wwPDB EM Validation Summary Report

Sep 9, 2026 – 10:42 pm BST

PDB ID	:	8B6F / pdb_00008b6f
EMDB ID	:	EMD-15865
Title	:	Cryo-EM structure of NADH:ubiquinone oxidoreductase (complex-I) from respiratory supercomplex of Tetrahymena thermophila
Authors	:	Muhleip, A.; Kock Flygaard, R.; Amunts, A.
Deposited on	:	2022-09-27
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

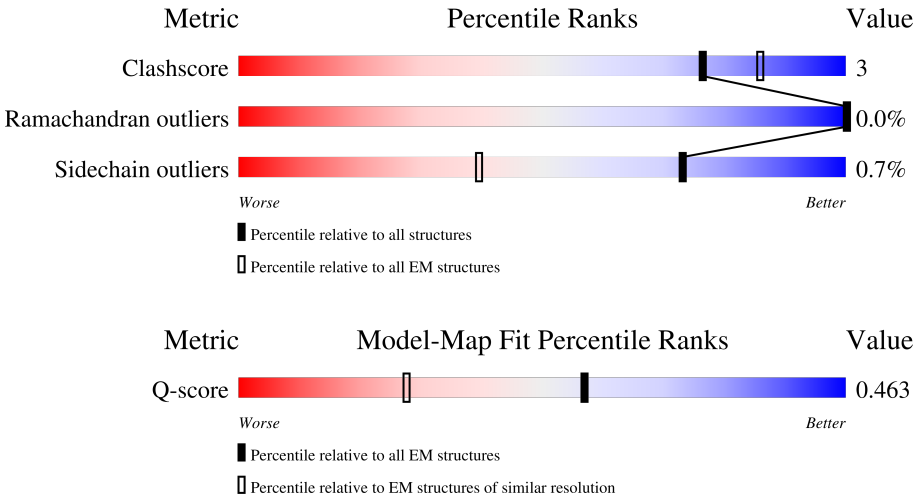
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	A0	516	9% 89% 8%
2	A1	362	88% 5% 7%
3	A2	317	7% 78% 7% 15%
4	A3	333	23% 79% 8% 13%

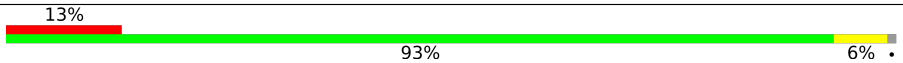
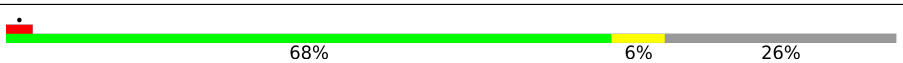
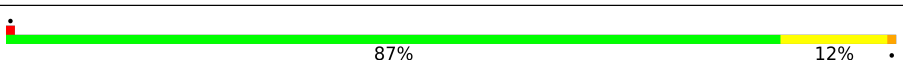
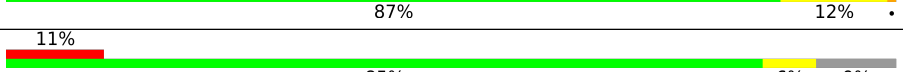
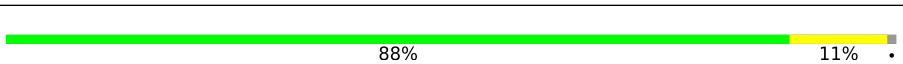
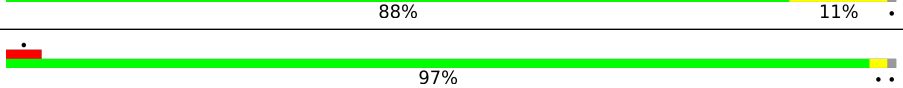
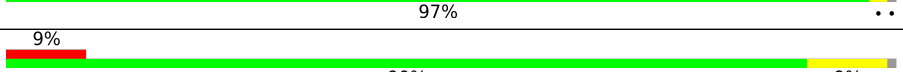
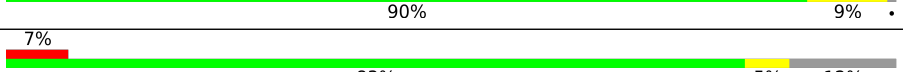
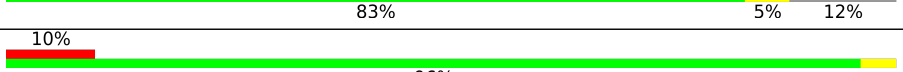
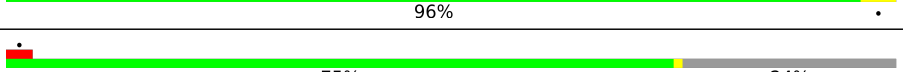
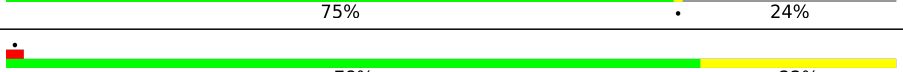
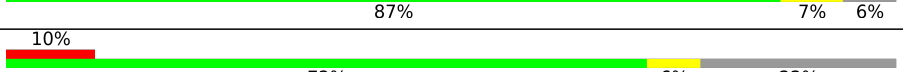
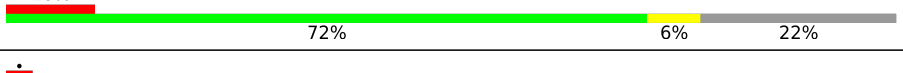
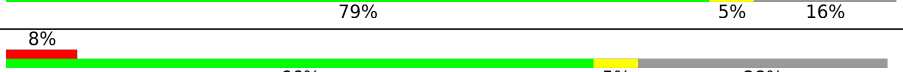
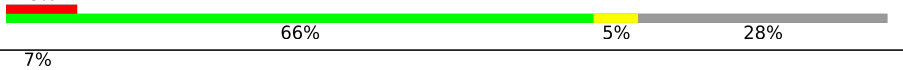
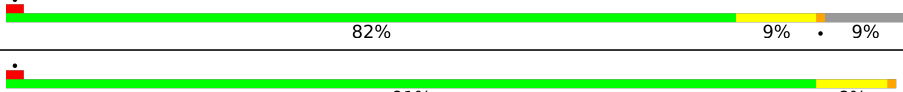
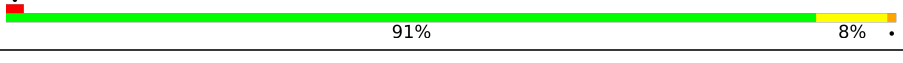
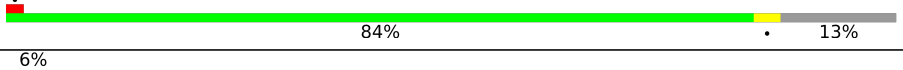
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Mol	Chain	Length	Quality of chain
5	A4	311	18% 96%
6	A5	282	7% 89% 11%
7	A6	251	83% 9% 8%
8	A7	238	50% 6% 44%
9	A8	217	7% 92% 7%
10	A9	231	6% 95% 5%
11	AA	750	10% 84% 11% 5%
12	AB	718	6% 86% 10%
13	AC	505	89% 10%
14	AD	474	17% 82% 11% 7%
15	AE	442	88% 12%
16	AF	360	89% 11%
17	AG	346	96%
18	AH	284	88% 11%
19	AI	274	16% 77% 8% 16%
20	AJ	255	93% 7%
21	AK	257	82% 8% 11%
22	AL	236	78% 14% 8%
23	AM	233	88% 10%
24	AN	206	71% 5% 24%
25	AO	198	87% 13%
26	AP	194	89% 9%
27	AQ	189	94% 5%
28	AR	185	6% 92% 5%
29	AS	172	93% 6%

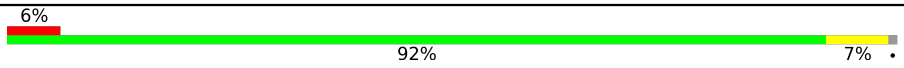
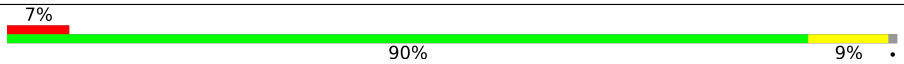
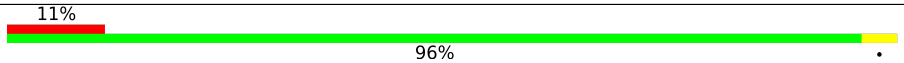
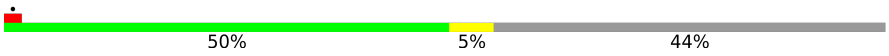
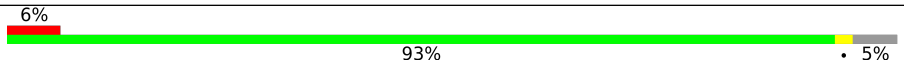
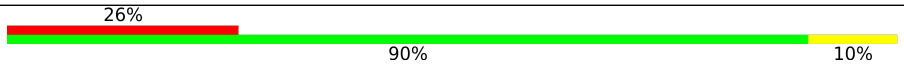
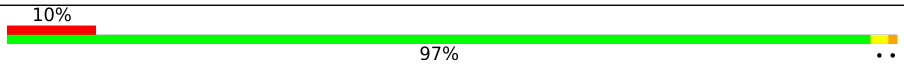
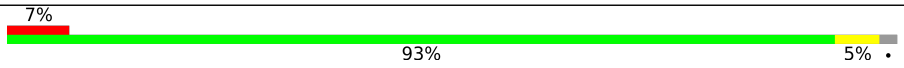
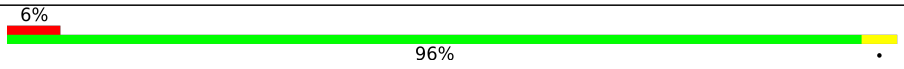
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Mol	Chain	Length	Quality of chain
30	AT	162	
31	AU	150	
32	AV	138	
33	AW	133	
34	AX	121	
35	AY	116	
36	AZ	103	
37	B0	94	
38	B1	93	
39	B2	94	
40	B3	83	
41	B4	73	
42	B5	71	
43	B6	59	
44	BA	212	
45	BB	214	
46	BC	207	
47	BD	205	
48	BE	189	
49	BF	188	
50	BG	175	
51	BH	178	
52	BI	172	
53	BJ	166	
54	BK	144	

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Mol	Chain	Length	Quality of chain
55	BL	143	
56	BM	135	
57	BN	135	
58	BO	136	
59	BP	129	
60	BQ	127	
61	BR	132	
62	BS	126	
63	BT	125	
64	BU	134	
65	BV	125	
66	BW	120	
67	BX	113	
68	BY	100	
69	BZ	102	

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
78	FES	AI	301	-	-	X	-
79	SF4	AB	803	-	-	X	-
79	SF4	AL	302	-	-	X	-

2 Entry composition (i)

There are 82 unique types of molecules in this entry. The entry contains 234355 atoms, of which 117595 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 Lipid-A-disaccharide synthase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A0	503	8090	2609	4019	699	750	13	0	0

- Molecule 2 is a protein called NAD-dependent epimerase/dehydratase family protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	A1	338	5368	1737	2650	475	494	12	0	0

- Molecule 3 is a protein called DnaJ domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	A2	269	4362	1392	2163	408	396	3	0	0

- Molecule 4 is a protein called Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	A3	291	4523	1438	2260	390	434	1	0	0

- Molecule 5 is a protein called RNase III domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	A4	311	4985	1583	2491	434	469	8	0	0

- Molecule 6 is a protein called 37S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	A5	282	4596	1478	2249	413	453	3	0	0

- Molecule 7 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	A6	230	Total	C	H	N	O	S	0	0
			3770	1241	1862	322	340	5		

- Molecule 8 is a protein called CX9C domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	A7	133	Total	C	H	N	O	S	0	0
			2124	682	1040	182	209	11		

- Molecule 9 is a protein called NDUTT15.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	A8	217	Total	C	H	N	O	S	0	0
			3597	1153	1803	305	328	8		

- Molecule 10 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	A9	231	Total	C	H	N	O	S	0	0
			3697	1219	1818	317	336	7		

- Molecule 11 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	AA	713	Total	C	H	N	O	S	0	0
			11919	4066	5978	855	1004	16		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	AB	688	Total	C	H	N	O	S	0	0
			10762	3410	5359	935	1030	28		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AC	505	Total	C	H	N	O	S	0	0
			8393	2859	4223	601	692	18		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	AD	441	Total	C	H	N	O	S	0	0
			6744	2140	3345	596	639	24		

- Molecule 15 is a protein called NADH dehydrogenase subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	AE	441	Total	C	H	N	O	S	0	0
			7126	2285	3539	620	658	24		

- Molecule 16 is a protein called Ymf65.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	AF	359	Total	C	H	N	O	S	0	0
			6216	2132	3148	435	494	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AF	208	VAL	GLY	conflict	UNP Q951A3

- Molecule 17 is a protein called Transcription factor apfi protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	AG	346	Total	C	H	N	O	S	0	0
			5531	1766	2727	481	549	8		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	AH	283	Total	C	H	N	O	S	0	0
			4656	1581	2350	334	379	12		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase 24 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	AI	231	Total	C	H	N	O	S	0	0
			3710	1173	1848	321	358	10		

- Molecule 20 is a protein called Ymf62.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	AJ	254	Total	C	H	N	O	S	0	0
			4316	1478	2156	305	373	4		

- Molecule 21 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	AK	230	Total	C	H	N	O	S	0	0
			3519	1117	1740	306	351	5		

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase 1, chain, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	AL	218	Total	C	H	N	O	S	0	0
			3501	1155	1689	299	347	11		

- Molecule 23 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AM	231	Total	C	H	N	O	S	0	0
			3558	1112	1788	316	335	7		

- Molecule 24 is a protein called ETC complex I subunit motif protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AN	157	Total	C	H	N	O	S	0	0
			2651	846	1329	221	249	6		

- Molecule 25 is a protein called NADH dehydrogenase subunit 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	AO	198	Total	C	H	N	O	S	0	0
			3363	1097	1680	268	312	6		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	AP	191	Total	C	H	N	O	S	0	0
			3104	1013	1505	301	280	5		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	AQ	187	Total	C	H	N	O	S	0	0
			3084	1027	1496	254	303	4		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	AR	181	Total	C	H	N	O	S	0	0
			2937	948	1445	267	269	8		

- Molecule 29 is a protein called NADH dehydrogenase, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	AS	172	Total	C	H	N	O	S	0	0
			2802	903	1382	253	256	8		

- Molecule 30 is a protein called NADH dehydrogenase subunit 10.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	AT	161	Total	C	H	N	O	S	0	0
			2549	822	1272	220	225	10		

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AU	149	Total	C	H	N	O	0	0
			2436	800	1209	213	214		

- Molecule 32 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AV	112	Total	C	H	N	O	0	0
			1829	586	904	158	181		

- Molecule 33 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	AW	98	Total	C	H	N	O	S	0	0
			1584	512	781	133	157	1		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	AX	121	Total	C	H	N	O	S	0	0
			2047	710	1020	143	170	4		

- Molecule 35 is a protein called Ymf58.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	AY	116	Total	C	H	N	O	S	0	0
			1944	648	987	142	163	4		

- Molecule 36 is a protein called Ribosomal protein L51/S25/CI-B8 domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	AZ	94	Total	C	H	N	O	S	0	0
			1552	491	775	140	144	2		

- Molecule 37 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B0	93	Total	C	H	N	O	0	0
			1607	531	802	139	135		

- Molecule 38 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	B1	92	Total	C	H	N	O	S	0	0
			1536	497	746	146	146	1		

- Molecule 39 is a protein called GRAM domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	B2	93	Total	C	H	N	O	S	0	0
			1485	480	728	129	142	6		

- Molecule 40 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	B3	73	Total	C	H	N	O	S	0	0
			1251	414	618	113	105	1		

- Molecule 41 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	B4	73	Total	C	H	N	O	S	0	0
			1247	408	623	111	104	1		

- Molecule 42 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	B5	54	Total	C	H	N	O	S	0	0
			917	305	464	71	75	2		

- Molecule 43 is a protein called ND1b.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	B6	59	Total	C	H	N	O	S	0	0
			1043	362	528	78	72	3		

- Molecule 44 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	BA	199	Total	C	H	N	O	S	0	0
			3289	1071	1638	285	292	3		

- Molecule 45 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	BB	167	Total	C	H	N	O	S	0	0
			2626	848	1280	228	265	5		

- Molecule 46 is a protein called NDUB8.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	BC	173	Total	C	H	N	O	S	0	0
			2848	928	1406	244	264	6		

- Molecule 47 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	BD	148	Total	C	H	N	O	S	0	0
			2414	764	1223	211	214	2		

- Molecule 48 is a protein called NDUPH2.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	BE	168	Total	C	H	N	O	S	0	0
			2807	930	1385	227	260	5		

- Molecule 49 is a protein called NDUB10.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	BF	177	Total	C	H	N	O	S	0	0
			2961	934	1486	267	270	4		

- Molecule 50 is a protein called NDUA13.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	BG	160	Total	C	H	N	O	S	0	0
			2725	858	1376	256	227	8		

- Molecule 51 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	BH	178	Total	C	H	N	O	S	0	0
			3036	1015	1554	215	247	5		

- Molecule 52 is a protein called 2 iron, 2 sulfur cluster-binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	BI	149	Total	C	H	N	O	S	0	0
			2318	731	1139	211	227	10		

- Molecule 53 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	BJ	144	Total	C	H	N	O	S	0	0
			2361	767	1156	205	226	7		

- Molecule 54 is a protein called COX assembly mitochondrial protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	BK	109	Total	C	H	N	O	S	0	0
			1757	562	854	161	174	6		

- Molecule 55 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	BL	142	Total	C	H	N	O	S	0	0
			2325	770	1138	202	209	6		

- Molecule 56 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	BM	128	Total	C	H	N	O	S	0	0
			2074	695	1002	194	180	3		

- Molecule 57 is a protein called PH domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BN	133	Total	C	H	N	O	0	0
			2229	716	1126	196	191		

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	BO	136	Total	C	H	N	O	S	0	0
			2156	690	1058	190	208	10		

- Molecule 59 is a protein called NDUB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	BP	72	Total	C	H	N	O	S	0	0
			1194	404	590	100	96	4		

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	BQ	101	Total	C	H	N	O	S	0	0
			1674	547	829	140	153	5		

- Molecule 61 is a protein called Zinc-finger protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	BR	91	Total	C	H	N	O	S	0	0
			1449	460	719	129	137	4		

- Molecule 62 is a protein called NDUB4.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	BS	120	Total	C	H	N	O	S	0	0
			1907	621	941	167	175	3		

- Molecule 63 is a protein called NDUB15.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	BT	125	Total	C	H	N	O	S	0	0
			2016	696	953	172	190	5		

- Molecule 64 is a protein called NDUTT16.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	BU	134	Total	C	H	N	O	S	0	0
			2176	683	1094	194	204	1		

- Molecule 65 is a protein called NDUTT17.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	BV	125	Total	C	H	N	O	S	0	0
			2001	632	1014	177	177	1		

- Molecule 66 is a protein called CHCH domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	BW	118	Total	C	H	N	O	S	0	0
			1848	603	893	167	179	6		

- Molecule 67 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BX	96	Total	C	H	N	O	0	0
			1552	512	755	139	146		

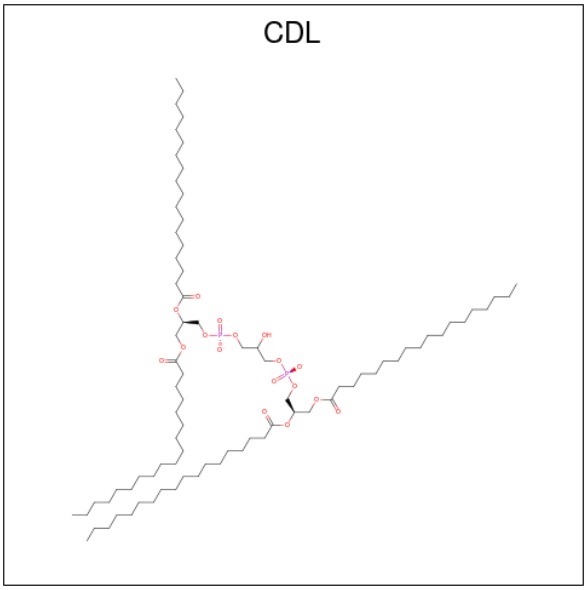
- Molecule 68 is a protein called Ymf57.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	BY	100	Total	C	H	N	O	S	0	0
			1806	620	917	128	138	3		

- Molecule 69 is a protein called Complex I-MNLL.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	BZ	102	Total	C	H	N	O	S	0	0
			1690	553	840	139	150	8		

- Molecule 70 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



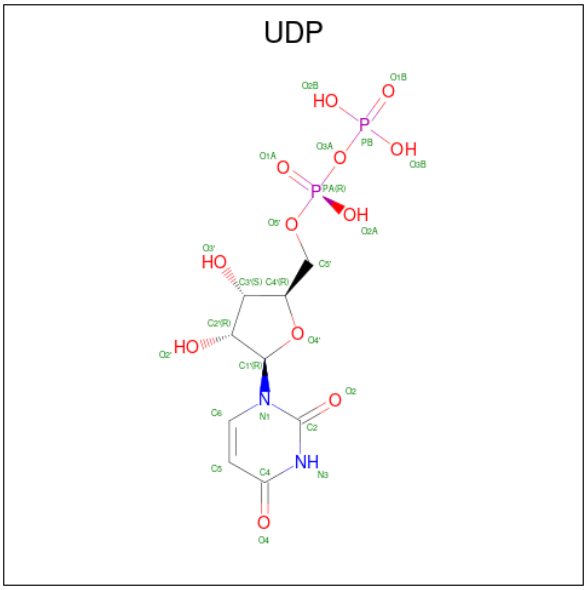
Mol	Chain	Residues	Atoms					AltConf
70	A0	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	A0	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	A1	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	AA	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	AA	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	AC	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	AC	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	AF	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	AF	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	AM	1	Total	C	H	O	P	0
			256	81	156	17	2	

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Mol	Chain	Residues	Atoms					AltConf
70	AP	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	B0	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	B0	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	B1	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	BC	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	BC	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	BE	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	BG	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	BL	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	BT	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	BV	1	Total	C	H	O	P	0
			256	81	156	17	2	
70	BY	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 71 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).

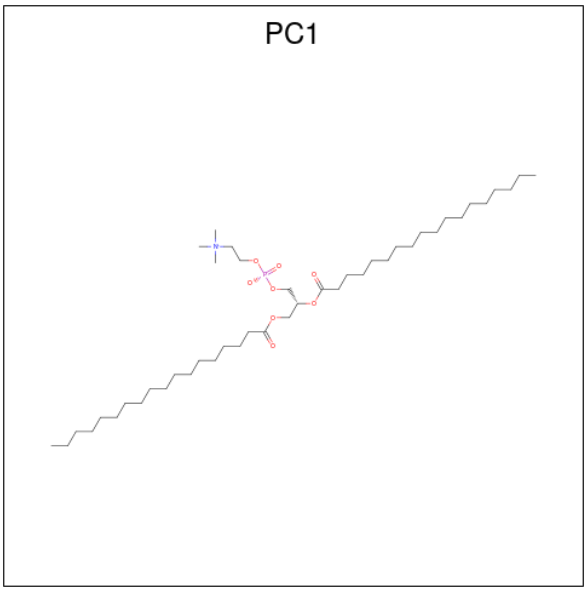


Mol	Chain	Residues	Atoms						AltConf
71	A0	1	Total	C	H	N	O	P	0
			36	9	11	2	12	2	

- Molecule 72 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
72	A0	1	Total	Mg	0
			1	1	
72	A8	1	Total	Mg	0
			1	1	

- Molecule 73 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



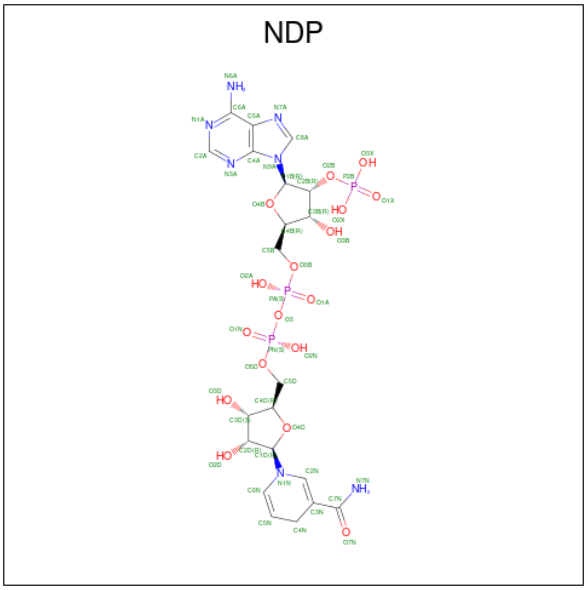
Mol	Chain	Residues	Atoms						AltConf
73	A0	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	A1	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	A1	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	A2	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	A6	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	A6	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

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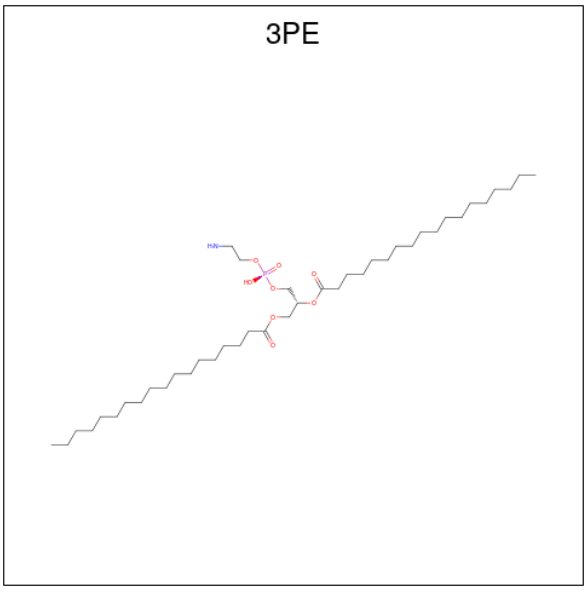
Mol	Chain	Residues	Atoms						AltConf
73	A9	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	A9	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	AA	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	AA	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	AA	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	AA	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	AA	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	AH	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	AJ	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	AL	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	AM	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	AQ	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	AU	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	AU	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	B1	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	B1	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	BQ	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	BS	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	BS	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	BT	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
73	BY	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

- Molecule 74 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



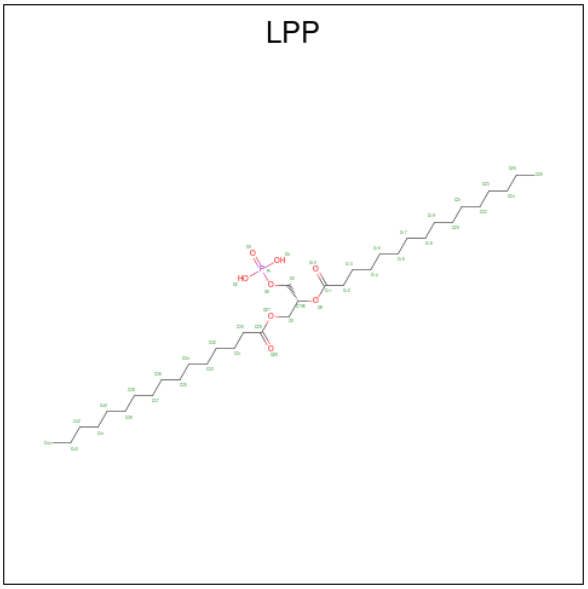
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
74	A1	1	74	21	26	7	17	3	0

- Molecule 75 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



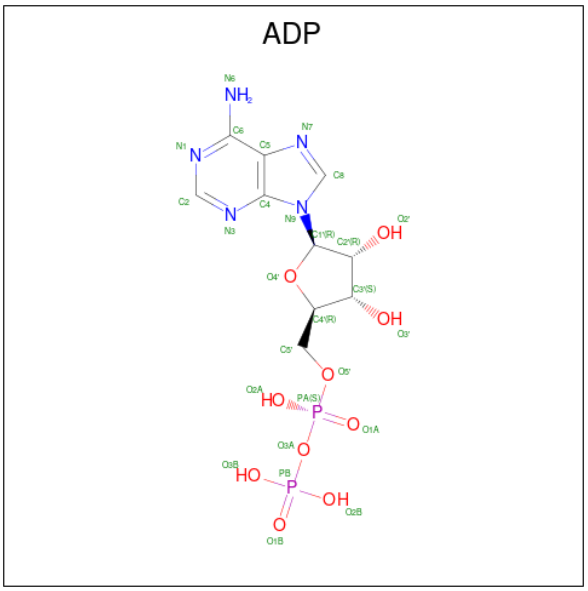
Mol	Chain	Residues	Atoms						AltConf
75	A2	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
75	A9	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
75	A9	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
75	AJ	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
75	BA	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
75	BP	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 76 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$).



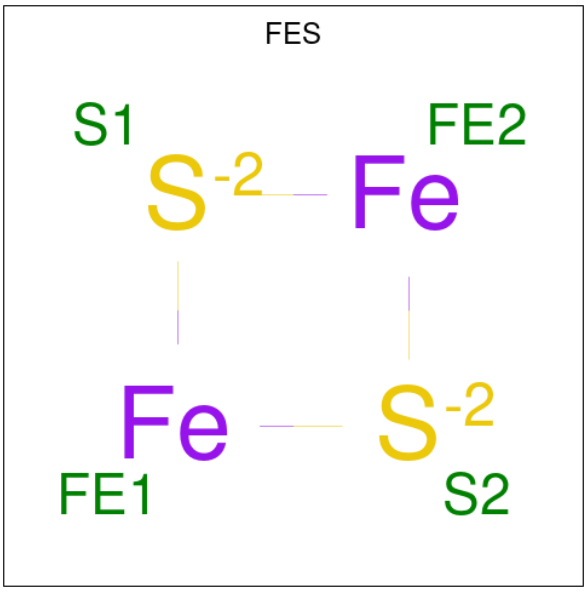
Mol	Chain	Residues	Atoms					AltConf
76	A6	1	Total	C	H	O	P	0
			111	35	67	8	1	
76	AA	1	Total	C	H	O	P	0
			111	35	67	8	1	
76	AL	1	Total	C	H	O	P	0
			111	35	67	8	1	
76	BN	1	Total	C	H	O	P	0
			111	35	67	8	1	

- Molecule 77 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
77	A8	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
77	AQ	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 78 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



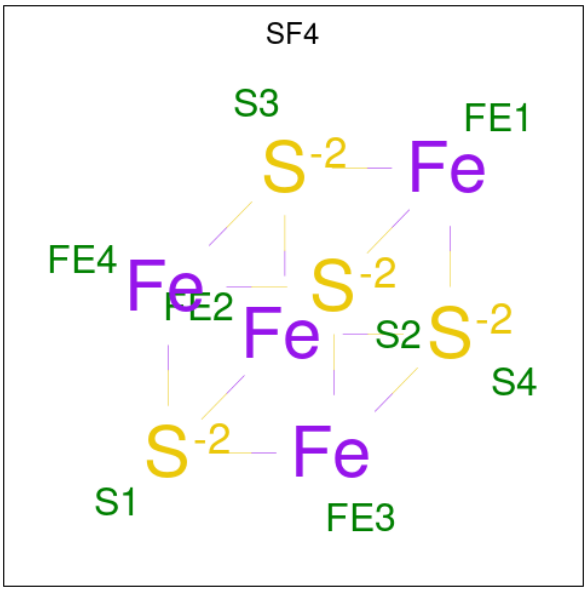
Mol	Chain	Residues	Atoms			AltConf
78	AB	1	Total	Fe	S	0
			4	2	2	

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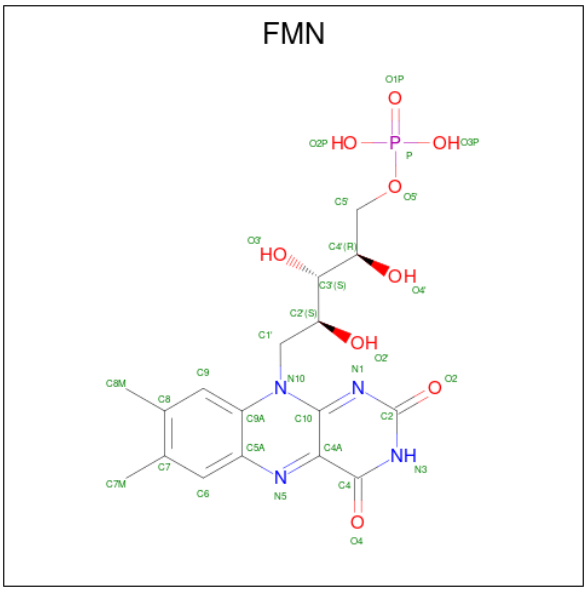
Mol	Chain	Residues	Atoms	AltConf
78	AI	1	Total Fe S 4 2 2	0
78	BI	1	Total Fe S 4 2 2	0

- Molecule 79 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



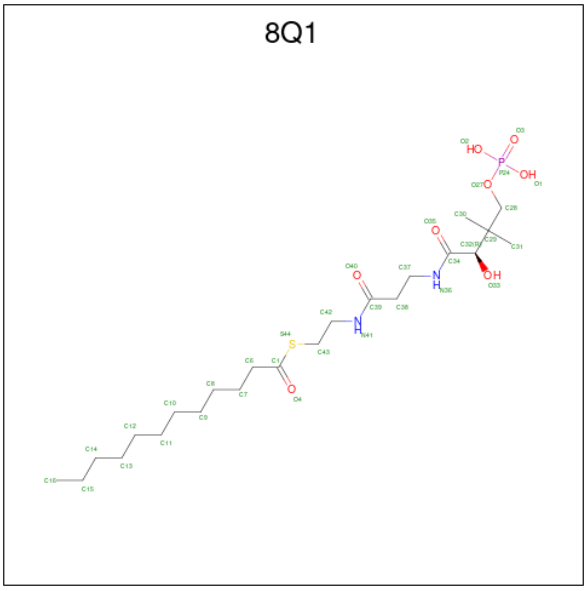
Mol	Chain	Residues	Atoms	AltConf
79	AB	1	Total Fe S 8 4 4	0
79	AB	1	Total Fe S 8 4 4	0
79	AD	1	Total Fe S 8 4 4	0
79	AL	1	Total Fe S 8 4 4	0
79	AL	1	Total Fe S 8 4 4	0
79	AT	1	Total Fe S 8 4 4	0

- Molecule 80 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
80	AD	1	Total	C	H	N	O	P	0
			49	17	18	4	9	1	

- Molecule 81 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
81	AS	1	Total	C	H	N	O	P	S	0
			77	23	43	2	7	1	1	

- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by

depositor).

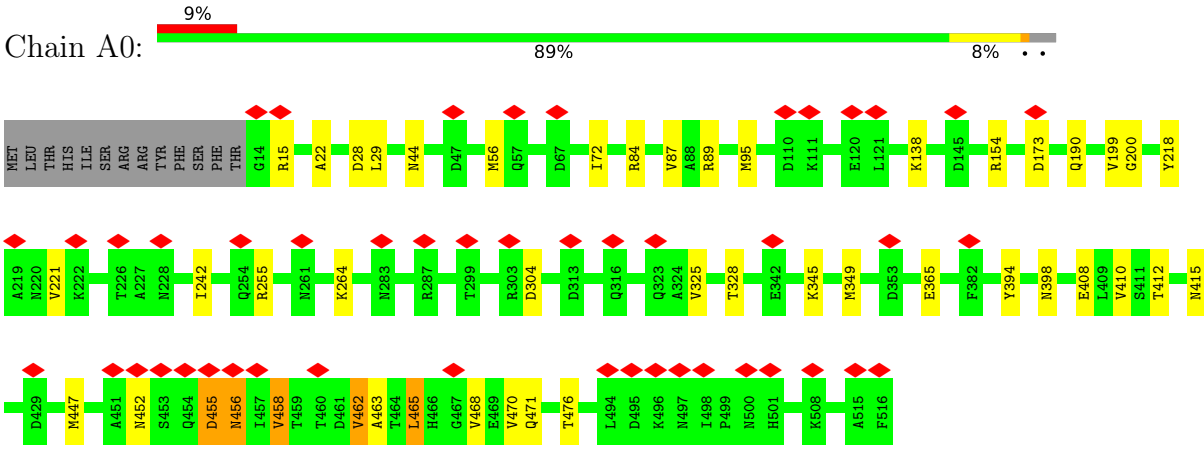
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
82	BR	1	1	1	0

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.

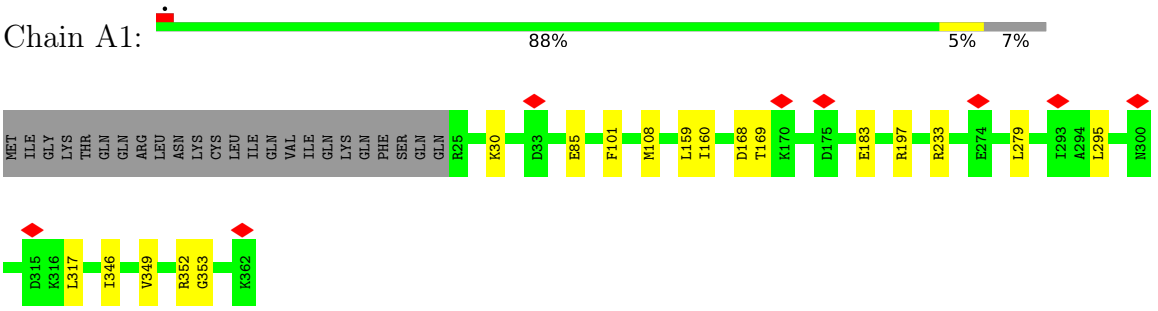
• Molecule 1: Lipid-A-disaccharide synthase

Chain A0:



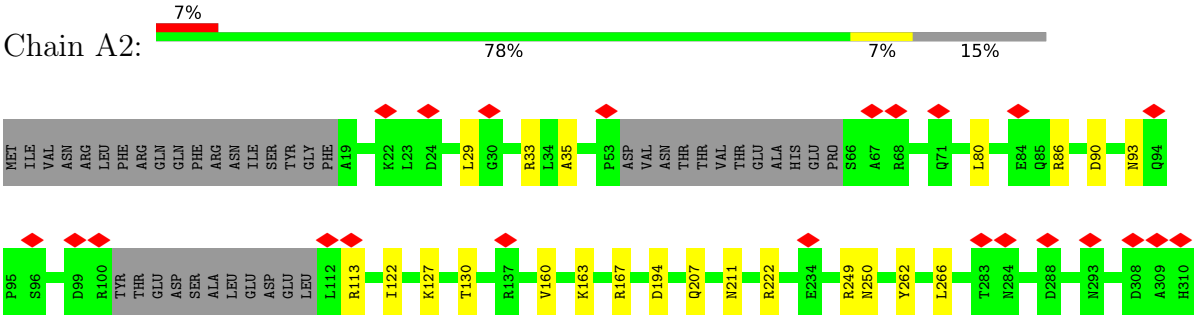
• Molecule 2: NAD-dependent epimerase/dehydratase family protein

Chain A1:



• Molecule 3: DnaJ domain protein

Chain A2:

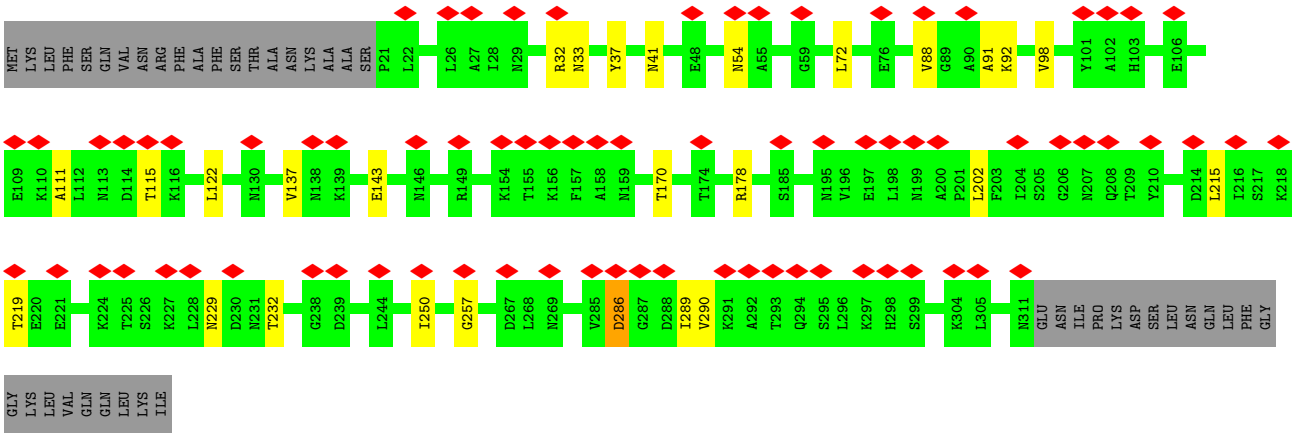




• Molecule 4: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II

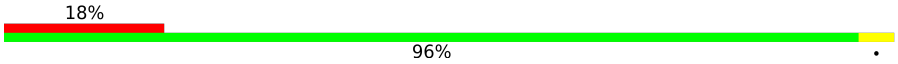
Chain A3:

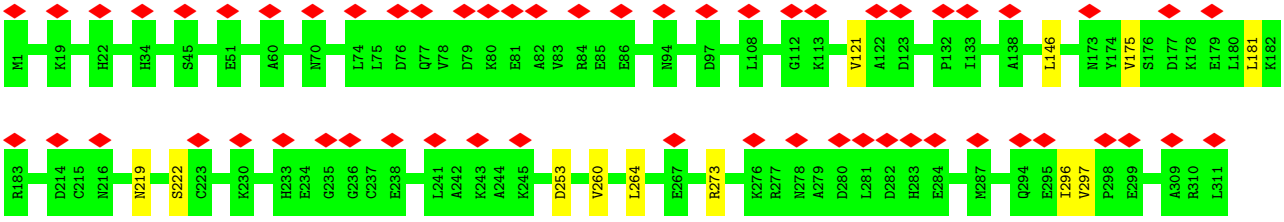




• Molecule 5: RNase III domain-containing protein

Chain A4:

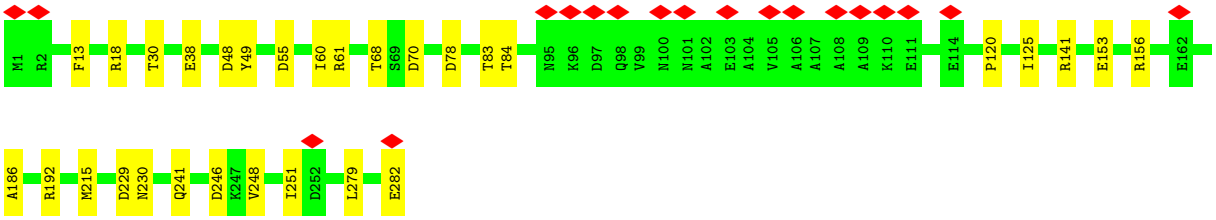




• Molecule 6: 37S ribosomal protein S25, mitochondrial

Chain A5:

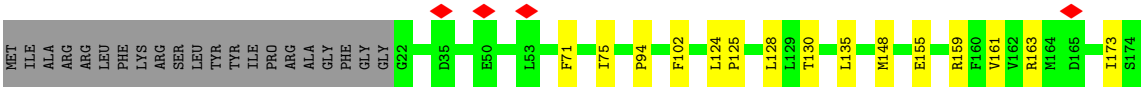


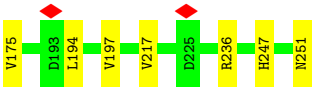


• Molecule 7: Transmembrane protein, putative

Chain A6:

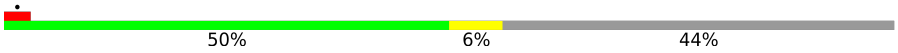




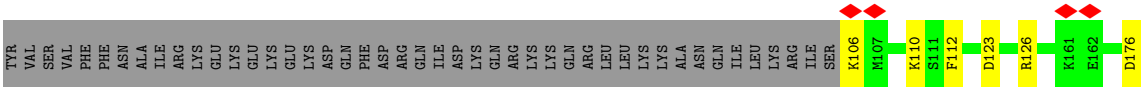


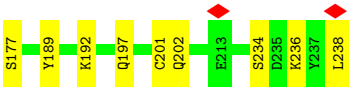
• Molecule 8: CX9C domain-containing protein

Chain A7:



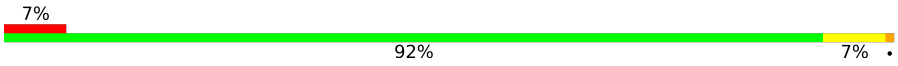


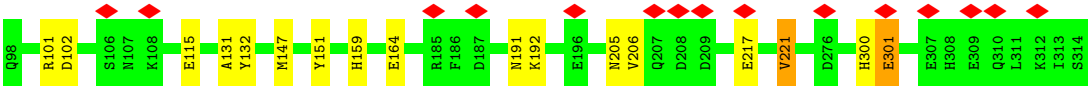




• Molecule 9: NDUTT15

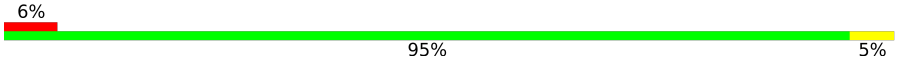
Chain A8:

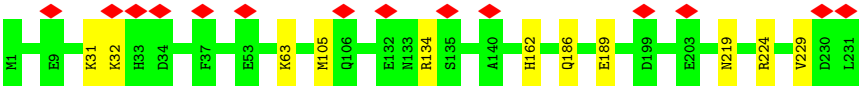




• Molecule 10: Transmembrane protein, putative

Chain A9:

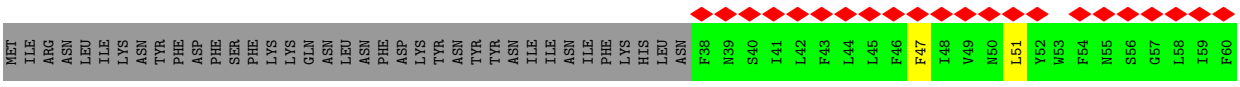


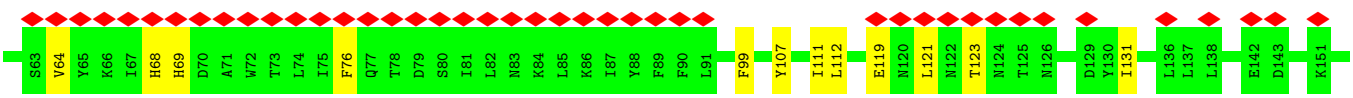


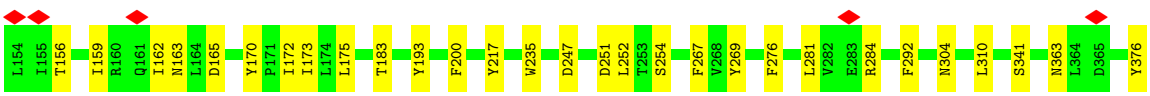
• Molecule 11: NADH dehydrogenase subunit 5

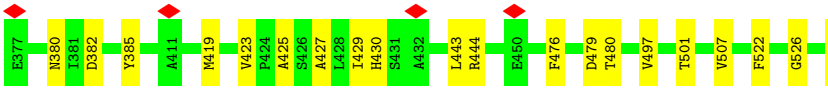
Chain AA:





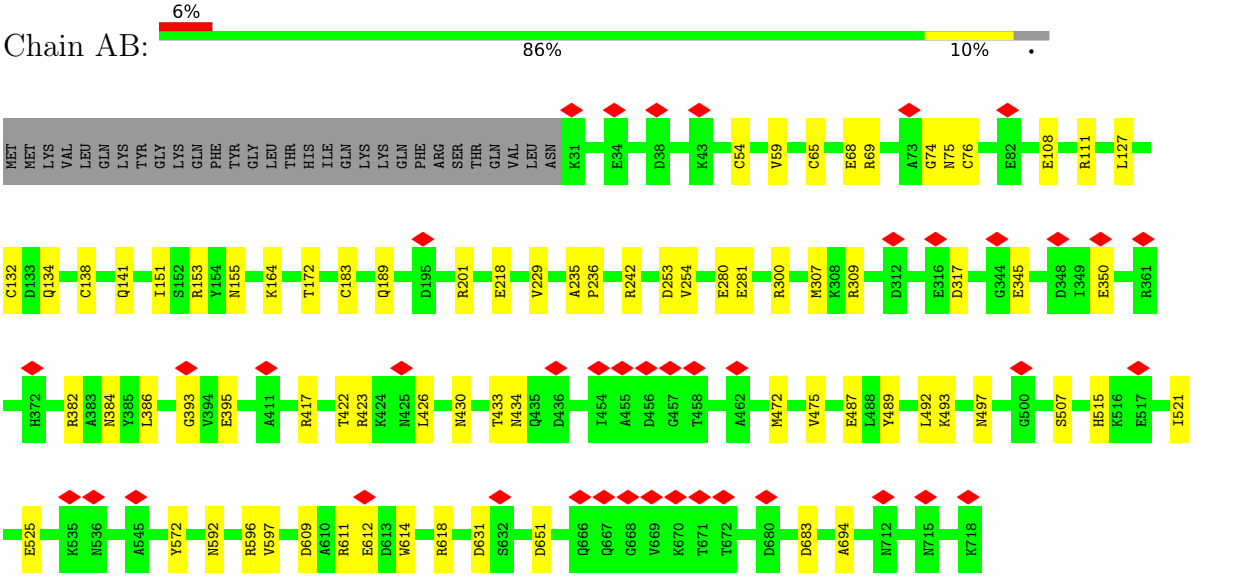




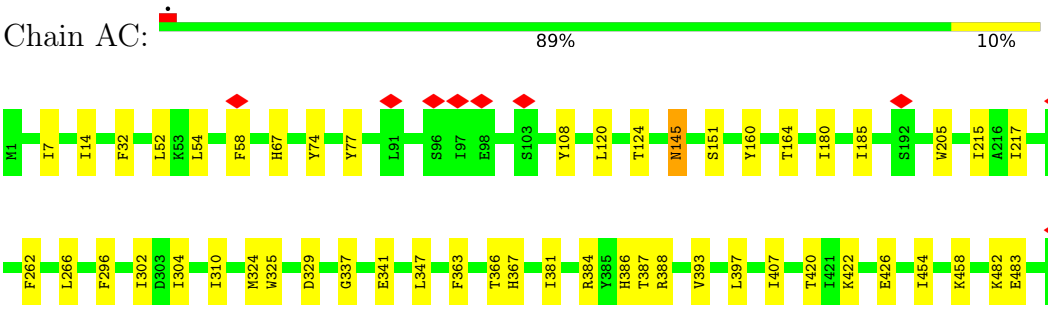




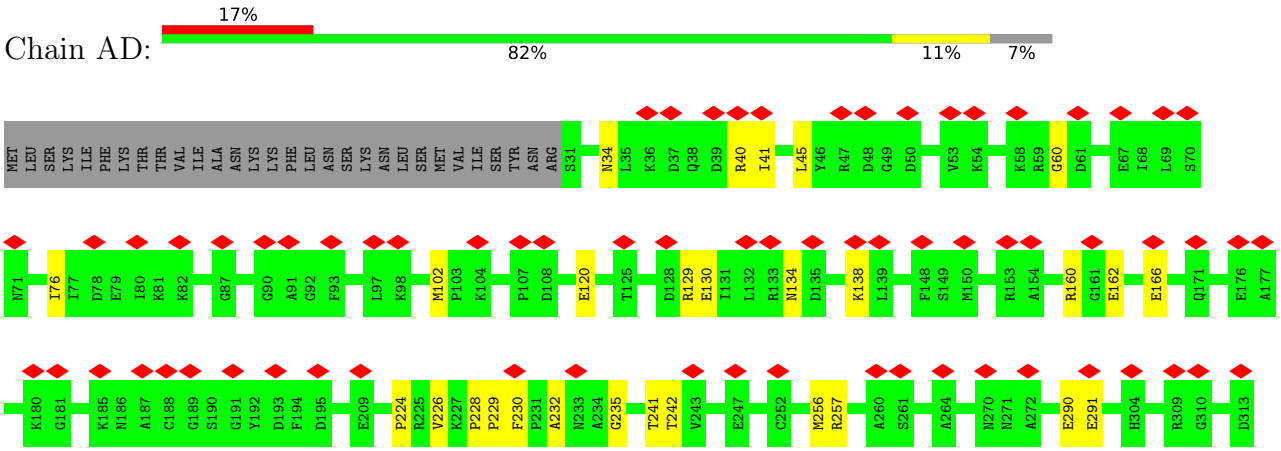
• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit

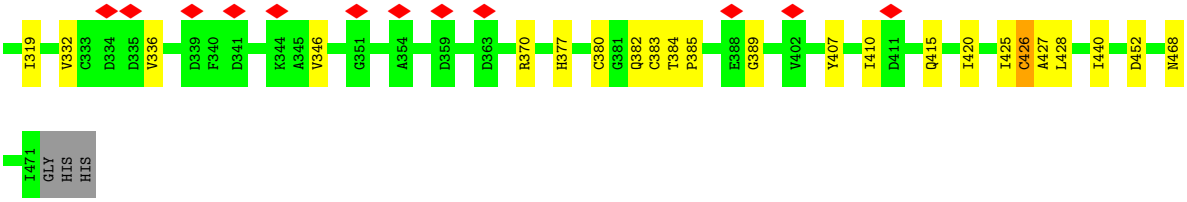


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

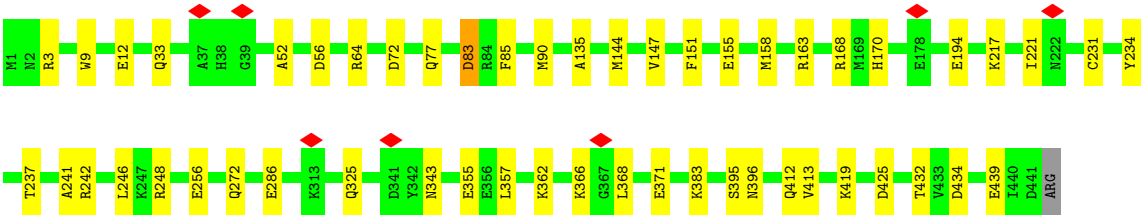




• Molecule 15: NADH dehydrogenase subunit 7

Chain AE:

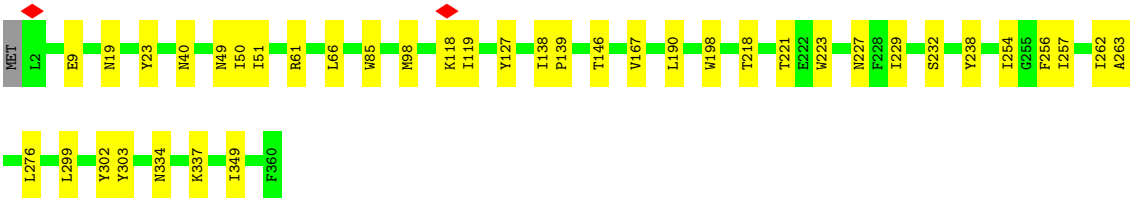




• Molecule 16: Ymf65

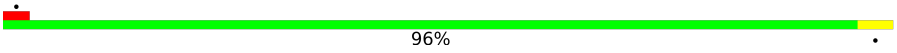
Chain AF:

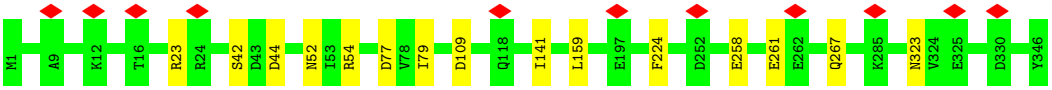




• Molecule 17: Transcription factor apfi protein, putative

Chain AG:

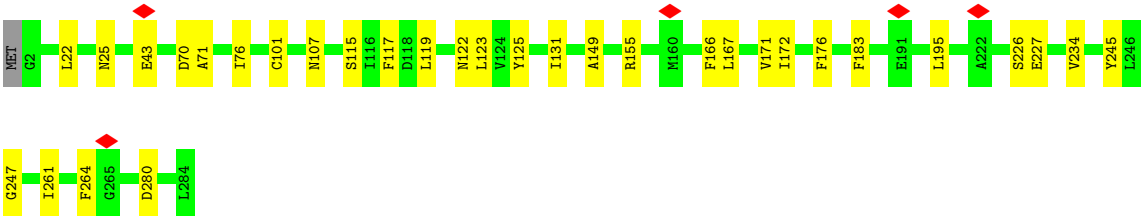




• Molecule 18: NADH-ubiquinone oxidoreductase chain 1

Chain AH:

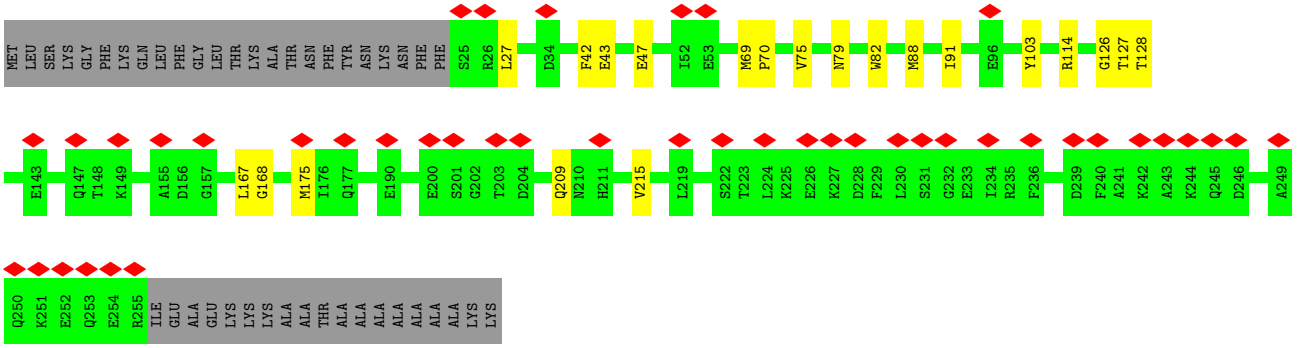




• Molecule 19: NADH-ubiquinone oxidoreductase 24 kDa subunit

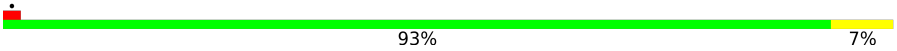
Chain AI:

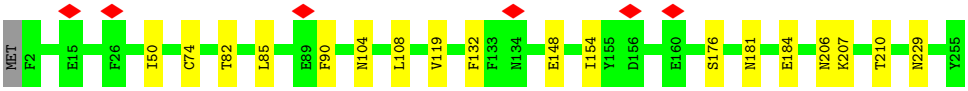




• Molecule 20: Ymf62

Chain AJ:

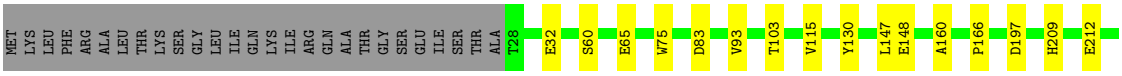




• Molecule 21: Gamma-carbonic anhydrase

Chain AK:

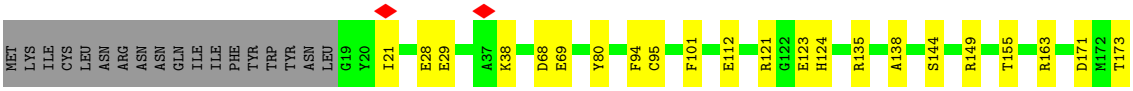


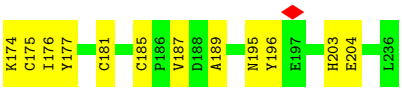


• Molecule 22: NADH-ubiquinone oxidoreductase 1, chain, putative

Chain AL:



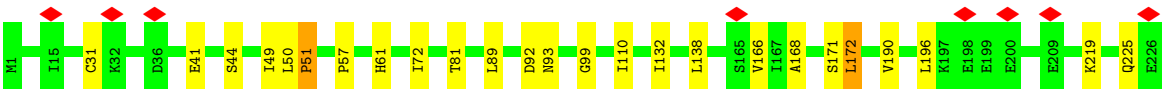


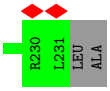


• Molecule 23: Gamma-carbonic anhydrase

Chain AM:



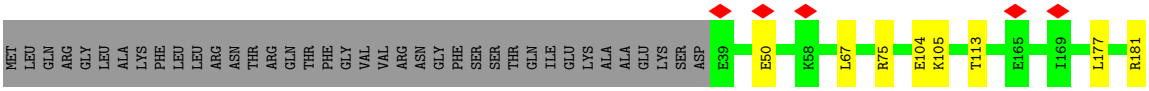


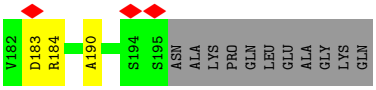


• Molecule 24: ETC complex I subunit motif protein

Chain AN:







• Molecule 25: NADH dehydrogenase subunit 9

Chain AO:

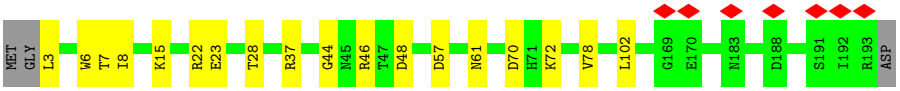




• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

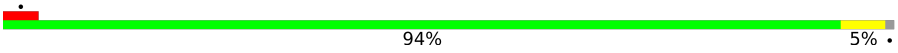
Chain AP:

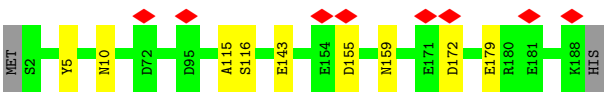




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

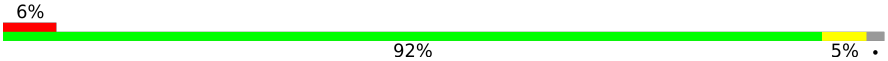
Chain AQ:

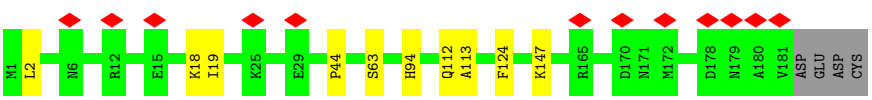




• Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

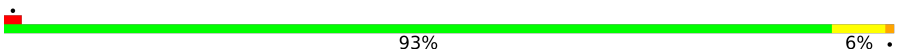
Chain AR:

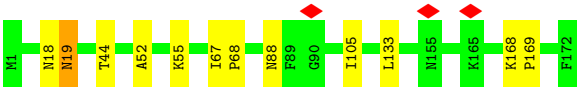




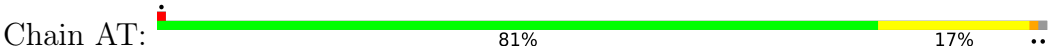
• Molecule 29: NADH dehydrogenase, putative

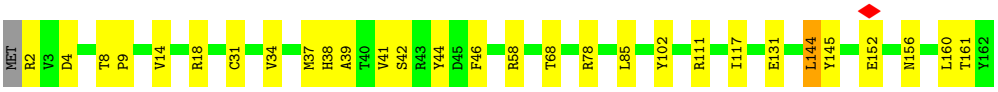
Chain AS:



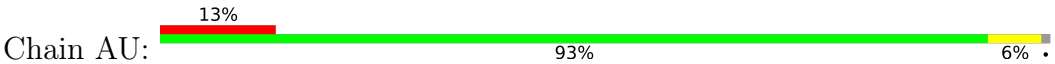


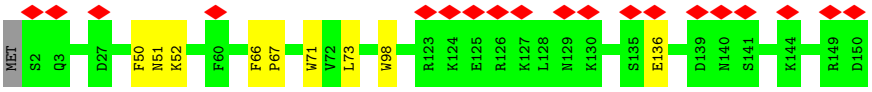
• Molecule 30: NADH dehydrogenase subunit 10



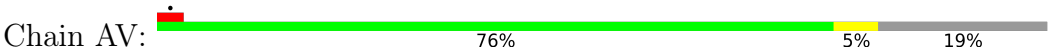


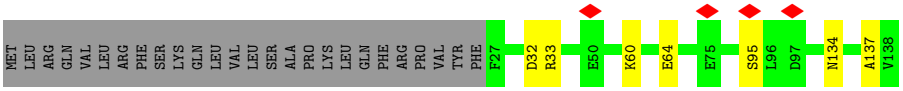
• Molecule 31: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit





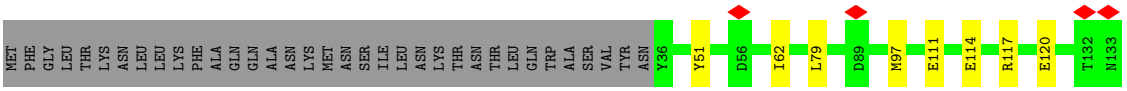
• Molecule 32: Acyl carrier protein



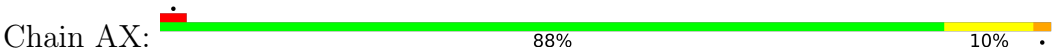


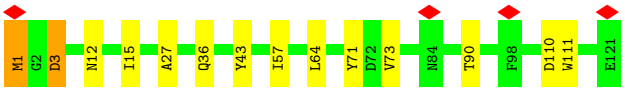
• Molecule 33: Acyl carrier protein



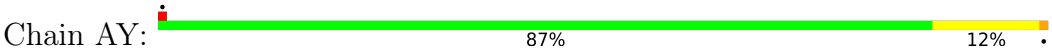


• Molecule 34: NADH-ubiquinone oxidoreductase chain 3





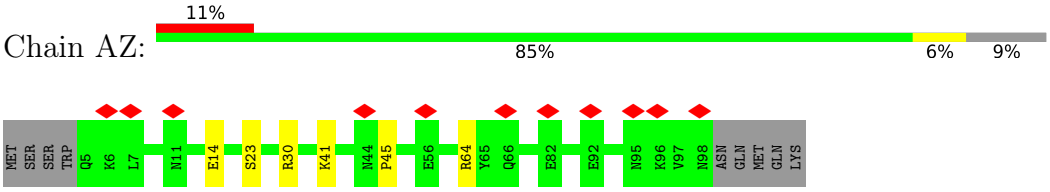
• Molecule 35: Ymf58





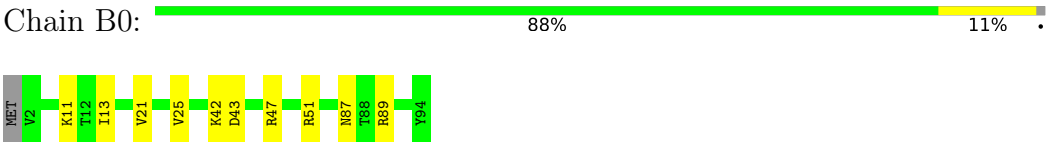
• Molecule 36: Ribosomal protein L51/S25/CI-B8 domain protein

Chain AZ:



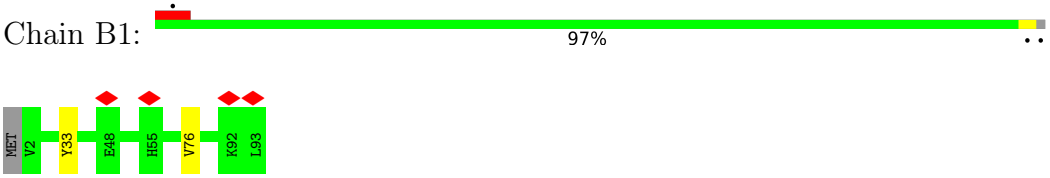
• Molecule 37: Transmembrane protein, putative

Chain B0:



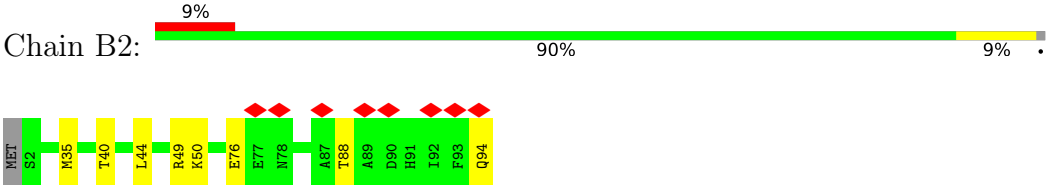
• Molecule 38: ATP synthase subunit e, mitochondrial

Chain B1:



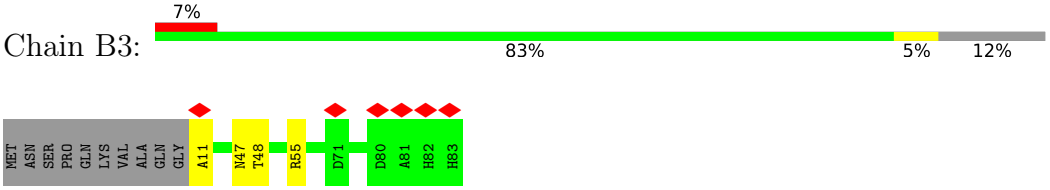
• Molecule 39: GRAM domain protein

Chain B2:



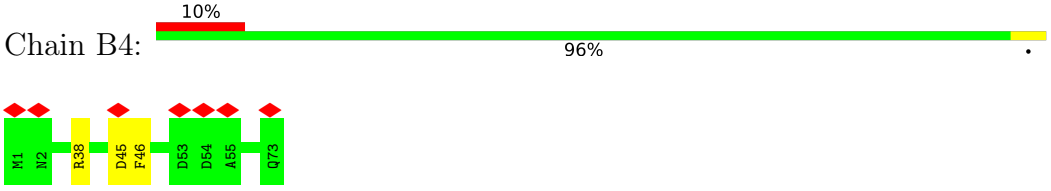
• Molecule 40: Transmembrane protein, putative

Chain B3:



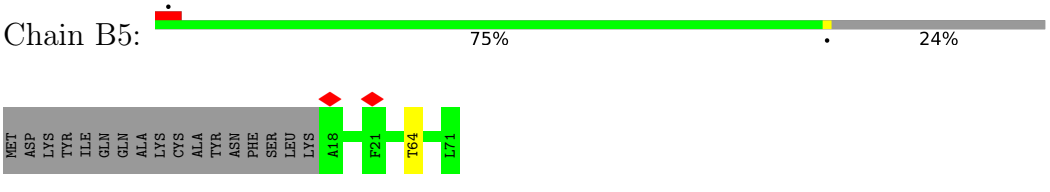
• Molecule 41: Transmembrane protein, putative

Chain B4:



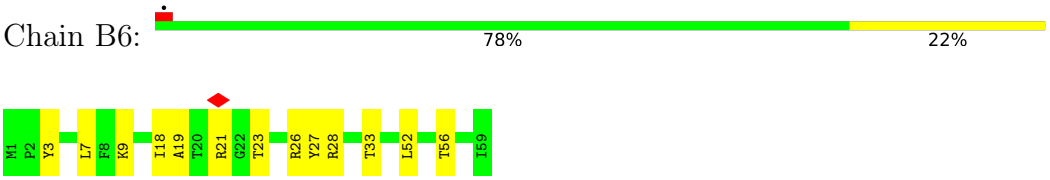
• Molecule 42: Transmembrane protein, putative

Chain B5:



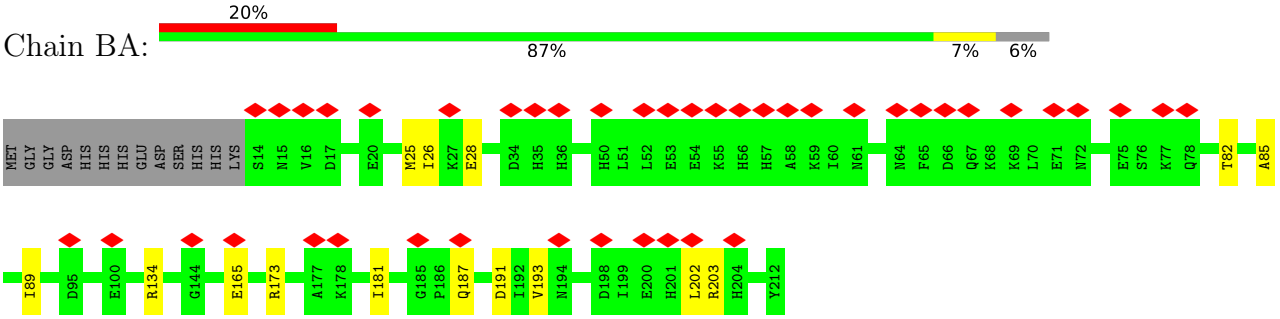
• Molecule 43: ND1b

Chain B6:



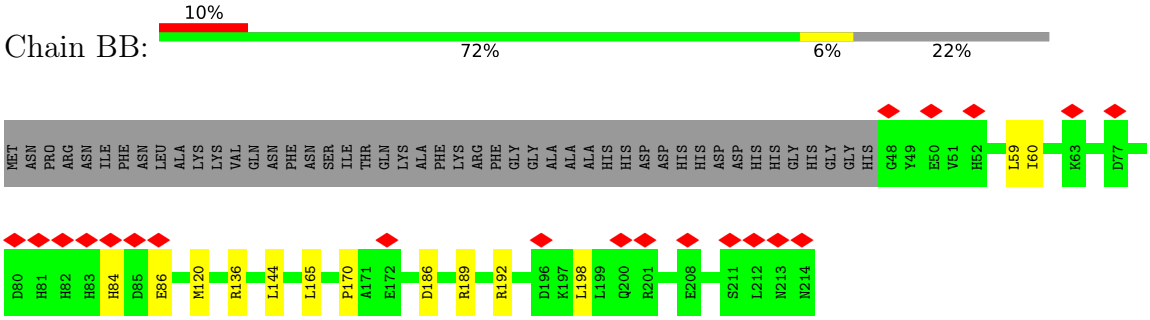
• Molecule 44: Transmembrane protein

Chain BA:



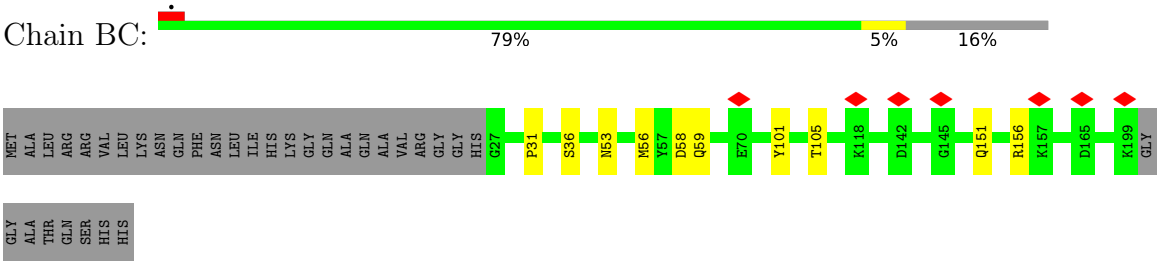
• Molecule 45: Transmembrane protein, putative

Chain BB:



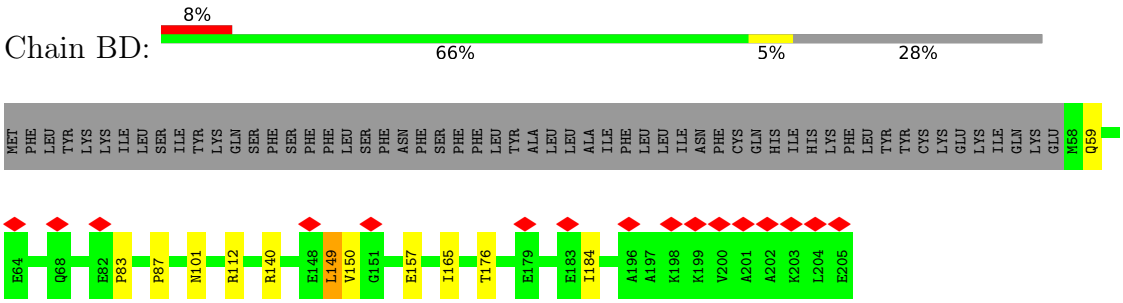
• Molecule 46: NDUB8

Chain BC:



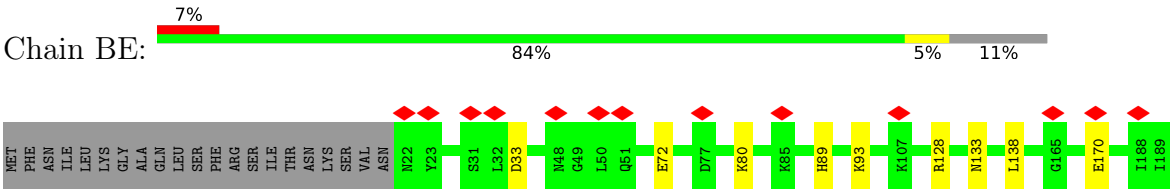
• Molecule 47: Transmembrane protein, putative

Chain BD:



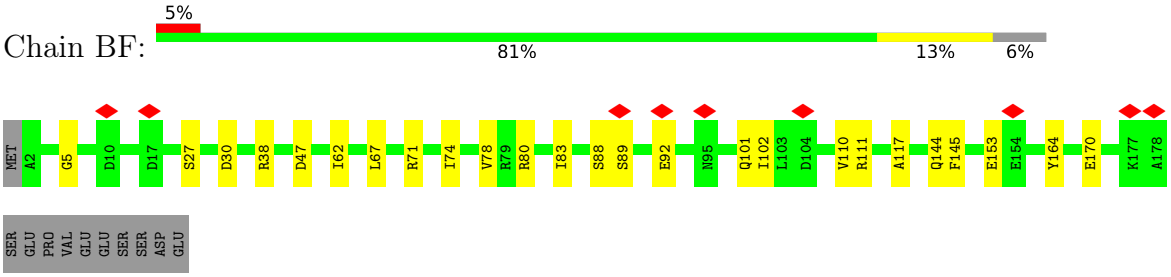
• Molecule 48: NDUPH2

Chain BE:



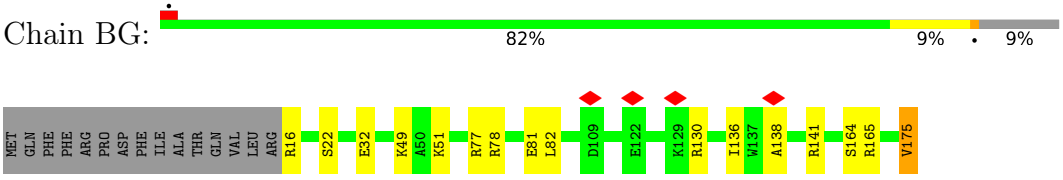
• Molecule 49: NDUB10

Chain BF:



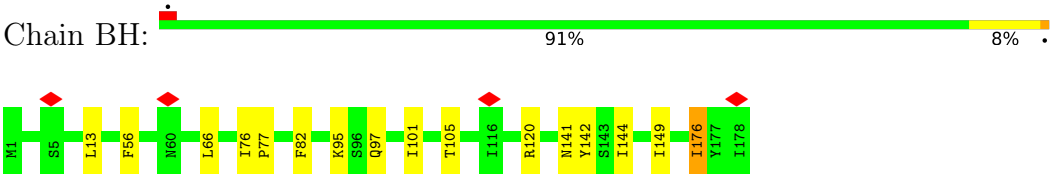
• Molecule 50: NDUA13

Chain BG:



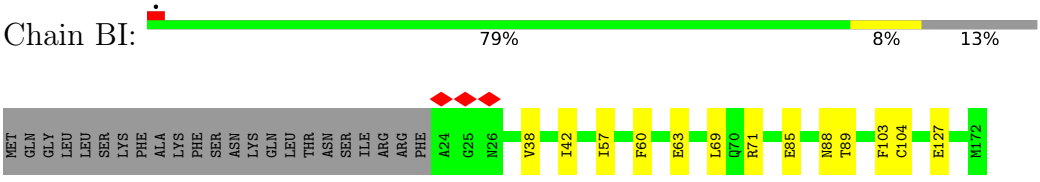
• Molecule 51: NADH dehydrogenase subunit 2

Chain BH:



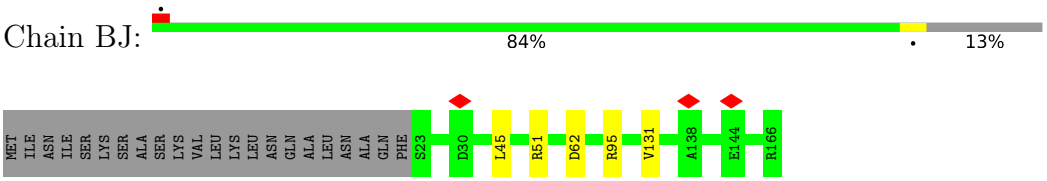
• Molecule 52: 2 iron, 2 sulfur cluster-binding protein

Chain BI:



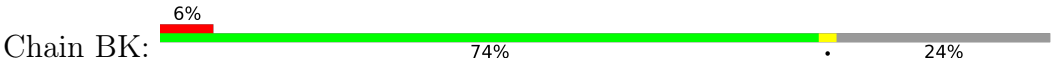
• Molecule 53: Thioredoxin

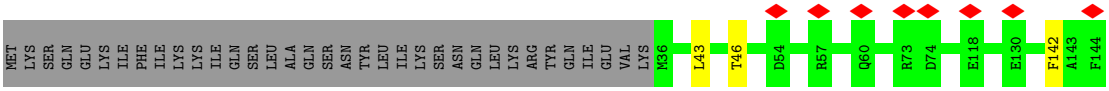
Chain BJ:



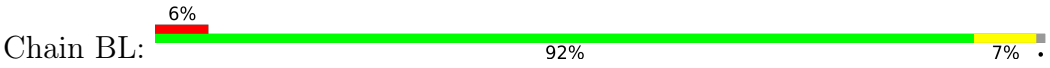
• Molecule 54: COX assembly mitochondrial protein

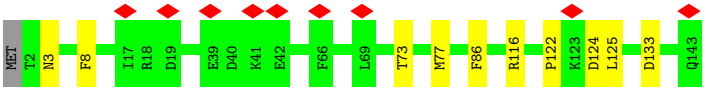
Chain BK:



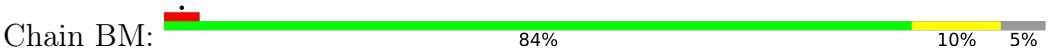


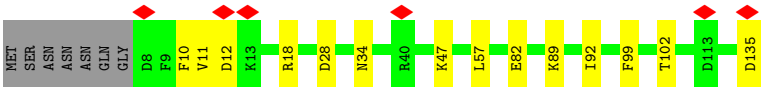
• Molecule 55: Transmembrane protein, putative



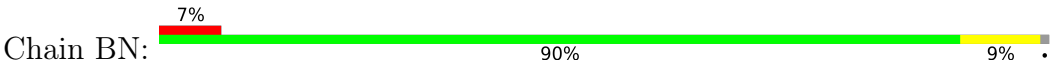


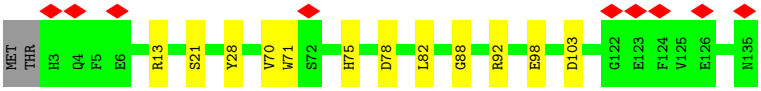
• Molecule 56: Transmembrane protein, putative





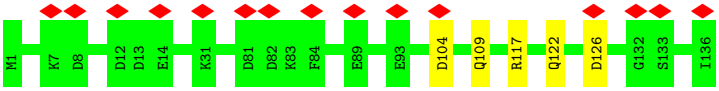
• Molecule 57: PH domain-containing protein





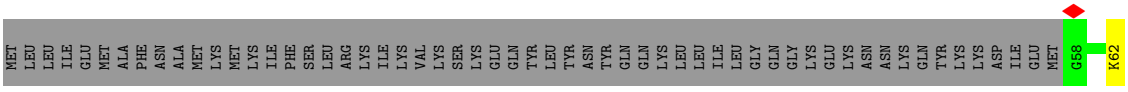
• Molecule 58: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8





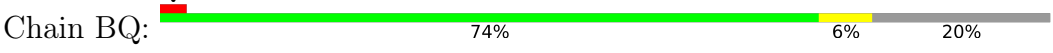
• Molecule 59: NDUB6

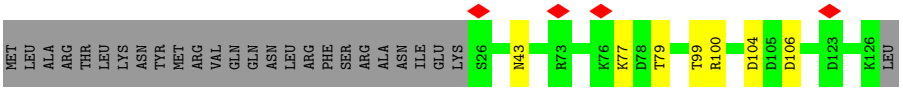






• Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

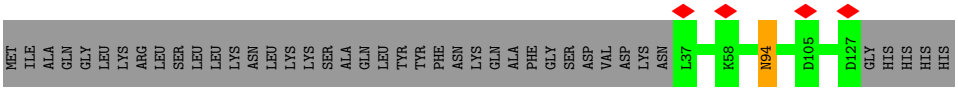




• Molecule 61: Zinc-finger protein

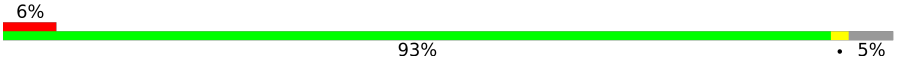
Chain BR:





• Molecule 62: NDUB4

Chain BS:

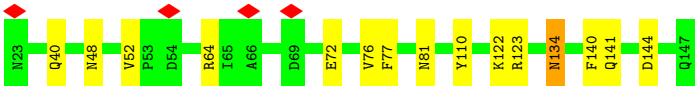




• Molecule 63: NDUB15

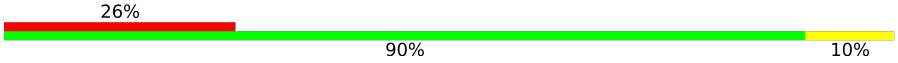
Chain BT:

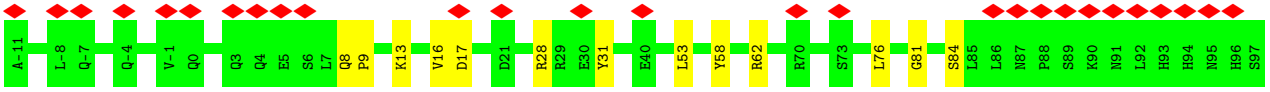


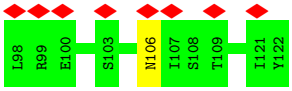


• Molecule 64: NDUTT16

Chain BU:

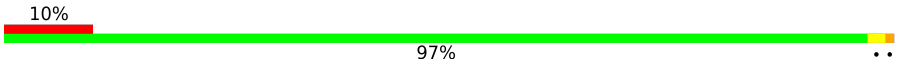


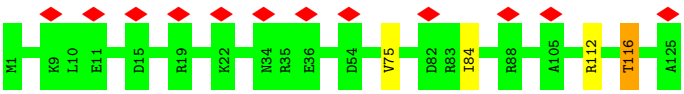




• Molecule 65: NDUTT17

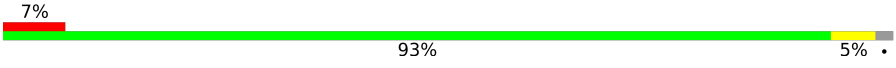
Chain BV:

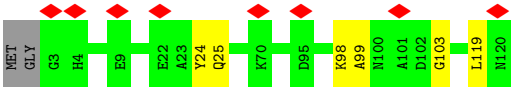




• Molecule 66: CHCH domain-containing protein

Chain BW:

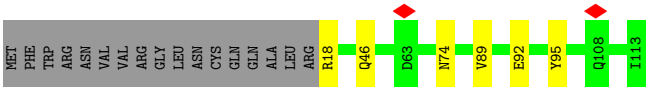




• Molecule 67: Transmembrane protein, putative

Chain BX:





• Molecule 68: Ymf57

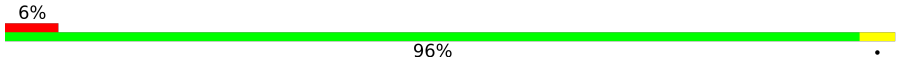
Chain BY:

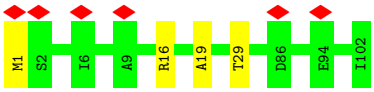




• Molecule 69: Complex I-MNLL

Chain BZ:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138746	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 ($e^-/Å^2$)	25.66	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	5.836	Depositor
Minimum map value	-2.721	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.179	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	600.0, 600.0, 600.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.25, 1.25, 1.25	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: FMN, 3PE, MG, ADP, PC1, 8Q1, SF4, FES, NDP, ZN, LPP, CDL, UDP

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	A0	0.10	0/4166	0.26	0/5634
2	A1	0.13	0/2789	0.26	0/3777
3	A2	0.10	0/2248	0.20	0/3027
4	A3	0.09	0/2308	0.28	0/3134
5	A4	0.09	0/2542	0.21	0/3441
6	A5	0.09	0/2408	0.22	0/3269
7	A6	0.11	0/1963	0.22	0/2658
8	A7	0.11	0/1108	0.22	0/1488
9	A8	0.09	0/1833	0.21	0/2479
10	A9	0.10	0/1935	0.22	0/2616
11	AA	0.12	0/6132	0.26	0/8343
12	AB	0.11	0/5511	0.27	0/7465
13	AC	0.12	0/4303	0.26	0/5844
14	AD	0.16	0/3474	0.30	0/4699
15	AE	0.13	0/3669	0.30	0/4955
16	AF	0.12	0/3168	0.25	0/4307
17	AG	0.10	0/2865	0.23	0/3877
18	AH	0.12	0/2377	0.23	0/3234
19	AI	0.11	0/1899	0.26	0/2563
20	AJ	0.11	0/2224	0.23	0/3025
21	AK	0.11	0/1816	0.25	0/2475
22	AL	0.19	0/1867	0.41	0/2538
23	AM	0.13	0/1801	0.31	0/2449
24	AN	0.10	0/1351	0.20	0/1817
25	AO	0.10	0/1720	0.25	0/2322
26	AP	0.10	0/1654	0.23	0/2240
27	AQ	0.11	0/1636	0.23	0/2214
28	AR	0.09	0/1535	0.23	0/2077
29	AS	0.10	0/1458	0.23	0/1965
30	AT	0.17	0/1310	0.45	0/1779
31	AU	0.10	0/1261	0.20	0/1698
32	AV	0.11	0/941	0.22	0/1272

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	AW	0.11	0/819	0.21	0/1110
34	AX	0.10	0/1061	0.22	0/1441
35	AY	0.11	0/982	0.27	0/1335
36	AZ	0.10	0/790	0.24	0/1066
37	B0	0.12	0/833	0.23	0/1132
38	B1	0.10	0/812	0.21	0/1093
39	B2	0.11	0/776	0.21	0/1048
40	B3	0.11	0/654	0.22	0/884
41	B4	0.07	0/642	0.19	0/865
42	B5	0.11	0/466	0.21	0/630
43	B6	0.13	0/535	0.23	0/727
44	BA	0.10	0/1696	0.22	0/2292
45	BB	0.11	0/1376	0.21	0/1862
46	BC	0.12	0/1479	0.32	0/1996
47	BD	0.11	0/1216	0.21	0/1643
48	BE	0.10	0/1462	0.22	0/1981
49	BF	0.11	0/1503	0.24	0/2018
50	BG	0.10	0/1379	0.22	0/1841
51	BH	0.12	0/1519	0.26	0/2058
52	BI	0.13	0/1203	0.25	0/1630
53	BJ	0.11	0/1234	0.22	0/1662
54	BK	0.10	0/923	0.20	0/1239
55	BL	0.10	0/1223	0.21	0/1648
56	BM	0.11	0/1110	0.25	0/1502
57	BN	0.12	0/1132	0.23	0/1534
58	BO	0.09	0/1120	0.21	0/1500
59	BP	0.15	0/631	0.25	0/860
60	BQ	0.11	0/868	0.21	0/1170
61	BR	0.10	0/747	0.22	0/1011
62	BS	0.12	0/991	0.20	0/1333
63	BT	0.10	0/1106	0.23	0/1504
64	BU	0.09	0/1102	0.22	0/1486
65	BV	0.10	0/1003	0.21	0/1353
66	BW	0.12	0/983	0.20	0/1327
67	BX	0.11	0/821	0.21	0/1111
68	BY	0.11	0/916	0.26	0/1224
69	BZ	0.10	0/873	0.20	0/1175
All	All	0.11	0/115258	0.25	0/155972

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	4071	4019	4018	32	0
2	A1	2718	2650	2649	11	0
3	A2	2199	2163	2160	13	0
4	A3	2263	2260	2260	15	0
5	A4	2494	2491	2491	9	0
6	A5	2347	2249	2249	23	0
7	A6	1908	1862	1861	14	0
8	A7	1084	1040	1039	14	0
9	A8	1794	1803	1800	12	0
10	A9	1879	1818	1818	7	0
11	AA	5941	5978	5977	50	0
12	AB	5403	5359	5358	48	0
13	AC	4170	4223	4223	35	0
14	AD	3399	3345	3345	33	0
15	AE	3587	3539	3539	38	0
16	AF	3068	3148	3147	32	0
17	AG	2804	2727	2727	13	0
18	AH	2306	2350	2349	22	0
19	AI	1862	1848	1847	15	0
20	AJ	2160	2156	2155	14	0
21	AK	1779	1740	1739	15	0
22	AL	1812	1689	1688	27	0
23	AM	1770	1788	1788	16	0
24	AN	1322	1329	1328	9	0
25	AO	1683	1680	1680	17	0
26	AP	1599	1505	1504	13	0
27	AQ	1588	1496	1495	6	0
28	AR	1492	1445	1445	6	0
29	AS	1420	1382	1382	6	0
30	AT	1277	1272	1271	20	0
31	AU	1227	1209	1208	5	0
32	AV	925	904	903	5	0
33	AW	803	781	780	6	0
34	AX	1027	1020	1020	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	AY	957	987	987	14	0
36	AZ	777	775	774	3	0
37	B0	805	802	801	7	0
38	B1	790	746	745	2	0
39	B2	757	728	727	8	0
40	B3	633	618	617	4	0
41	B4	624	623	623	3	0
42	B5	453	464	463	1	0
43	B6	515	528	528	11	0
44	BA	1651	1638	1637	11	0
45	BB	1346	1280	1279	11	0
46	BC	1442	1406	1405	7	0
47	BD	1191	1223	1222	12	0
48	BE	1422	1385	1384	5	0
49	BF	1475	1486	1485	20	0
50	BG	1349	1376	1375	14	0
51	BH	1482	1554	1554	15	0
52	BI	1179	1139	1134	10	0
53	BJ	1205	1156	1155	3	0
54	BK	903	854	853	2	0
55	BL	1187	1138	1137	9	0
56	BM	1072	1002	1001	11	0
57	BN	1103	1126	1125	10	0
58	BO	1098	1058	1058	3	0
59	BP	604	590	589	7	0
60	BQ	845	829	828	7	0
61	BR	730	719	718	1	0
62	BS	966	941	940	4	0
63	BT	1063	953	950	8	0
64	BU	1082	1094	1094	9	0
65	BV	987	1014	1014	2	0
66	BW	955	893	892	5	0
67	BX	797	755	754	6	0
68	BY	889	917	917	10	0
69	BZ	850	840	840	4	0
70	A0	200	312	312	1	0
70	A1	100	156	156	0	0
70	AA	200	312	312	3	0
70	AC	200	312	312	0	0
70	AF	200	312	312	0	0
70	AM	100	156	156	0	0
70	AP	100	156	156	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	B0	200	312	312	1	0
70	B1	100	156	156	0	0
70	BC	200	312	312	0	0
70	BE	100	156	156	1	0
70	BG	100	156	156	0	0
70	BL	100	156	156	1	0
70	BT	100	156	156	0	0
70	BV	100	156	156	0	0
70	BY	100	156	156	0	0
71	A0	25	11	11	2	0
72	A0	1	0	0	0	0
72	A8	1	0	0	0	0
73	A0	54	88	88	0	0
73	A1	108	176	176	0	0
73	A2	54	88	88	0	0
73	A6	108	176	176	2	0
73	A9	108	176	176	0	0
73	AA	270	440	440	0	0
73	AH	54	88	88	0	0
73	AJ	54	88	88	0	0
73	AL	54	88	88	2	0
73	AM	54	88	88	0	0
73	AQ	54	88	88	0	0
73	AU	108	176	176	0	0
73	B1	108	176	176	0	0
73	BQ	54	88	88	0	0
73	BS	108	176	176	1	0
73	BT	54	88	88	1	0
73	BY	54	88	88	0	0
74	A1	48	26	25	0	0
75	A2	51	82	82	0	0
75	A9	102	164	164	1	0
75	AJ	51	82	82	0	0
75	BA	51	82	82	1	0
75	BP	51	82	82	0	0
76	A6	44	67	67	0	0
76	AA	44	67	67	1	0
76	AL	44	67	67	2	0
76	BN	44	67	67	0	0
77	A8	27	12	12	0	0
77	AQ	27	12	12	0	0
78	AB	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
78	AI	4	0	0	2	0
78	BI	4	0	0	1	0
79	AB	16	0	0	3	0
79	AD	8	0	0	1	0
79	AL	16	0	0	6	0
79	AT	8	0	0	0	0
80	AD	31	18	19	0	0
81	AS	34	43	0	2	0
82	BR	1	0	0	0	0
All	All	116760	117595	117495	696	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 3.

The worst 5 of 696 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)
26:AP:3:LEU:N	70:AP:301:CDL:OA3	1.70	1.23
17:AG:54:ARG:O	23:AM:225:GLN:NE2	2.11	0.82
24:AN:105:LYS:NZ	25:AO:52:GLU:OE2	2.14	0.80
14:AD:40:ARG:NH1	14:AD:290:GLU:O	2.16	0.79
70:AP:301:CDL:OA4	70:AP:301:CDL:O1	2.00	0.79

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	A0	501/516 (97%)	486 (97%)	15 (3%)	0	100	100
2	A1	336/362 (93%)	329 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A2	263/317 (83%)	260 (99%)	3 (1%)	0	100	100
4	A3	289/333 (87%)	285 (99%)	4 (1%)	0	100	100
5	A4	309/311 (99%)	302 (98%)	7 (2%)	0	100	100
6	A5	280/282 (99%)	279 (100%)	1 (0%)	0	100	100
7	A6	228/251 (91%)	224 (98%)	4 (2%)	0	100	100
8	A7	131/238 (55%)	129 (98%)	2 (2%)	0	100	100
9	A8	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
10	A9	229/231 (99%)	227 (99%)	2 (1%)	0	100	100
11	AA	711/750 (95%)	691 (97%)	19 (3%)	1 (0%)	48	77
12	AB	686/718 (96%)	671 (98%)	15 (2%)	0	100	100
13	AC	503/505 (100%)	490 (97%)	13 (3%)	0	100	100
14	AD	439/474 (93%)	425 (97%)	14 (3%)	0	100	100
15	AE	439/442 (99%)	430 (98%)	9 (2%)	0	100	100
16	AF	357/360 (99%)	348 (98%)	9 (2%)	0	100	100
17	AG	344/346 (99%)	339 (98%)	5 (2%)	0	100	100
18	AH	281/284 (99%)	273 (97%)	8 (3%)	0	100	100
19	AI	229/274 (84%)	228 (100%)	1 (0%)	0	100	100
20	AJ	252/255 (99%)	246 (98%)	6 (2%)	0	100	100
21	AK	228/257 (89%)	220 (96%)	8 (4%)	0	100	100
22	AL	216/236 (92%)	209 (97%)	7 (3%)	0	100	100
23	AM	229/233 (98%)	220 (96%)	8 (4%)	1 (0%)	30	60
24	AN	155/206 (75%)	155 (100%)	0	0	100	100
25	AO	196/198 (99%)	192 (98%)	4 (2%)	0	100	100
26	AP	189/194 (97%)	183 (97%)	6 (3%)	0	100	100
27	AQ	185/189 (98%)	182 (98%)	3 (2%)	0	100	100
28	AR	179/185 (97%)	177 (99%)	2 (1%)	0	100	100
29	AS	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
30	AT	159/162 (98%)	152 (96%)	7 (4%)	0	100	100
31	AU	147/150 (98%)	145 (99%)	2 (1%)	0	100	100
32	AV	110/138 (80%)	109 (99%)	1 (1%)	0	100	100
33	AW	96/133 (72%)	94 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	AX	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
35	AY	114/116 (98%)	114 (100%)	0	0	100	100
36	AZ	92/103 (89%)	89 (97%)	3 (3%)	0	100	100
37	B0	91/94 (97%)	91 (100%)	0	0	100	100
38	B1	90/93 (97%)	89 (99%)	1 (1%)	0	100	100
39	B2	91/94 (97%)	89 (98%)	2 (2%)	0	100	100
40	B3	71/83 (86%)	68 (96%)	3 (4%)	0	100	100
41	B4	71/73 (97%)	71 (100%)	0	0	100	100
42	B5	52/71 (73%)	52 (100%)	0	0	100	100
43	B6	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
44	BA	197/212 (93%)	194 (98%)	3 (2%)	0	100	100
45	BB	165/214 (77%)	164 (99%)	1 (1%)	0	100	100
46	BC	171/207 (83%)	170 (99%)	1 (1%)	0	100	100
47	BD	146/205 (71%)	145 (99%)	1 (1%)	0	100	100
48	BE	166/189 (88%)	160 (96%)	6 (4%)	0	100	100
49	BF	175/188 (93%)	167 (95%)	8 (5%)	0	100	100
50	BG	158/175 (90%)	154 (98%)	4 (2%)	0	100	100
51	BH	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
52	BI	147/172 (86%)	145 (99%)	2 (1%)	0	100	100
53	BJ	142/166 (86%)	142 (100%)	0	0	100	100
54	BK	107/144 (74%)	106 (99%)	1 (1%)	0	100	100
55	BL	140/143 (98%)	137 (98%)	3 (2%)	0	100	100
56	BM	126/135 (93%)	119 (94%)	7 (6%)	0	100	100
57	BN	131/135 (97%)	128 (98%)	3 (2%)	0	100	100
58	BO	134/136 (98%)	133 (99%)	1 (1%)	0	100	100
59	BP	70/129 (54%)	69 (99%)	1 (1%)	0	100	100
60	BQ	99/127 (78%)	97 (98%)	2 (2%)	0	100	100
61	BR	89/132 (67%)	88 (99%)	1 (1%)	0	100	100
62	BS	118/126 (94%)	115 (98%)	3 (2%)	0	100	100
63	BT	123/125 (98%)	123 (100%)	0	0	100	100
64	BU	132/134 (98%)	131 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	BV	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
66	BW	116/120 (97%)	111 (96%)	5 (4%)	0	100	100
67	BX	94/113 (83%)	93 (99%)	1 (1%)	0	100	100
68	BY	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
69	BZ	100/102 (98%)	100 (100%)	0	0	100	100
All	All	13572/14758 (92%)	13286 (98%)	284 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	AA	119	GLU
23	AM	51	PRO

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	A0	441/454 (97%)	434 (98%)	7 (2%)	55	83
2	A1	288/311 (93%)	287 (100%)	1 (0%)	86	95
3	A2	225/270 (83%)	224 (100%)	1 (0%)	84	94
4	A3	244/280 (87%)	242 (99%)	2 (1%)	73	90
5	A4	275/275 (100%)	275 (100%)	0	100	100
6	A5	257/257 (100%)	257 (100%)	0	100	100
7	A6	207/223 (93%)	206 (100%)	1 (0%)	81	93
8	A7	122/224 (54%)	122 (100%)	0	100	100
9	A8	195/195 (100%)	193 (99%)	2 (1%)	68	88
10	A9	199/199 (100%)	196 (98%)	3 (2%)	57	84
11	AA	657/694 (95%)	649 (99%)	8 (1%)	63	87
12	AB	589/617 (96%)	587 (100%)	2 (0%)	86	95
13	AC	463/463 (100%)	461 (100%)	2 (0%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	AD	361/392 (92%)	359 (99%)	2 (1%)	78 92
15	AE	398/399 (100%)	395 (99%)	3 (1%)	73 90
16	AF	346/347 (100%)	346 (100%)	0	100 100
17	AG	309/309 (100%)	308 (100%)	1 (0%)	86 95
18	AH	249/250 (100%)	244 (98%)	5 (2%)	48 80
19	AI	206/236 (87%)	205 (100%)	1 (0%)	81 93
20	AJ	243/244 (100%)	243 (100%)	0	100 100
21	AK	196/218 (90%)	194 (99%)	2 (1%)	68 88
22	AL	197/215 (92%)	193 (98%)	4 (2%)	48 80
23	AM	196/197 (100%)	194 (99%)	2 (1%)	68 88
24	AN	146/186 (78%)	146 (100%)	0	100 100
25	AO	191/191 (100%)	191 (100%)	0	100 100
26	AP	168/170 (99%)	168 (100%)	0	100 100
27	AQ	170/172 (99%)	169 (99%)	1 (1%)	78 92
28	AR	159/163 (98%)	158 (99%)	1 (1%)	78 92
29	AS	154/154 (100%)	153 (99%)	1 (1%)	78 92
30	AT	136/137 (99%)	132 (97%)	4 (3%)	37 73
31	AU	132/133 (99%)	130 (98%)	2 (2%)	57 84
32	AV	104/129 (81%)	104 (100%)	0	100 100
33	AW	87/119 (73%)	87 (100%)	0	100 100
34	AX	112/112 (100%)	109 (97%)	3 (3%)	39 74
35	AY	108/108 (100%)	107 (99%)	1 (1%)	70 89
36	AZ	84/93 (90%)	84 (100%)	0	100 100
37	B0	88/89 (99%)	88 (100%)	0	100 100
38	B1	83/84 (99%)	82 (99%)	1 (1%)	63 87
39	B2	82/83 (99%)	82 (100%)	0	100 100
40	B3	66/74 (89%)	66 (100%)	0	100 100
41	B4	65/65 (100%)	65 (100%)	0	100 100
42	B5	48/63 (76%)	48 (100%)	0	100 100
43	B6	55/55 (100%)	54 (98%)	1 (2%)	51 82
44	BA	179/190 (94%)	179 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
45	BB	145/182 (80%)	145 (100%)	0	100 100
46	BC	155/180 (86%)	154 (99%)	1 (1%)	78 92
47	BD	124/179 (69%)	123 (99%)	1 (1%)	73 90
48	BE	159/178 (89%)	157 (99%)	2 (1%)	61 86
49	BF	161/172 (94%)	161 (100%)	0	100 100
50	BG	142/156 (91%)	141 (99%)	1 (1%)	76 91
51	BH	170/170 (100%)	169 (99%)	1 (1%)	78 92
52	BI	131/152 (86%)	131 (100%)	0	100 100
53	BJ	128/147 (87%)	128 (100%)	0	100 100
54	BK	97/131 (74%)	97 (100%)	0	100 100
55	BL	124/125 (99%)	124 (100%)	0	100 100
56	BM	108/114 (95%)	107 (99%)	1 (1%)	70 89
57	BN	120/122 (98%)	120 (100%)	0	100 100
58	BO	122/122 (100%)	122 (100%)	0	100 100
59	BP	64/117 (55%)	64 (100%)	0	100 100
60	BQ	93/117 (80%)	92 (99%)	1 (1%)	65 87
61	BR	81/116 (70%)	80 (99%)	1 (1%)	63 87
62	BS	103/109 (94%)	103 (100%)	0	100 100
63	BT	110/110 (100%)	104 (94%)	6 (6%)	19 51
64	BU	121/121 (100%)	121 (100%)	0	100 100
65	BV	102/102 (100%)	101 (99%)	1 (1%)	68 88
66	BW	98/99 (99%)	98 (100%)	0	100 100
67	BX	81/97 (84%)	81 (100%)	0	100 100
68	BY	98/98 (100%)	98 (100%)	0	100 100
69	BZ	89/89 (100%)	89 (100%)	0	100 100
All	All	12206/13144 (93%)	12126 (99%)	80 (1%)	73 91

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	AU	73	LEU
60	BQ	99	THR
34	AX	3	ASP

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Mol	Chain	Res	Type
47	BD	149	LEU
63	BT	52	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
44	BA	135	ASN
58	BO	109	GLN
45	BB	92	HIS
52	BI	53	GLN
64	BU	112	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 77 ligands modelled in this entry, 3 are monoatomic - leaving 74 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	$\#\|Z\| > 2$
73	PC1	A0	605	-	53,53,53	1.07	3 (5%)	59,61,61	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
73	PC1	AA	906	-	53,53,53	1.06	3 (5%)	59,61,61	0.68	1 (1%)
75	3PE	A9	602	-	50,50,50	1.09	5 (10%)	53,55,55	1.01	5 (9%)
73	PC1	A6	303	-	53,53,53	1.07	3 (5%)	59,61,61	0.60	1 (1%)
70	CDL	AA	901	-	99,99,99	1.19	7 (7%)	105,111,111	0.74	2 (1%)
70	CDL	BV	201	-	99,99,99	1.17	7 (7%)	105,111,111	0.66	0
75	3PE	AJ	502	-	50,50,50	1.05	5 (10%)	53,55,55	0.71	1 (1%)
73	PC1	AU	202	-	53,53,53	1.06	3 (5%)	59,61,61	0.62	0
70	CDL	AC	801	-	99,99,99	1.15	7 (7%)	105,111,111	0.74	2 (1%)
73	PC1	A9	601	-	53,53,53	1.07	3 (5%)	59,61,61	0.58	1 (1%)
73	PC1	A9	604	-	53,53,53	1.05	3 (5%)	59,61,61	0.63	0
70	CDL	A0	602	-	99,99,99	1.19	8 (8%)	105,111,111	0.75	2 (1%)
73	PC1	AA	907	-	53,53,53	1.07	3 (5%)	59,61,61	0.56	1 (1%)
73	PC1	B1	401	-	53,53,53	1.07	3 (5%)	59,61,61	0.68	1 (1%)
73	PC1	BS	1302	-	53,53,53	1.06	3 (5%)	59,61,61	0.60	1 (1%)
75	3PE	BA	301	-	50,50,50	1.06	5 (10%)	53,55,55	0.58	0
73	PC1	A1	403	-	53,53,53	1.09	3 (5%)	59,61,61	0.62	1 (1%)
73	PC1	B1	403	-	53,53,53	1.07	3 (5%)	59,61,61	0.54	0
76	LPP	AA	902	-	43,43,43	0.91	3 (6%)	47,48,48	0.71	1 (2%)
77	ADP	A8	401	72	27,29,29	3.24	10 (37%)	42,45,45	3.08	15 (35%)
76	LPP	A6	301	-	43,43,43	0.90	3 (6%)	47,48,48	0.93	1 (2%)
73	PC1	AM	302	-	53,53,53	1.06	3 (5%)	59,61,61	0.62	1 (1%)
79	SF4	AB	803	12	0,12,12	-	-	-		
73	PC1	AH	301	-	53,53,53	1.07	3 (5%)	59,61,61	0.60	0
79	SF4	AL	301	22	0,12,12	-	-	-		
73	PC1	AA	904	-	53,53,53	1.04	3 (5%)	59,61,61	0.72	1 (1%)
79	SF4	AL	302	22	0,12,12	-	-	-		
73	PC1	BY	202	-	53,53,53	1.06	3 (5%)	59,61,61	0.61	1 (1%)
73	PC1	AU	201	-	53,53,53	1.06	3 (5%)	59,61,61	0.58	0
73	PC1	A1	404	-	53,53,53	1.06	3 (5%)	59,61,61	0.75	2 (3%)
73	PC1	A2	402	-	53,53,53	1.05	3 (5%)	59,61,61	0.62	0
79	SF4	AT	201	30	0,12,12	-	-	-		
71	UDP	A0	603	72	24,26,26	3.62	14 (58%)	37,40,40	1.49	5 (13%)
73	PC1	AA	903	-	53,53,53	1.06	3 (5%)	59,61,61	0.64	1 (1%)
70	CDL	B1	402	-	99,99,99	1.19	7 (7%)	105,111,111	0.64	1 (0%)
70	CDL	A1	402	-	99,99,99	1.20	7 (7%)	105,111,111	0.68	2 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
70	CDL	BC	301	-	99,99,99	1.18	7 (7%)	105,111,111	0.74	1 (0%)
74	NDP	A1	401	-	49,52,52	3.91	23 (46%)	66,80,80	1.70	11 (16%)
70	CDL	AF	402	-	99,99,99	1.19	7 (7%)	105,111,111	0.70	2 (1%)
73	PC1	A6	302	-	53,53,53	1.08	3 (5%)	59,61,61	0.66	1 (1%)
70	CDL	AF	401	-	99,99,99	1.19	8 (8%)	105,111,111	0.74	1 (0%)
70	CDL	BT	201	-	99,99,99	1.21	8 (8%)	105,111,111	0.67	2 (1%)
78	FES	AI	301	19	0,4,4	-	-	-		
70	CDL	AA	908	-	99,99,99	1.16	6 (6%)	105,111,111	0.68	1 (0%)
70	CDL	BG	201	-	99,99,99	1.19	7 (7%)	105,111,111	0.73	3 (2%)
73	PC1	BQ	401	-	53,53,53	1.06	3 (5%)	59,61,61	0.58	0
79	SF4	AD	501	14	0,12,12	-	-	-		
73	PC1	AA	905	-	53,53,53	1.06	3 (5%)	59,61,61	0.58	0
75	3PE	A9	603	-	50,50,50	1.07	5 (10%)	53,55,55	0.66	1 (1%)
75	3PE	A2	401	-	50,50,50	1.07	5 (10%)	53,55,55	0.65	1 (1%)
75	3PE	BP	201	-	50,50,50	1.07	5 (10%)	53,55,55	0.71	1 (1%)
80	FMN	AD	502	-	33,33,33	0.72	0	48,50,50	0.78	0
70	CDL	AM	301	-	99,99,99	1.21	9 (9%)	105,111,111	0.69	2 (1%)
77	ADP	AQ	201	-	27,29,29	3.24	10 (37%)	42,45,45	3.11	15 (35%)
73	PC1	AQ	202	-	53,53,53	1.09	3 (5%)	59,61,61	0.63	1 (1%)
73	PC1	BT	202	-	53,53,53	1.06	3 (5%)	59,61,61	0.71	2 (3%)
78	FES	AB	801	12	0,4,4	-	-	-		
81	8Q1	AS	200	-	27,33,34	1.59	4 (14%)	32,40,43	1.53	6 (18%)
70	CDL	AC	802	-	99,99,99	1.18	7 (7%)	105,111,111	0.67	0
70	CDL	A0	601	-	99,99,99	1.17	7 (7%)	105,111,111	0.77	1 (0%)
73	PC1	AJ	501	-	53,53,53	1.06	3 (5%)	59,61,61	0.64	1 (1%)
70	CDL	AP	301	-	99,99,99	1.17	6 (6%)	105,111,111	0.75	0
70	CDL	BL	301	-	99,99,99	1.18	7 (7%)	105,111,111	0.72	2 (1%)
70	CDL	B0	102	-	99,99,99	1.19	7 (7%)	105,111,111	0.68	2 (1%)
70	CDL	BC	302	-	99,99,99	1.19	7 (7%)	105,111,111	0.73	1 (0%)
79	SF4	AB	802	12	0,12,12	-	-	-		
70	CDL	BY	201	-	99,99,99	1.20	8 (8%)	105,111,111	0.73	2 (1%)
76	LPP	AL	304	-	43,43,43	0.90	3 (6%)	47,48,48	0.68	1 (2%)
76	LPP	BN	301	-	43,43,43	0.90	3 (6%)	47,48,48	0.73	1 (2%)
70	CDL	BE	201	-	99,99,99	1.19	8 (8%)	105,111,111	0.74	2 (1%)
70	CDL	B0	101	-	99,99,99	1.19	7 (7%)	105,111,111	0.72	2 (1%)
73	PC1	AL	303	-	53,53,53	1.06	3 (5%)	59,61,61	0.72	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
78	FES	BI	201	52	0,4,4	-	-	-		
73	PC1	BS	1301	-	53,53,53	1.04	3 (5%)	59,61,61	0.66	2 (3%)

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
73	PC1	A0	605	-	-	14/57/57/57	-
73	PC1	AA	906	-	-	20/57/57/57	-
75	3PE	A9	602	-	-	16/54/54/54	-
73	PC1	A6	303	-	-	9/57/57/57	-
70	CDL	AA	901	-	-	23/110/110/110	-
70	CDL	BV	201	-	-	18/110/110/110	-
75	3PE	AJ	502	-	-	12/54/54/54	-
73	PC1	AU	202	-	-	13/57/57/57	-
70	CDL	AC	801	-	-	25/110/110/110	-
73	PC1	A9	601	-	-	15/57/57/57	-
73	PC1	A9	604	-	-	20/57/57/57	-
70	CDL	A0	602	-	-	25/110/110/110	-
73	PC1	AA	907	-	-	21/57/57/57	-
73	PC1	B1	401	-	-	18/57/57/57	-
73	PC1	BS	1302	-	-	10/57/57/57	-
75	3PE	BA	301	-	-	19/54/54/54	-
73	PC1	A1	403	-	-	6/57/57/57	-
73	PC1	B1	403	-	-	15/57/57/57	-
76	LPP	AA	902	-	-	10/45/45/45	-
77	ADP	A8	401	72	-	0/16/32/32	0/3/3/3
76	LPP	A6	301	-	-	9/45/45/45	-
73	PC1	AM	302	-	-	17/57/57/57	-
79	SF4	AB	803	12	-	-	0/6/5/5
73	PC1	AH	301	-	-	8/57/57/57	-
79	SF4	AL	301	22	-	-	0/6/5/5
73	PC1	AA	904	-	-	15/57/57/57	-
79	SF4	AL	302	22	-	-	0/6/5/5
73	PC1	BY	202	-	-	12/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
73	PC1	AU	201	-	-	12/57/57/57	-
73	PC1	A1	404	-	-	13/57/57/57	-
73	PC1	A2	402	-	-	8/57/57/57	-
79	SF4	AT	201	30	-	-	0/6/5/5
71	UDP	A0	603	72	-	7/16/32/32	0/2/2/2
73	PC1	AA	903	-	-	14/57/57/57	-
70	CDL	B1	402	-	-	26/110/110/110	-
70	CDL	A1	402	-	-	33/110/110/110	-
70	CDL	BC	301	-	-	19/110/110/110	-
74	NDP	A1	401	-	-	7/34/77/77	0/5/5/5
70	CDL	AF	402	-	-	27/110/110/110	-
73	PC1	A6	302	-	-	11/57/57/57	-
70	CDL	AF	401	-	-	20/110/110/110	-
70	CDL	BT	201	-	-	21/110/110/110	-
78	FES	AI	301	19	-	-	0/1/1/1
70	CDL	AA	908	-	-	31/110/110/110	-
70	CDL	BG	201	-	-	36/110/110/110	-
73	PC1	BQ	401	-	-	21/57/57/57	-
79	SF4	AD	501	14	-	-	0/6/5/5
73	PC1	AA	905	-	-	17/57/57/57	-
75	3PE	A9	603	-	-	7/54/54/54	-
75	3PE	A2	401	-	-	8/54/54/54	-
75	3PE	BP	201	-	-	13/54/54/54	-
80	FMN	AD	502	-	-	7/18/18/18	0/3/3/3
70	CDL	AM	301	-	-	26/110/110/110	-
77	ADP	AQ	201	-	-	1/16/32/32	0/3/3/3
73	PC1	AQ	202	-	-	18/57/57/57	-
73	PC1	BT	202	-	-	13/57/57/57	-
81	8Q1	AS	200	-	-	10/38/40/41	-
78	FES	AB	801	12	-	-	0/1/1/1
70	CDL	AC	802	-	-	26/110/110/110	-
70	CDL	A0	601	-	-	21/110/110/110	-
73	PC1	AJ	501	-	-	17/57/57/57	-
70	CDL	AP	301	-	-	24/110/110/110	-
70	CDL	BL	301	-	-	17/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	CDL	B0	102	-	-	21/110/110/110	-
70	CDL	BC	302	-	-	23/110/110/110	-
79	SF4	AB	802	12	-	-	0/6/5/5
70	CDL	BY	201	-	-	21/110/110/110	-
76	LPP	AL	304	-	-	4/45/45/45	-
76	LPP	BN	301	-	-	7/45/45/45	-
70	CDL	BE	201	-	-	31/110/110/110	-
70	CDL	B0	101	-	-	30/110/110/110	-
73	PC1	AL	303	-	-	9/57/57/57	-
78	FES	BI	201	52	-	-	0/1/1/1
73	PC1	BS	1301	-	-	16/57/57/57	-

The worst 5 of 343 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	A1	401	NDP	C6N-C5N	12.07	1.54	1.33
77	AQ	201	ADP	C2'-C3'	-11.05	1.23	1.53
77	A8	401	ADP	C2'-C3'	-10.99	1.23	1.53
74	A1	401	NDP	C2D-C3D	-10.66	1.24	1.53
74	A1	401	NDP	C2B-C1B	-8.74	1.30	1.53

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
77	A8	401	ADP	C1'-N9-C8	-9.25	106.25	127.14
77	AQ	201	ADP	C1'-N9-C8	-9.20	106.36	127.14
77	AQ	201	ADP	C4-N9-C1'	7.93	145.50	126.59
77	A8	401	ADP	C4-N9-C1'	7.93	145.48	126.59
77	A8	401	ADP	N6-C6-N1	-6.63	103.83	118.35

There are no chirality outliers.

5 of 1063 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	A0	601	CDL	C11-CA5-OA6-CA4
70	A0	601	CDL	CB3-OB5-PB2-OB4
70	A0	601	CDL	C51-CB5-OB6-CB4
70	A0	602	CDL	C1-CB2-OB2-PB2
70	A0	602	CDL	OB5-CB3-CB4-OB6

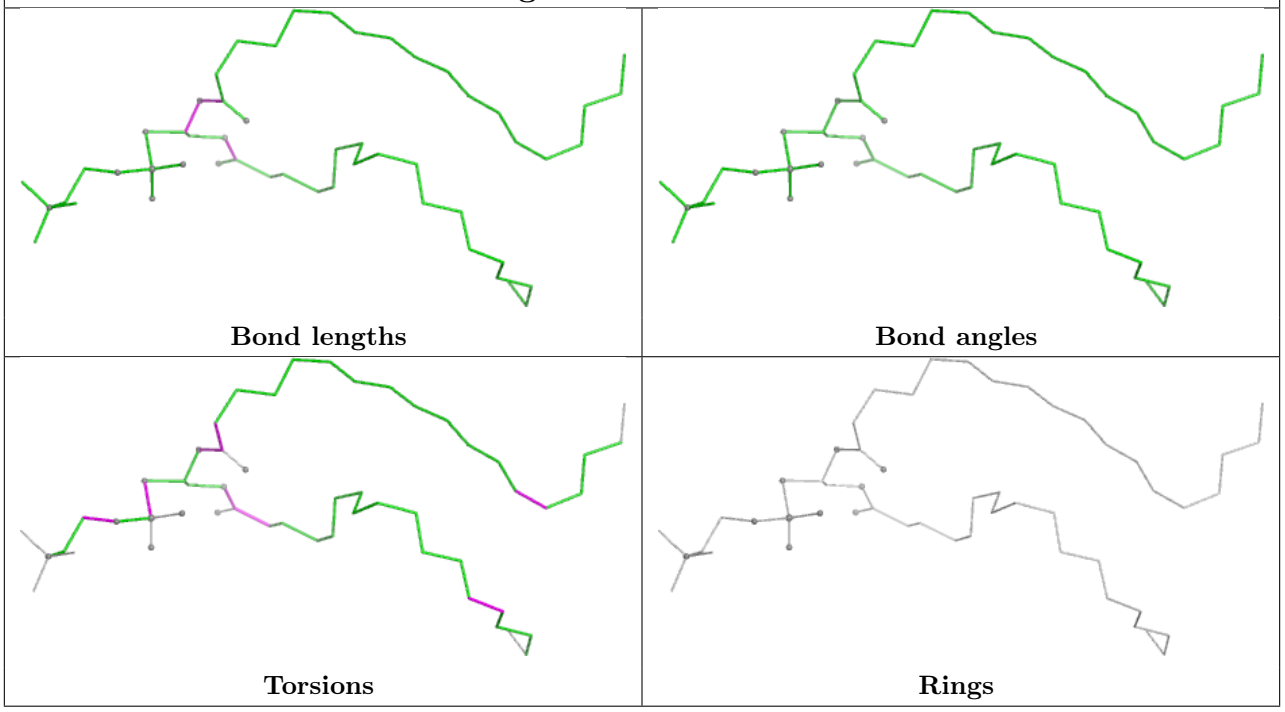
There are no ring outliers.

25 monomers are involved in 39 short contacts:

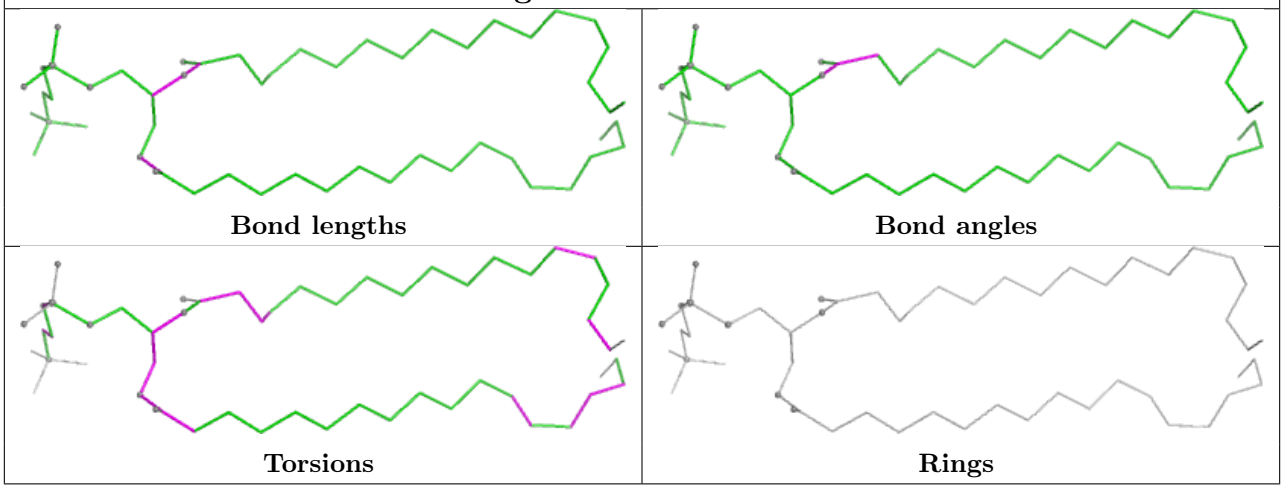
Mol	Chain	Res	Type	Clashes	Symm-Clashes
75	A9	602	3PE	1	0
73	A6	303	PC1	2	0
70	AA	901	CDL	2	0
70	A0	602	CDL	1	0
75	BA	301	3PE	1	0
76	AA	902	LPP	1	0
79	AB	803	SF4	2	0
79	AL	301	SF4	1	0
79	AL	302	SF4	5	0
71	A0	603	UDP	2	0
78	AI	301	FES	2	0
70	AA	908	CDL	1	0
79	AD	501	SF4	1	0
73	BT	202	PC1	1	0
78	AB	801	FES	1	0
81	AS	200	8Q1	2	0
70	AP	301	CDL	3	0
70	BL	301	CDL	1	0
70	B0	102	CDL	1	0
79	AB	802	SF4	1	0
76	AL	304	LPP	2	0
70	BE	201	CDL	1	0
73	AL	303	PC1	2	0
78	BI	201	FES	1	0
73	BS	1301	PC1	1	0

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

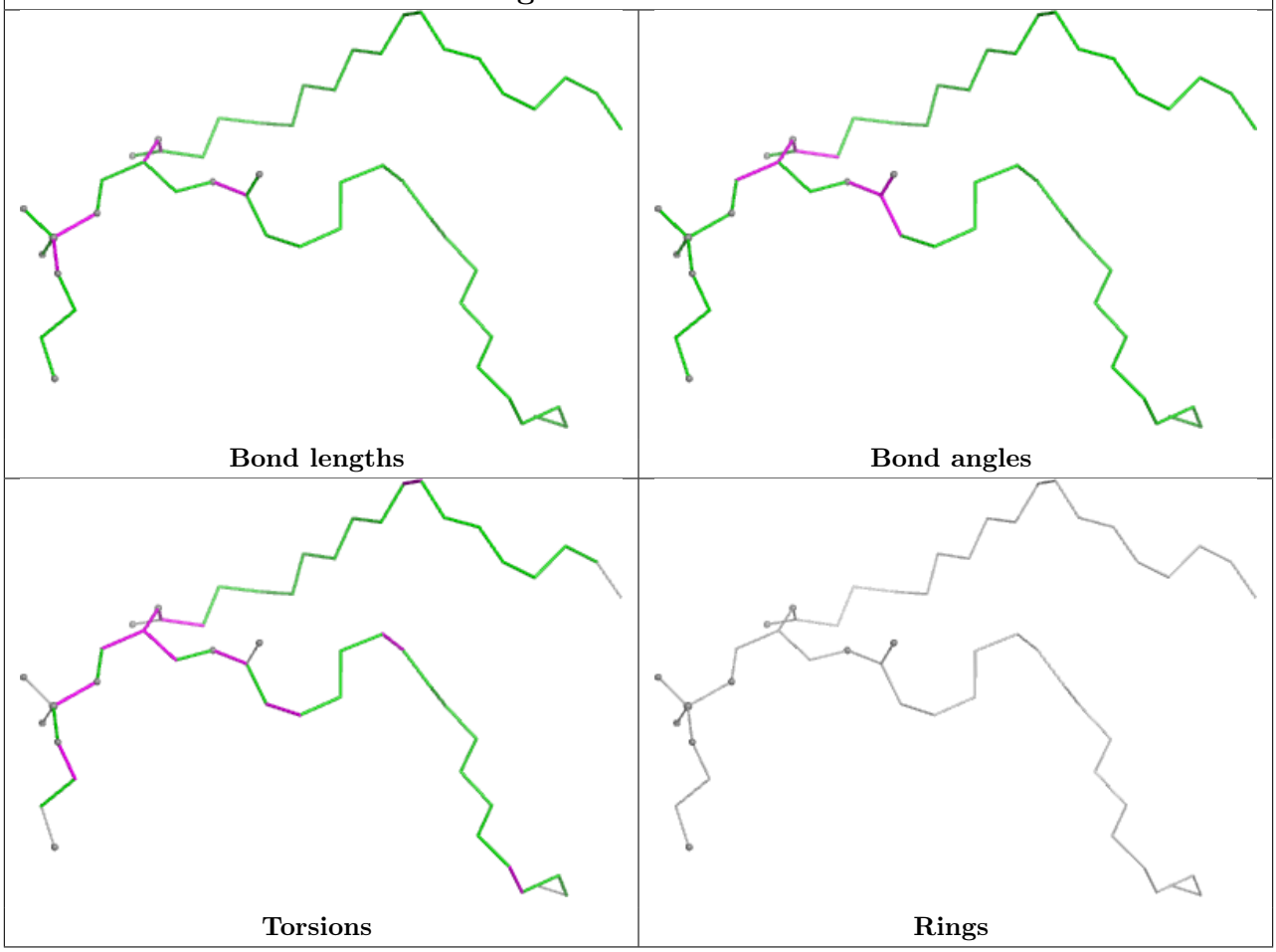
Ligand PC1 A0 605



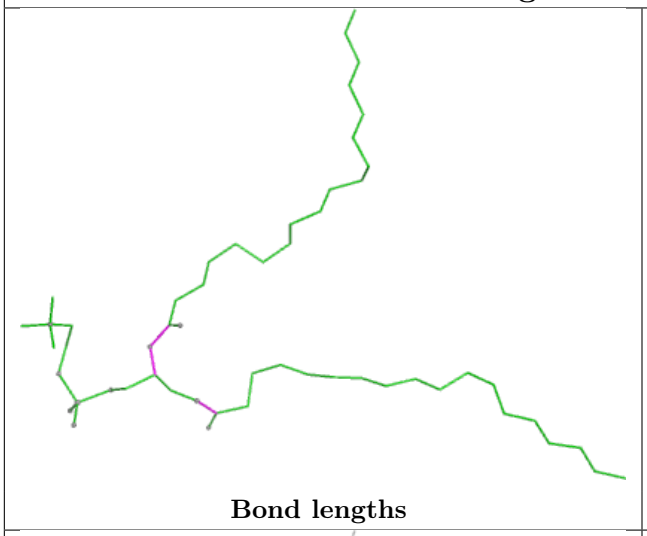
Ligand PC1 AA 906



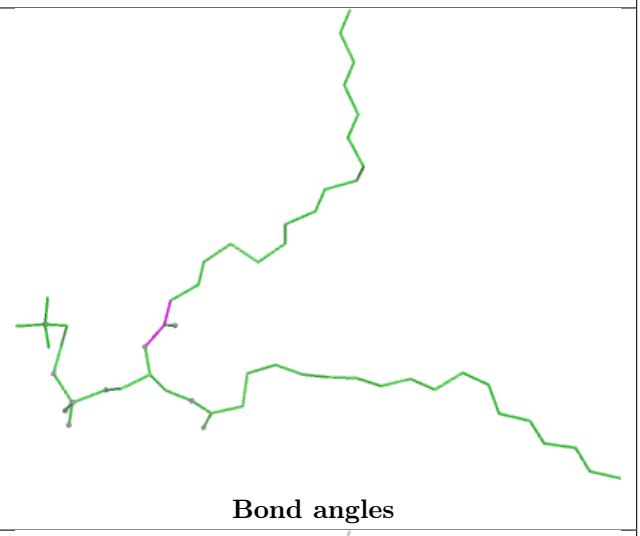
Ligand 3PE A9 602



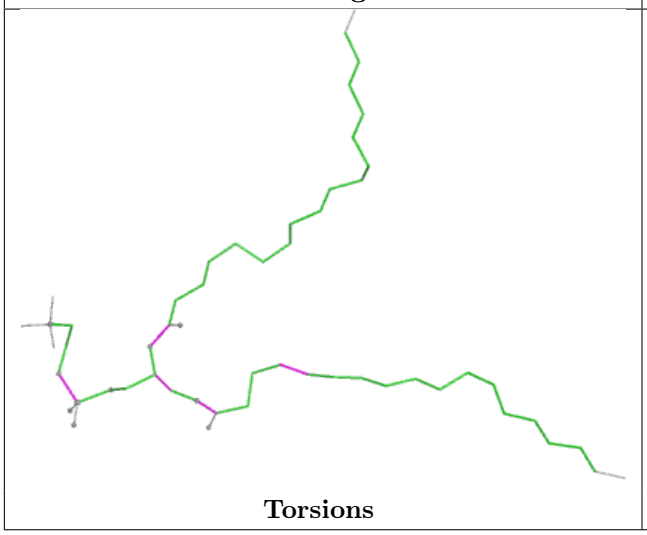
Ligand PC1 A6 303



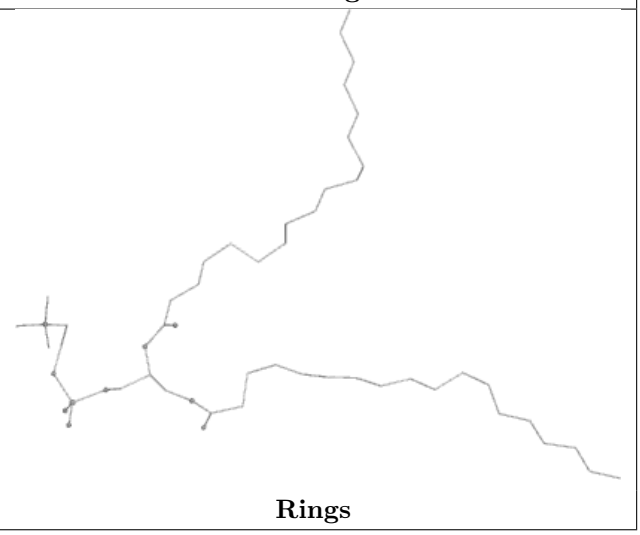
Bond lengths



Bond angles

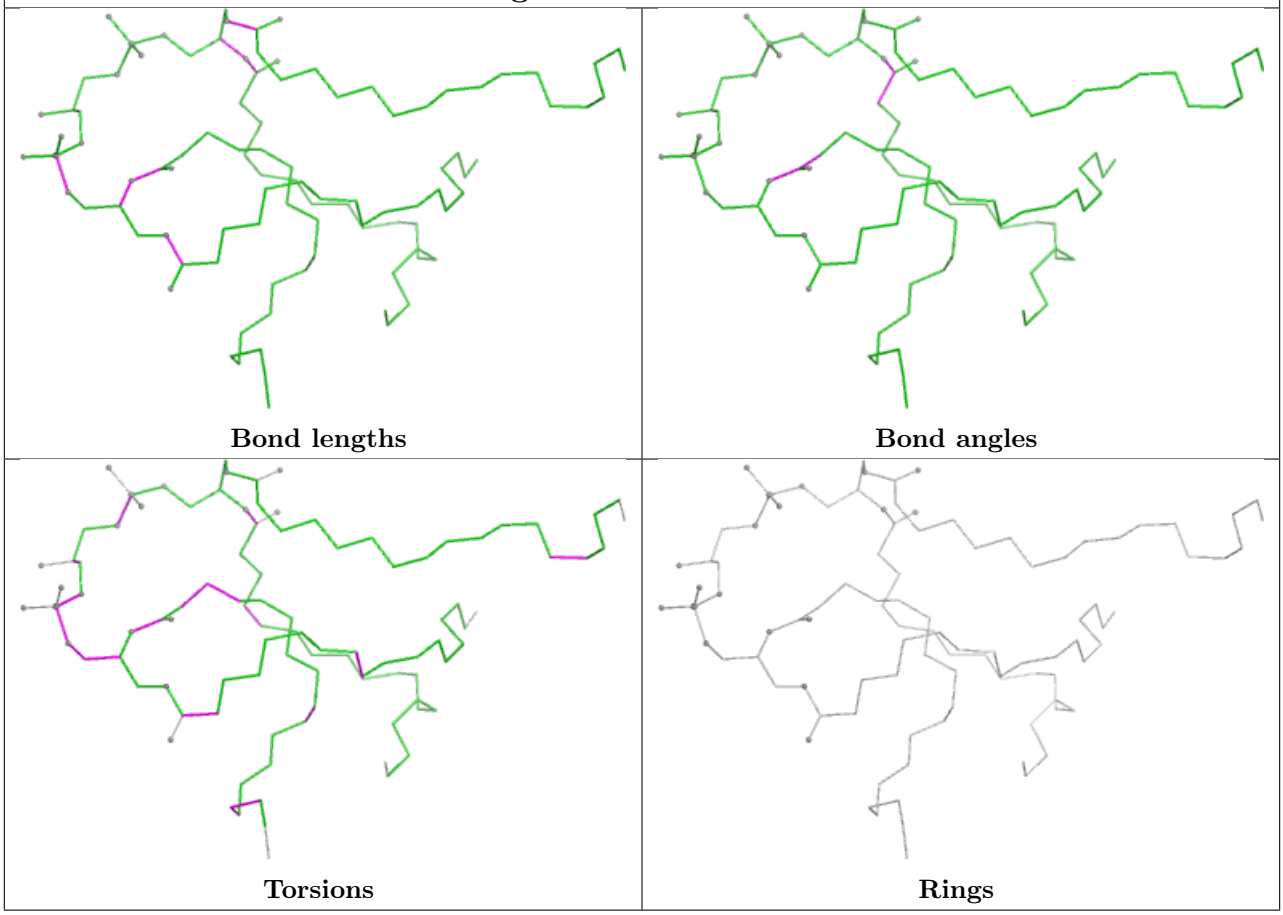


Torsions

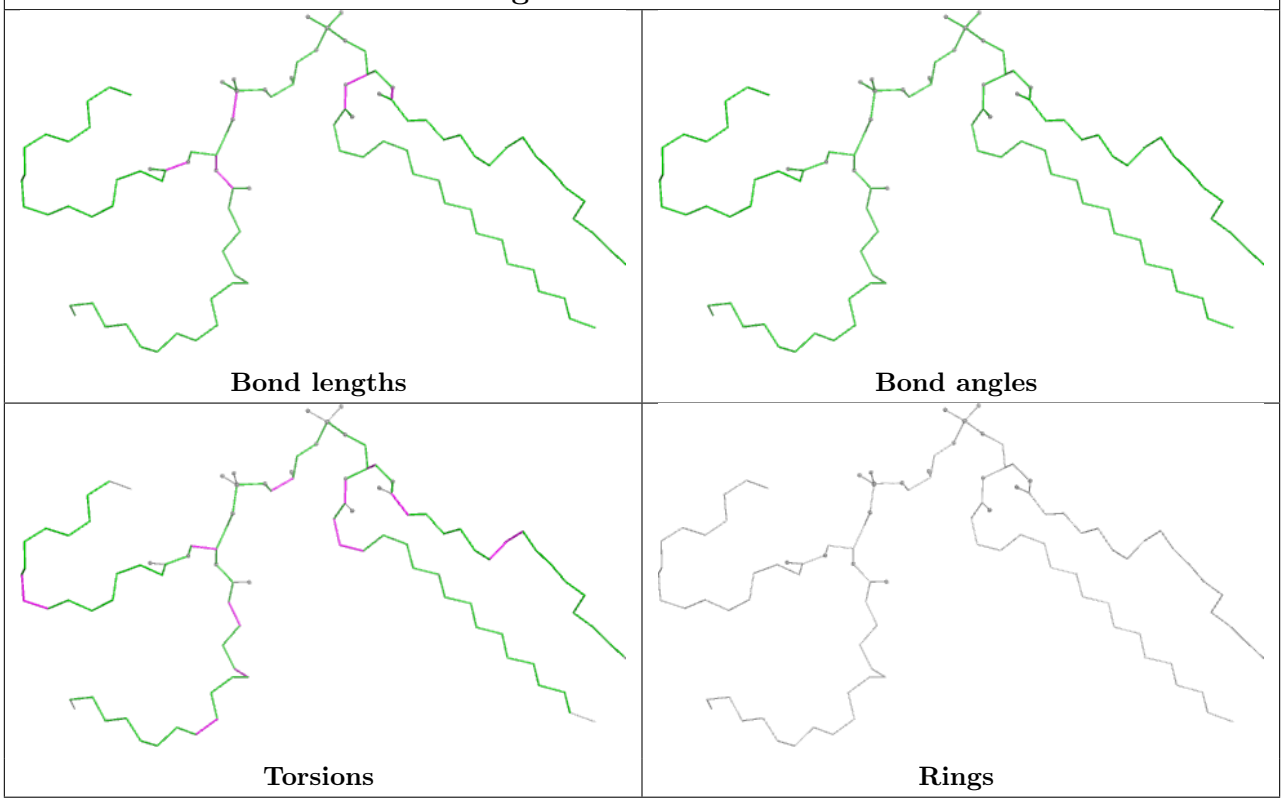


Rings

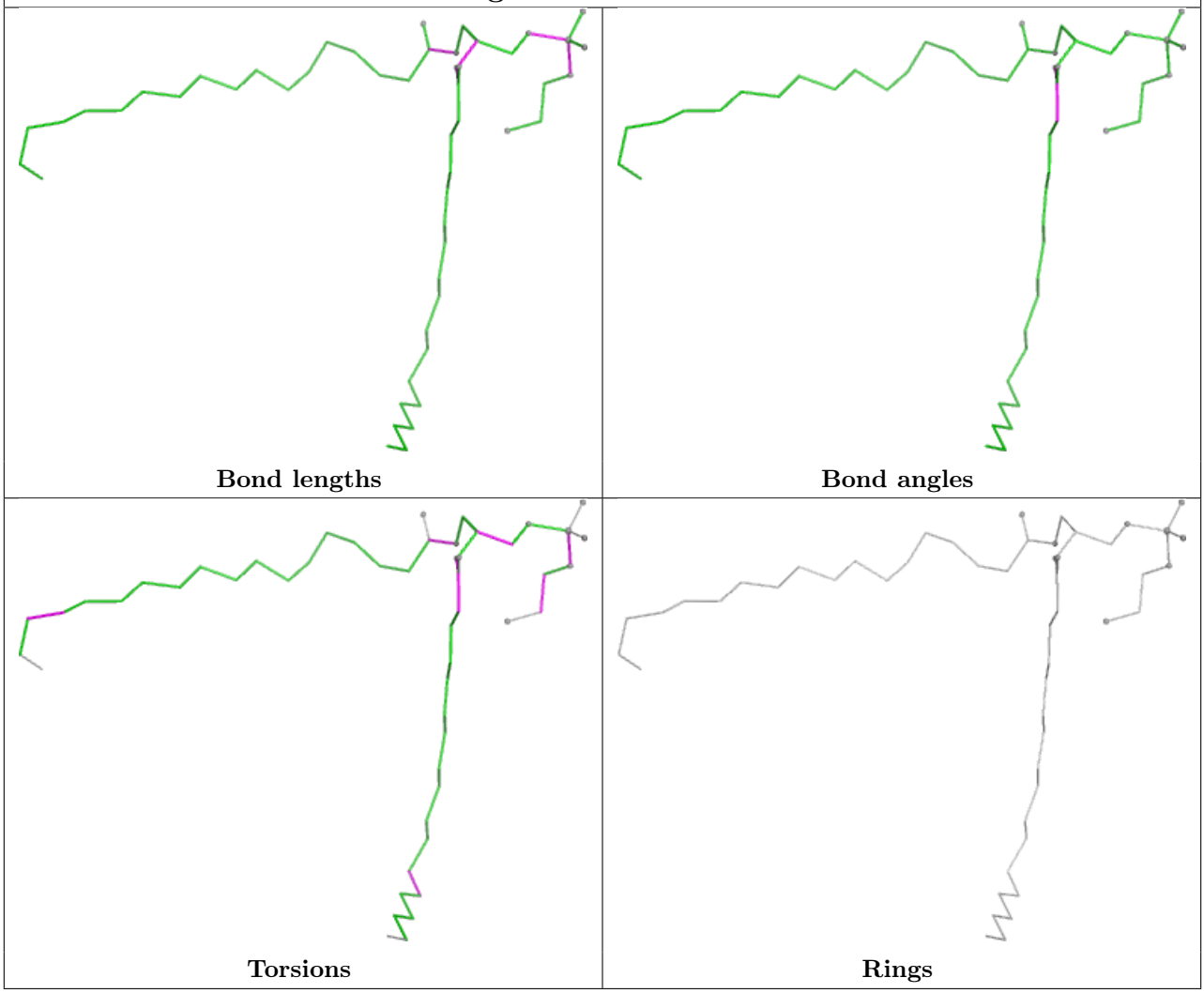
Ligand CDL AA 901



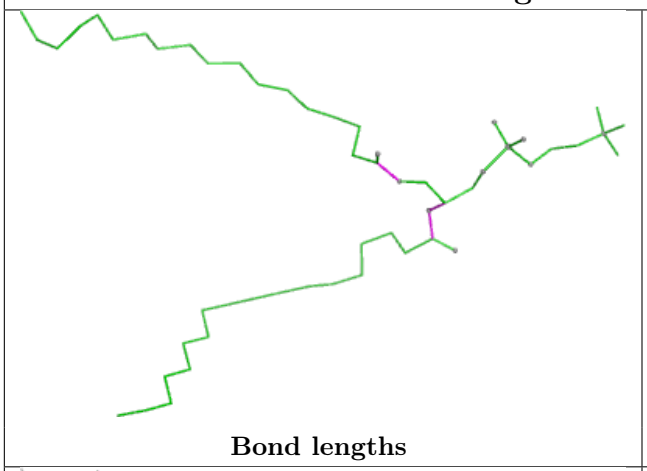
Ligand CDL BV 201



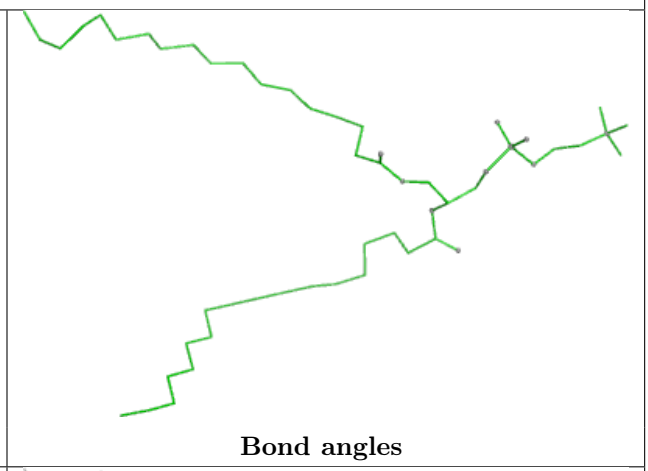
Ligand 3PE AJ 502



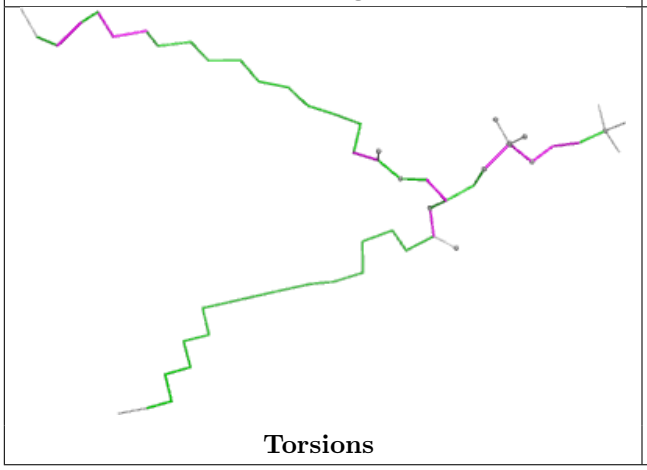
Ligand PC1 AU 202



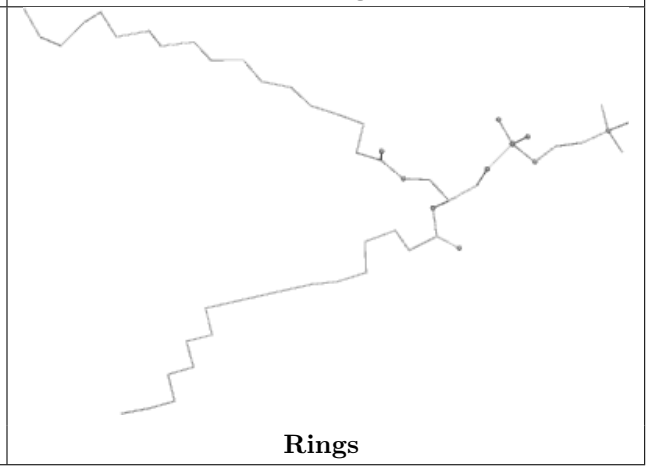
Bond lengths



Bond angles

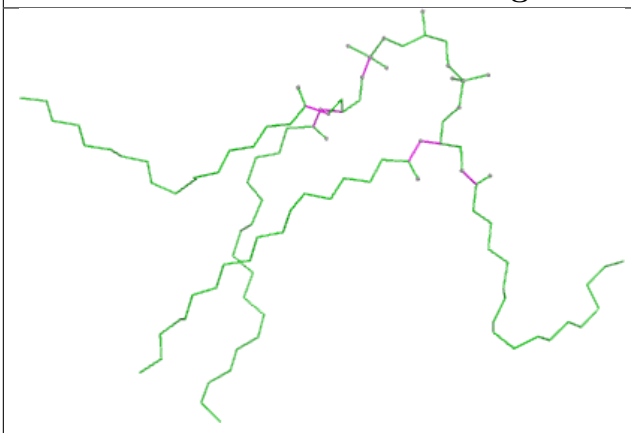


Torsions



Rings

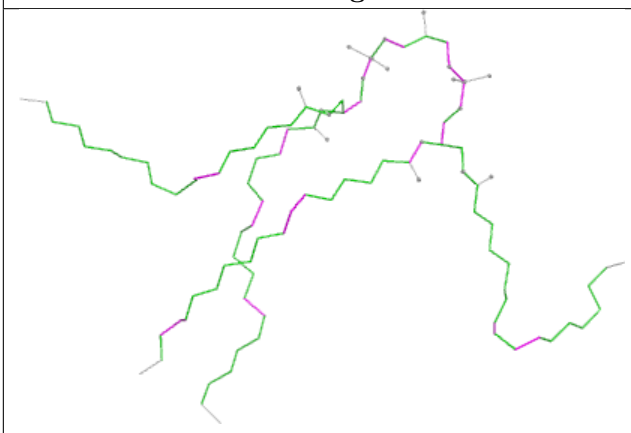
Ligand CDL AC 801



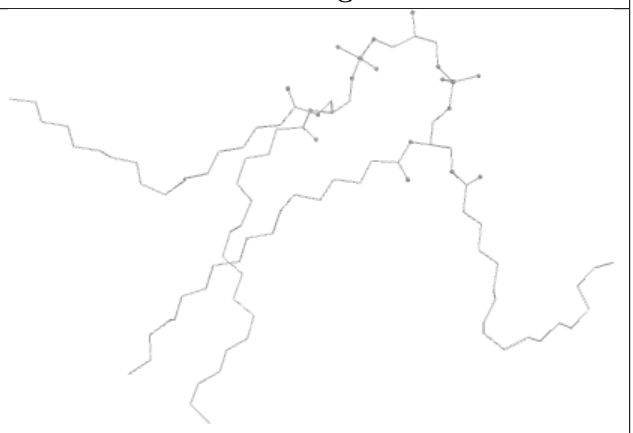
Bond lengths



Bond angles

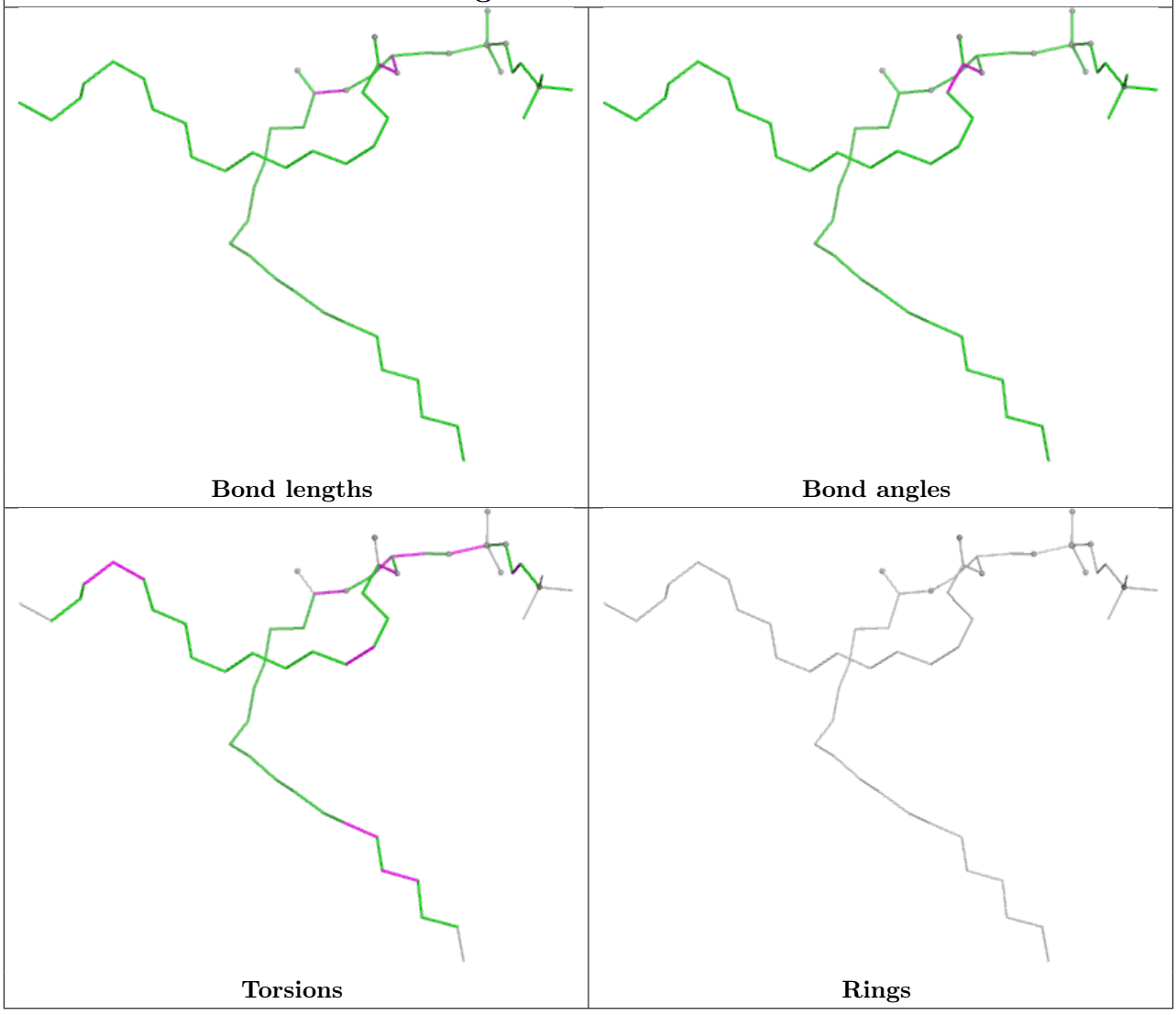


Torsions

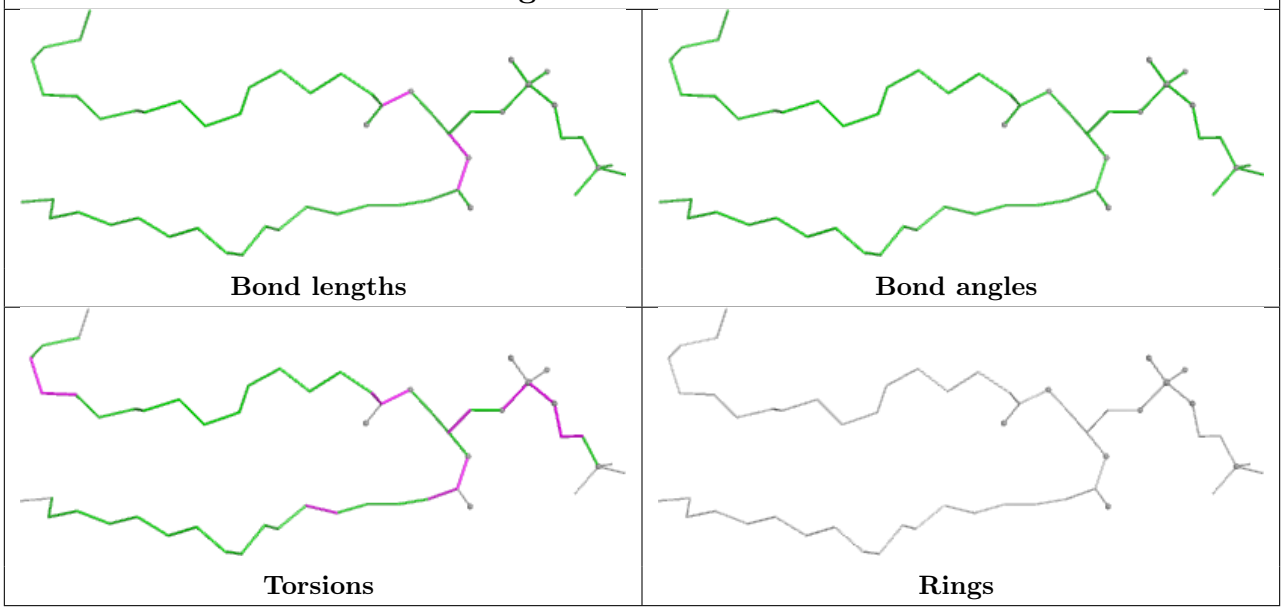


Rings

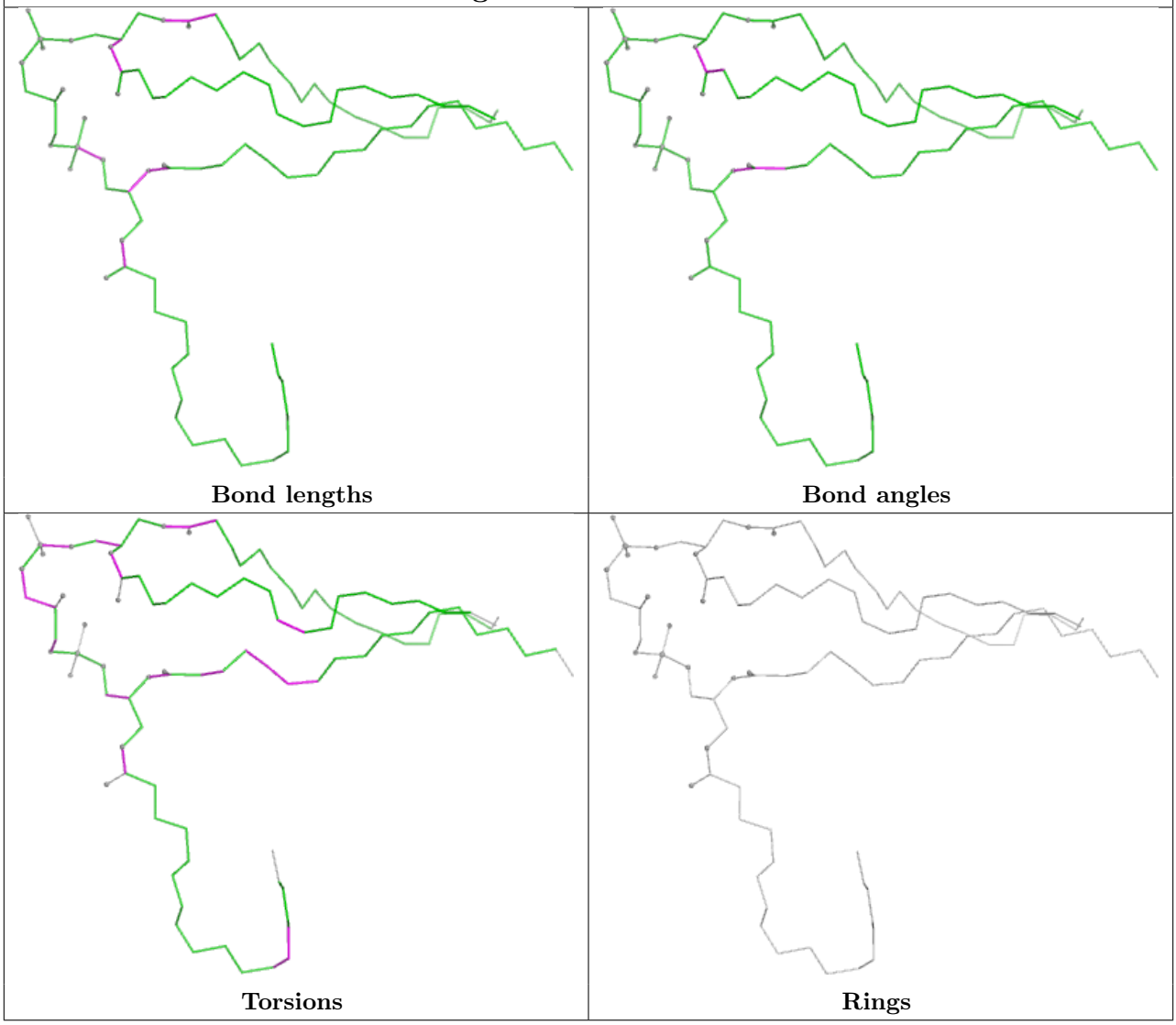
Ligand PC1 A9 601



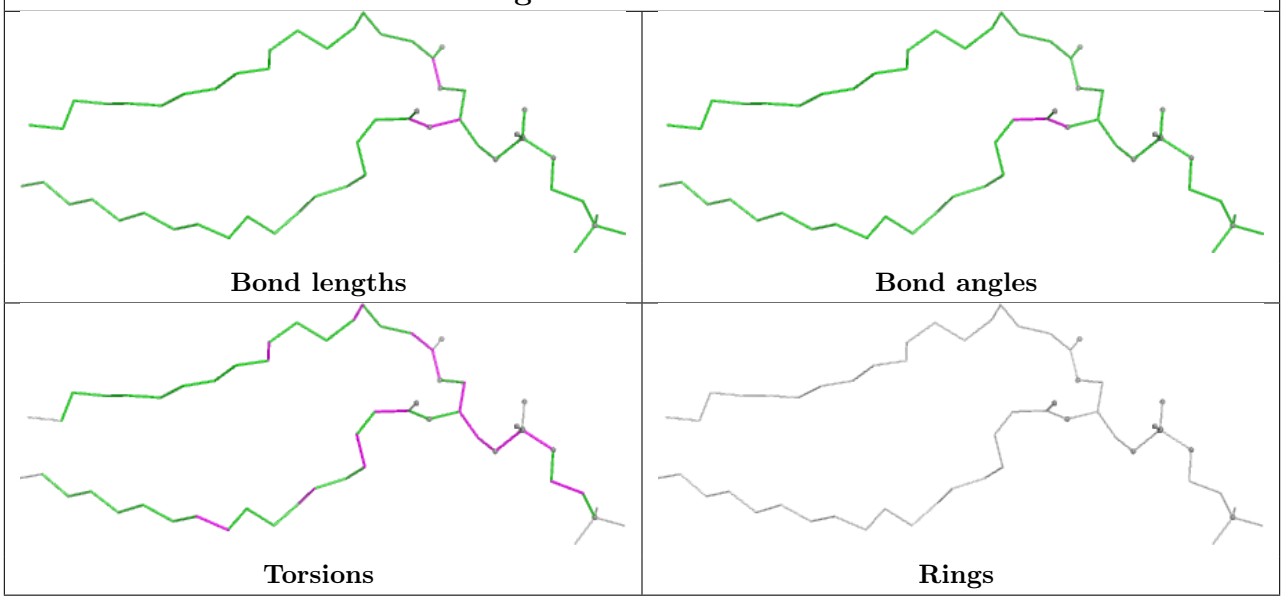
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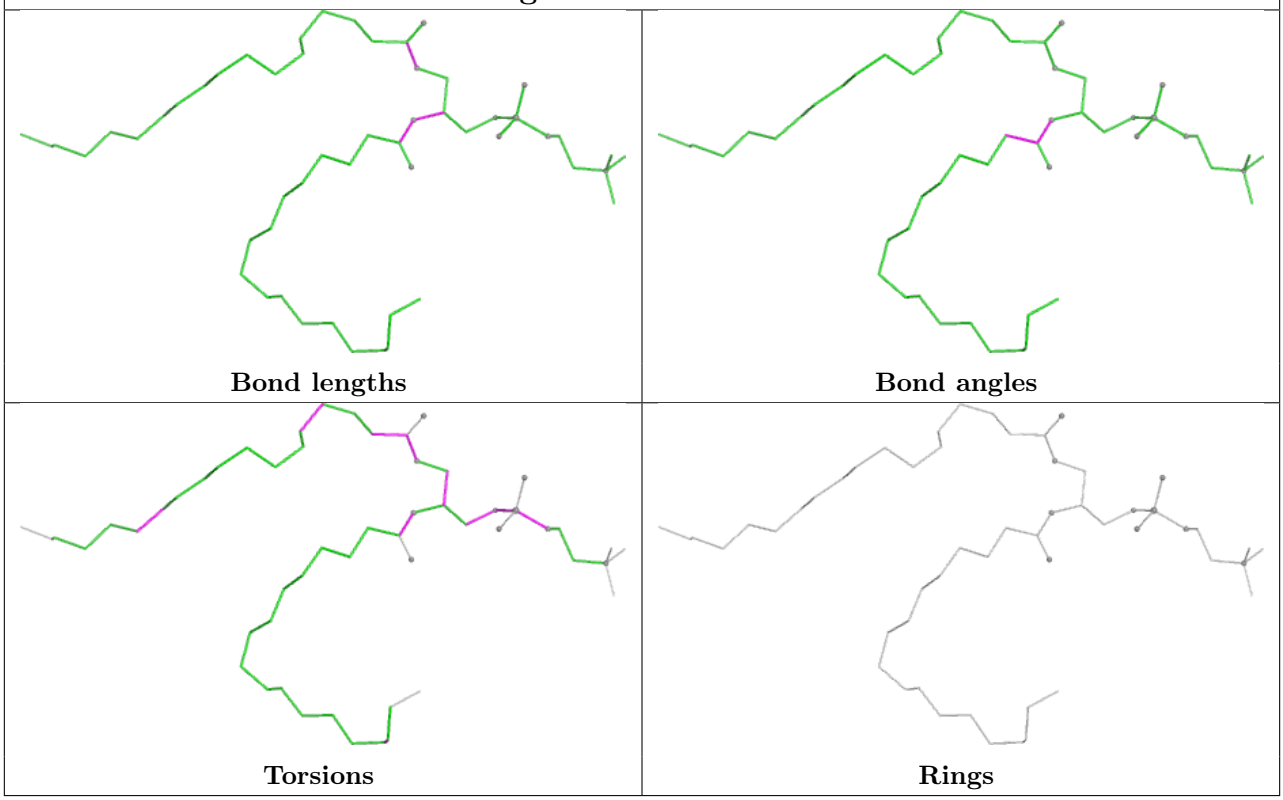
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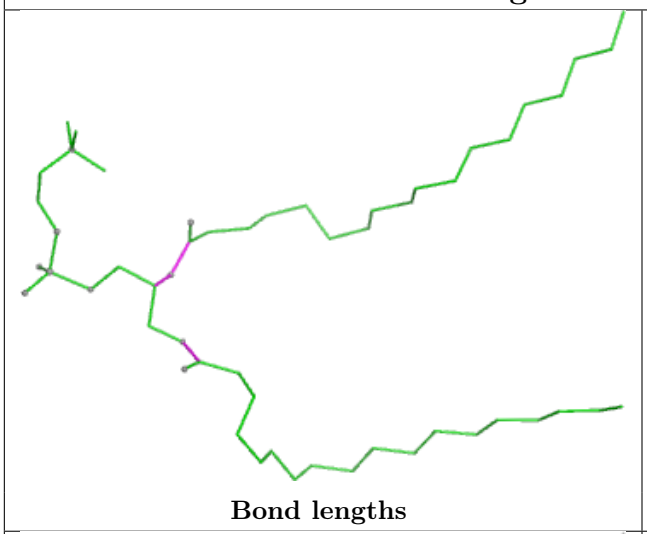
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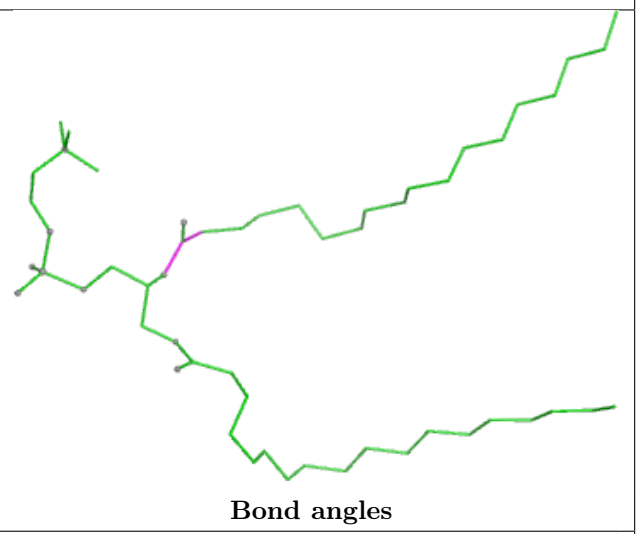
Bond lengths | **Bond angles**

Torsions | **Rings**

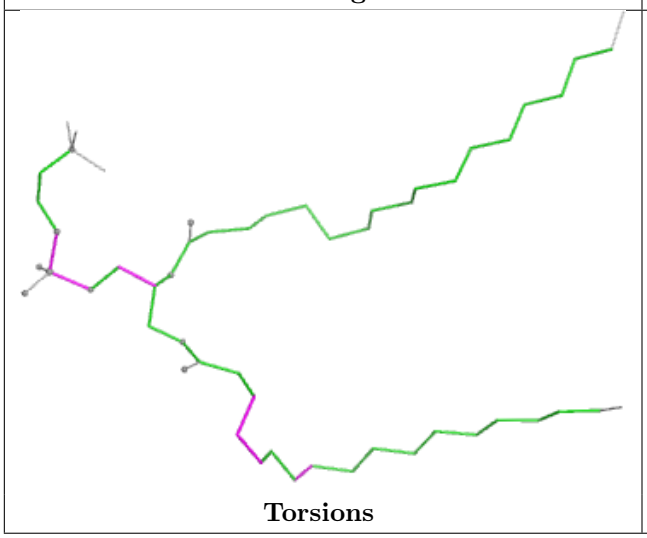
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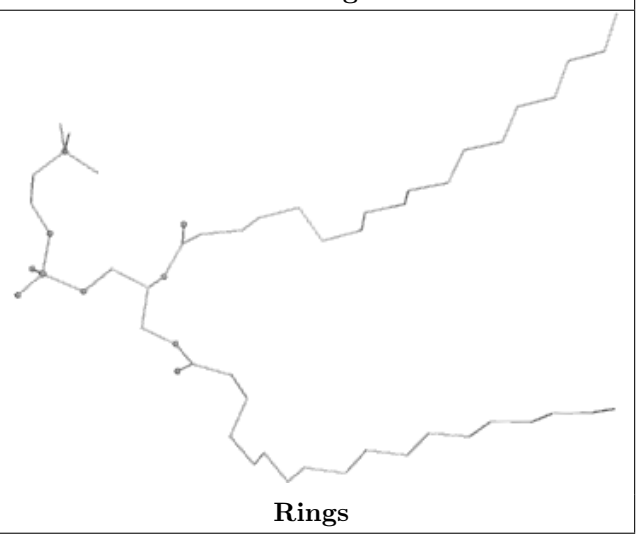
Bond lengths



Bond angles

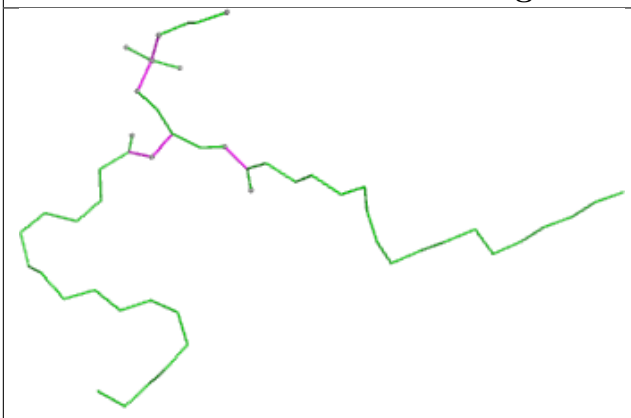


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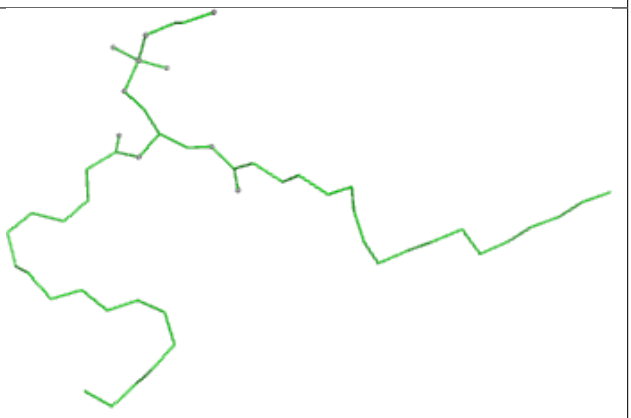


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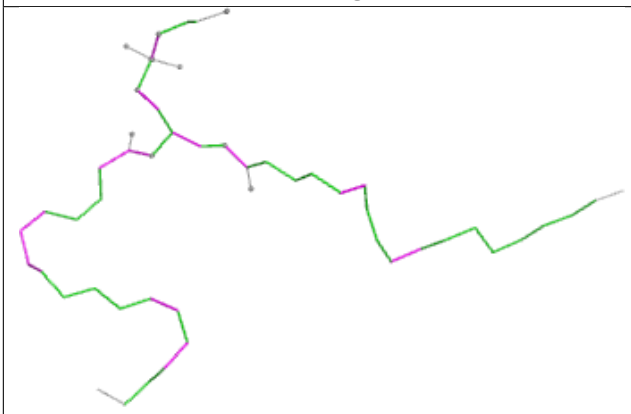
Ligand 3PE BA 301



Bond lengths



Bond angles

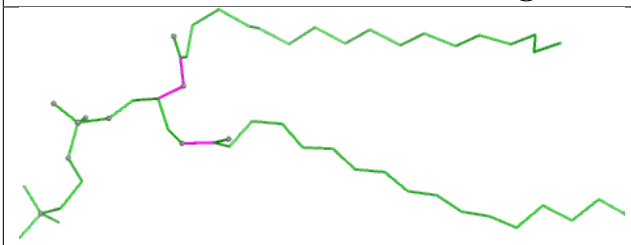


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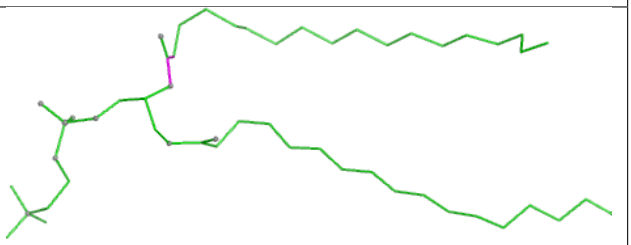


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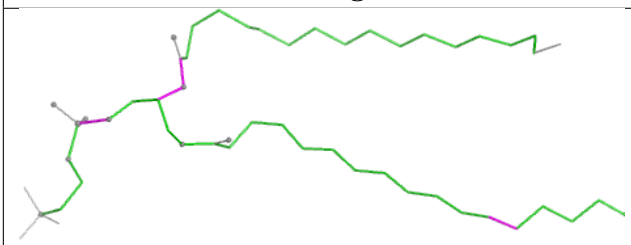
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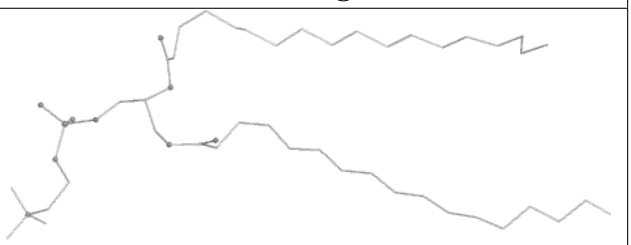
Bond lengths



Bond angles

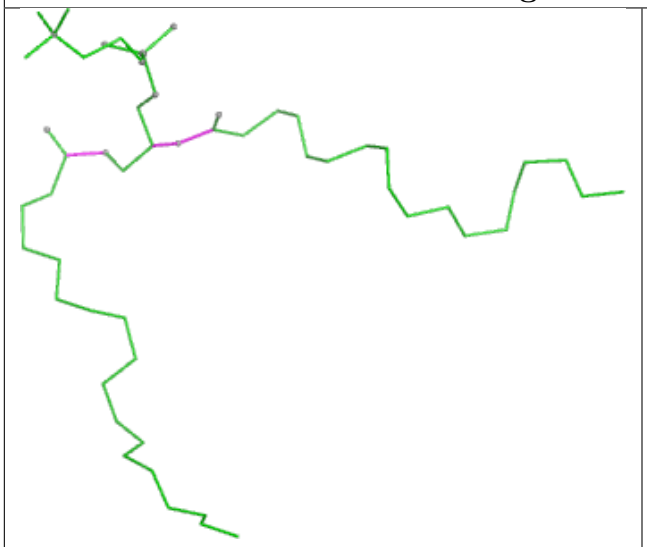


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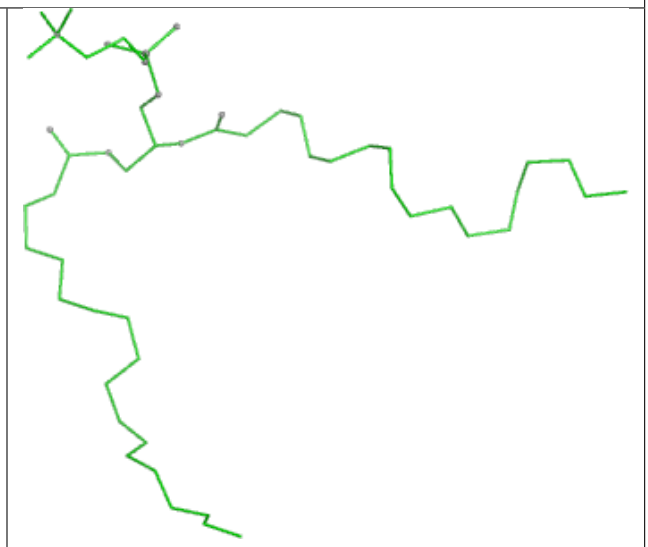


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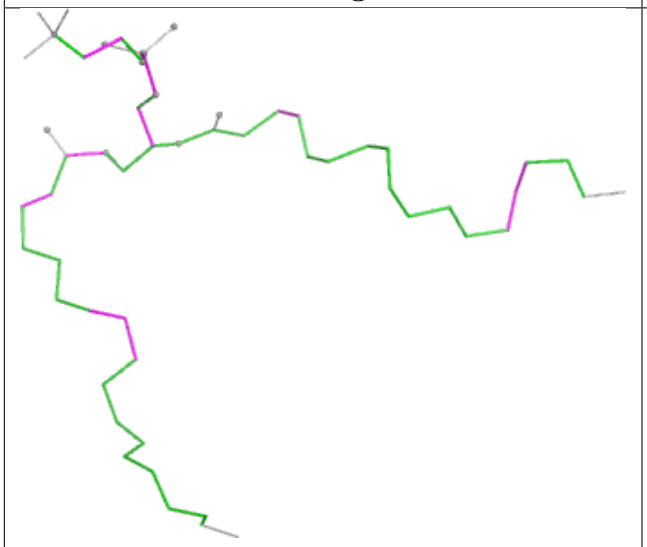
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Bond lengths



Bond angles

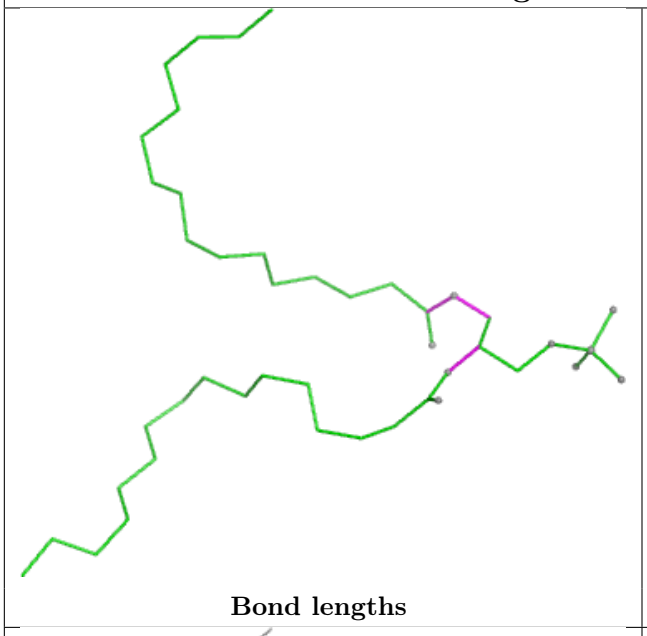


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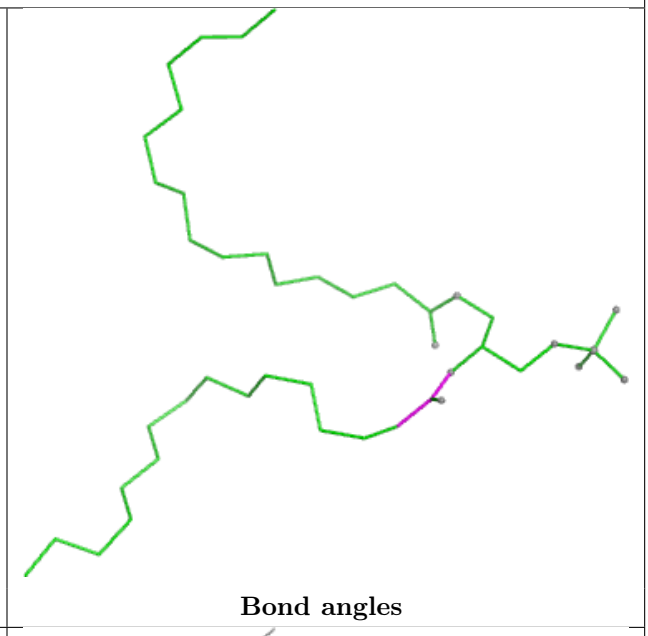


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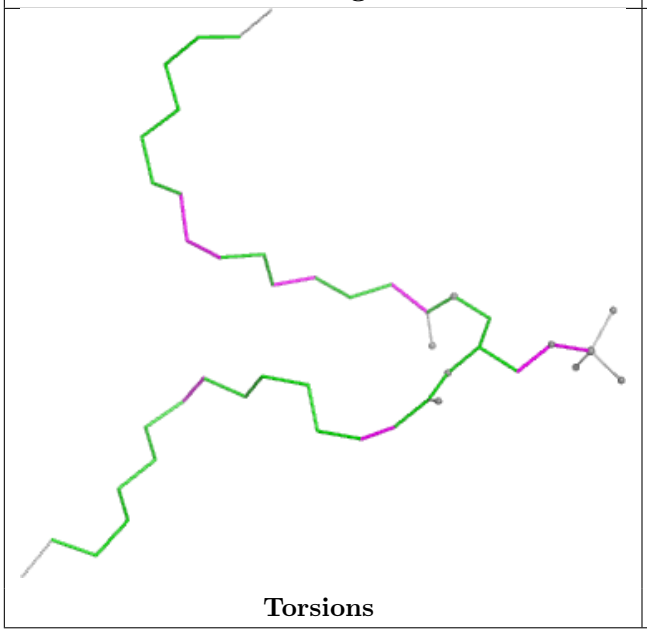
Ligand LPP AA 902



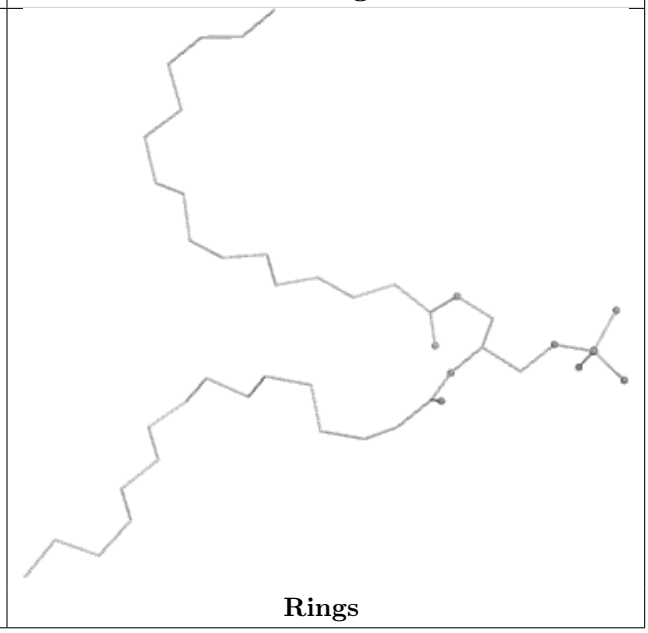
Bond lengths



Bond angles

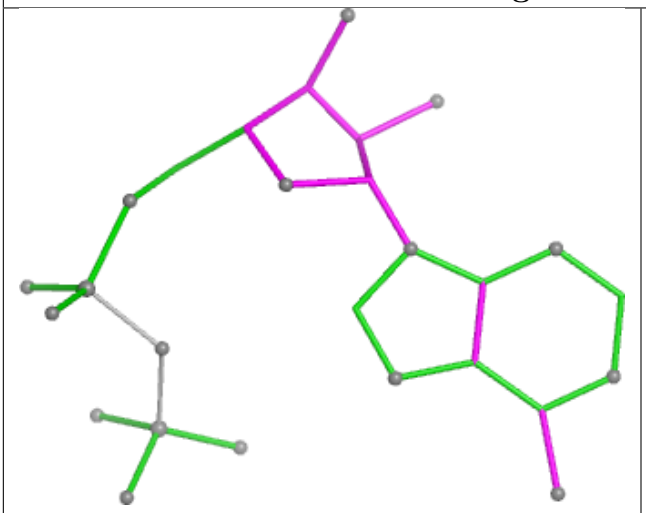


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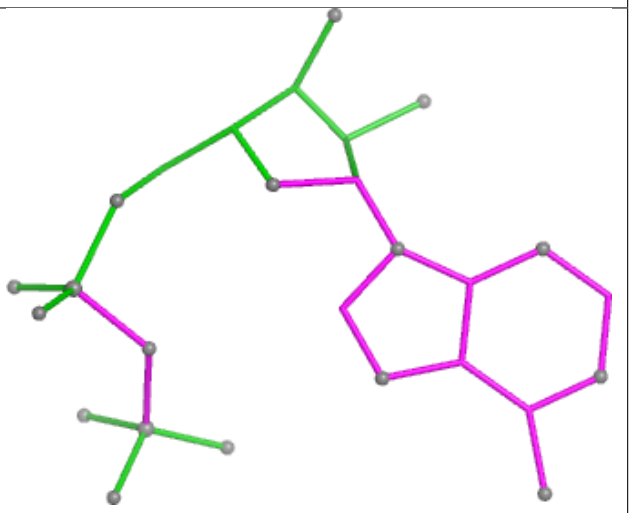


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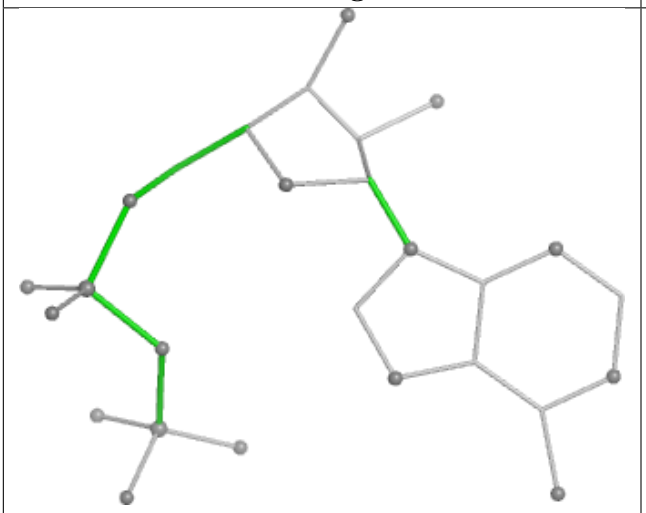
Ligand ADP A8 401



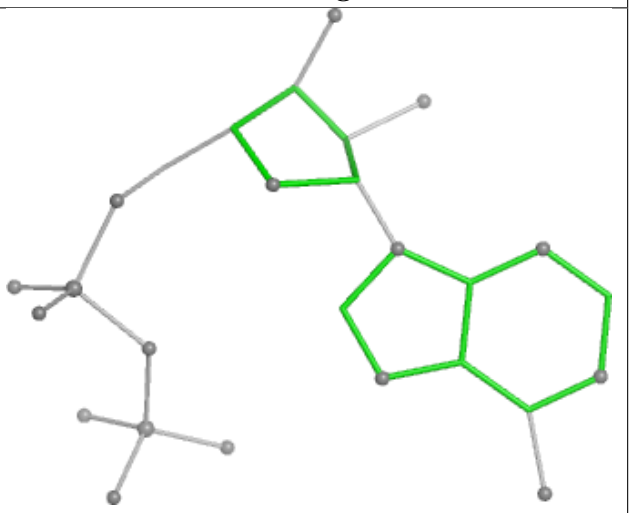
Bond lengths



Bond angles

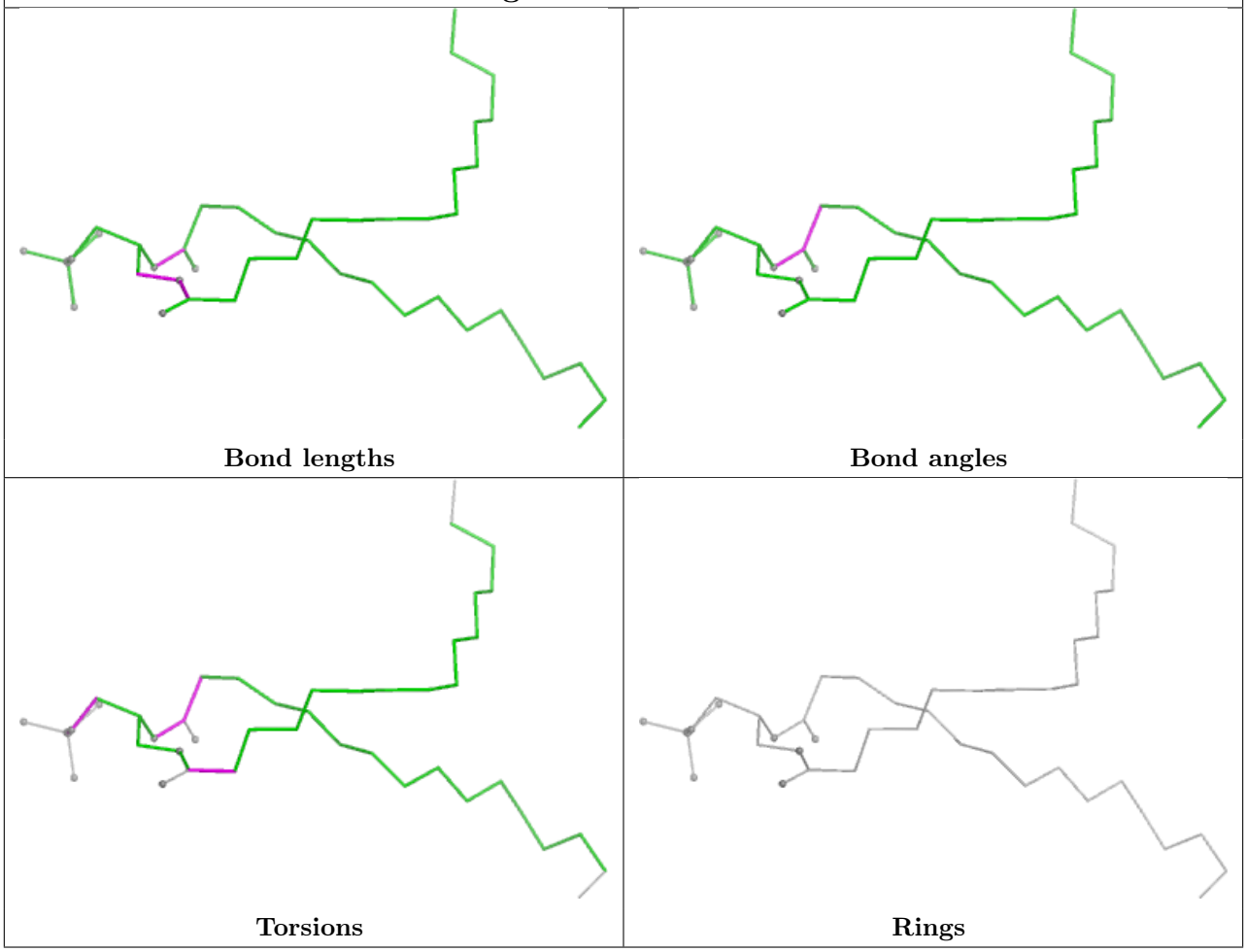


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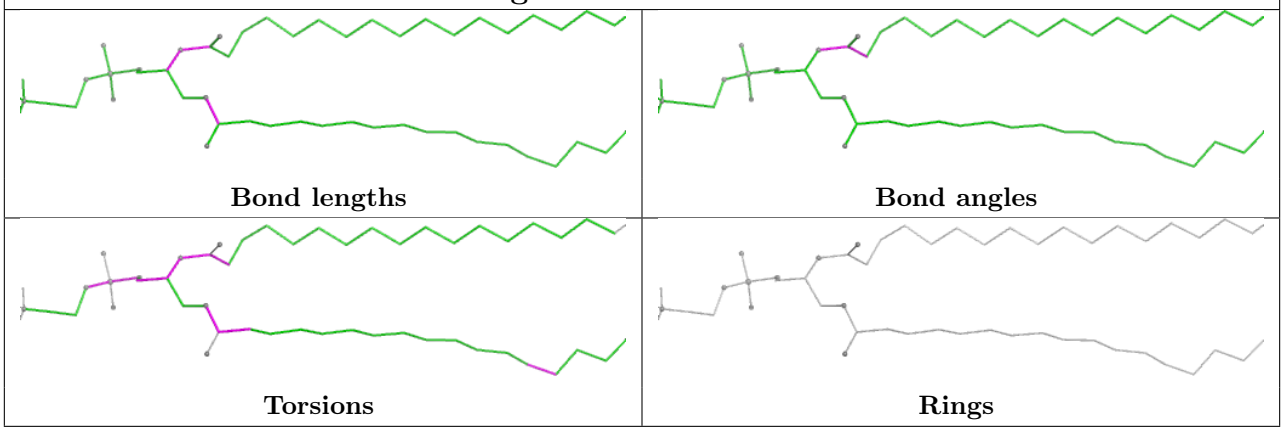


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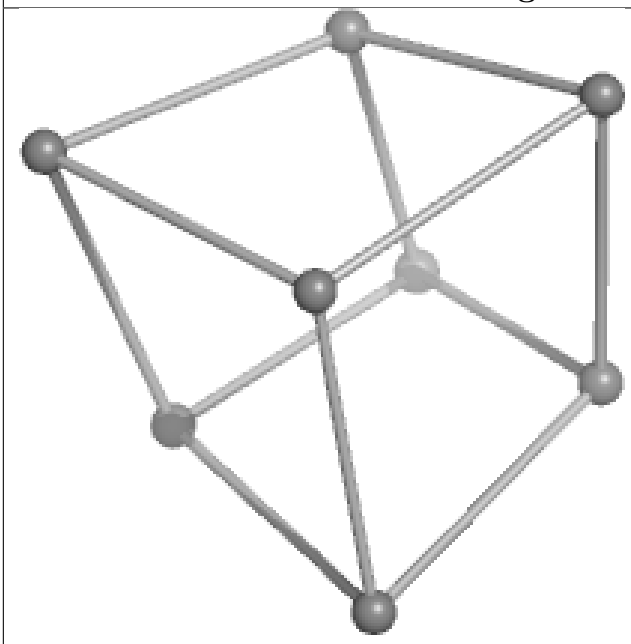
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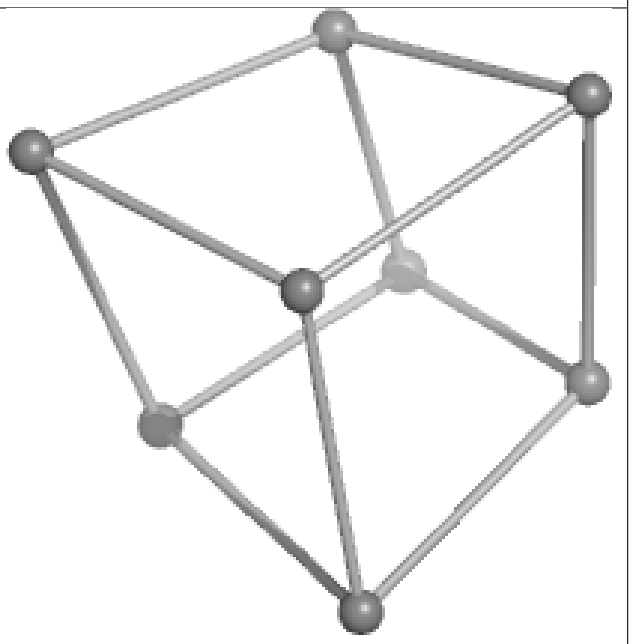
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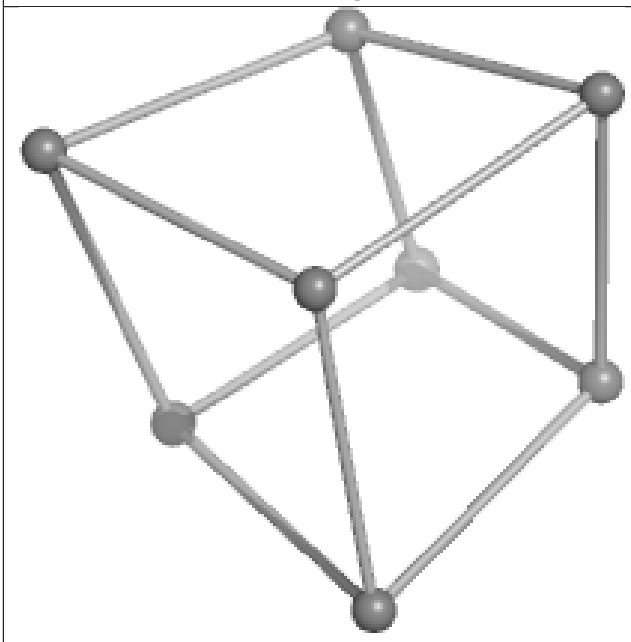
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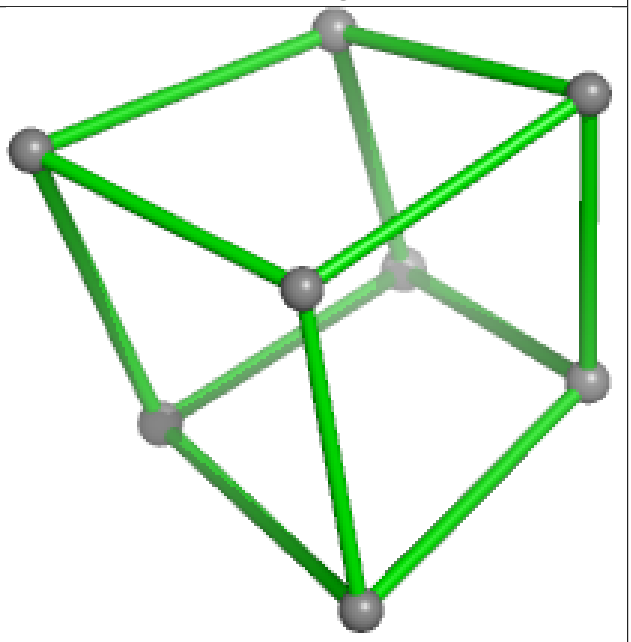
Bond lengths



Bond angles

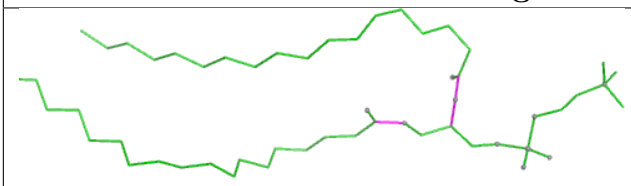


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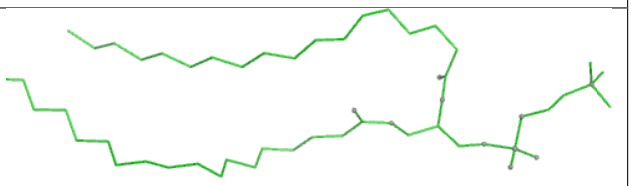


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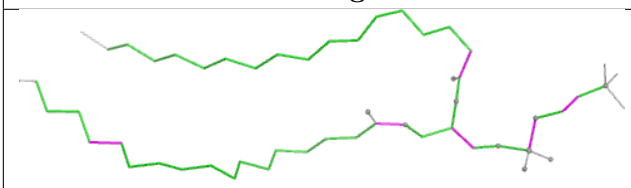
Ligand PC1 AH 301



Bond lengths



Bond angles

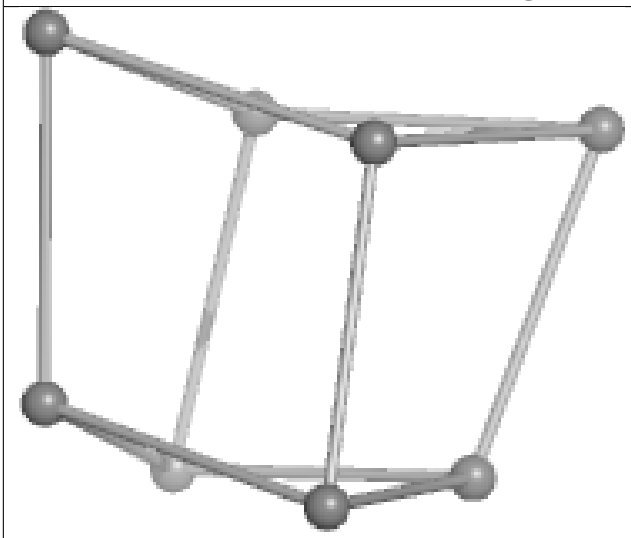


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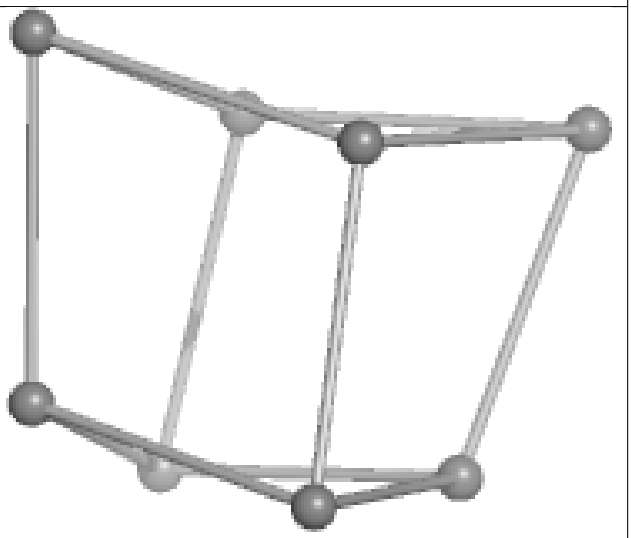


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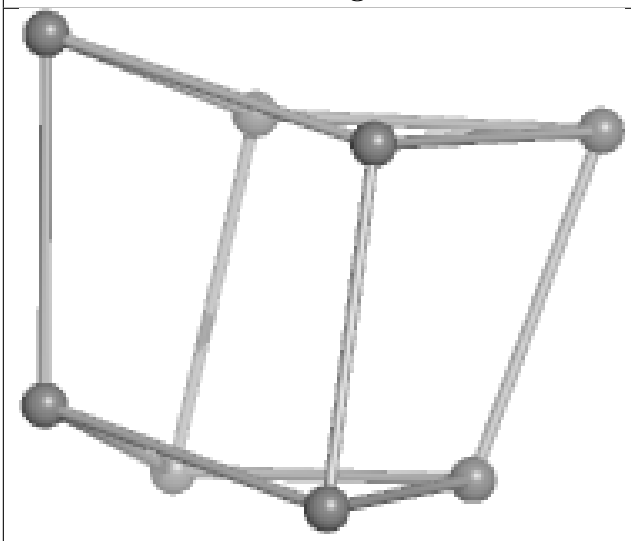
Ligand SF4 AL 301



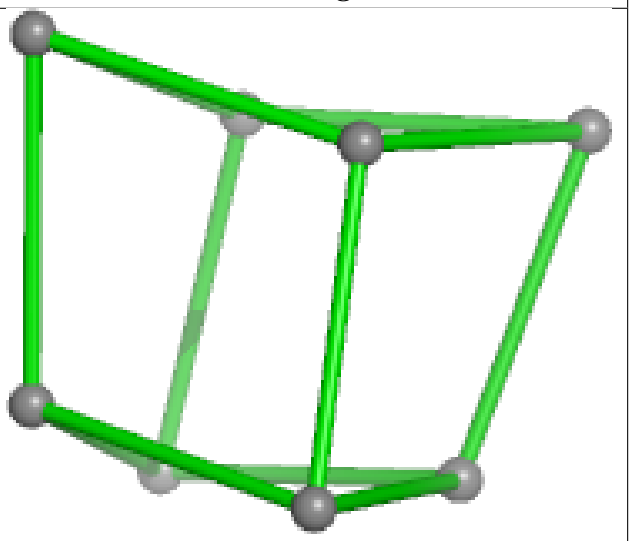
Bond lengths



Bond angles

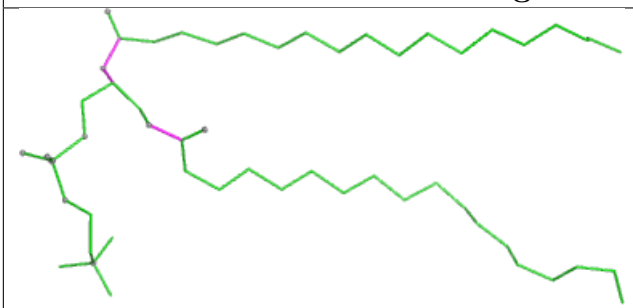


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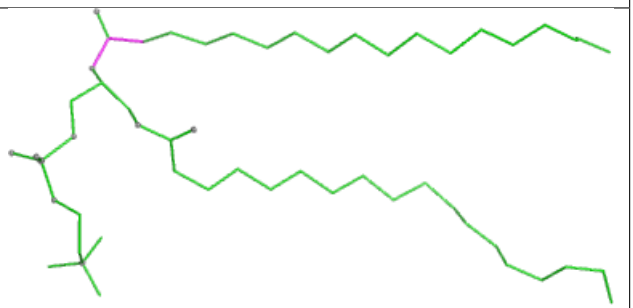


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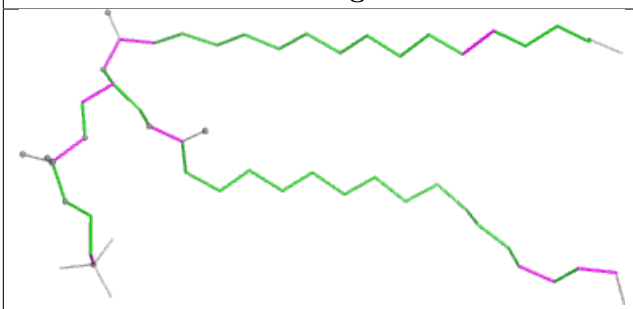
Ligand PC1 AA 904



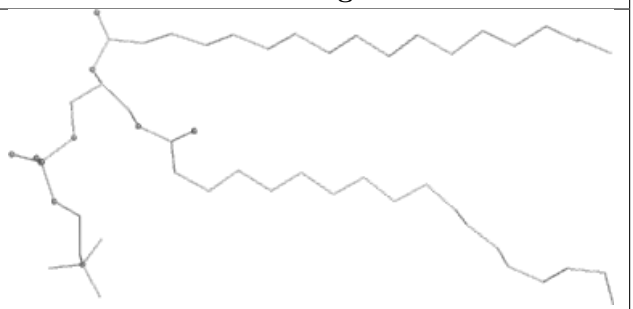
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Bond angles

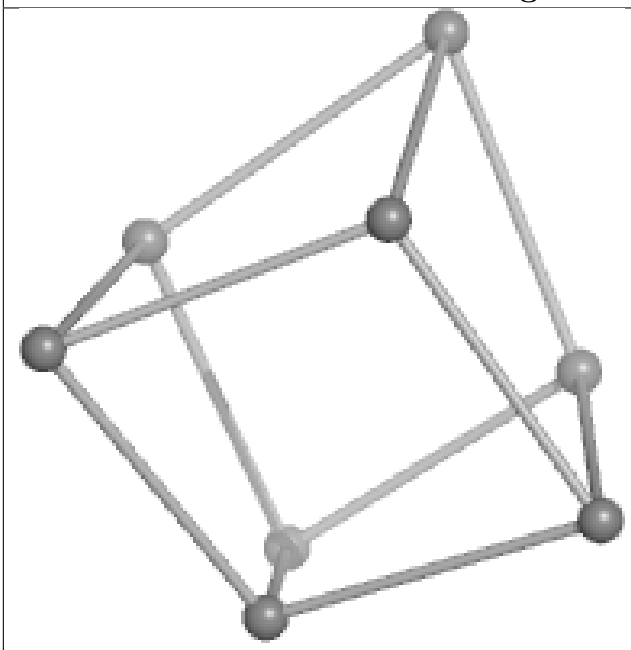


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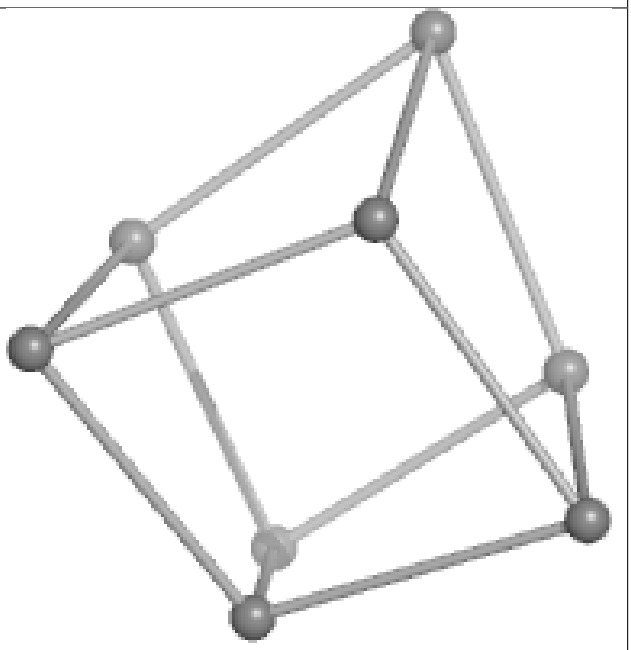


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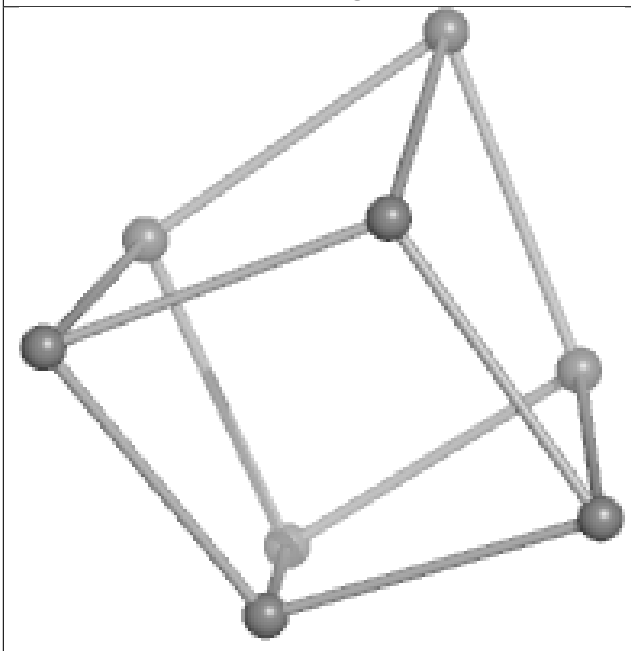
Ligand SF4 AL 302



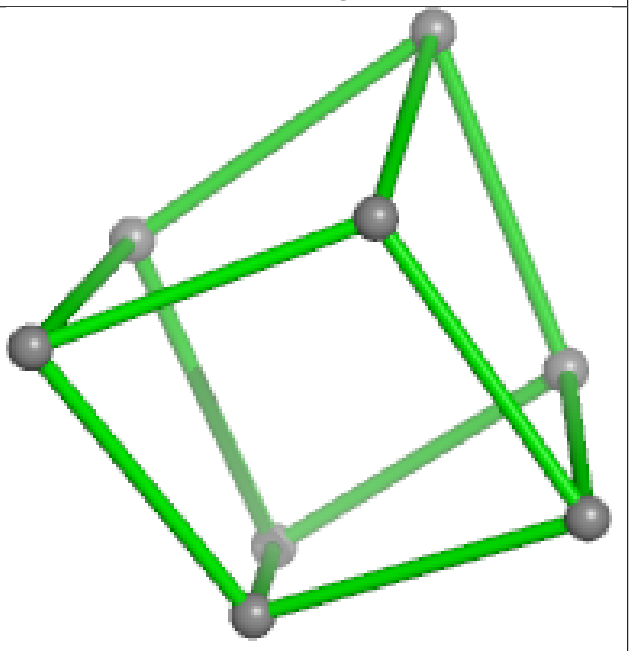
Bond lengths



Bond angles

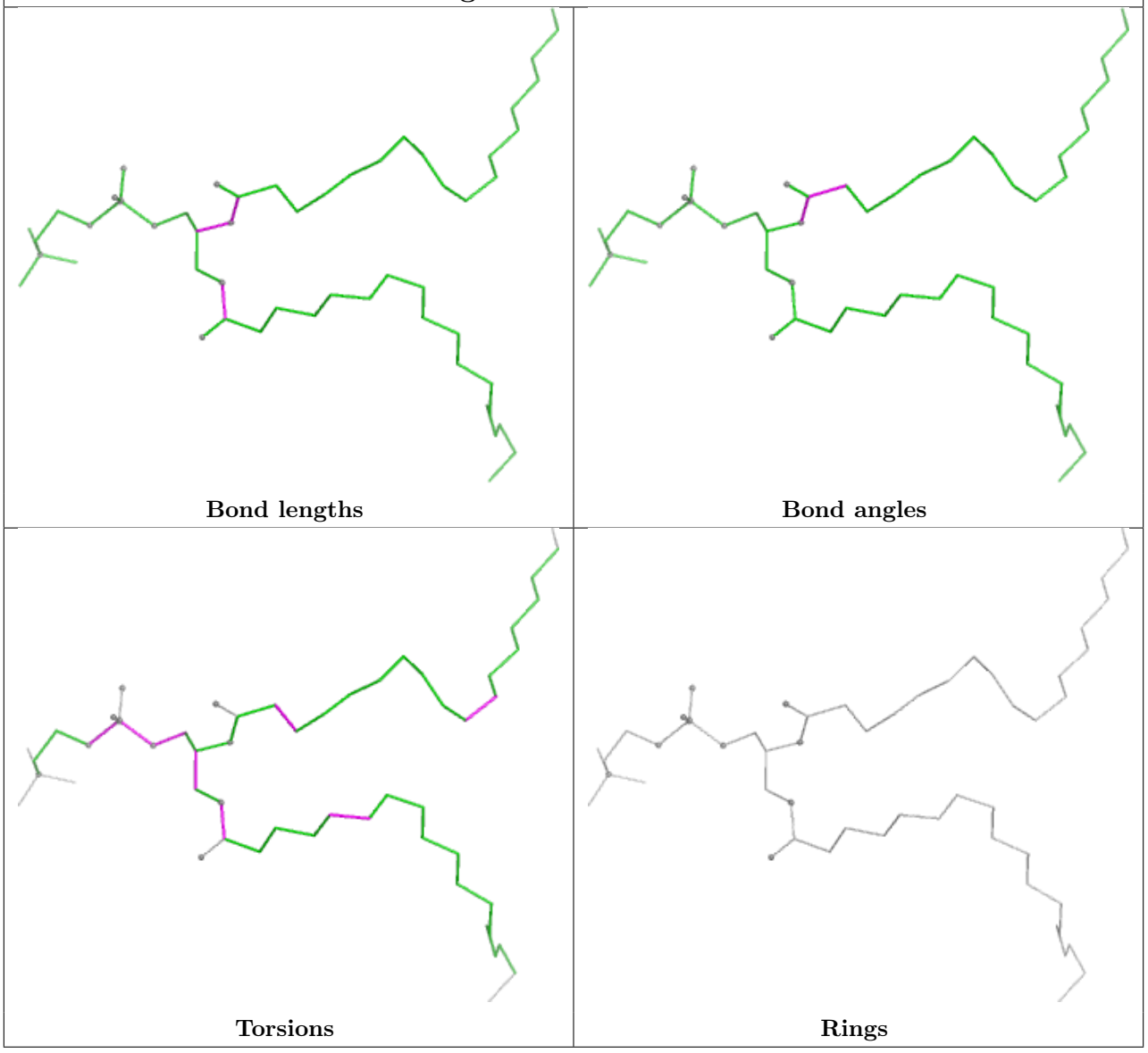


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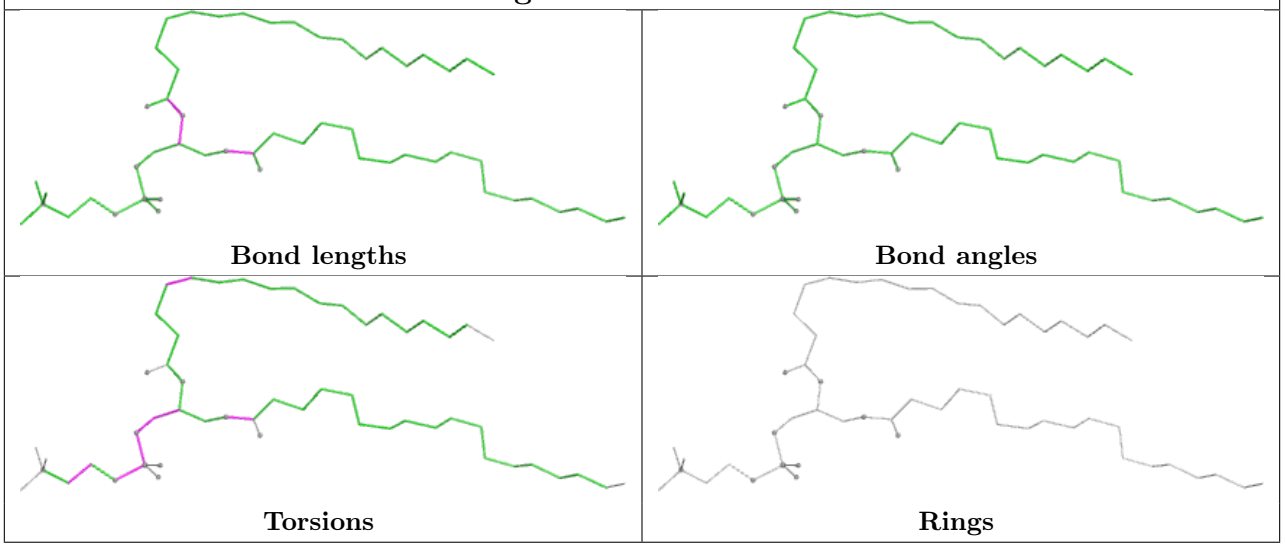


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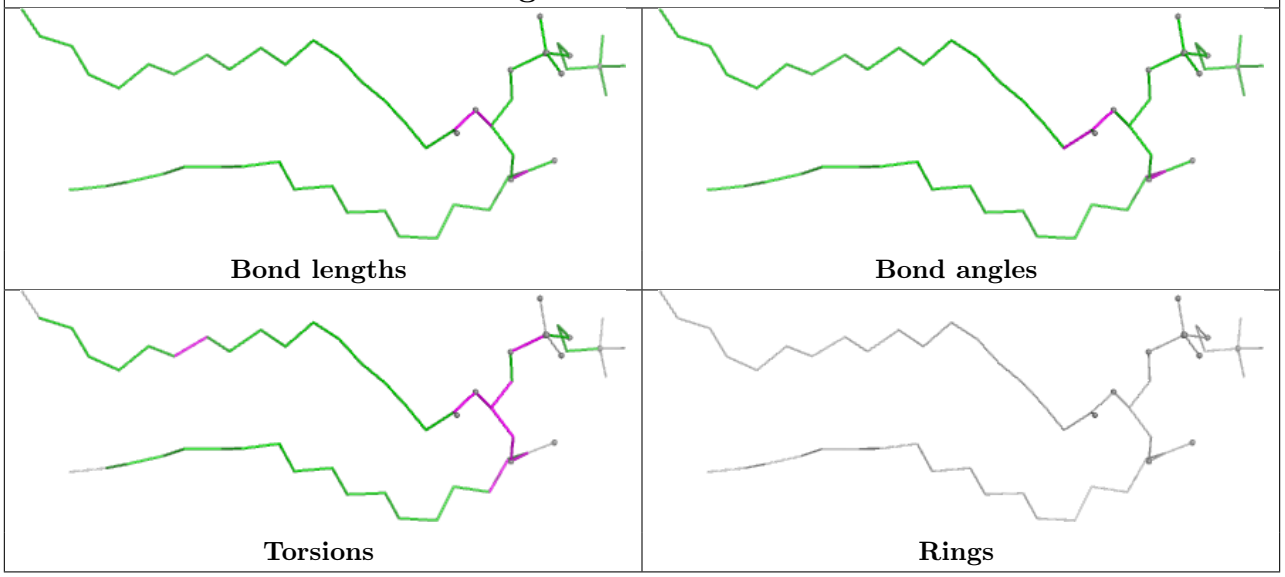
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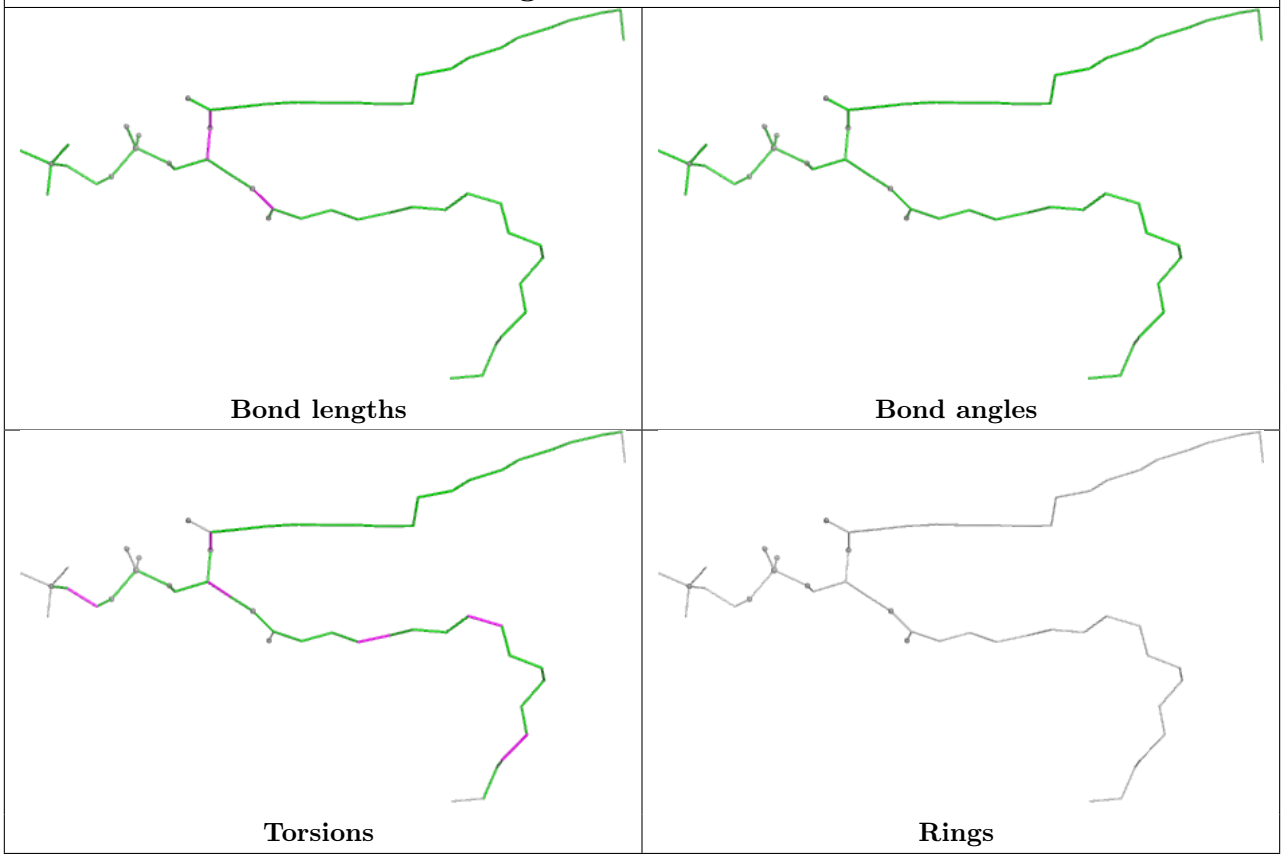
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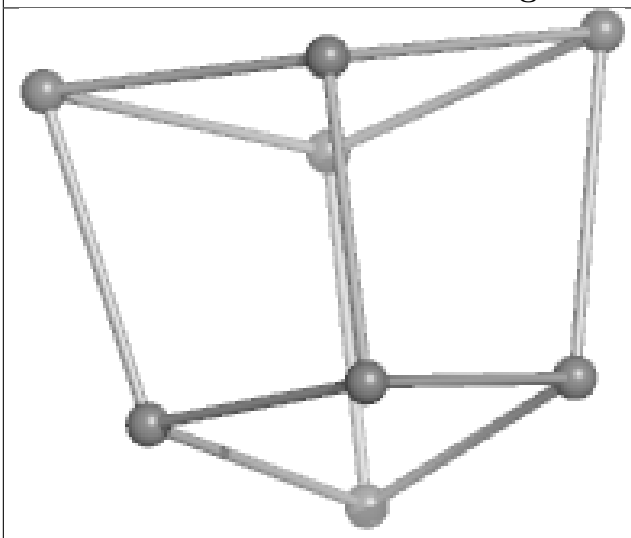
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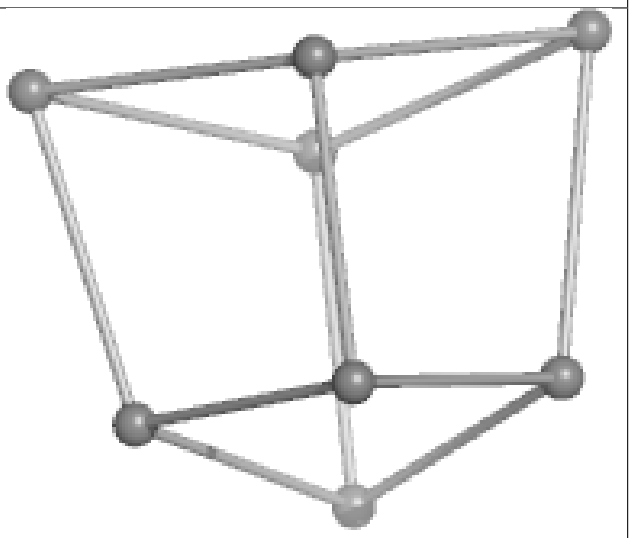
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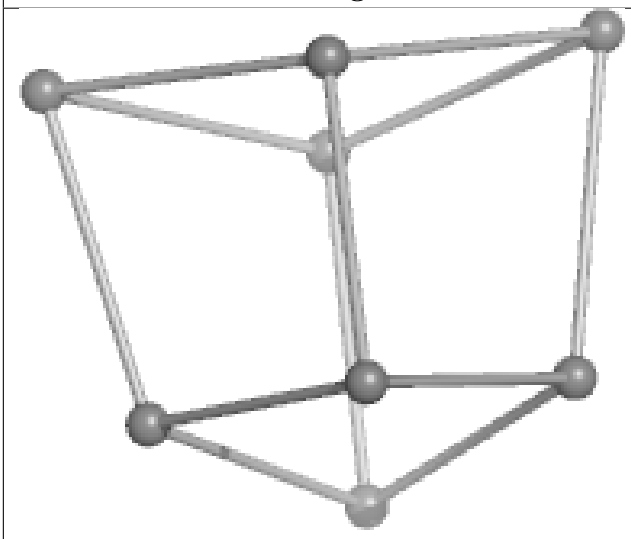
Ligand SF4 AT 201



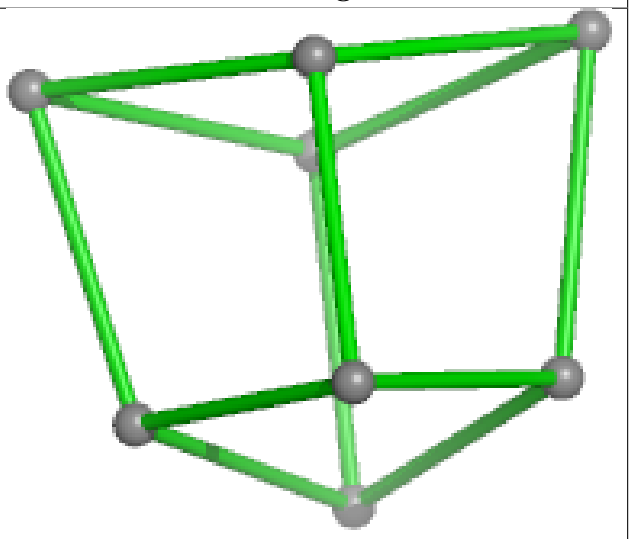
Bond lengths



Bond angles

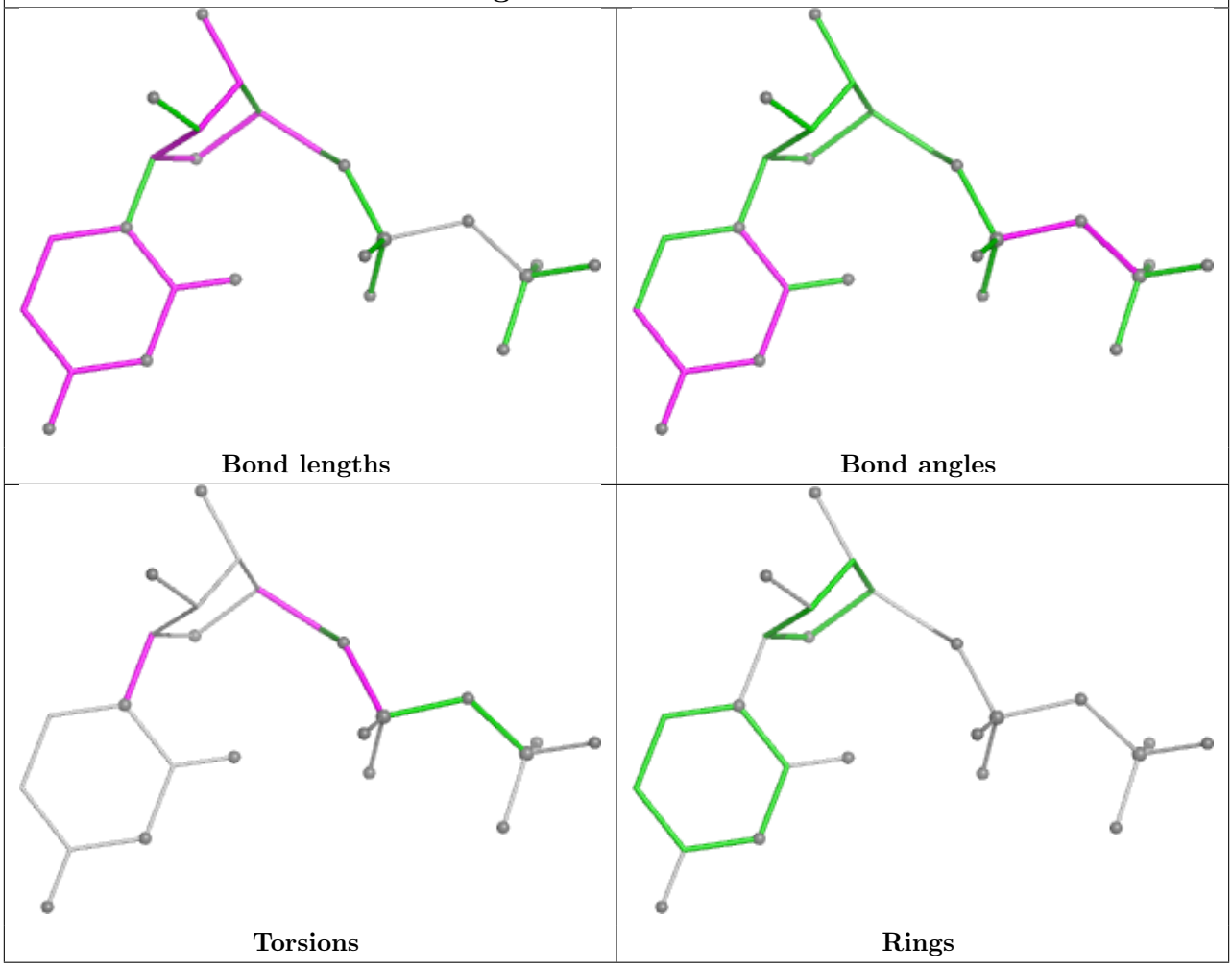


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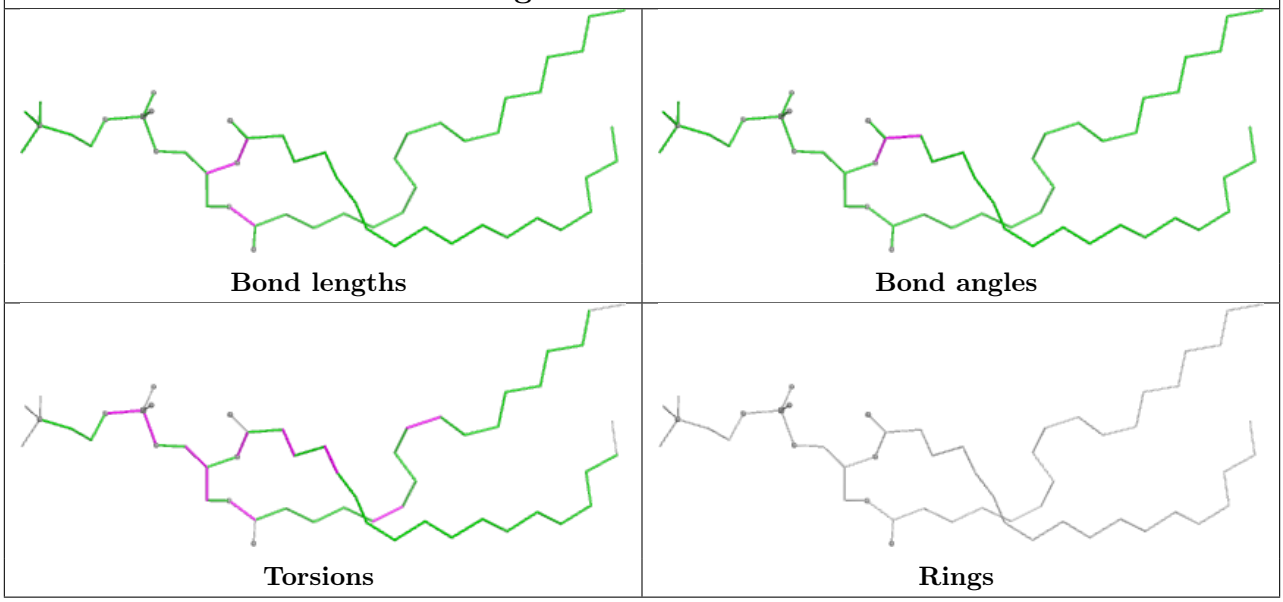


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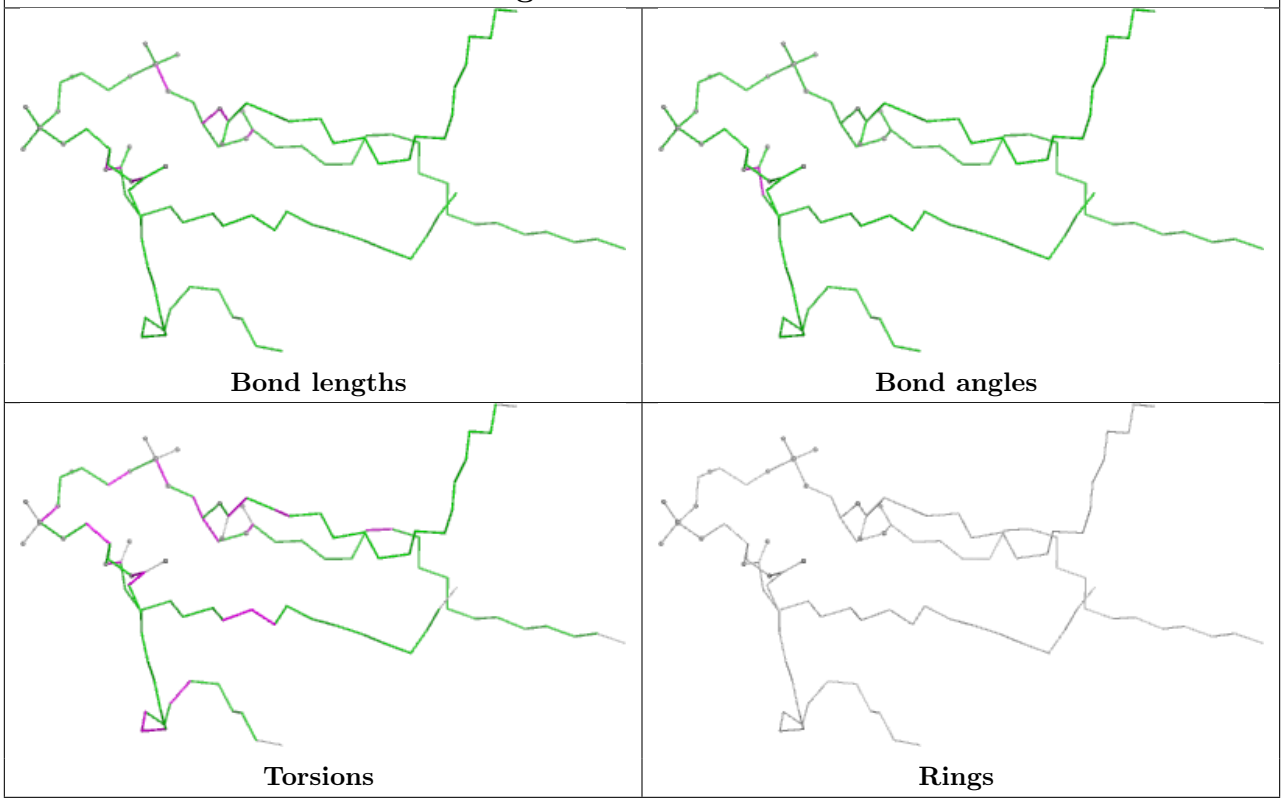
Ligand UDP A0 603



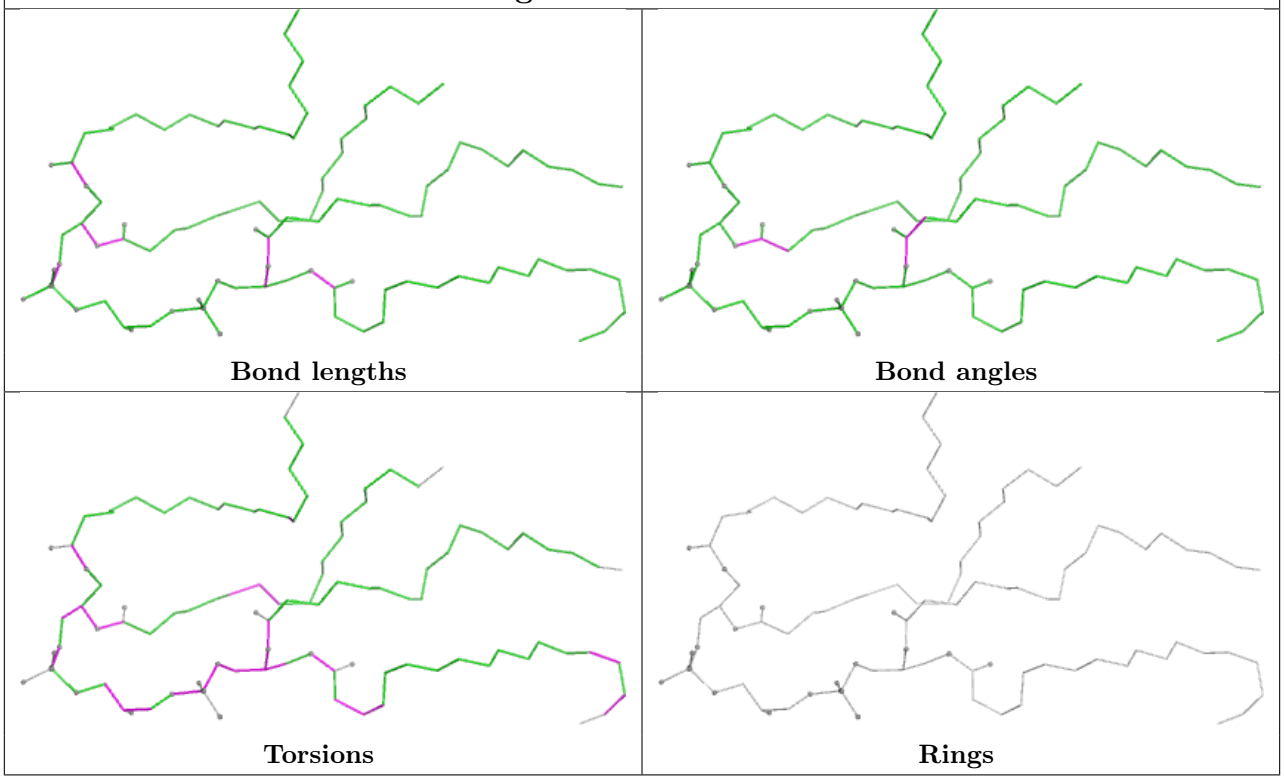
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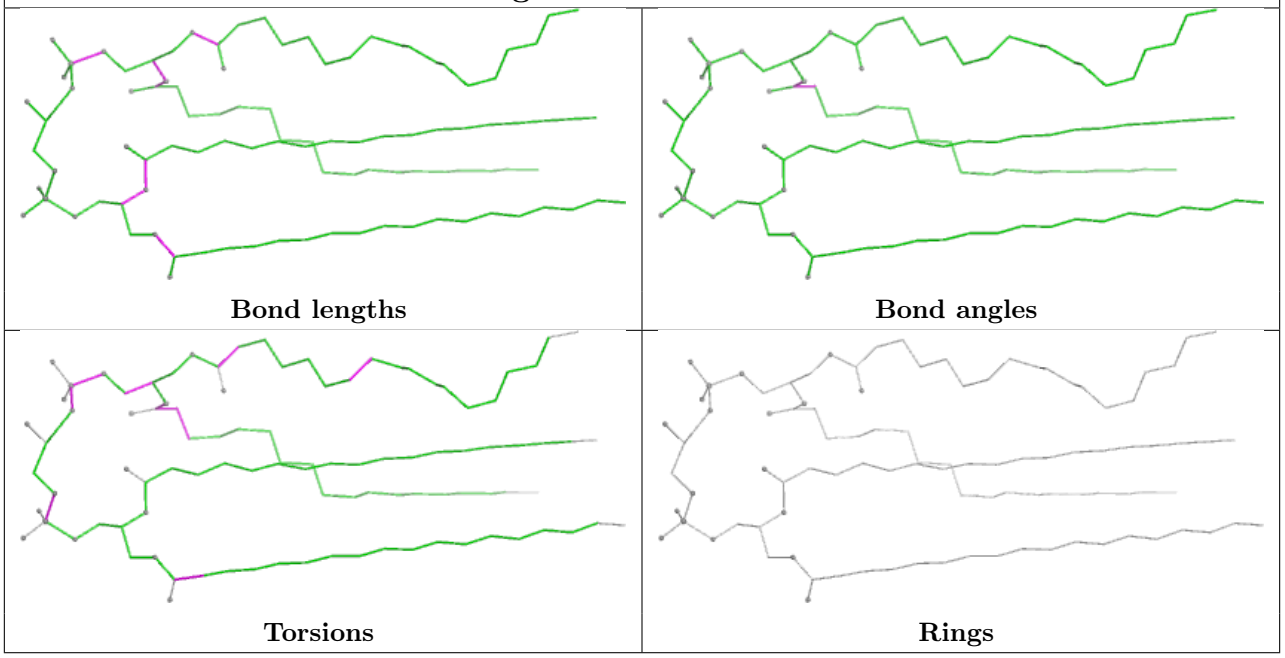
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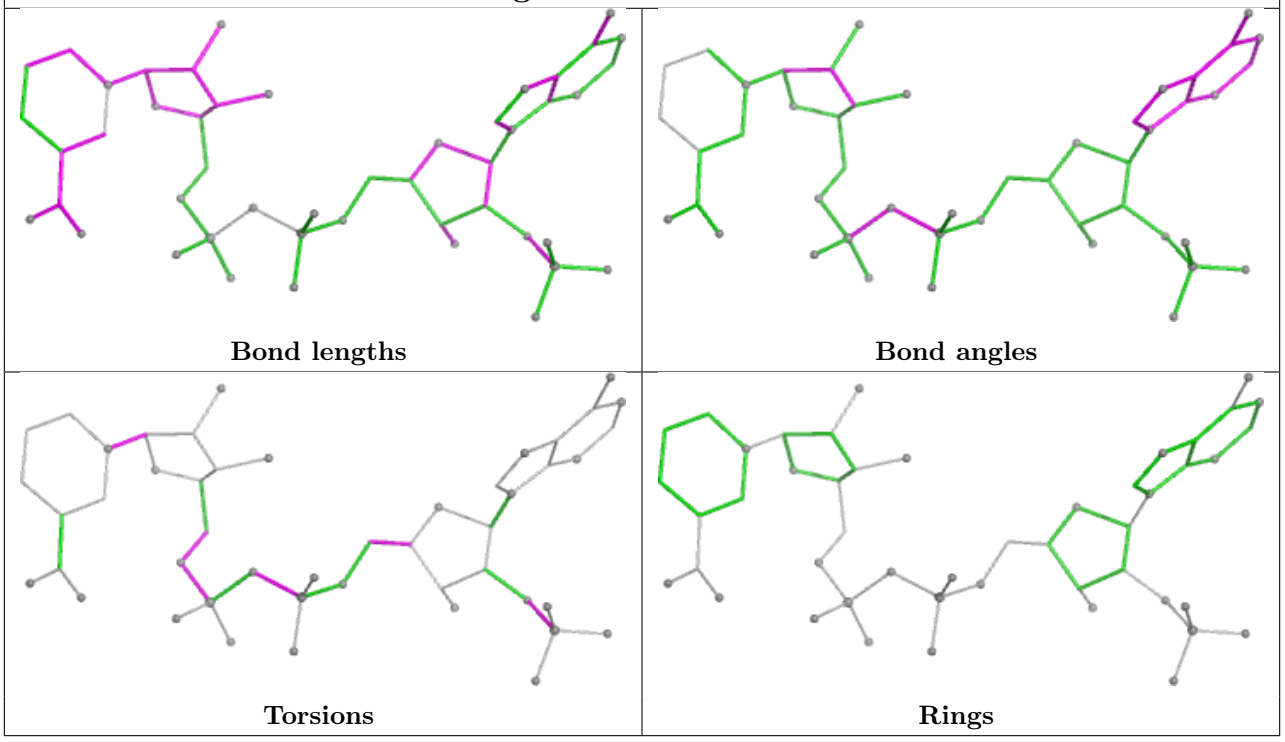
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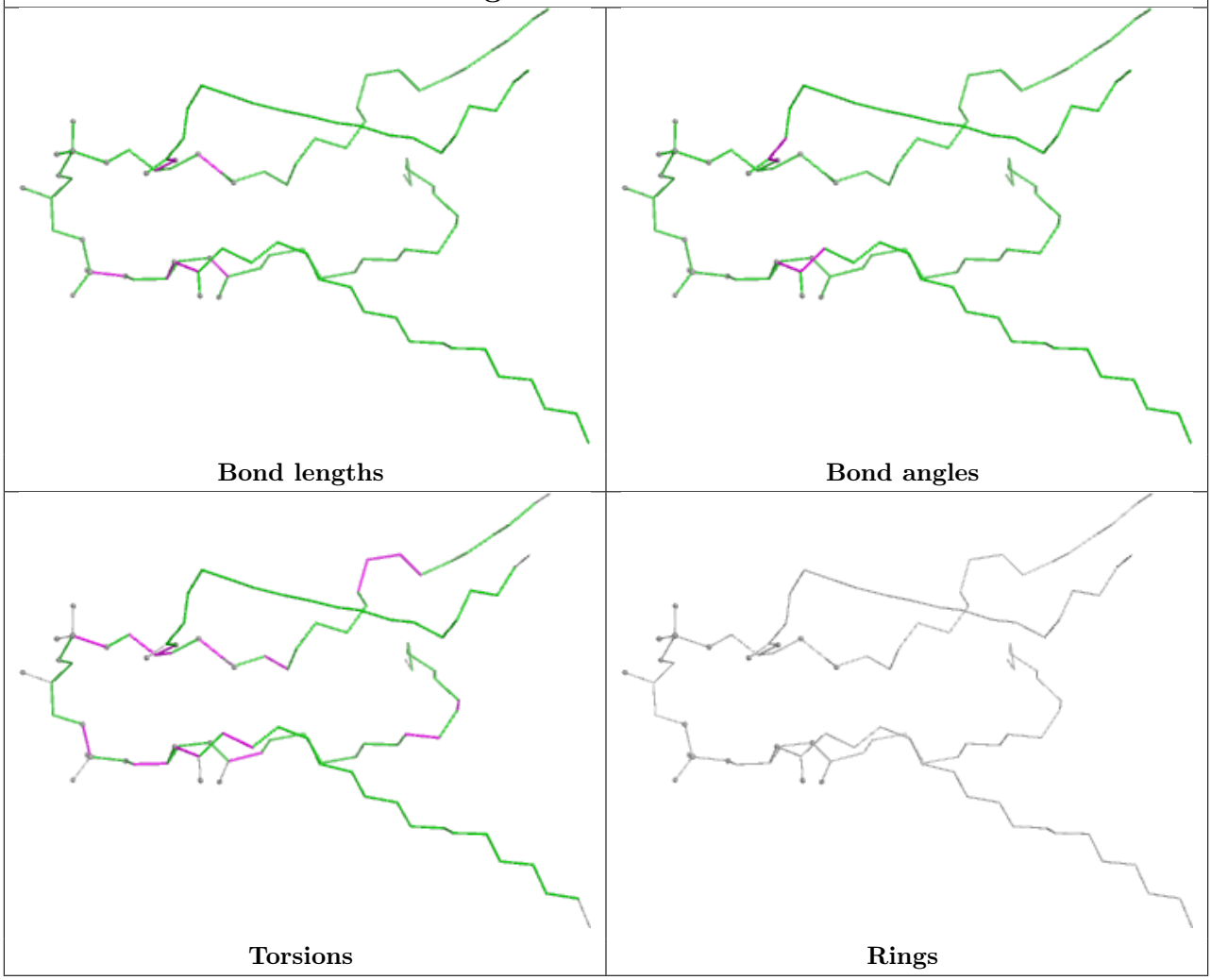
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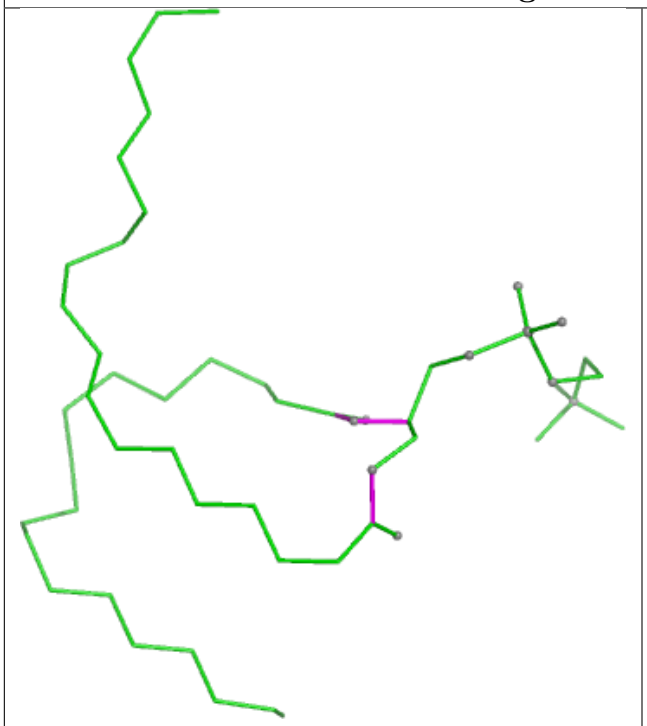
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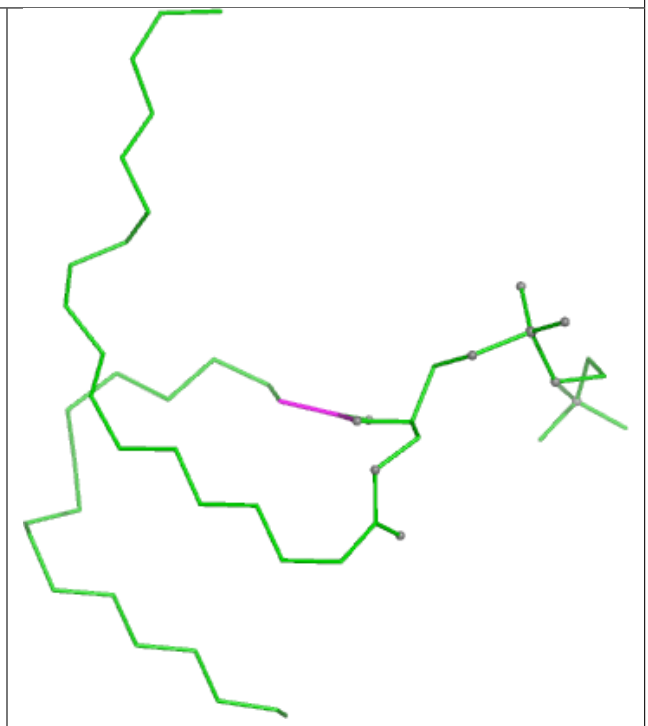
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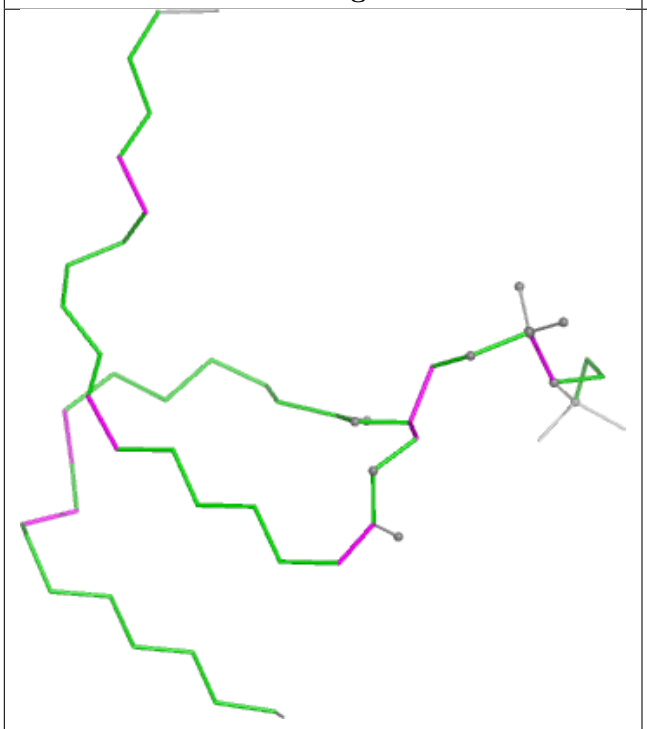
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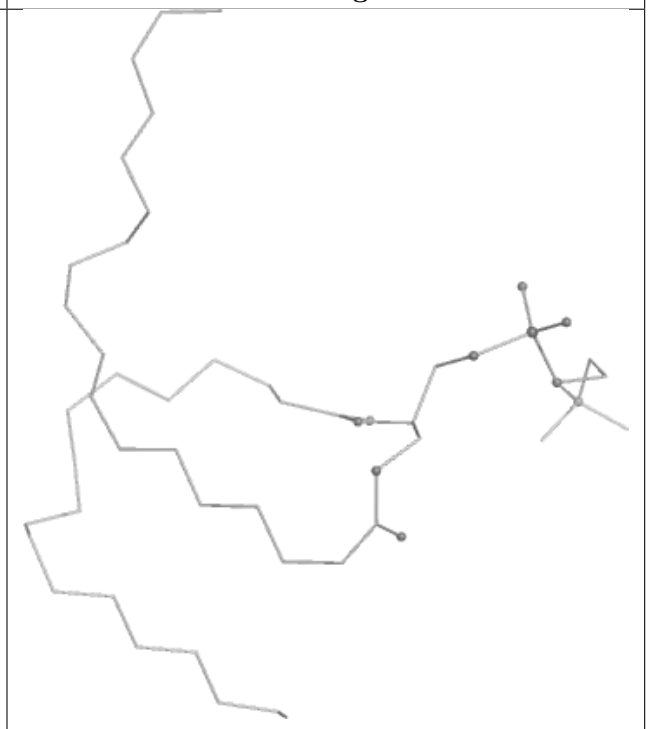
Bond lengths



Bond angles



Torsions



Rings

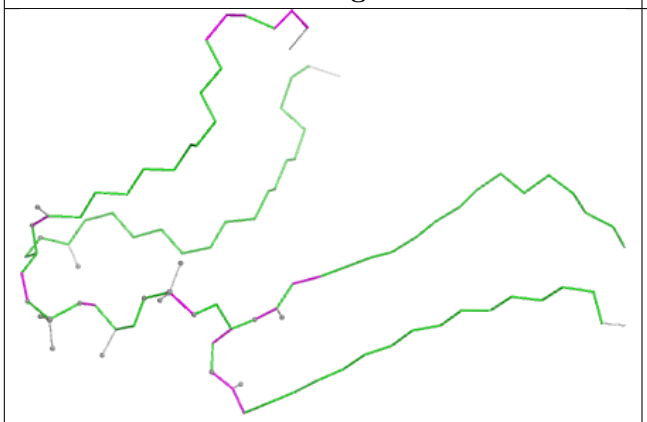
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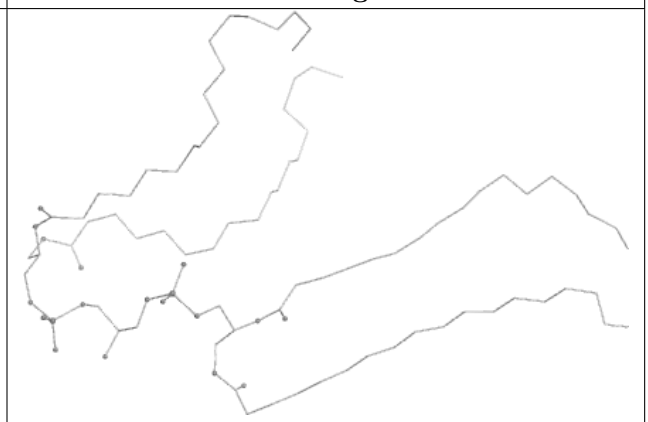
Bond lengths



Bond angles

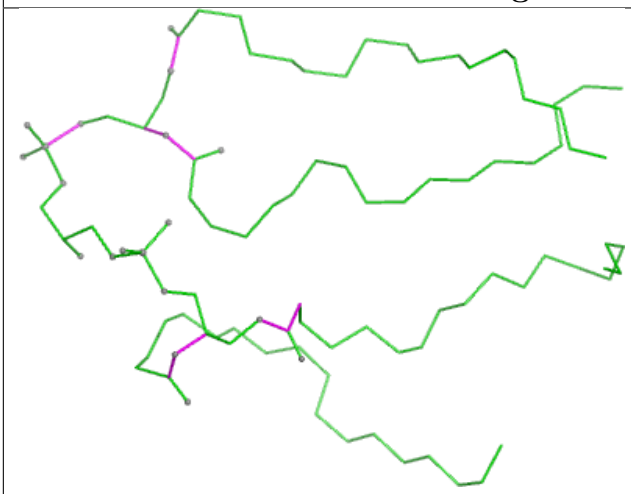


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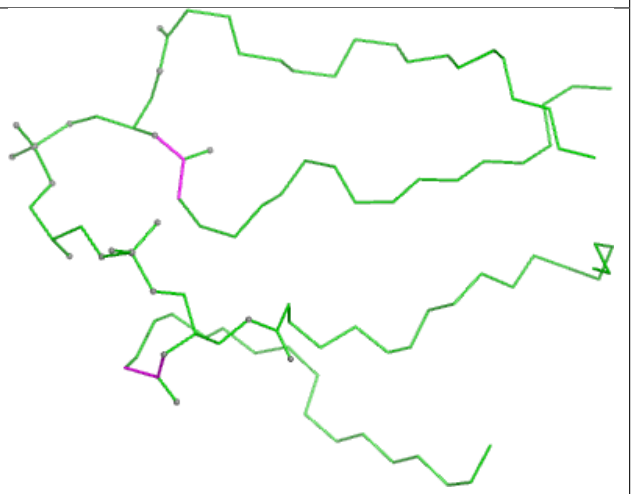


Rings

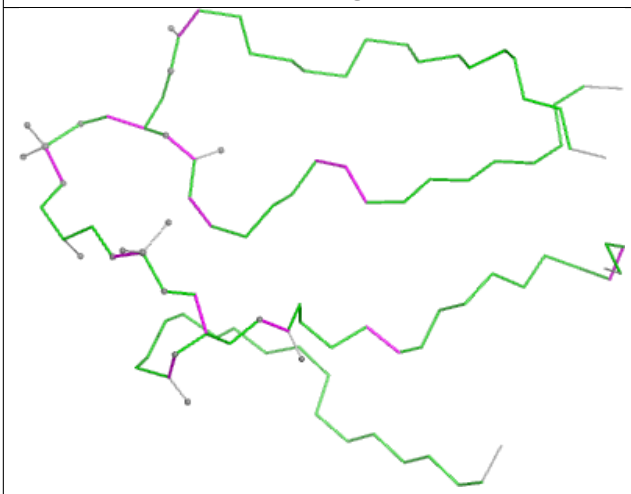
Ligand CDL BT 201



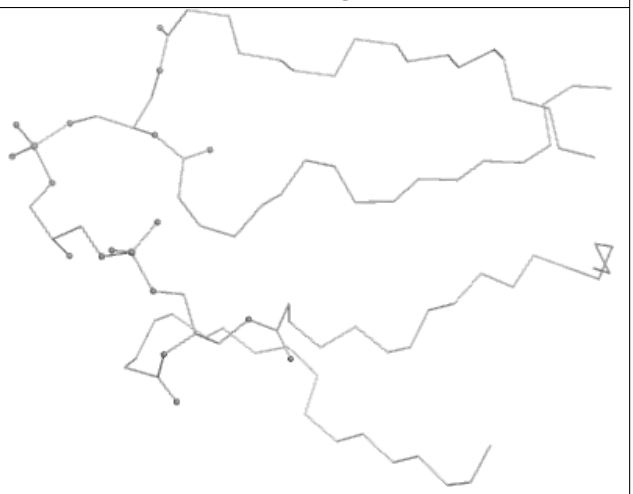
Bond lengths



Bond angles

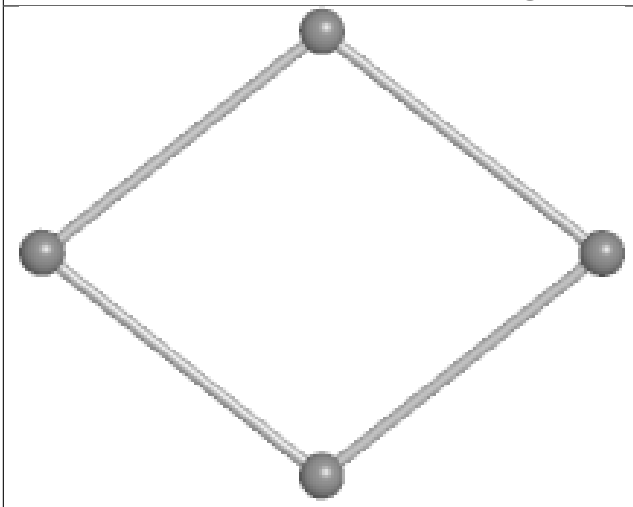


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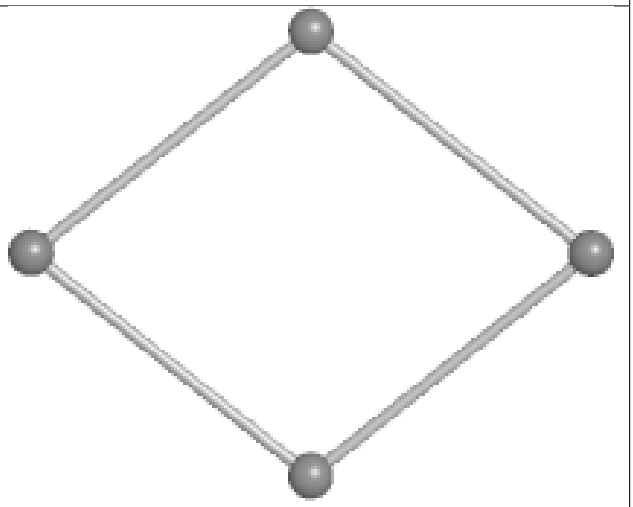


Rings

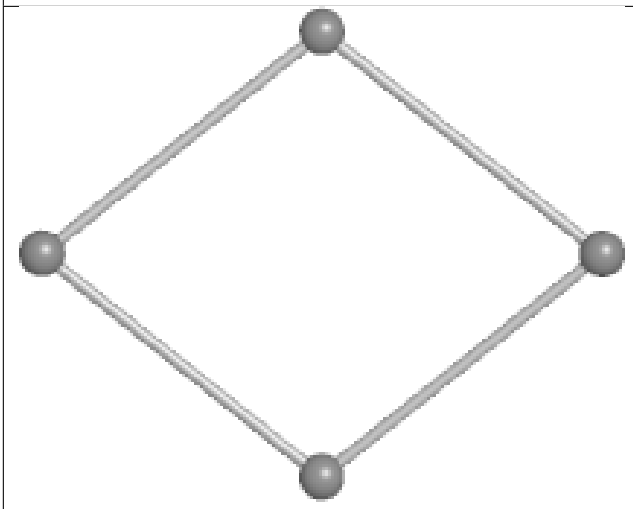
Ligand FES AI 301



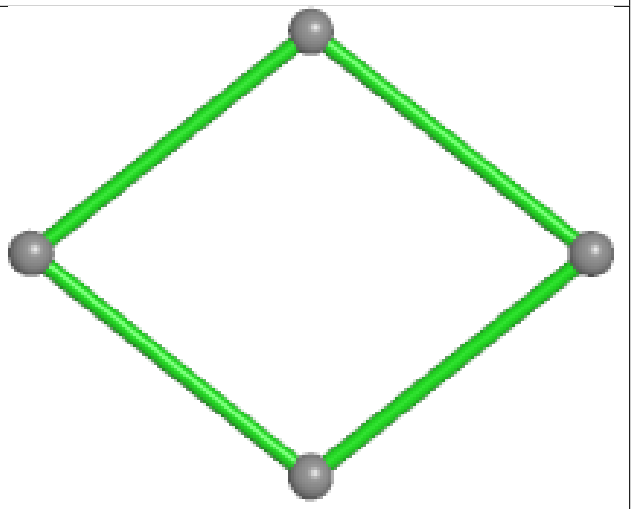
Bond lengths



Bond angles

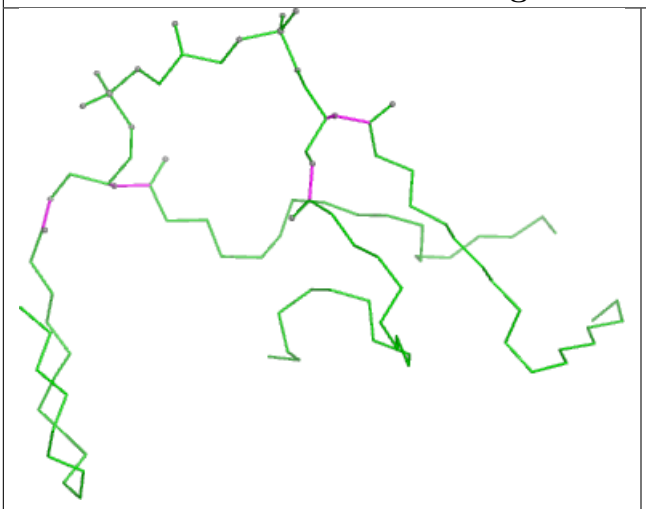


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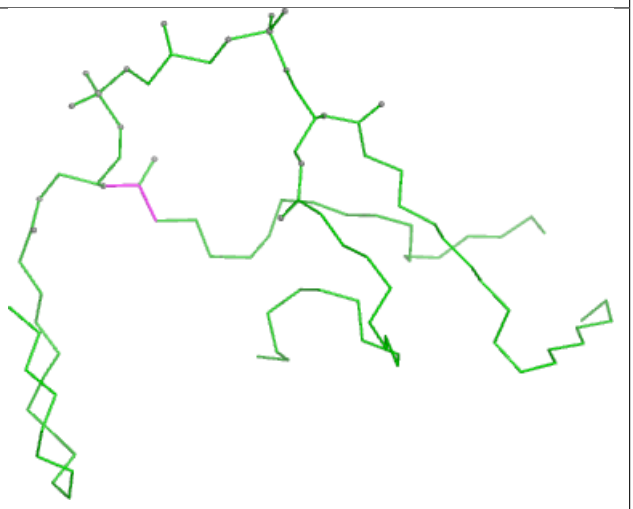


Rings

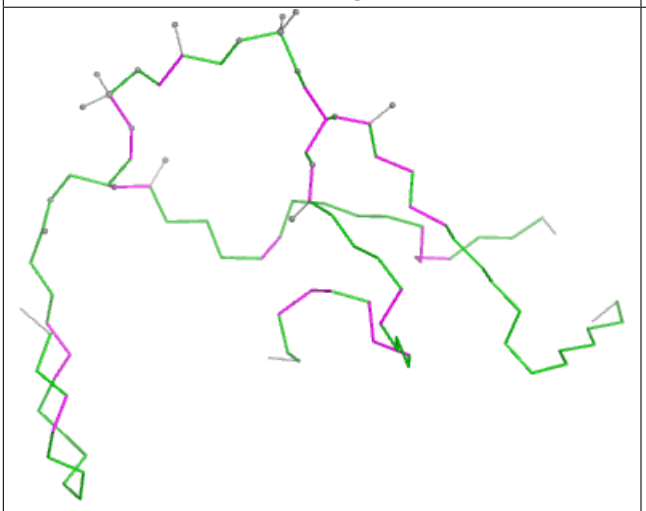
Ligand CDL AA 908



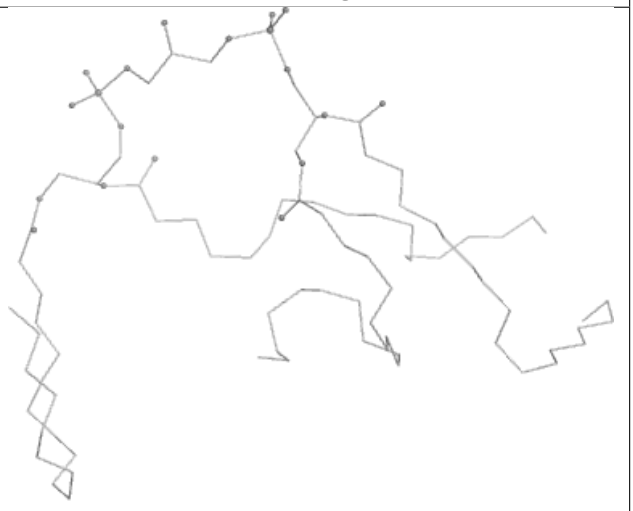
Bond lengths



Bond angles



Torsions



Rings

Ligand CDL BG 201



Bond lengths



Bond angles

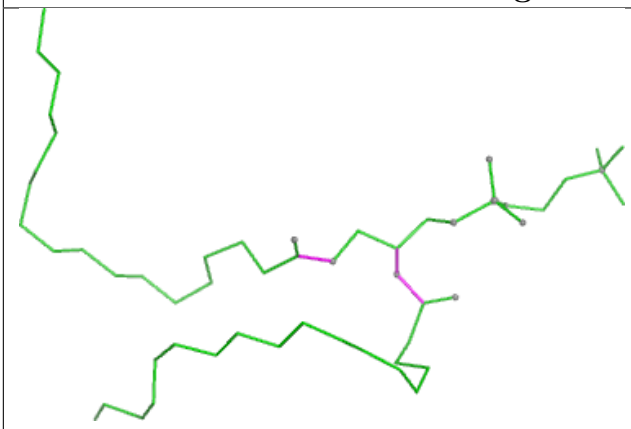


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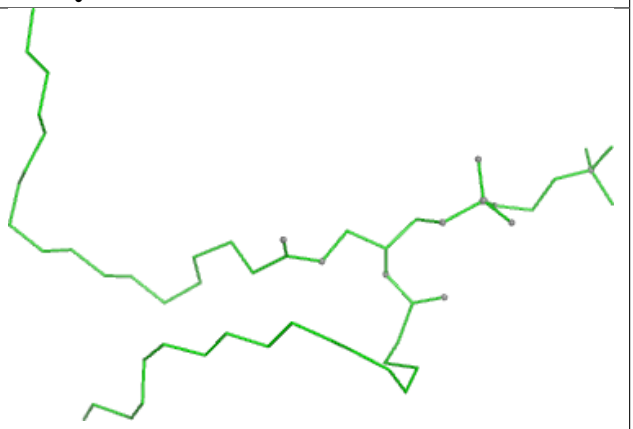


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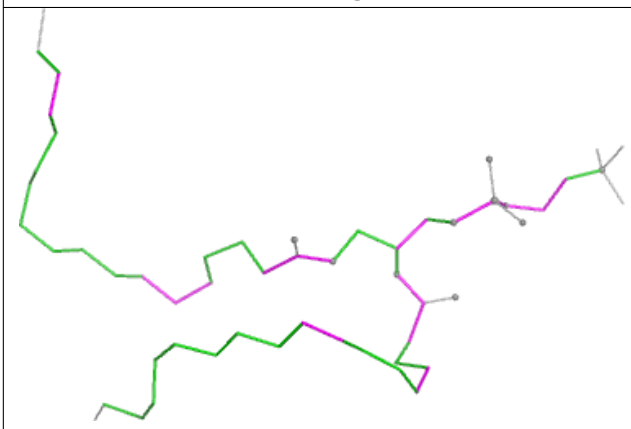
Ligand PC1 BQ 401



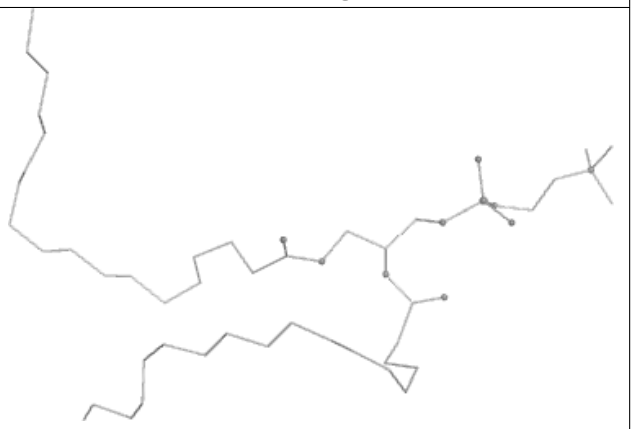
Bond lengths



Bond angles

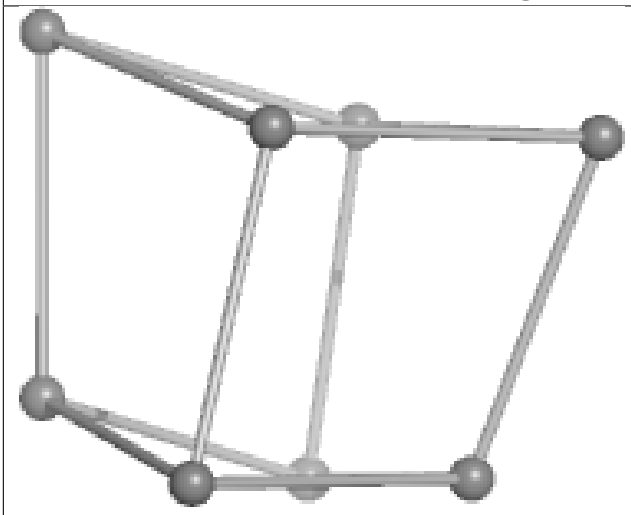


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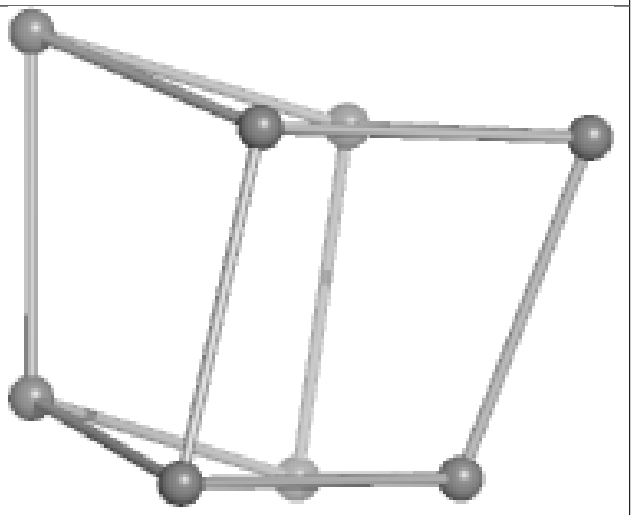


Rings

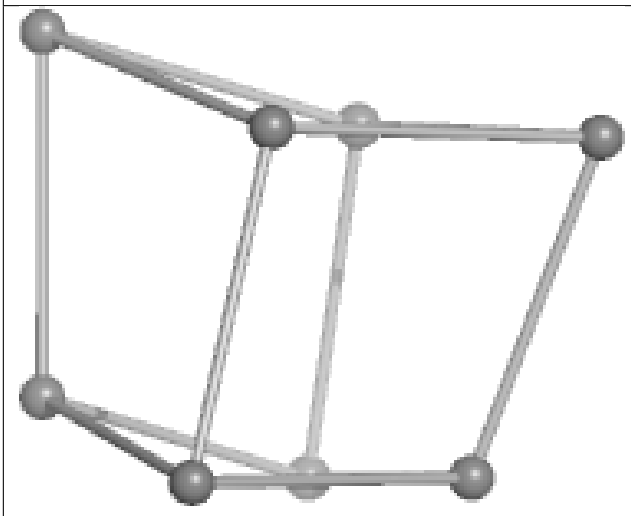
Ligand SF4 AD 501



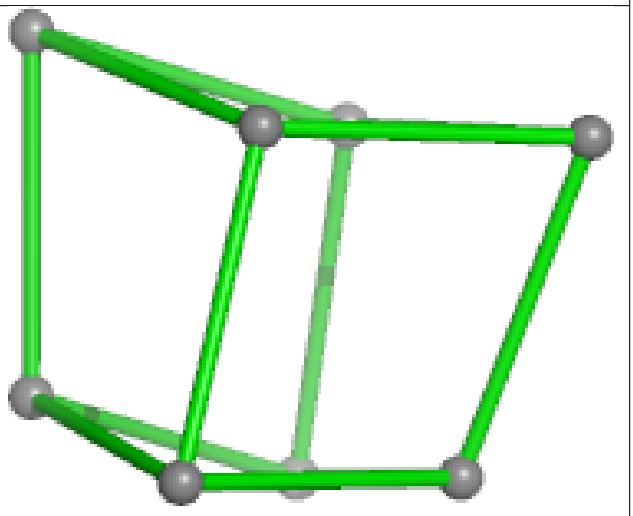
Bond lengths



Bond angles

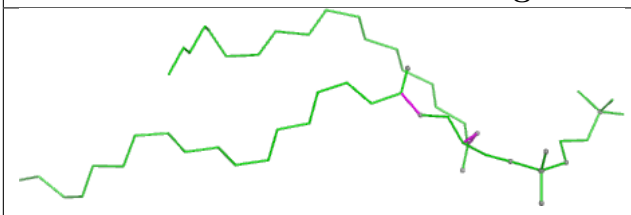


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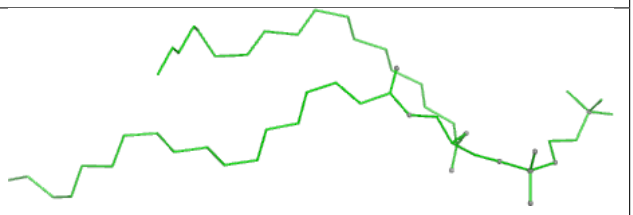


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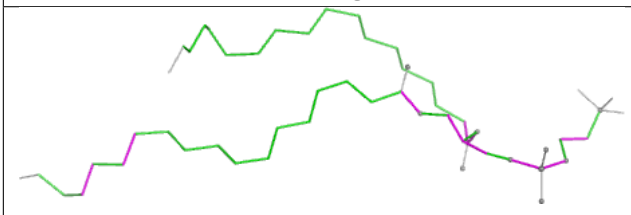
Ligand PC1 AA 905



Bond lengths



Bond angles

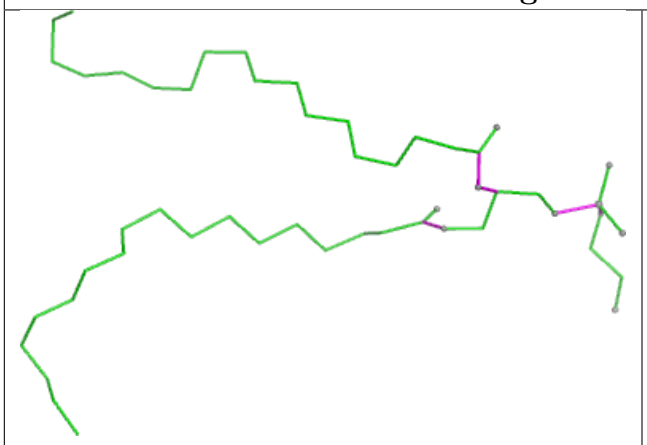


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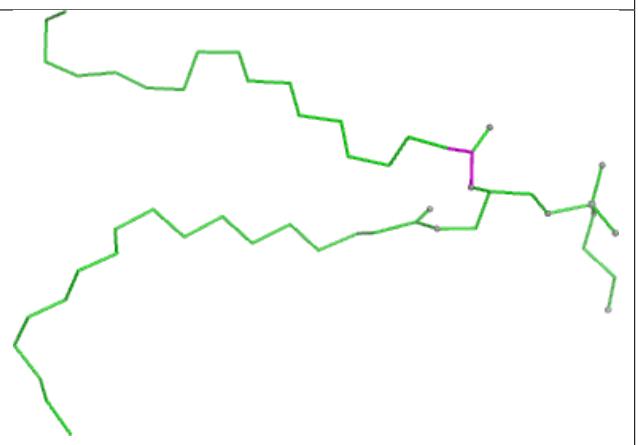


Rings

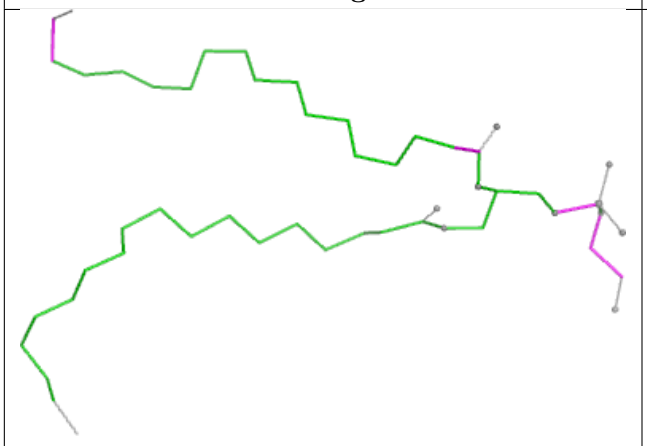
Ligand 3PE A9 603



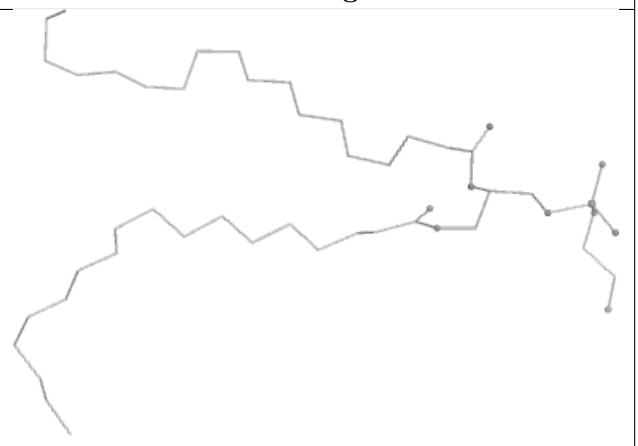
Bond lengths



Bond angles

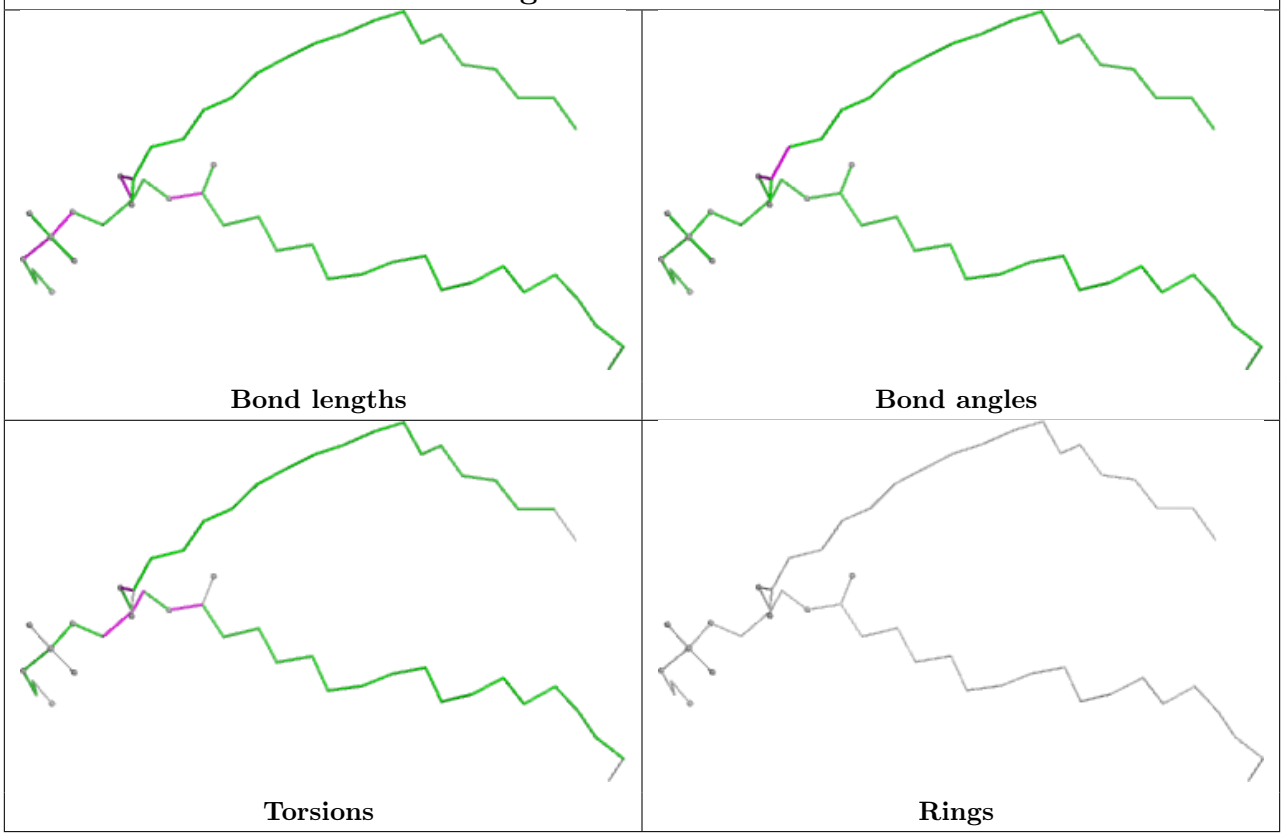


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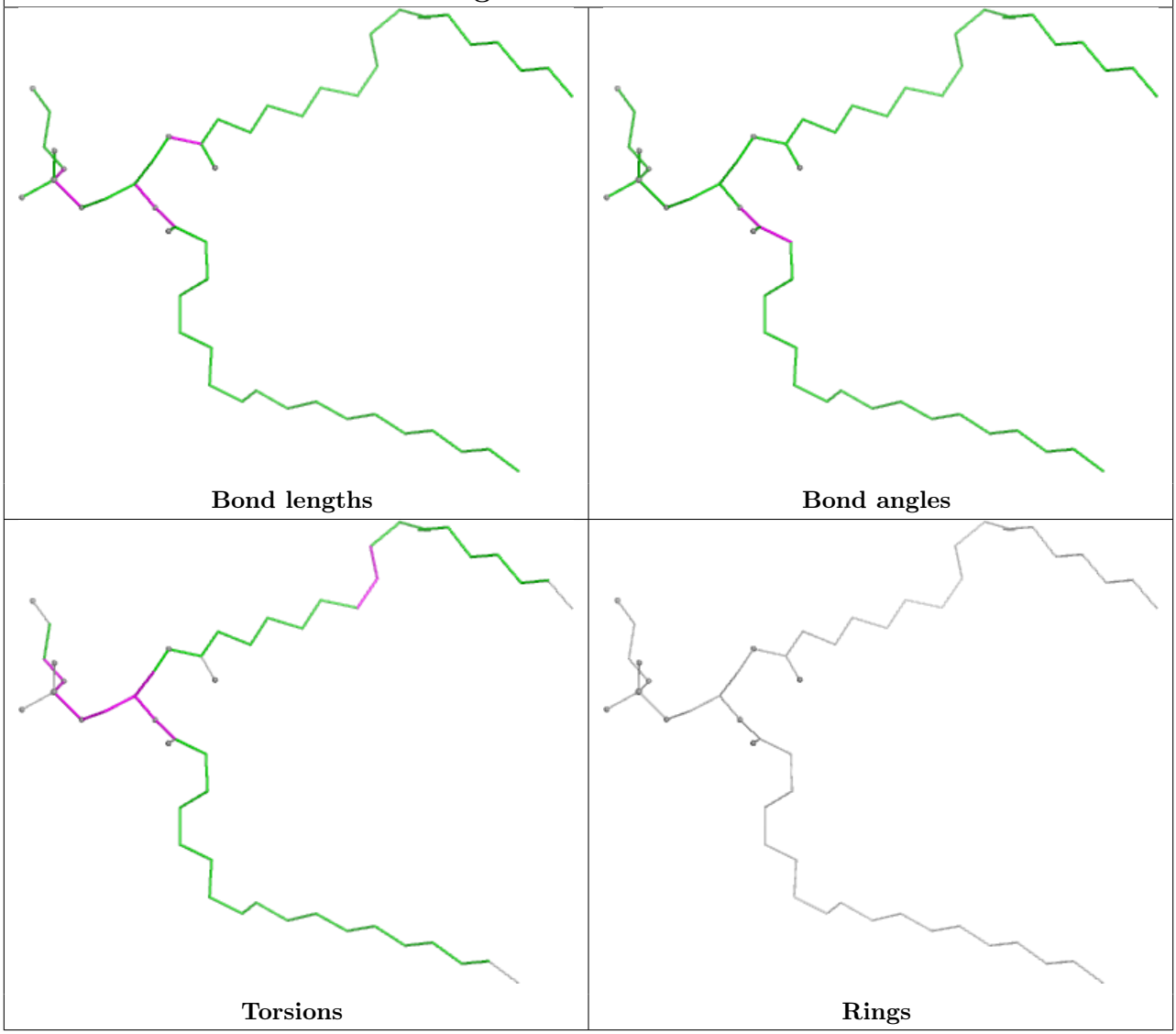


Rings

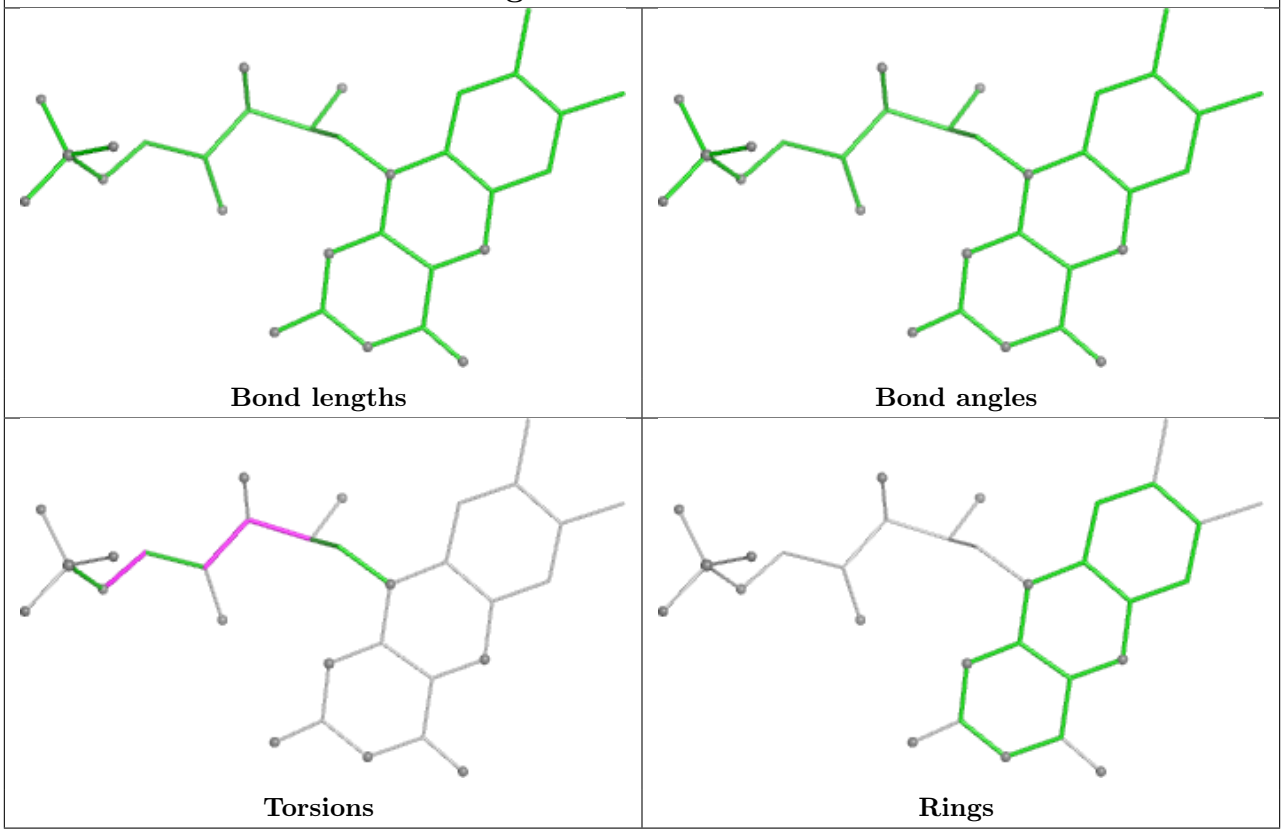
Ligand 3PE A2 401



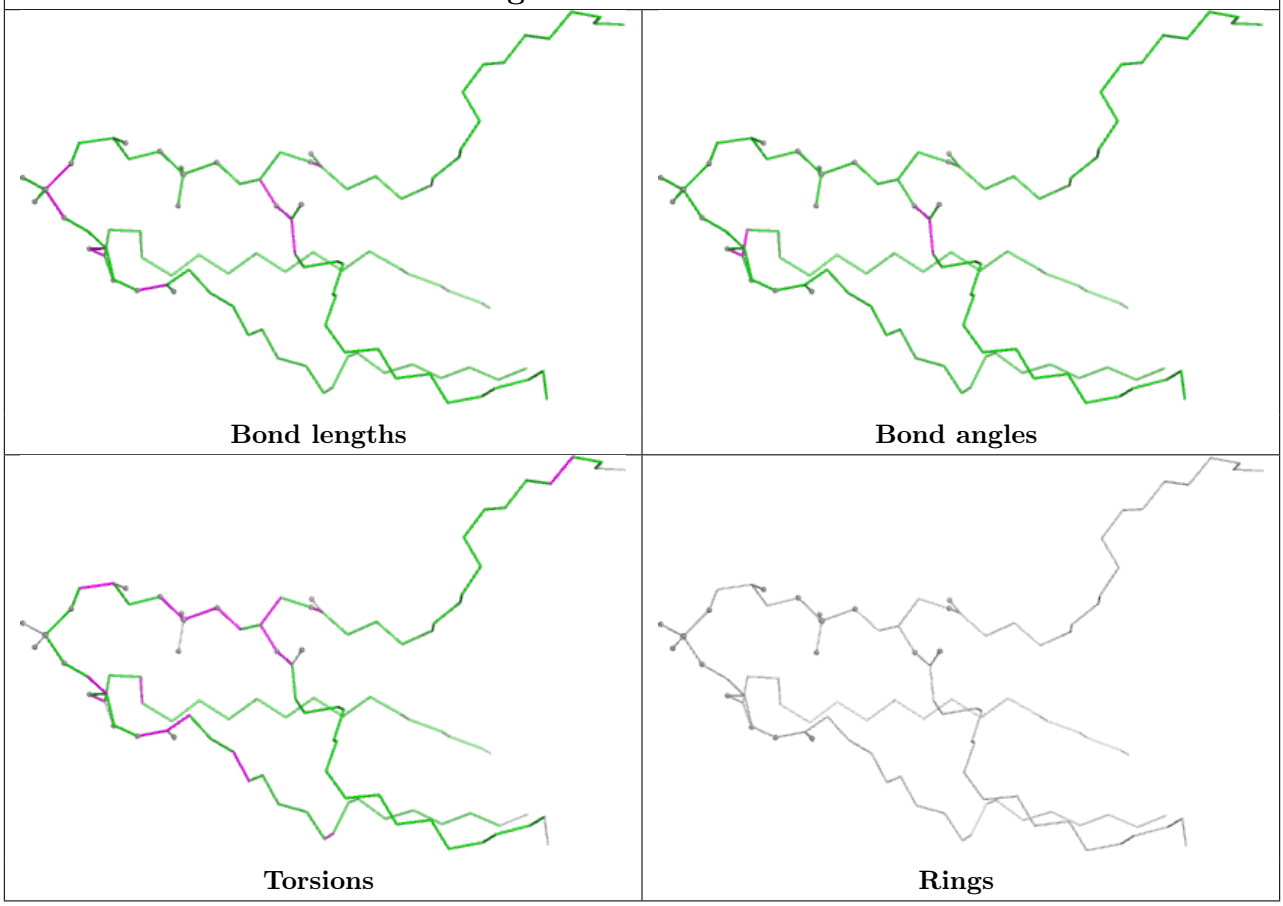
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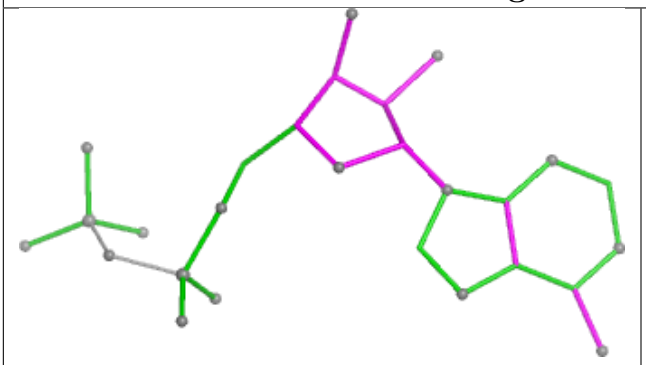
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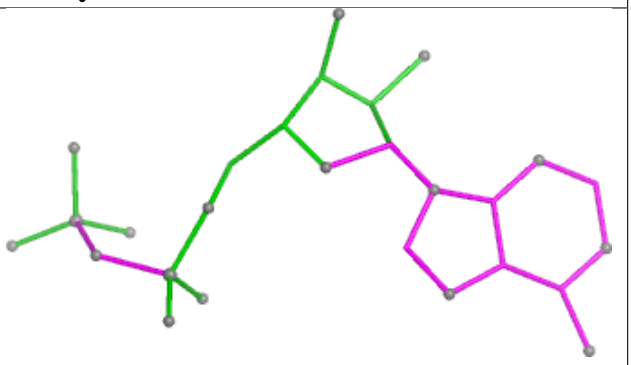
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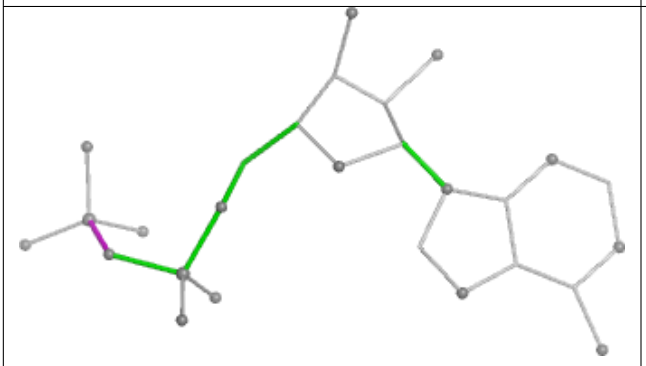
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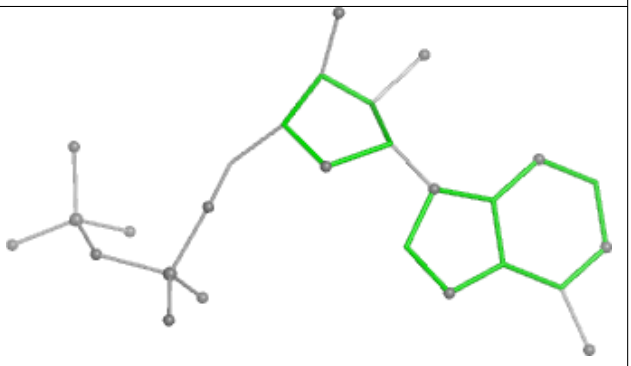
Bond lengths



Bond angles

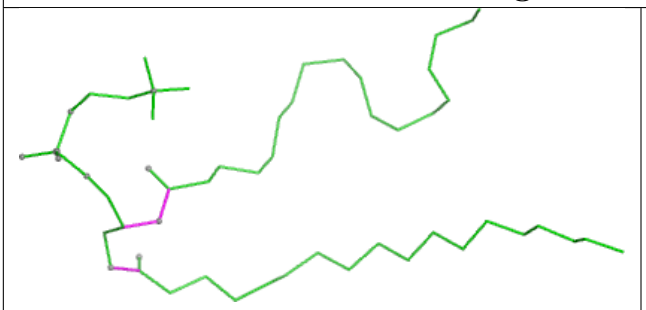


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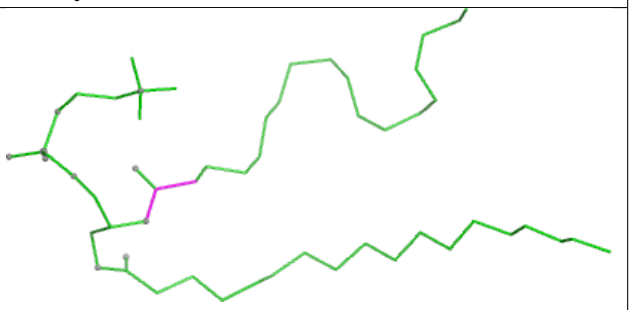


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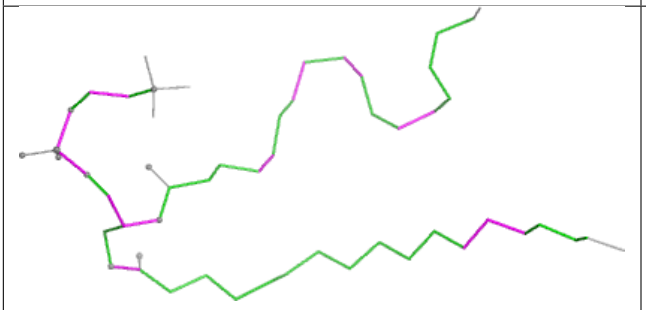
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Bond lengths



Bond angles

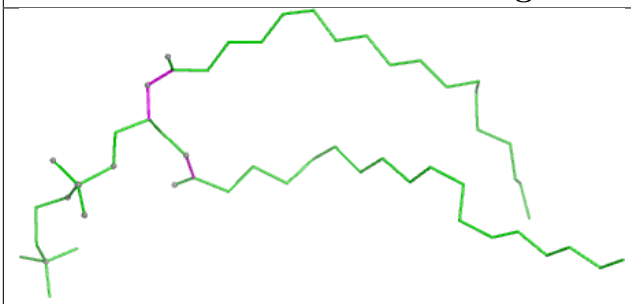


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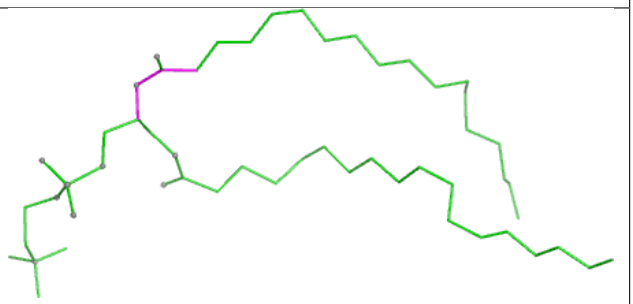


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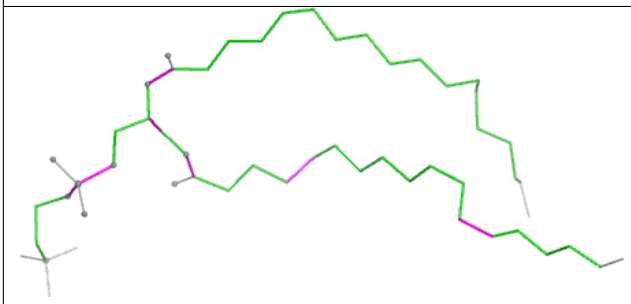
Ligand PC1 BT 202



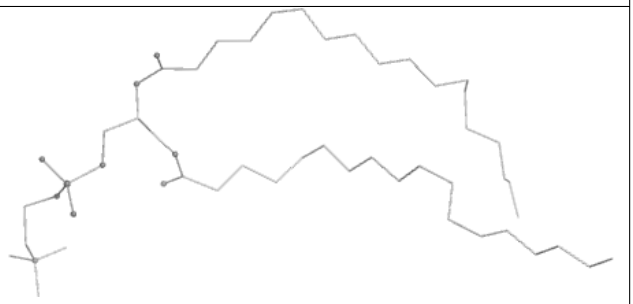
Bond lengths



Bond angles

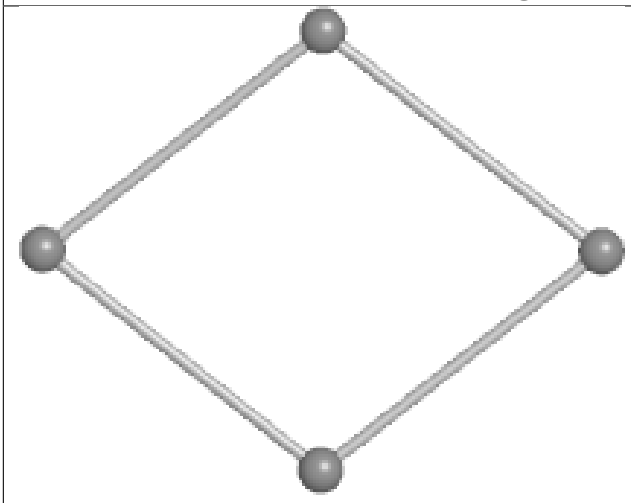


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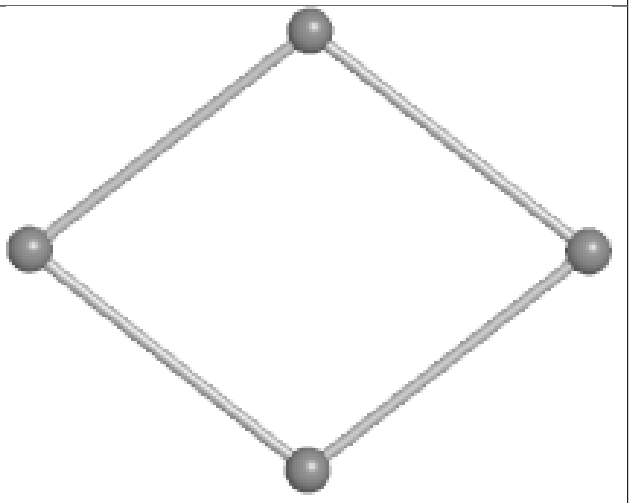


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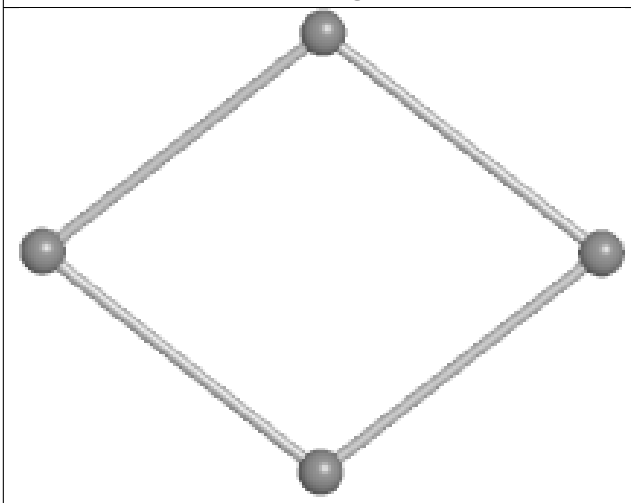
Ligand FES AB 801



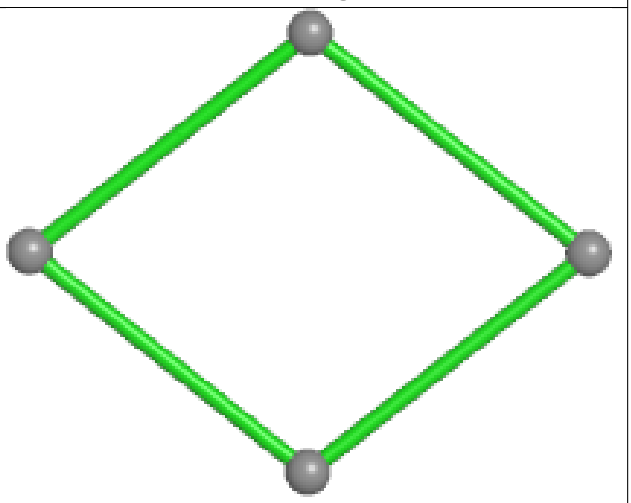
Bond lengths



Bond angles

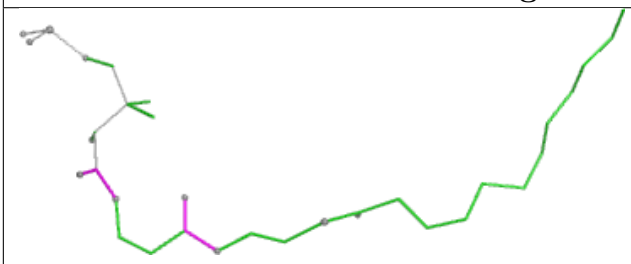


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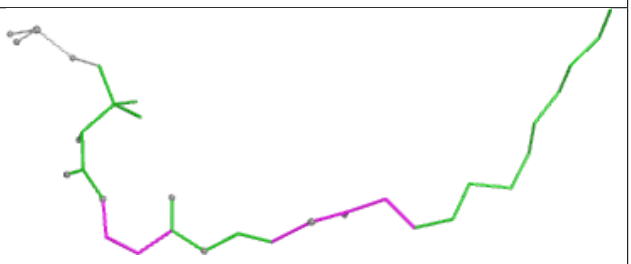


Rings

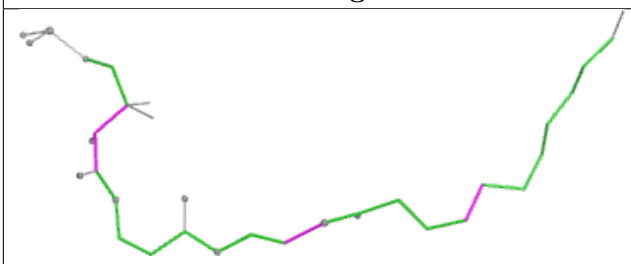
Ligand 8Q1 AS 200



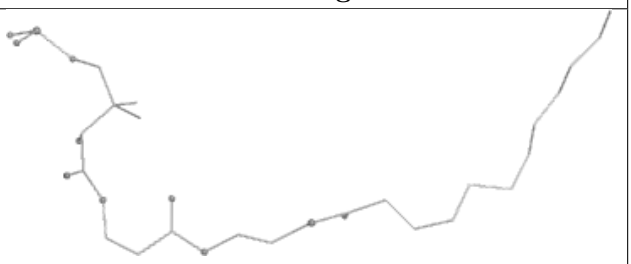
Bond lengths



Bond angles

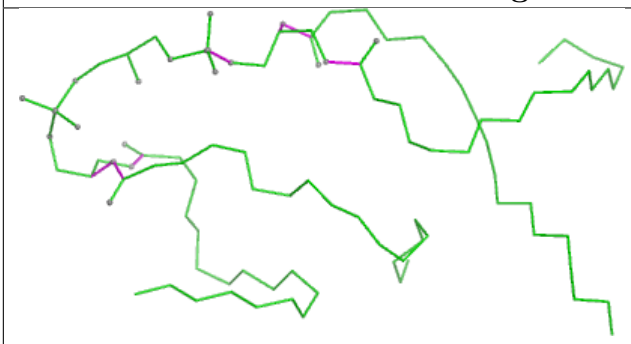


Torsions

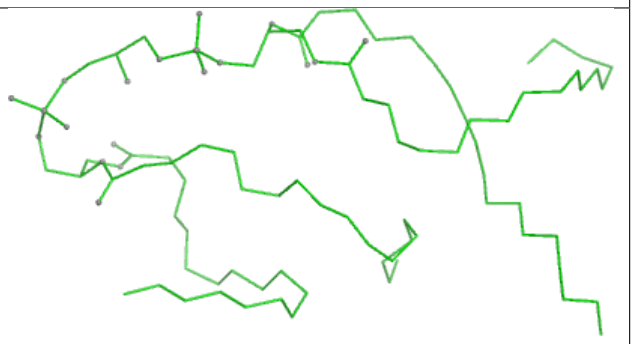


Rings

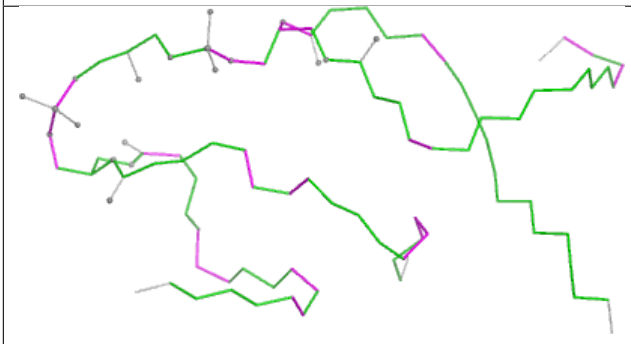
Ligand CDL AC 802



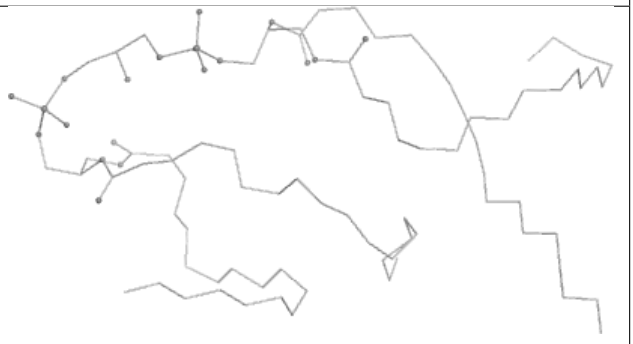
Bond lengths



Bond angles

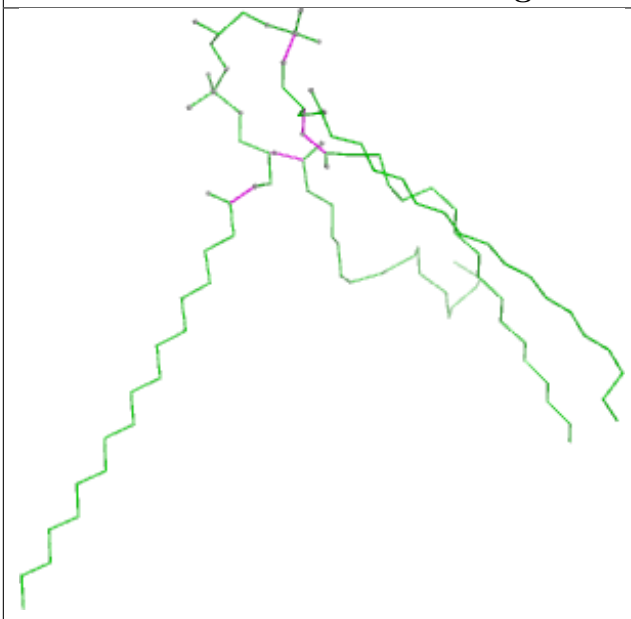


Torsions

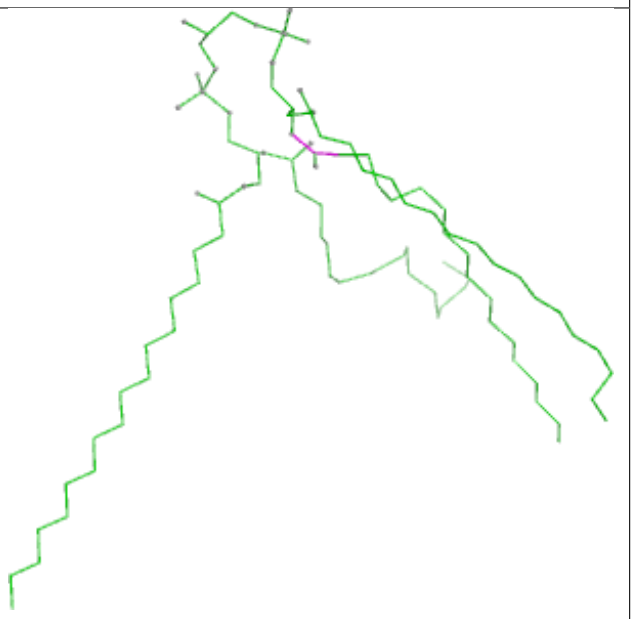


Rings

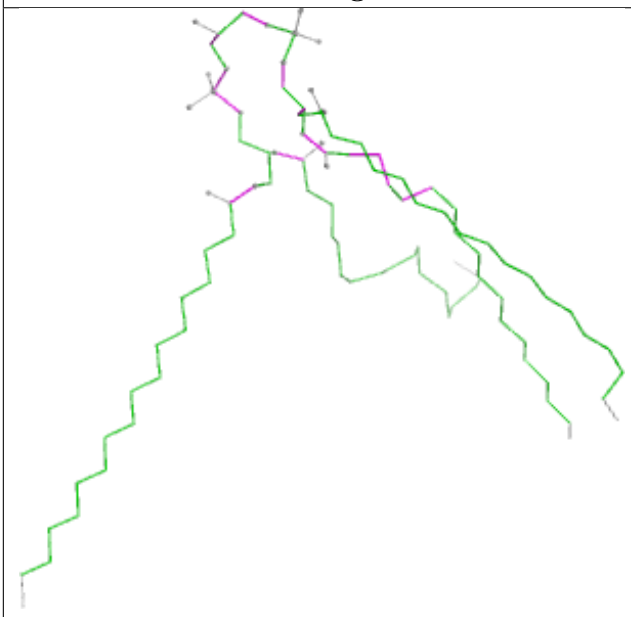
Ligand CDL A0 601



Bond lengths



Bond angles

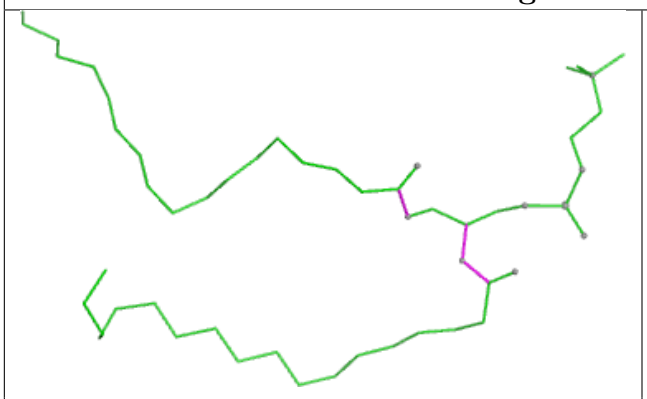


Torsions

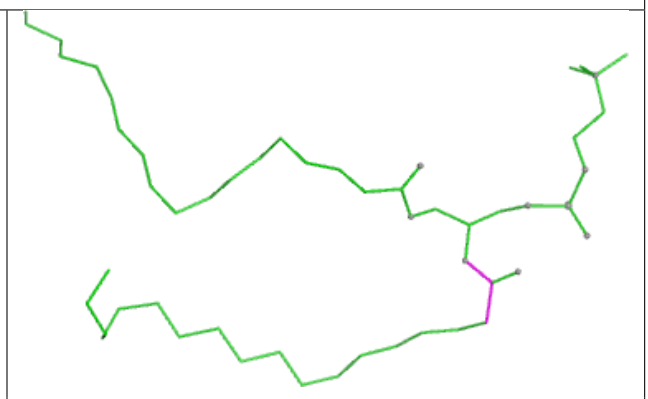


Rings

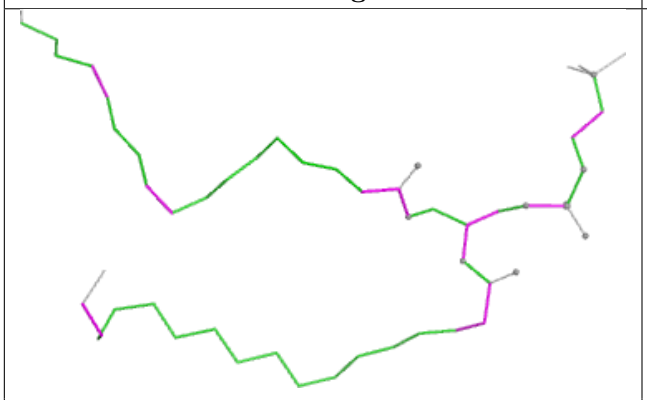
Ligand PC1 AJ 501



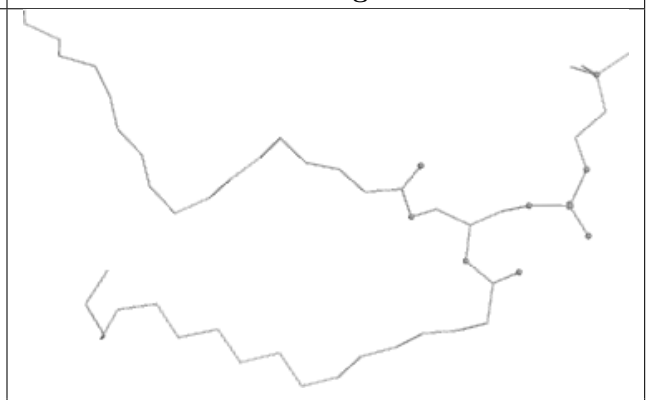
Bond lengths



Bond angles



Torsions

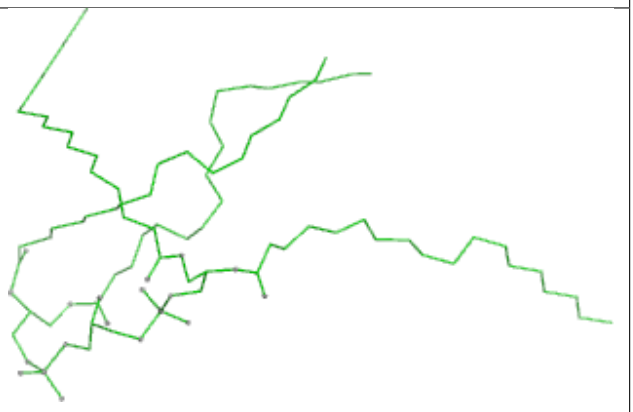


Rings

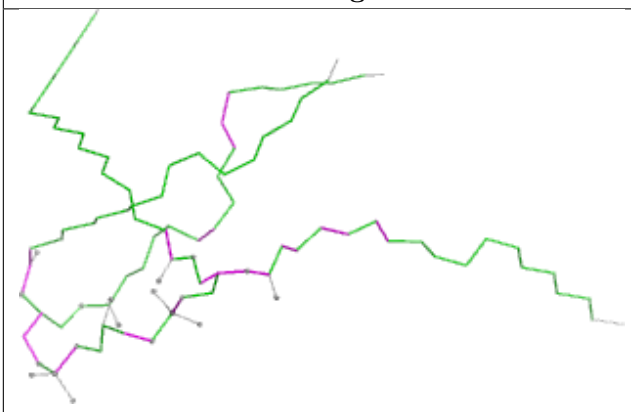
Ligand CDL AP 301



Bond lengths



Bond angles



Torsions



Rings

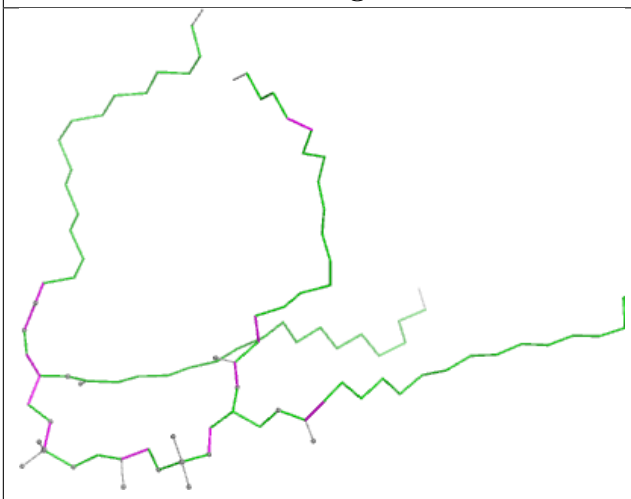
Ligand CDL BL 301



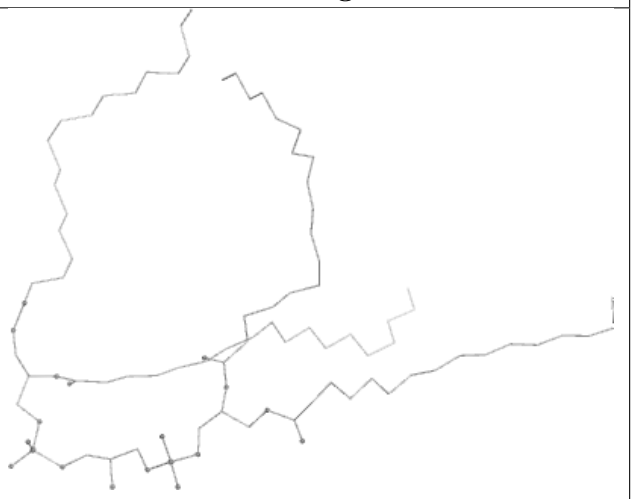
Bond lengths



Bond angles

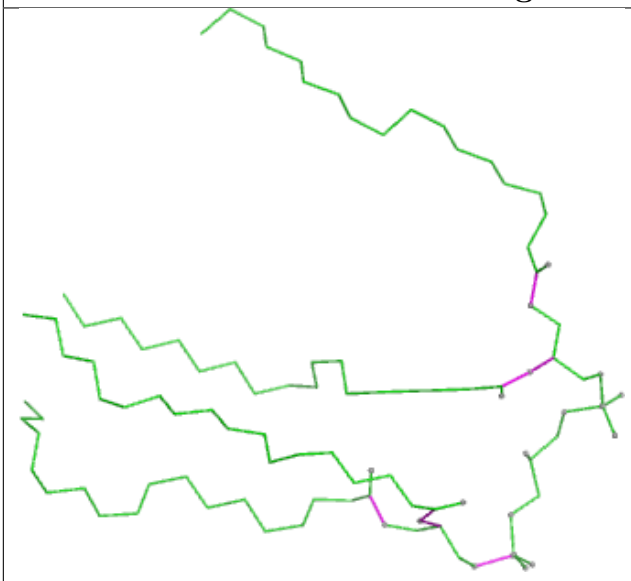


Torsions



Rings

Ligand CDL B0 102



Bond lengths



Bond angles

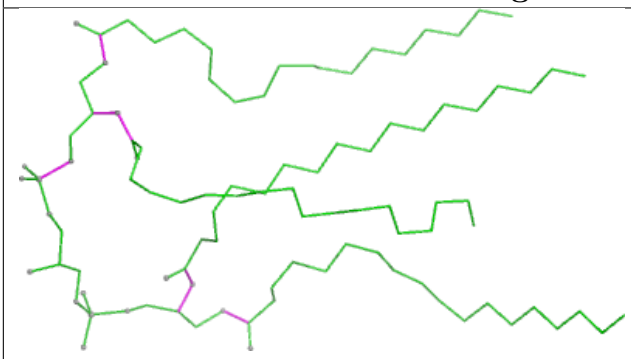


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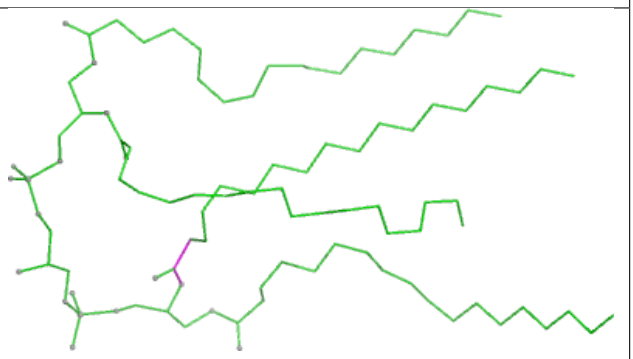


Rings

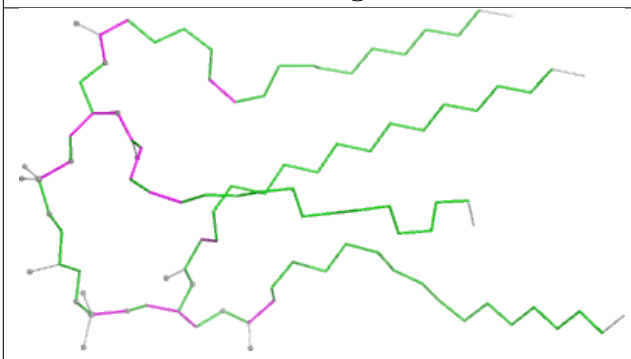
Ligand CDL BC 302



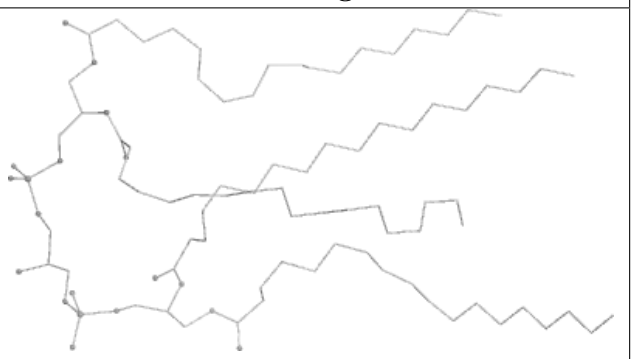
Bond lengths



Bond angles

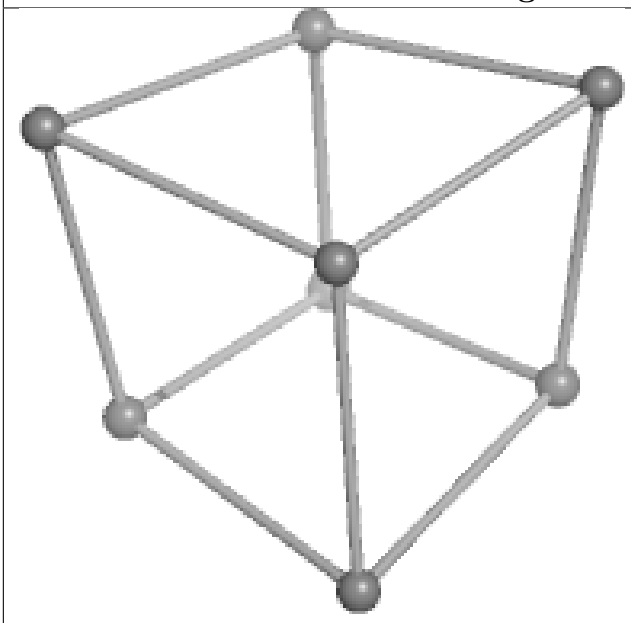


Torsions

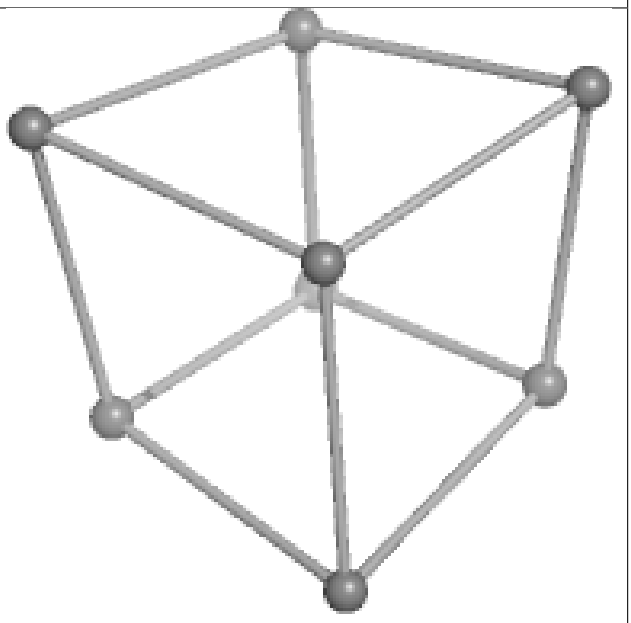


Rings

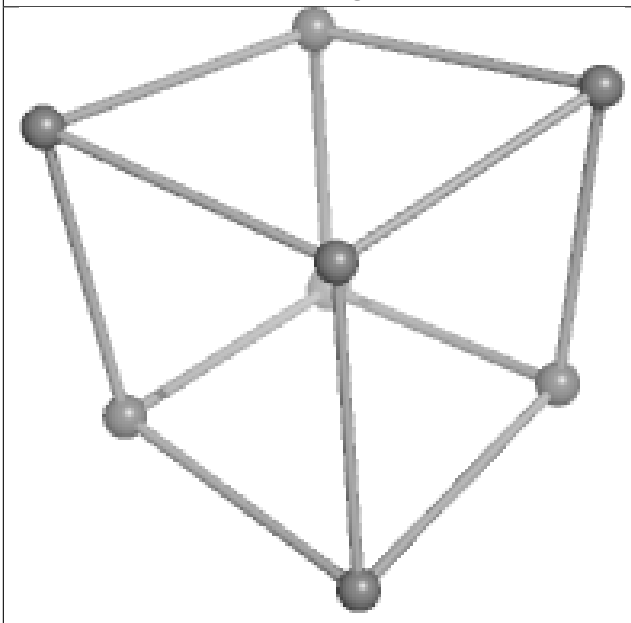
Ligand SF4 AB 802



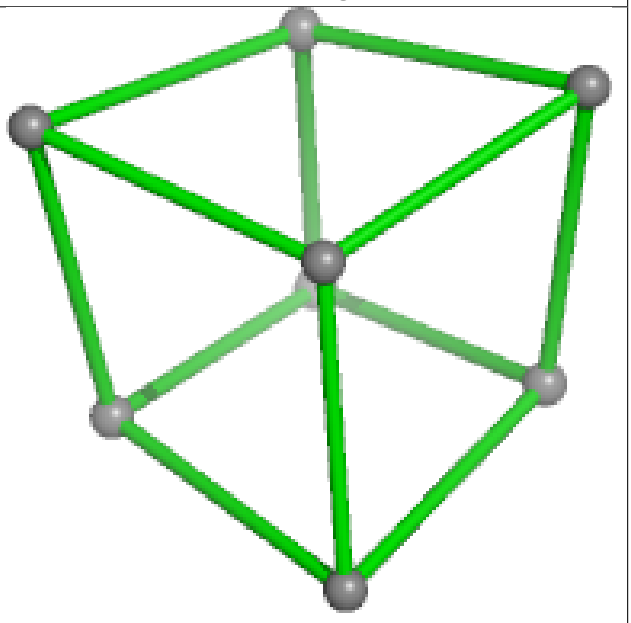
Bond lengths



Bond angles

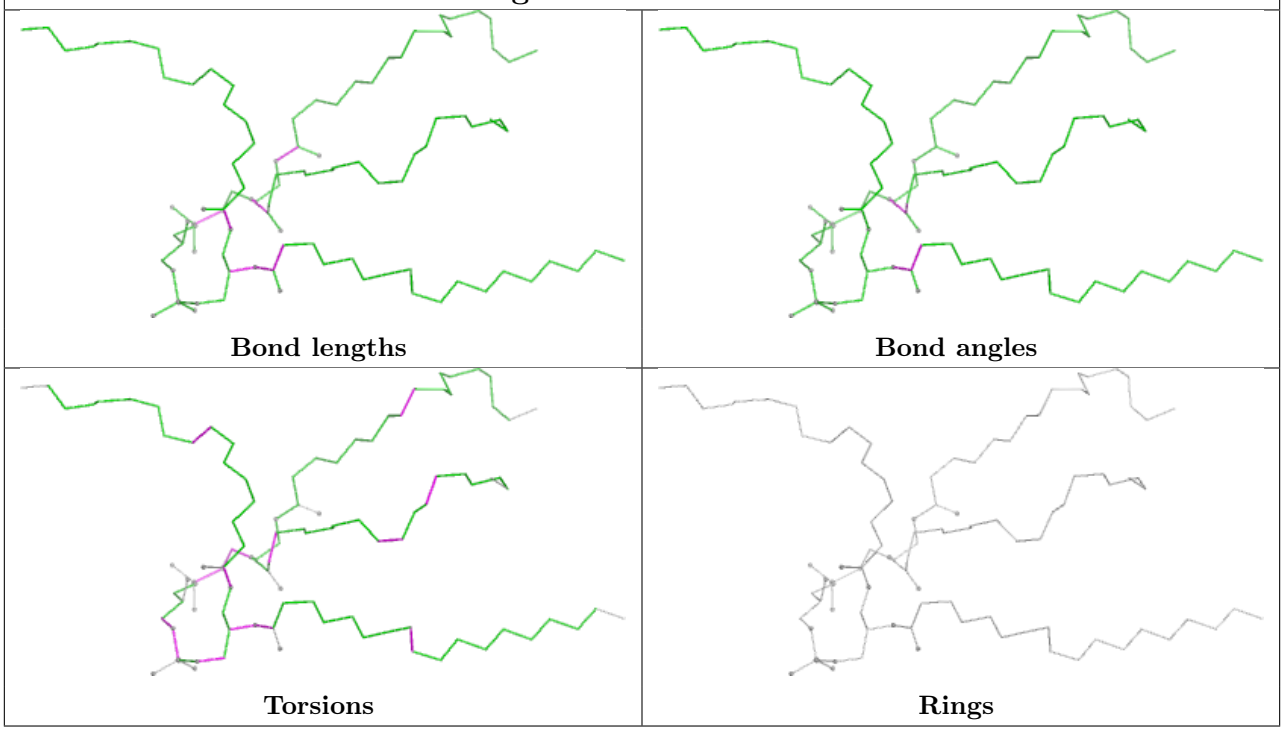


Torsions

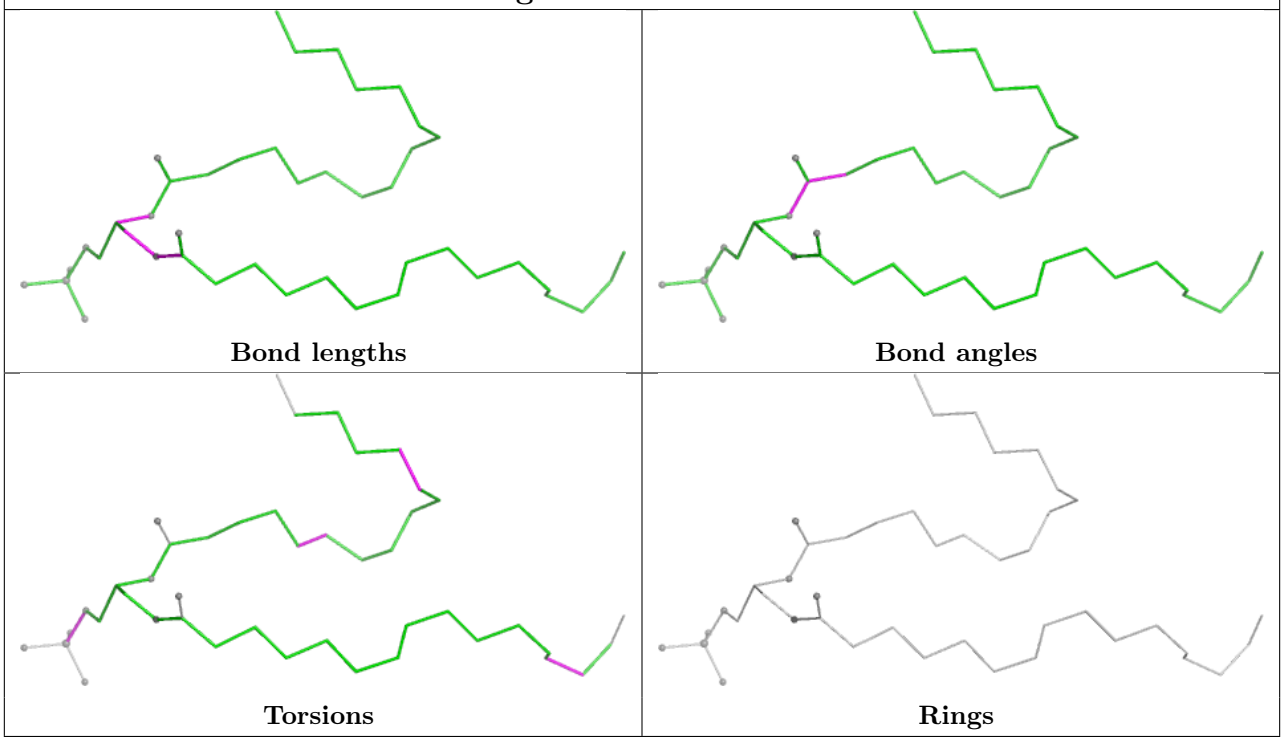


Rings

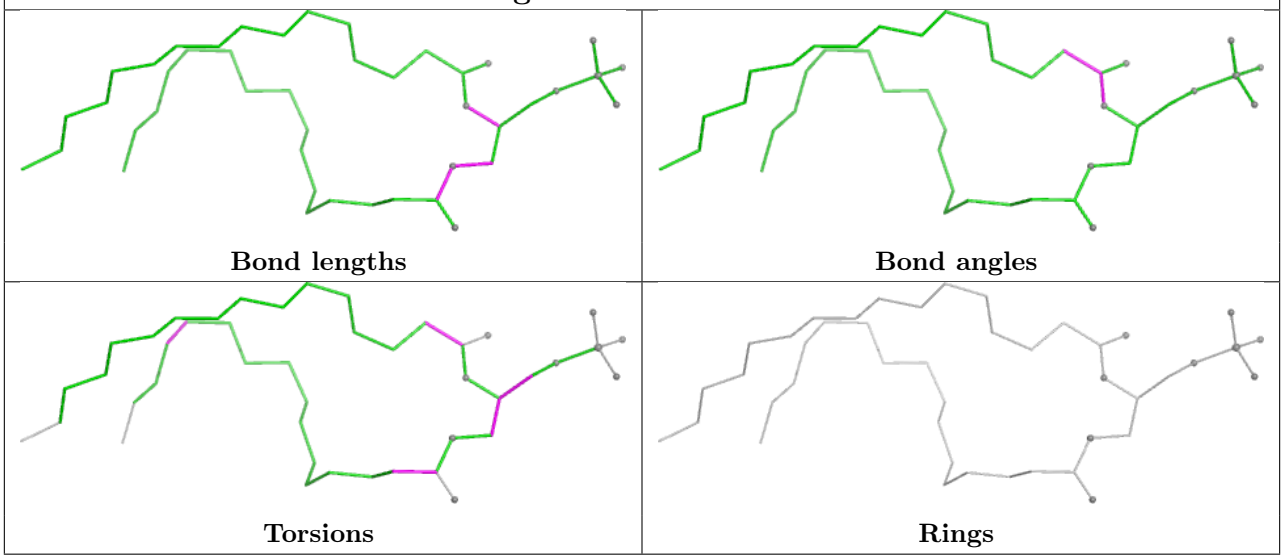
Ligand CDL BY 201



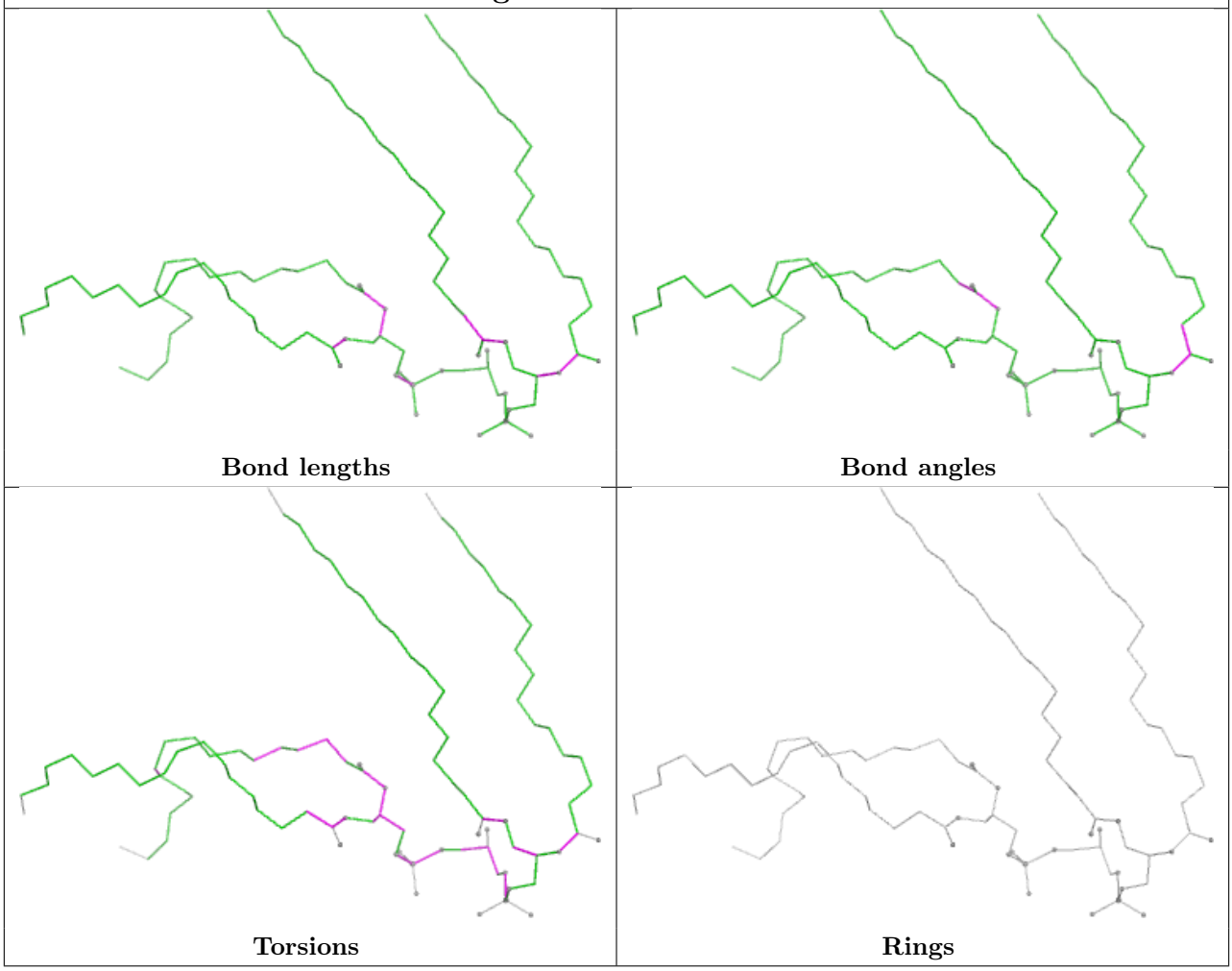
Ligand LPP AL 304



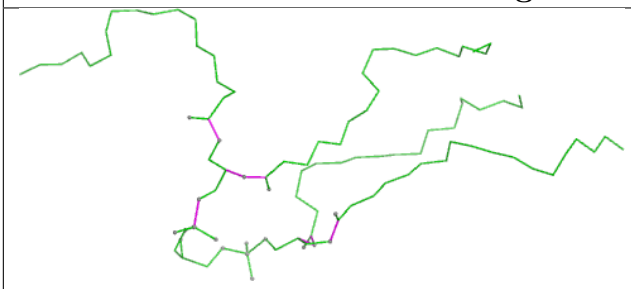
Ligand LPP BN 301



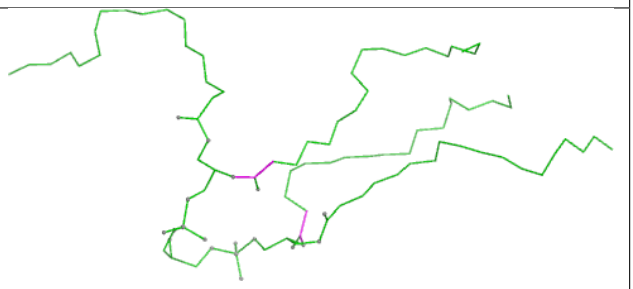
Ligand CDL BE 201



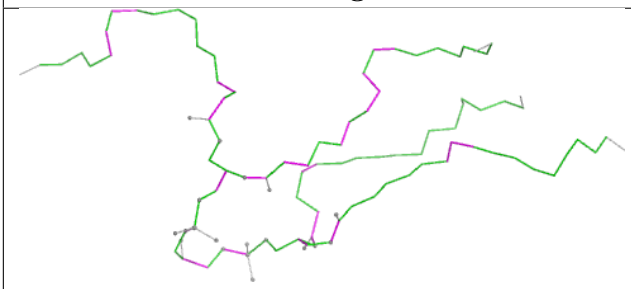
Ligand CDL B0 101



Bond lengths



Bond angles

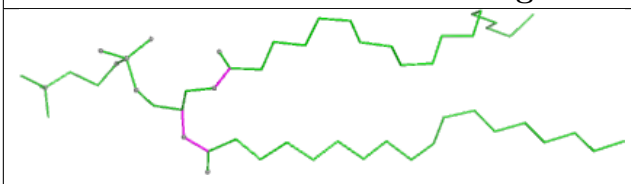


Torsions

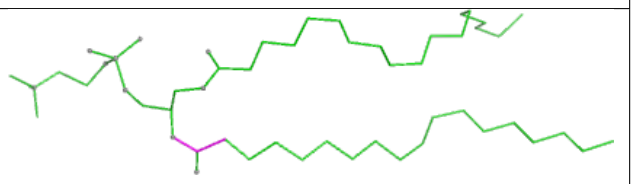


Rings

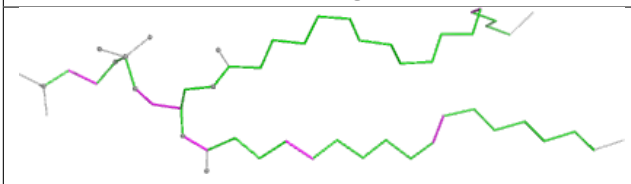
Ligand PC1 AL 303



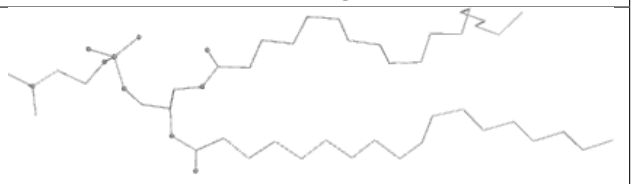
Bond lengths



Bond angles

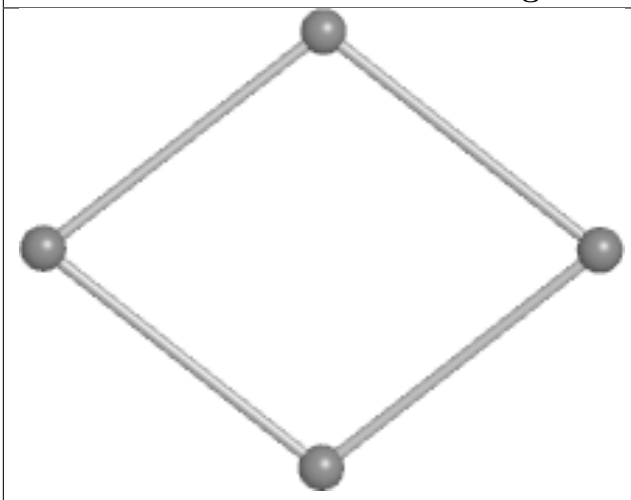


Torsions

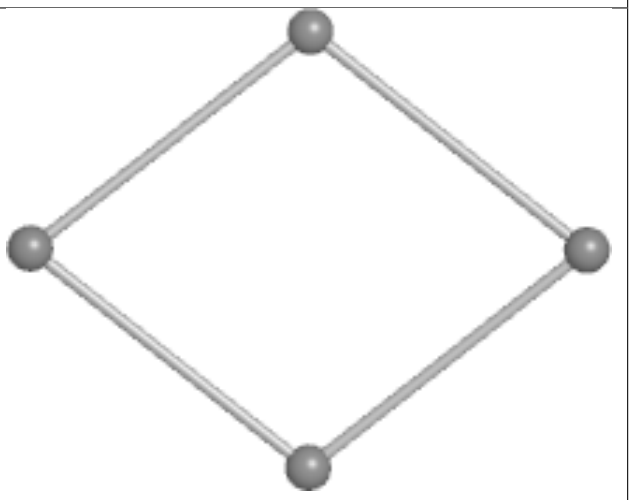


Rings

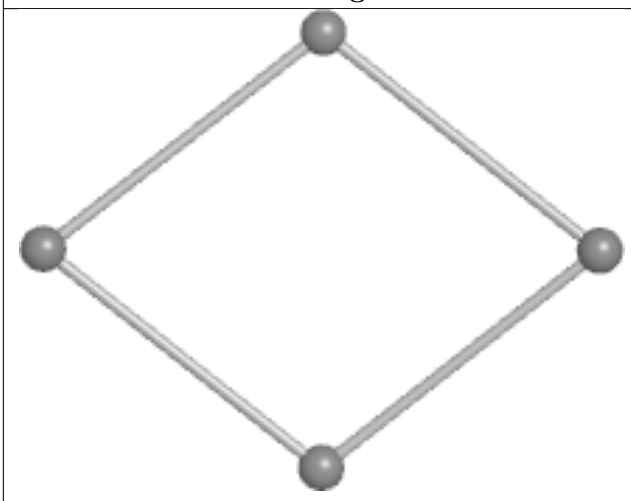
Ligand FES BI 201



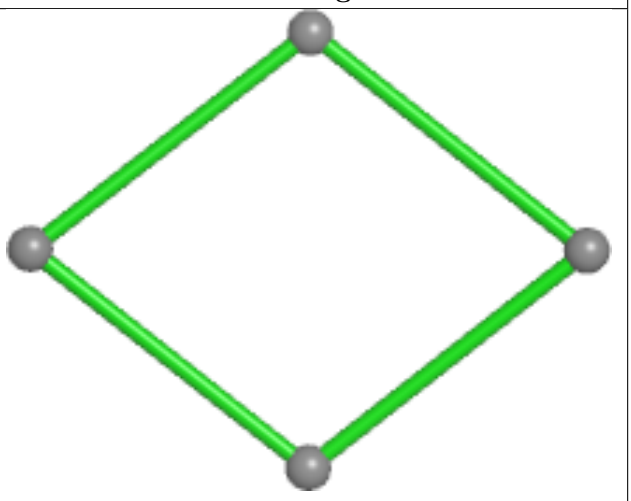
Bond lengths



Bond angles

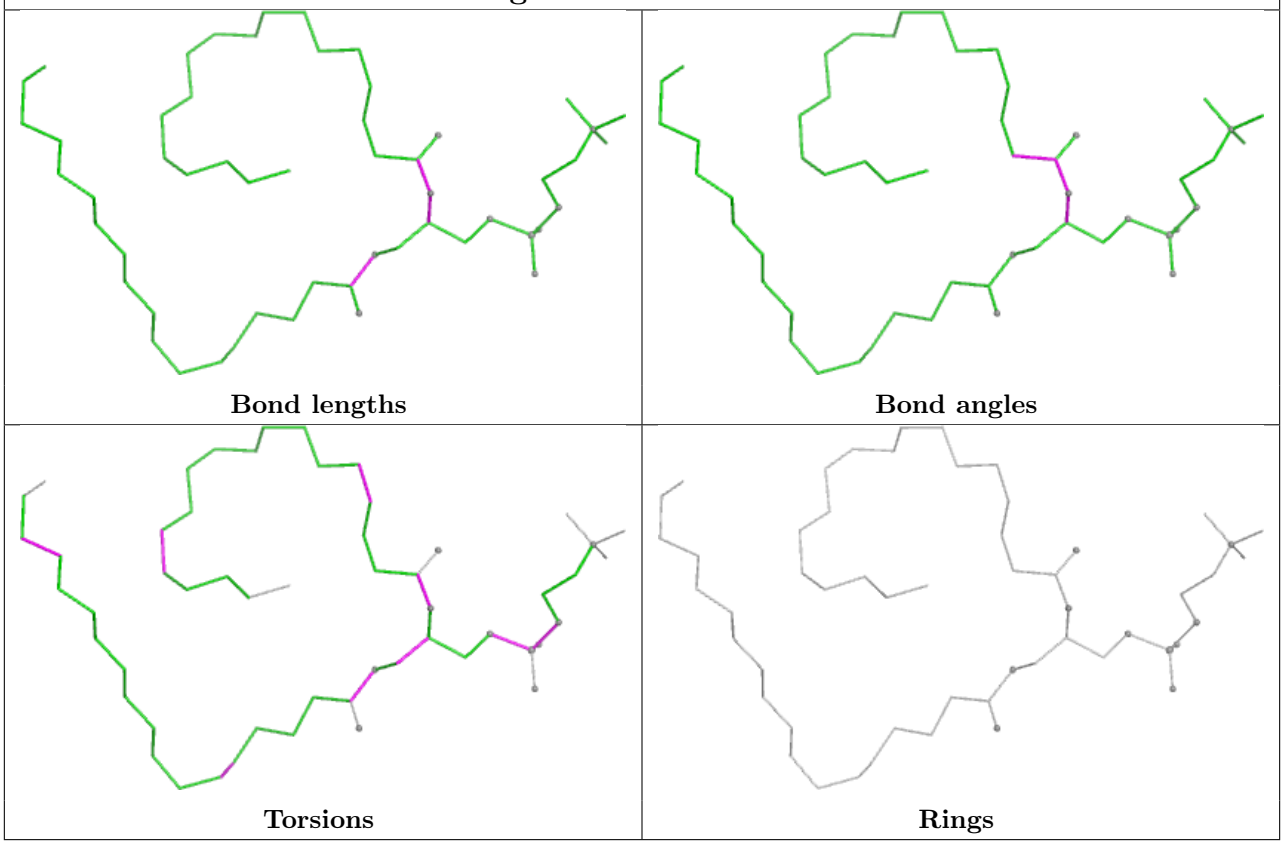


Torsions



Rings

Ligand PC1 BS 1301



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.

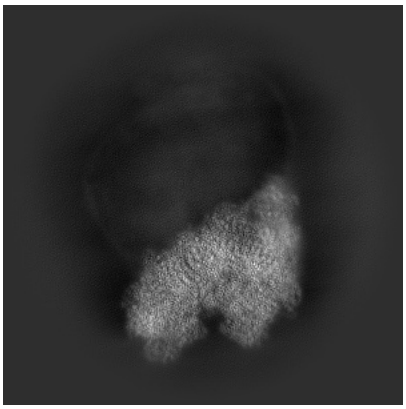
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15865. These allow visual inspection of the internal detail of the map and identification of artifacts.

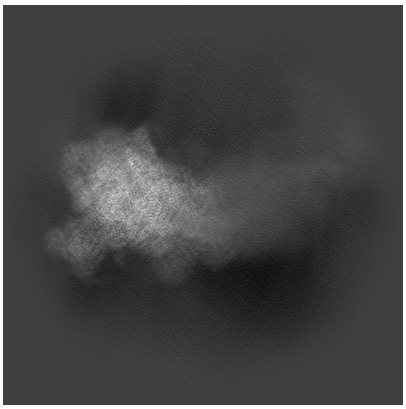
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

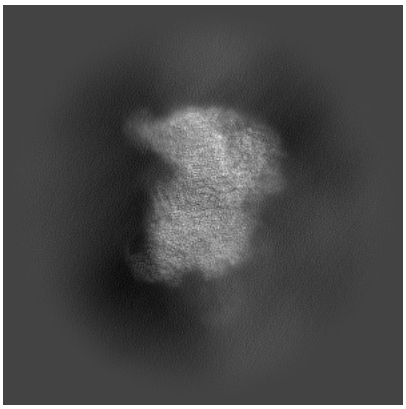
6.1.1 Primary map



X

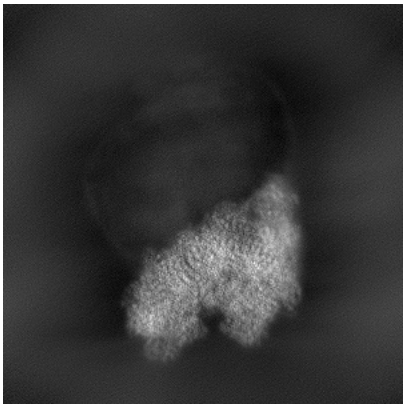


Y

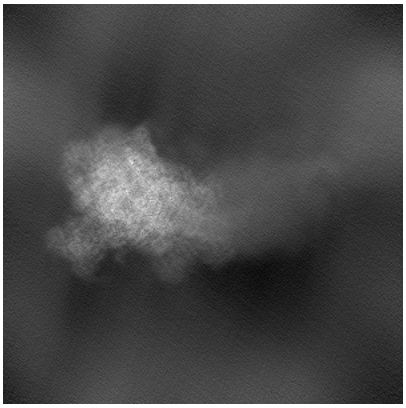


Z

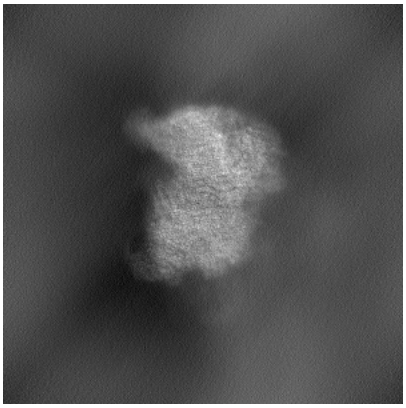
6.1.2 Raw map



X



Y

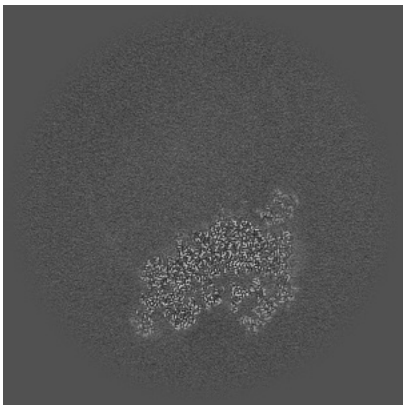


Z

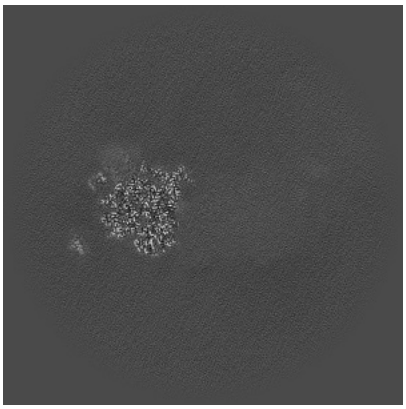
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

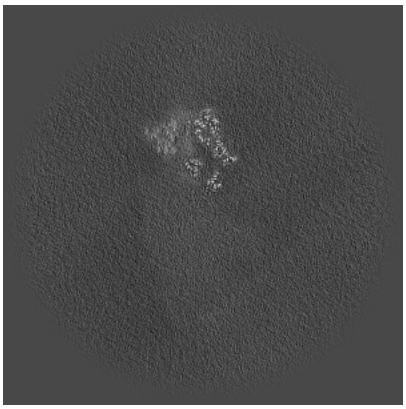
6.2.1 Primary map



X Index: 240

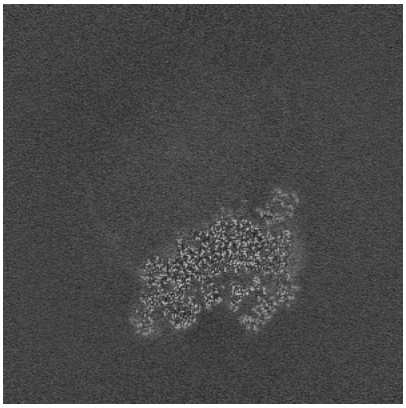


Y Index: 240

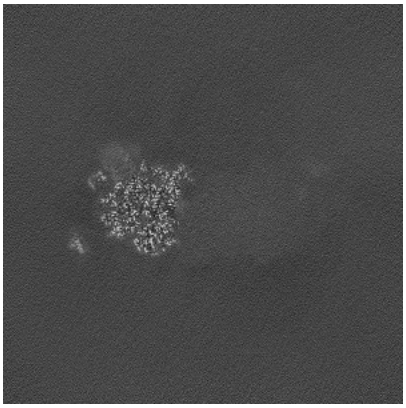


Z Index: 240

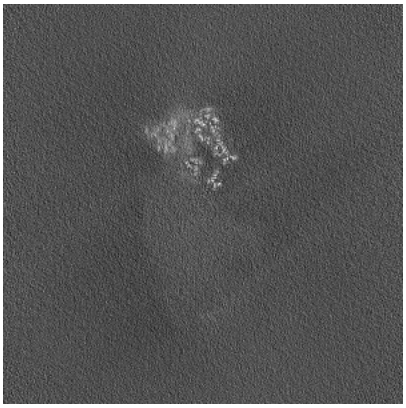
6.2.2 Raw map



X Index: 240



Y Index: 240

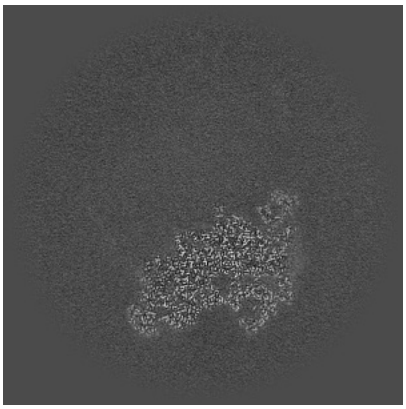


Z Index: 240

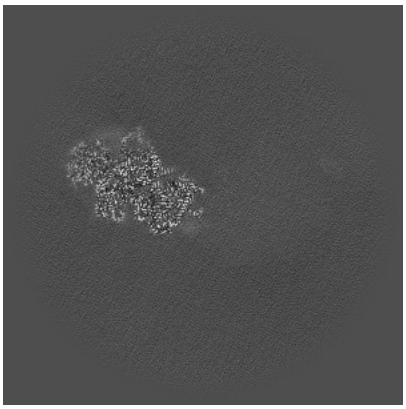
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

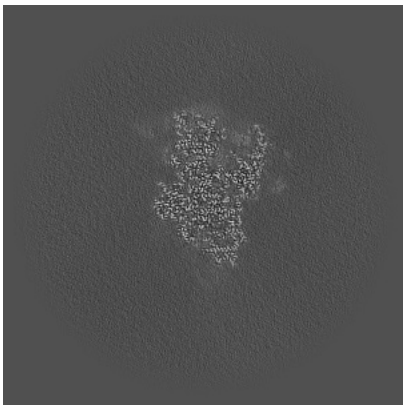
6.3.1 Primary map



X Index: 243

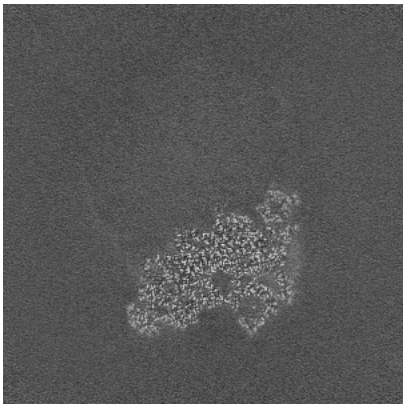


Y Index: 278

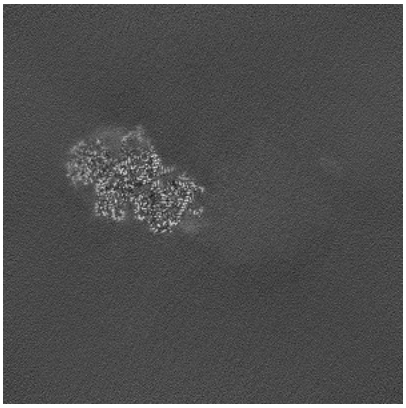


Z Index: 177

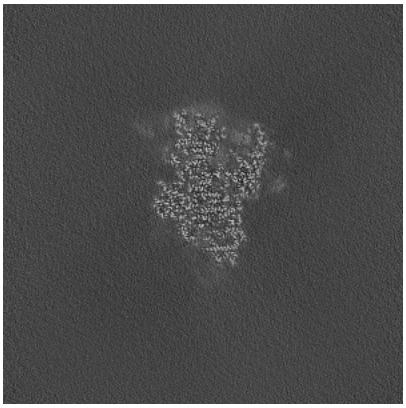
6.3.2 Raw map



X Index: 244



Y Index: 278

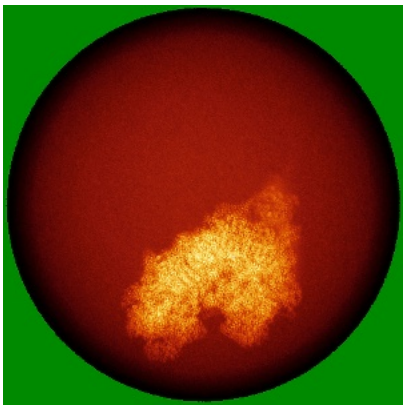


Z Index: 177

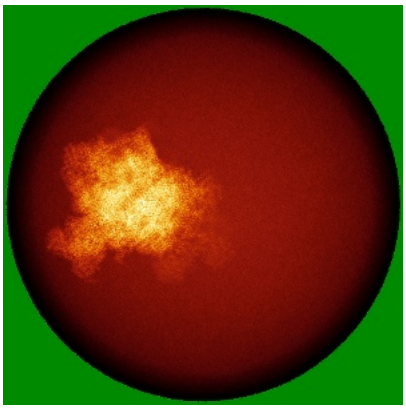
The images above show the largest variance slices of the map in three orthogonal directions.

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

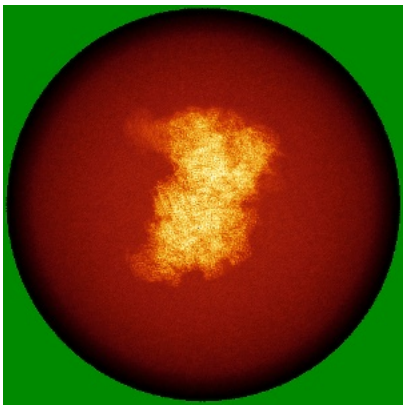
6.4.1 Primary map



X

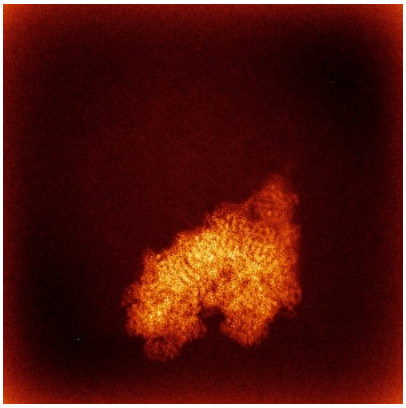


Y

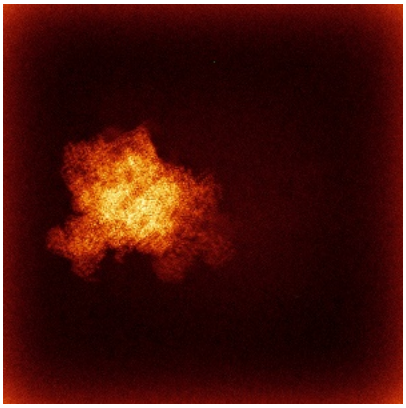


Z

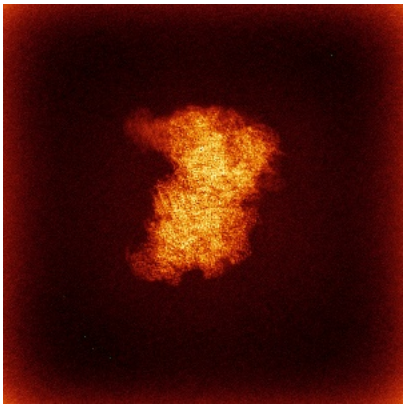
6.4.2 Raw map



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

6.5.2 Raw map



X Y Z

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

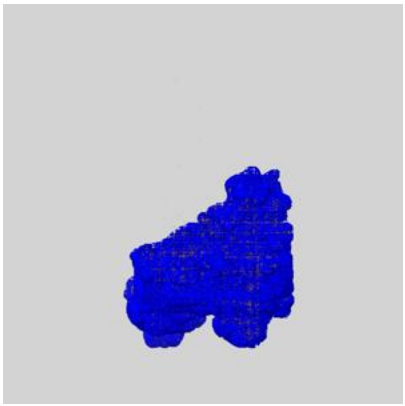
6.6 Mask visualisation

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

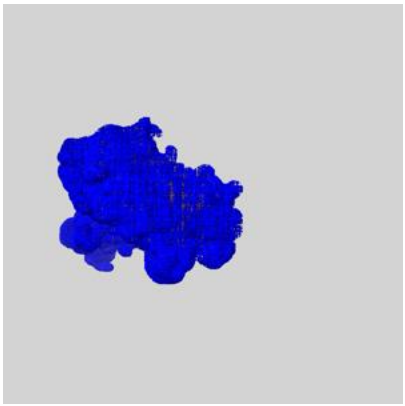
A mask typically either:

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

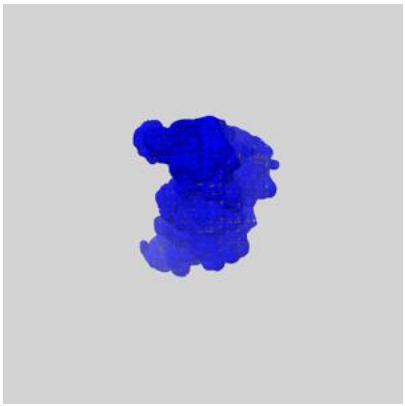
6.6.1 emd_15865_msk_1.map



X



Y

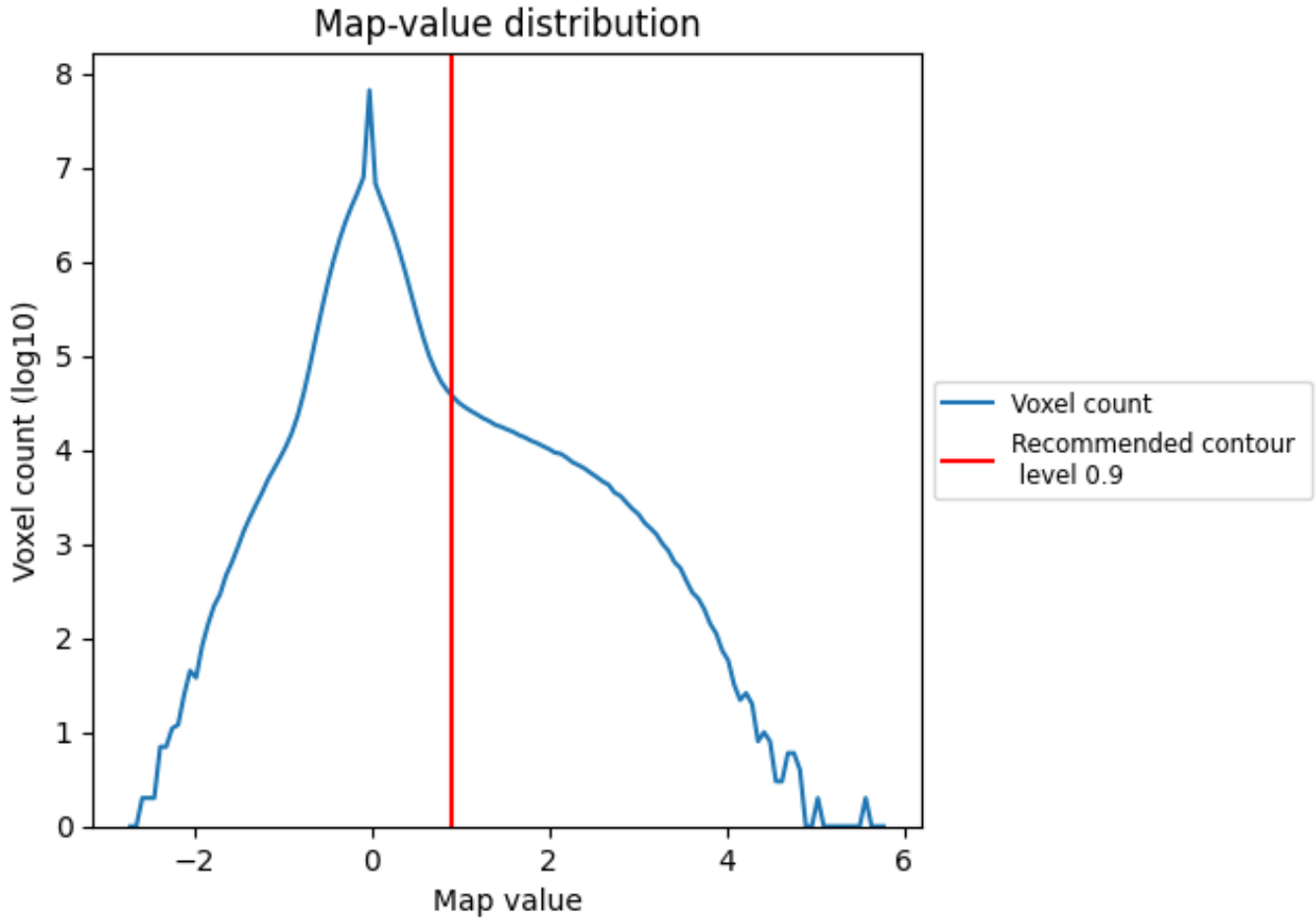


Z

7 Map analysis

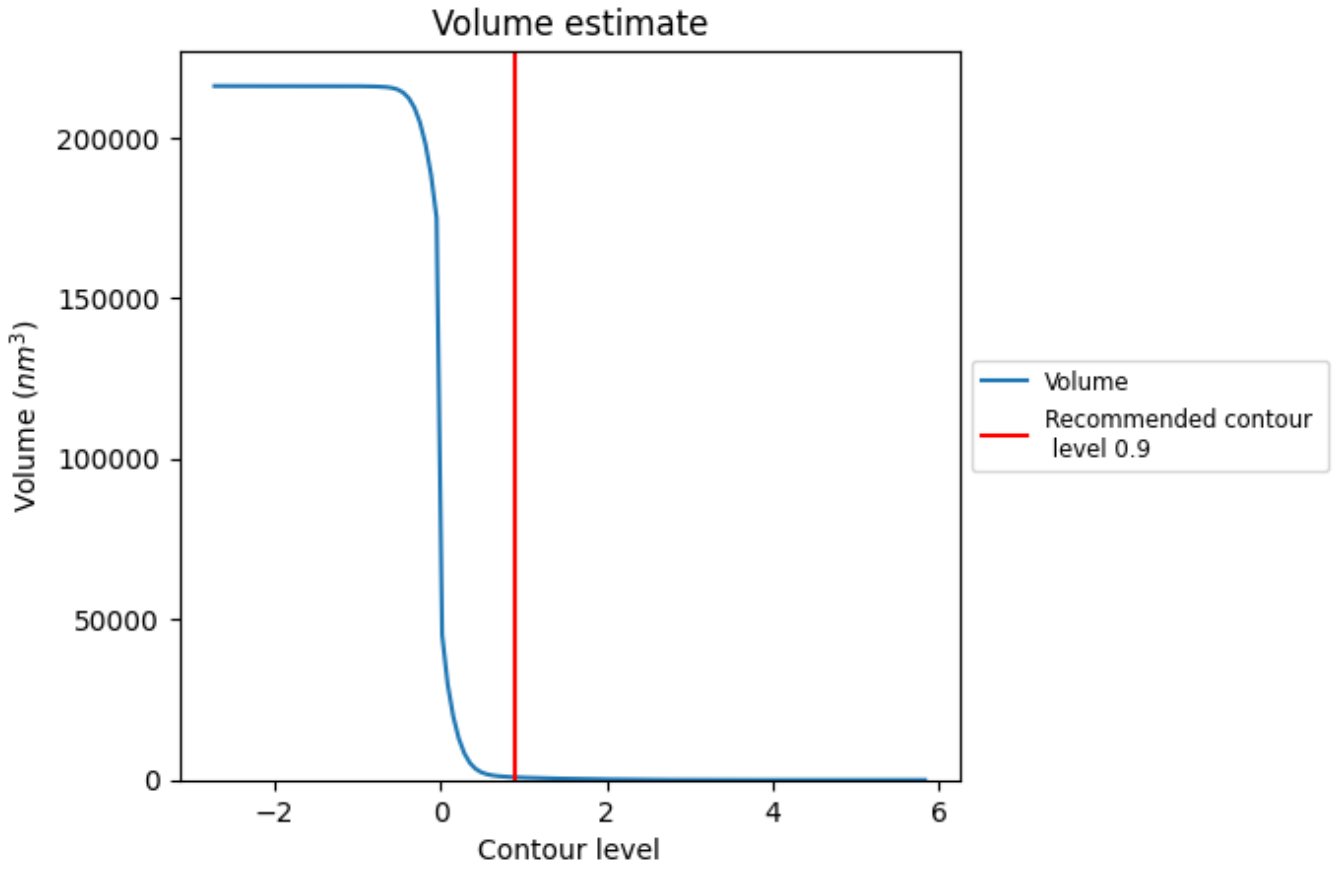
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

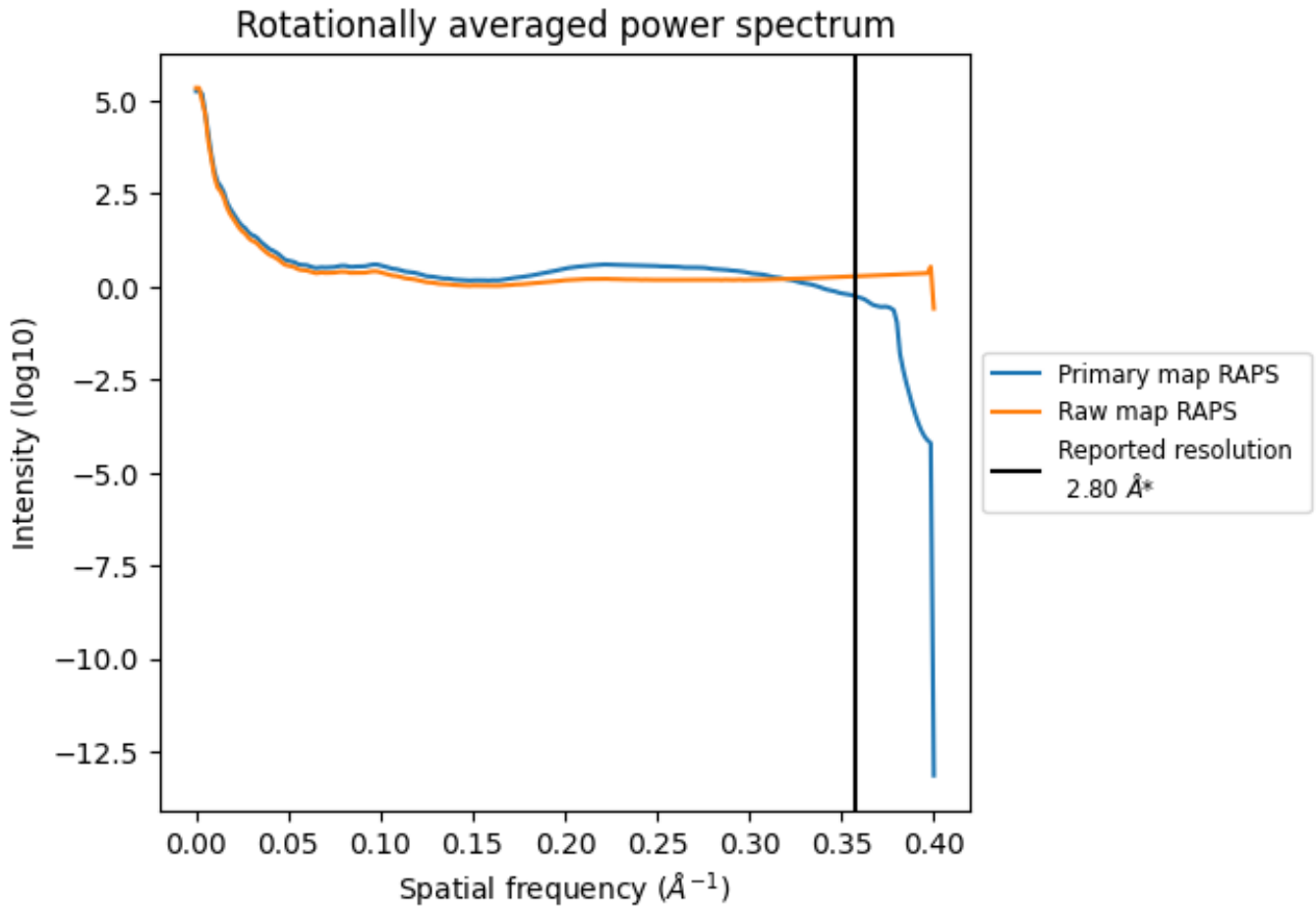
7.2 Volume estimate (i)



The volume at the recommended contour level is 843 nm^3; this corresponds to an approximate mass of 762 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)

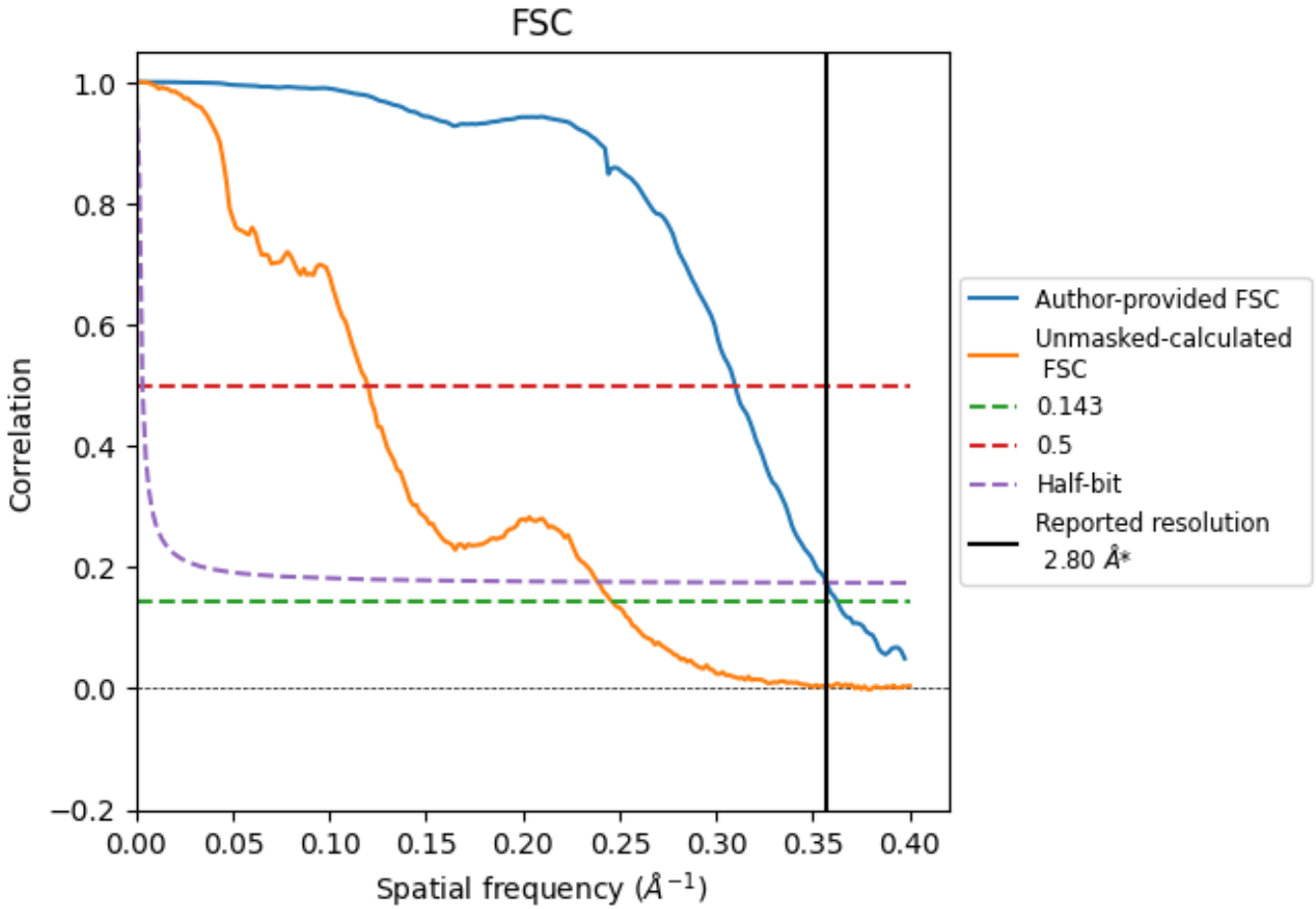


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

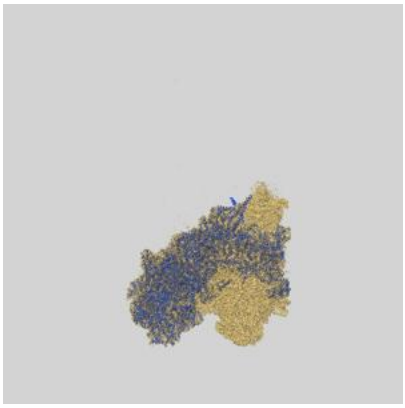
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.76	3.23	2.80
Unmasked-calculated*	4.06	8.35	4.19

*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 4.06 differs from the reported value 2.8 by more than 10 %

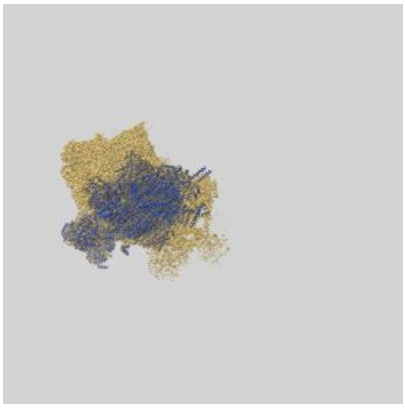
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15865 and PDB model 8B6F. Per-residue inclusion information can be found in section 3 on page 26.

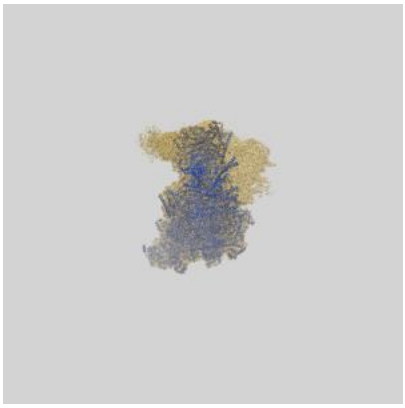
9.1 Map-model overlay



X



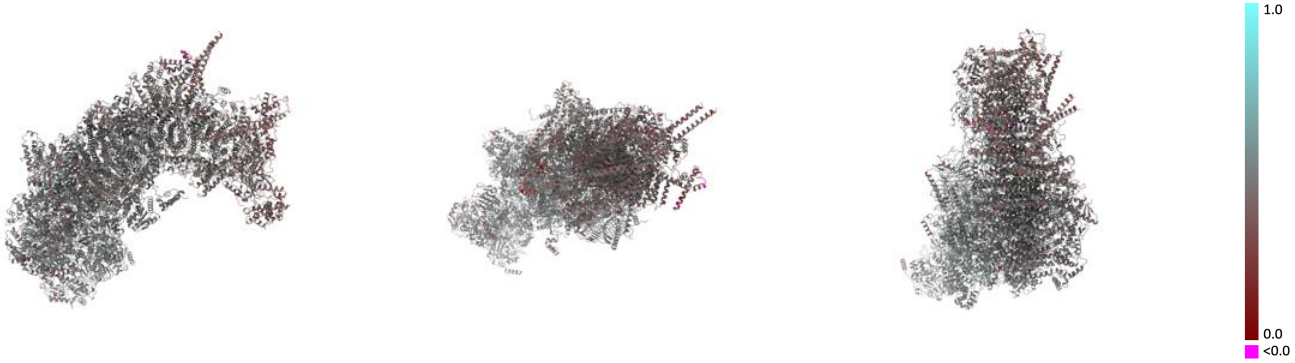
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9 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.

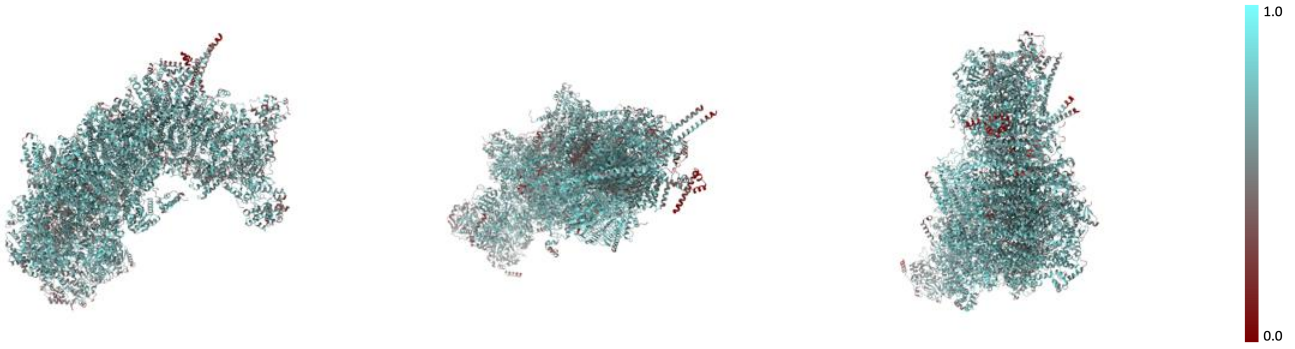
9.2 Q-score mapped to coordinate model



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.

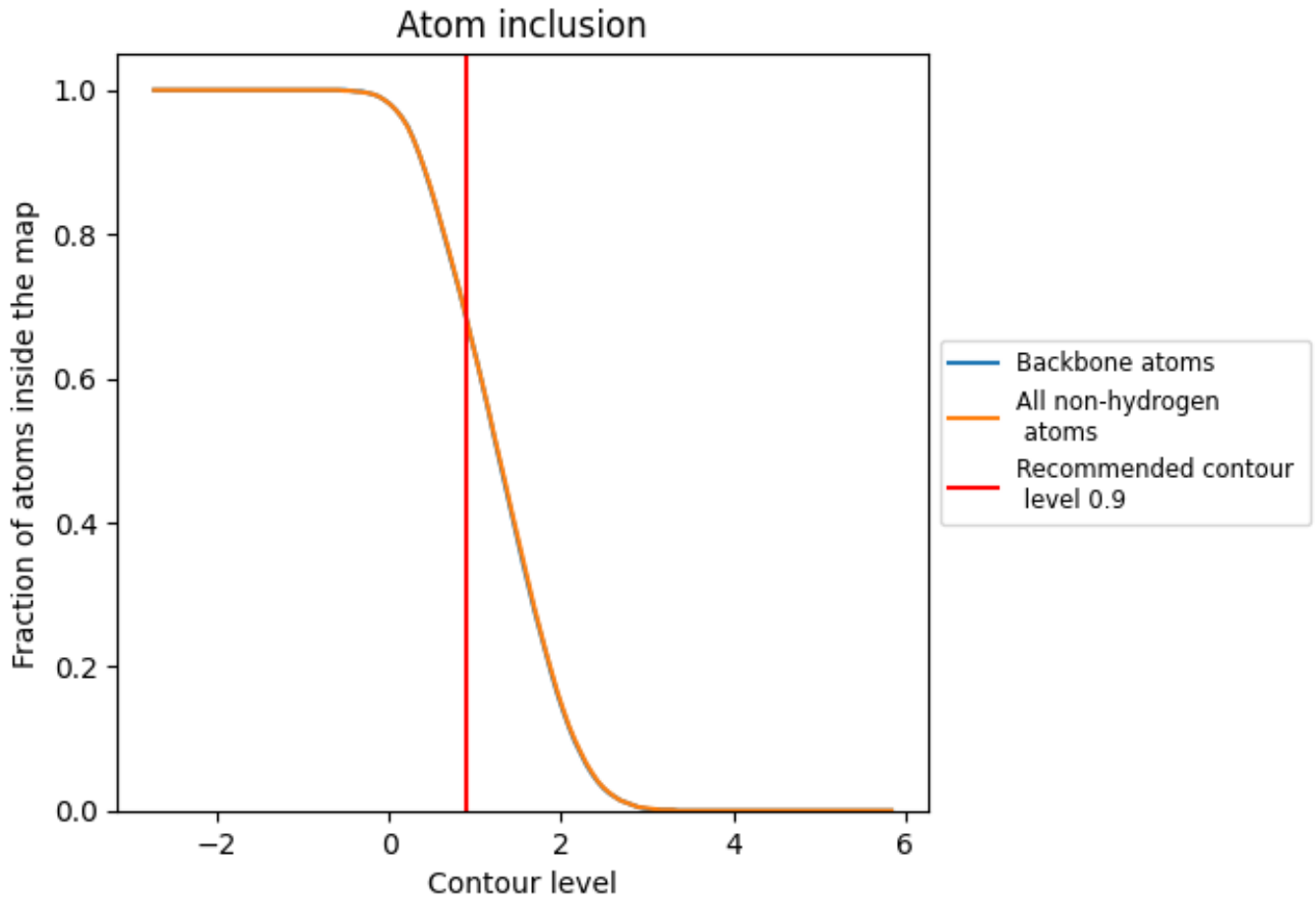
9.3 Atom inclusion mapped to coordinate model



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 (0.9).

9.4 Atom inclusion (i)



At the recommended contour level, 68% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6850	0.4630
A0	0.6510	0.4540
A1	0.7180	0.4840
A2	0.6830	0.4610
A3	0.5250	0.4510
A4	0.5720	0.3870
A5	0.7200	0.4890
A6	0.6880	0.4230
A7	0.7030	0.4540
A8	0.7050	0.5010
A9	0.6710	0.4470
AA	0.6540	0.4260
AB	0.6810	0.4860
AC	0.7300	0.4560
AD	0.6030	0.4830
AE	0.7770	0.5050
AF	0.7440	0.4730
AG	0.7320	0.4920
AH	0.7330	0.4880
AI	0.5940	0.4700
AJ	0.7320	0.4760
AK	0.7860	0.4980
AL	0.7750	0.5100
AM	0.7110	0.4730
AN	0.7220	0.5010
AO	0.7760	0.5070
AP	0.7300	0.4960
AQ	0.7220	0.4490
AR	0.7110	0.5000
AS	0.7760	0.4920
AT	0.7850	0.5010
AU	0.6610	0.4630
AV	0.7020	0.4770
AW	0.7040	0.4570
AX	0.7480	0.4870



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Chain	Atom inclusion	Q-score
AY	0.7590	0.4970
AZ	0.6130	0.4490
B0	0.6870	0.4590
B1	0.6490	0.4560
B2	0.6810	0.4490
B3	0.7020	0.4380
B4	0.6300	0.4390
B5	0.6950	0.4610
B6	0.7880	0.5130
BA	0.5750	0.3710
BB	0.6560	0.4170
BC	0.6560	0.4260
BD	0.6600	0.4210
BE	0.6510	0.4250
BF	0.7190	0.4340
BG	0.7080	0.4670
BH	0.7700	0.4720
BI	0.7840	0.4840
BJ	0.7350	0.4660
BK	0.6760	0.4410
BL	0.6770	0.4640
BM	0.7490	0.4790
BN	0.6820	0.4520
BO	0.6460	0.4250
BP	0.7360	0.4550
BQ	0.6620	0.4510
BR	0.7480	0.5090
BS	0.6650	0.4120
BT	0.6930	0.4480
BU	0.5560	0.4140
BV	0.6830	0.4420
BW	0.6900	0.4210
BX	0.7190	0.4580
BY	0.7080	0.4600
BZ	0.7220	0.4640