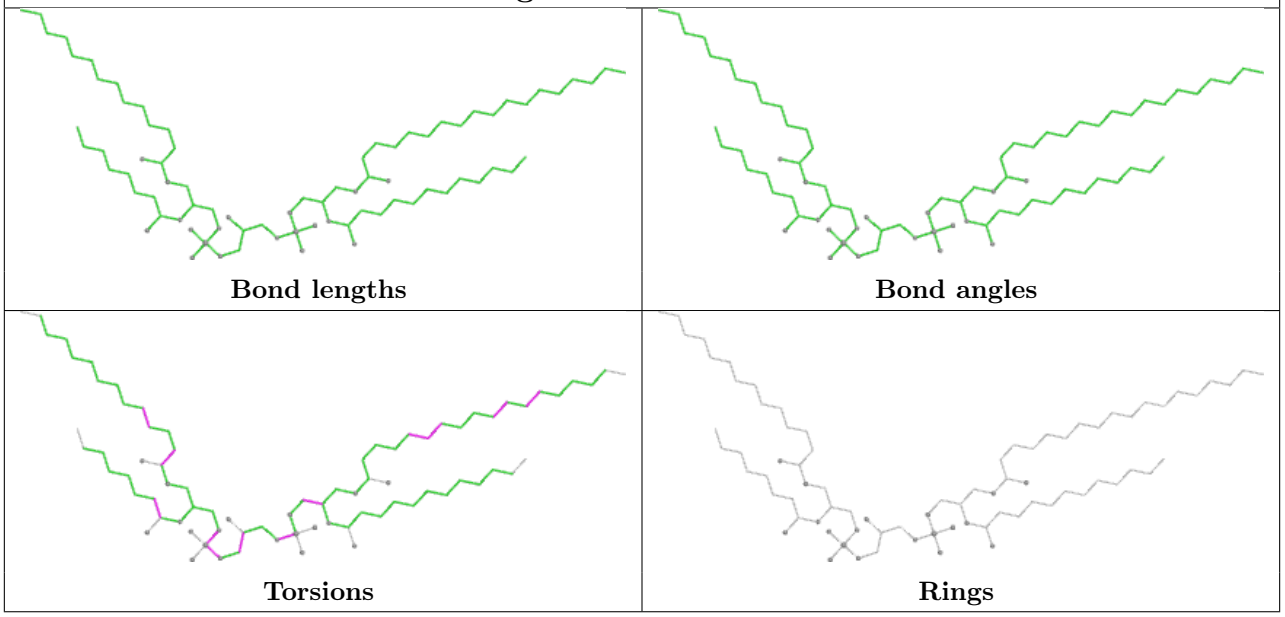
Ligand CDL 4L 201



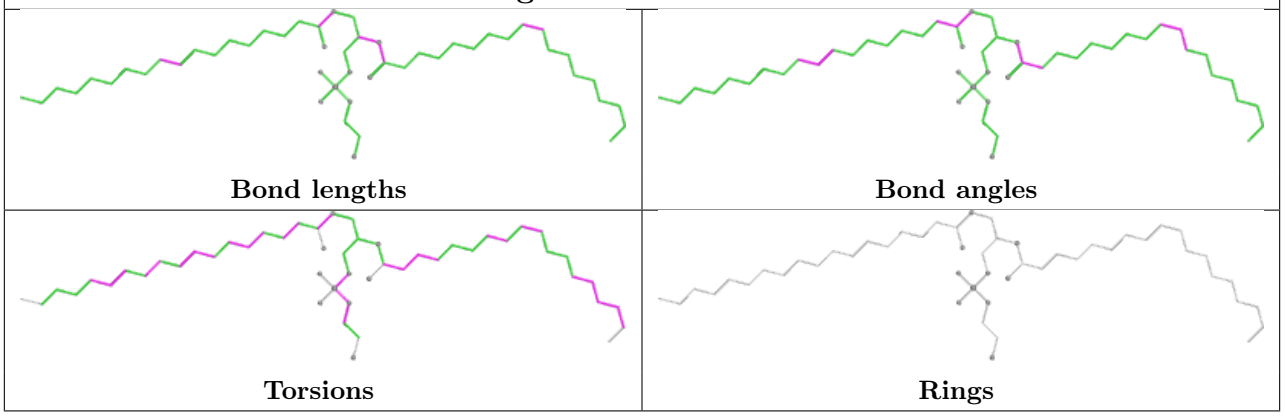
Ligand CDL A8 301



Ligand CDL B4 201



Ligand PEE N3 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

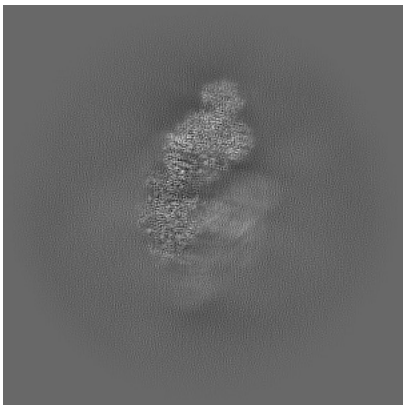
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-61173. These allow visual inspection of the internal detail of the map and identification of artifacts.

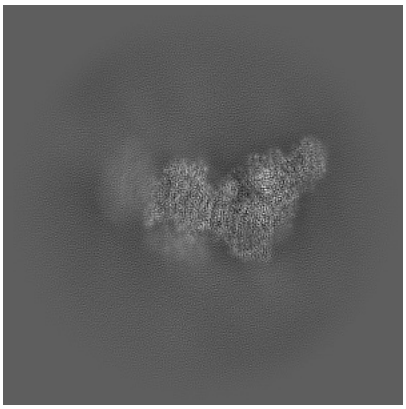
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

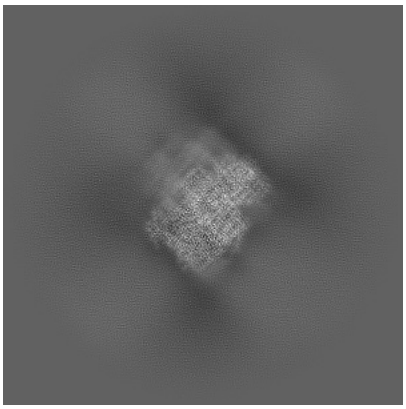
6.1.1 Primary map



X

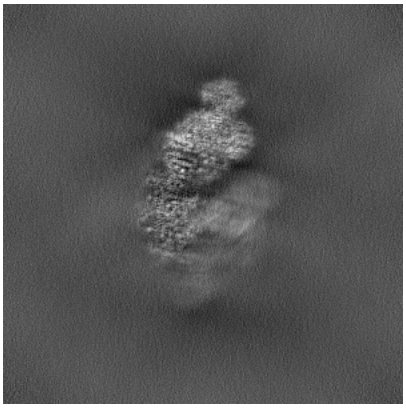


Y

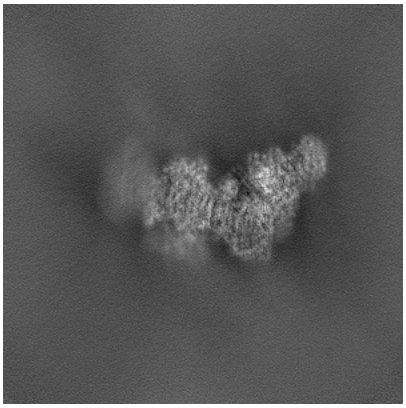


Z

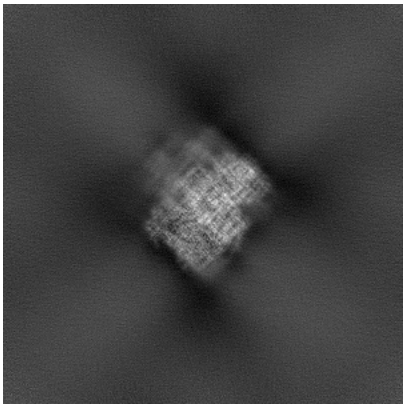
6.1.2 Raw map



X



Y

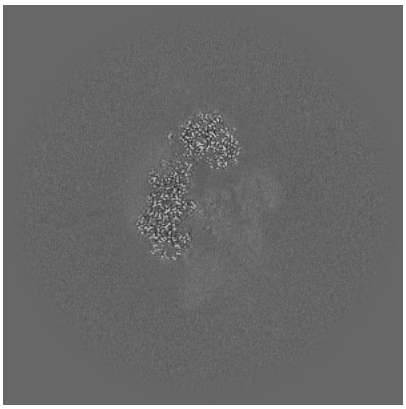


Z

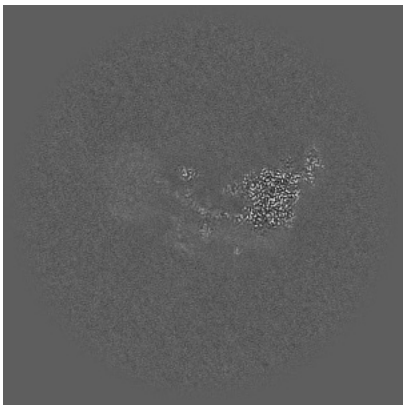
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

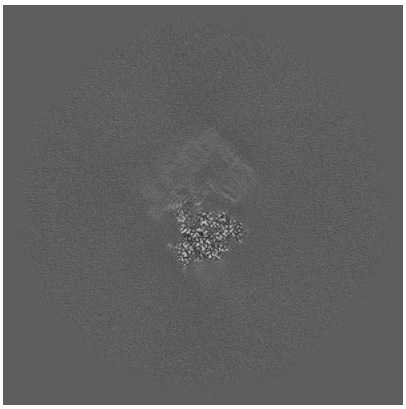
6.2.1 Primary map



X Index: 240

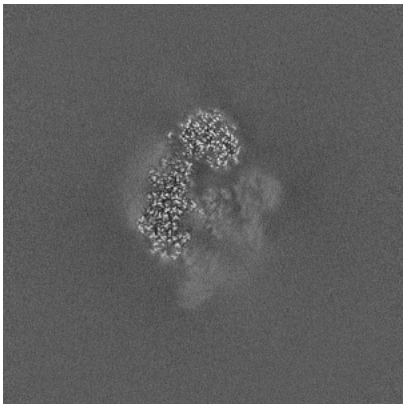


Y Index: 240

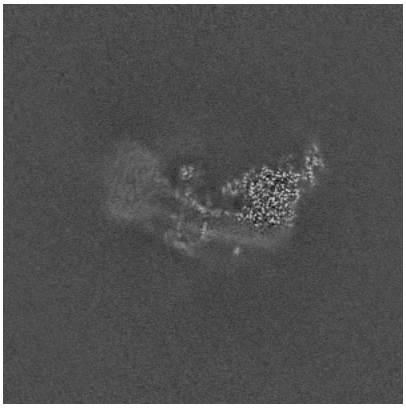


Z Index: 240

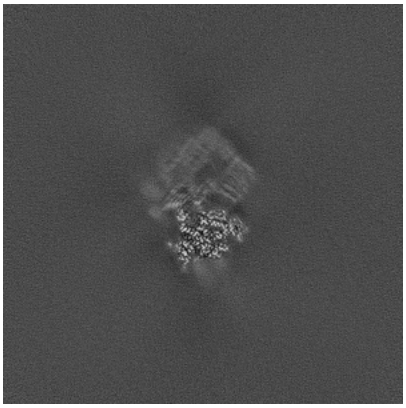
6.2.2 Raw map



X Index: 240



Y Index: 240

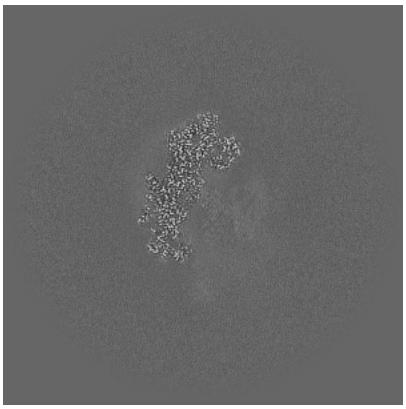


Z Index: 240

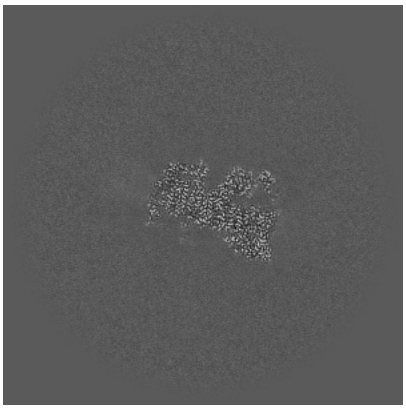
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

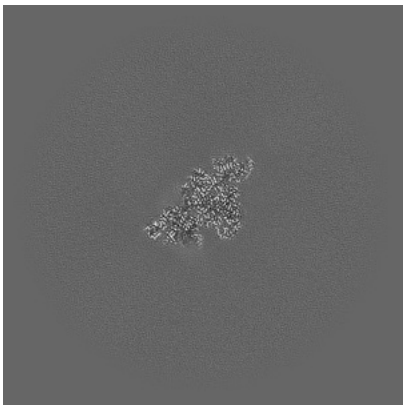
6.3.1 Primary map



X Index: 229

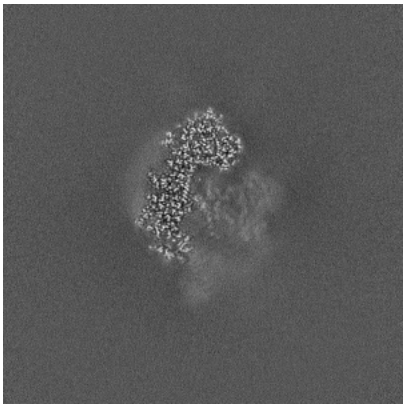


Y Index: 206

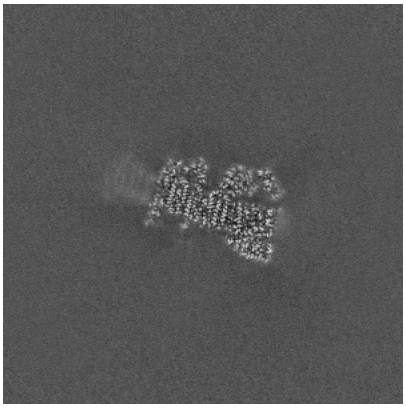


Z Index: 314

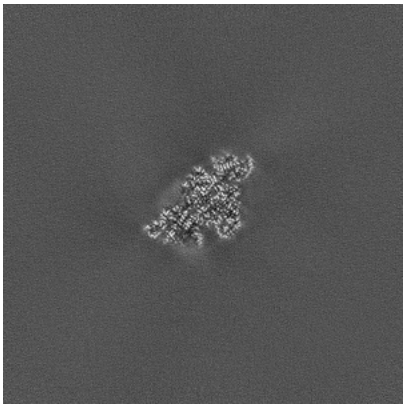
6.3.2 Raw map



X Index: 235



Y Index: 208

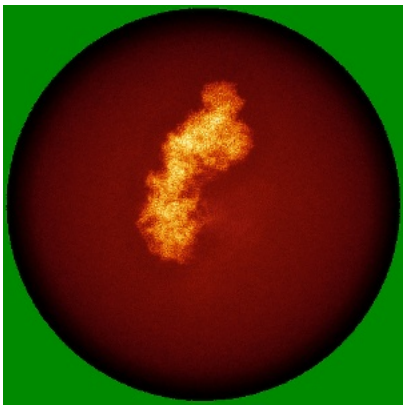


Z Index: 314

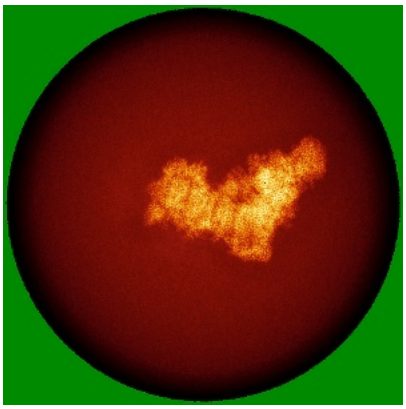
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

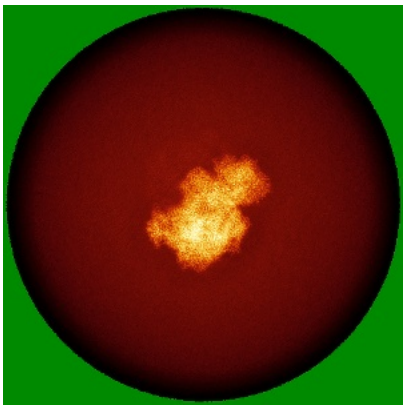
6.4.1 Primary map



X

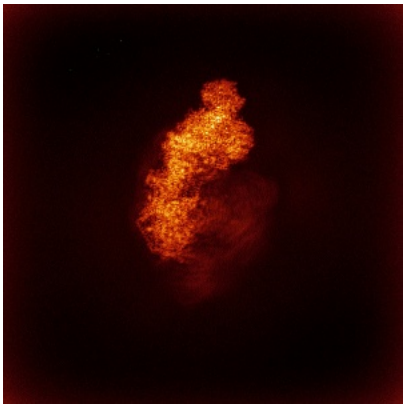


Y

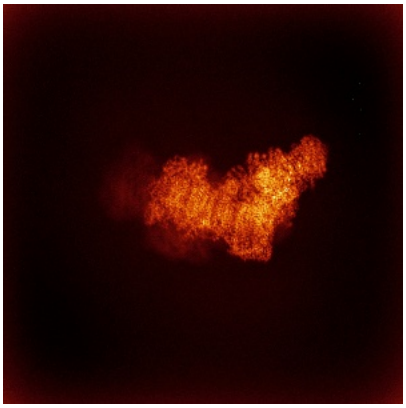


Z

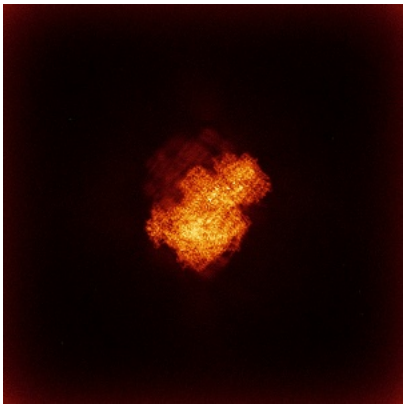
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.62. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

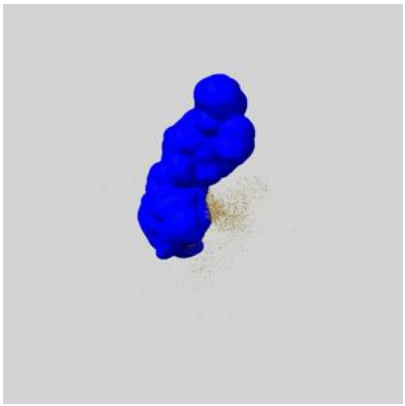
6.6 Mask visualisation

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

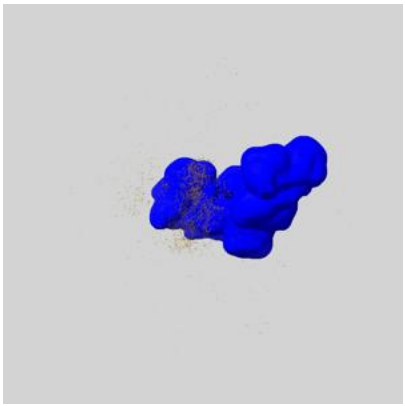
A mask typically either:

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

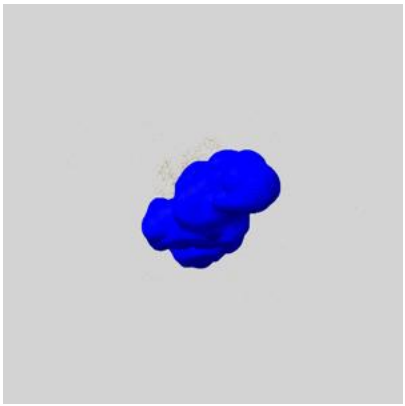
6.6.1 emd_61173_msk_1.map



X



Y

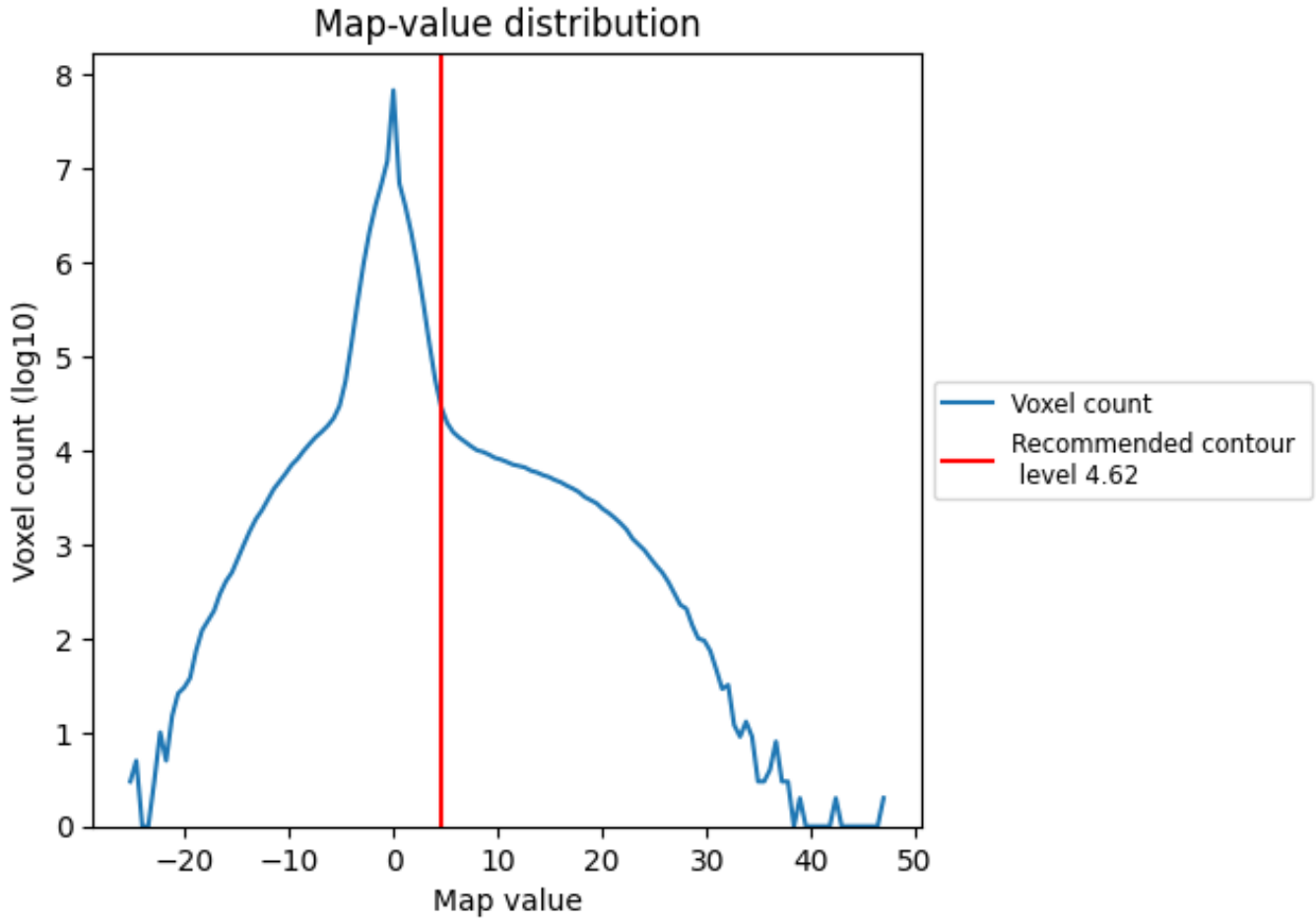


Z

7 Map analysis

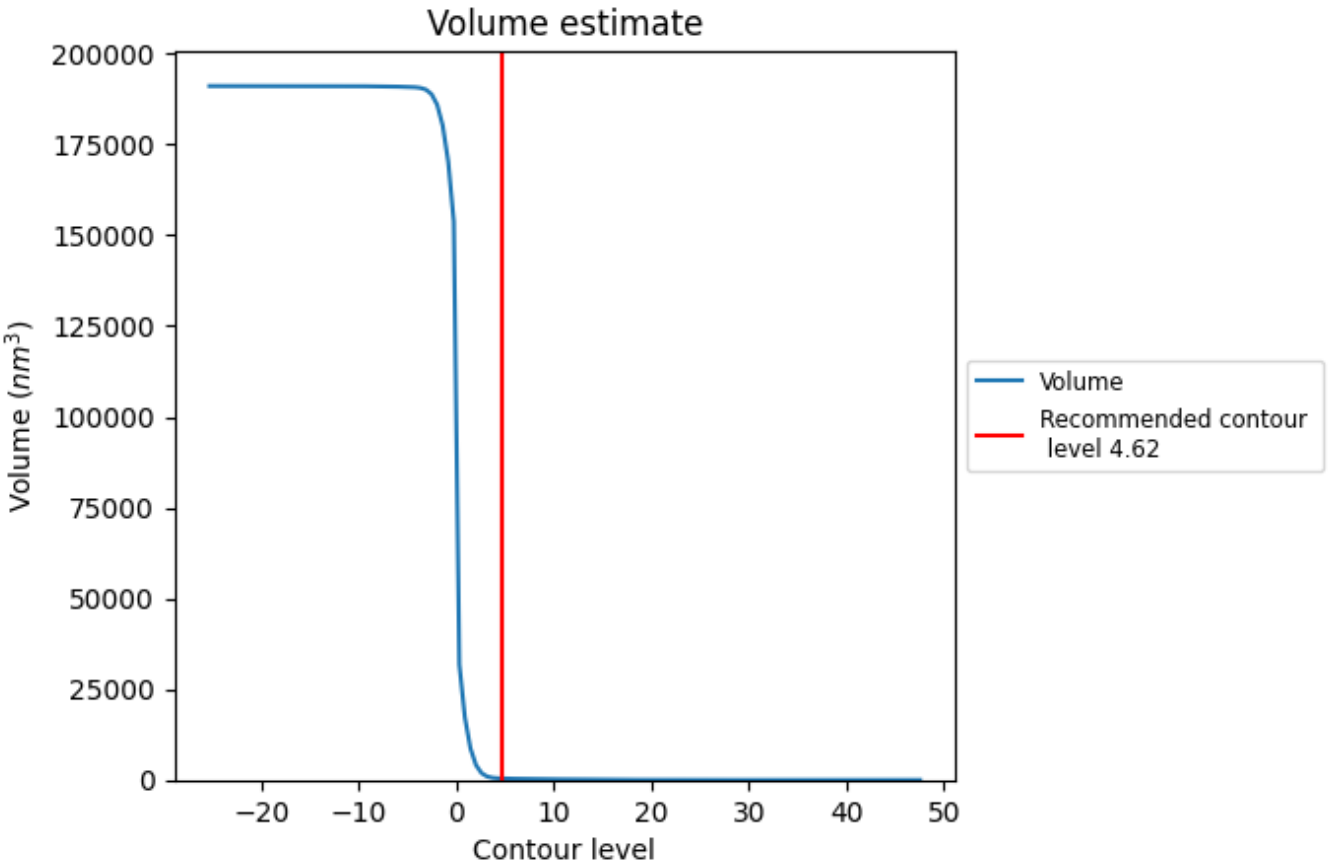
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

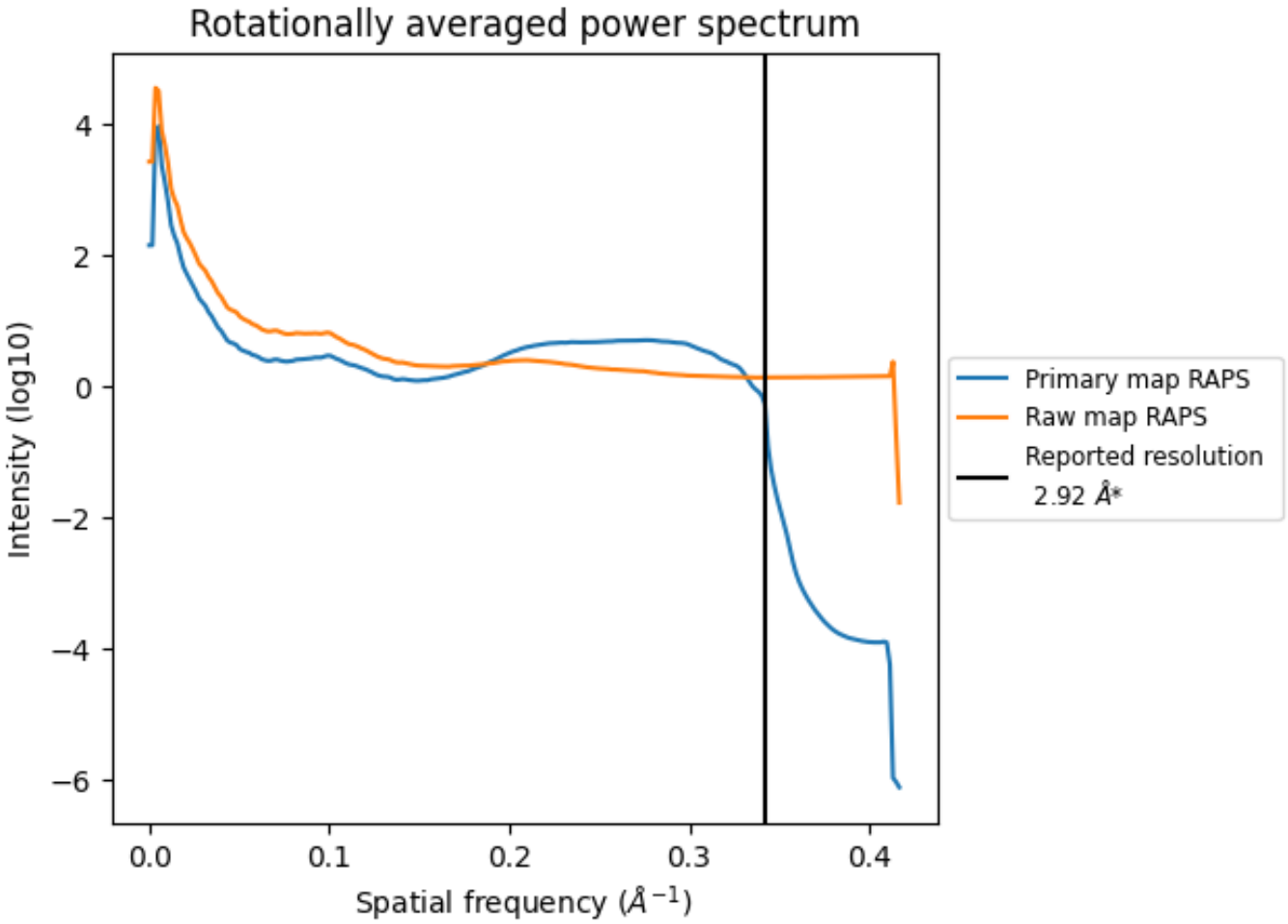
7.2 Volume estimate (i)



The volume at the recommended contour level is 419 nm^3; this corresponds to an approximate mass of 379 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 (i)

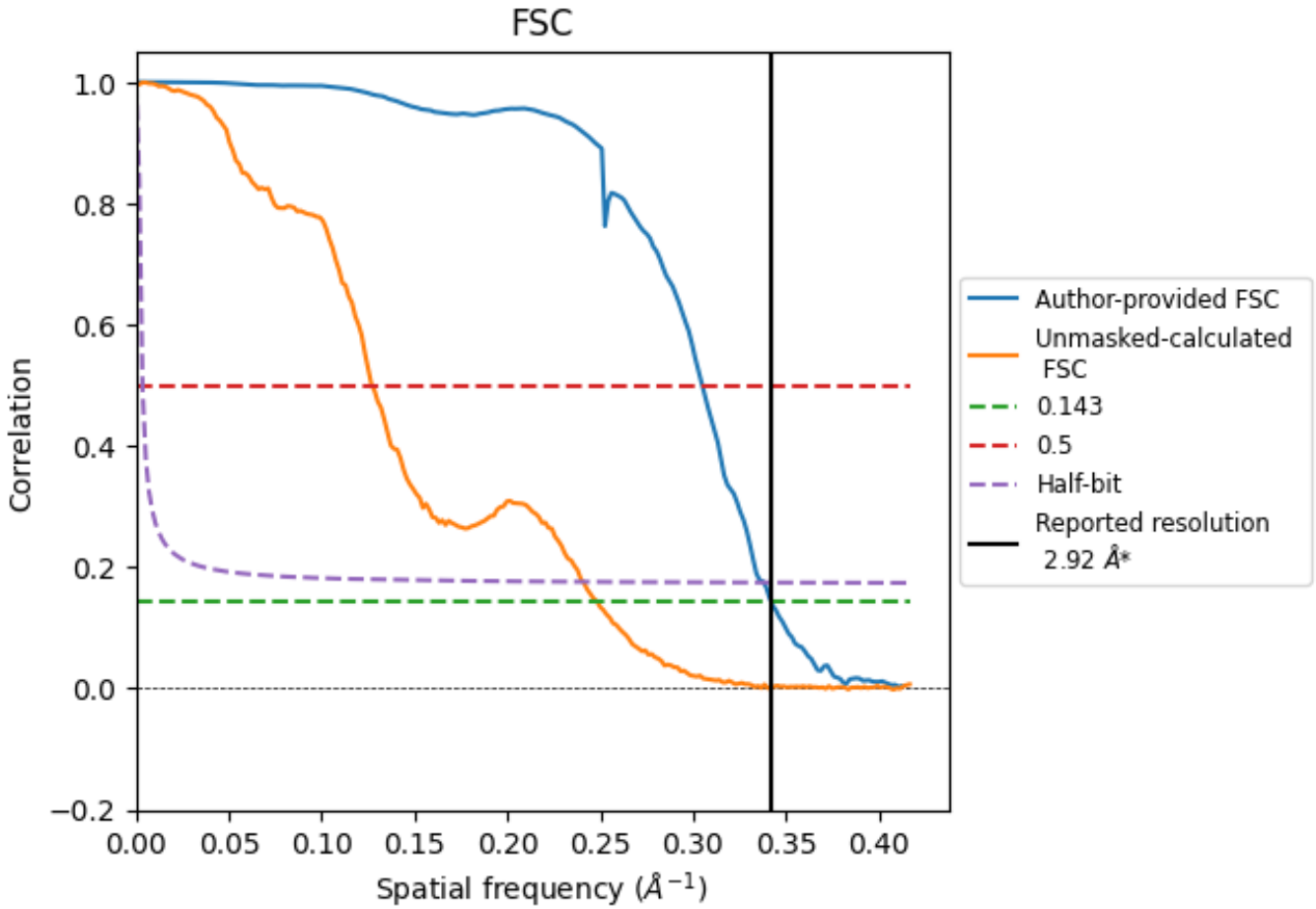


*Reported resolution corresponds to spatial frequency of 0.342 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.342 Å^{-1}

8.2 Resolution estimates (i)

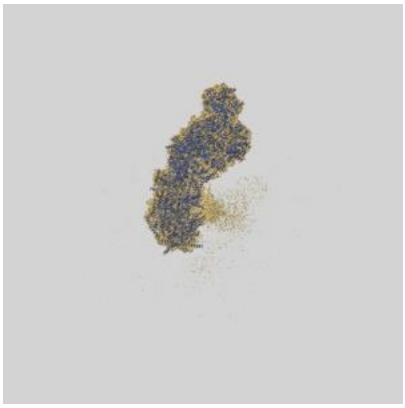
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	2.92	3.28	2.96
Unmasked-calculated*	4.03	7.87	4.15

*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 4.03 differs from the reported value 2.92 by more than 10 %

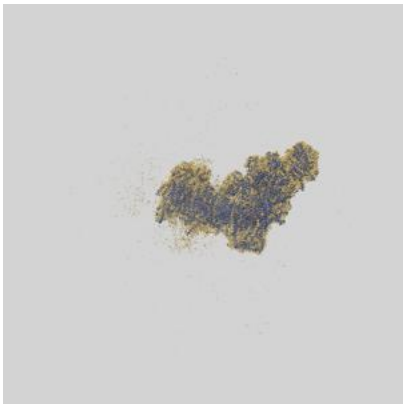
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-61173 and PDB model 9J6H. Per-residue inclusion information can be found in section 3 on page 22.

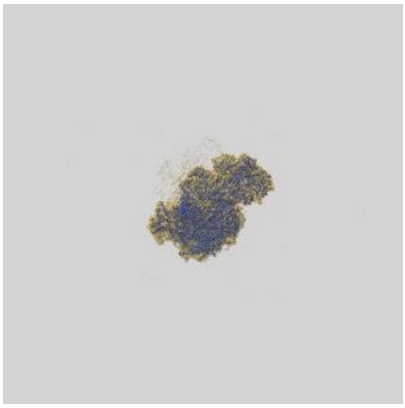
9.1 Map-model overlay



X



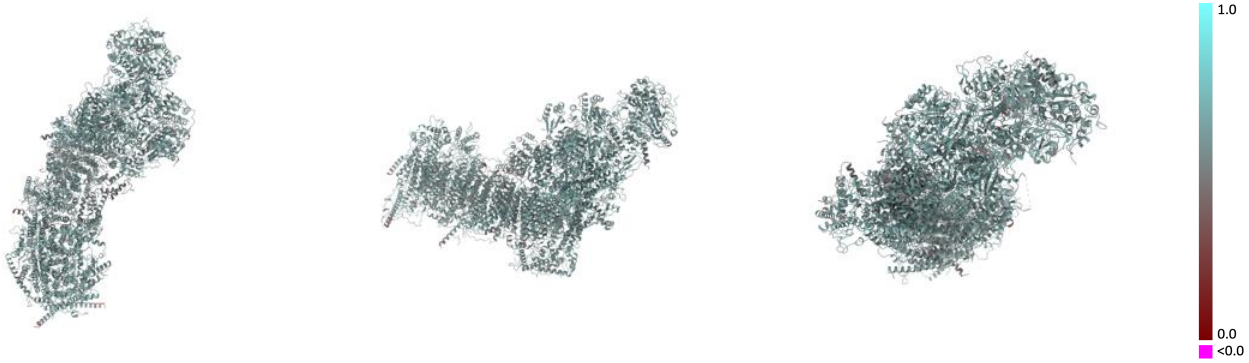
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.62 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.

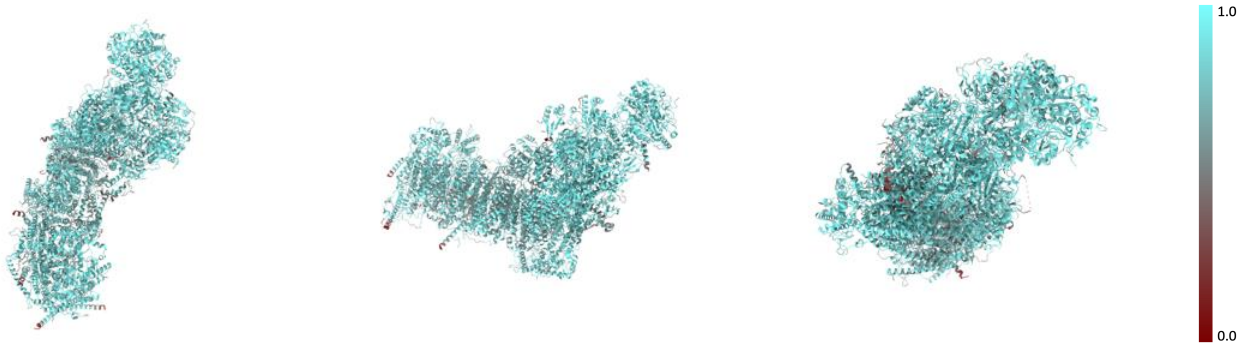
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

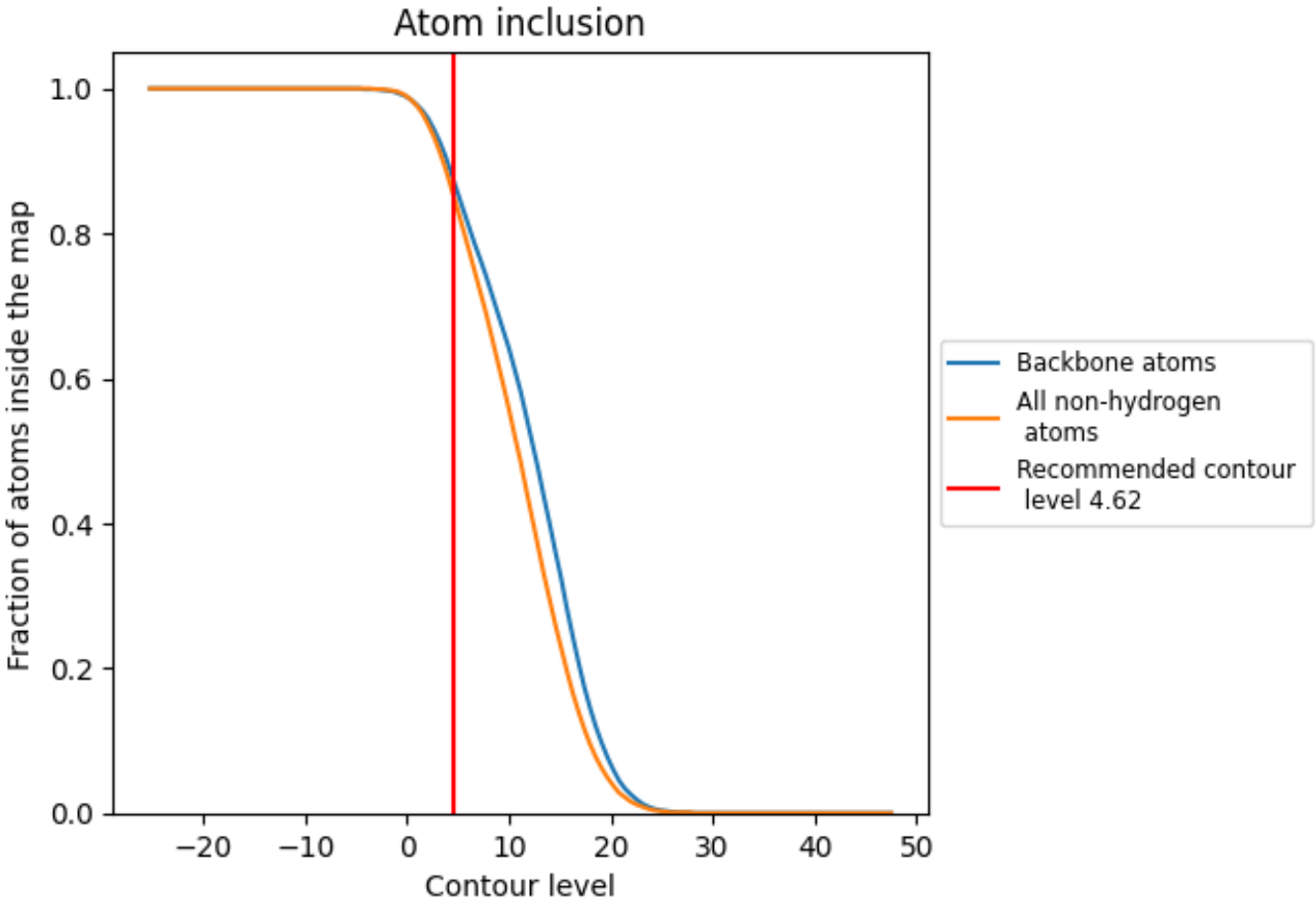
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (4.62).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (4.62) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8490	0.5820
4L	0.8500	0.5950
A1	0.8980	0.5900
A2	0.8080	0.5600
A3	0.8490	0.5750
A5	0.8450	0.5860
A6	0.8340	0.5780
A7	0.7390	0.5630
A8	0.8710	0.5840
A9	0.8800	0.5940
AB	0.6730	0.4910
AC	0.8470	0.5890
AK	0.7830	0.5550
AL	0.7850	0.5660
AM	0.7580	0.5770
AN	0.8580	0.5760
B1	0.7420	0.5610
B2	0.8100	0.5720
B3	0.7490	0.5490
B4	0.7880	0.5700
B5	0.8730	0.5980
B6	0.7530	0.5500
B7	0.8110	0.5630
B8	0.8470	0.5860
B9	0.8680	0.5850
BK	0.8270	0.5770
BL	0.8200	0.5730
CA	0.7800	0.5580
CB	0.8530	0.5880
N1	0.8710	0.5860
N2	0.8840	0.5950
N3	0.8750	0.5940
N4	0.8700	0.5940
N5	0.8620	0.5920
N6	0.7740	0.5500



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
S1	0.8690	0.5810
S2	0.9000	0.6020
S3	0.9200	0.6140
S4	0.8440	0.5920
S5	0.8110	0.5690
S6	0.8210	0.5810
S7	0.9010	0.6050
S8	0.9400	0.6160
V1	0.8680	0.5740
V2	0.8420	0.5660
V3	0.8370	0.5700