wwPDB EM Validation Summary Report

Mar 4, 2024 – 10:52 PM JST

PDB ID	:	8J9J
EMDB ID	:	EMD-36109
Title	:	Cryo-EM structure of Euglena gracilis complex I, NADH state
Authors	:	Wu, M.C.; He, Z.X.; Tian, H.T.; Hu, Y.Q.; Han, F.Z.; Zhou, L.
Deposited on	:	2023-05-03
Resolution	:	3.03 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:

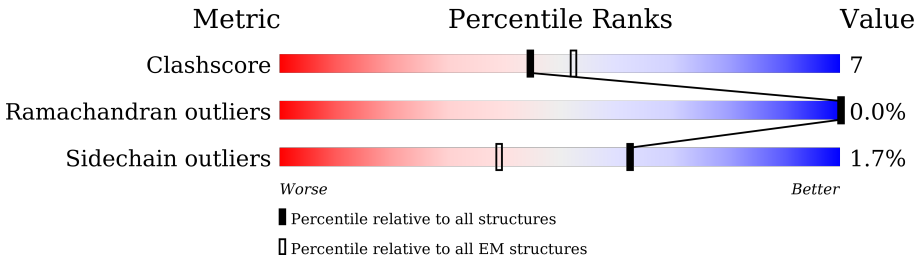
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.03 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1A	385	72% 18% • 9%
2	1B	527	5% 82% 18%
3	2B	142	5% 78% 20% •
4	4L	171	51% 12% 37%
5	A1	141	13% 85% 12% •
6	A2	193	7% 90% 10% •
7	A3	125	9% 89% 10% ••
8	A5	184	8% 77% 7% 16%

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Mol	Chain	Length	Quality of chain
9	A6	437	23% 81% 15%
10	A7	136	7% 84% 16%
11	A8	223	8% 78% 22%
12	A9	489	7% 83% 16%
13	AB	134	8% 56% 10% 34%
14	AC	134	8% 59% 10% 31%
15	AL	281	11% 82% 12% 6%
16	AM	198	7% 81% 12% 7%
17	AN	287	10% 95% 5%
18	B2	145	7% 62% 10% 28%
19	B3	62	21% 79% 18%
20	B4	171	9% 86% 14%
21	B5	140	85% 14%
22	B6	91	12% 87% 13%
23	B7	97	7% 74% 25%
24	B8	176	74% 7% 16%
25	B9	158	5% 76% 19%
26	BL	144	11% 86% 13%
27	BM	112	9% 78% 22%
28	C4	185	11% 80% 18%
29	E1	483	15% 77% 16% 7%
30	E2	467	20% 85% 14%
31	E3	434	21% 85% 14%
32	E4	368	17% 79% 15% 5%
33	E5	290	77% 73% 21% 5%

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Mol	Chain	Length	Quality of chain
34	E6	371	26% 77% 8% 14%
35	E8	205	23% 80% 19%
36	EA	126	87% 11%
37	EB	101	12% 89% 11%
38	EC	101	16% 66% 18% 16%
39	ED	151	17% 77% 14% 9%
40	FX	325	5% 58% 14% 27%
41	G1	436	8% 76% 16% 8%
42	G2	267	12% 75% 13% 12%
43	G3	261	85% 15%
44	N1	670	37% 9% 54%
45	N2	300	71% 26%
46	N3	293	30% 12% 59%
46	N6	293	8% 39% 13% 47%
47	N4	478	72% 27%
48	N5	584	73% 26%
49	S2	395	77% 21%
50	S3	277	64% 25% 10%
51	S4	208	75% 17% 9%
52	S5	122	11% 89% 11%
53	S6	147	79% 20%
54	S7	207	7% 82% 15%
55	S8	212	67% 18% 14%
56	U1	12	58% 92% 8%
56	U2	12	50% 100%

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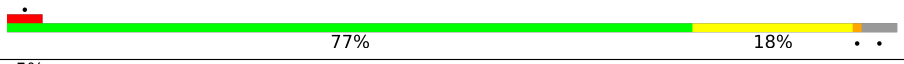
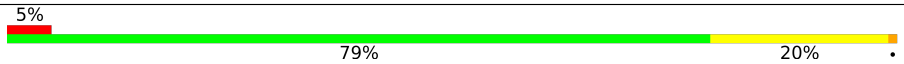
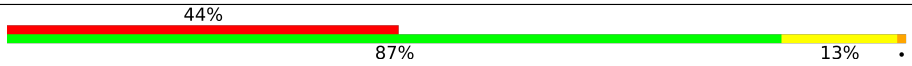
Mol	Chain	Length	Quality of chain
57	V1	526	
58	V2	225	
59	E7	246	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
61	SF4	S8	297	-	-	X	-

2 Entry composition (i)

There are 71 unique types of molecules in this entry. The entry contains 226179 atoms, of which 112544 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 NDUFS1A.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	1A	352	5501	1753	2700	488	537	23	0	0

- Molecule 2 is a protein called NDUFS1B.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	1B	525	8357	2679	4159	743	765	11	1	0

- Molecule 3 is a protein called ND2B.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	2B	140	2059	712	989	172	183	3	0	0

- Molecule 4 is a protein called ND4L.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	4L	108	1768	606	878	133	145	6	0	0

- Molecule 5 is a protein called NDUFA1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	A1	137	2097	684	1026	192	192	3	0	0

- Molecule 6 is a protein called NDUFA2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	A2	192	2967	942	1474	267	280	4	0	0

- Molecule 7 is a protein called NDUFA3.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	A3	124	Total	C	H	N	O	S	0	0
			2089	678	1039	191	175	6		

- Molecule 8 is a protein called NDUFA5.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	A5	154	Total	C	H	N	O	S	0	0
			2509	794	1248	221	244	2		

- Molecule 9 is a protein called NDUFA6.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	A6	423	Total	C	H	N	O	S	0	0
			6608	2091	3280	601	632	4		

- Molecule 10 is a protein called NDUFA7.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	A7	136	Total	C	H	N	O	S	0	0
			2272	735	1118	219	194	6		

- Molecule 11 is a protein called NDUFA8.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	A8	223	Total	C	H	N	O	S	0	0
			3548	1160	1726	315	334	13		

- Molecule 12 is a protein called NDUFA9.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	A9	484	Total	C	H	N	O	S	0	0
			7679	2449	3850	662	700	18		

- Molecule 13 is a protein called NDUFAB1-alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AB	88	Total	C	H	N	O	S	0	0
			1367	437	673	114	139	4		

- Molecule 14 is a protein called NDUFAB1-beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	AC	92	Total	C	H	N	O	S	0	0
			1418	461	697	116	140	4		

- Molecule 15 is a protein called NDUFA12.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	AL	265	Total	C	H	N	O	S	0	0
			4409	1439	2172	414	379	5		

- Molecule 16 is a protein called NDUFA13.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	AM	184	Total	C	H	N	O	S	0	0
			2935	953	1448	264	263	7		

- Molecule 17 is a protein called NDUFA11.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	AN	287	Total	C	H	N	O	S	0	0
			4573	1501	2267	396	399	10		

- Molecule 18 is a protein called NDUFB2.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	B2	105	Total	C	H	N	O	S	0	0
			1770	604	857	142	166	1		

- Molecule 19 is a protein called NDUFB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	B3	61	Total	C	H	N	O	S	0	0
			758	292	309	88	68	1		

- Molecule 20 is a protein called NDUFB4.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	B4	171	Total	C	H	N	O	S	0	0
			2735	885	1358	250	236	6		

- Molecule 21 is a protein called NDUFB5.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	B5	140	Total	C	H	N	O	S	0	0
			2181	708	1069	207	195	2		

- Molecule 22 is a protein called NDUFB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	B6	91	Total	C	H	N	O	S	0	0
			1520	509	747	132	128	4		

- Molecule 23 is a protein called NDUFB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	B7	97	Total	C	H	N	O	S	0	0
			1692	536	835	165	149	7		

- Molecule 24 is a protein called NDUFB8.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	B8	147	Total	C	H	N	O	S	0	0
			2351	804	1127	199	213	8		

- Molecule 25 is a protein called NDUFB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	B9	151	Total	C	H	N	O	S	0	0
			2443	795	1207	216	222	3		

- Molecule 26 is a protein called NDUFB10.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	BL	144	Total	C	H	N	O	S	0	0
			2406	786	1179	215	216	10		

- Molecule 27 is a protein called NDUFB11.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	BM	112	Total	C	H	N	O	S	0	0
			1737	577	827	164	167	2		

- Molecule 28 is a protein called NDUFC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	C4	183	Total	C	H	N	O	S	0	0
			3062	1000	1517	268	271	6		

- Molecule 29 is a protein called NDUEG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	E1	450	Total	C	H	N	O	S	0	0
			7008	2244	3496	601	654	13		

- Molecule 30 is a protein called NDUEG2.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	E2	466	Total	C	H	N	O	S	0	0
			7103	2286	3540	618	655	4		

- Molecule 31 is a protein called NDUEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	E3	432	Total	C	H	N	O	S	0	0
			6518	2071	3263	565	612	7		

- Molecule 32 is a protein called NDUEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	E4	351	Total	C	H	N	O	S	0	0
			5502	1774	2732	477	504	15		

- Molecule 33 is a protein called NDUEG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	E5	276	Total	C	H	N	O	S	0	0
			4046	1265	2069	341	369	2		

- Molecule 34 is a protein called NDUEG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	E6	318	Total	C	H	N	O	S	0	0
			5228	1703	2554	477	482	12		

- Molecule 35 is a protein called NDUEG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	E8	205	Total	C	H	N	O	S	0	0
			3354	1100	1663	288	292	11		

- Molecule 36 is a protein called NDUEG10.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	EA	124	Total	C	H	N	O	S	0	0
			1793	630	832	172	156	3		

- Molecule 37 is a protein called NDUEG11.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	EB	101	Total	C	H	N	O	S	0	0
			1405	473	631	150	144	7		

- Molecule 38 is a protein called NDUEG12.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	EC	85	Total	C	H	N	O	S	0	0
			1323	424	663	116	118	2		

- Molecule 39 is a protein called NDUEG13.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	ED	138	Total	C	H	N	O	S	0	0
			2273	736	1131	205	196	5		

- Molecule 40 is a protein called NDUFX.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	FX	237	Total	C	H	N	O	S	0	0
			3816	1263	1849	338	359	7		

- Molecule 41 is a protein called NDUCA1.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	G1	403	Total	C	H	N	O	S	0	0
			6146	1979	2999	558	594	16		

- Molecule 42 is a protein called NDUCA2.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	G2	236	Total	C	H	N	O	S	0	0
			3650	1138	1846	323	338	5		

- Molecule 43 is a protein called NDUCA3.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	G3	261	Total	C	H	N	O	S	0	0
			3905	1226	1944	356	373	6		

- Molecule 44 is a protein called ND1.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	N1	310	Total	C	H	N	O	S	0	0
			5331	1783	2726	380	435	7		

- Molecule 45 is a protein called ND2A.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	N2	296	Total	C	H	N	O	S	0	0
			5101	1725	2589	362	418	7		

- Molecule 46 is a protein called ND3.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	N3	121	Total	C	H	N	O	S	0	0
			2094	720	1057	143	172	2		
46	N6	154	Total	C	H	N	O	S	0	0
			2642	857	1385	187	210	3		

- Molecule 47 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	N4	478	Total	C	H	N	O	S	0	0
			8215	2743	4214	582	663	13		

- Molecule 48 is a protein called ND5.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	N5	584	Total	C	H	N	O	S	0	0
			9869	3293	5032	711	808	25		

- Molecule 49 is a protein called NDUFS2.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	S2	394	Total	C	H	N	O	S	0	0
			6274	2041	3101	541	569	22		

- Molecule 50 is a protein called NDUFS3.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	S3	248	Total	C	H	N	O	S	0	0
			3978	1307	1928	346	384	13		

- Molecule 51 is a protein called NDUFS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	S4	190	Total	C	H	N	O	S	0	0
			3038	956	1502	300	273	7		

- Molecule 52 is a protein called NDUFS5.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	S5	122	Total	C	H	N	O	S	0	0
			1886	625	895	173	188	5		

- Molecule 53 is a protein called NDUFS6.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	S6	147	Total	C	H	N	O	S	0	0
			2392	759	1192	225	208	8		

- Molecule 54 is a protein called NDUFS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	S7	201	Total	C	H	N	O	S	0	0
			3045	975	1500	272	284	14		

- Molecule 55 is a protein called NDUFS8.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	S8	182	Total	C	H	N	O	S	0	0
			2843	915	1392	245	275	16		

- Molecule 56 is a protein called UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	U1	12	Total 76	C 36	H 16	N 12	O 12	0	0
56	U2	12	Total 76	C 36	H 16	N 12	O 12	0	0

- Molecule 57 is a protein called NDUFV1.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	V1	504	Total 7724	C 2463	H 3827	N 680	O 727	S 27	0	0

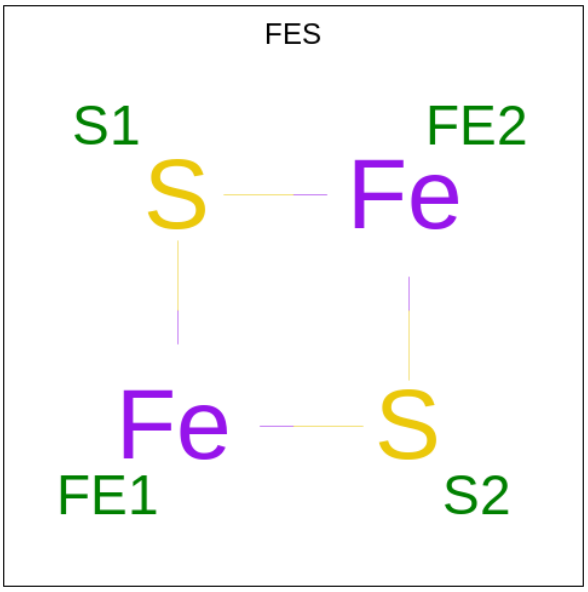
- Molecule 58 is a protein called NDUFV2.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	V2	225	Total 3460	C 1124	H 1701	N 299	O 319	S 17	0	0

- Molecule 59 is a protein called NDUEG7.

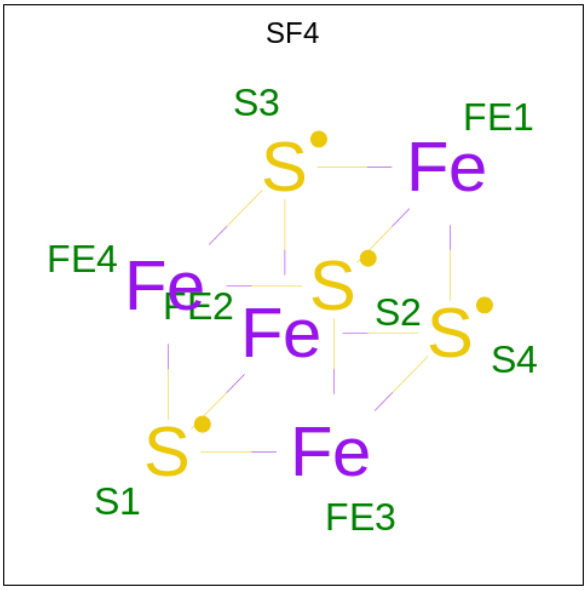
Mol	Chain	Residues	Atoms						AltConf	Trace
59	E7	246	Total 3780	C 1205	H 1892	N 332	O 344	S 7	0	0

- Molecule 60 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
60	1A	1	Total Fe S 4 2 2	0
60	V2	1	Total Fe S 4 2 2	0

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

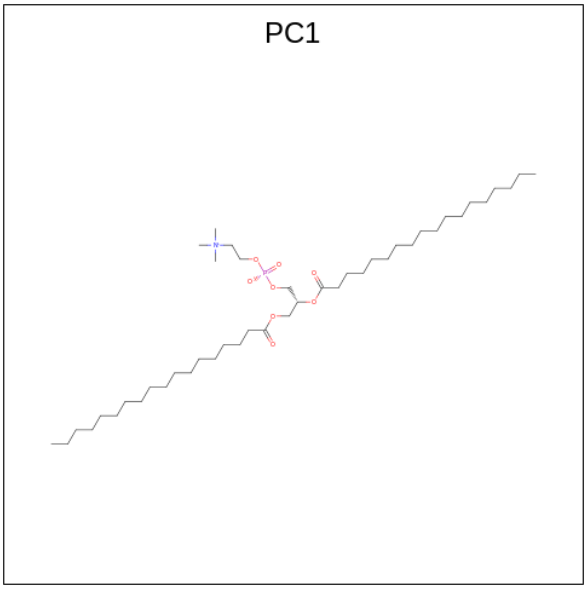


Mol	Chain	Residues	Atoms	AltConf
61	1A	1	Total Fe S 8 4 4	0
61	1A	1	Total Fe S 8 4 4	0
61	S7	1	Total Fe S 8 4 4	0
61	S8	1	Total Fe S 8 4 4	0
61	S8	1	Total Fe S 8 4 4	0
61	V1	1	Total Fe S 8 4 4	0

- Molecule 62 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
62	1A	1	Total K 1 1	0

- Molecule 63 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
63	A1	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
63	A1	1	Total	C	H	N	O	P	0
			67	21	36	1	8	1	
63	A9	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
63	A9	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
63	AL	1	Total	C	H	N	O	P	0
			127	40	77	1	8	1	
63	AM	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
63	AM	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
63	AN	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
63	B5	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
63	B5	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
63	C4	1	Total	C	H	N	O	P	0
			88	28	50	1	8	1	
63	E4	1	Total	C	H	N	O	P	0
			130	41	79	1	8	1	

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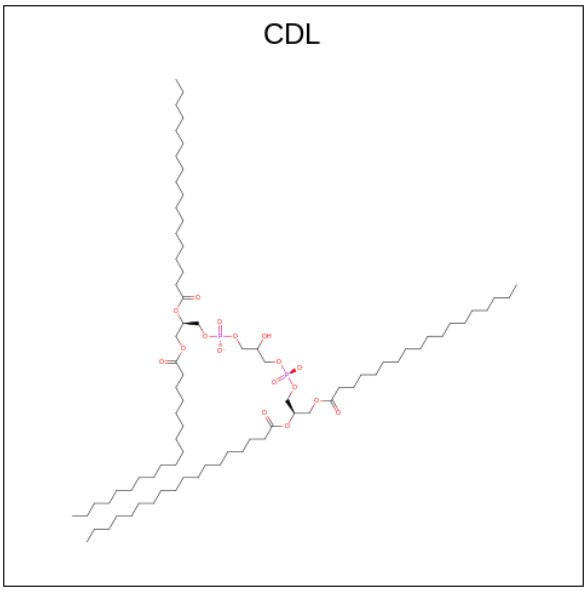
Mol	Chain	Residues	Atoms						AltConf
63	E8	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
63	E8	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
63	E8	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
63	E8	1	Total	C	H	N	O	P	0
			64	20	34	1	8	1	
63	ED	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
63	N1	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
63	N1	1	Total	C	H	N	O	P	0
			94	30	54	1	8	1	
63	N2	1	Total	C	H	N	O	P	0
			85	27	48	1	8	1	
63	N3	1	Total	C	H	N	O	P	0
			103	32	61	1	8	1	
63	N4	1	Total	C	H	N	O	P	0
			91	29	52	1	8	1	
63	N4	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
63	N5	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
63	N5	1	Total	C	H	N	O	P	0
			97	31	56	1	8	1	
63	N5	1	Total	C	H	N	O	P	0
			82	26	46	1	8	1	

- Molecule 64 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms					AltConf
64	A3	1	Total	C	H	O	P	0
			118	39	60	17	2	
64	AL	1	Total	C	H	O	P	0
			148	49	80	17	2	
64	AL	1	Total	C	H	O	P	0
			136	45	72	17	2	
64	AL	1	Total	C	H	O	P	0
			154	51	84	17	2	
64	AM	1	Total	C	H	O	P	0
			163	53	91	17	2	
64	AM	1	Total	C	H	O	P	0
			163	53	91	17	2	
64	AM	1	Total	C	H	O	P	0
			163	53	91	17	2	
64	B3	1	Total	C	H	O	P	0
			139	46	74	17	2	
64	B5	1	Total	C	H	O	P	0
			118	39	60	17	2	
64	C4	1	Total	C	H	O	P	0
			235	75	141	17	2	
64	C4	1	Total	C	H	O	P	0
			151	50	82	17	2	
64	E6	1	Total	C	H	O	P	0
			136	45	72	17	2	
64	EA	1	Total	C	H	O	P	0
			121	40	62	17	2	
64	EA	1	Total	C	H	O	P	0
			109	36	54	17	2	

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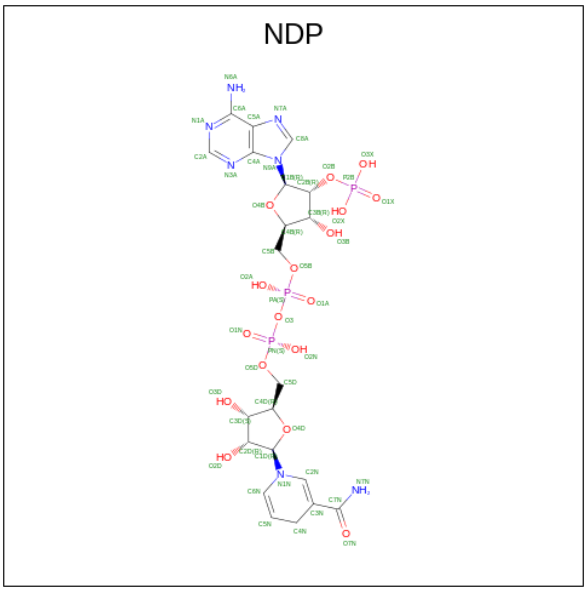
Mol	Chain	Residues	Atoms					AltConf
64	N4	1	Total	C	H	O	P	0
			247	79	149	17	2	
64	N5	1	Total	C	H	O	P	0
			157	51	87	17	2	
64	N5	1	Total	C	H	O	P	0
			229	74	136	17	2	
64	E7	1	Total	C	H	O	P	0
			148	49	80	17	2	

- Molecule 65 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

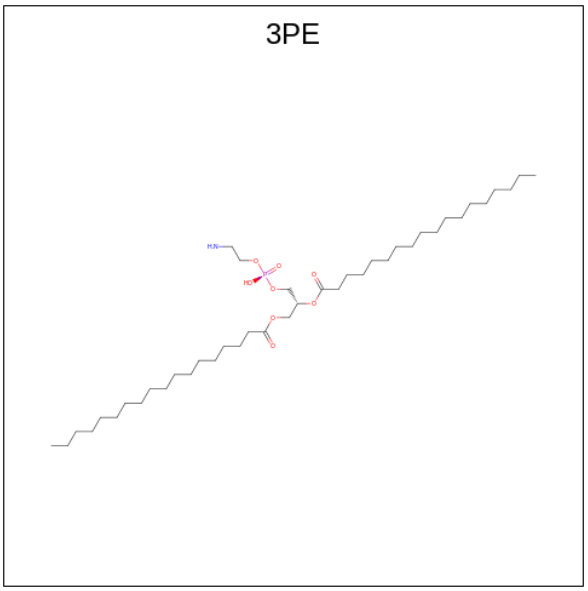


Mol	Chain	Residues	Atoms						AltConf
65	A9	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

- Molecule 66 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 67 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
67	AN	1	Total	C	H	N	O	P	0
			132	41	81	1	8	1	

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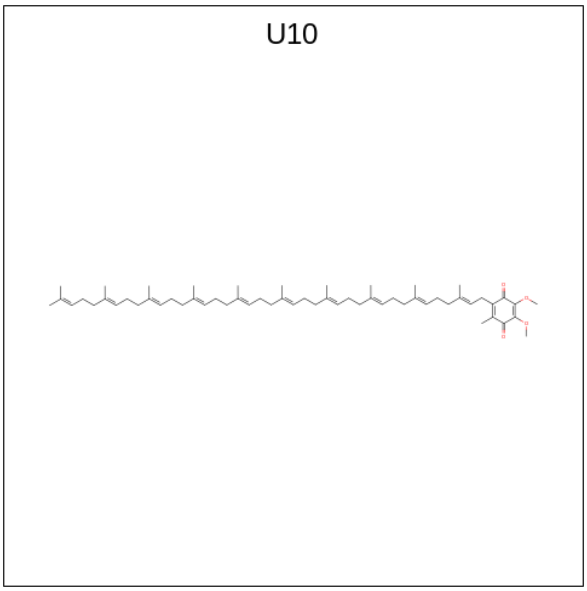
Mol	Chain	Residues	Atoms						AltConf
67	G1	1	Total	C	H	N	O	P	0
			96	30	56	1	8	1	
67	N4	1	Total	C	H	N	O	P	0
			96	31	55	1	8	1	
67	N5	1	Total	C	H	N	O	P	0
			132	41	81	1	8	1	

- Molecule 68 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

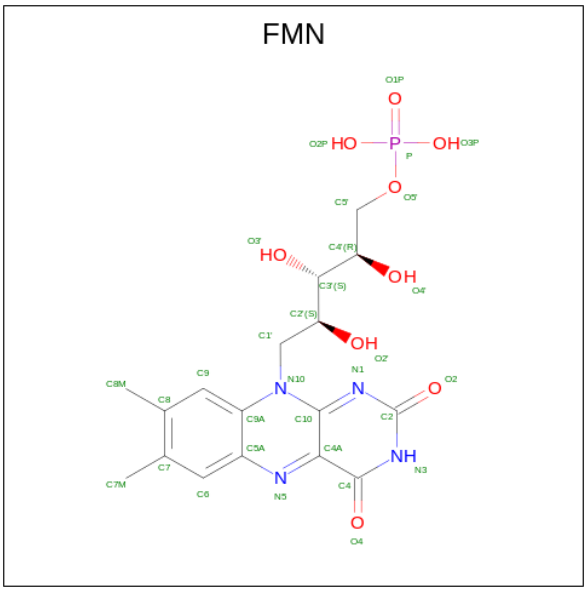


Mol	Chain	Residues	Atoms				AltConf
68	N4	1	Total	C	H	O	0
			98	39	55	4	

- Molecule 69 is ZINC ION (three-letter code: ZN) (formula: Zn).

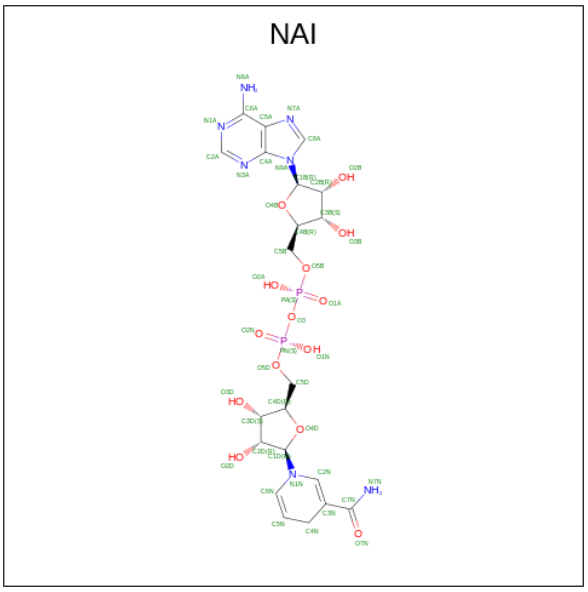
Mol	Chain	Residues	Atoms		AltConf
69	S6	1	Total	Zn	0
			1	1	
69	E7	1	Total	Zn	0
			1	1	

- Molecule 70 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms						AltConf
70	V1	1	Total	C	H	N	O	P	0
			50	17	19	4	9	1	

- Molecule 71 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



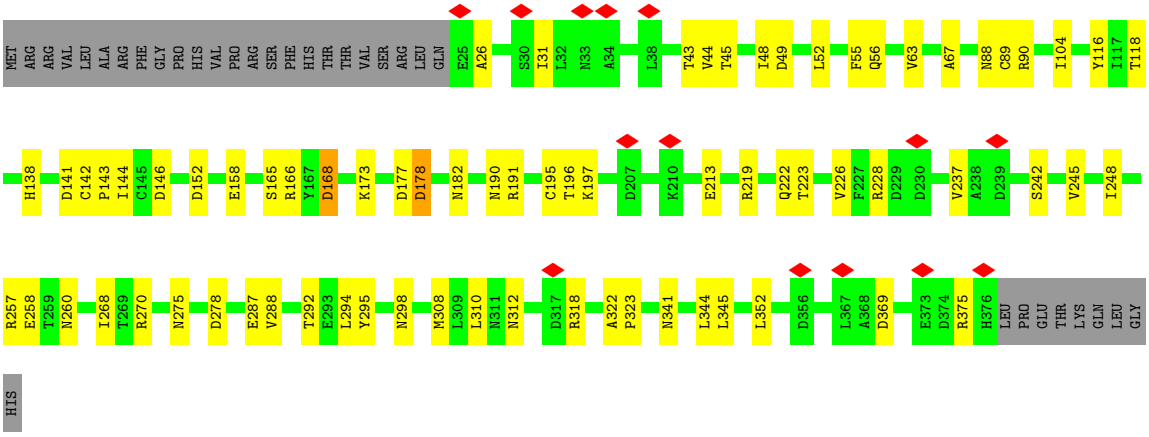
Mol	Chain	Residues	Atoms					AltConf
71	V1	1	Total	C	N	O	P	0
			44	21	7	14	2	

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.

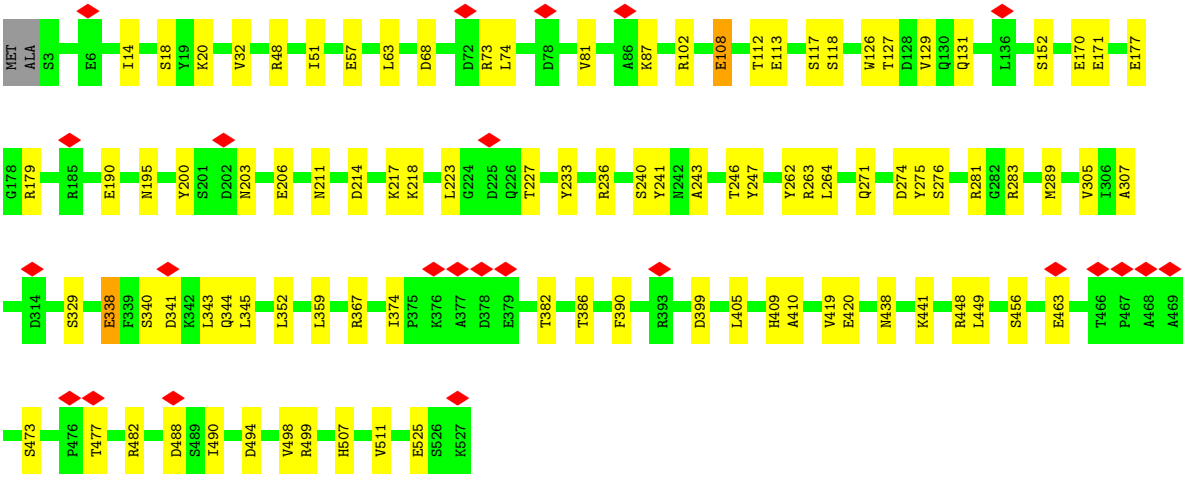
- Molecule 1: NDUFS1A

Chain 1A:



- Molecule 2: NDUFS1B

Chain 1B:



- Molecule 3: ND2B

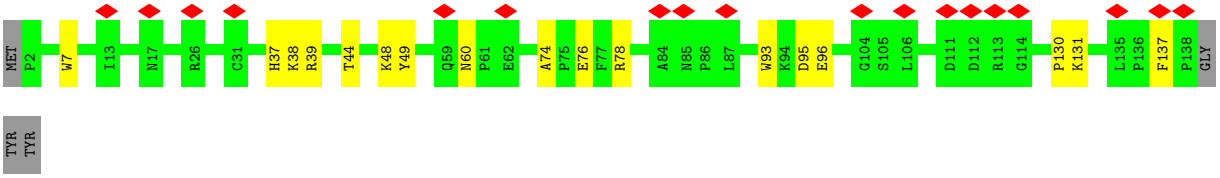
Chain 2B:

• Molecule 4: ND4L

Chain 4L:

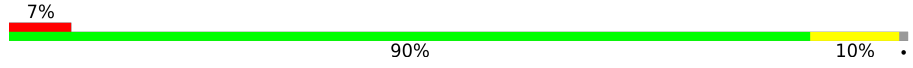
• Molecule 5: NDUFA1

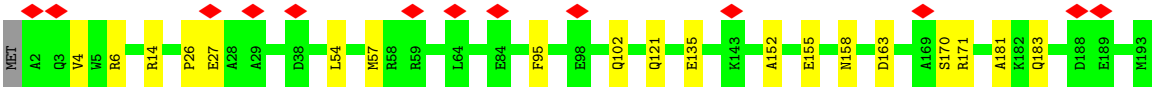
Chain A1:



• Molecule 6: NDUFA2

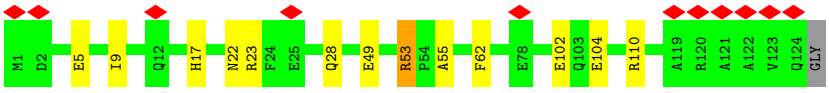
Chain A2:





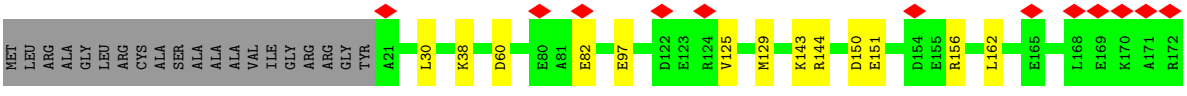
• Molecule 7: NDUFA3

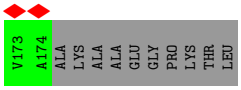
Chain A3:



• Molecule 8: NDUFA5

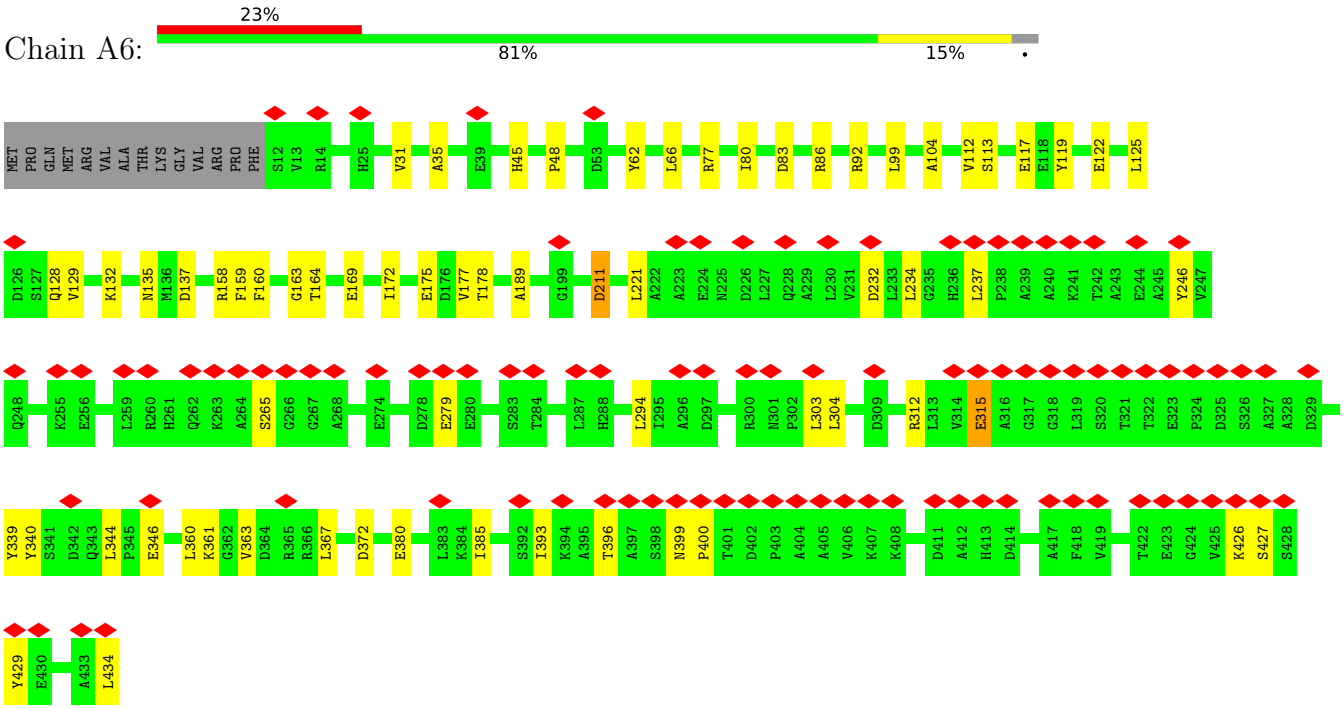
Chain A5:





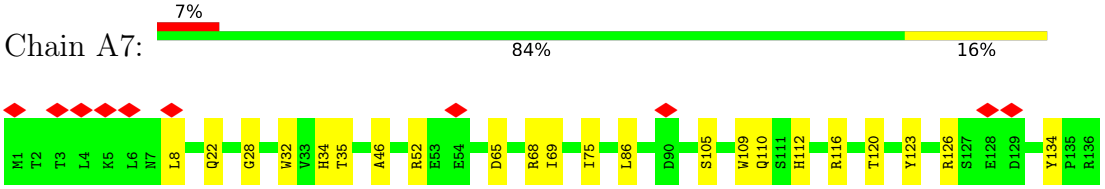
• Molecule 9: NDUFA6

Chain A6:



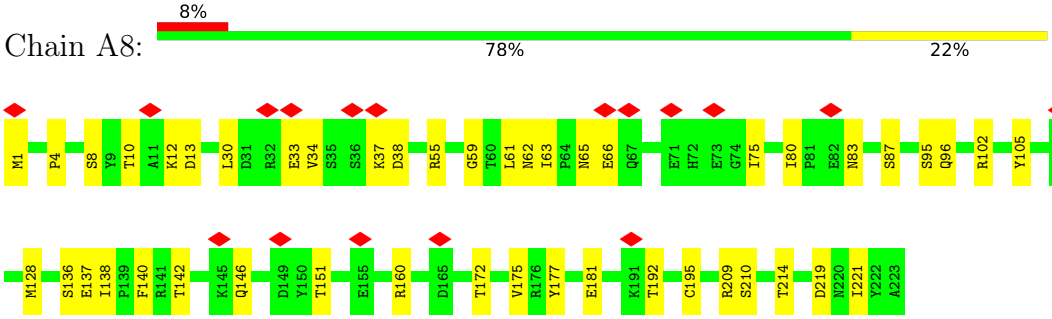
• Molecule 10: NDUFA7

Chain A7:



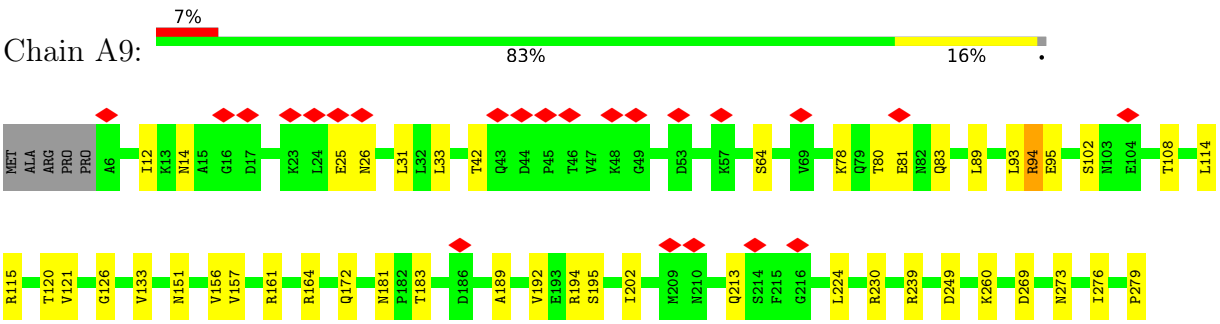
• Molecule 11: NDUFA8

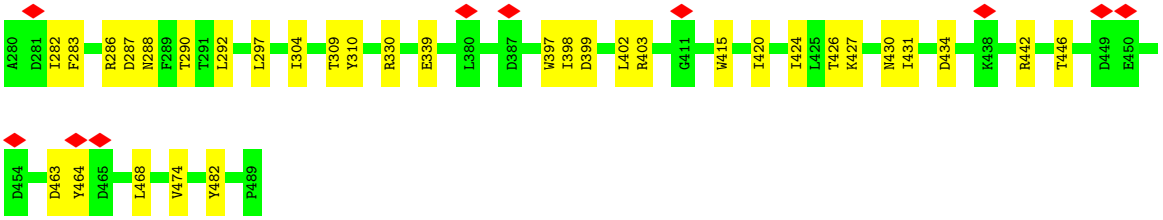
Chain A8:



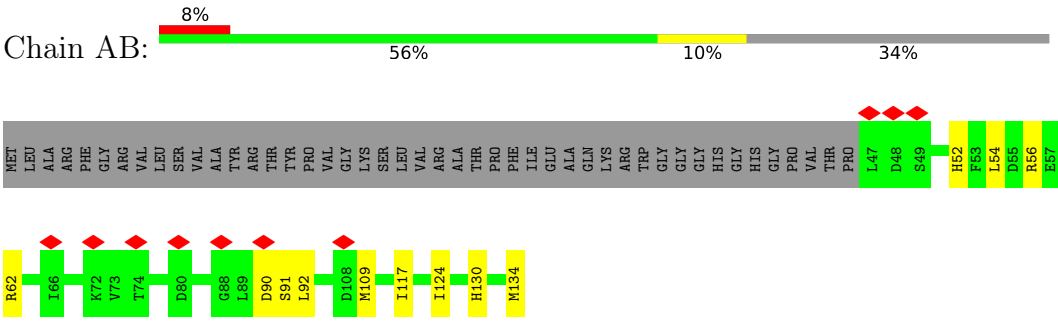
• Molecule 12: NDUFA9

Chain A9:

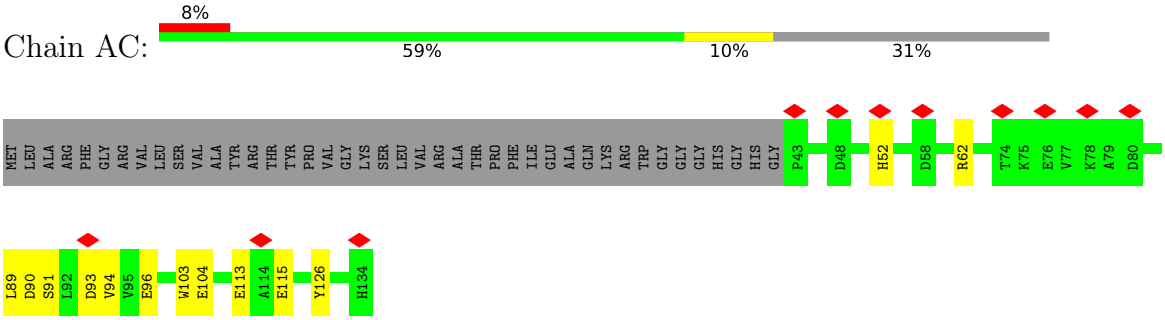




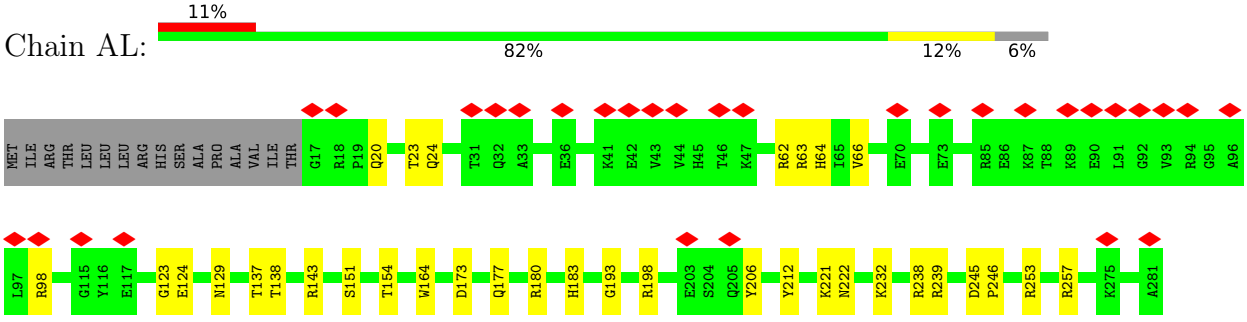
• Molecule 13: NDUFAB1-alpha



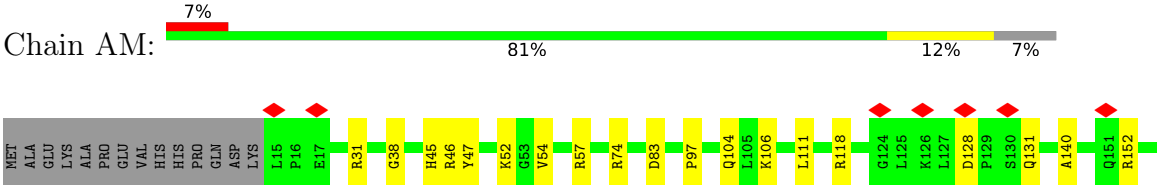
• Molecule 14: NDUFAB1-beta

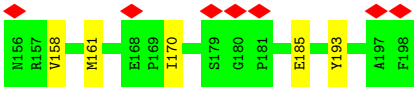


• Molecule 15: NDUFA12



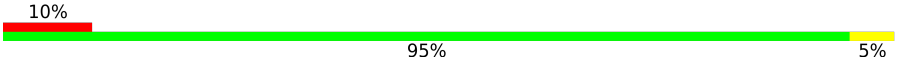
• Molecule 16: NDUFA13

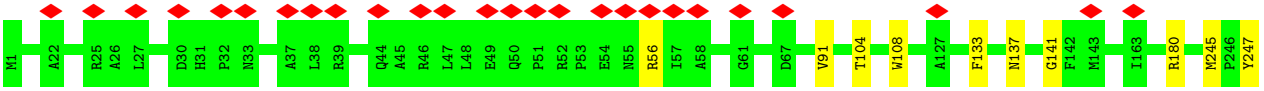




• Molecule 17: NDUFA11

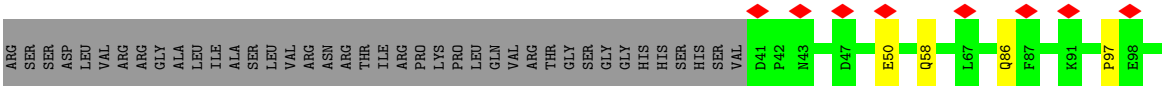
Chain AN:

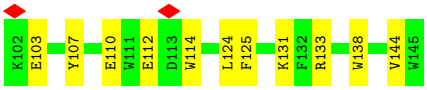




• Molecule 18: NDUFB2

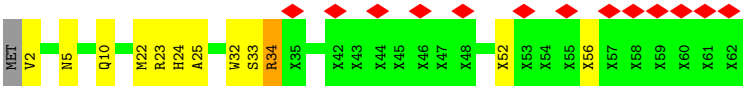
Chain B2:





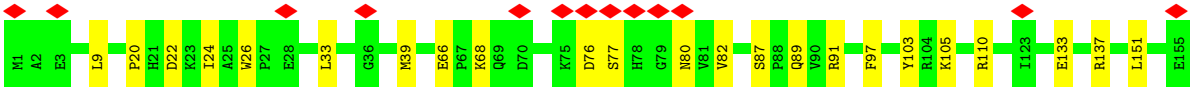
• Molecule 19: NDUFB3

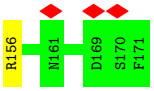
Chain B3:



• Molecule 20: NDUFB4

Chain B4:

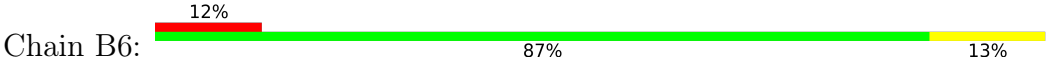


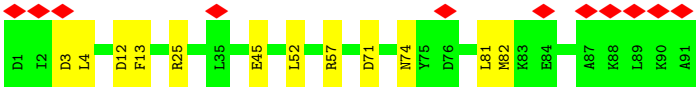


• Molecule 21: NDUFB5

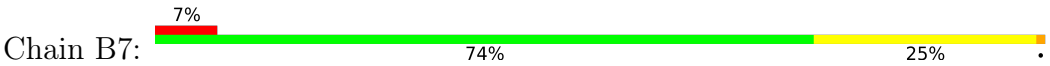
Chain B5:

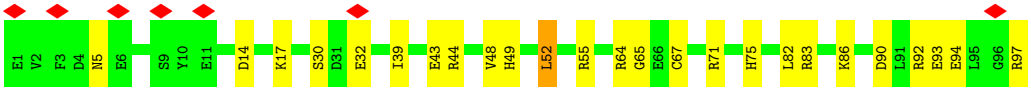
• Molecule 22: NDUFB6



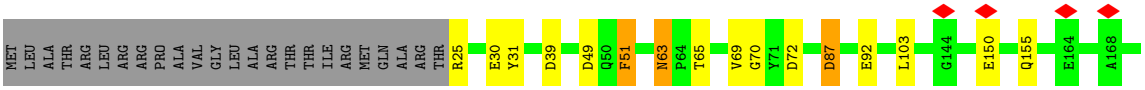


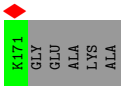
• Molecule 23: NDUFB7



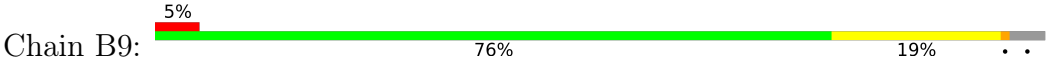


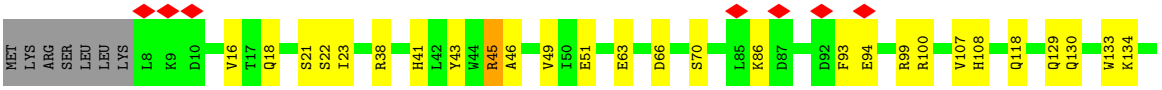
• Molecule 24: NDUFB8

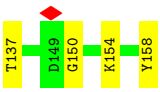




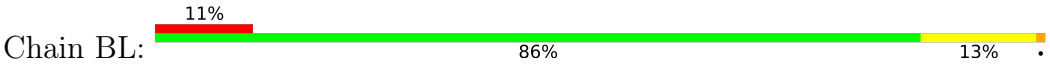
• Molecule 25: NDUFB9

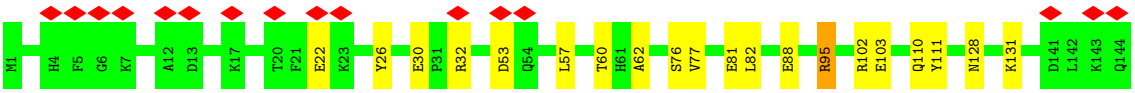






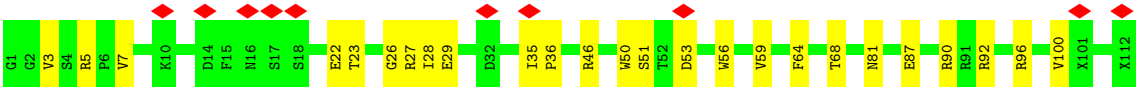
• Molecule 26: NDUFB10





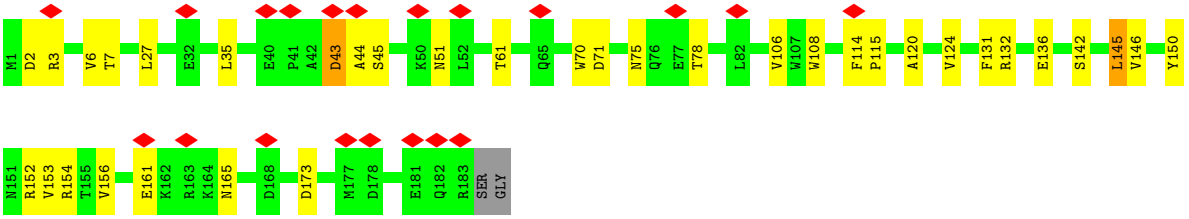
• Molecule 27: NDUFB11

Chain BM:



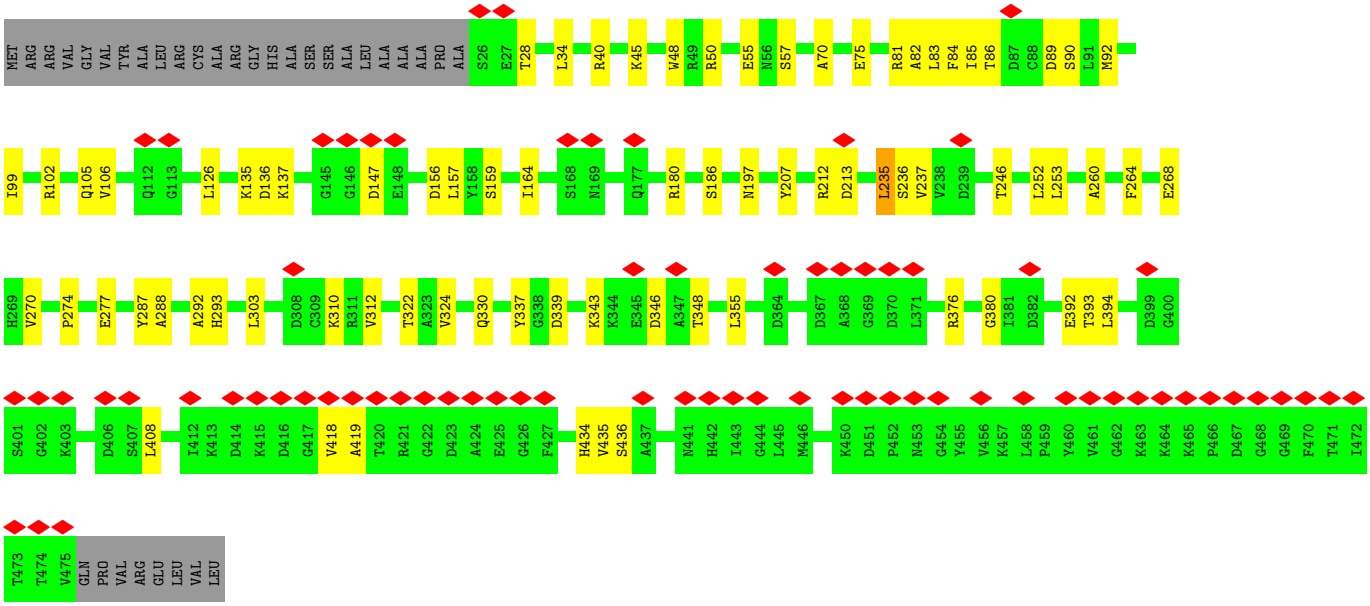
• Molecule 28: NDUFC2

Chain C4:



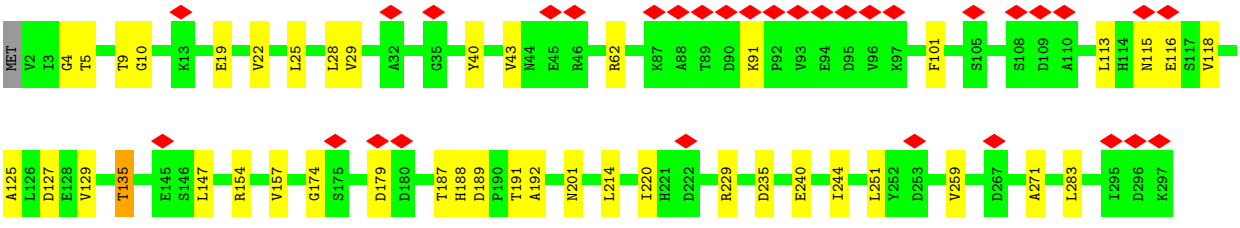
• Molecule 29: NDUEG1

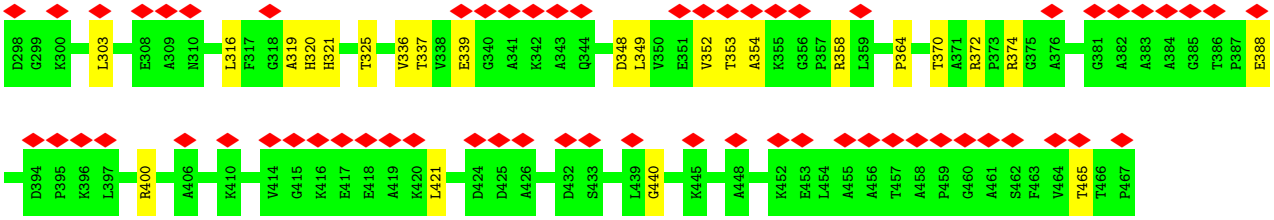
Chain E1:



• Molecule 30: NDUEG2

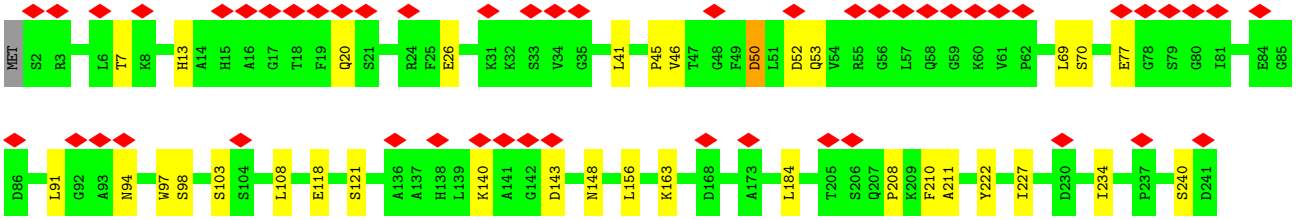
Chain E2:





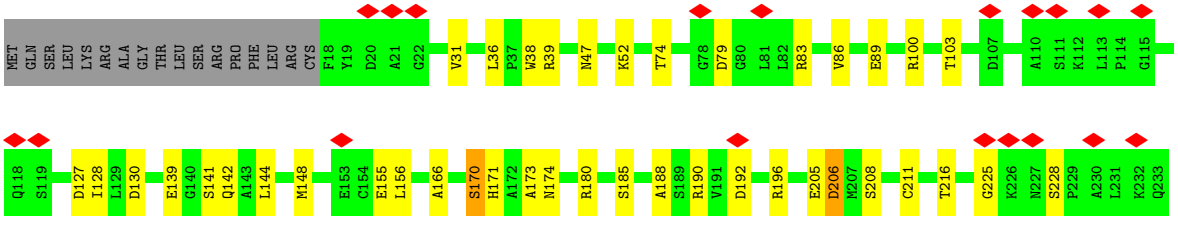
• Molecule 31: NDUEG3

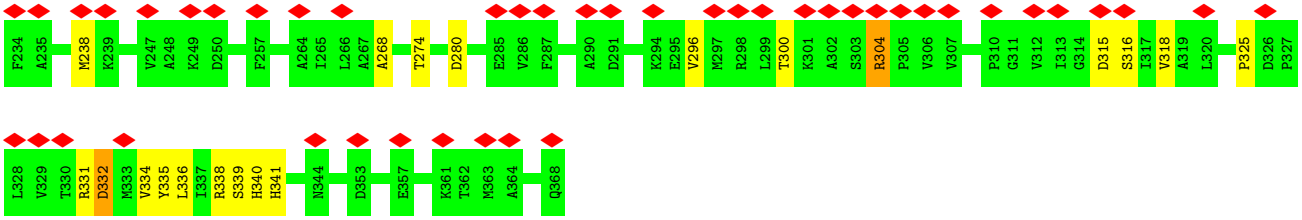
Chain E3:



• Molecule 32: NDUEG4

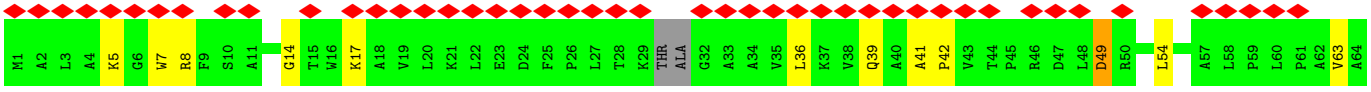
Chain E4:

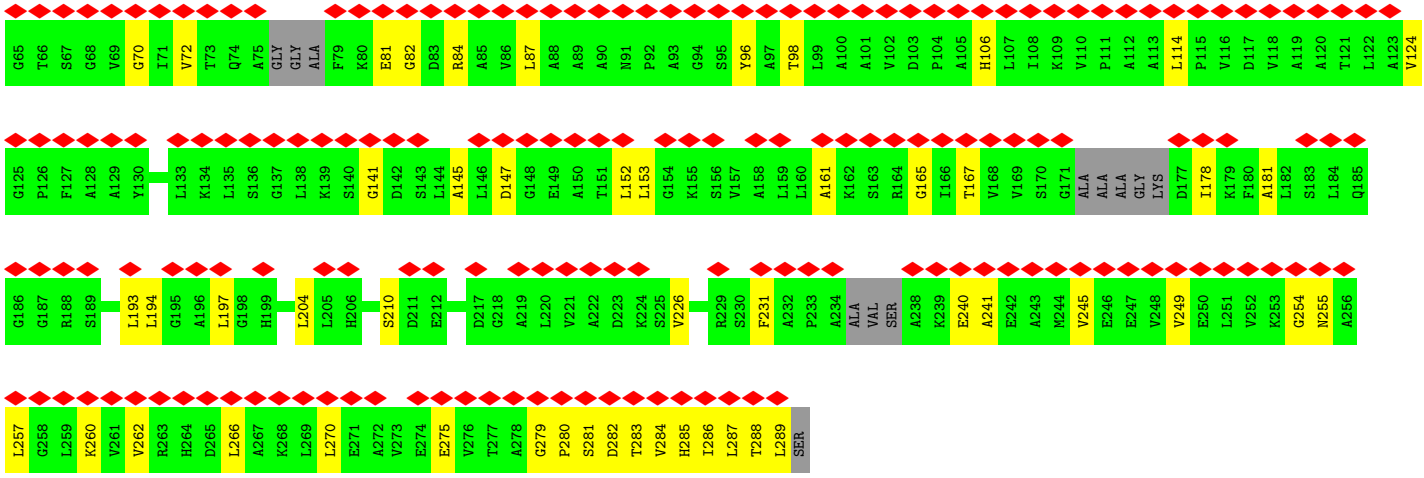




• Molecule 33: NDUEG5

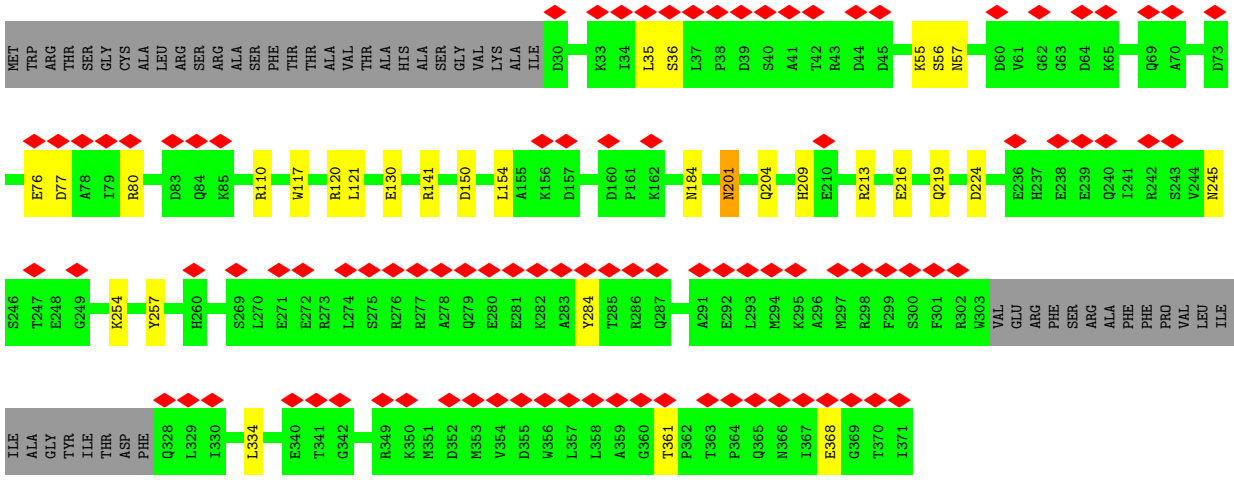
Chain E5:





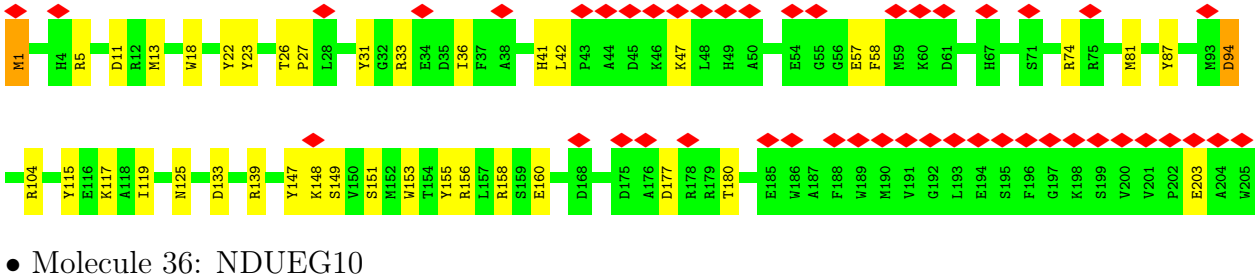
• Molecule 34: NDUEG6

Chain E6:



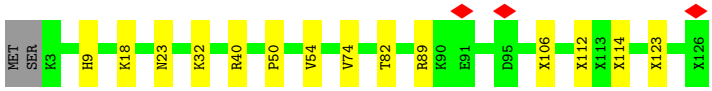
• Molecule 35: NDUEG8

Chain E8:



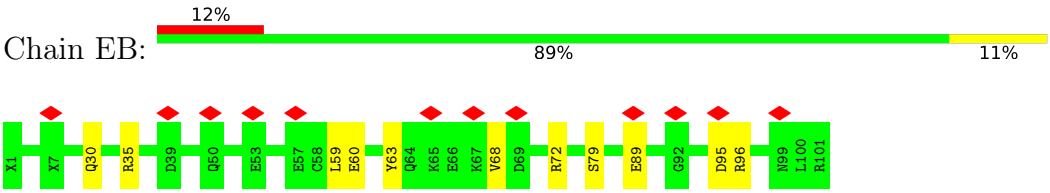
• Molecule 36: NDUEG10

Chain EA:



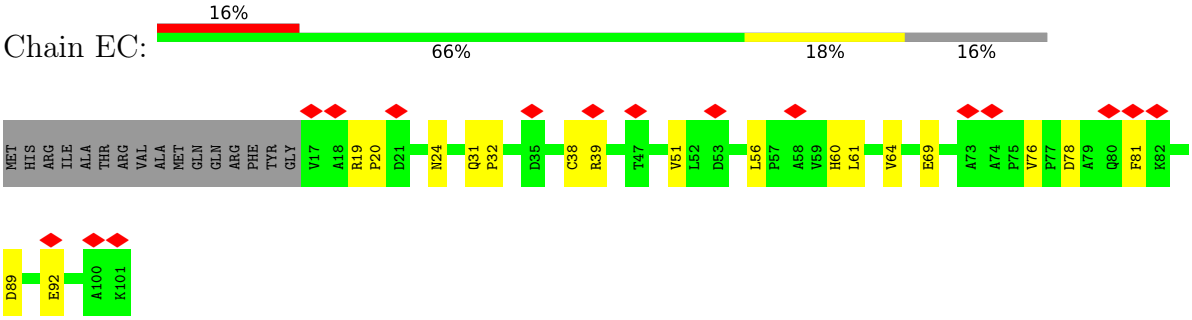
• Molecule 37: NDUEG11

Chain EB:



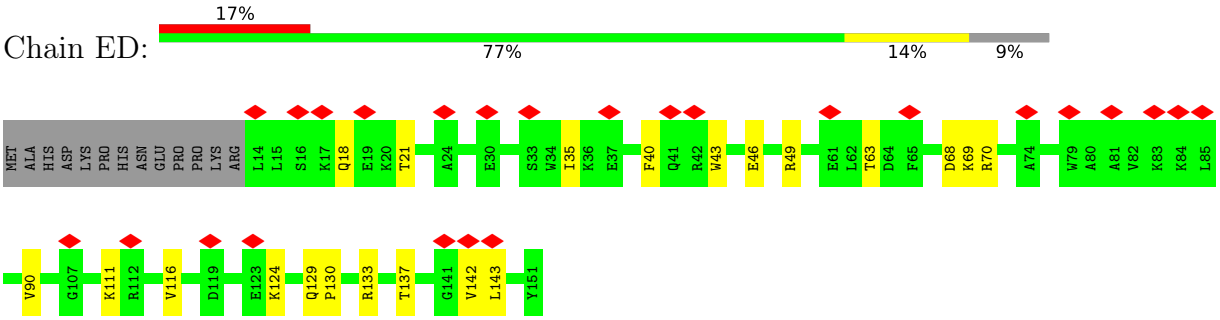
• Molecule 38: NDUEG12

Chain EC:



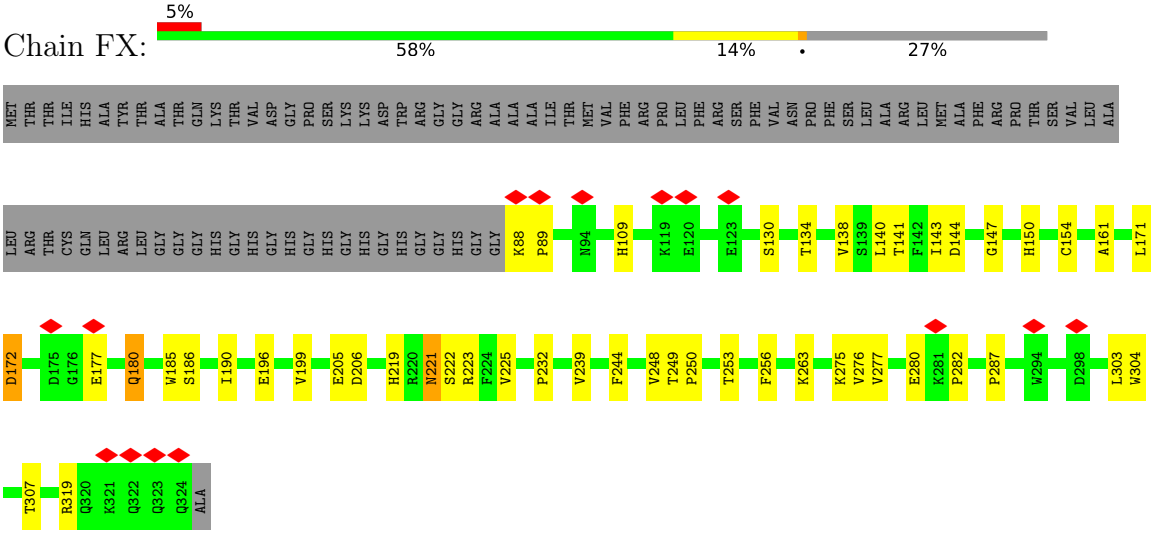
• Molecule 39: NDUEG13

Chain ED:



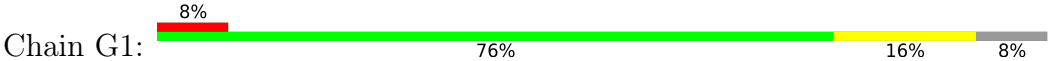
• Molecule 40: NDUFX

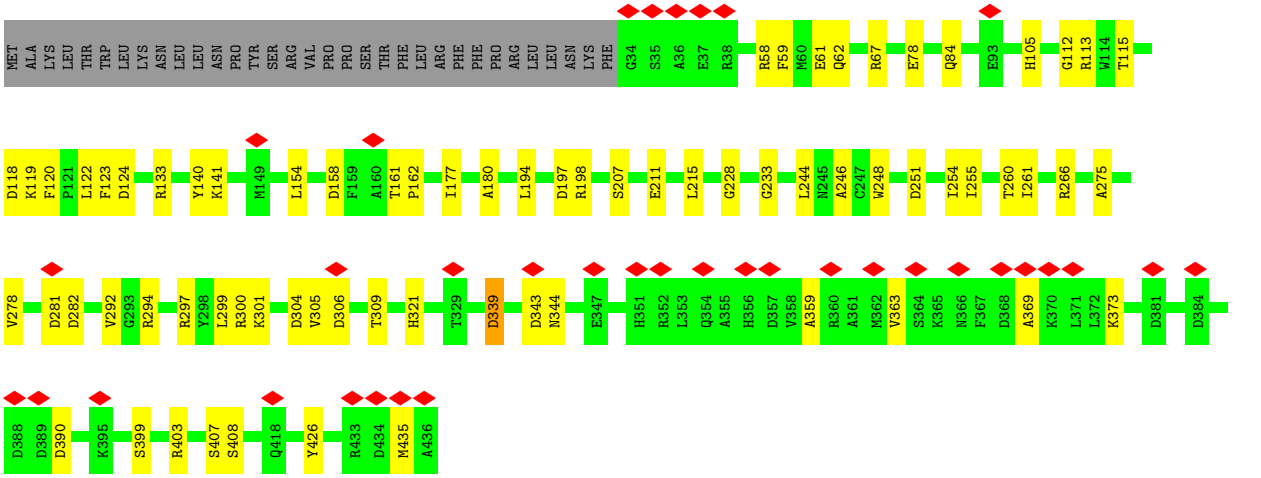
Chain FX:



• Molecule 41: NDUCA1

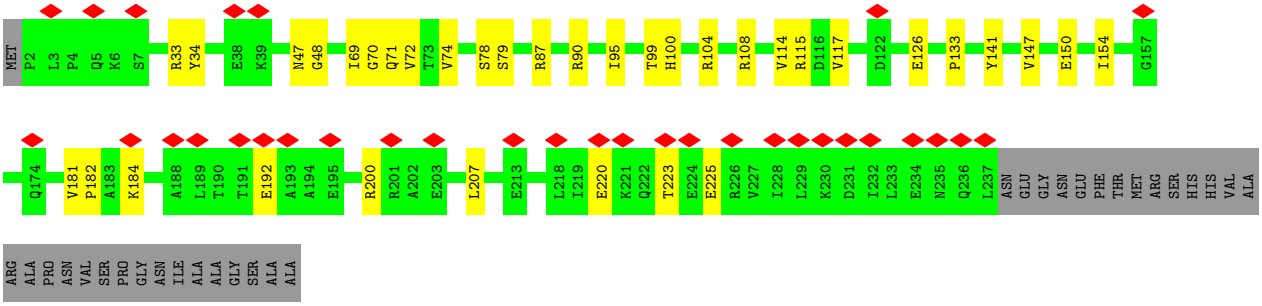
Chain G1:





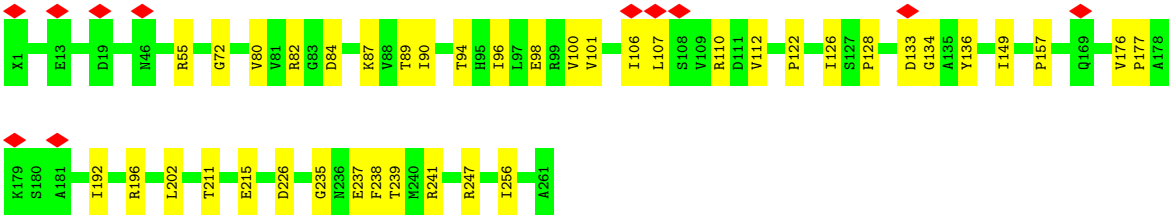
- Molecule 42: NDUCA2

Chain G2:



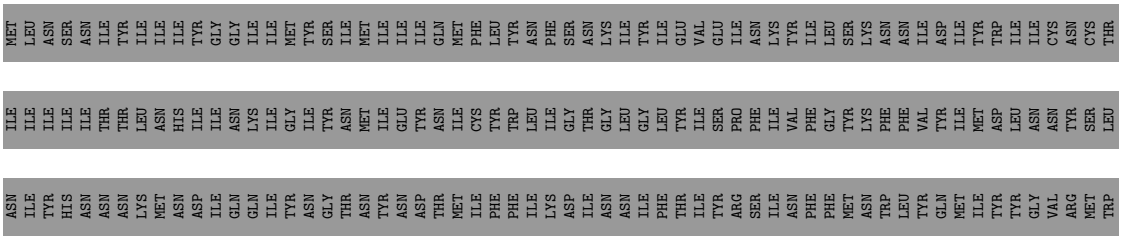
- Molecule 43: NDUCA3

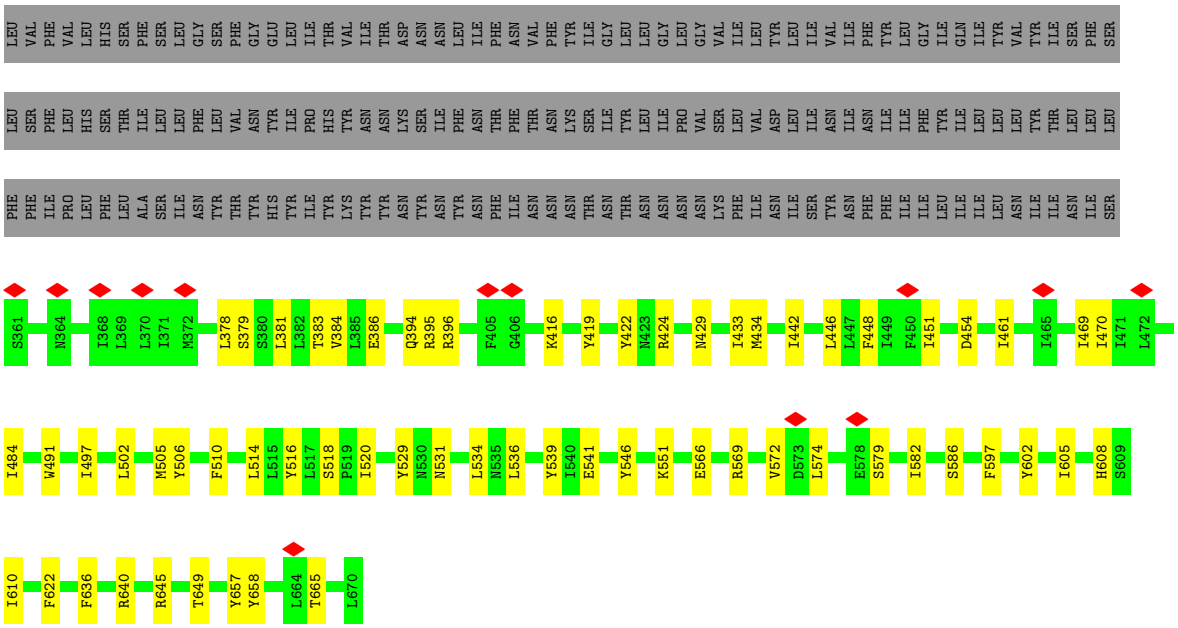
Chain G3:



- Molecule 44: ND1

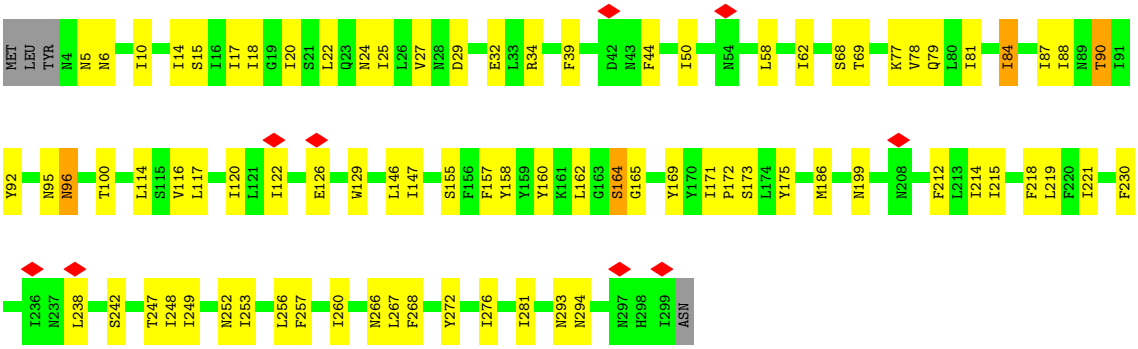
Chain N1:





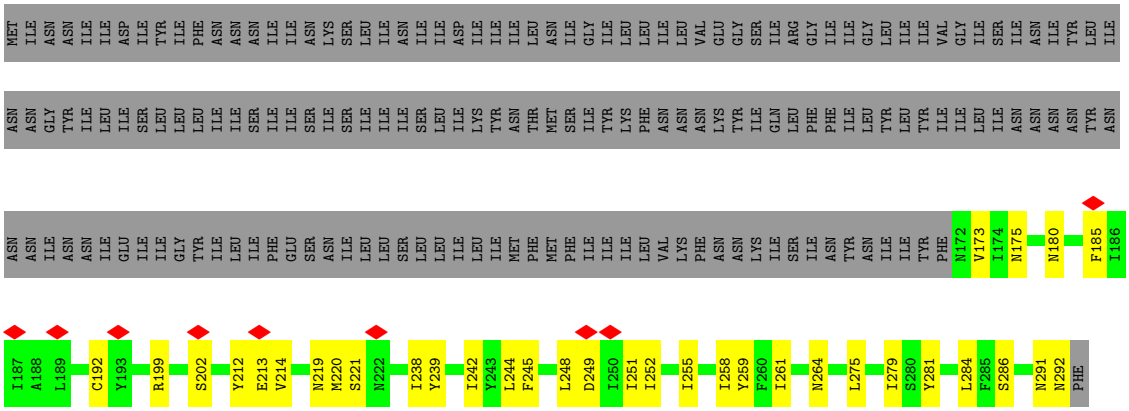
• Molecule 45: ND2A

Chain N2:



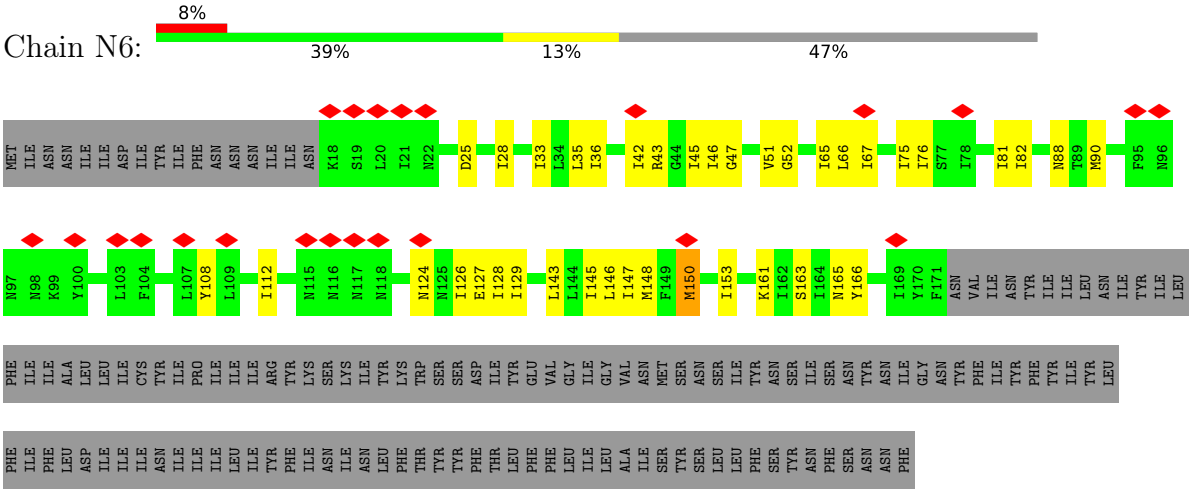
• Molecule 46: ND3

Chain N3:



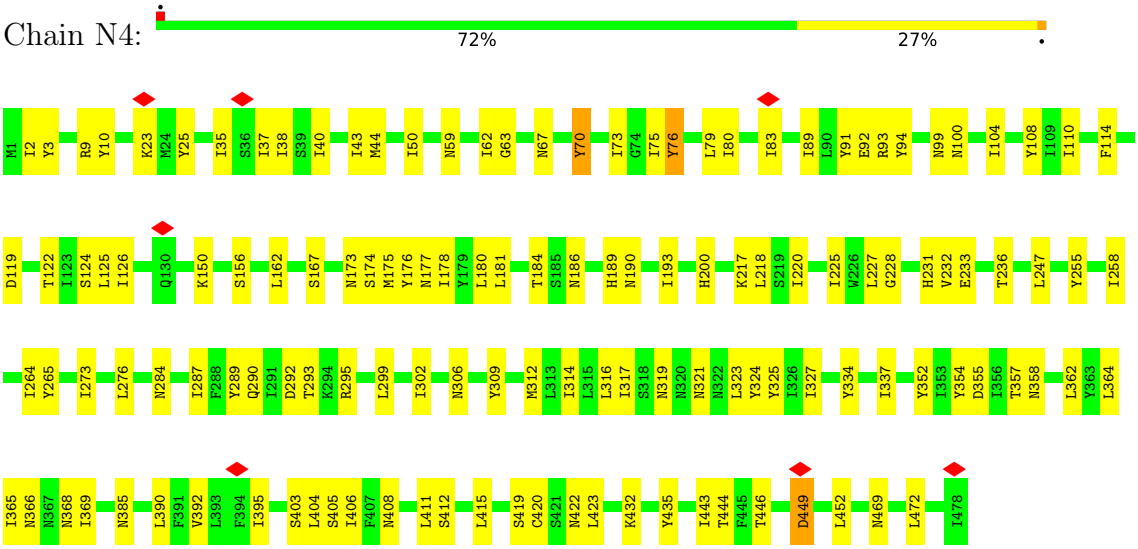
• Molecule 46: ND3

Chain N6:



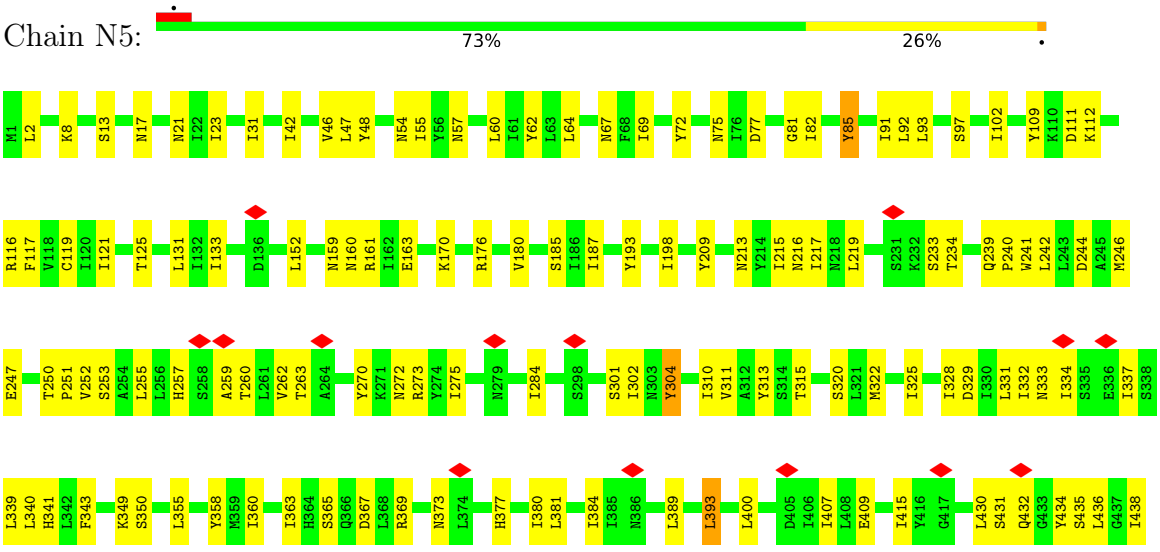
• Molecule 47: NADH-ubiquinone oxidoreductase chain 4

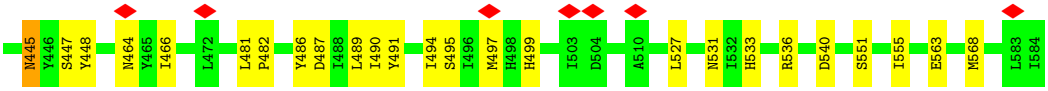
Chain N4:



• Molecule 48: ND5

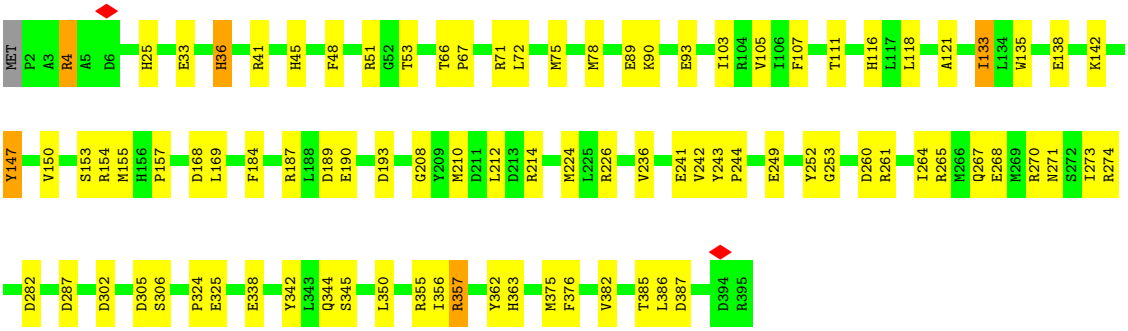
Chain N5:





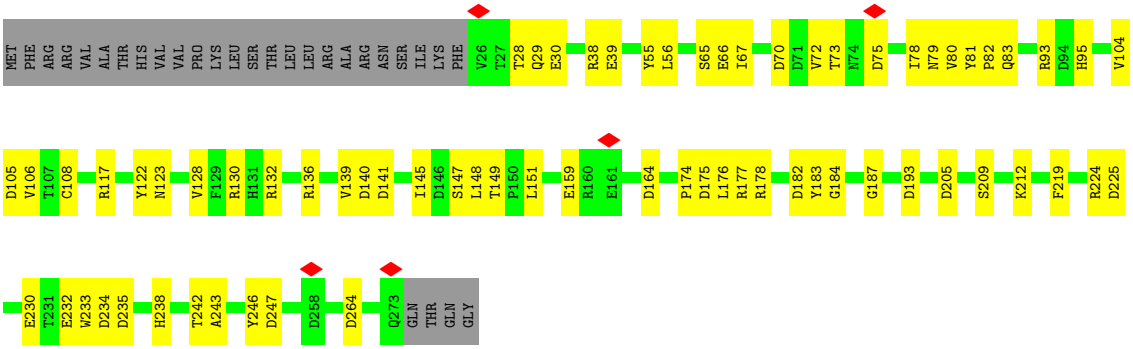
• Molecule 49: NDUFS2

Chain S2:



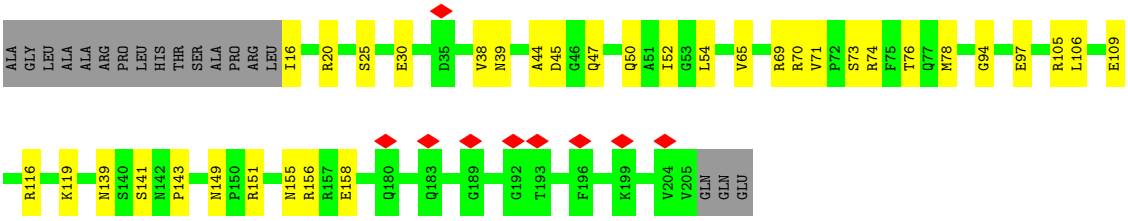
• Molecule 50: NDUFS3

Chain S3:



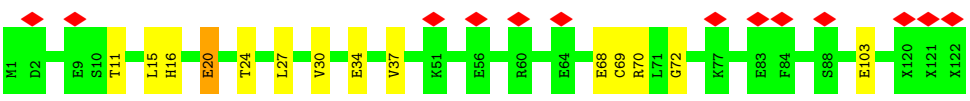
• Molecule 51: NDUFS4

Chain S4:



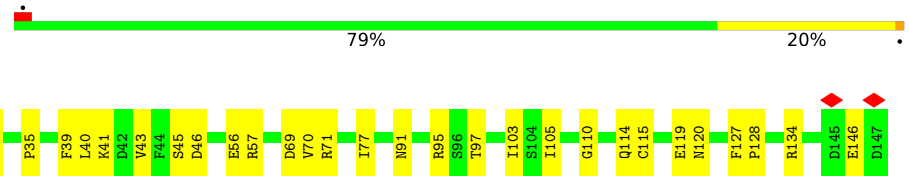
• Molecule 52: NDUFS5

Chain S5:



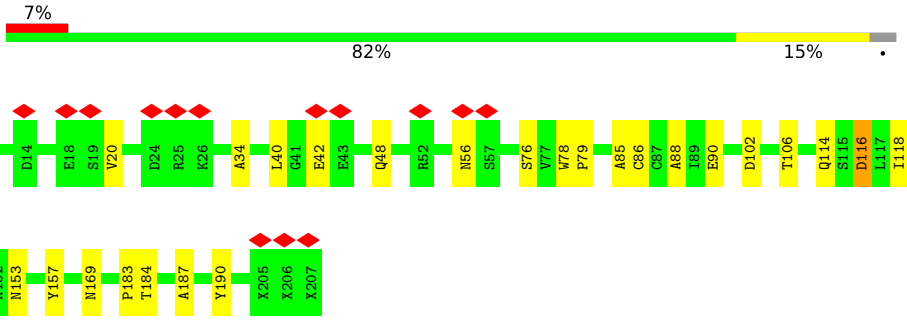
• Molecule 53: NDUFS6

Chain S6:



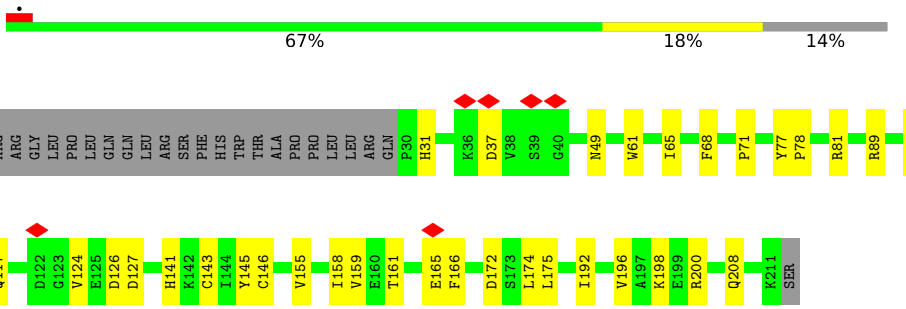
• Molecule 54: NDUFS7

Chain S7:



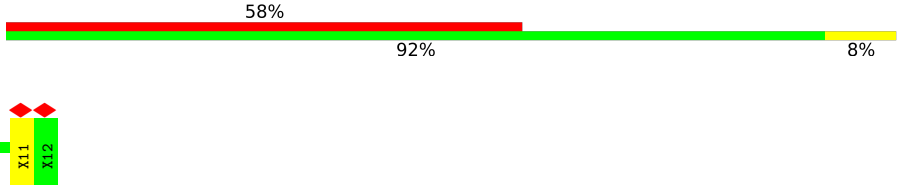
• Molecule 55: NDUFS8

Chain S8:



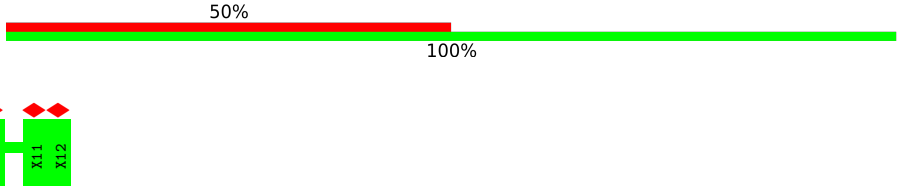
• Molecule 56: UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK

Chain U1:



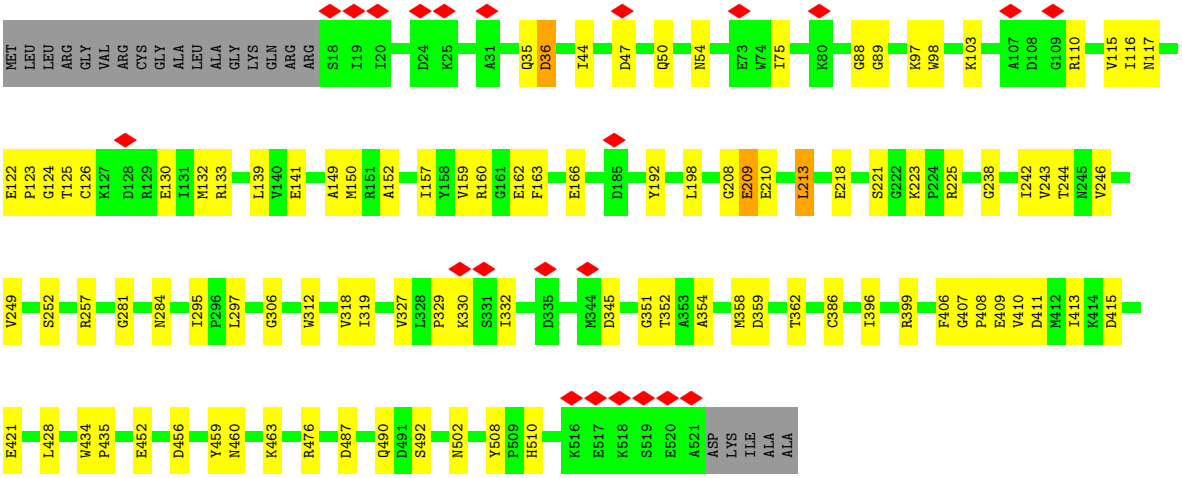
• Molecule 56: UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK

Chain U2:

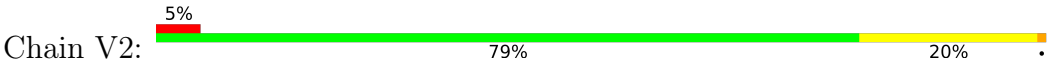


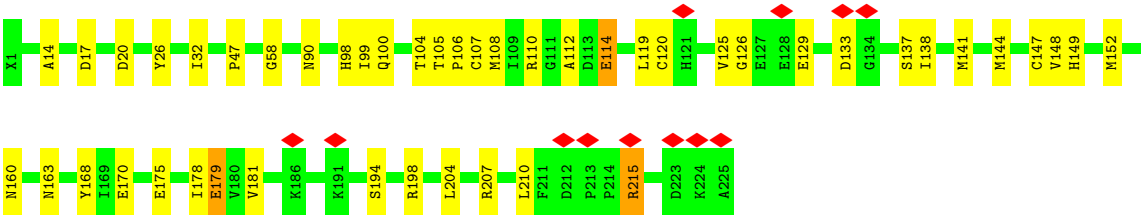
• Molecule 57: NDUFV1

Chain V1:

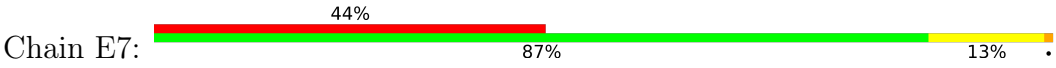


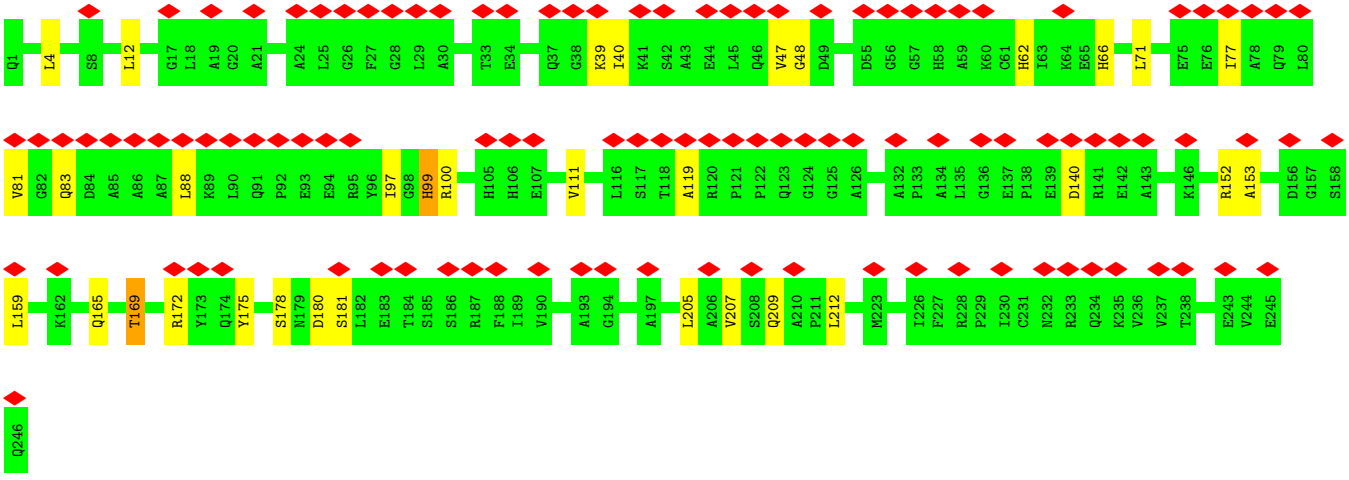
- Molecule 58: NDUFV2





- Molecule 59: NDUEG7





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	76643	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 ($e^-/Å^2$)	61.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	41.632	Depositor
Minimum map value	-19.553	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.993	Depositor
Recommended contour level	5.0	Depositor
Map size (Å)	446.4, 446.4, 446.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	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: K, U10, NDP, SF4, ZN, 3PE, ZMP, FES, FMN, PC1, 2MR, NAI, CDL

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	1A	0.27	0/2858	0.50	0/3878
2	1B	0.27	0/4306	0.49	0/5854
3	2B	0.28	0/958	0.43	0/1306
4	4L	0.27	0/924	0.42	0/1261
5	A1	0.25	0/1108	0.46	0/1511
6	A2	0.25	0/1530	0.49	0/2089
7	A3	0.27	0/1079	0.53	0/1453
8	A5	0.26	0/1282	0.50	0/1737
9	A6	0.25	0/3395	0.49	0/4608
10	A7	0.26	0/1194	0.54	0/1619
11	A8	0.27	0/1879	0.46	0/2543
12	A9	0.27	0/3920	0.50	0/5335
13	AB	0.26	0/704	0.42	0/951
14	AC	0.26	0/736	0.41	0/1000
15	AL	0.26	0/2317	0.52	0/3136
16	AM	0.27	0/1533	0.48	0/2079
17	AN	0.26	0/2382	0.47	0/3249
18	B2	0.25	0/947	0.43	0/1291
19	B3	0.27	0/326	0.50	0/441
20	B4	0.27	0/1419	0.49	0/1922
21	B5	0.27	0/1111	0.49	0/1505
22	B6	0.28	0/803	0.46	0/1087
23	B7	0.26	0/877	0.53	0/1172
24	B8	0.28	0/1273	0.42	0/1733
25	B9	0.27	0/1274	0.48	0/1728
26	BL	0.28	0/1266	0.49	0/1710
27	BM	0.29	0/876	0.53	0/1192
28	C4	0.26	0/1592	0.47	0/2158
29	E1	0.26	0/3596	0.47	0/4879
30	E2	0.26	0/3658	0.48	0/4983
31	E3	0.25	0/3320	0.46	0/4520
32	E4	0.26	0/2850	0.47	0/3884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	E5	0.27	0/2004	0.49	0/2721
34	E6	0.24	0/2750	0.46	0/3724
35	E8	0.26	0/1747	0.49	0/2367
36	EA	0.26	0/858	0.45	0/1163
37	EB	0.24	0/650	0.51	0/863
38	EC	0.26	0/676	0.45	0/925
39	ED	0.25	0/1176	0.49	0/1590
40	FX	0.27	0/2035	0.45	0/2763
41	G1	0.27	0/3234	0.50	0/4401
42	G2	0.27	0/1832	0.53	0/2476
43	G3	0.27	0/1957	0.53	0/2646
44	N1	0.27	0/2672	0.44	0/3639
45	N2	0.28	0/2582	0.42	0/3530
46	N3	0.29	0/1068	0.43	0/1456
46	N6	0.26	0/1275	0.43	0/1730
47	N4	0.29	0/4105	0.43	0/5594
48	N5	0.28	0/4963	0.44	0/6758
49	S2	0.29	0/3244	0.52	0/4403
50	S3	0.28	0/2112	0.52	0/2874
51	S4	0.27	0/1573	0.56	0/2107
52	S5	0.26	0/960	0.47	0/1291
53	S6	0.27	0/1232	0.51	0/1659
54	S7	0.27	0/1558	0.50	0/2120
55	S8	0.28	0/1485	0.50	0/2010
57	V1	0.27	0/3990	0.49	0/5394
58	V2	0.27	0/1787	0.47	0/2428
59	E7	0.26	0/1931	0.48	0/2618
All	All	0.27	0/112749	0.48	0/153064

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
12	A9	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	A9	286	ARG	Peptide

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	1A	2801	2700	2710	50	0
2	1B	4198	4159	4175	66	0
3	2B	1070	989	1009	23	0
4	4L	890	878	880	16	0
5	A1	1071	1026	1030	12	0
6	A2	1493	1474	1478	15	0
7	A3	1050	1039	1041	14	0
8	A5	1261	1248	1251	8	0
9	A6	3328	3280	3293	59	0
10	A7	1154	1118	1123	23	0
11	A8	1822	1726	1736	41	0
12	A9	3829	3850	3857	60	0
13	AB	694	673	677	9	0
14	AC	721	697	702	9	0
15	AL	2237	2172	2180	25	0
16	AM	1487	1448	1452	25	0
17	AN	2306	2267	2275	11	0
18	B2	913	857	858	15	0
19	B3	449	309	312	9	0
20	B4	1377	1358	1364	20	0
21	B5	1112	1069	1075	19	0
22	B6	773	747	751	14	0
23	B7	857	835	841	14	0
24	B8	1224	1127	1136	19	0
25	B9	1236	1207	1212	27	0
26	BL	1227	1179	1185	14	0
27	BM	910	827	830	20	0
28	C4	1545	1517	1519	26	0
29	E1	3512	3496	3510	49	0
30	E2	3563	3540	3554	42	0
31	E3	3255	3263	3279	42	0
32	E4	2770	2732	2742	47	0
33	E5	1977	2069	2075	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	E6	2674	2554	2562	20	0
35	E8	1691	1663	1668	32	0
36	EA	961	832	836	11	0
37	EB	774	631	636	9	0
38	EC	660	663	666	12	0
39	ED	1142	1131	1134	16	0
40	FX	1967	1849	1858	36	0
41	G1	3147	2999	3015	53	0
42	G2	1804	1846	1850	30	0
43	G3	1961	1944	1950	32	0
44	N1	2605	2726	2729	51	0
45	N2	2512	2589	2592	70	0
46	N3	1037	1057	1057	29	0
46	N6	1257	1385	1385	40	0
47	N4	4001	4214	4224	101	0
48	N5	4837	5032	5046	123	0
49	S2	3173	3101	3114	62	0
50	S3	2050	1928	1936	54	0
51	S4	1536	1502	1505	31	0
52	S5	991	895	898	9	0
53	S6	1200	1192	1198	25	0
54	S7	1545	1500	1503	22	0
55	S8	1451	1392	1397	35	0
56	U1	60	16	18	1	0
56	U2	60	16	17	0	0
57	V1	3897	3827	3837	74	0
58	V2	1759	1701	1711	29	0
59	E7	1888	1892	1903	23	0
60	1A	4	0	0	0	0
60	V2	4	0	0	0	0
61	1A	16	0	0	1	0
61	S7	8	0	0	0	0
61	S8	16	0	0	4	0
61	V1	8	0	0	0	0
62	1A	1	0	0	0	0
63	A1	80	111	111	3	0
63	A9	66	80	80	2	0
63	AL	50	77	77	0	0
63	AM	97	148	148	1	0
63	AN	48	73	73	0	0
63	B5	108	176	176	2	0
63	C4	38	50	50	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	E4	51	79	79	0	0
63	E8	171	250	250	2	0
63	ED	54	88	88	0	0
63	N1	89	129	129	0	0
63	N2	37	48	48	0	0
63	N3	42	61	61	1	0
63	N4	72	92	92	0	0
63	N5	131	190	190	3	0
64	A3	58	60	60	2	0
64	AL	202	236	236	2	0
64	AM	216	273	273	10	0
64	B3	65	74	74	2	0
64	B5	58	60	60	1	0
64	C4	163	223	223	1	0
64	E6	64	72	72	0	0
64	E7	68	80	80	0	0
64	EA	114	116	116	0	0
64	N4	98	149	149	5	0
64	N5	163	223	223	2	0
65	A9	48	26	26	2	0
66	AB	36	0	47	8	0
66	AC	36	0	47	7	0
67	AN	51	81	82	0	0
67	G1	40	56	57	1	0
67	N4	41	55	56	0	0
67	N5	51	81	82	1	0
68	N4	43	55	55	10	0
69	E7	1	0	0	0	0
69	S6	1	0	0	0	0
70	V1	31	19	19	5	0
71	V1	44	0	27	12	0
All	All	113635	112544	113073	1540	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 1540 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)
25:B9:137:THR:HG22	27:BM:23:THR:HG21	1.48	0.95
33:E5:287:LEU:O	33:E5:289:LEU:N	1.98	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B2:50:GLU:O	39:ED:70:ARG:NH2	2.04	0.91
44:N1:657:TYR:HH	46:N3:286:SER:HG	1.11	0.90
10:A7:34:HIS:O	49:S2:142:LYS:NZ	2.05	0.87

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	1A	350/385 (91%)	340 (97%)	10 (3%)	0	100	100
2	1B	523/527 (99%)	506 (97%)	17 (3%)	0	100	100
3	2B	112/142 (79%)	105 (94%)	7 (6%)	0	100	100
4	4L	106/171 (62%)	103 (97%)	3 (3%)	0	100	100
5	A1	135/141 (96%)	126 (93%)	9 (7%)	0	100	100
6	A2	190/193 (98%)	184 (97%)	6 (3%)	0	100	100
7	A3	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
8	A5	152/184 (83%)	147 (97%)	5 (3%)	0	100	100
9	A6	421/437 (96%)	409 (97%)	12 (3%)	0	100	100
10	A7	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
11	A8	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
12	A9	482/489 (99%)	465 (96%)	17 (4%)	0	100	100
13	AB	86/134 (64%)	84 (98%)	2 (2%)	0	100	100
14	AC	90/134 (67%)	89 (99%)	1 (1%)	0	100	100
15	AL	263/281 (94%)	243 (92%)	20 (8%)	0	100	100
16	AM	182/198 (92%)	175 (96%)	7 (4%)	0	100	100
17	AN	285/287 (99%)	282 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	B2	103/145 (71%)	103 (100%)	0	0	100	100
19	B3	32/62 (52%)	31 (97%)	0	1 (3%)	4	20
20	B4	169/171 (99%)	157 (93%)	12 (7%)	0	100	100
21	B5	132/140 (94%)	129 (98%)	3 (2%)	0	100	100
22	B6	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
23	B7	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
24	B8	145/176 (82%)	137 (94%)	8 (6%)	0	100	100
25	B9	149/158 (94%)	146 (98%)	3 (2%)	0	100	100
26	BL	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
27	BM	99/112 (88%)	98 (99%)	1 (1%)	0	100	100
28	C4	181/185 (98%)	178 (98%)	3 (2%)	0	100	100
29	E1	448/483 (93%)	434 (97%)	14 (3%)	0	100	100
30	E2	464/467 (99%)	447 (96%)	16 (3%)	1 (0%)	47	80
31	E3	430/434 (99%)	423 (98%)	7 (2%)	0	100	100
32	E4	349/368 (95%)	343 (98%)	6 (2%)	0	100	100
33	E5	266/290 (92%)	242 (91%)	23 (9%)	1 (0%)	34	69
34	E6	314/371 (85%)	312 (99%)	2 (1%)	0	100	100
35	E8	203/205 (99%)	192 (95%)	11 (5%)	0	100	100
36	EA	96/126 (76%)	91 (95%)	5 (5%)	0	100	100
37	EB	73/101 (72%)	72 (99%)	1 (1%)	0	100	100
38	EC	83/101 (82%)	77 (93%)	6 (7%)	0	100	100
39	ED	136/151 (90%)	127 (93%)	9 (7%)	0	100	100
40	FX	235/325 (72%)	223 (95%)	11 (5%)	1 (0%)	34	69
41	G1	401/436 (92%)	387 (96%)	14 (4%)	0	100	100
42	G2	234/267 (88%)	218 (93%)	16 (7%)	0	100	100
43	G3	253/261 (97%)	234 (92%)	19 (8%)	0	100	100
44	N1	308/670 (46%)	290 (94%)	18 (6%)	0	100	100
45	N2	294/300 (98%)	278 (95%)	16 (5%)	0	100	100
46	N3	119/293 (41%)	115 (97%)	4 (3%)	0	100	100
46	N6	152/293 (52%)	148 (97%)	4 (3%)	0	100	100
47	N4	476/478 (100%)	464 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
48	N5	582/584 (100%)	558 (96%)	24 (4%)	0	100 100
49	S2	391/395 (99%)	377 (96%)	13 (3%)	1 (0%)	41 74
50	S3	246/277 (89%)	237 (96%)	9 (4%)	0	100 100
51	S4	188/208 (90%)	180 (96%)	8 (4%)	0	100 100
52	S5	110/122 (90%)	108 (98%)	2 (2%)	0	100 100
53	S6	145/147 (99%)	141 (97%)	4 (3%)	0	100 100
54	S7	195/207 (94%)	188 (96%)	7 (4%)	0	100 100
55	S8	180/212 (85%)	174 (97%)	6 (3%)	0	100 100
57	V1	502/526 (95%)	480 (96%)	22 (4%)	0	100 100
58	V2	220/225 (98%)	214 (97%)	6 (3%)	0	100 100
59	E7	244/246 (99%)	235 (96%)	9 (4%)	0	100 100
All	All	13527/15237 (89%)	13024 (96%)	498 (4%)	5 (0%)	100 100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	B3	34	ARG
30	E2	370	THR
33	E5	288	THR
49	S2	36	HIS
40	FX	276	VAL

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	1A	310/340 (91%)	303 (98%)	7 (2%)	50 78
2	1B	453/454 (100%)	448 (99%)	5 (1%)	73 90
3	2B	109/111 (98%)	106 (97%)	3 (3%)	43 75
4	4L	96/151 (64%)	94 (98%)	2 (2%)	53 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	A1	115/118 (98%)	113 (98%)	2 (2%)	60 84
6	A2	159/160 (99%)	159 (100%)	0	100 100
7	A3	104/104 (100%)	103 (99%)	1 (1%)	76 91
8	A5	134/152 (88%)	130 (97%)	4 (3%)	41 73
9	A6	346/358 (97%)	344 (99%)	2 (1%)	86 94
10	A7	119/119 (100%)	118 (99%)	1 (1%)	81 92
11	A8	196/196 (100%)	193 (98%)	3 (2%)	65 86
12	A9	420/424 (99%)	414 (99%)	6 (1%)	67 86
13	AB	79/114 (69%)	78 (99%)	1 (1%)	69 88
14	AC	80/111 (72%)	79 (99%)	1 (1%)	69 88
15	AL	228/242 (94%)	225 (99%)	3 (1%)	69 88
16	AM	156/168 (93%)	156 (100%)	0	100 100
17	AN	241/241 (100%)	239 (99%)	2 (1%)	81 92
18	B2	97/131 (74%)	97 (100%)	0	100 100
19	B3	30/31 (97%)	30 (100%)	0	100 100
20	B4	144/144 (100%)	143 (99%)	1 (1%)	84 93
21	B5	108/108 (100%)	106 (98%)	2 (2%)	57 82
22	B6	82/82 (100%)	81 (99%)	1 (1%)	71 89
23	B7	93/93 (100%)	88 (95%)	5 (5%)	22 55
24	B8	127/148 (86%)	124 (98%)	3 (2%)	49 78
25	B9	132/139 (95%)	129 (98%)	3 (2%)	50 78
26	BL	132/132 (100%)	129 (98%)	3 (2%)	50 78
27	BM	93/93 (100%)	92 (99%)	1 (1%)	73 90
28	C4	166/167 (99%)	163 (98%)	3 (2%)	59 83
29	E1	381/404 (94%)	379 (100%)	2 (0%)	88 95
30	E2	379/380 (100%)	373 (98%)	6 (2%)	62 85
31	E3	339/341 (99%)	331 (98%)	8 (2%)	49 78
32	E4	302/317 (95%)	291 (96%)	11 (4%)	35 68
33	E5	200/205 (98%)	197 (98%)	3 (2%)	65 86
34	E6	272/314 (87%)	269 (99%)	3 (1%)	73 90
35	E8	179/179 (100%)	176 (98%)	3 (2%)	60 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	EA	84/86 (98%)	84 (100%)	0	100	100
37	EB	70/70 (100%)	70 (100%)	0	100	100
38	EC	73/86 (85%)	73 (100%)	0	100	100
39	ED	121/133 (91%)	120 (99%)	1 (1%)	81	92
40	FX	212/276 (77%)	208 (98%)	4 (2%)	57	82
41	G1	333/365 (91%)	324 (97%)	9 (3%)	44	75
42	G2	192/214 (90%)	190 (99%)	2 (1%)	76	91
43	G3	202/202 (100%)	201 (100%)	1 (0%)	88	95
44	N1	295/639 (46%)	291 (99%)	4 (1%)	67	86
45	N2	285/289 (99%)	274 (96%)	11 (4%)	32	66
46	N3	116/281 (41%)	114 (98%)	2 (2%)	60	84
46	N6	147/281 (52%)	144 (98%)	3 (2%)	55	81
47	N4	455/455 (100%)	446 (98%)	9 (2%)	55	81
48	N5	546/546 (100%)	534 (98%)	12 (2%)	52	79
49	S2	335/336 (100%)	325 (97%)	10 (3%)	41	73
50	S3	224/250 (90%)	218 (97%)	6 (3%)	44	75
51	S4	159/172 (92%)	157 (99%)	2 (1%)	69	88
52	S5	102/102 (100%)	101 (99%)	1 (1%)	76	91
53	S6	130/130 (100%)	129 (99%)	1 (1%)	81	92
54	S7	165/171 (96%)	161 (98%)	4 (2%)	49	78
55	S8	160/187 (86%)	159 (99%)	1 (1%)	86	94
57	V1	412/427 (96%)	405 (98%)	7 (2%)	60	84
58	V2	190/190 (100%)	180 (95%)	10 (5%)	22	56
59	E7	192/192 (100%)	189 (98%)	3 (2%)	62	85
All	All	11801/13051 (90%)	11597 (98%)	204 (2%)	62	84

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	G2	71	GLN
47	N4	449	ASP
58	V2	179	GLU
44	N1	531	ASN
45	N2	173	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 191 such sidechains are listed below:

Mol	Chain	Res	Type
41	G1	117	ASN
47	N4	209	ASN
42	G2	36	HIS
45	N2	28	ASN
48	N5	21	ASN

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	$\#\|Z\| > 2$
49	2MR	S2	154	49	10,12,13	2.45	2 (20%)	5,13,15	0.92	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
49	2MR	S2	154	49	-	1/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	154	2MR	CZ-NH2	5.21	1.45	1.33
49	S2	154	2MR	CZ-NE	5.12	1.45	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	S2	154	2MR	CG-CD-NE-CZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 65 ligands modelled in this entry, 3 are monoatomic - leaving 62 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	$\#\|Z\| > 2$
64	CDL	N4	501	-	97,97,99	0.31	0	103,109,111	0.28	0
61	SF4	1A	403	1	0,12,12	-	-	-		
64	CDL	N5	603	-	69,69,99	0.35	0	75,81,111	0.30	0
63	PC1	A9	561	-	32,32,53	0.36	0	38,40,61	0.32	0
64	CDL	E7	301	-	67,67,99	0.36	0	73,79,111	0.31	0
63	PC1	C4	203	-	37,37,53	0.35	0	43,45,61	0.29	0
63	PC1	AN	301	-	47,47,53	0.32	0	53,55,61	0.30	0
67	3PE	N5	607	-	50,50,50	0.30	0	53,55,55	0.29	0
64	CDL	A3	201	-	57,57,99	0.38	0	63,69,111	0.34	0
63	PC1	N5	606	-	35,35,53	0.35	0	41,43,61	0.32	0
63	PC1	N2	301	-	36,36,53	0.34	0	42,44,61	0.36	0
60	FES	1A	401	1	0,4,4	-	-	-		
63	PC1	N4	502	-	38,38,53	0.34	0	44,46,61	0.31	0
64	CDL	B3	102	-	64,64,99	0.37	0	70,76,111	0.34	0
64	CDL	EA	202	-	54,54,99	0.39	0	60,66,111	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
67	3PE	N4	504	-	40,40,50	0.34	0	43,45,55	0.32	0
64	CDL	C4	202	-	93,93,99	0.32	0	99,105,111	0.30	0
64	CDL	AM	217	-	71,71,99	0.36	0	77,83,111	0.33	0
63	PC1	AM	220	-	47,47,53	0.31	0	53,55,61	0.25	0
66	ZMP	AB	150	13	29,35,36	0.66	1 (3%)	34,42,45	0.87	1 (2%)
64	CDL	C4	204	-	68,68,99	0.35	0	74,80,111	0.32	0
64	CDL	EA	201	-	58,58,99	0.38	0	64,70,111	0.34	0
67	3PE	AN	302	-	50,50,50	0.30	0	53,55,55	0.28	0
64	CDL	AL	303	-	63,63,99	0.37	0	69,75,111	0.31	0
64	CDL	AM	215	-	71,71,99	0.35	0	77,83,111	0.31	0
61	SF4	V1	580	57	0,12,12	-	-	-		
70	FMN	V1	579	-	33,33,33	0.27	0	48,50,50	0.41	0
61	SF4	S8	297	55	0,12,12	-	-	-		
61	SF4	S7	301	54	0,12,12	-	-	-		
63	PC1	N1	701	-	48,48,53	0.30	0	54,56,61	0.28	0
67	3PE	G1	516	-	39,39,50	0.34	0	42,44,55	0.31	0
64	CDL	AL	304	-	69,69,99	0.35	0	75,81,111	0.32	0
64	CDL	B5	201	-	57,57,99	0.38	0	63,69,111	0.34	0
64	CDL	AL	302	-	67,67,99	0.36	0	73,79,111	0.34	0
64	CDL	N5	608	-	92,92,99	0.31	0	98,104,111	0.30	0
63	PC1	B5	203	-	53,53,53	0.31	0	59,61,61	0.31	0
63	PC1	E8	301	-	53,53,53	0.30	0	59,61,61	0.31	0
63	PC1	N4	503	-	32,32,53	0.36	0	38,40,61	0.34	0
63	PC1	B5	202	-	53,53,53	0.30	0	59,61,61	0.30	0
68	U10	N4	505	-	43,43,63	2.44	16 (37%)	52,55,79	1.68	15 (28%)
64	CDL	AM	216	-	71,71,99	0.35	0	77,83,111	0.37	0
63	PC1	A1	203	-	30,30,53	0.37	0	36,38,61	0.34	0
63	PC1	E8	303	-	32,32,53	0.36	0	38,40,61	0.35	0
63	PC1	A1	202	-	48,48,53	0.32	0	54,56,61	0.31	0
63	PC1	E8	304	-	29,29,53	0.38	0	35,37,61	0.33	0
63	PC1	N5	605	-	40,40,53	0.33	0	46,48,61	0.29	0
65	NDP	A9	559	-	45,52,52	0.54	0	53,80,80	0.53	1 (1%)
60	FES	V2	301	57,58	0,4,4	-	-	-		
61	SF4	1A	402	1	0,12,12	-	-	-		
63	PC1	A9	560	-	32,32,53	0.37	0	38,40,61	0.33	0
63	PC1	N5	601	-	53,53,53	0.29	0	59,61,61	0.29	0
63	PC1	AM	218	-	48,48,53	0.32	0	54,56,61	0.29	0
63	PC1	E4	401	-	50,50,53	0.30	0	56,58,61	0.31	0
63	PC1	E8	302	-	53,53,53	0.30	0	59,61,61	0.28	0
63	PC1	N3	301	-	41,41,53	0.33	0	47,49,61	0.31	0
64	CDL	E6	431	-	63,63,99	0.37	0	69,75,111	0.31	0
71	NAI	V1	581	-	42,48,48	0.51	0	47,73,73	0.56	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
63	PC1	ED	201	-	53,53,53	0.30	0	59,61,61	0.28	0
63	PC1	N1	702	-	39,39,53	0.34	0	45,47,61	0.32	0
61	SF4	S8	298	55	0,12,12	-	-	-		
63	PC1	AL	301	-	49,49,53	0.31	0	55,57,61	0.29	0
66	ZMP	AC	201	14	29,35,36	0.65	1 (3%)	34,42,45	0.76	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
64	CDL	N4	501	-	-	18/108/108/110	-
61	SF4	1A	403	1	-	-	0/6/5/5
64	CDL	N5	603	-	-	14/80/80/110	-
63	PC1	A9	561	-	-	8/36/36/57	-
64	CDL	E7	301	-	-	18/78/78/110	-
63	PC1	C4	203	-	-	8/41/41/57	-
63	PC1	AN	301	-	-	13/51/51/57	-
67	3PE	N5	607	-	-	8/54/54/54	-
64	CDL	A3	201	-	-	11/68/68/110	-
63	PC1	N5	606	-	-	7/39/39/57	-
63	PC1	N2	301	-	-	15/40/40/57	-
63	PC1	N4	502	-	-	17/42/42/57	-
64	CDL	B3	102	-	-	13/75/75/110	-
64	CDL	EA	202	-	-	18/65/65/110	-
67	3PE	N4	504	-	-	10/44/44/54	-
60	FES	1A	401	1	-	-	0/1/1/1
64	CDL	C4	202	-	-	18/104/104/110	-
64	CDL	AM	217	-	-	20/82/82/110	-
63	PC1	AM	220	-	-	8/51/51/57	-
66	ZMP	AB	150	13	-	22/40/42/43	-
64	CDL	C4	204	-	-	13/79/79/110	-
64	CDL	EA	201	-	-	11/69/69/110	-
67	3PE	AN	302	-	-	9/54/54/54	-
64	CDL	AL	303	-	-	15/74/74/110	-
64	CDL	AM	215	-	-	17/82/82/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	SF4	V1	580	57	-	-	0/6/5/5
70	FMN	V1	579	-	-	2/18/18/18	0/3/3/3
61	SF4	S8	297	55	-	-	0/6/5/5
63	PC1	N1	701	-	-	17/52/52/57	-
61	SF4	S7	301	54	-	-	0/6/5/5
67	3PE	G1	516	-	-	8/43/43/54	-
64	CDL	AL	304	-	-	28/80/80/110	-
64	CDL	B5	201	-	-	13/68/68/110	-
64	CDL	AL	302	-	-	9/78/78/110	-
64	CDL	N5	608	-	-	20/103/103/110	-
63	PC1	B5	203	-	-	22/57/57/57	-
63	PC1	E8	301	-	-	12/57/57/57	-
63	PC1	N4	503	-	-	6/36/36/57	-
63	PC1	B5	202	-	-	14/57/57/57	-
68	U10	N4	505	-	-	12/39/63/87	0/1/1/1
64	CDL	AM	216	-	-	14/82/82/110	-
63	PC1	A1	203	-	-	8/34/34/57	-
63	PC1	E8	303	-	-	5/36/36/57	-
63	PC1	A1	202	-	-	16/52/52/57	-
63	PC1	E8	304	-	-	9/33/33/57	-
63	PC1	N5	605	-	-	11/44/44/57	-
65	NDP	A9	559	-	-	7/30/77/77	0/5/5/5
60	FES	V2	301	57,58	-	-	0/1/1/1
61	SF4	1A	402	1	-	-	0/6/5/5
63	PC1	A9	560	-	-	12/36/36/57	-
63	PC1	N5	601	-	-	9/57/57/57	-
63	PC1	AM	218	-	-	17/52/52/57	-
63	PC1	E4	401	-	-	11/54/54/57	-
63	PC1	E8	302	-	-	20/57/57/57	-
63	PC1	N3	301	-	-	11/45/45/57	-
64	CDL	E6	431	-	-	24/74/74/110	-
71	NAI	V1	581	-	-	8/25/72/72	0/5/5/5
63	PC1	ED	201	-	-	12/57/57/57	-
63	PC1	N1	702	-	-	11/43/43/57	-
61	SF4	S8	298	55	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	PC1	AL	301	-	-	11/53/53/57	-
66	ZMP	AC	201	14	-	18/40/42/43	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	N4	505	U10	C6-C1	10.34	1.54	1.35
68	N4	505	U10	C4-C3	4.19	1.53	1.36
68	N4	505	U10	C7-C8	3.10	1.55	1.50
68	N4	505	U10	C7-C6	3.09	1.56	1.51
68	N4	505	U10	C31-C29	2.62	1.56	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
68	N4	505	U10	C7-C8-C9	-3.65	120.72	126.79
68	N4	505	U10	C7-C6-C5	3.45	122.63	118.48
68	N4	505	U10	C15-C14-C16	3.42	121.03	115.27
68	N4	505	U10	C30-C29-C31	2.94	120.22	115.27
68	N4	505	U10	C22-C23-C24	-2.90	120.67	127.66

There are no chirality outliers.

5 of 708 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	A1	203	PC1	C11-O13-P-O12
63	A1	203	PC1	C11-O13-P-O14
63	A1	203	PC1	C1-O11-P-O12
63	A9	560	PC1	C1-O11-P-O12
63	A9	560	PC1	C1-O11-P-O14

There are no ring outliers.

32 monomers are involved in 86 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	N4	501	CDL	5	0
61	1A	403	SF4	1	0
64	N5	603	CDL	1	0
67	N5	607	3PE	1	0
64	A3	201	CDL	2	0

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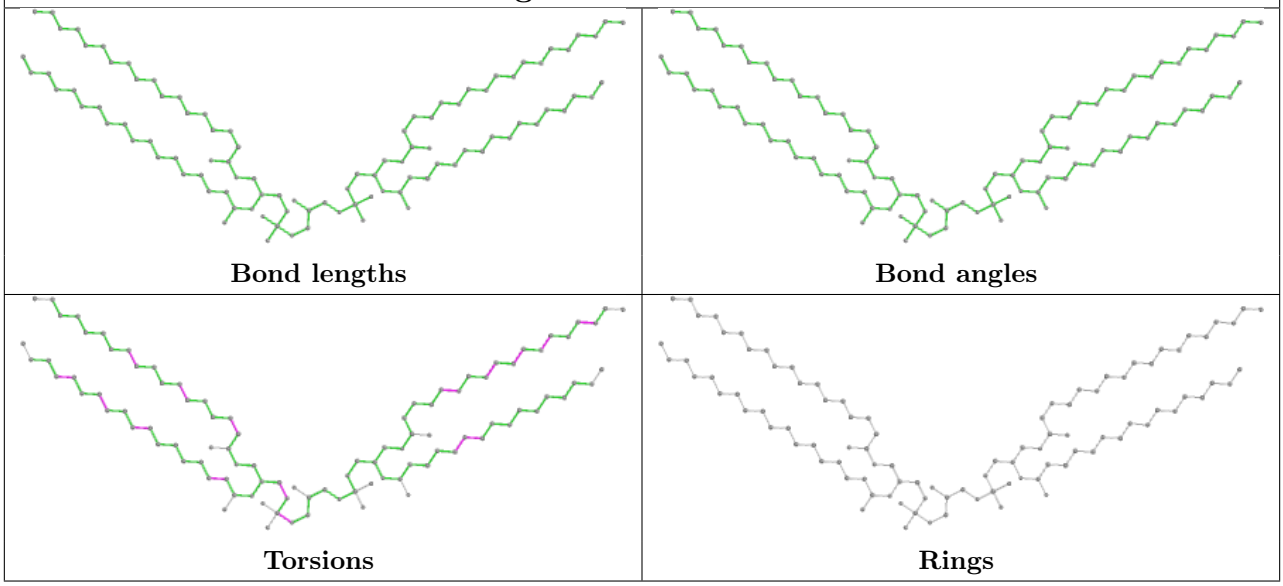
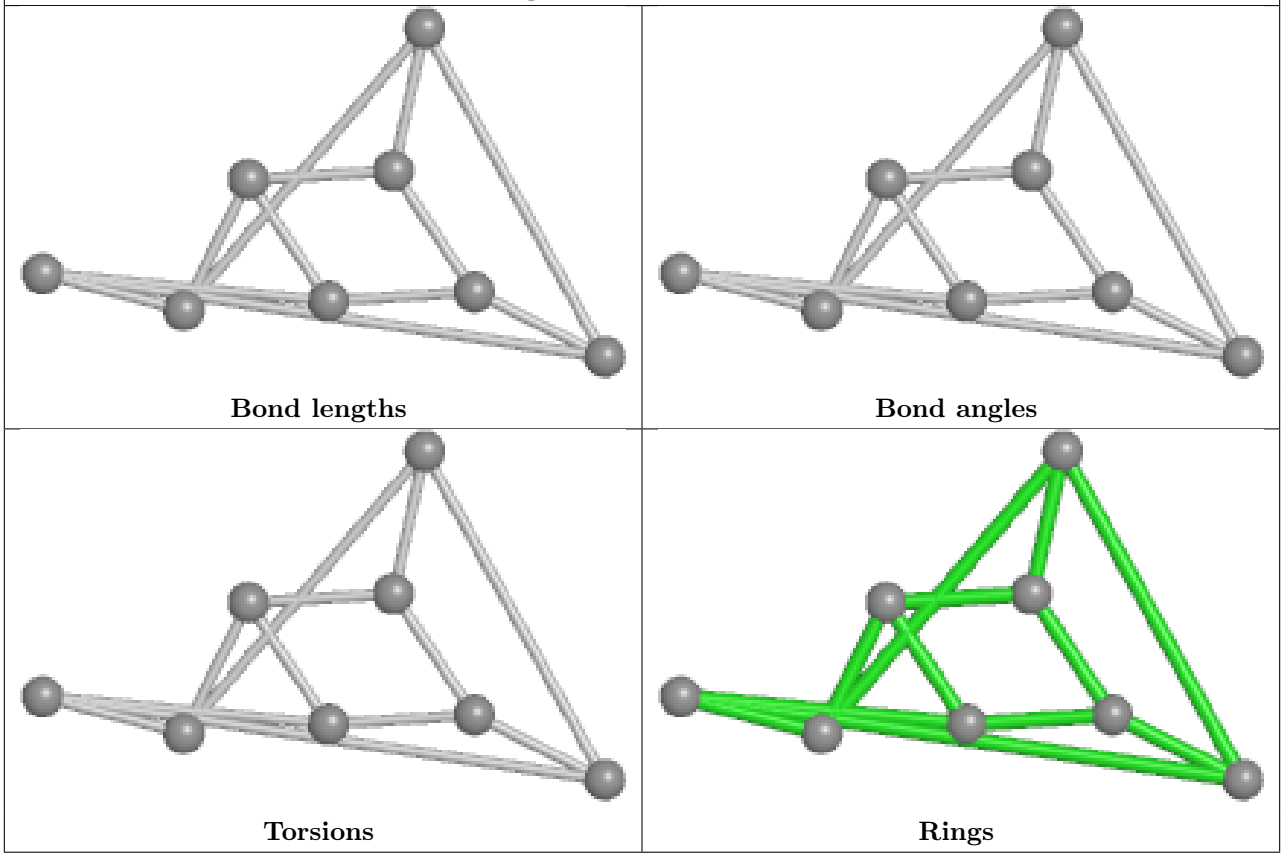
Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	B3	102	CDL	2	0
64	C4	202	CDL	1	0
64	AM	217	CDL	2	0
63	AM	220	PC1	1	0
66	AB	150	ZMP	8	0
64	AL	303	CDL	2	0
64	AM	215	CDL	5	0
70	V1	579	FMN	5	0
61	S8	297	SF4	3	0
67	G1	516	3PE	1	0
64	B5	201	CDL	1	0
64	N5	608	CDL	1	0
63	B5	203	PC1	1	0
63	E8	301	PC1	2	0
63	B5	202	PC1	1	0
68	N4	505	U10	10	0
64	AM	216	CDL	3	0
63	A1	203	PC1	2	0
63	A1	202	PC1	1	0
63	N5	605	PC1	1	0
65	A9	559	NDP	2	0
63	A9	560	PC1	2	0
63	N5	601	PC1	2	0
63	N3	301	PC1	1	0
71	V1	581	NAI	12	0
61	S8	298	SF4	1	0
66	AC	201	ZMP	7	0

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

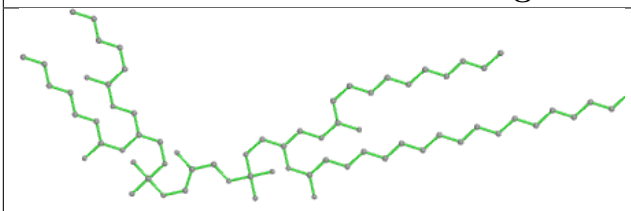
Ligand CDL N4 501



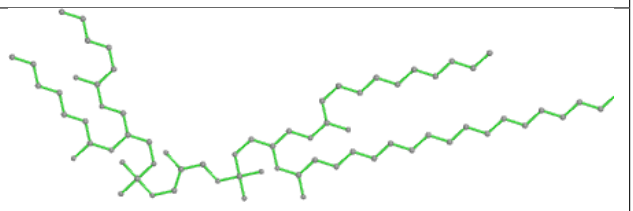
Ligand SF4 1A 403



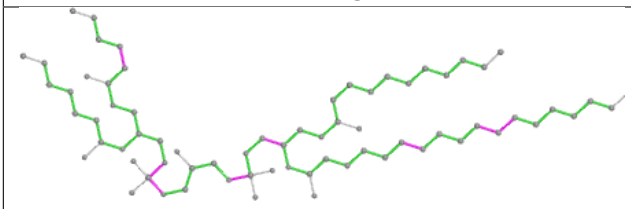
Ligand CDL N5 603



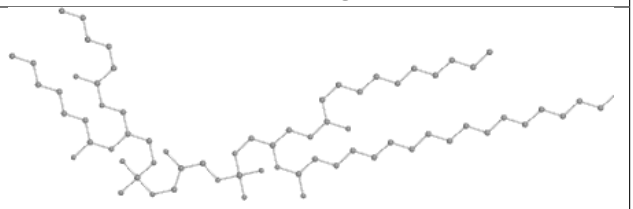
Bond lengths



Bond angles

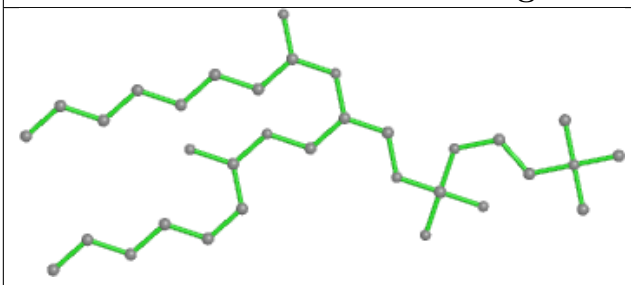


Torsions

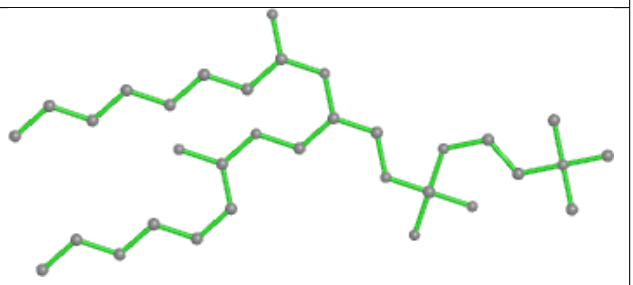


Rings

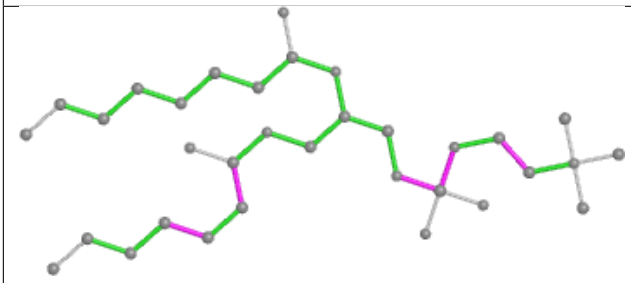
Ligand PC1 A9 561



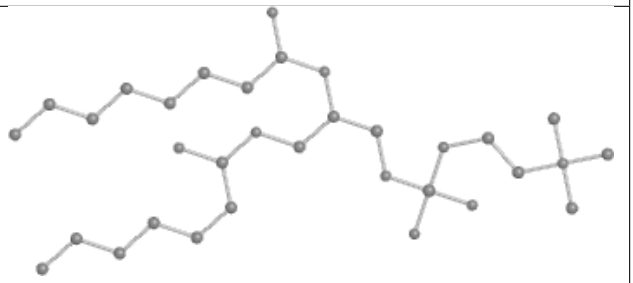
Bond lengths



Bond angles

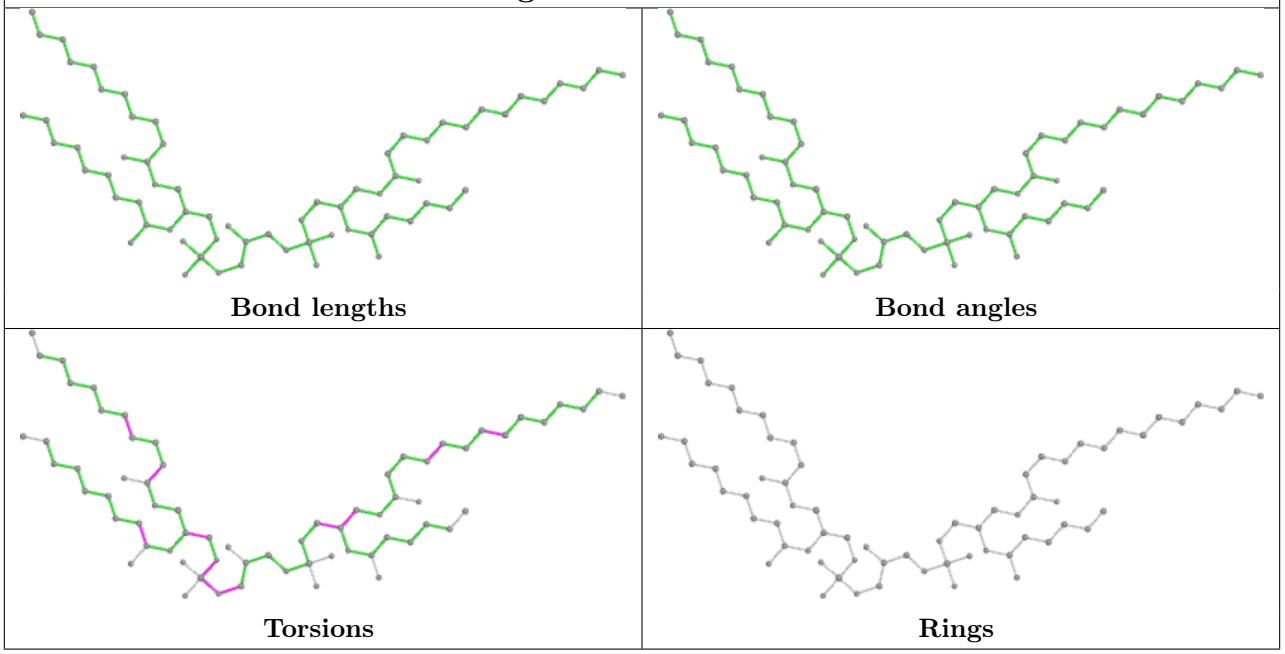


Torsions

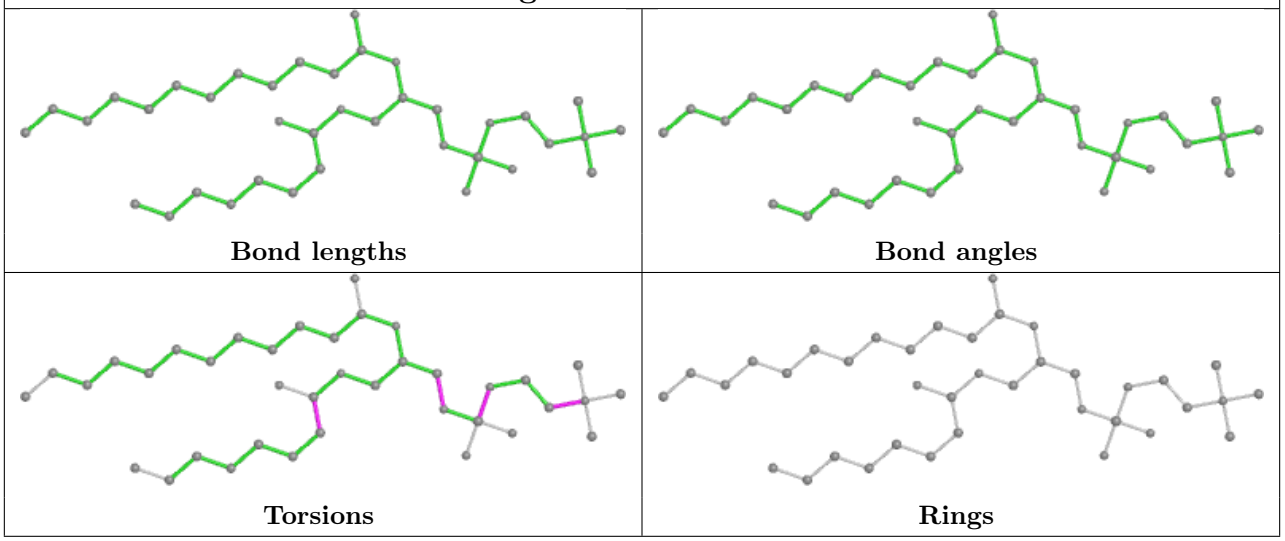


Rings

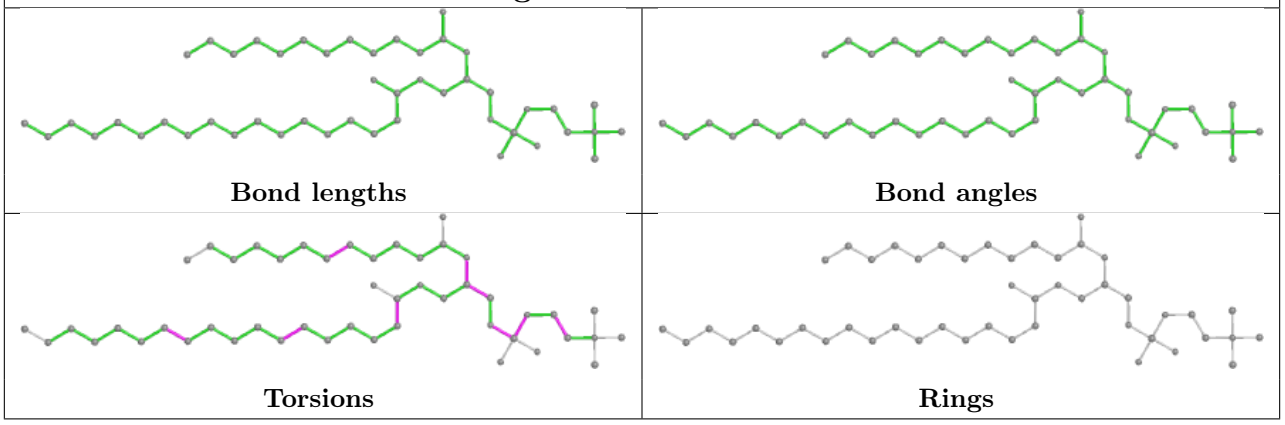
Ligand CDL E7 301



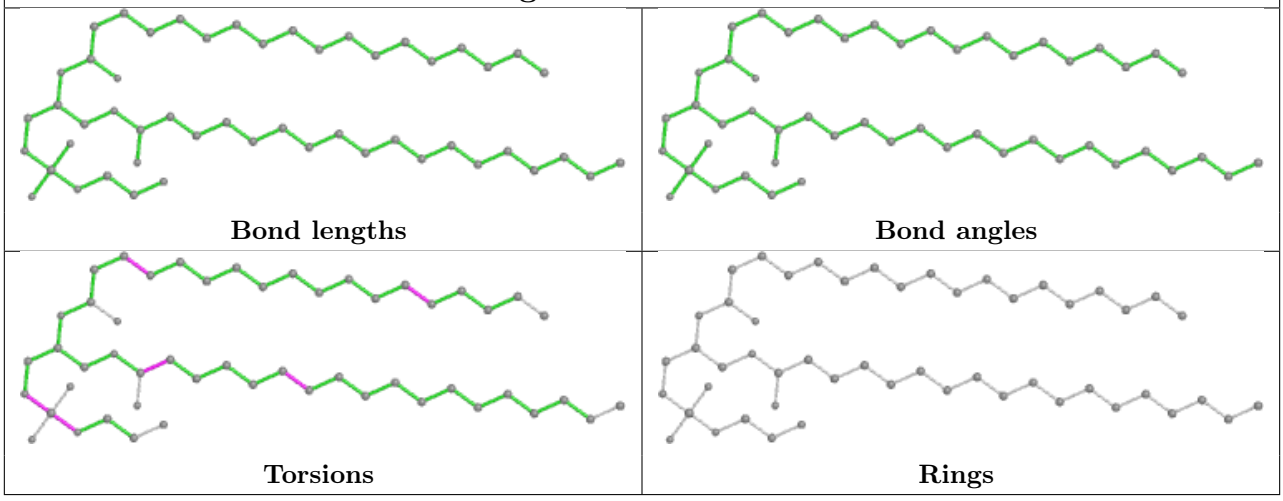
Ligand PC1 C4 203



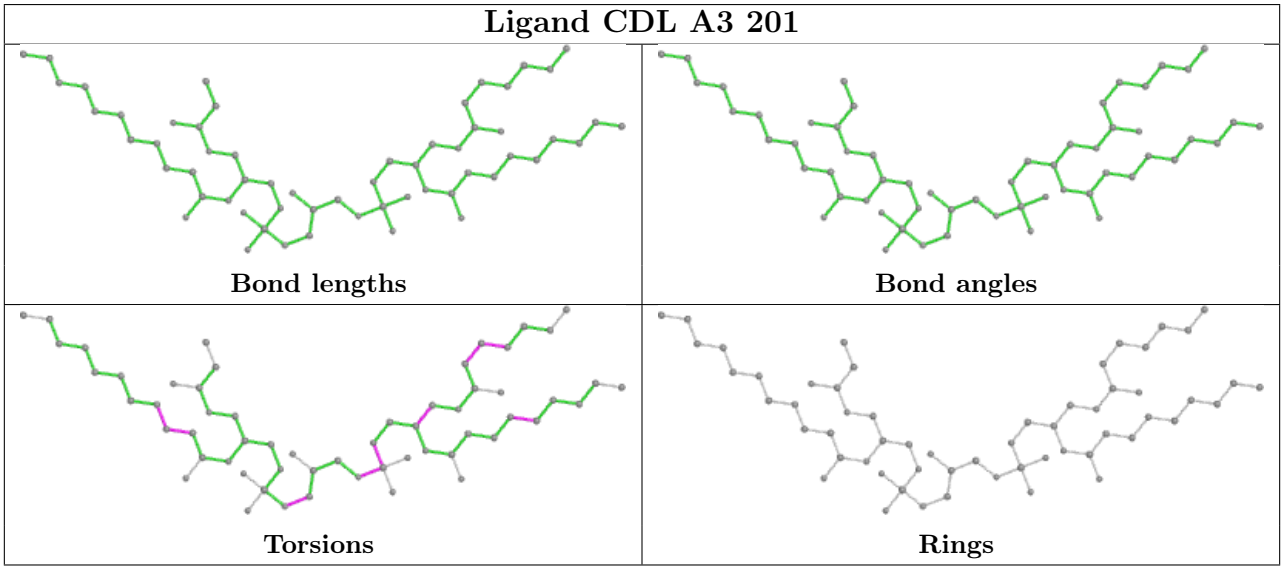
Ligand PC1 AN 301



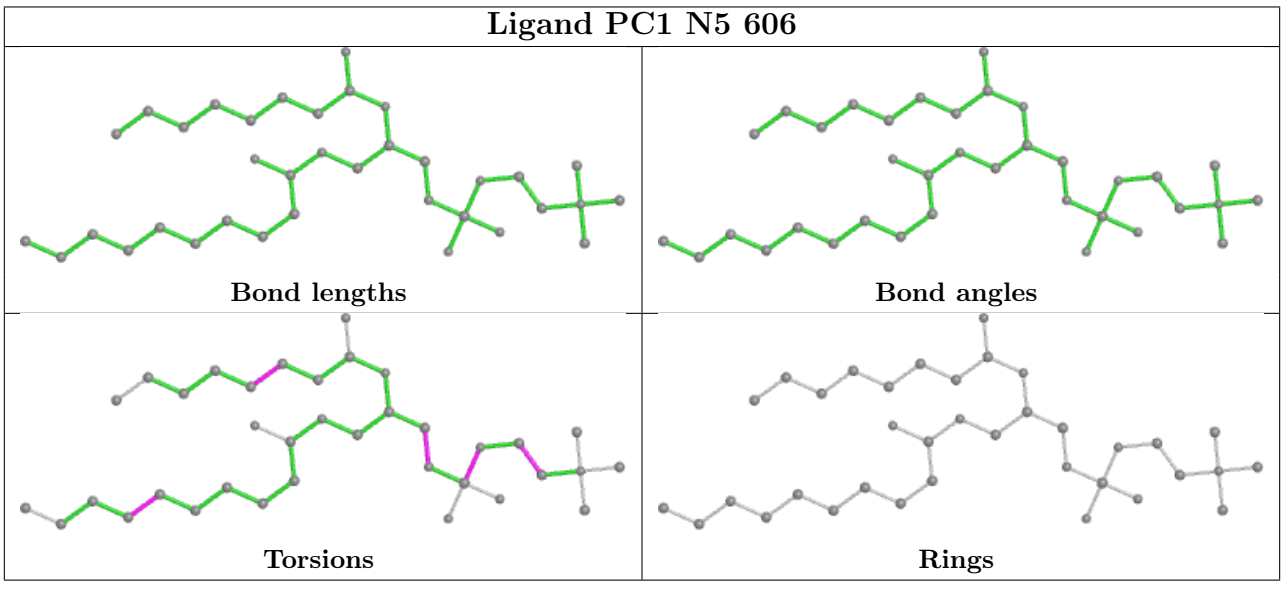
Ligand 3PE N5 607



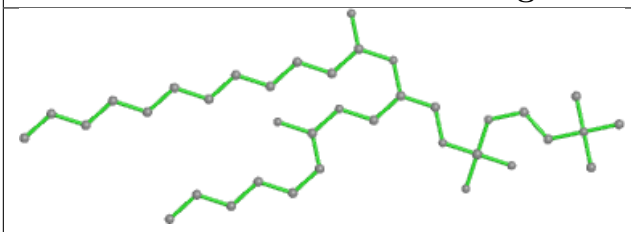
Ligand CDL A3 201



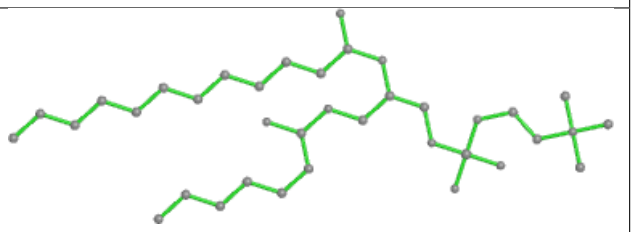
Ligand PC1 N5 606



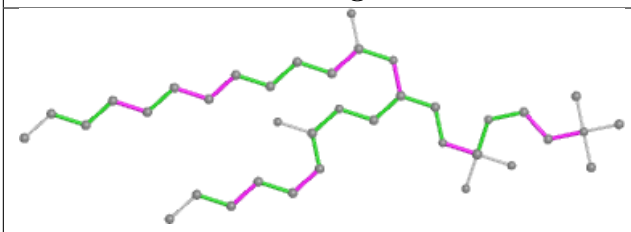
Ligand PC1 N2 301



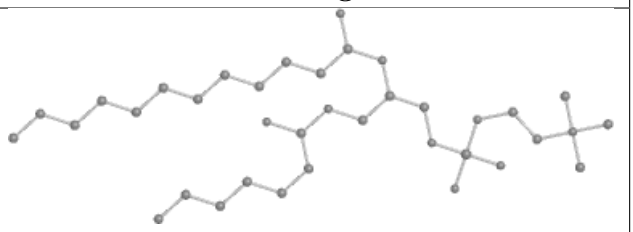
Bond lengths



Bond angles

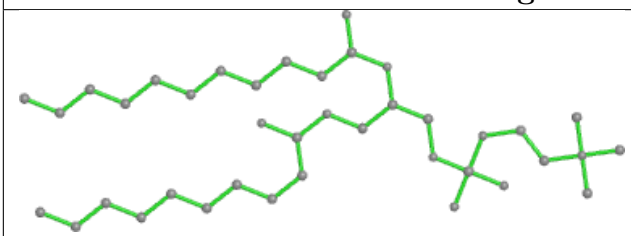


Torsions

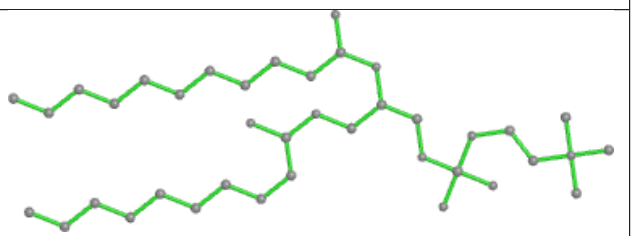


Rings

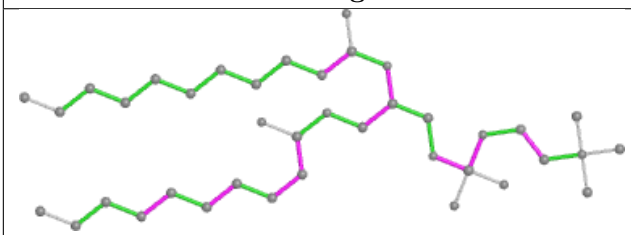
Ligand PC1 N4 502



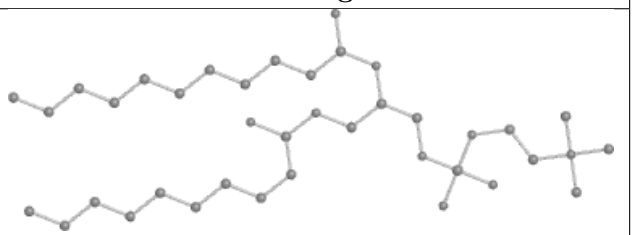
Bond lengths



Bond angles

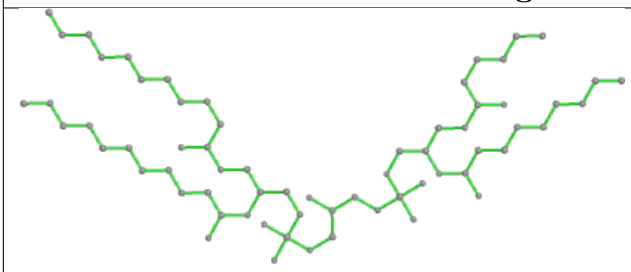


Torsions

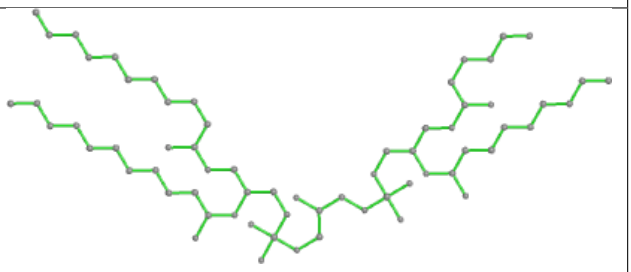


Rings

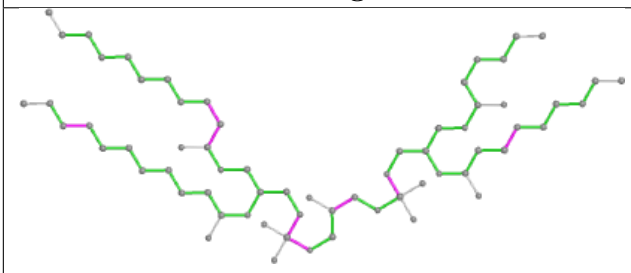
Ligand CDL B3 102



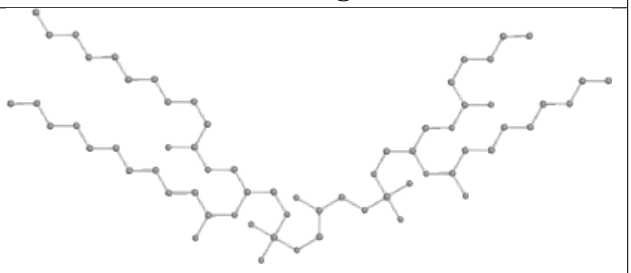
Bond lengths



Bond angles

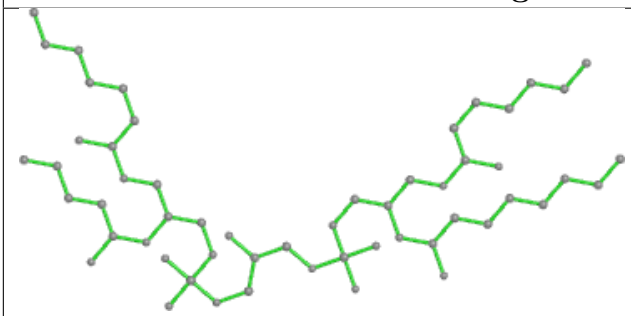


Torsions

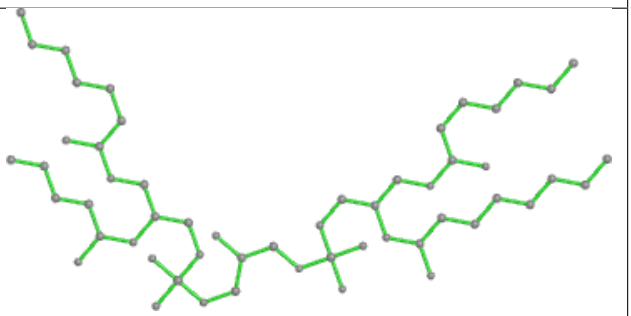


Rings

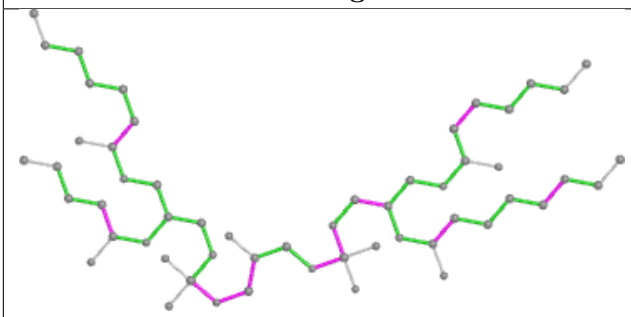
Ligand CDL EA 202



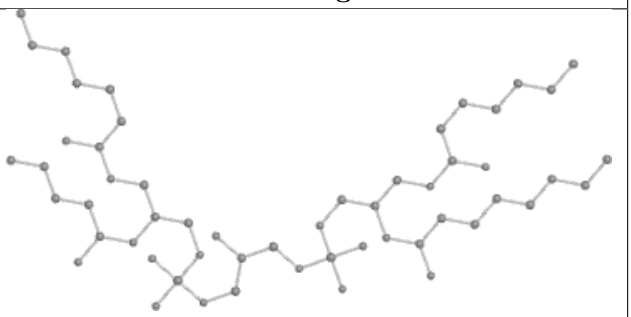
Bond lengths



Bond angles

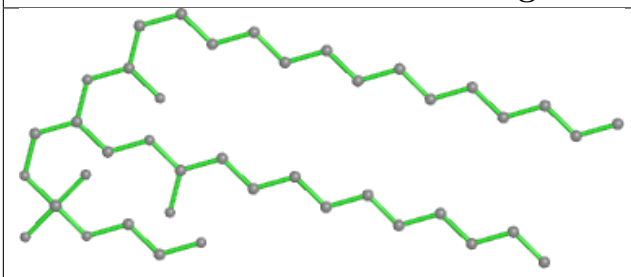


Torsions

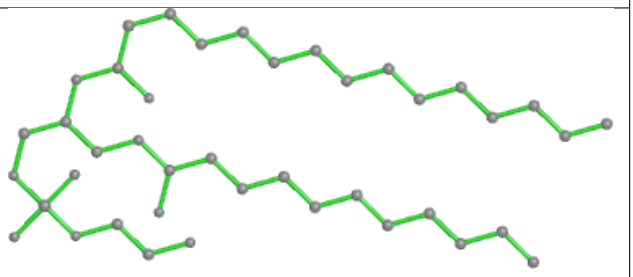


Rings

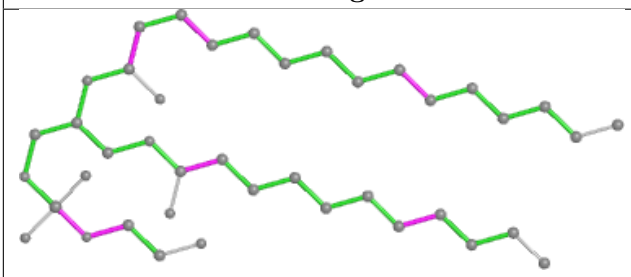
Ligand 3PE N4 504



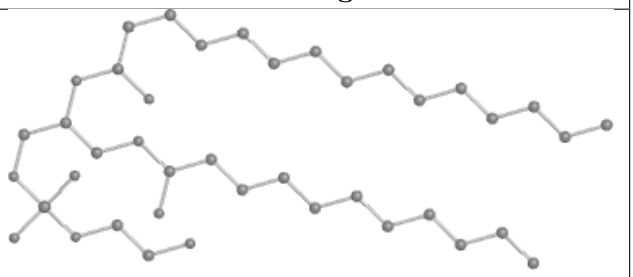
Bond lengths



Bond angles

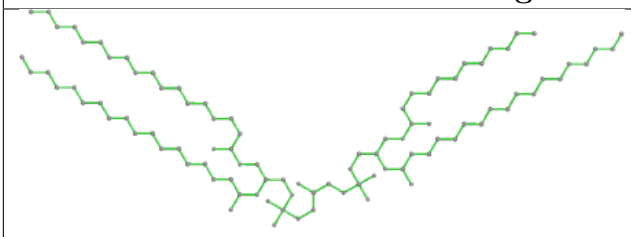


Torsions

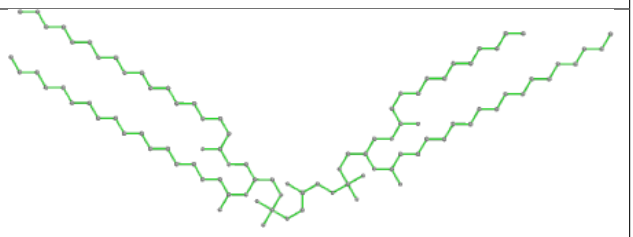


Rings

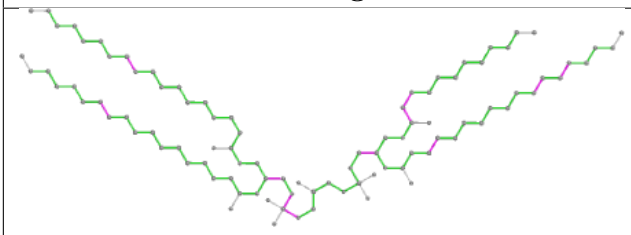
Ligand CDL C4 202



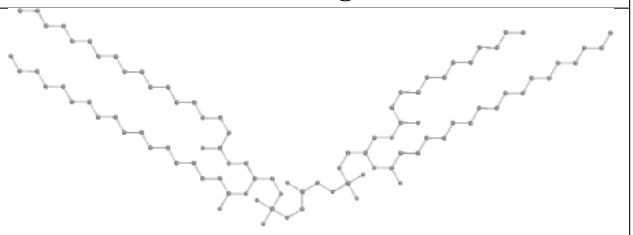
Bond lengths



Bond angles

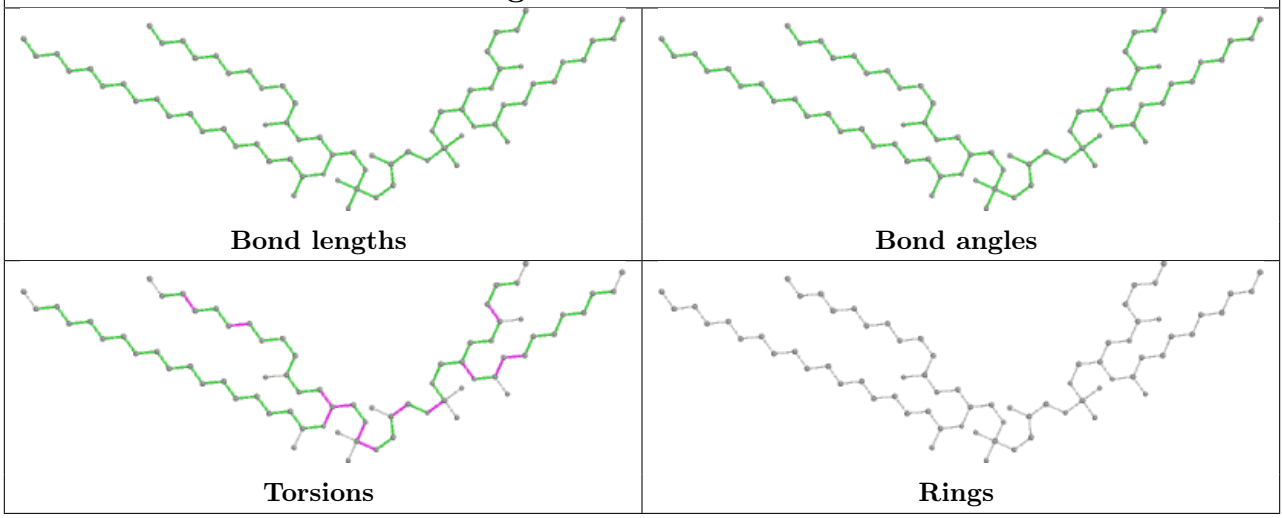


Torsions

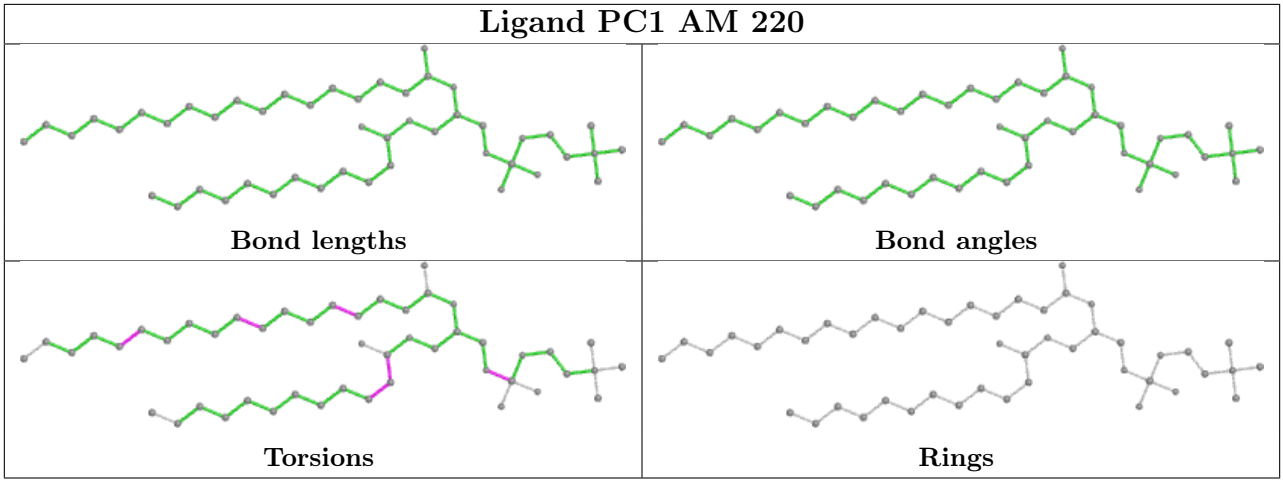


Rings

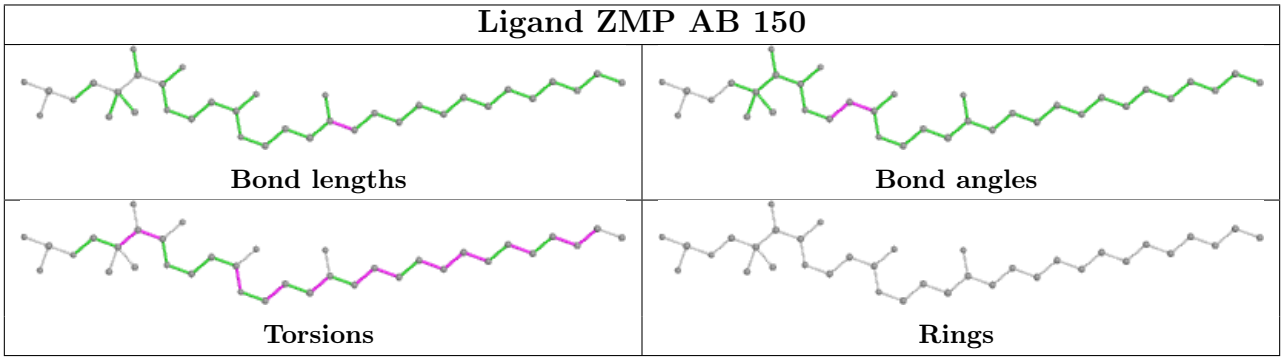
Ligand CDL AM 217



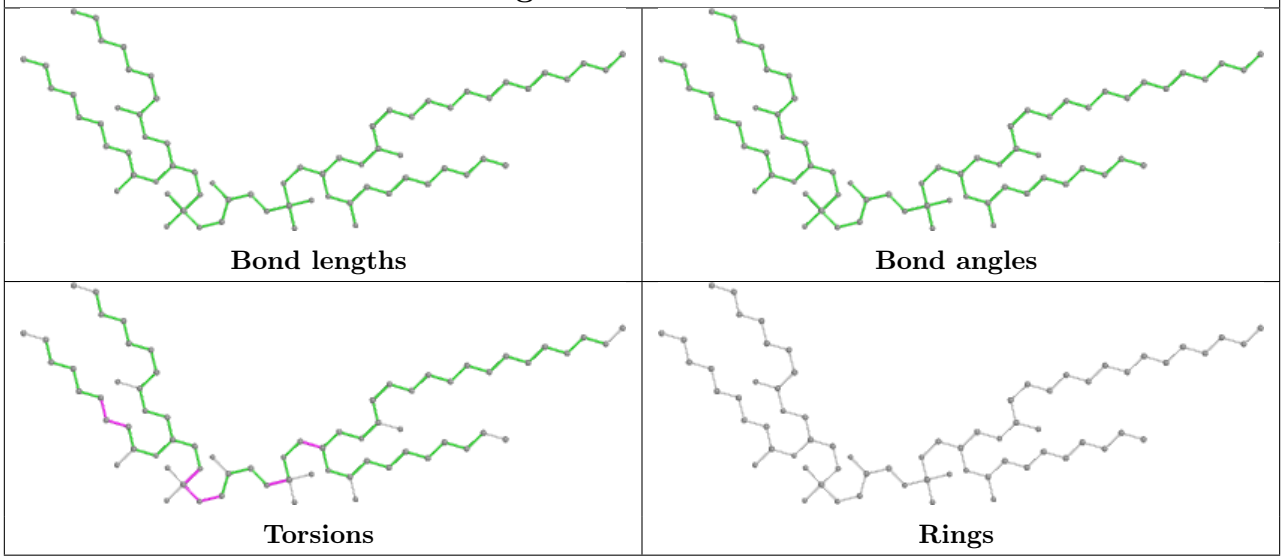
Ligand PC1 AM 220



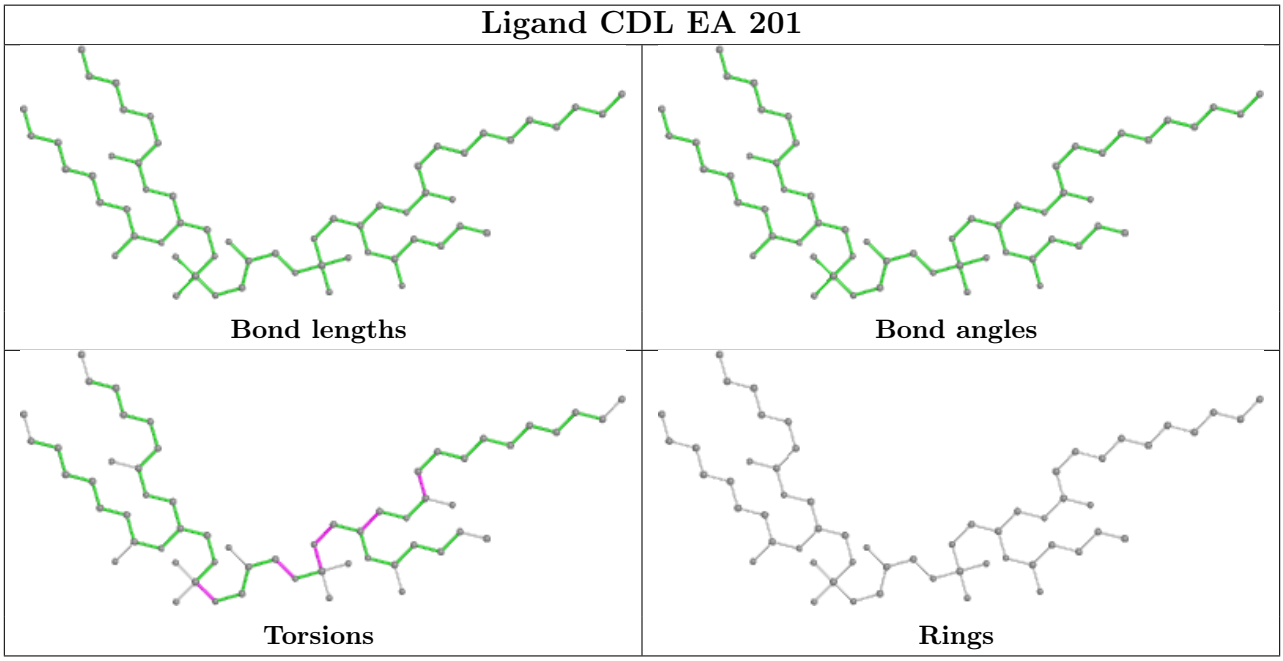
Ligand ZMP AB 150



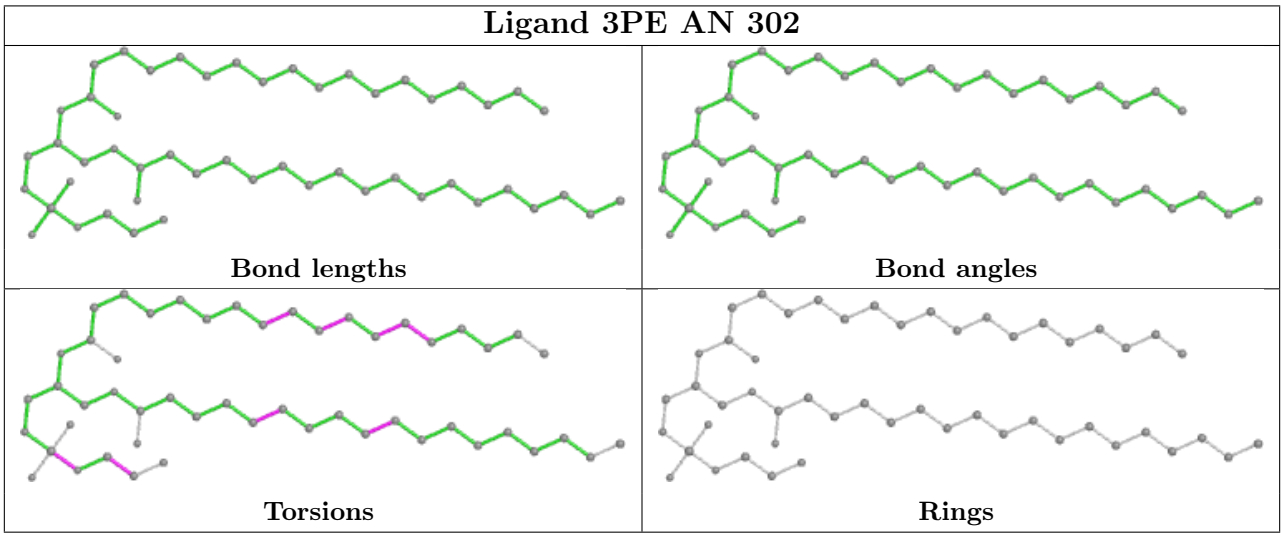
Ligand CDL C4 204



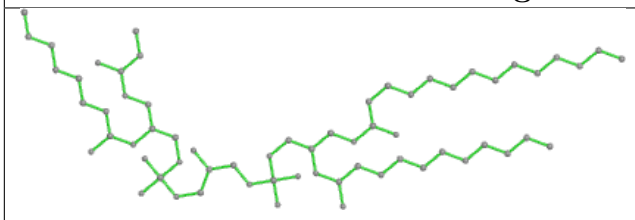
Ligand CDL EA 201



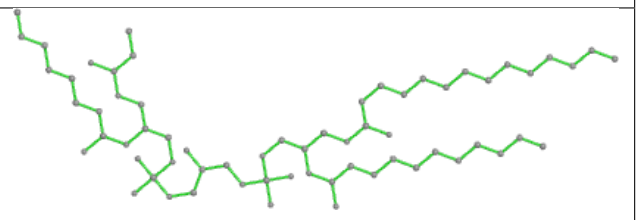
Ligand 3PE AN 302



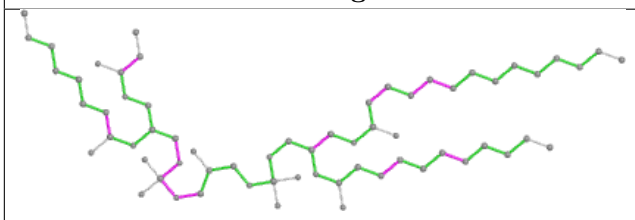
Ligand CDL AL 303



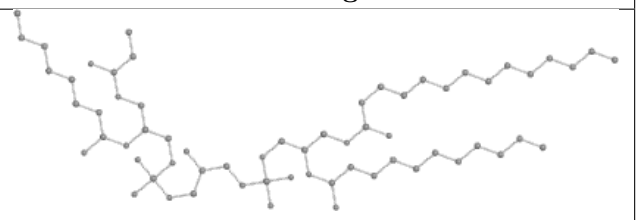
Bond lengths



Bond angles

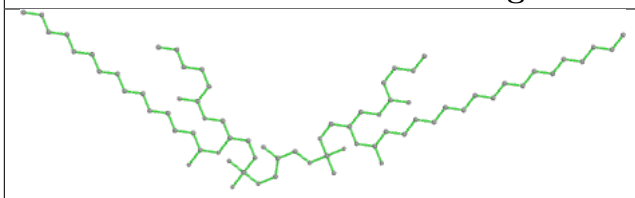


Torsions

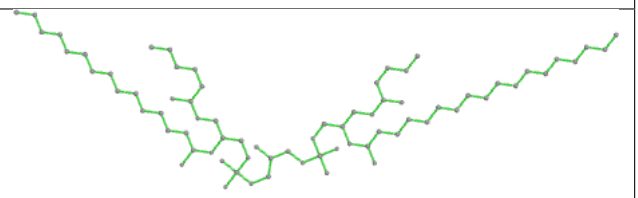


Rings

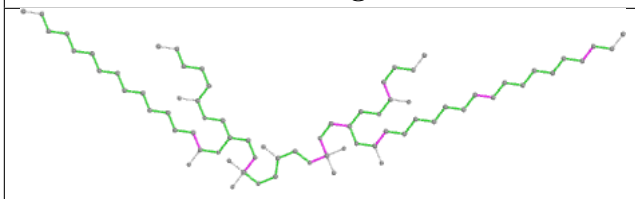
Ligand CDL AM 215



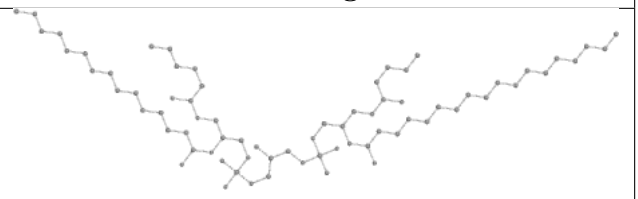
Bond lengths



Bond angles

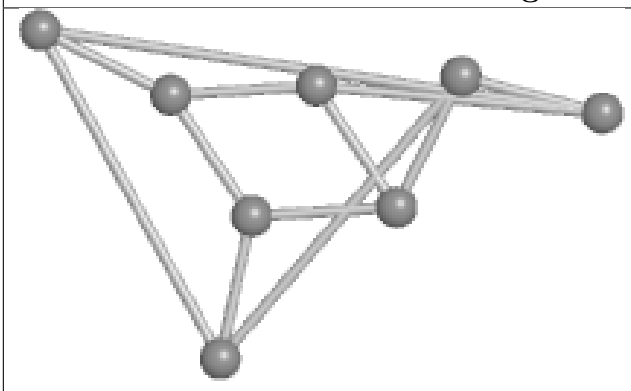


Torsions

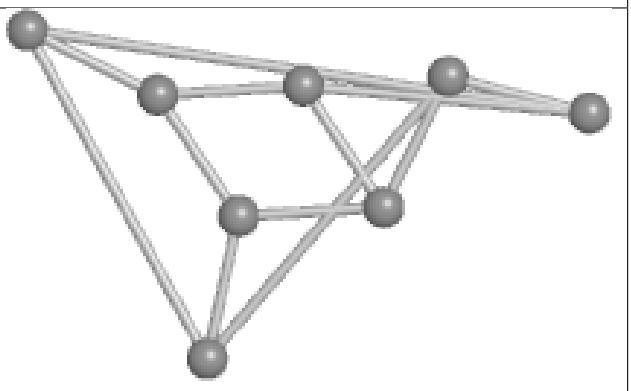


Rings

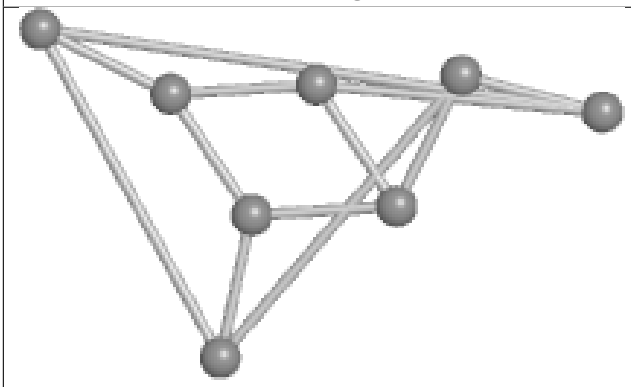
Ligand SF4 V1 580



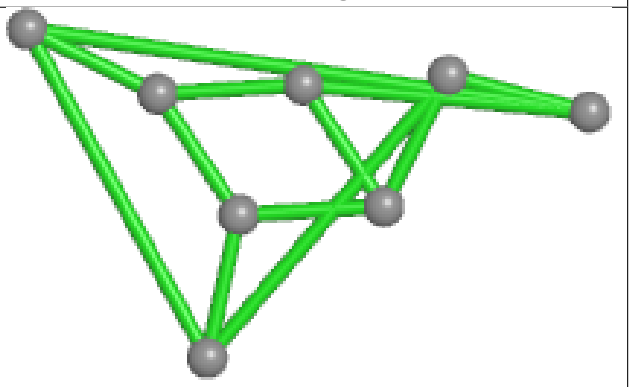
Bond lengths



Bond angles

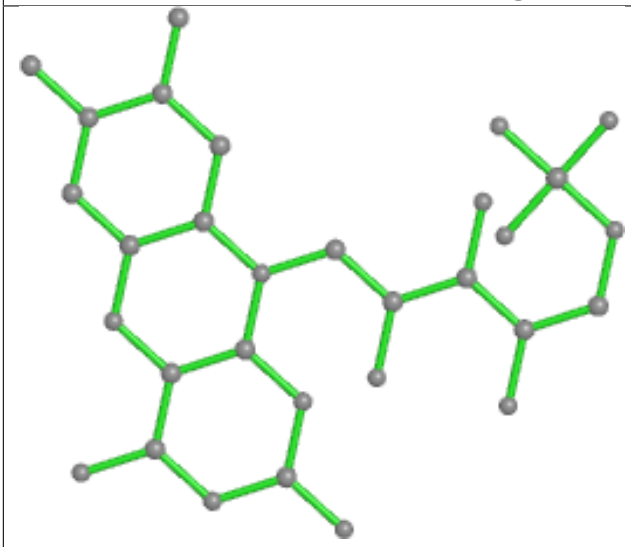


Torsions

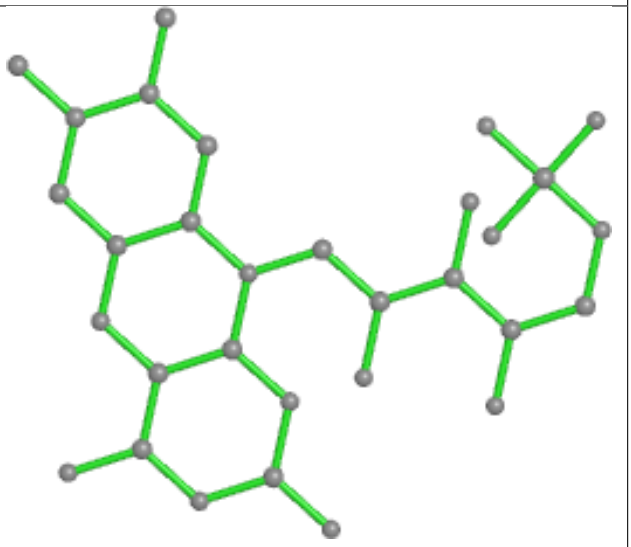


Rings

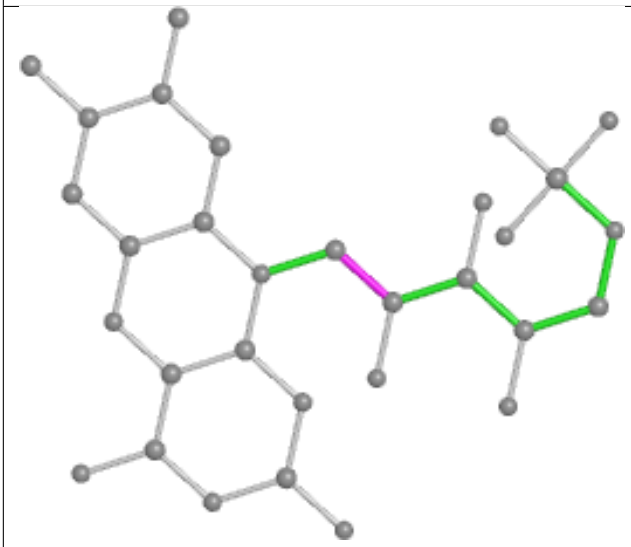
Ligand FMN V1 579



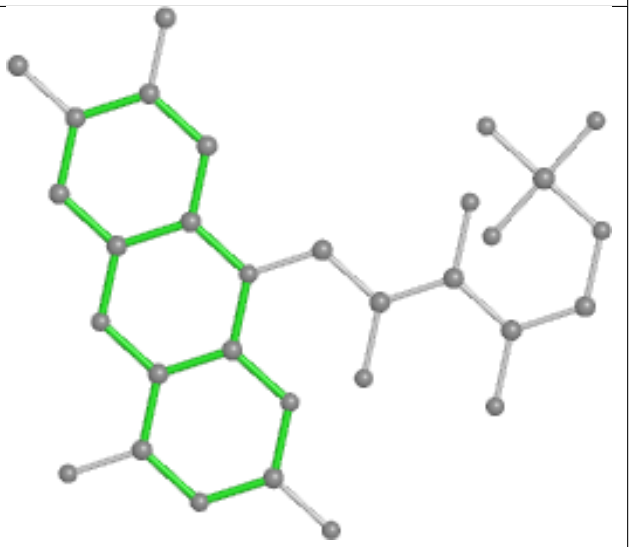
Bond lengths



Bond angles

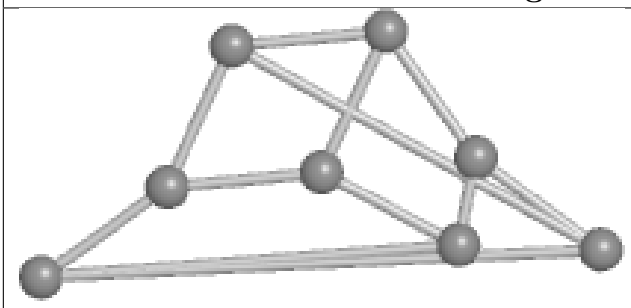


Torsions

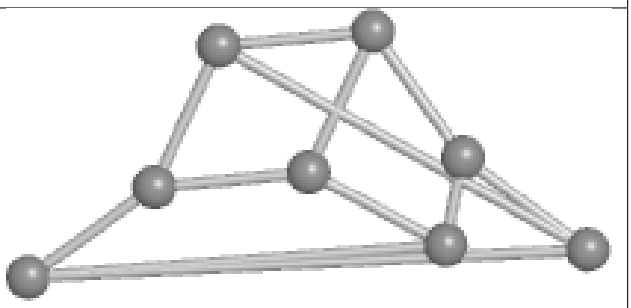


Rings

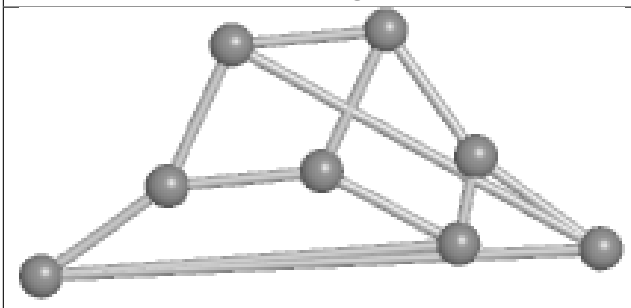
Ligand SF4 S8 297



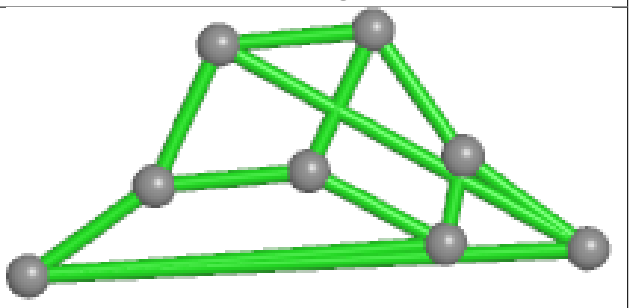
Bond lengths



Bond angles

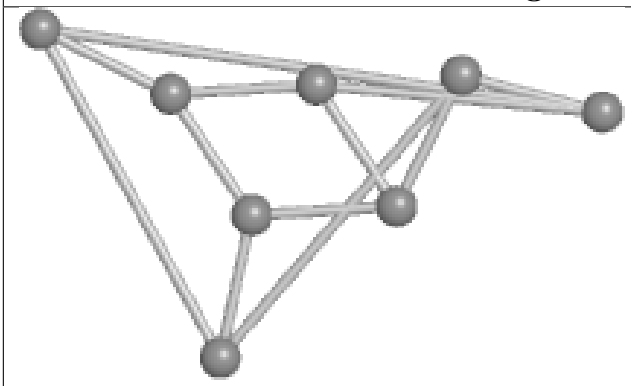


Torsions

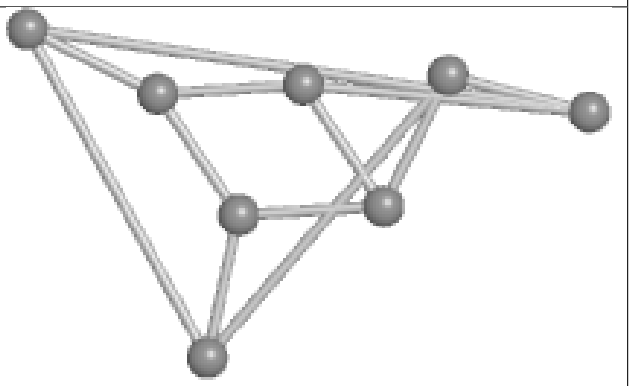


Rings

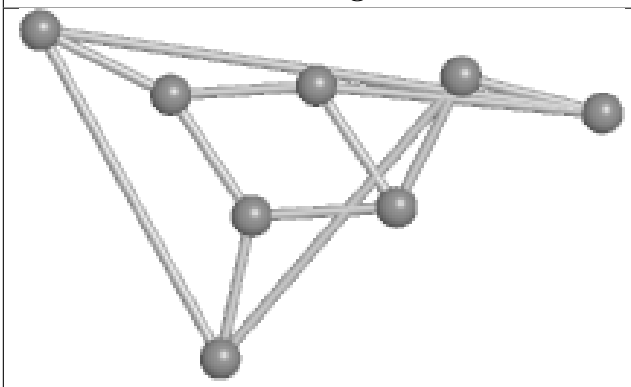
Ligand SF4 S7 301



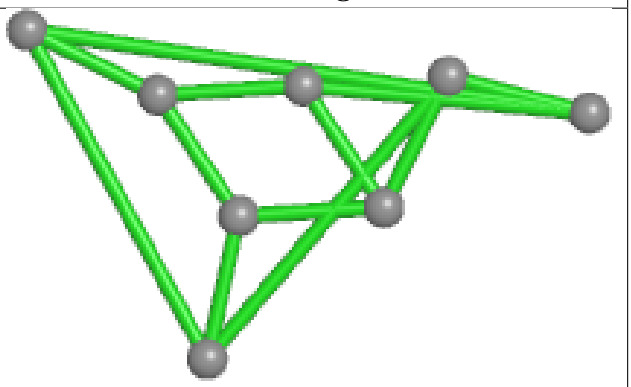
Bond lengths



Bond angles

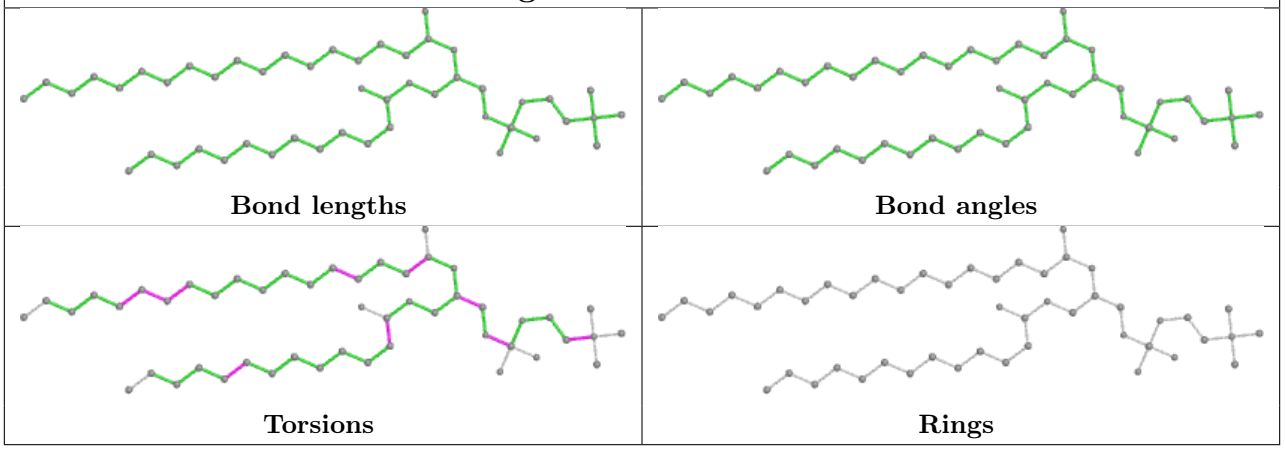


Torsions

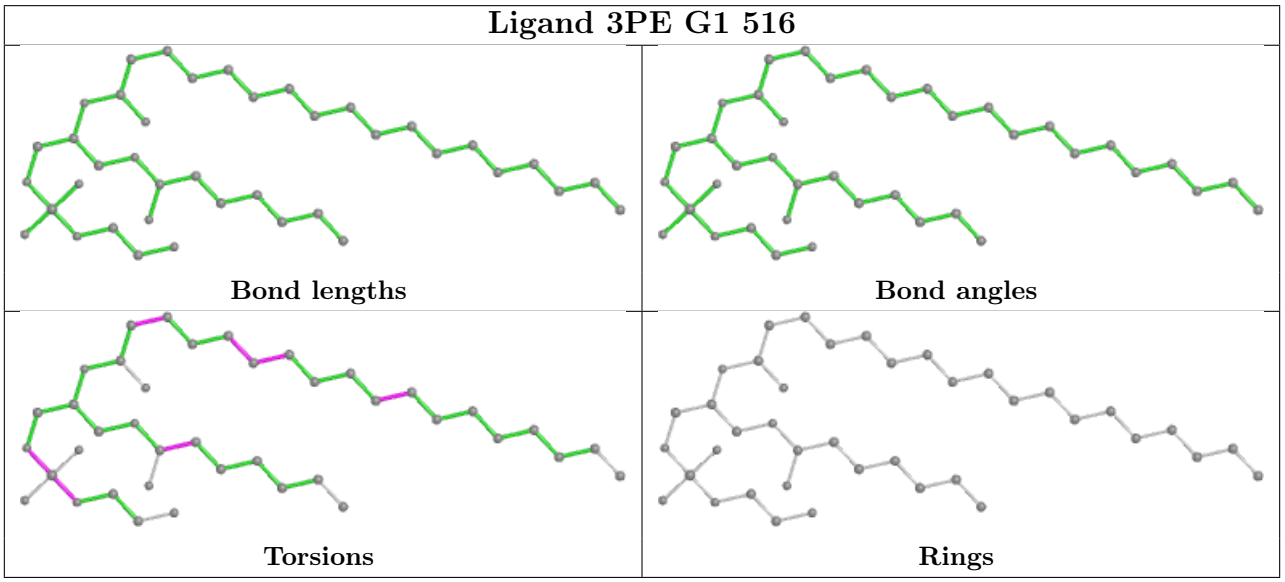


Rings

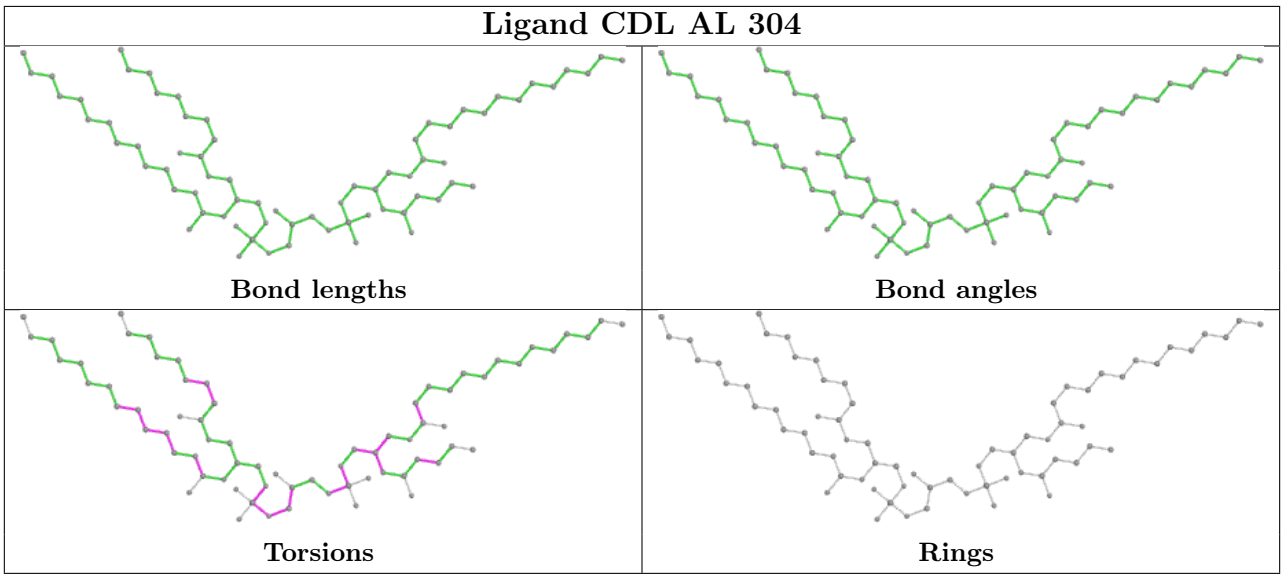
Ligand PC1 N1 701



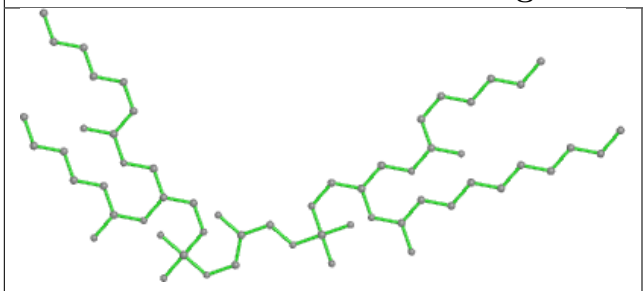
Ligand 3PE G1 516



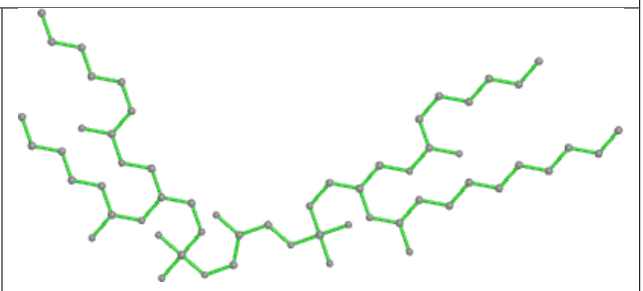
Ligand CDL AL 304



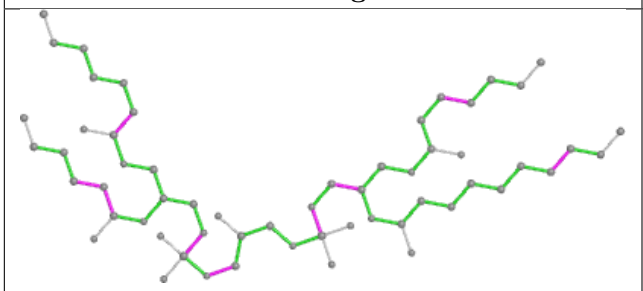
Ligand CDL B5 201



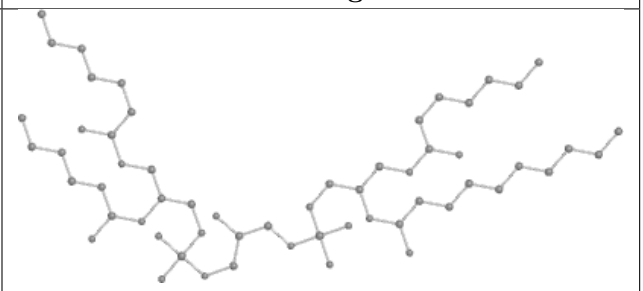
Bond lengths



Bond angles

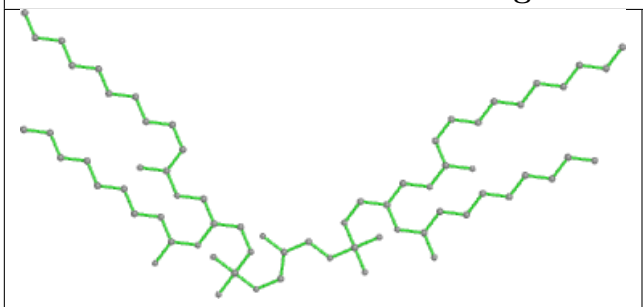


Torsions

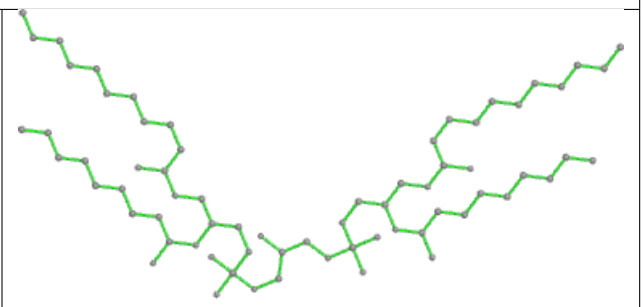


Rings

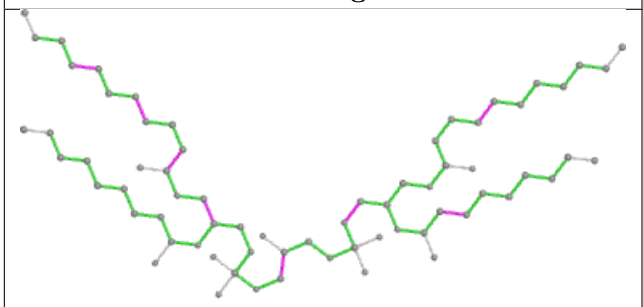
Ligand CDL AL 302



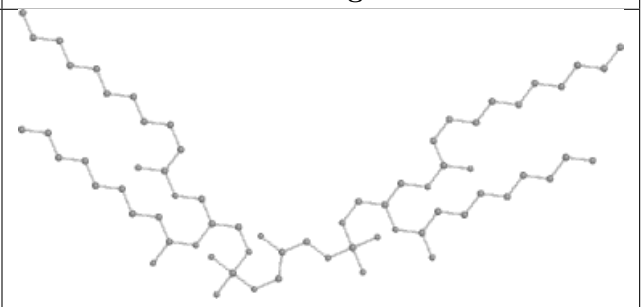
Bond lengths



Bond angles

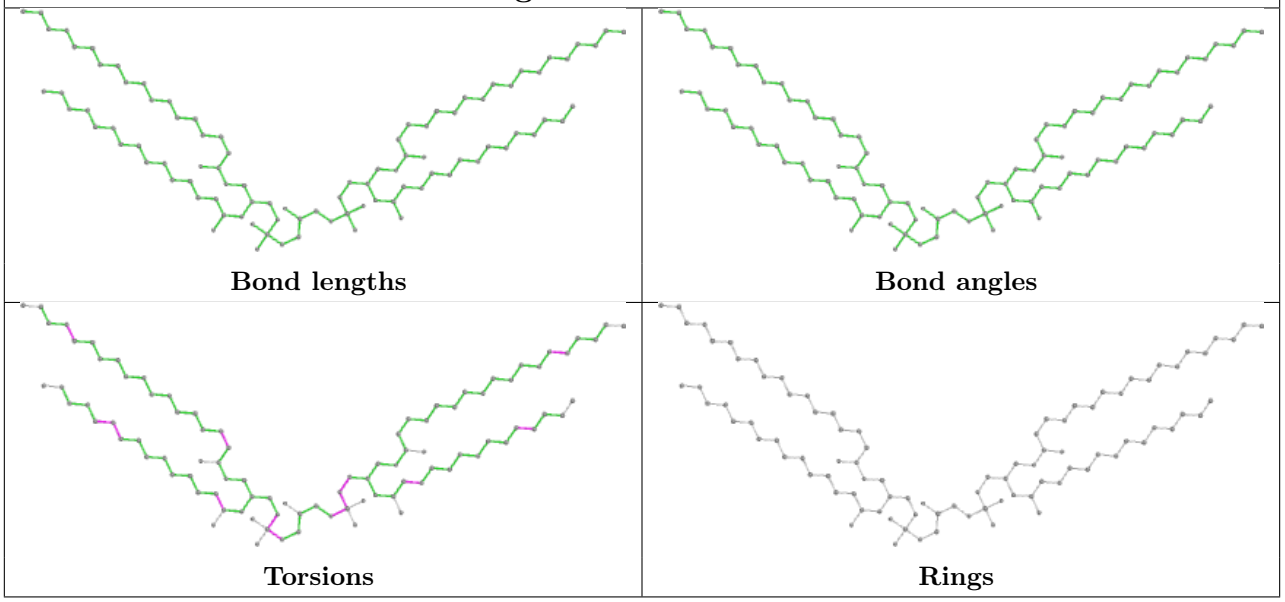


Torsions

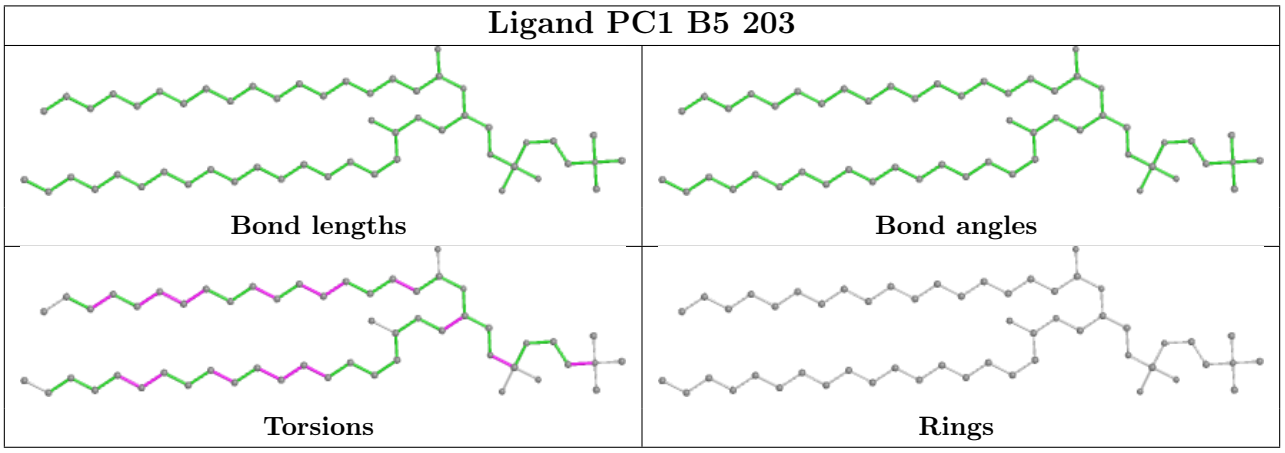


Rings

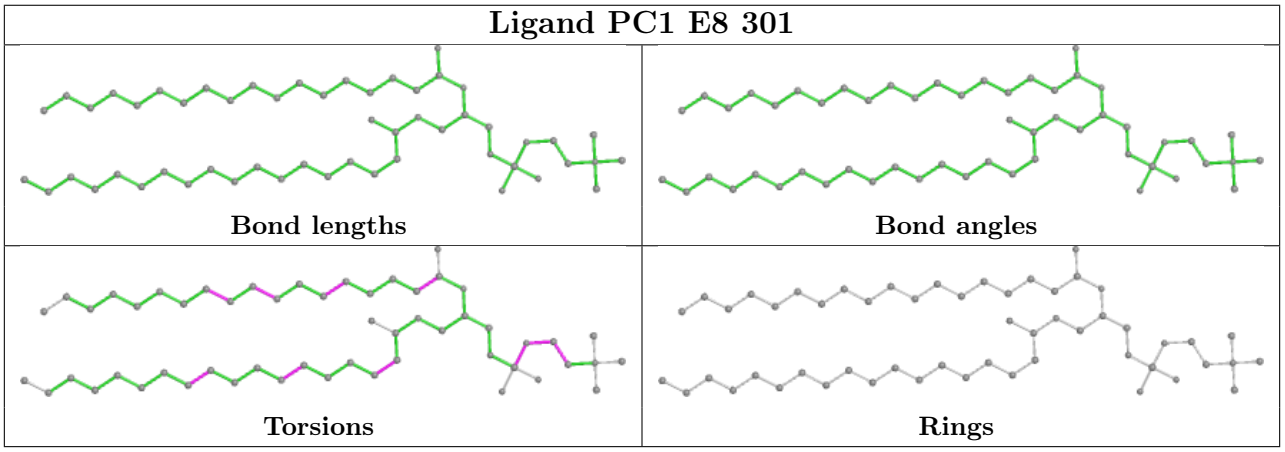
Ligand CDL N5 608



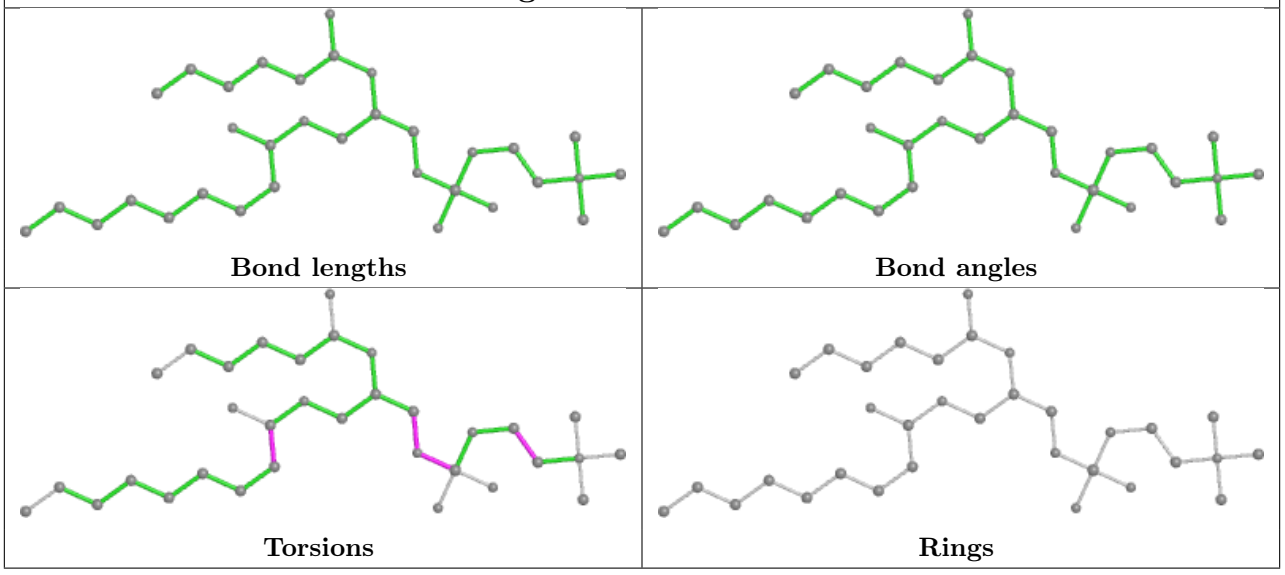
Ligand PC1 B5 203



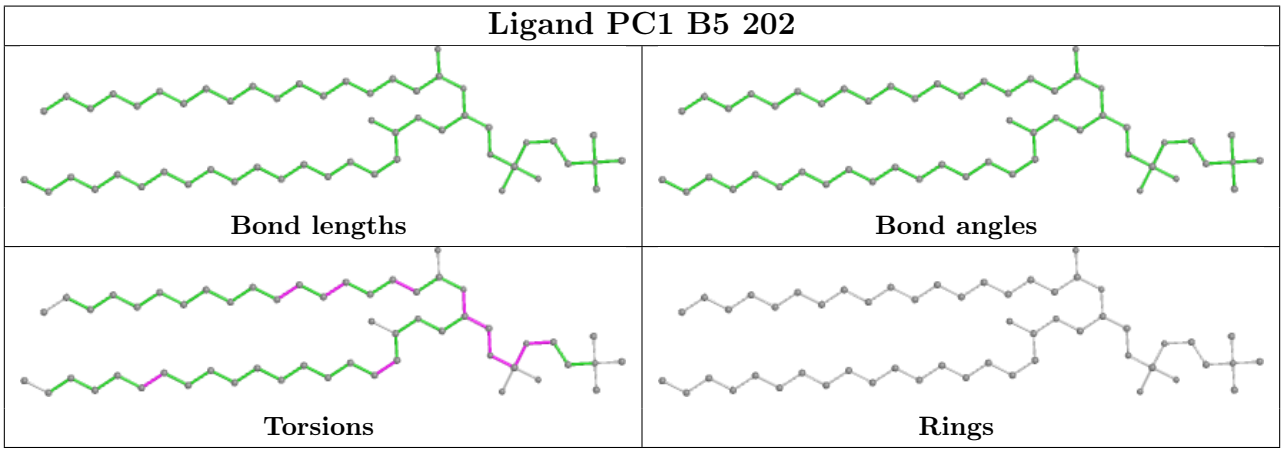
Ligand PC1 E8 301



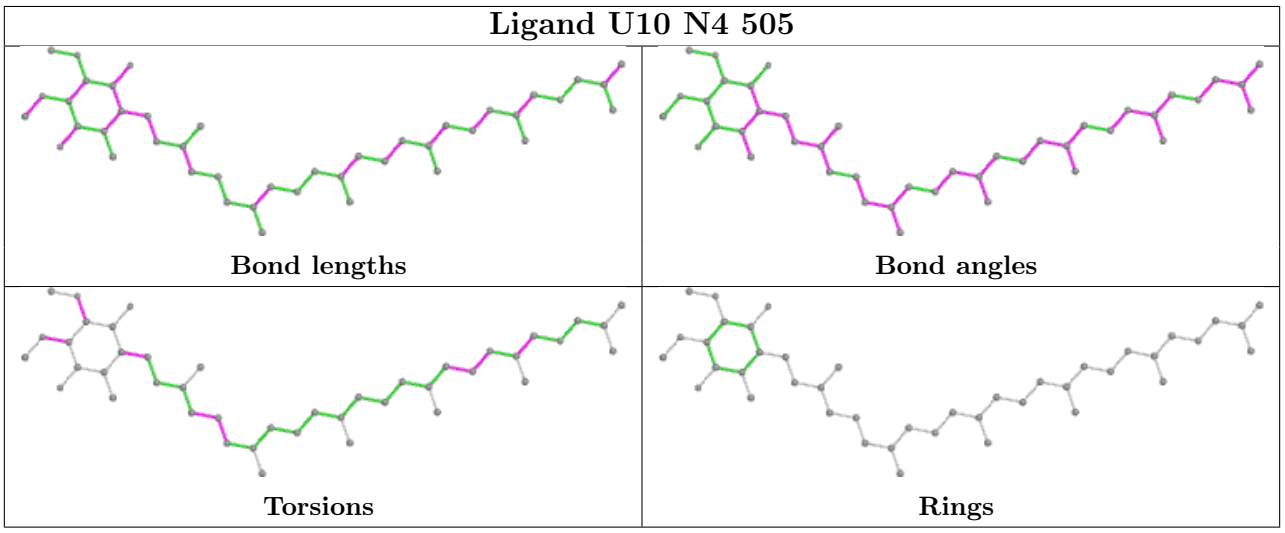
Ligand PC1 N4 503



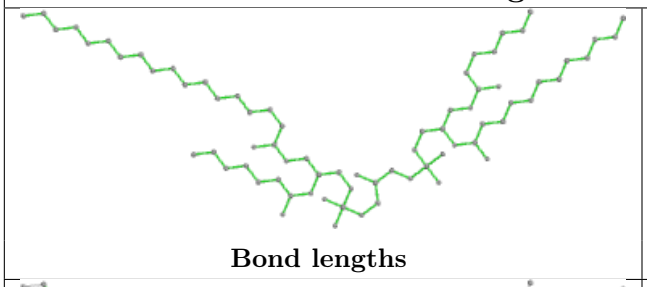
Ligand PC1 B5 202



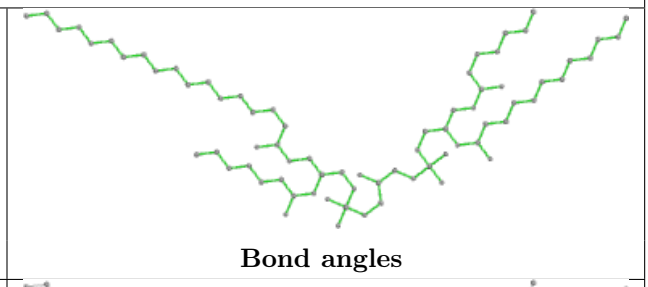
Ligand U10 N4 505



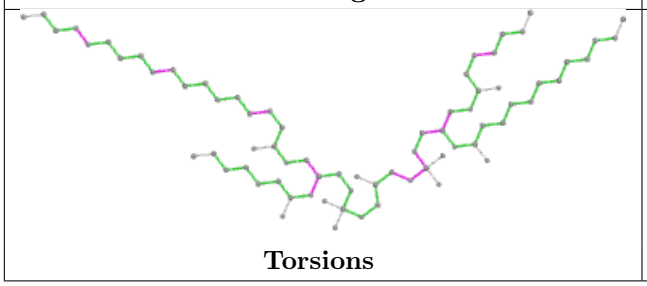
Ligand CDL AM 216



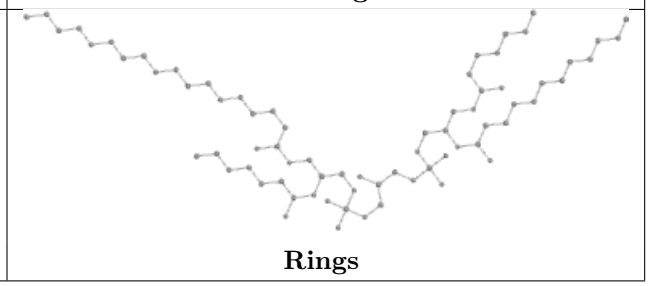
Bond lengths



Bond angles

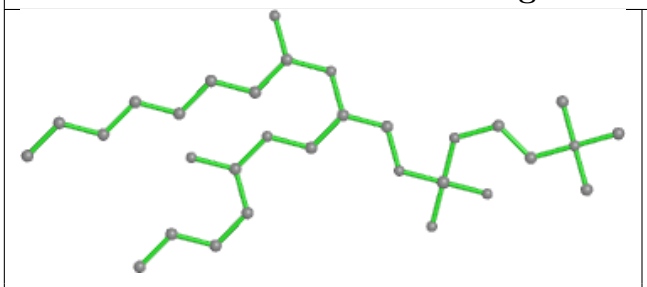


Torsions

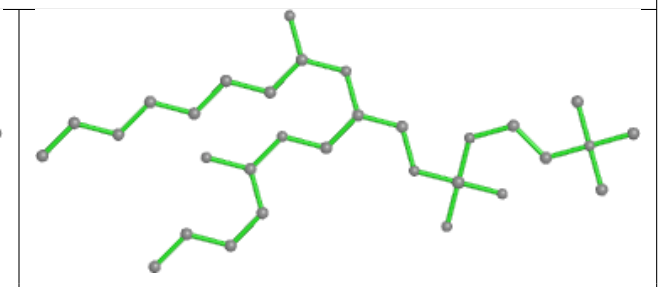


Rings

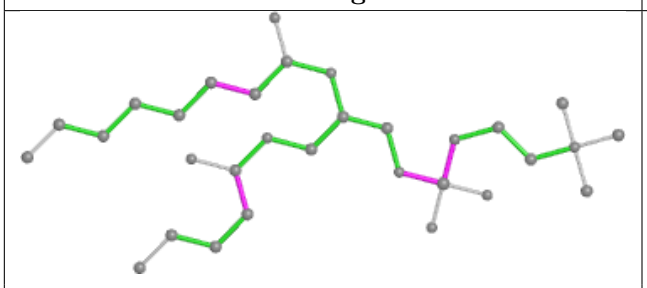
Ligand PC1 A1 203



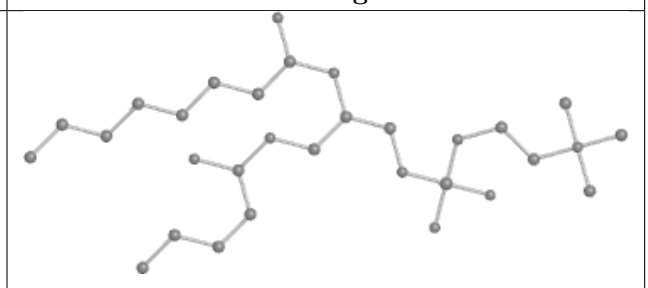
Bond lengths



Bond angles

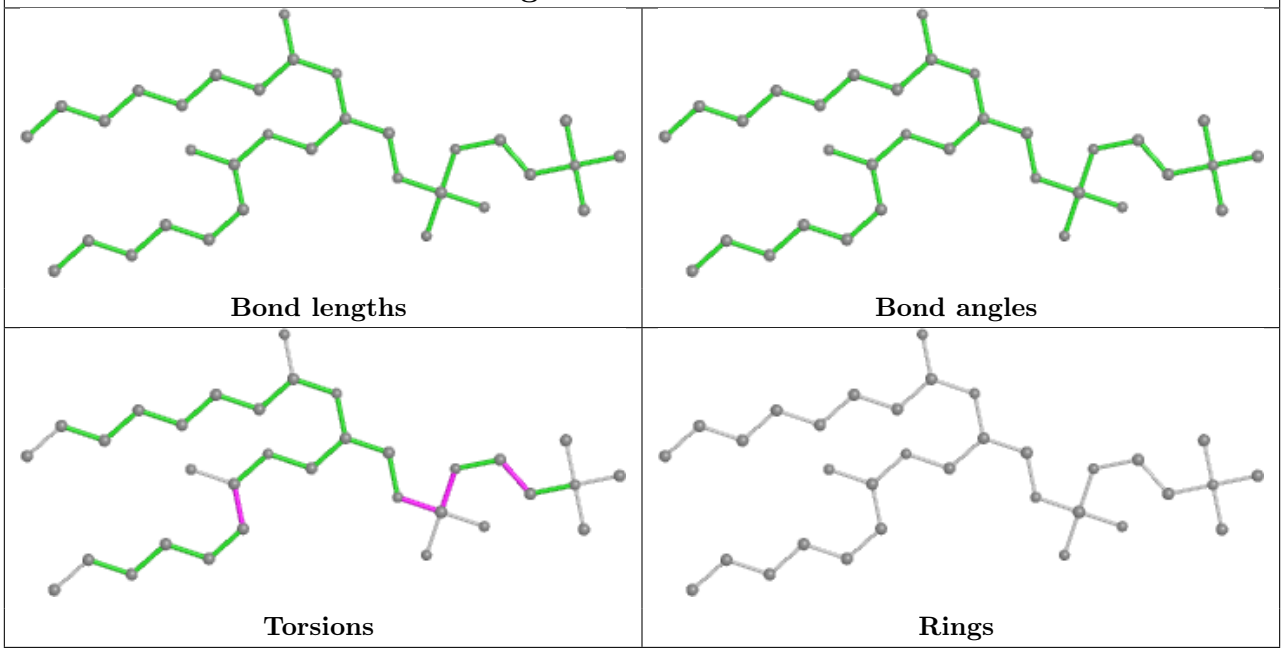


Torsions

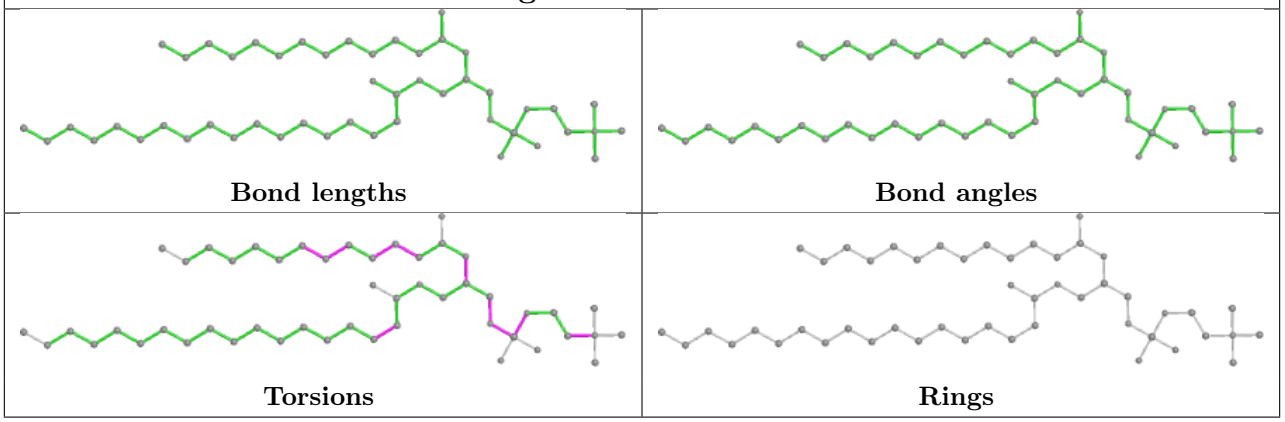


Rings

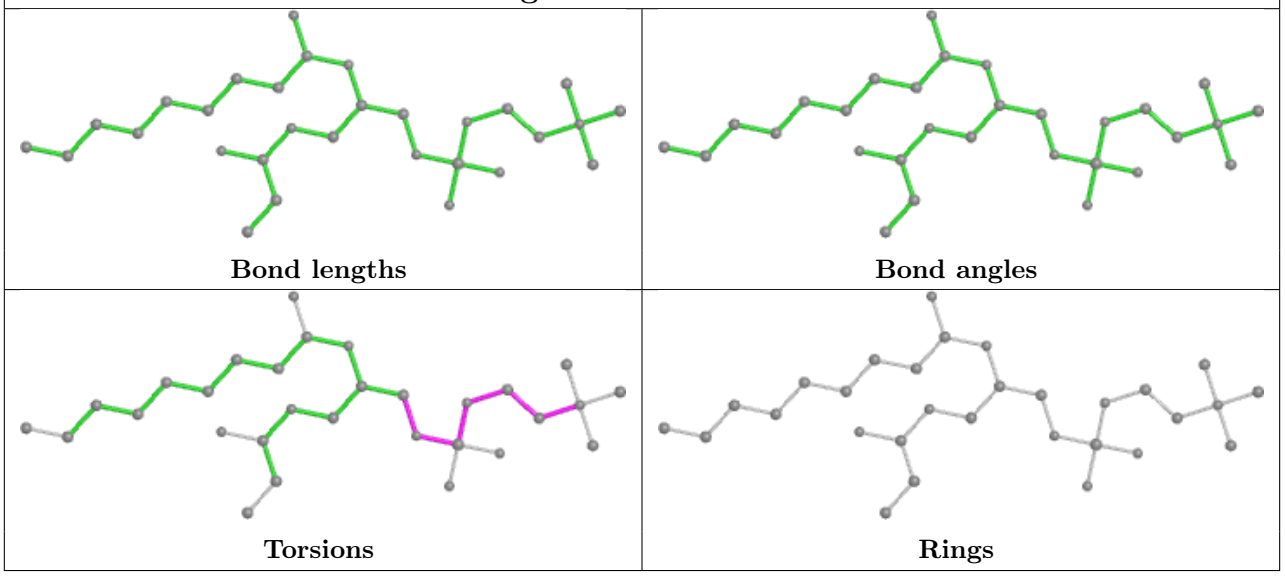
Ligand PC1 E8 303



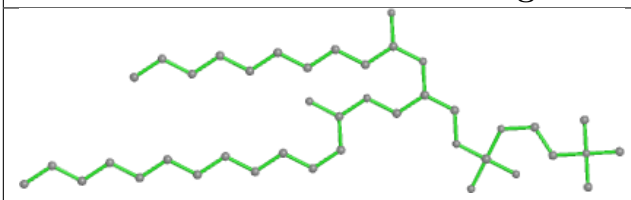
Ligand PC1 A1 202



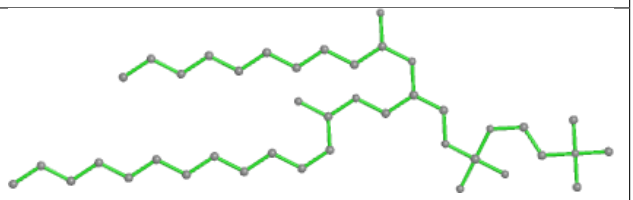
Ligand PC1 E8 304



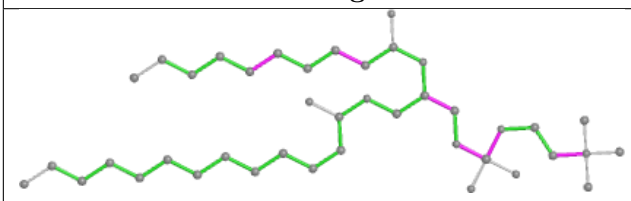
Ligand PC1 N5 605



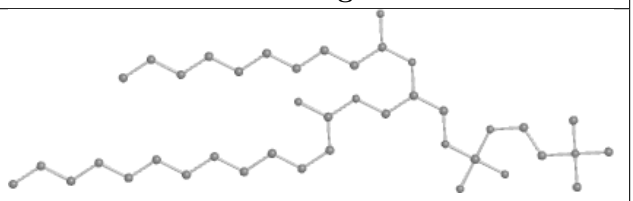
Bond lengths



Bond angles

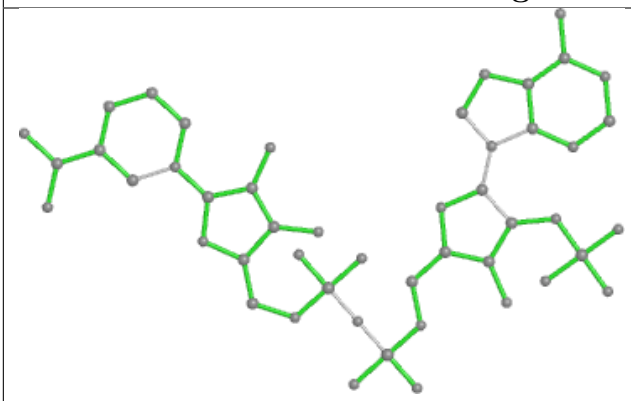


Torsions

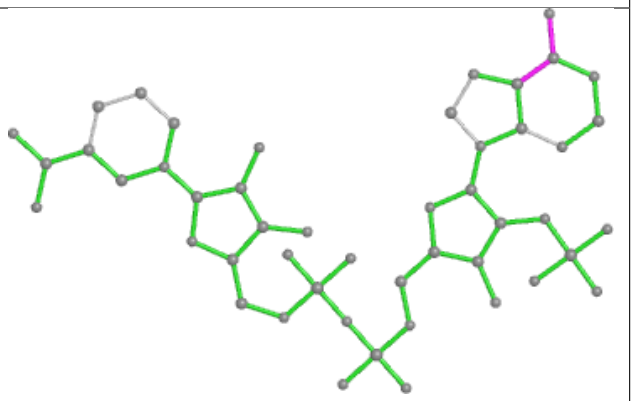


Rings

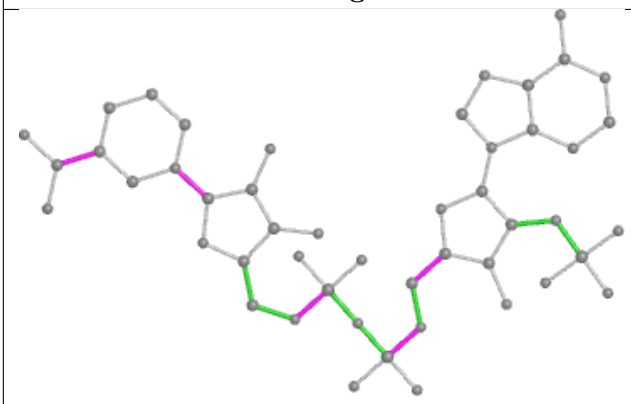
Ligand NDP A9 559



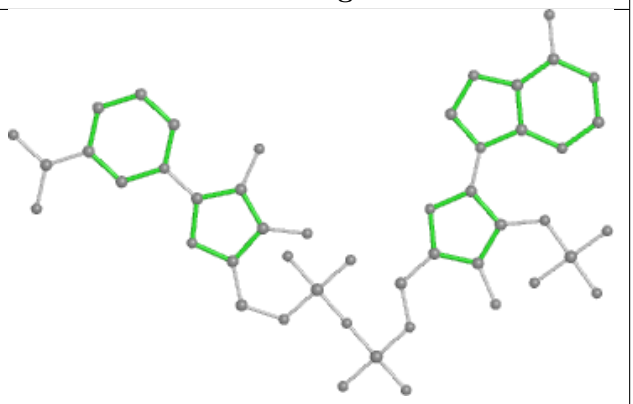
Bond lengths



Bond angles

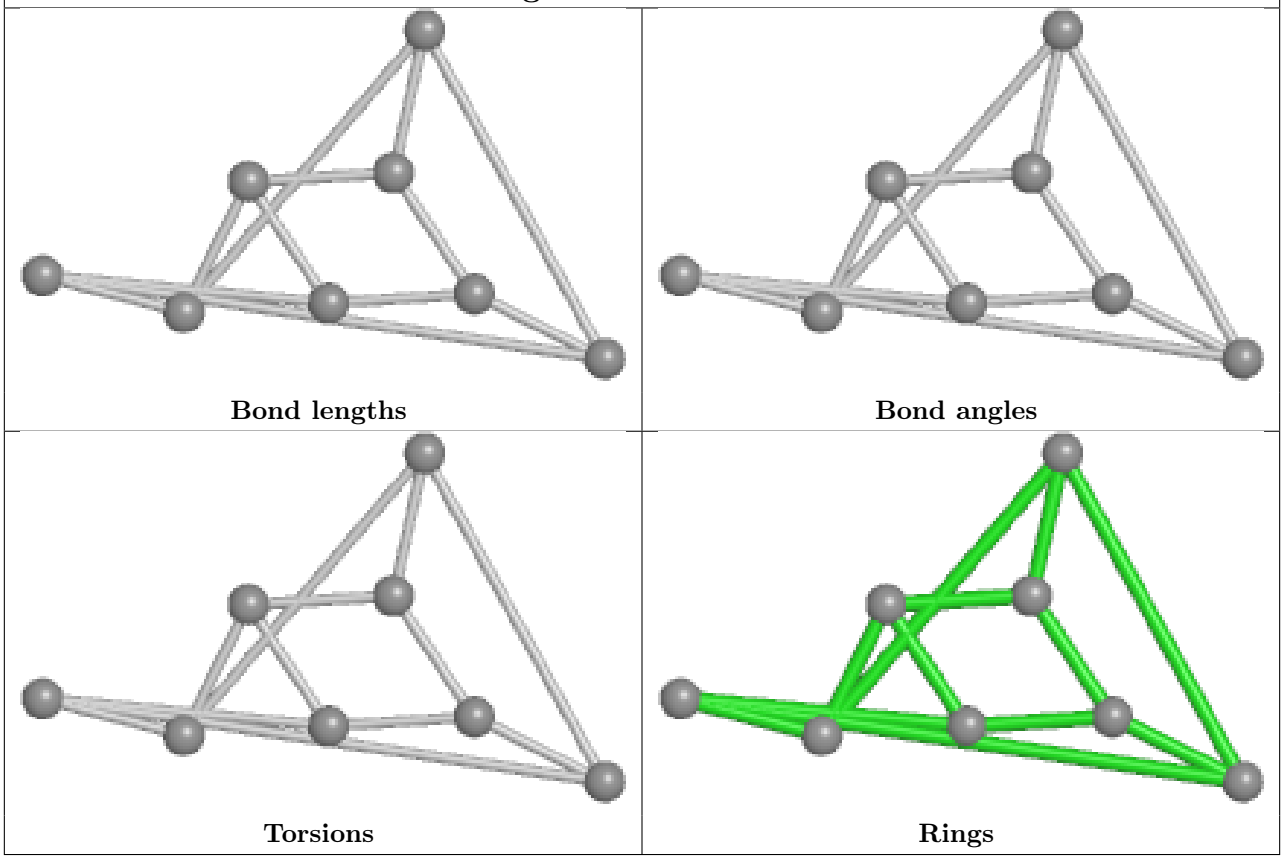


Torsions

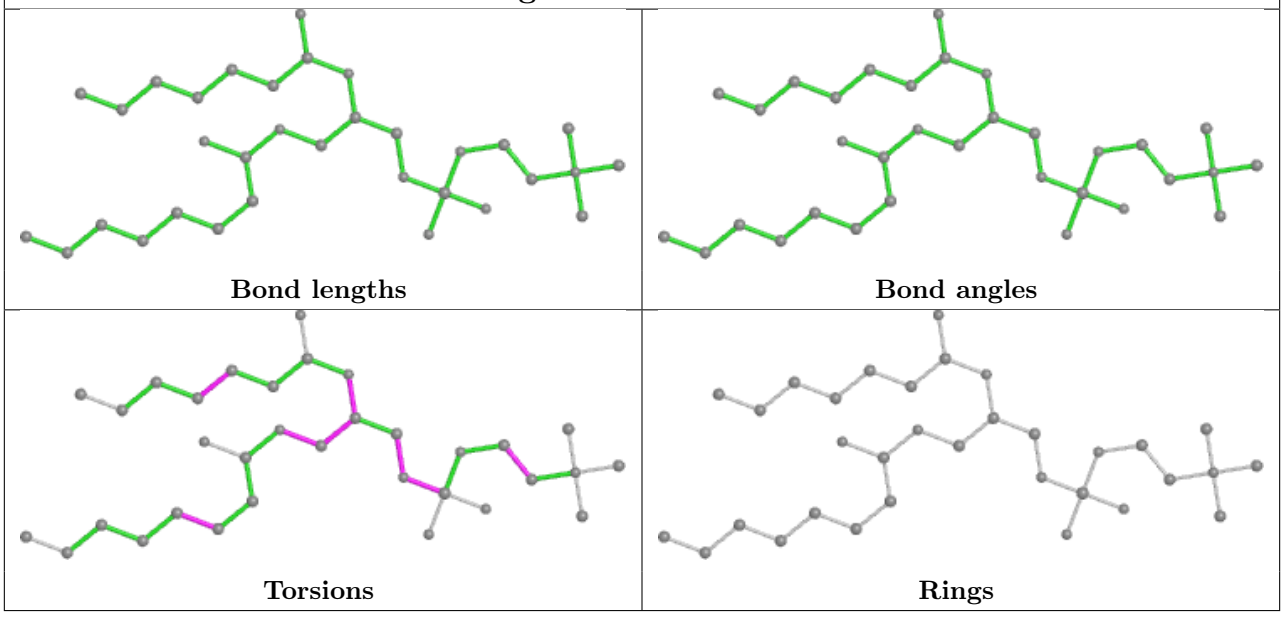


Rings

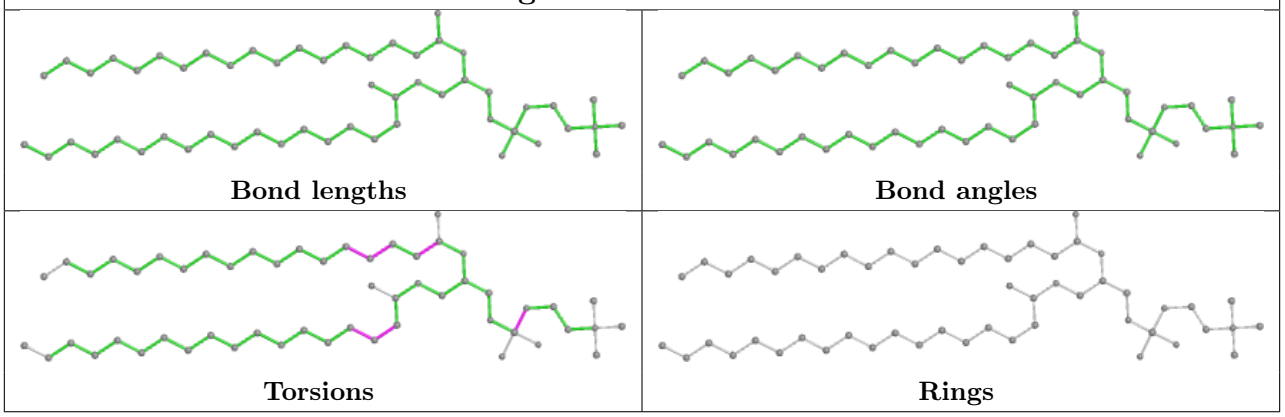
Ligand SF4 1A 402



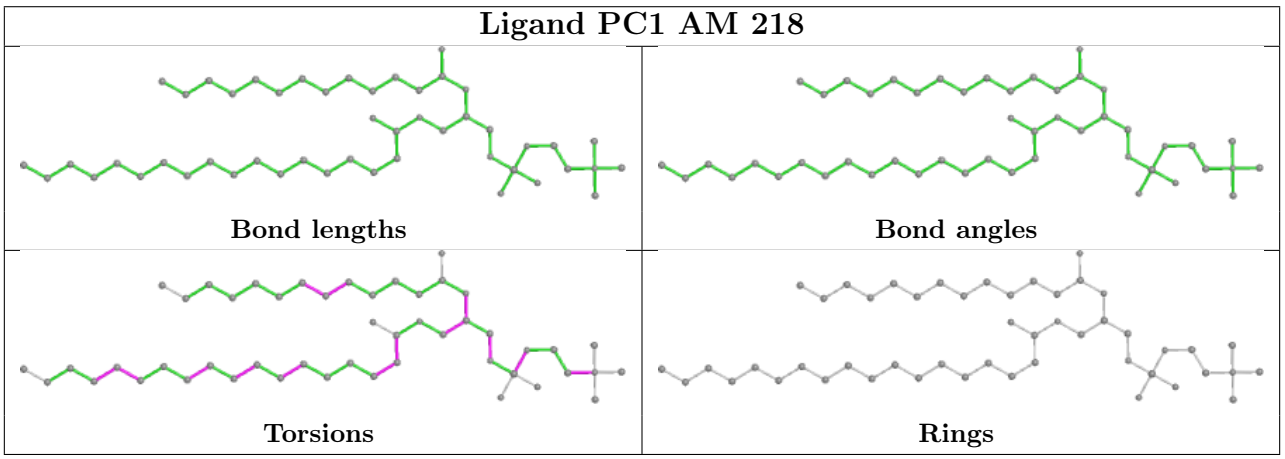
Ligand PC1 A9 560



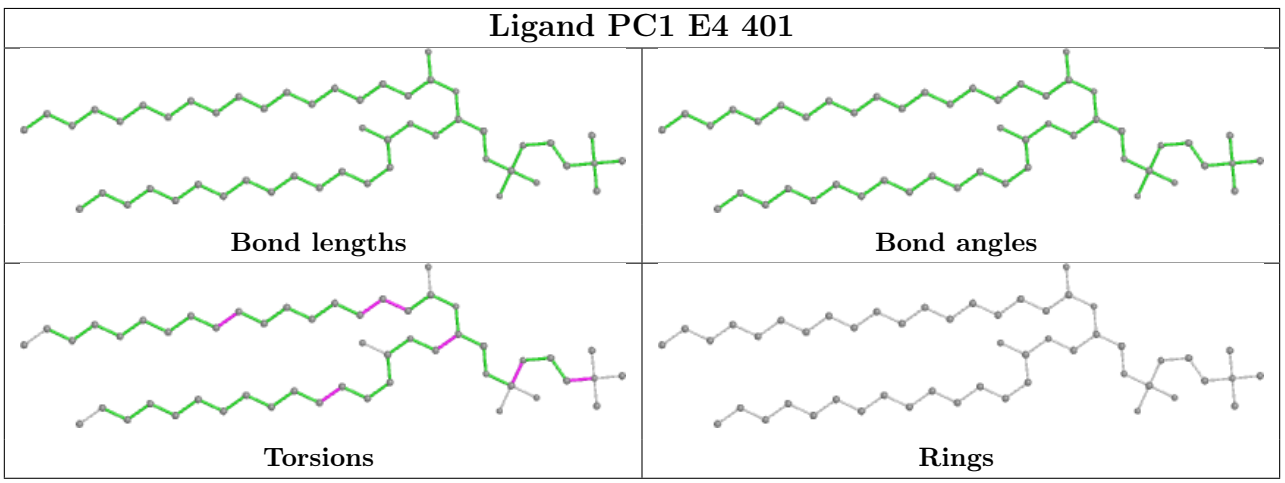
Ligand PC1 N5 601



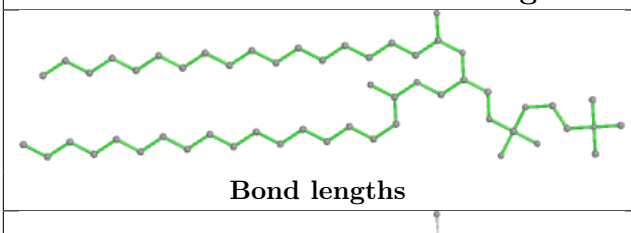
Ligand PC1 AM 218



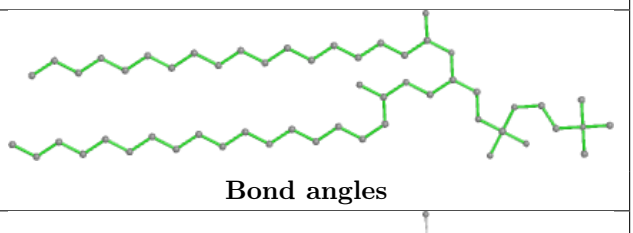
Ligand PC1 E4 401



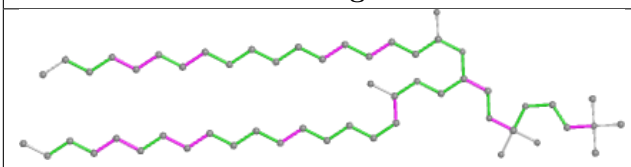
Ligand PC1 E8 302



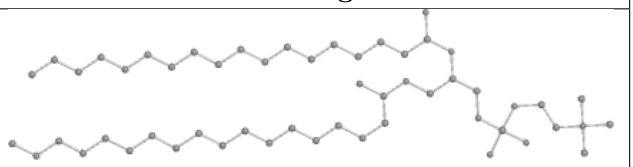
Bond lengths



Bond angles

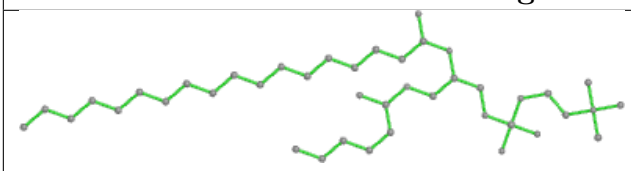


Torsions

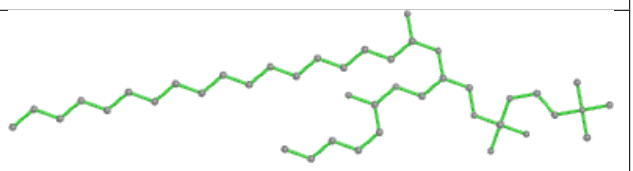


Rings

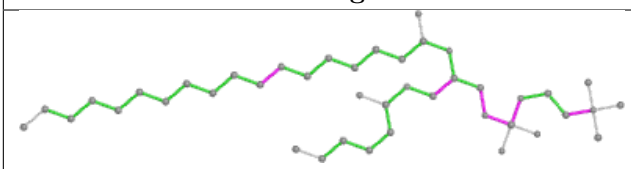
Ligand PC1 N3 301



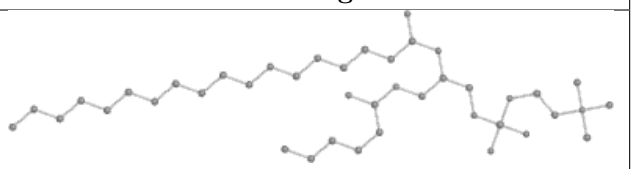
Bond lengths



Bond angles

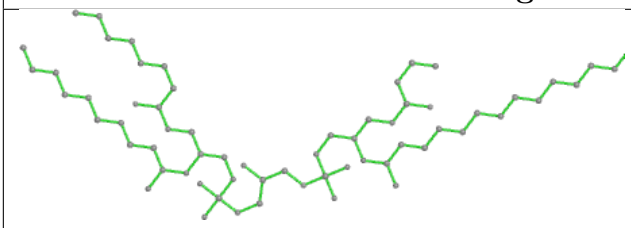


Torsions

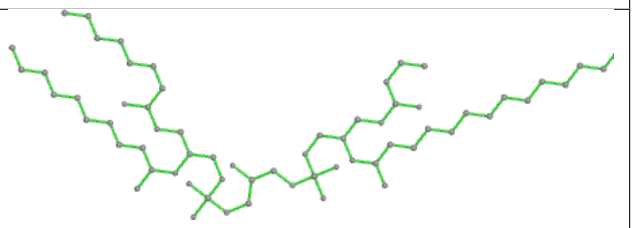


Rings

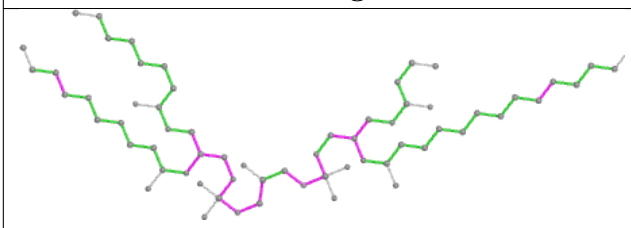
Ligand CDL E6 431



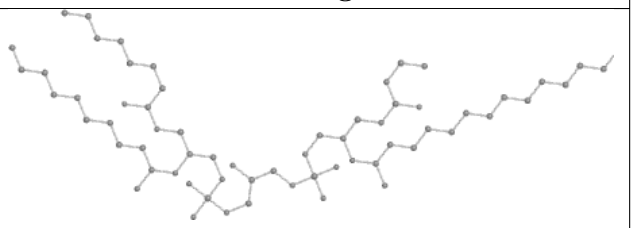
Bond lengths



Bond angles

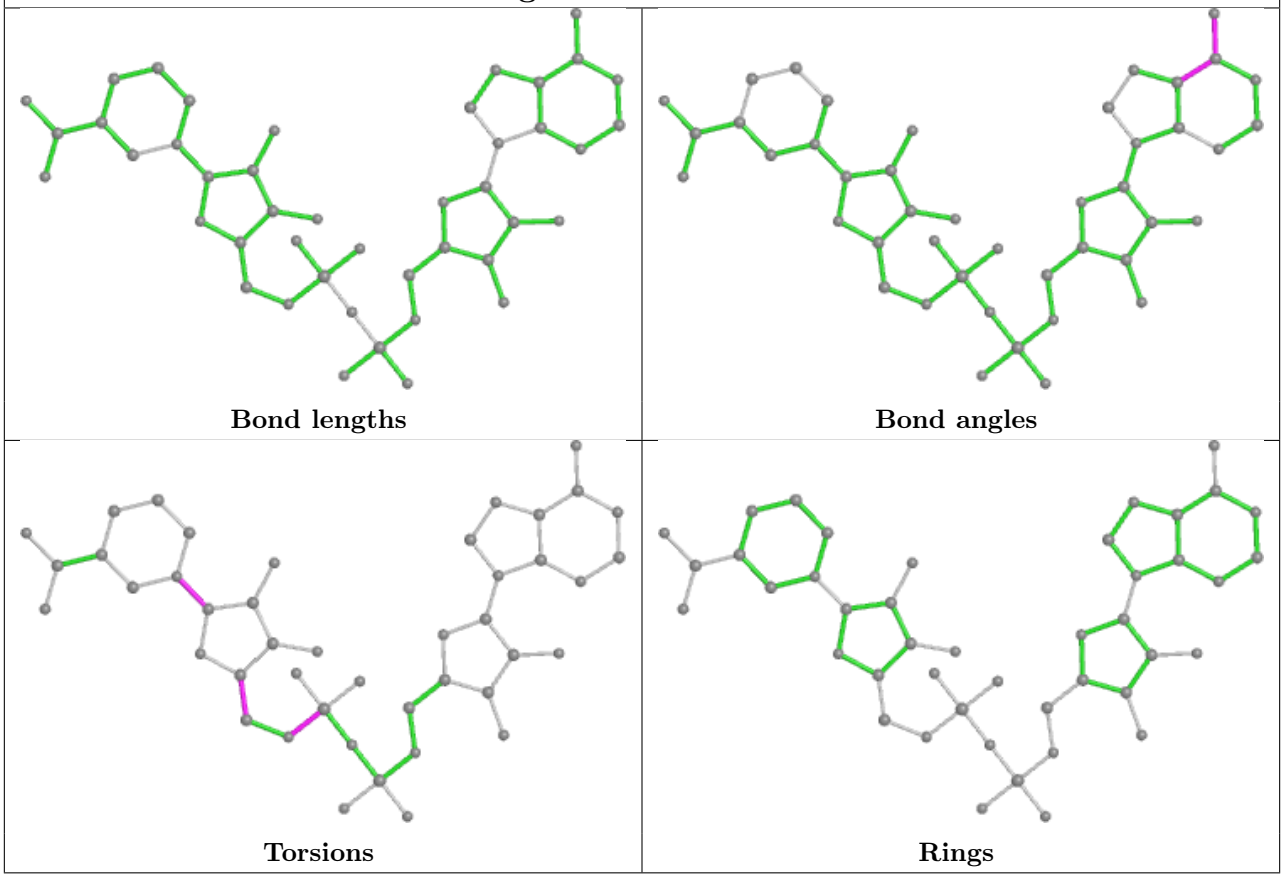


Torsions

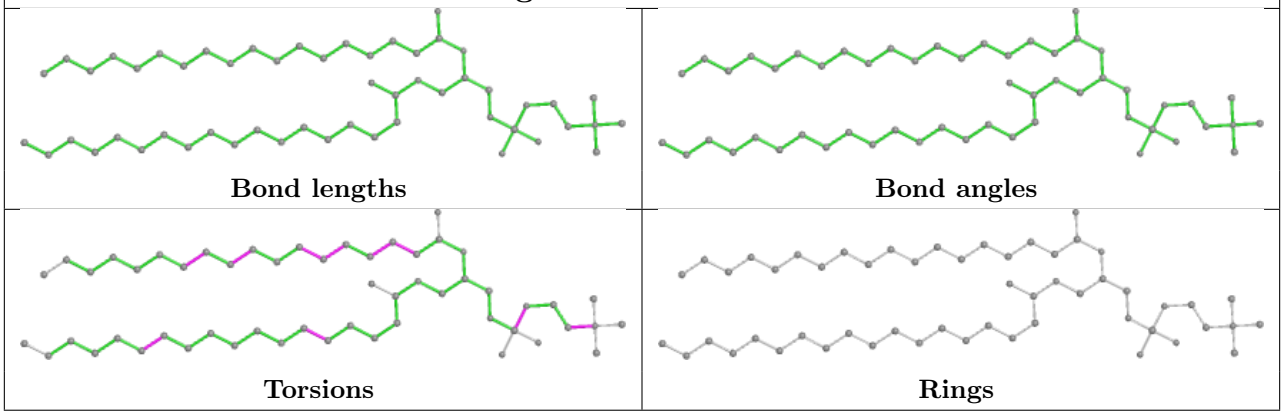


Rings

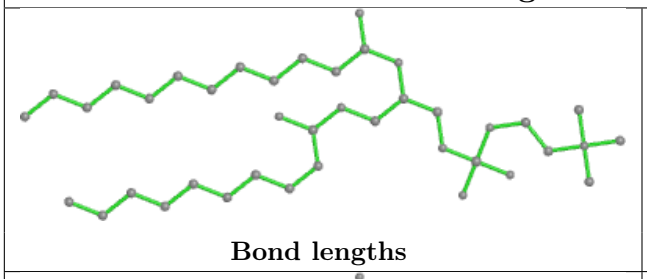
Ligand NAI V1 581



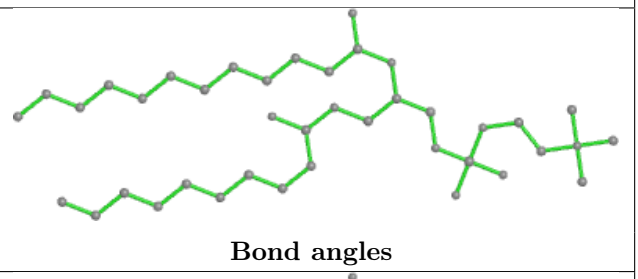
Ligand PC1 ED 201



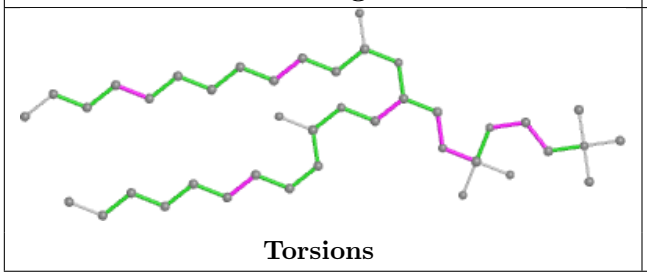
Ligand PC1 N1 702



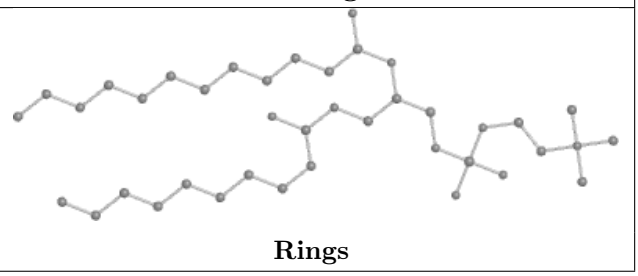
Bond lengths



Bond angles

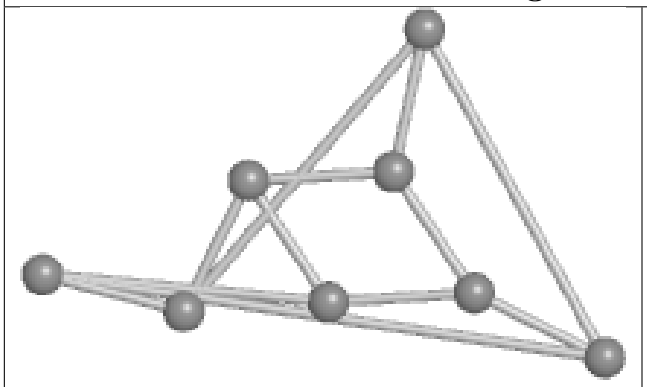


Torsions

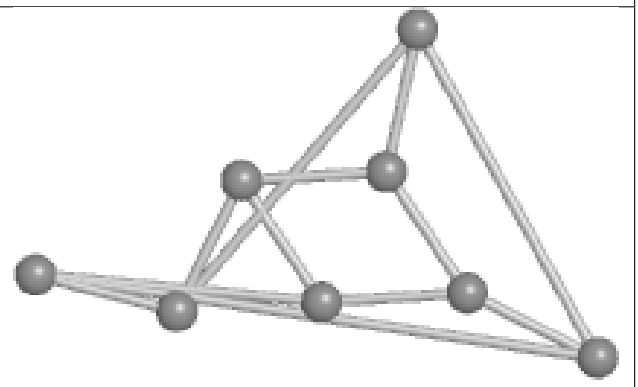


Rings

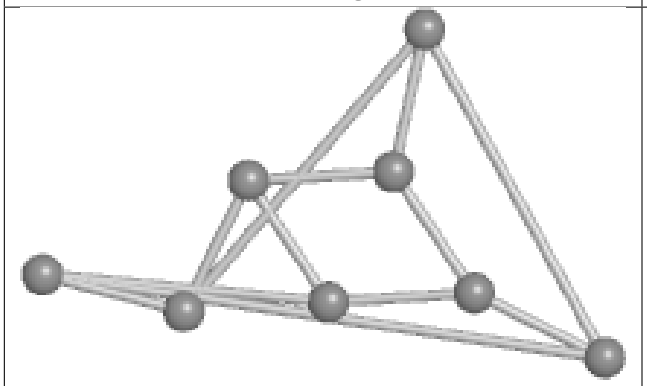
Ligand SF4 S8 298



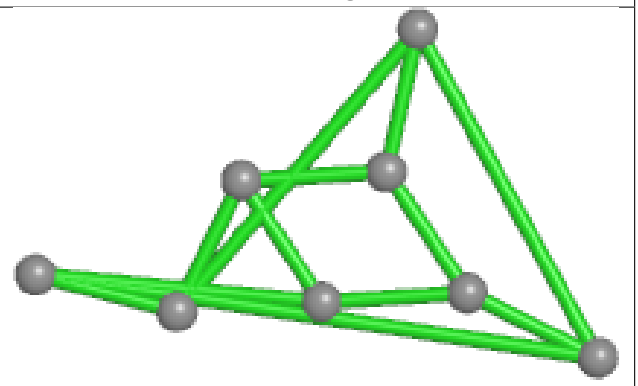
Bond lengths



Bond angles

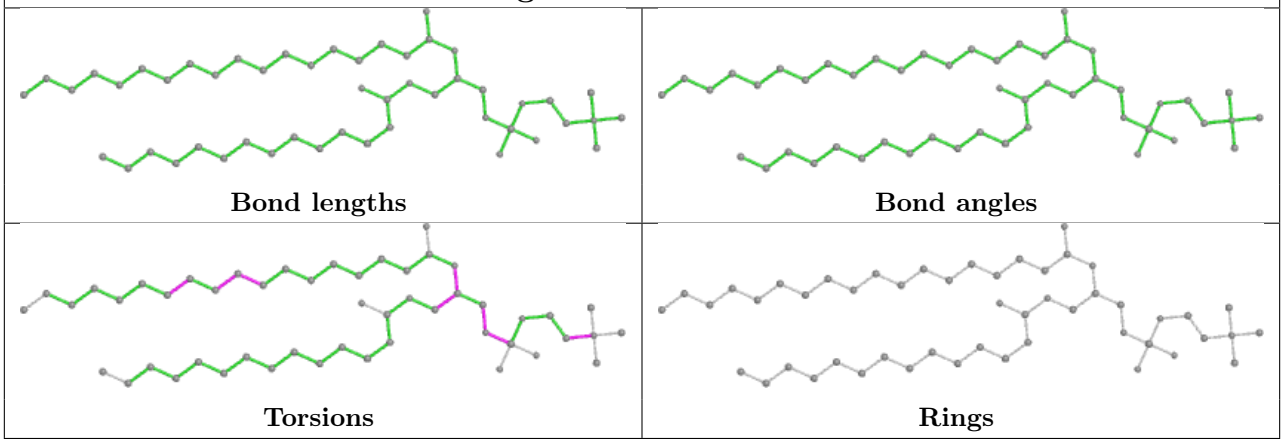


Torsions

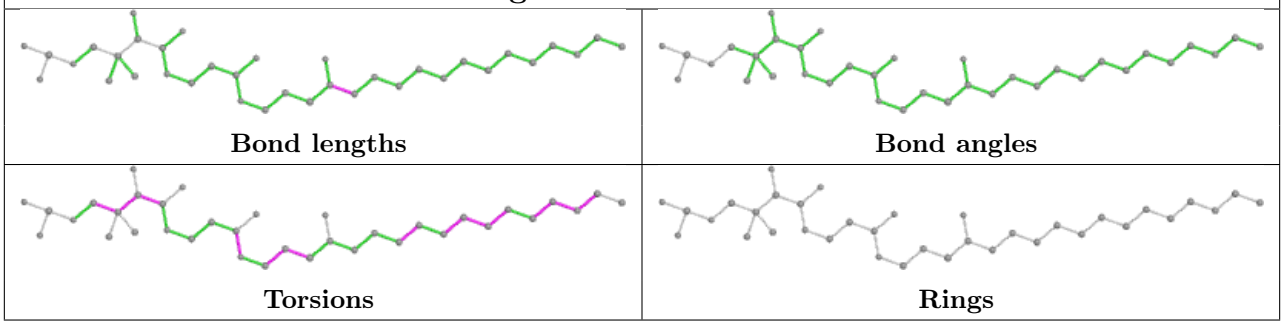


Rings

Ligand PC1 AL 301



Ligand ZMP AC 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.

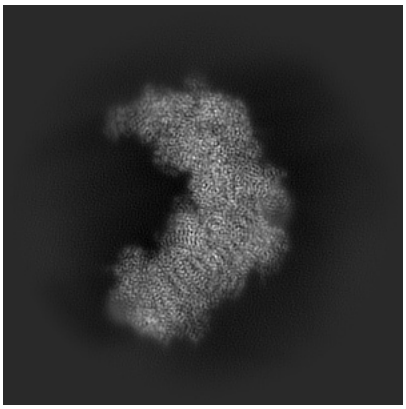
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36109. These allow visual inspection of the internal detail of the map and identification of artifacts.

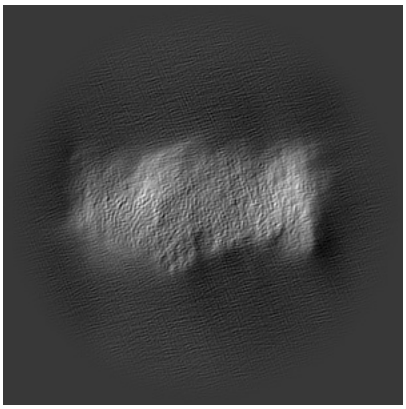
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

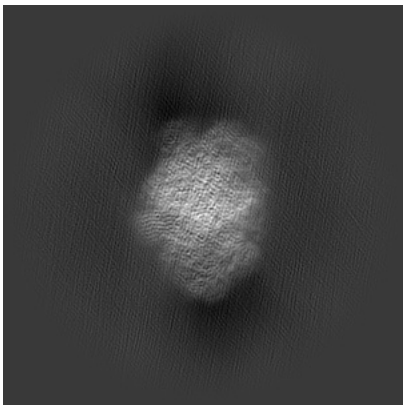
6.1.1 Primary map



X

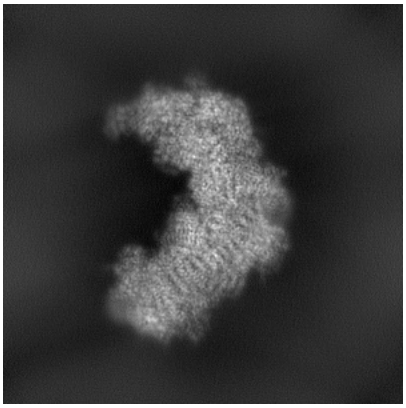


Y

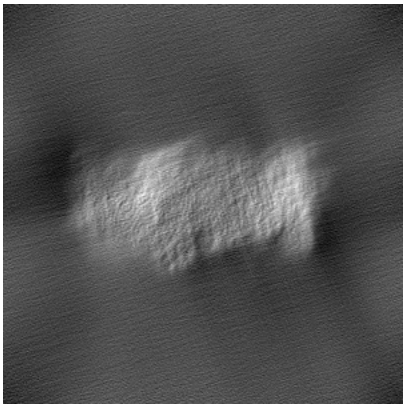


Z

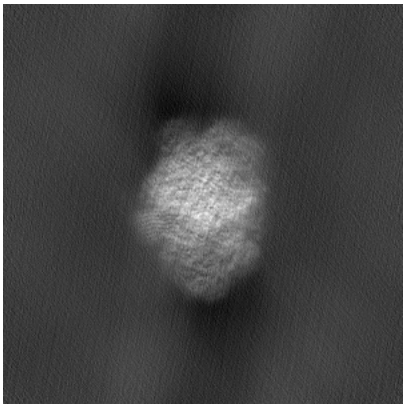
6.1.2 Raw map



X



Y

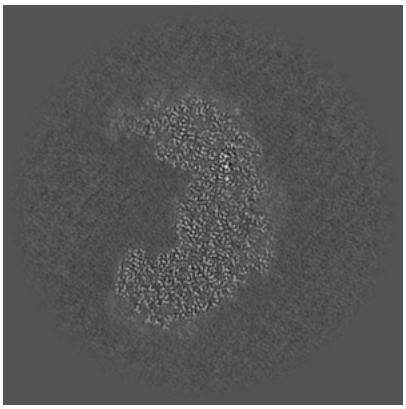


Z

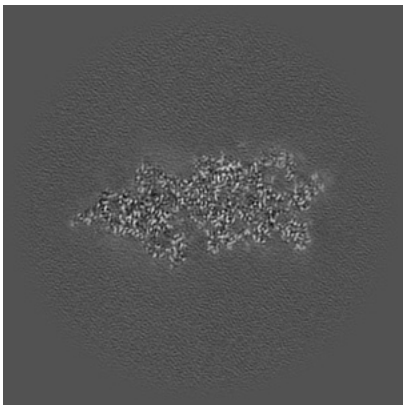
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

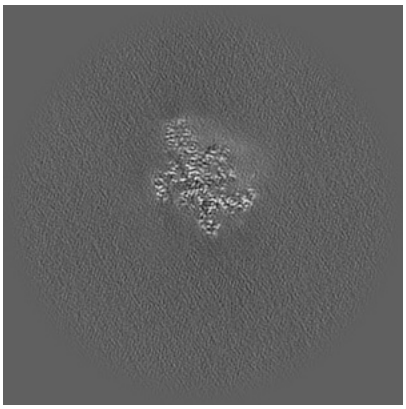
6.2.1 Primary map



X Index: 240

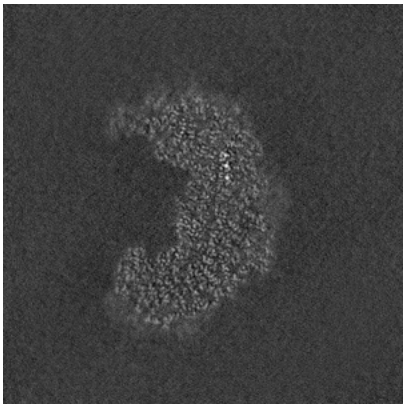


Y Index: 240

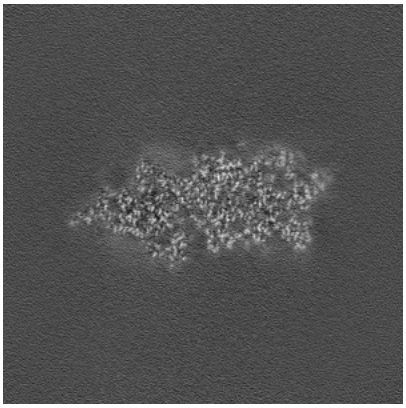


Z Index: 240

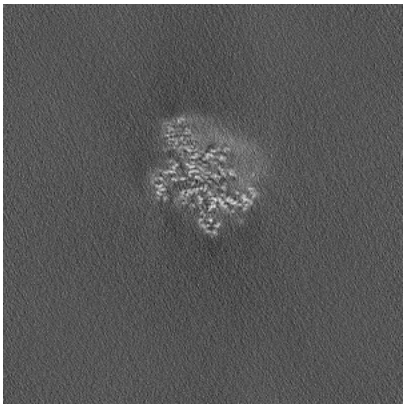
6.2.2 Raw map



X Index: 240



Y Index: 240

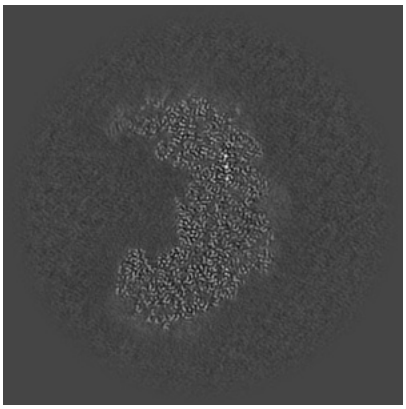


Z Index: 240

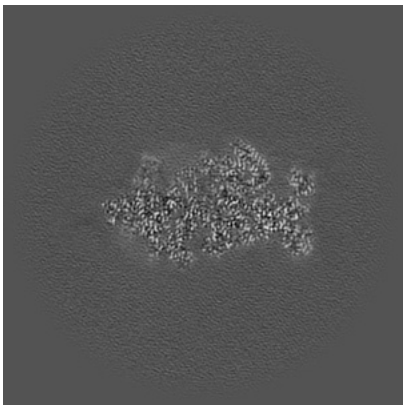
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

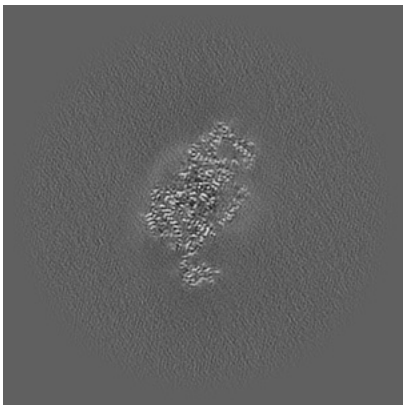
6.3.1 Primary map



X Index: 241

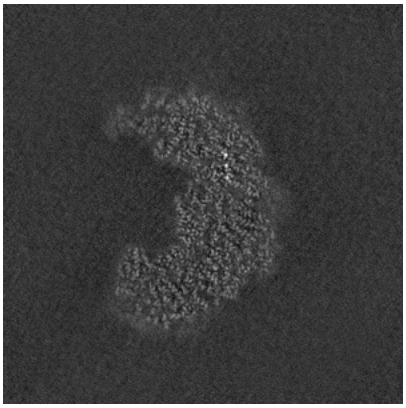


Y Index: 254

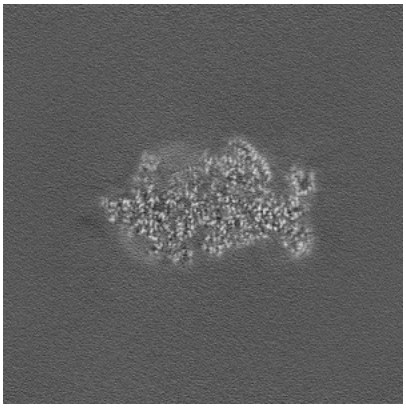


Z Index: 183

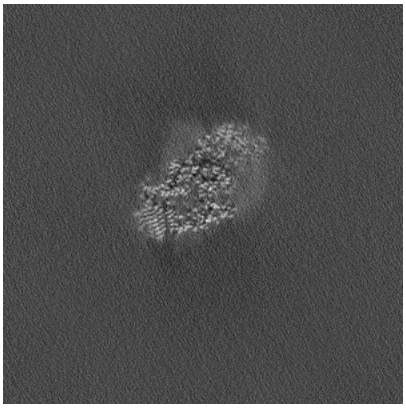
6.3.2 Raw map



X Index: 242



Y Index: 255

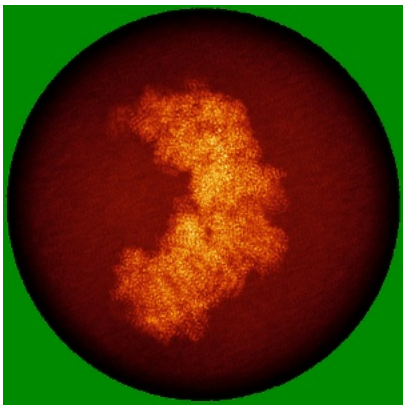


Z Index: 211

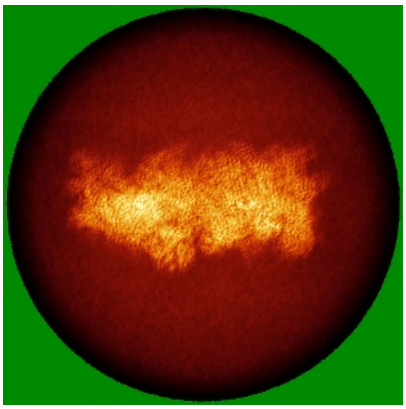
The images above show the largest variance slices of the map in three orthogonal directions.

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

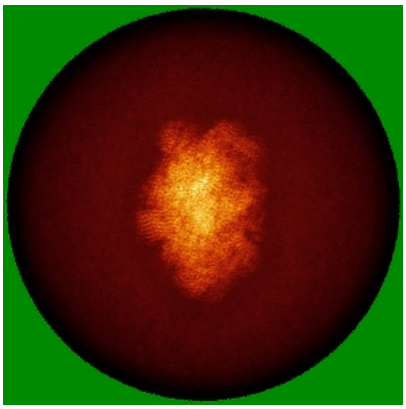
6.4.1 Primary map



X

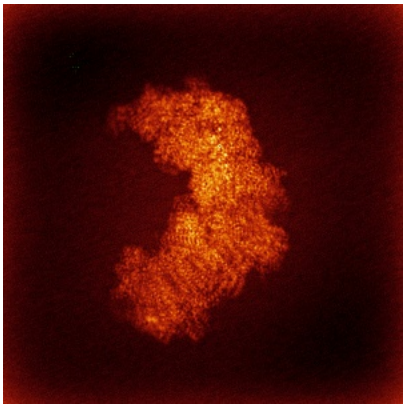


Y

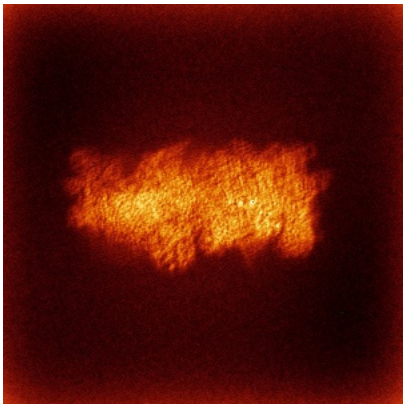


Z

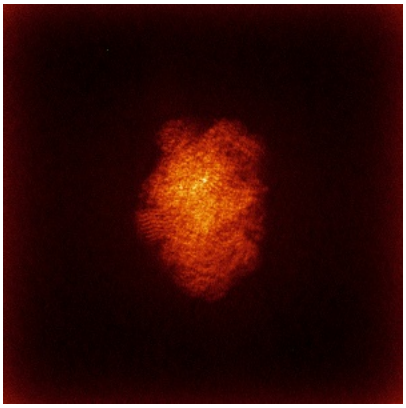
6.4.2 Raw map



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 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

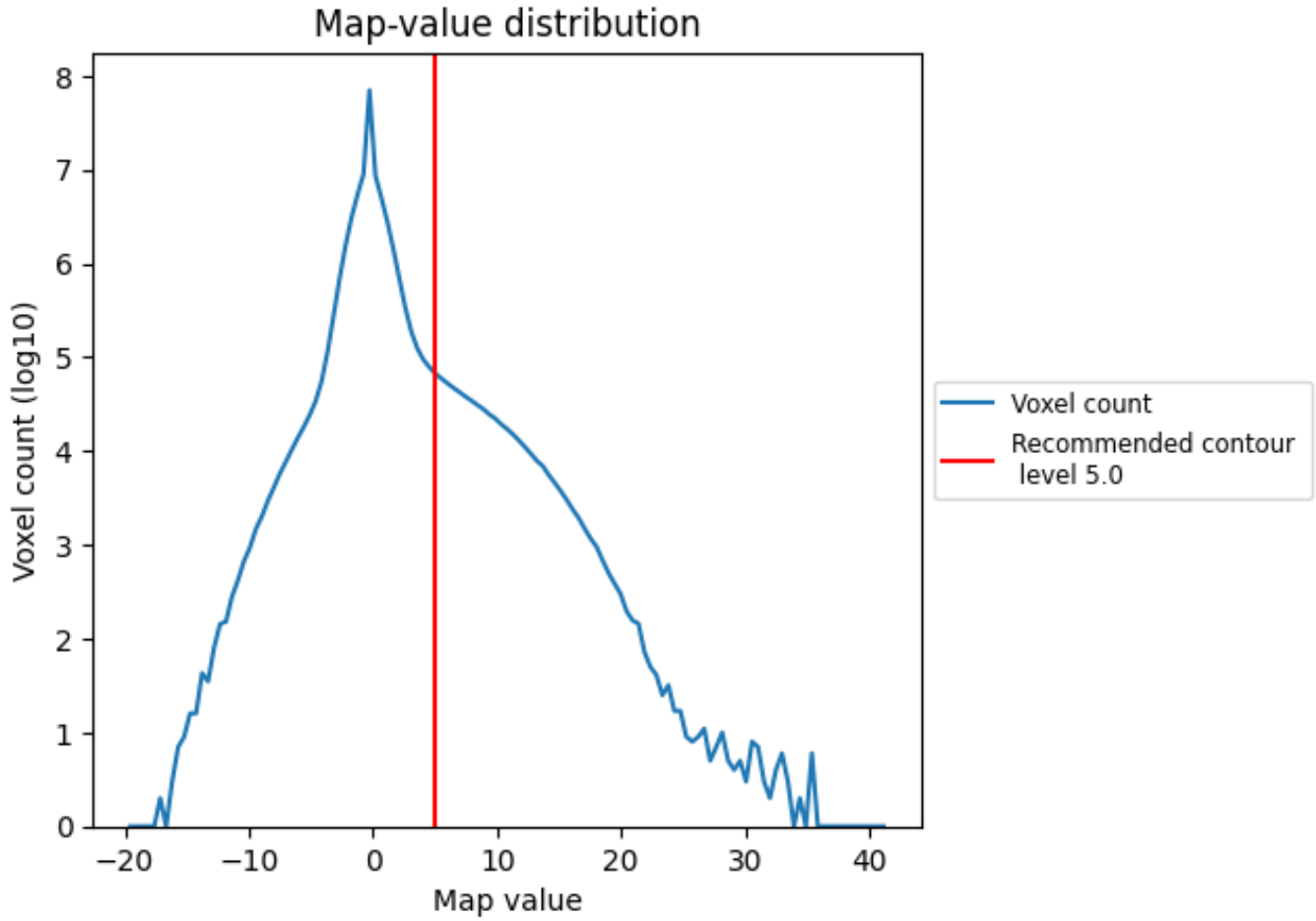
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

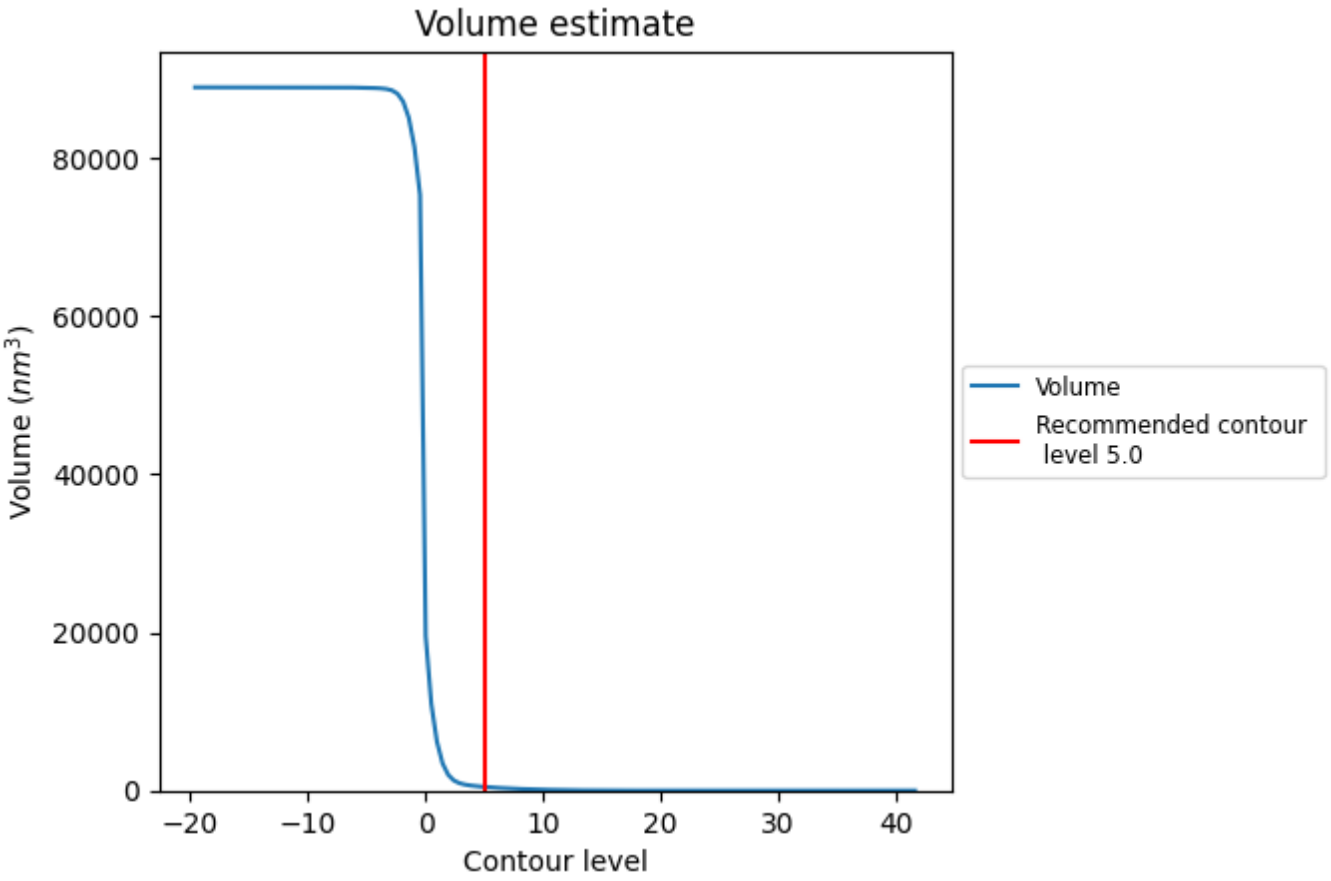
This section contains the results of statistical analysis of the map.

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.

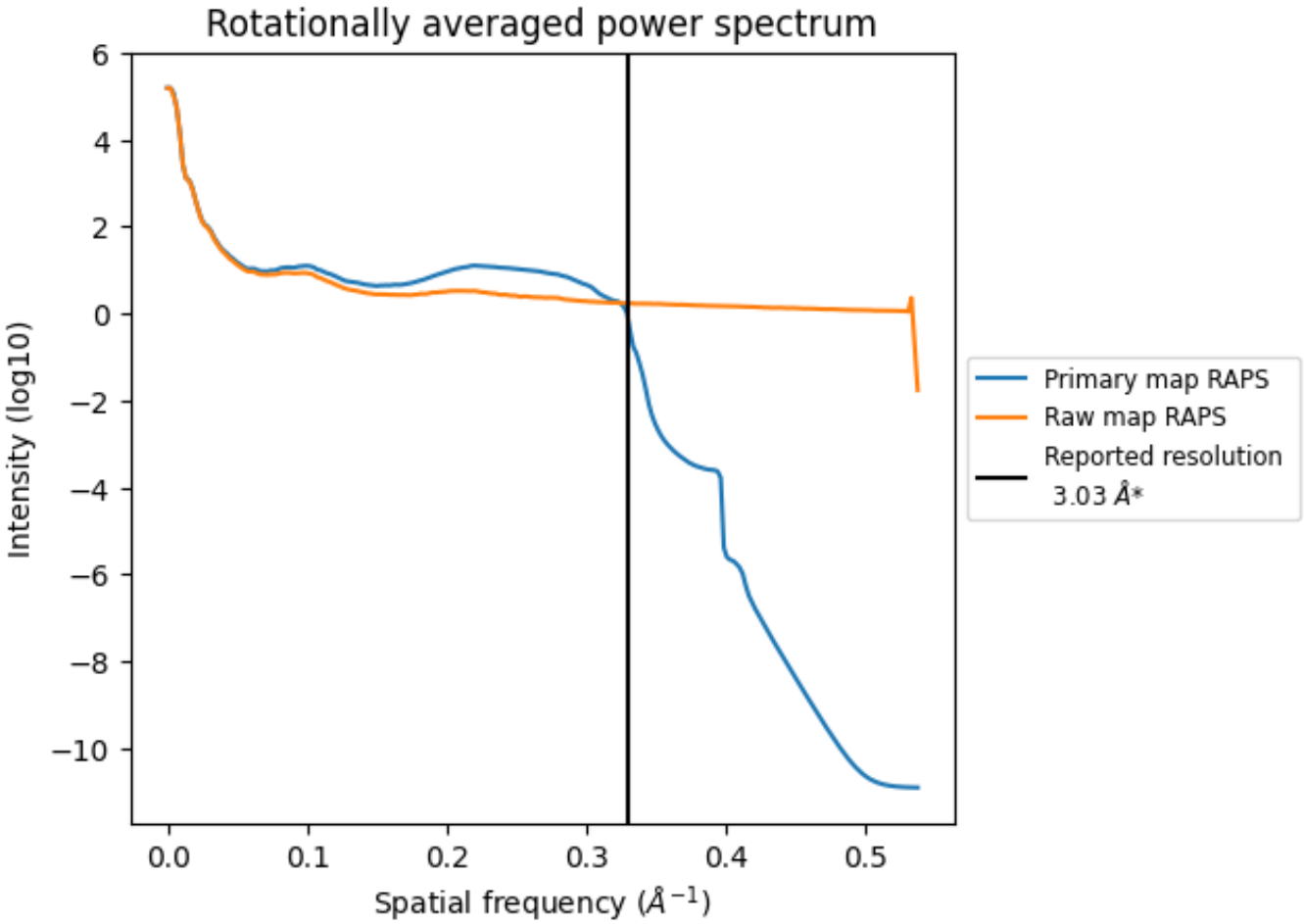
7.2 Volume estimate (i)



The volume at the recommended contour level is 468 nm^3; this corresponds to an approximate mass of 422 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)

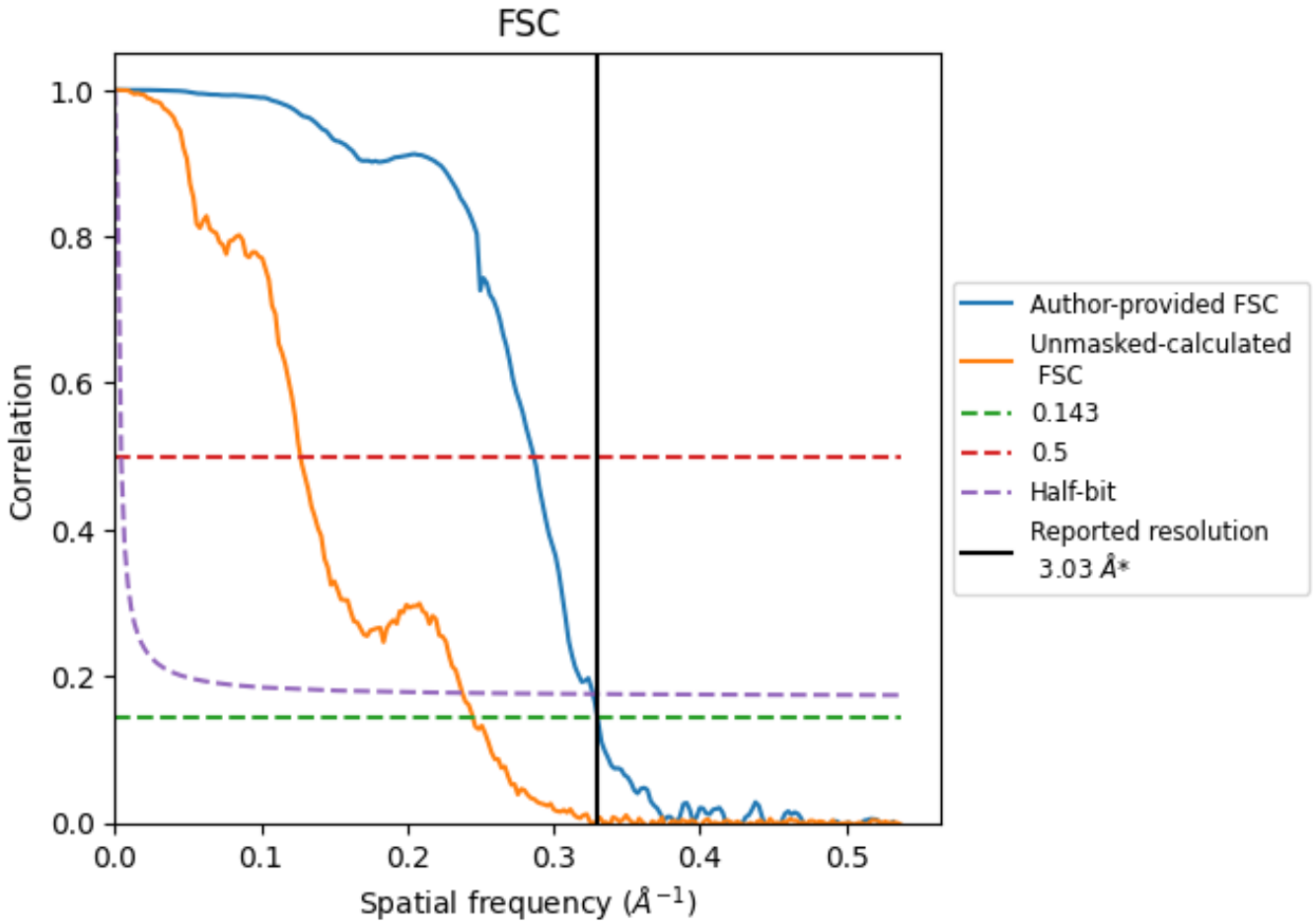


*Reported resolution corresponds to spatial frequency of 0.330 Å^{-1}

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 0.330 Å^{-1}

8.2 Resolution estimates (i)

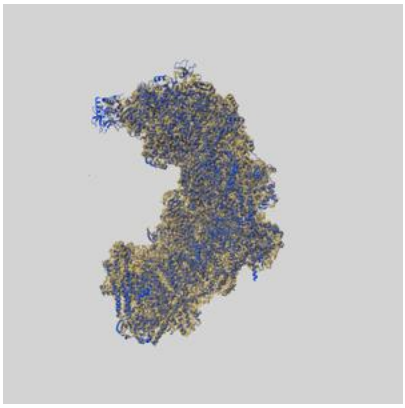
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	3.03	3.49	3.06
Unmasked-calculated*	4.08	7.88	4.21

*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 4.08 differs from the reported value 3.03 by more than 10 %

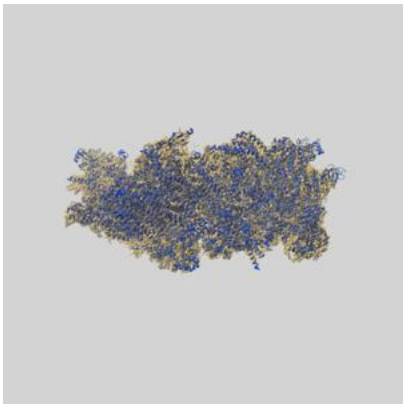
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36109 and PDB model 8J9J. Per-residue inclusion information can be found in section 3 on page 23.

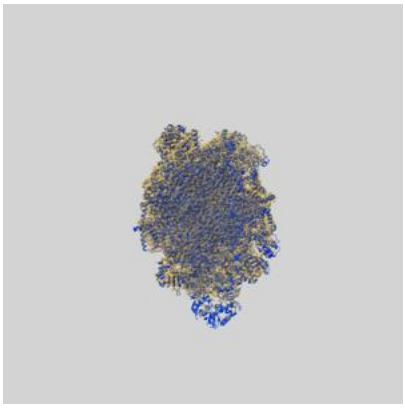
9.1 Map-model overlay



X



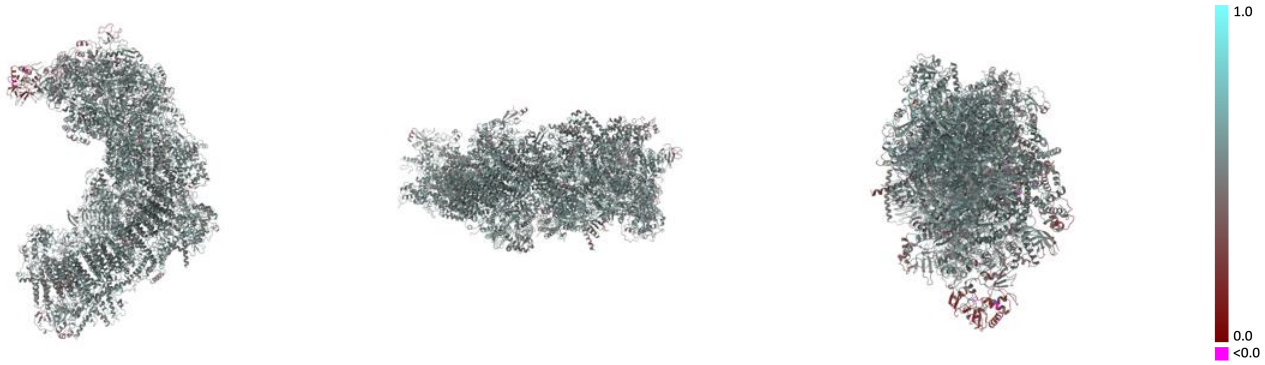
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

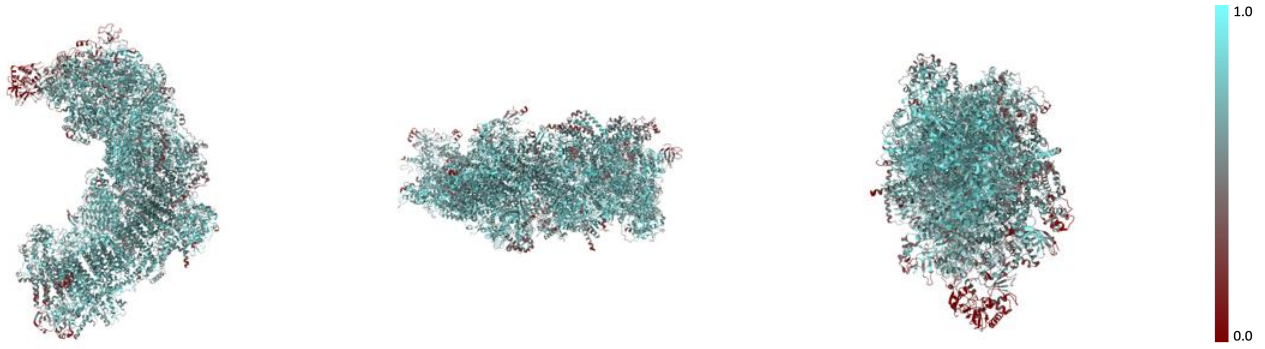
9.2 Q-score mapped to coordinate model



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.

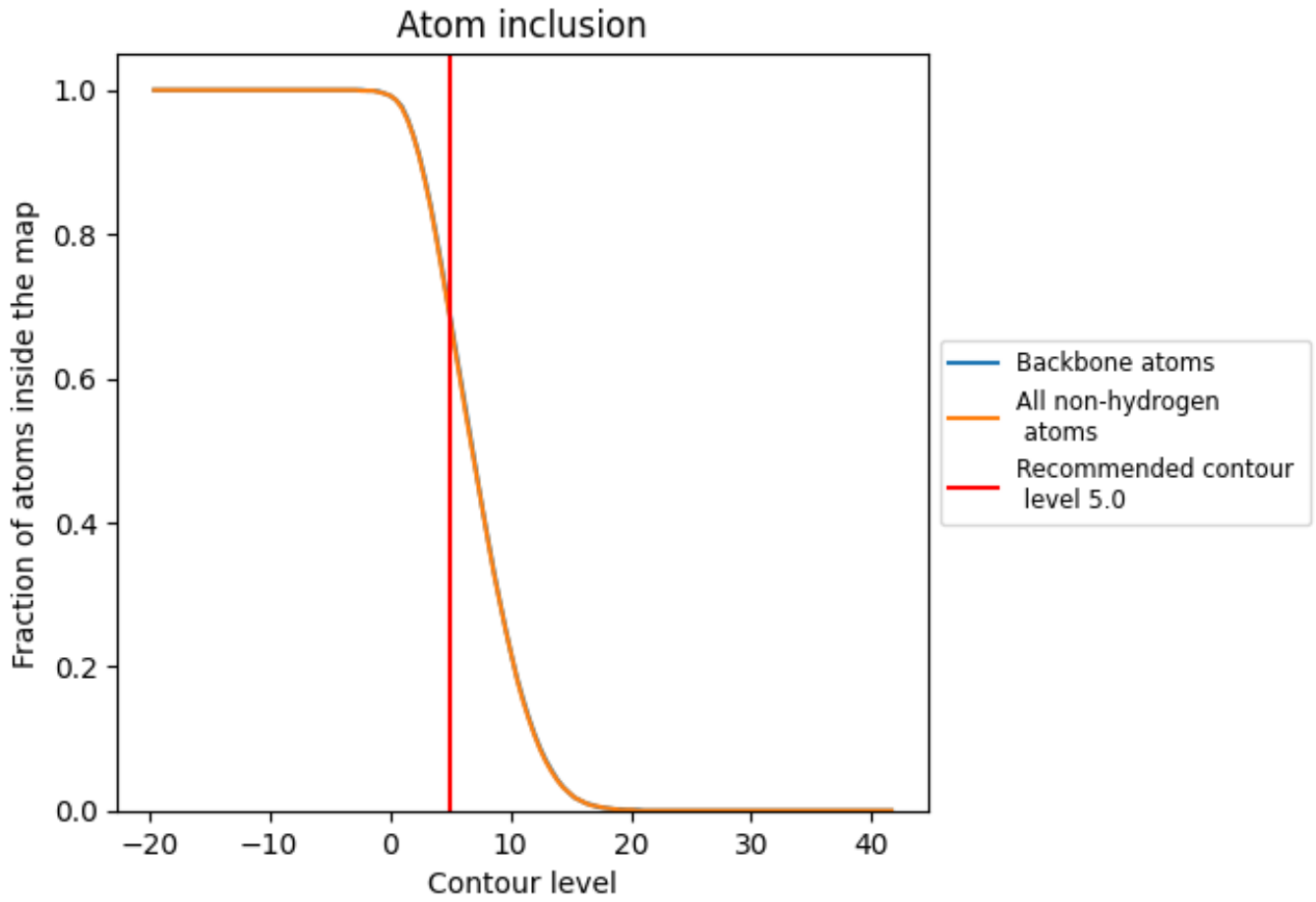
9.3 Atom inclusion mapped to coordinate model



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 (5.0).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (5.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.5310
1A	0.7740	0.5520
1B	0.7650	0.5520
2B	0.7530	0.5500
4L	0.7580	0.5550
A1	0.6010	0.5150
A2	0.7160	0.5450
A3	0.7040	0.5380
A5	0.7070	0.5240
A6	0.6070	0.5050
A7	0.7800	0.5580
A8	0.7210	0.5270
A9	0.7230	0.5360
AB	0.6720	0.5390
AC	0.6660	0.5430
AL	0.6780	0.5390
AM	0.6390	0.5220
AN	0.6640	0.5320
B2	0.7130	0.5450
B3	0.6530	0.5270
B4	0.7300	0.5410
B5	0.7140	0.5340
B6	0.7120	0.5420
B7	0.7310	0.5310
B8	0.7680	0.5540
B9	0.7450	0.5530
BL	0.7280	0.5310
BM	0.7410	0.5460
C4	0.6710	0.5330
E1	0.6680	0.5160
E2	0.6130	0.5020
E3	0.5980	0.5050
E4	0.6400	0.5360
E5	0.1700	0.3130
E6	0.5780	0.5030

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Chain	Atom inclusion	Q-score
E7	0.4490	0.4710
E8	0.5760	0.5010
EA	0.7550	0.5570
EB	0.6830	0.5350
EC	0.5790	0.5140
ED	0.6060	0.5130
FX	0.7730	0.5560
G1	0.7360	0.5520
G2	0.6790	0.5310
G3	0.7150	0.5390
N1	0.6910	0.5350
N2	0.7650	0.5540
N3	0.6990	0.5490
N4	0.7490	0.5480
N5	0.7090	0.5390
N6	0.6400	0.5200
S2	0.8060	0.5640
S3	0.8000	0.5580
S4	0.7480	0.5540
S5	0.6870	0.5320
S6	0.7910	0.5640
S7	0.7590	0.5510
S8	0.7810	0.5590
U1	0.4330	0.4740
U2	0.4830	0.4840
V1	0.7460	0.5390
V2	0.7500	0.5420