wwPDB EM Validation Summary Report (i)

Aug 6, 2026 – 02:05 AM JST

PDB ID	:	6KHI / pdb_00006khi
EMDB ID	:	EMD-9989
Title	:	Supercomplex for cylic electron transport in cyanobacteria
Authors	:	Pan, X.; Cao, D.; Xie, F.; Zhang, X.; Li, M.
Deposited on	:	2019-07-15
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

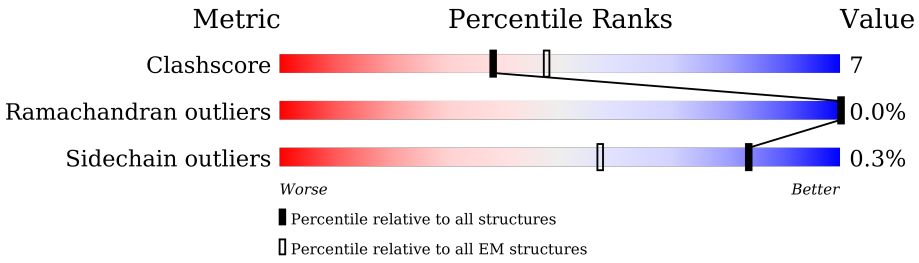
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

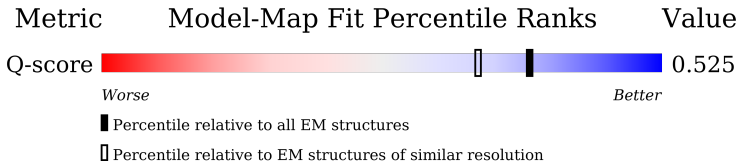
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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.





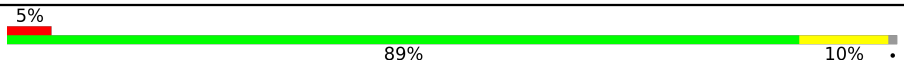
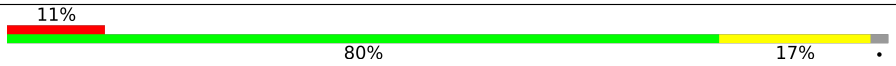
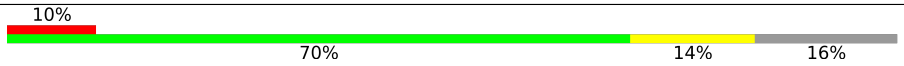
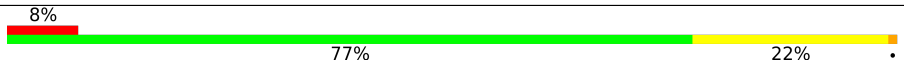
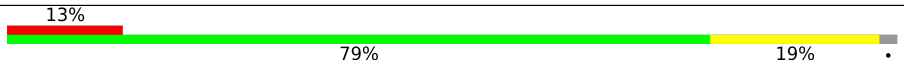
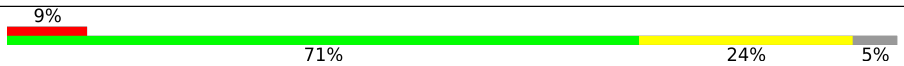
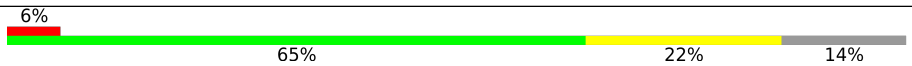
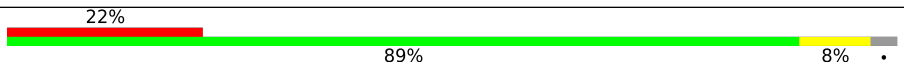
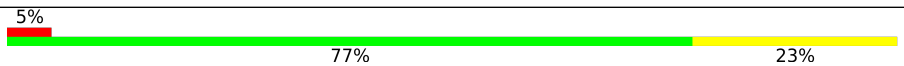
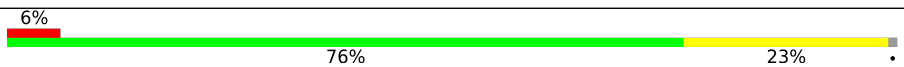
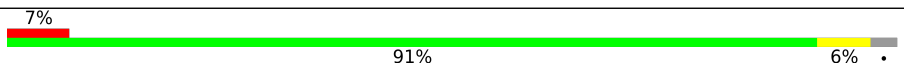
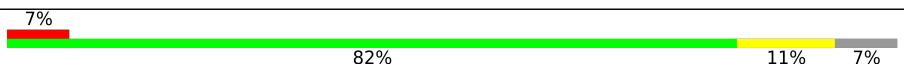
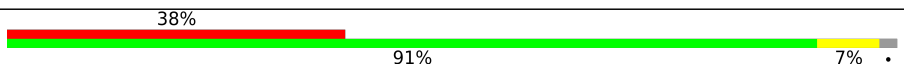
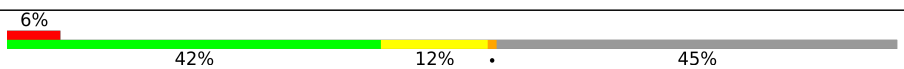
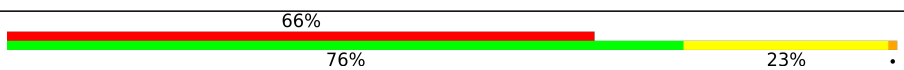
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	A	372	9% 81% 18%
2	B	515	79% 16%
3	C	132	7% 72% 19% 9%
4	D	529	5% 74% 22% 5%

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Mol	Chain	Length	Quality of chain
5	E	101	
6	F	656	
7	G	200	
8	H	394	
9	I	196	
10	J	168	
11	K	237	
12	L	76	
13	M	111	
14	N	150	
15	O	70	
16	P	44	
17	Q	45	
18	S	110	
19	V	146	
20	1	98	

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
24	BCR	D	602	-	X	-	-
24	BCR	D	603	-	X	-	-

2 Entry composition (i)

There are 27 unique types of molecules in this entry. The entry contains 32635 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NAD(P)H-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	366	2821	1893	439	478	11	0	0

- Molecule 2 is a protein called NAD(P)H-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	492	3724	2472	578	658	16	0	0

- Molecule 3 is a protein called NAD(P)H-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	120	971	665	149	153	4	0	0

- Molecule 4 is a protein called NAD(P)H-quinone oxidoreductase chain 4 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	504	3897	2614	606	655	22	0	0

- Molecule 5 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	100	775	512	127	133	3	0	0

- Molecule 6 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	641	4945	3285	778	845	37	0	0

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	169	Total	C	N	O	S	0	0
			1278	855	200	219	4		

- Molecule 8 is a protein called NAD(P)H-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	393	Total	C	N	O	S	0	0
			3177	2048	545	565	19		

- Molecule 9 is a protein called NAD(P)H-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	192	Total	C	N	O	S	0	0
			1537	979	264	281	13		

- Molecule 10 is a protein called NAD(P)H-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	160	Total	C	N	O	S	0	0
			1307	836	222	244	5		

- Molecule 11 is a protein called NAD(P)H-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	205	Total	C	N	O	S	0	0
			1590	1019	275	283	13		

- Molecule 12 is a protein called NAD(P)H-quinone oxidoreductase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	74	Total	C	N	O	S	0	0
			595	409	91	94	1		

- Molecule 13 is a protein called NAD(P)H-quinone oxidoreductase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	111	Total	C	N	O	S	0	0
			885	551	161	171	2		

- Molecule 14 is a protein called NAD(P)H-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	148	Total	C	N	O	S	0	0
			1165	758	201	205	1		

- Molecule 15 is a protein called NAD(P)H-quinone oxidoreductase subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	68	Total	C	N	O	0	0
			538	349	91	98		

- Molecule 16 is a protein called proton-translocating NADH-quinone dehydrogenase subunit P.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	41	Total	C	N	O	S	0	0
			321	212	52	55	2		

- Molecule 17 is a protein called proton-translocating NADH-quinone dehydrogenase subunit Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	44	Total	C	N	O	S	0	0
			333	222	53	56	2		

- Molecule 18 is a protein called Tlr0636 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	60	Total	C	N	O	S	0	0
			469	304	74	89	2		

- Molecule 19 is a protein called Tlr0472 protein.

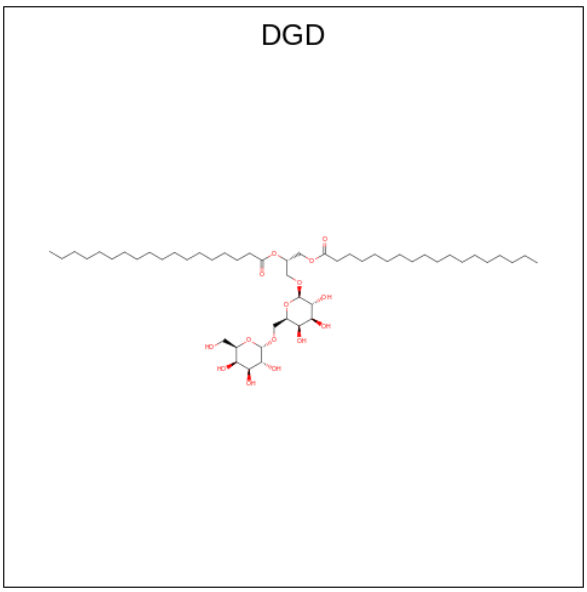
Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	109	Total	C	N	O	S	0	0
			838	545	139	150	4		

- Molecule 20 is a protein called Ferredoxin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1	98	Total	C	N	O	S	0	0
			756	468	117	165	6		

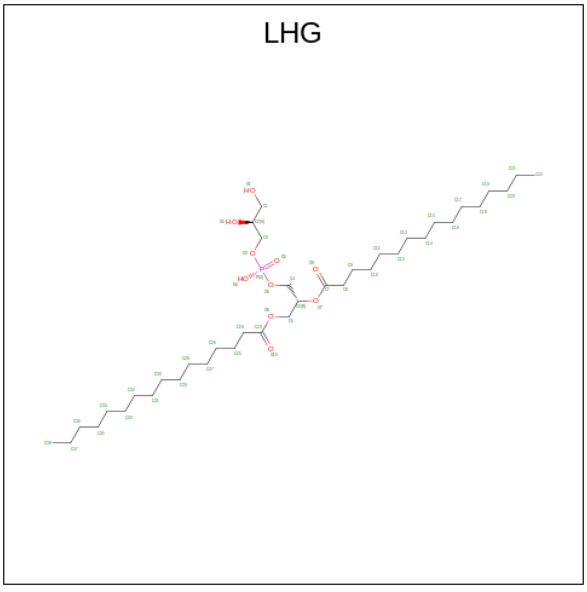
- Molecule 21 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:

$C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



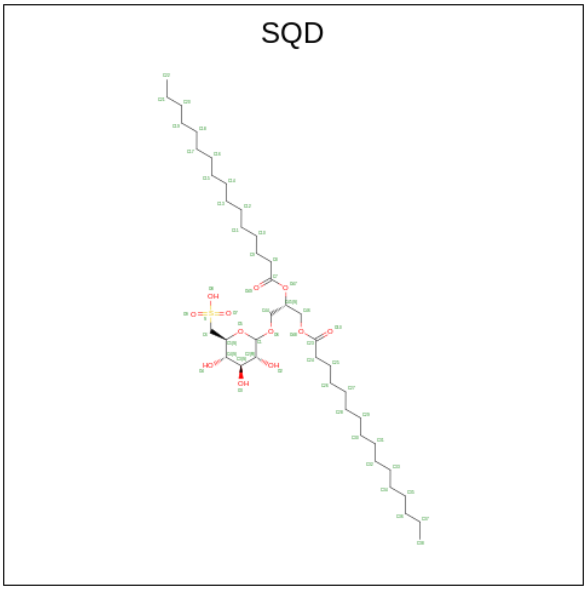
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C O 62 47 15	0
21	A	1	Total C O 62 47 15	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



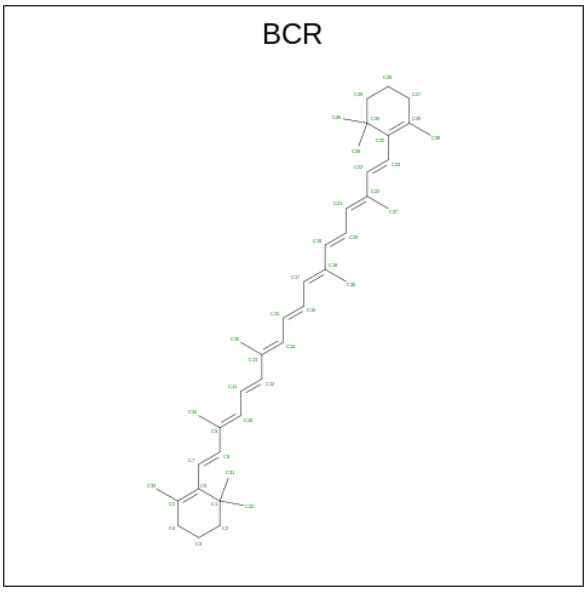
Mol	Chain	Residues	Atoms				AltConf
22	B	1	Total	C	O	P	0
			46	35	10	1	
22	C	1	Total	C	O	P	0
			43	32	10	1	
22	F	1	Total	C	O	P	0
			49	38	10	1	
22	F	1	Total	C	O	P	0
			36	25	10	1	
22	F	1	Total	C	O	P	0
			44	33	10	1	
22	I	1	Total	C	O	P	0
			44	33	10	1	

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



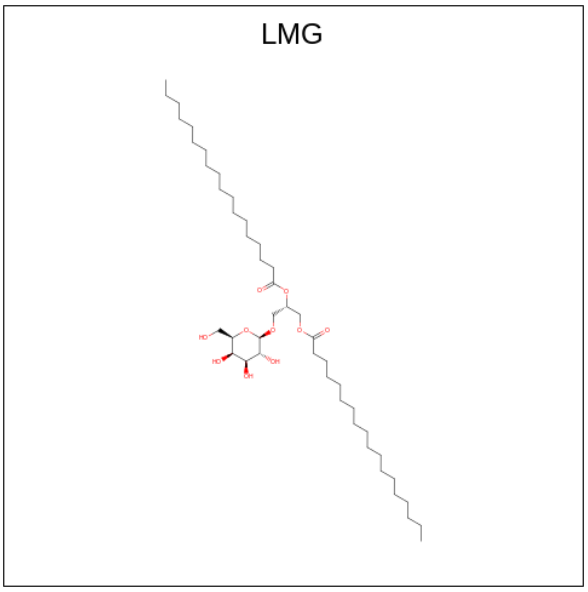
Mol	Chain	Residues	Atoms				AltConf
23	C	1	Total	C	O	S	0
			40	27	12	1	
23	D	1	Total	C	O	S	0
			54	41	12	1	
23	L	1	Total	C	O	S	0
			38	25	12	1	

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
24	D	1	Total C 40 40	0
24	D	1	Total C 40 40	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



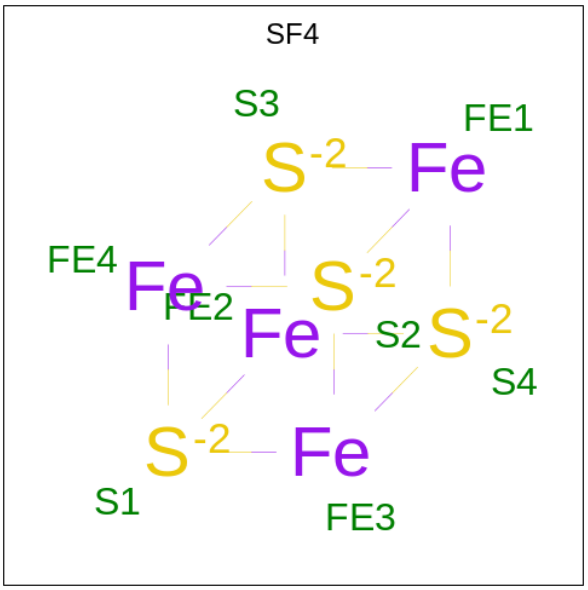
Mol	Chain	Residues	Atoms	AltConf
25	F	1	Total C O 47 37 10	0

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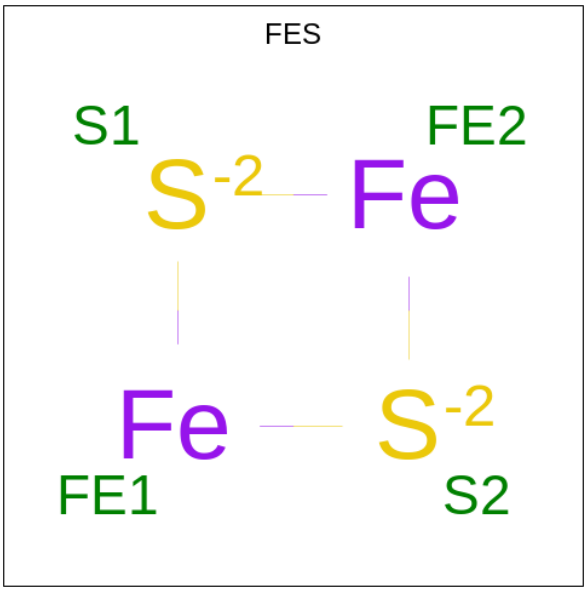
Mol	Chain	Residues	Atoms			AltConf
25	F	1	Total	C	O	0
			40	30	10	

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	I	1	Total	Fe	S	0
			8	4	4	
26	I	1	Total	Fe	S	0
			8	4	4	
26	K	1	Total	Fe	S	0
			8	4	4	

- Molecule 27 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

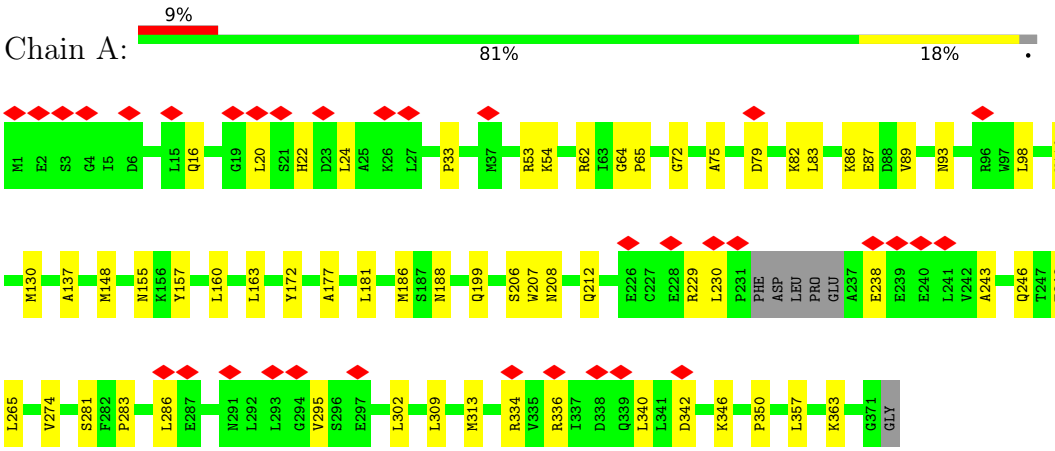


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
27	1	1	4	2	2	0

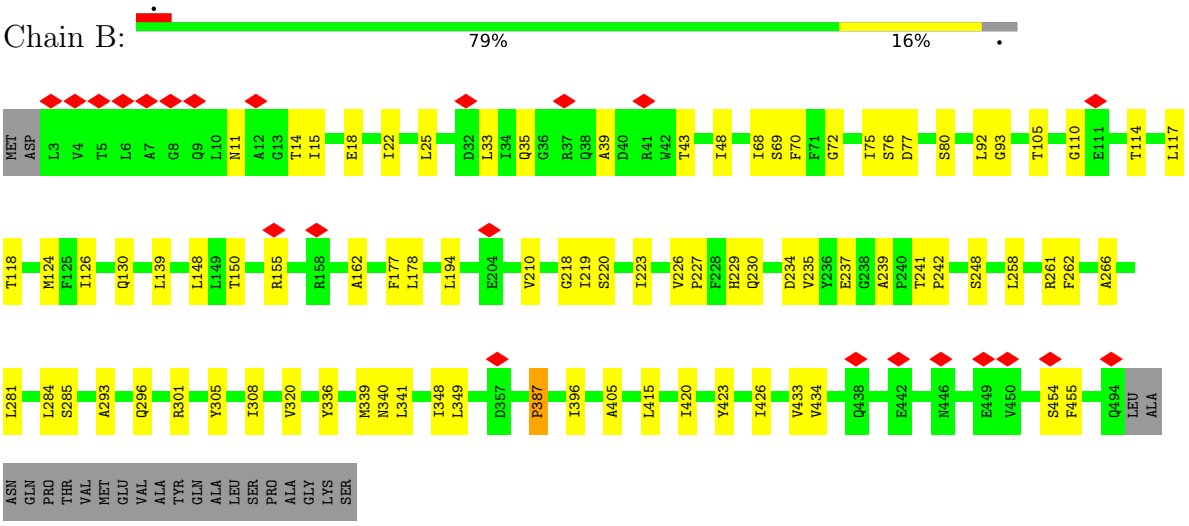
3 Residue-property plots

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

• Molecule 1: NAD(P)H-quinone oxidoreductase subunit 1

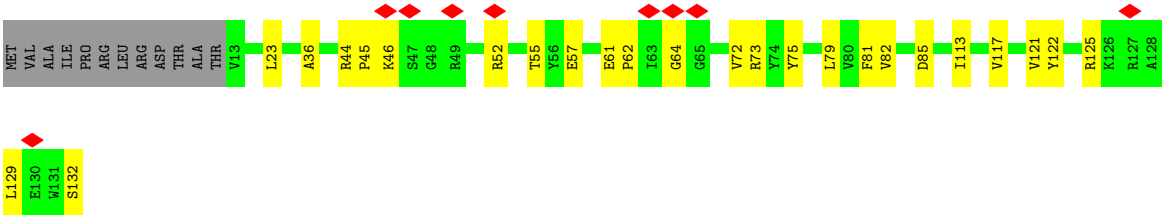


• Molecule 2: NAD(P)H-quinone oxidoreductase subunit 2

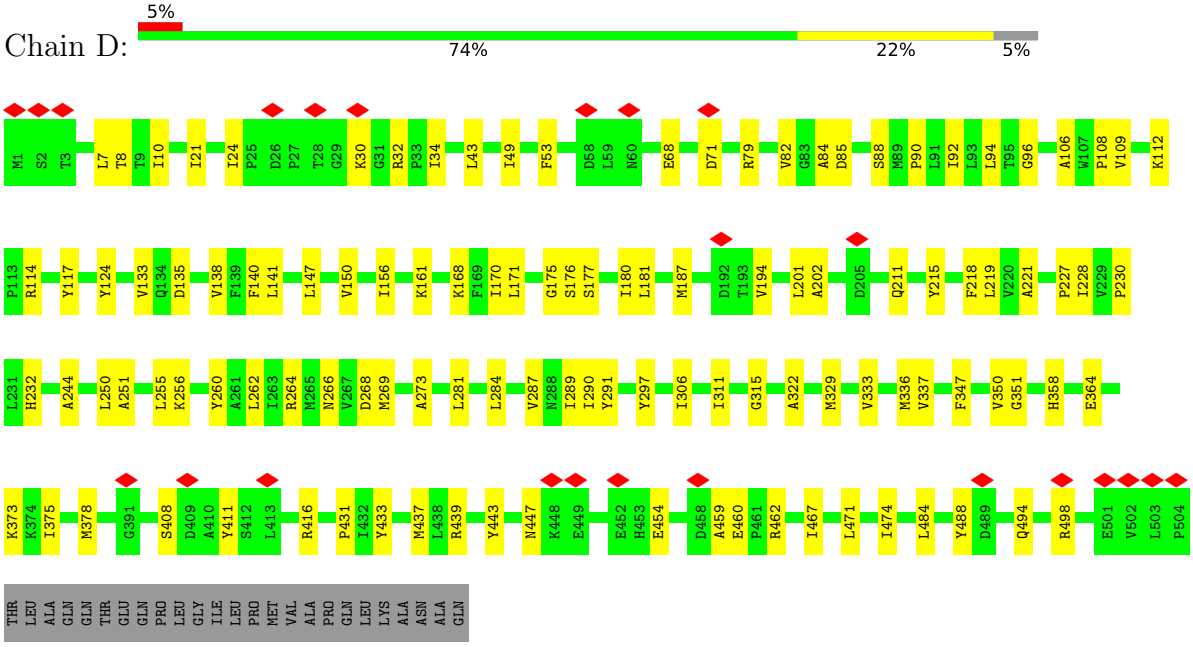


• Molecule 3: NAD(P)H-quinone oxidoreductase subunit 3

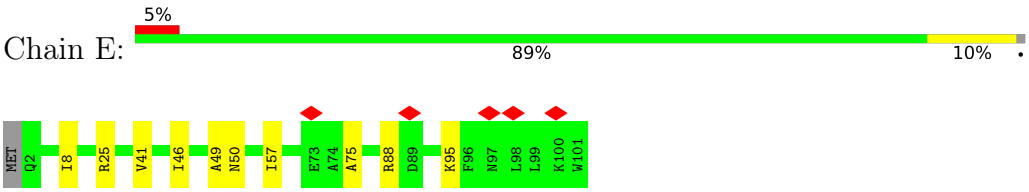




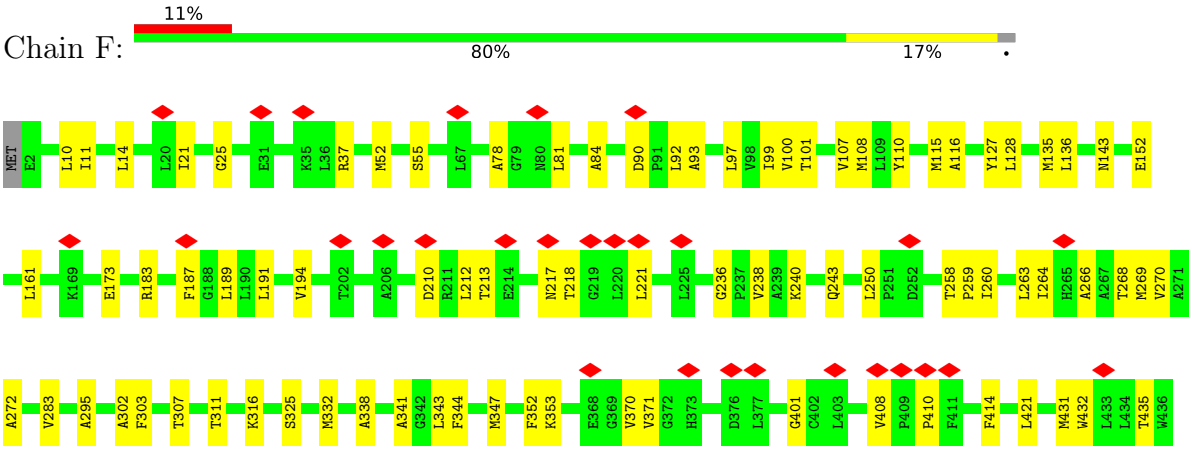
• Molecule 4: NAD(P)H-quinone oxidoreductase chain 4 1

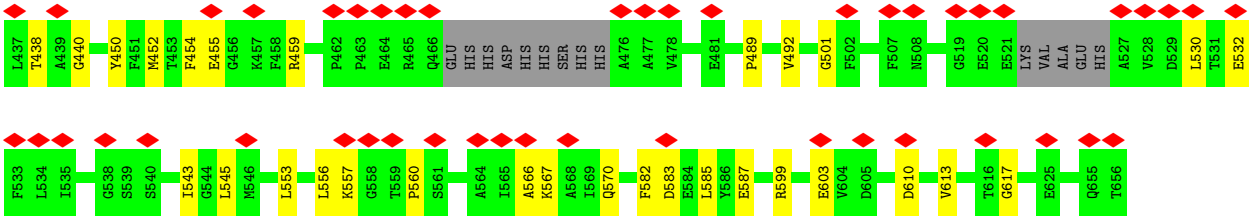


• Molecule 5: NAD(P)H-quinone oxidoreductase subunit 4L

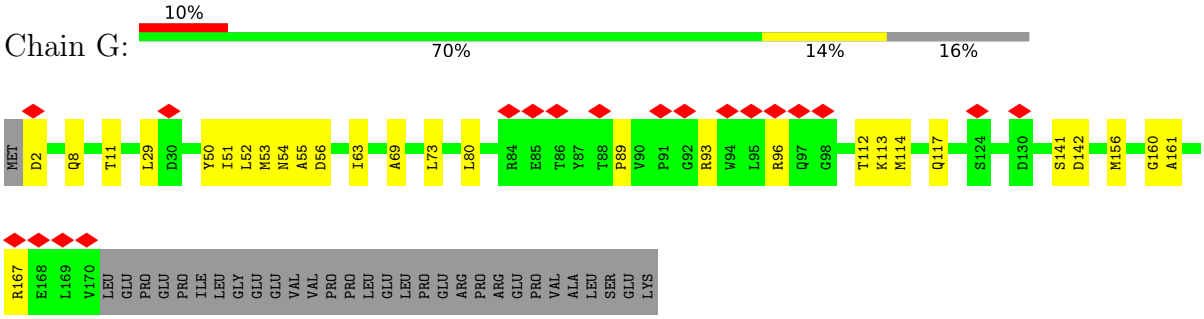


• Molecule 6: NADH dehydrogenase subunit 5

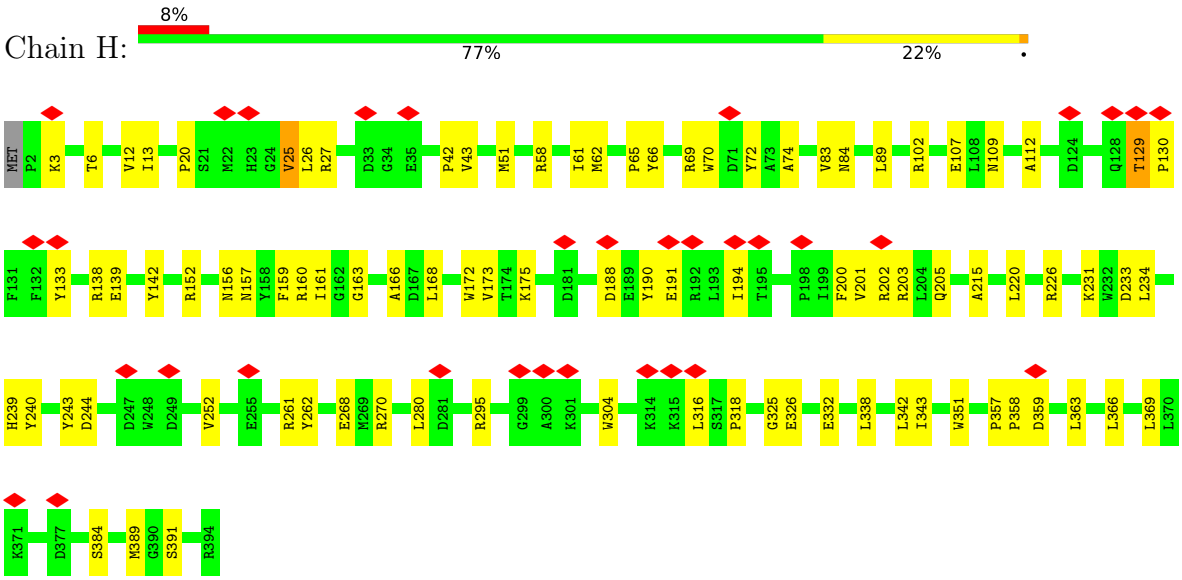




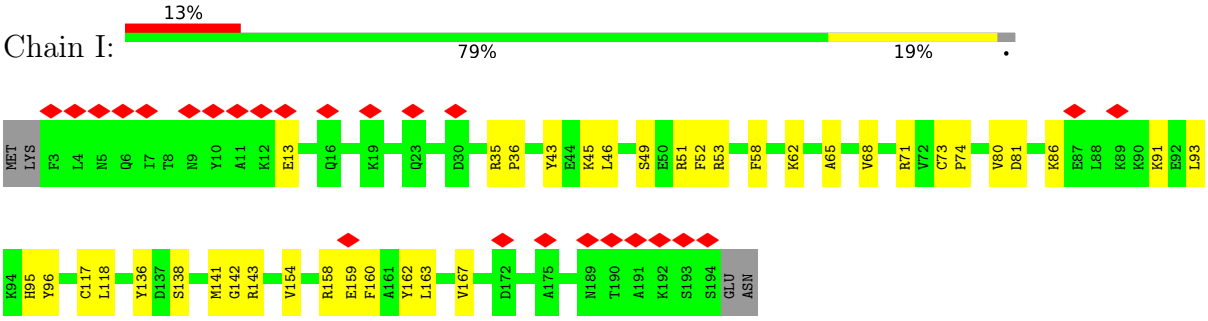
• Molecule 7: NADH-quinone oxidoreductase subunit J



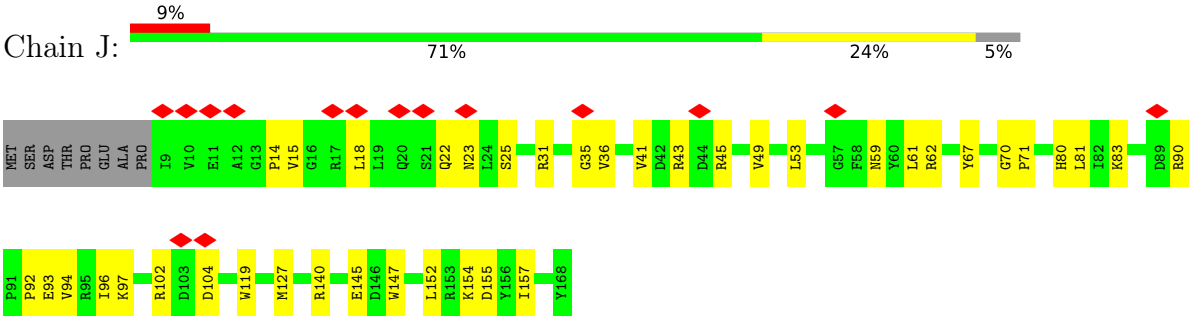
• Molecule 8: NAD(P)H-quinone oxidoreductase subunit H



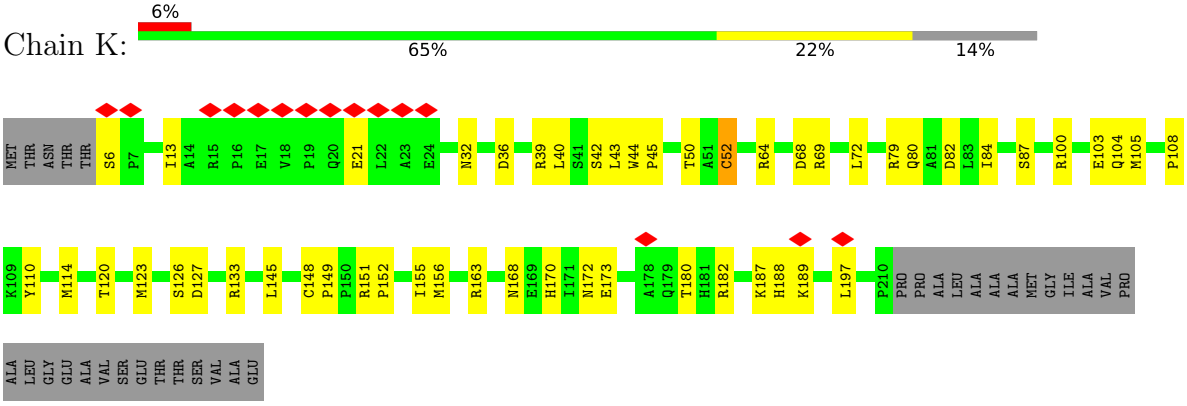
• Molecule 9: NAD(P)H-quinone oxidoreductase subunit I



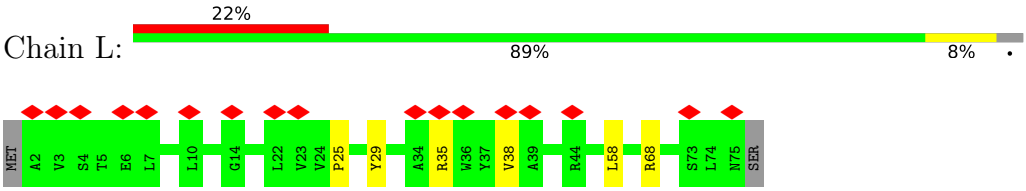
• Molecule 10: NAD(P)H-quinone oxidoreductase subunit J



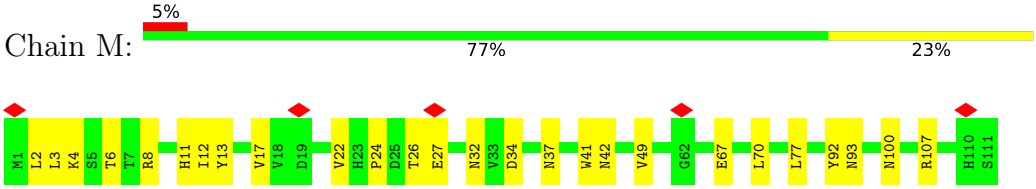
• Molecule 11: NAD(P)H-quinone oxidoreductase subunit K



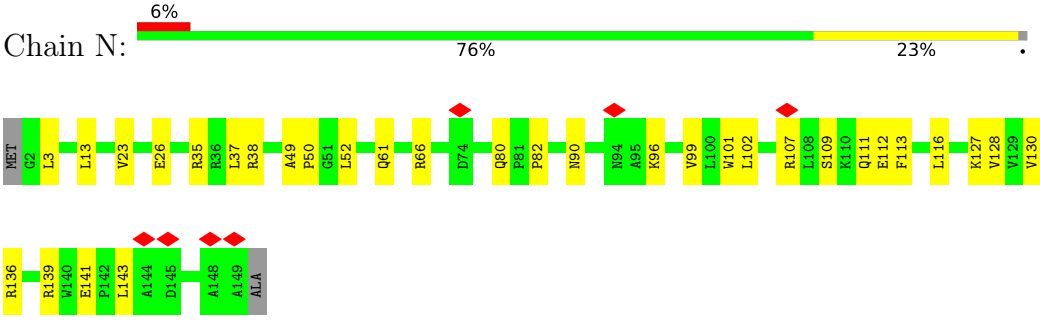
• Molecule 12: NAD(P)H-quinone oxidoreductase subunit L



• Molecule 13: NAD(P)H-quinone oxidoreductase subunit M

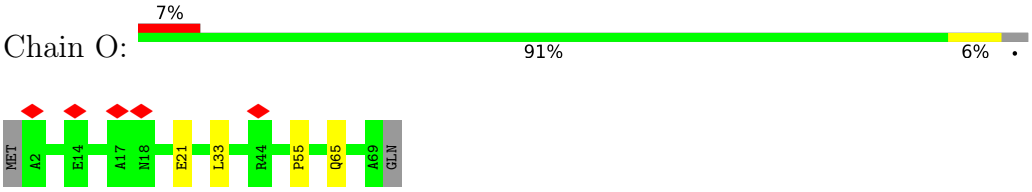


• Molecule 14: NAD(P)H-quinone oxidoreductase subunit N



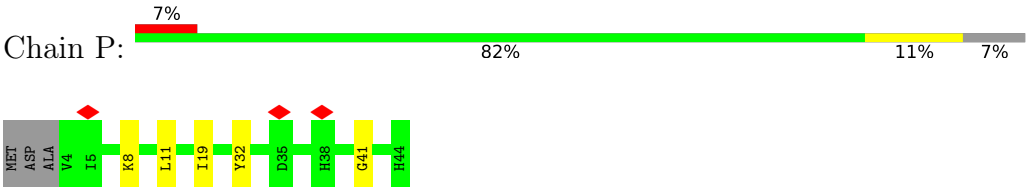
• Molecule 15: NAD(P)H-quinone oxidoreductase subunit O

Chain O:



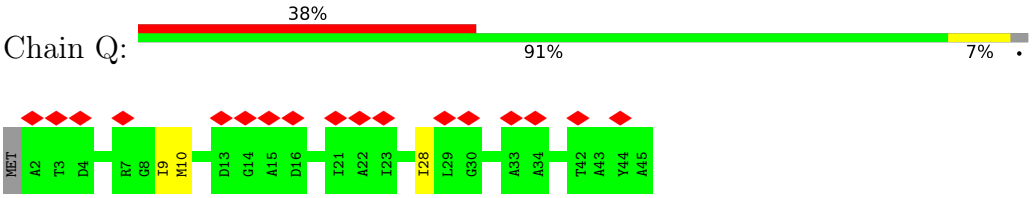
• Molecule 16: proton-translocating NADH-quinone dehydrogenase subunit P

Chain P:



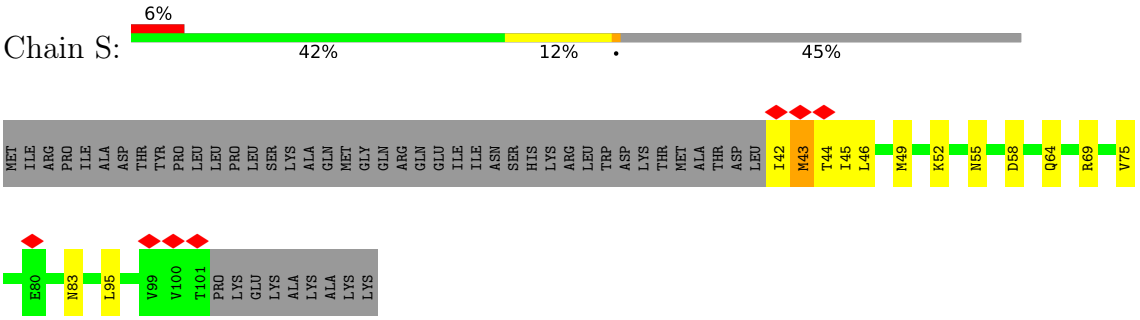
• Molecule 17: proton-translocating NADH-quinone dehydrogenase subunit Q

Chain Q:



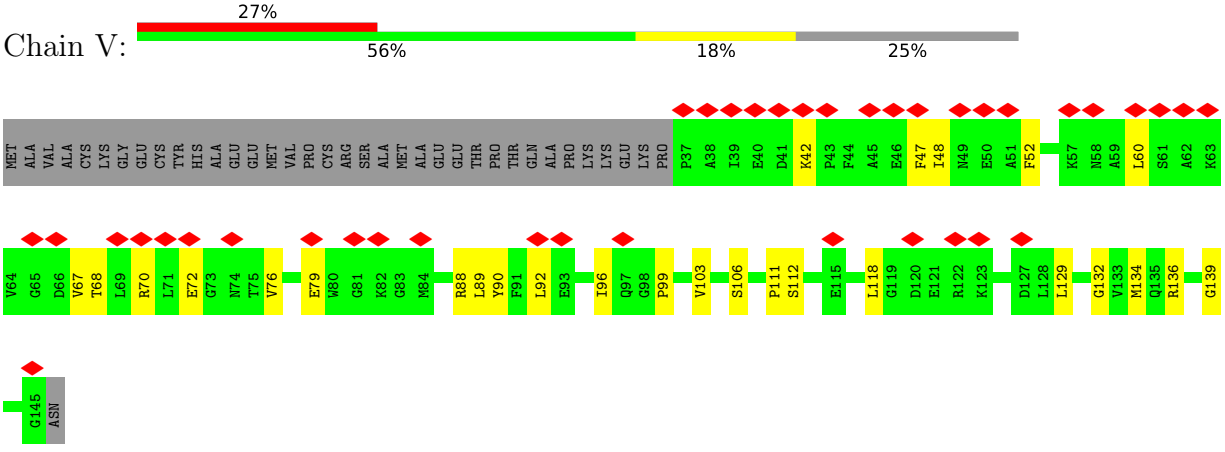
• Molecule 18: Tlr0636 protein

Chain S:



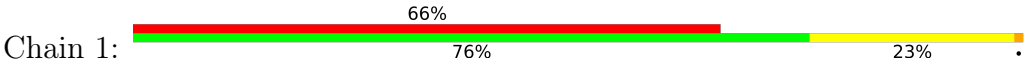
• Molecule 19: Tlr0472 protein

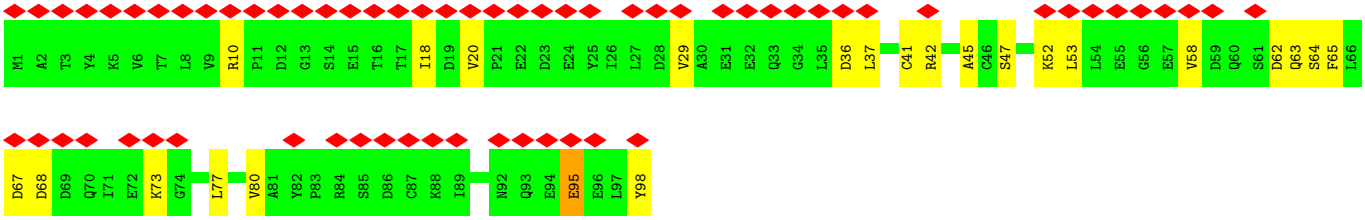
Chain V:



• Molecule 20: Ferredoxin-1

Chain 1:




M1 A2 T3 Y4 K5 V6 T7 L8 V9 R10 P11 D12 G13 S14 E15 T16 T17 I18 D19 V20 P21 E22 D23 E24 Y25 I26 L27 D28 V29 A30 E31 E32 Q33 G34 L35 D36 L37 C41 R42 A45 C46 S47 K52 L53 L54 E55 G56 E57 V58 D59 Q60 S61 D62 Q63 S64 F65 L66
D67 D68 D69 Q70 I71 E72 K73 G74 L77 V80 A81 Y82 P83 R84 S85 D86 C87 K88 I89 N92 Q93 E94 E95 E96 L97 Y98

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	152003	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 ($e^-/Å^2$)	60.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.417	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, LHG, FES, LMG, DGD, SF4, SQD

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	A	0.25	0/2891	0.56	0/3949
2	B	0.25	0/3810	0.52	1/5198 (0.0%)
3	C	0.25	0/1001	0.61	0/1365
4	D	0.25	0/4004	0.49	0/5464
5	E	0.22	0/785	0.45	0/1067
6	F	0.23	0/5087	0.51	0/6930
7	G	0.22	0/1304	0.44	0/1786
8	H	0.28	1/3260 (0.0%)	0.56	0/4417
9	I	0.29	0/1575	0.58	0/2135
10	J	0.22	0/1343	0.52	0/1829
11	K	0.31	0/1630	0.63	0/2218
12	L	0.21	0/615	0.52	0/842
13	M	0.21	0/901	0.54	0/1222
14	N	0.22	0/1197	0.50	0/1628
15	O	0.21	0/550	0.50	0/748
16	P	0.24	0/330	0.51	0/448
17	Q	0.17	0/342	0.38	0/466
18	S	0.22	0/478	0.55	2/652 (0.3%)
19	V	0.24	0/857	0.60	0/1155
20	1	0.20	0/766	0.46	0/1039
All	All	0.25	1/32726 (0.0%)	0.53	3/44558 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	129	THR	C-N	5.79	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	S	43	MET	CA-C-N	5.70	132.43	121.54
18	S	43	MET	C-N-CA	5.70	132.43	121.54
2	B	387	PRO	N-CA-C	5.24	117.10	110.70

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	A	2821	0	2958	44	0
2	B	3724	0	3861	58	0
3	C	971	0	1001	24	0
4	D	3897	0	4046	78	0
5	E	775	0	825	8	0
6	F	4945	0	4997	70	0
7	G	1278	0	1360	23	0
8	H	3177	0	3157	64	0
9	I	1537	0	1505	30	0
10	J	1307	0	1264	26	0
11	K	1590	0	1621	44	0
12	L	595	0	608	4	0
13	M	885	0	865	18	0
14	N	1165	0	1176	28	0
15	O	538	0	549	3	0
16	P	321	0	317	5	0
17	Q	333	0	333	2	0
18	S	469	0	473	8	0
19	V	838	0	845	17	0
20	1	756	0	714	17	0
21	A	124	0	170	3	0
22	B	46	0	62	0	0
22	C	43	0	59	3	0
22	F	129	0	177	0	0
22	I	44	0	61	0	0
23	C	40	0	44	2	0
23	D	54	0	78	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	L	38	0	40	2	0
24	D	80	0	112	7	0
25	F	87	0	114	4	0
26	I	16	0	0	1	0
26	K	8	0	0	0	0
27	1	4	0	0	0	0
All	All	32635	0	33392	490	0

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

The worst 5 of 490 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)
2:B:22:ILE:O	2:B:25:LEU:HB3	1.82	0.80
8:H:130:PRO:O	8:H:133:TYR:HB2	1.86	0.74
10:J:62:ARG:O	10:J:80:HIS:HB3	1.94	0.68
8:H:326:GLU:HA	8:H:342:LEU:O	1.96	0.66
3:C:73:ARG:HD2	3:C:132:SER:HA	1.78	0.65

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	A	362/372 (97%)	329 (91%)	33 (9%)	0	100	100
2	B	490/515 (95%)	465 (95%)	25 (5%)	0	100	100
3	C	118/132 (89%)	106 (90%)	12 (10%)	0	100	100
4	D	502/529 (95%)	474 (94%)	28 (6%)	0	100	100
5	E	98/101 (97%)	94 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	635/656 (97%)	574 (90%)	61 (10%)	0	100	100
7	G	167/200 (84%)	159 (95%)	8 (5%)	0	100	100
8	H	391/394 (99%)	342 (88%)	49 (12%)	0	100	100
9	I	190/196 (97%)	166 (87%)	24 (13%)	0	100	100
10	J	158/168 (94%)	135 (85%)	23 (15%)	0	100	100
11	K	203/237 (86%)	184 (91%)	18 (9%)	1 (0%)	24	60
12	L	72/76 (95%)	65 (90%)	7 (10%)	0	100	100
13	M	109/111 (98%)	93 (85%)	16 (15%)	0	100	100
14	N	146/150 (97%)	132 (90%)	14 (10%)	0	100	100
15	O	66/70 (94%)	61 (92%)	5 (8%)	0	100	100
16	P	39/44 (89%)	36 (92%)	3 (8%)	0	100	100
17	Q	42/45 (93%)	42 (100%)	0	0	100	100
18	S	58/110 (53%)	54 (93%)	4 (7%)	0	100	100
19	V	107/146 (73%)	86 (80%)	21 (20%)	0	100	100
20	1	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
All	All	4049/4350 (93%)	3686 (91%)	362 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	149	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	A	297/302 (98%)	297 (100%)	0	100	100
2	B	395/413 (96%)	395 (100%)	0	100	100
3	C	99/109 (91%)	98 (99%)	1 (1%)	68	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	404/424 (95%)	403 (100%)	1 (0%)	87 92
5	E	81/82 (99%)	81 (100%)	0	100 100
6	F	513/527 (97%)	512 (100%)	1 (0%)	87 92
7	G	137/166 (82%)	137 (100%)	0	100 100
8	H	337/338 (100%)	335 (99%)	2 (1%)	78 88
9	I	168/172 (98%)	168 (100%)	0	100 100
10	J	141/148 (95%)	141 (100%)	0	100 100
11	K	174/196 (89%)	171 (98%)	3 (2%)	53 78
12	L	61/63 (97%)	61 (100%)	0	100 100
13	M	96/96 (100%)	96 (100%)	0	100 100
14	N	119/120 (99%)	119 (100%)	0	100 100
15	O	57/59 (97%)	57 (100%)	0	100 100
16	P	35/37 (95%)	35 (100%)	0	100 100
17	Q	31/32 (97%)	31 (100%)	0	100 100
18	S	53/97 (55%)	53 (100%)	0	100 100
19	V	87/118 (74%)	87 (100%)	0	100 100
20	1	86/86 (100%)	85 (99%)	1 (1%)	63 82
All	All	3371/3585 (94%)	3362 (100%)	9 (0%)	84 91

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	120	THR
20	1	95	GLU
8	H	25	VAL
8	H	129	THR
11	K	50	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	305	ASN
10	J	87	ASN
19	V	49	ASN
8	H	310	GLN

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Mol	Chain	Res	Type
10	J	20	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)

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	LMG	F	703	-	40,40,55	0.93	1 (2%)	48,48,63	1.24	4 (8%)
26	SF4	K	301	11	0,12,12	-	-	-		
24	BCR	D	602	-	41,41,41	5.49	17 (41%)	56,56,56	5.54	36 (64%)
22	LHG	B	601	-	45,45,48	0.93	4 (8%)	48,51,54	1.09	2 (4%)
22	LHG	I	201	-	43,43,48	0.94	4 (9%)	46,49,54	1.08	2 (4%)
27	FES	1	101	20	0,4,4	-	-	-		
26	SF4	I	203	9	0,12,12	-	-	-		
22	LHG	F	705	-	43,43,48	0.95	4 (9%)	46,49,54	1.08	2 (4%)
21	DGD	A	401	-	63,63,67	1.22	5 (7%)	77,77,81	1.16	4 (5%)
22	LHG	C	202	-	42,42,48	0.95	4 (9%)	45,48,54	1.09	2 (4%)
26	SF4	I	202	9	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	DGD	A	402	-	63,63,67	1.23	6 (9%)	77,77,81	1.18	4 (5%)
24	BCR	D	603	-	41,41,41	5.53	17 (41%)	56,56,56	5.36	33 (58%)
25	LMG	F	701	-	47,47,55	0.87	2 (4%)	55,55,63	1.41	7 (12%)
23	SQD	D	601	-	53,54,54	1.90	11 (20%)	62,65,65	5.64	6 (9%)
22	LHG	F	704	-	35,35,48	1.04	4 (11%)	38,41,54	1.14	2 (5%)
23	SQD	L	101	-	37,38,54	2.19	10 (27%)	46,49,65	6.52	9 (19%)
22	LHG	F	702	-	48,48,48	0.90	4 (8%)	51,54,54	1.08	2 (3%)
23	SQD	C	201	-	39,40,54	2.18	11 (28%)	48,51,65	6.39	6 (12%)

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
25	LMG	F	703	-	-	14/35/55/70	0/1/1/1
26	SF4	K	301	11	-	-	0/6/5/5
24	BCR	D	602	-	-	16/29/63/63	0/2/2/2
22	LHG	B	601	-	-	23/50/50/53	-
22	LHG	I	201	-	-	19/48/48/53	-
27	FES	1	101	20	-	-	0/1/1/1
26	SF4	I	203	9	-	-	0/6/5/5
22	LHG	F	705	-	-	23/48/48/53	-
21	DGD	A	401	-	-	24/51/91/95	0/2/2/2
22	LHG	C	202	-	-	23/47/47/53	-
26	SF4	I	202	9	-	-	0/6/5/5
21	DGD	A	402	-	-	15/51/91/95	0/2/2/2
24	BCR	D	603	-	-	15/29/63/63	0/2/2/2
25	LMG	F	701	-	-	23/42/62/70	0/1/1/1
23	SQD	D	601	-	-	25/49/69/69	0/1/1/1
22	LHG	F	704	-	-	19/40/40/53	-
23	SQD	L	101	-	-	22/33/53/69	0/1/1/1
22	LHG	F	702	-	-	26/53/53/53	-
23	SQD	C	201	-	-	15/35/55/69	0/1/1/1

The worst 5 of 104 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	602	BCR	C10-C9	14.87	1.55	1.35
24	D	603	BCR	C10-C9	14.76	1.55	1.35
24	D	603	BCR	C14-C13	14.53	1.55	1.35
24	D	603	BCR	C17-C18	14.50	1.55	1.35
24	D	602	BCR	C14-C13	13.85	1.54	1.35

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	601	SQD	O9-S-C6	29.71	142.25	106.94
23	C	201	SQD	O9-S-C6	29.68	142.22	106.94
23	L	101	SQD	O9-S-C6	29.64	142.17	106.94
23	C	201	SQD	O7-S-C6	-28.12	73.52	106.94
23	D	601	SQD	O7-S-C6	-28.00	73.66	106.94

There are no chirality outliers.

5 of 302 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	601	LHG	C3-O3-P-O5
22	B	601	LHG	C4-O6-P-O3
22	B	601	LHG	C4-O6-P-O4
22	B	601	LHG	C4-O6-P-O5
22	C	202	LHG	O1-C1-C2-O2

There are no ring outliers.

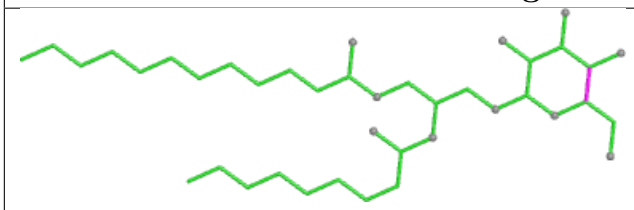
11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	F	703	LMG	2	0
24	D	602	BCR	3	0
21	A	401	DGD	1	0
22	C	202	LHG	3	0
26	I	202	SF4	1	0
21	A	402	DGD	2	0
24	D	603	BCR	4	0
25	F	701	LMG	2	0
23	D	601	SQD	4	0
23	L	101	SQD	2	0
23	C	201	SQD	2	0

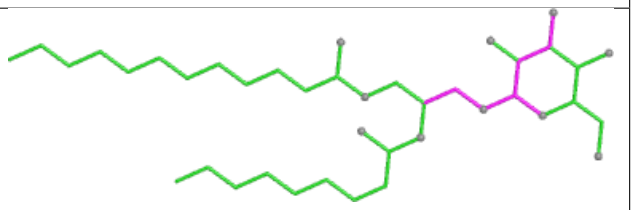
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

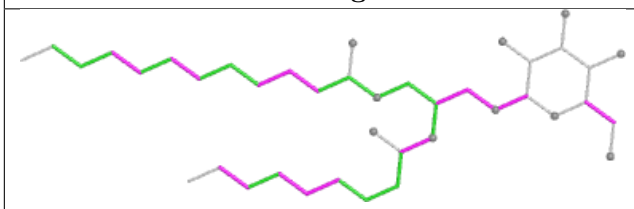
Ligand LMG F 703



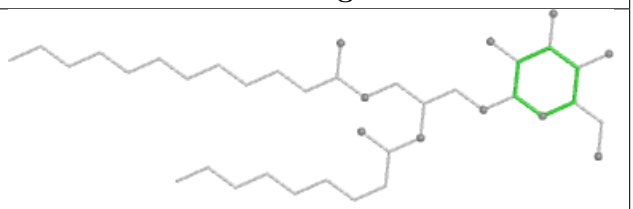
Bond lengths



Bond angles

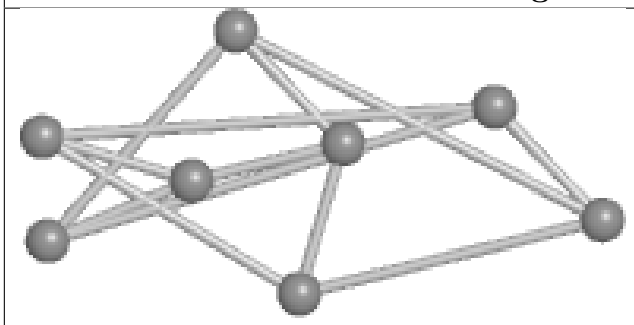


Torsions

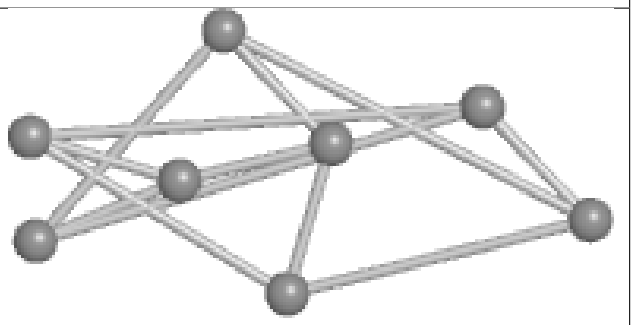


Rings

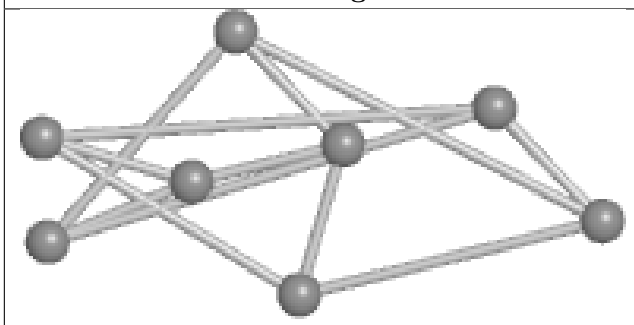
Ligand SF4 K 301



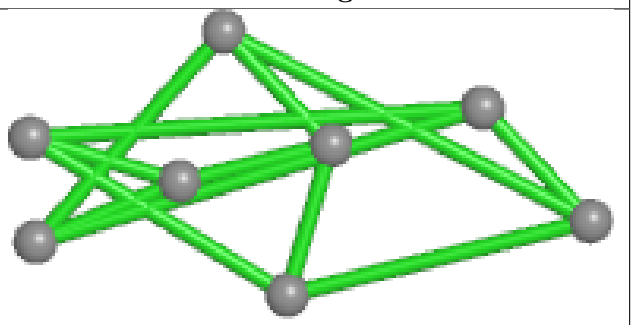
Bond lengths



Bond angles



Torsions

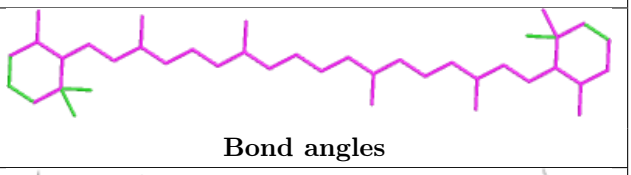


Rings

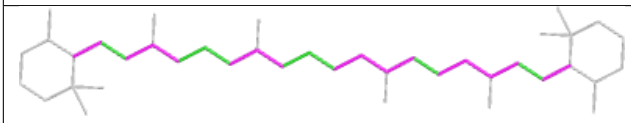
Ligand BCR D 602



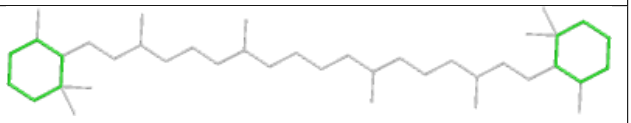
Bond lengths



Bond angles

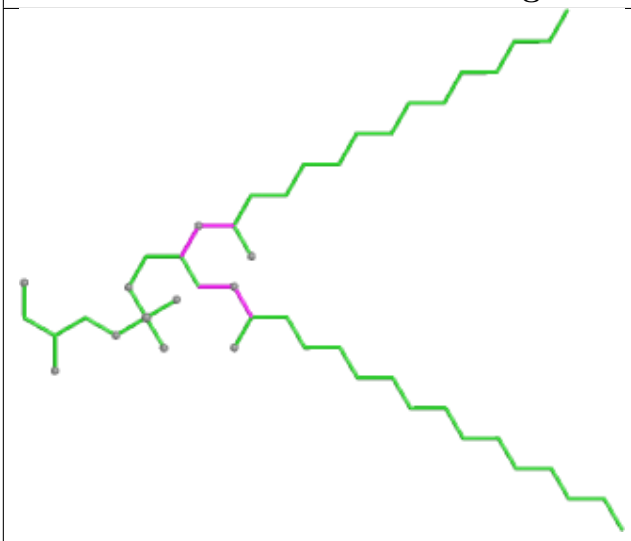


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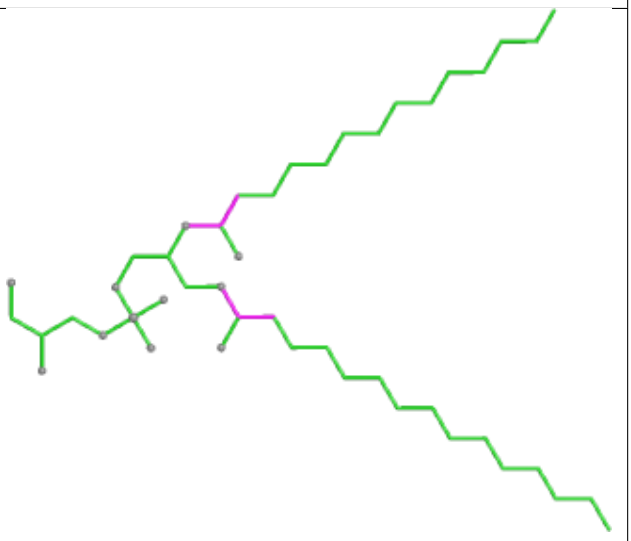


Rings

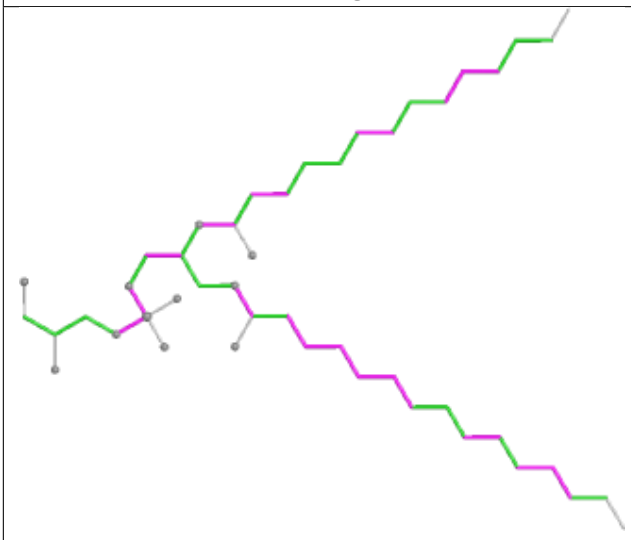
Ligand LHG B 601



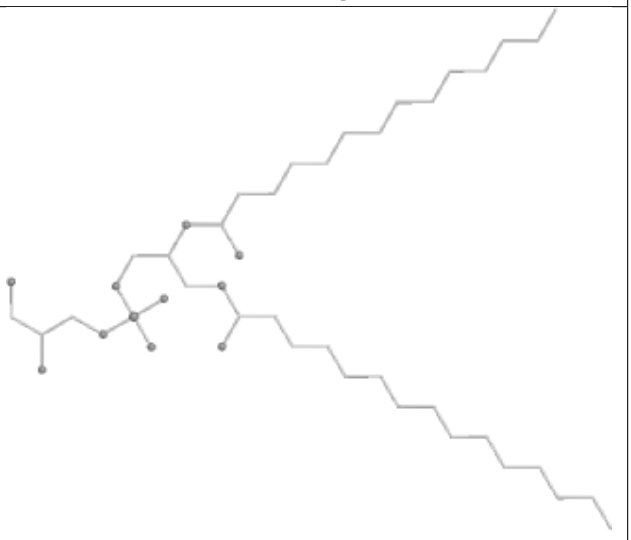
Bond lengths



Bond angles

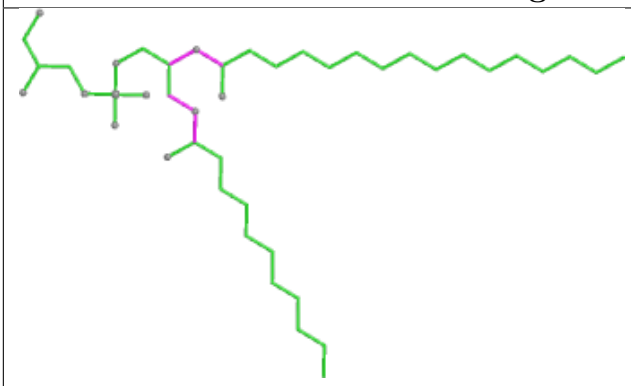


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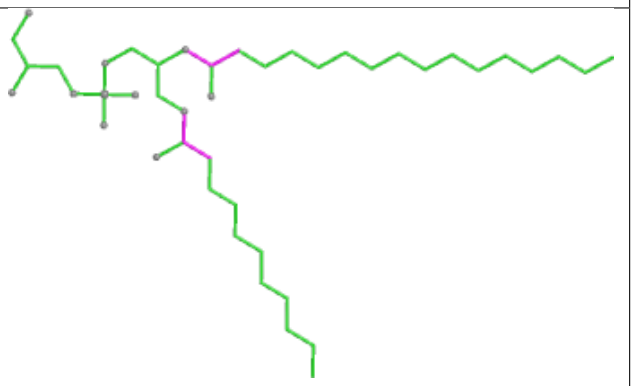


Rings

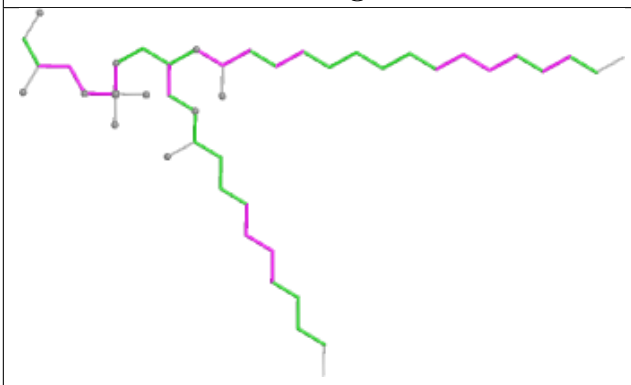
Ligand LHG I 201



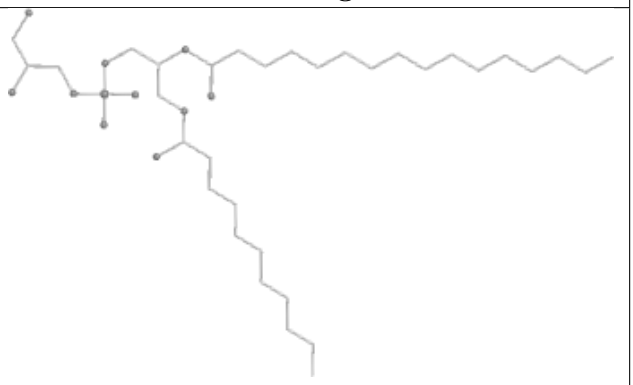
Bond lengths



Bond angles

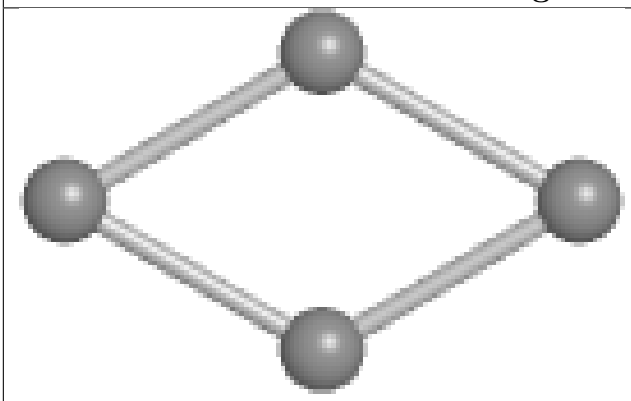


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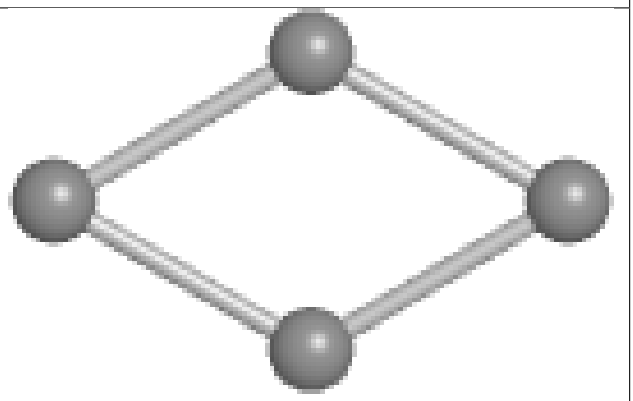


Rings

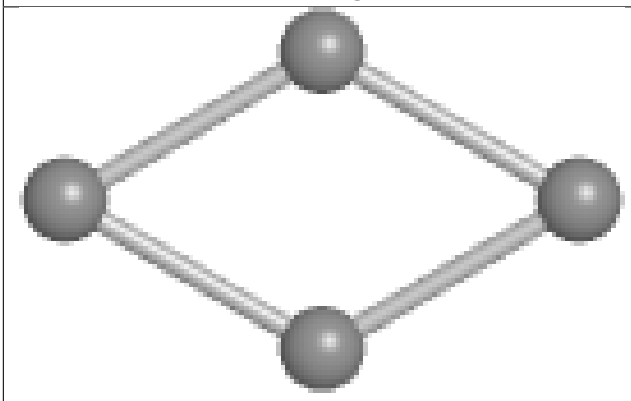
Ligand FES 1 101



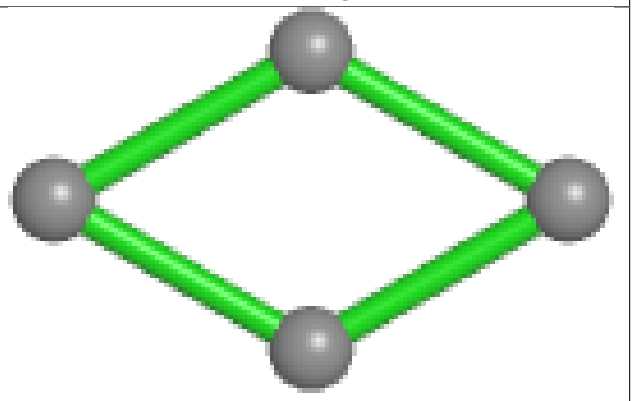
Bond lengths



Bond angles

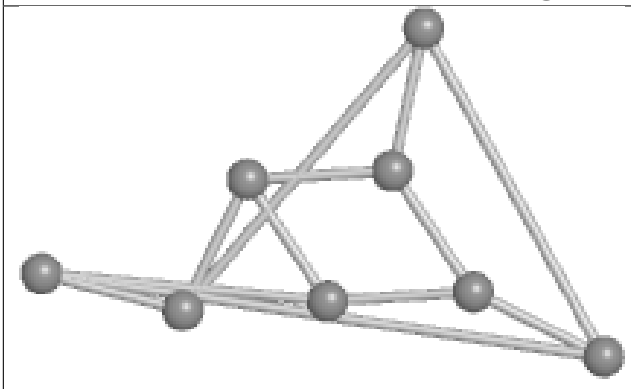


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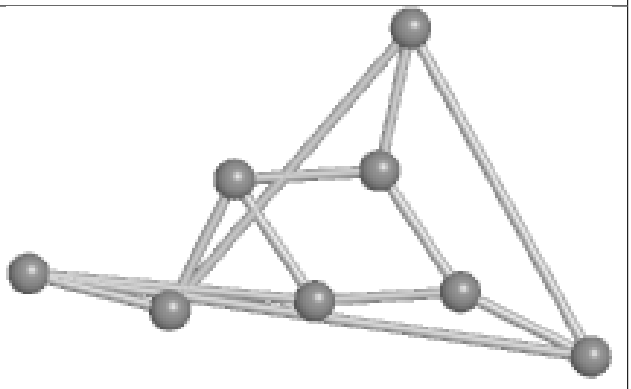


Rings

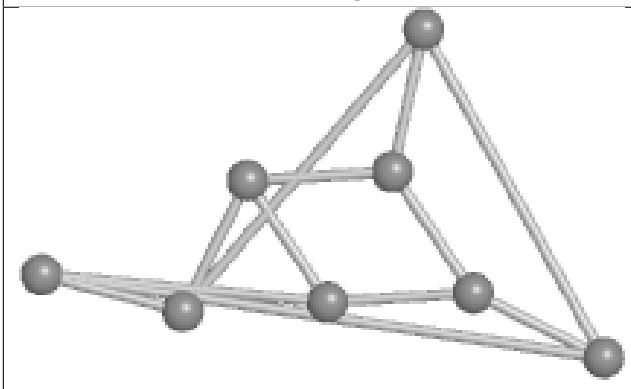
Ligand SF4 I 203



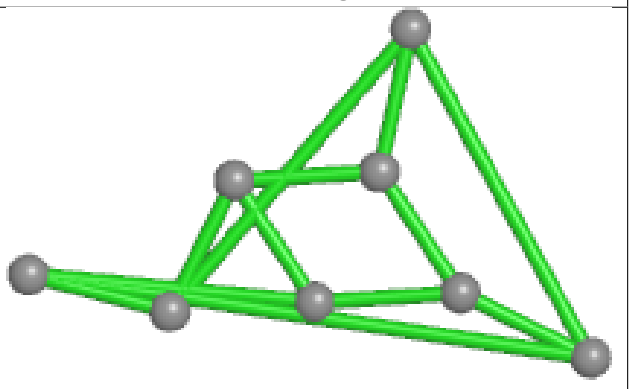
Bond lengths



Bond angles

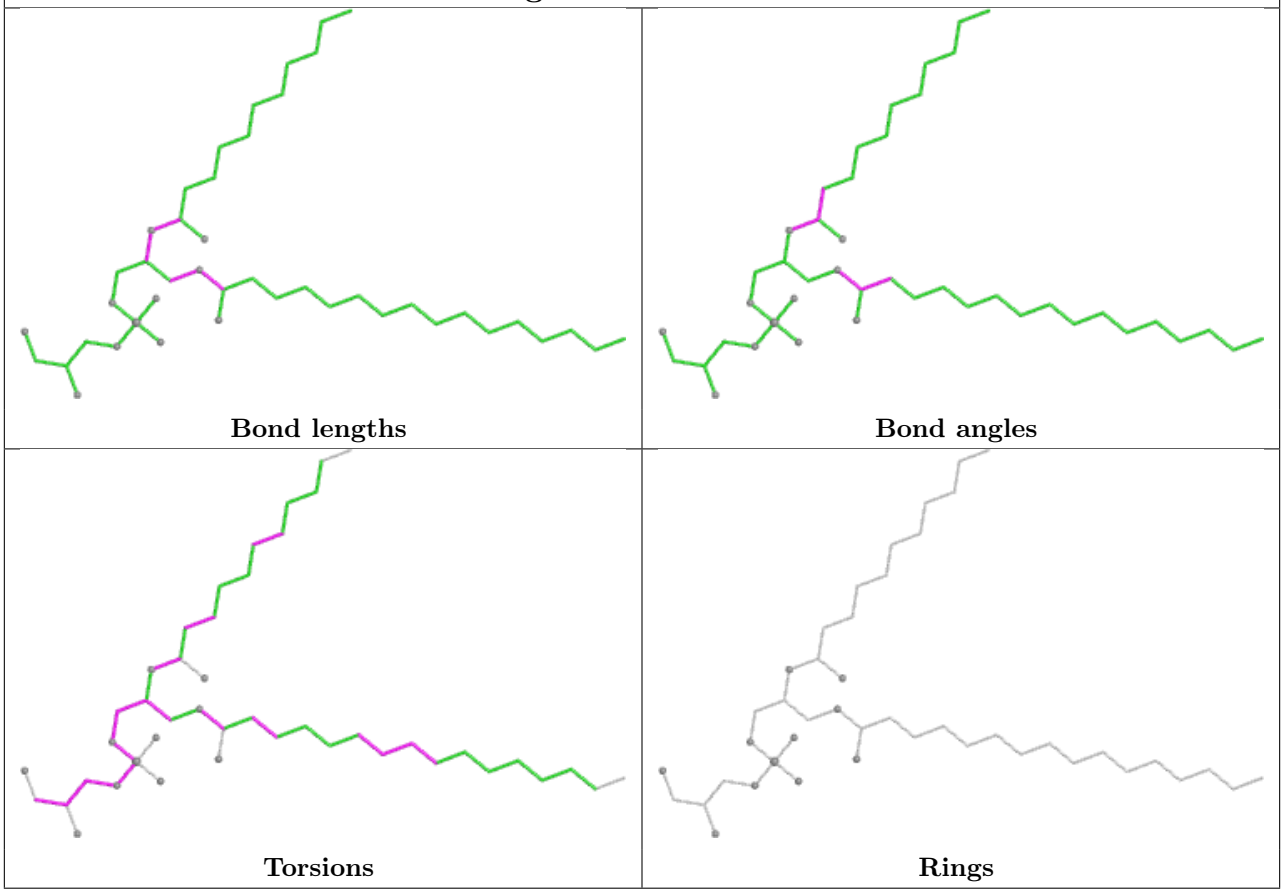


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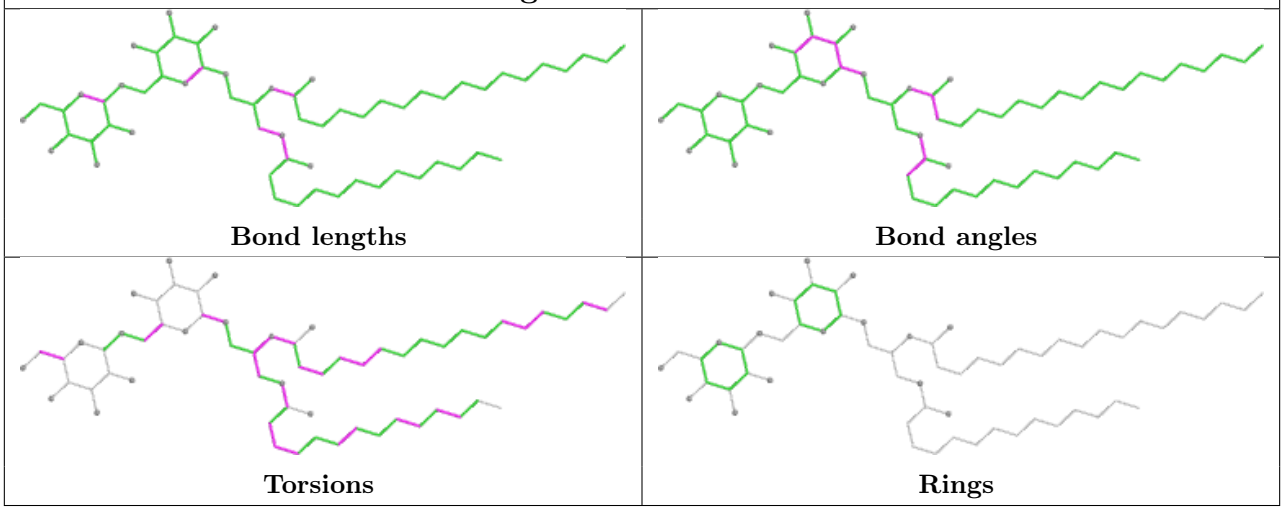


Rings

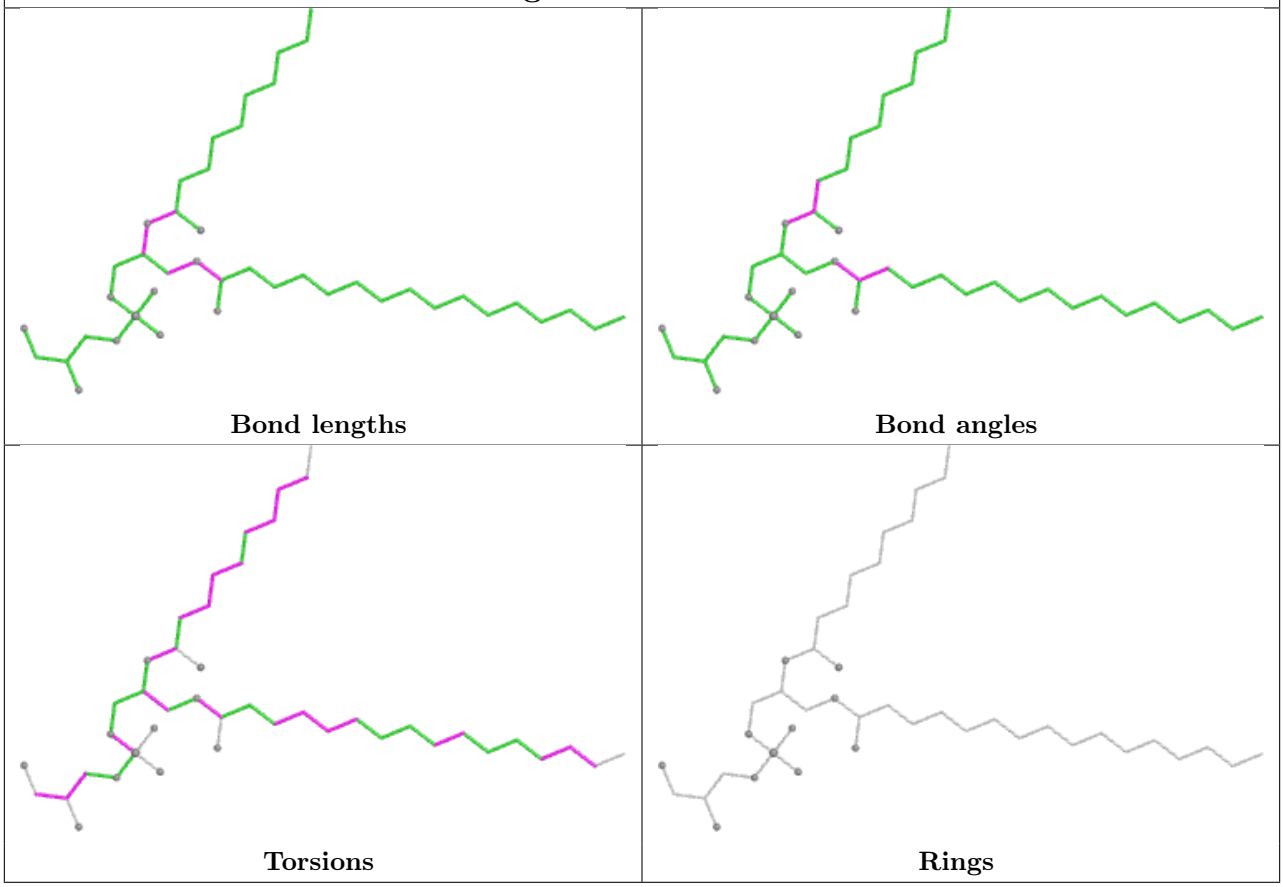
Ligand LHG F 705



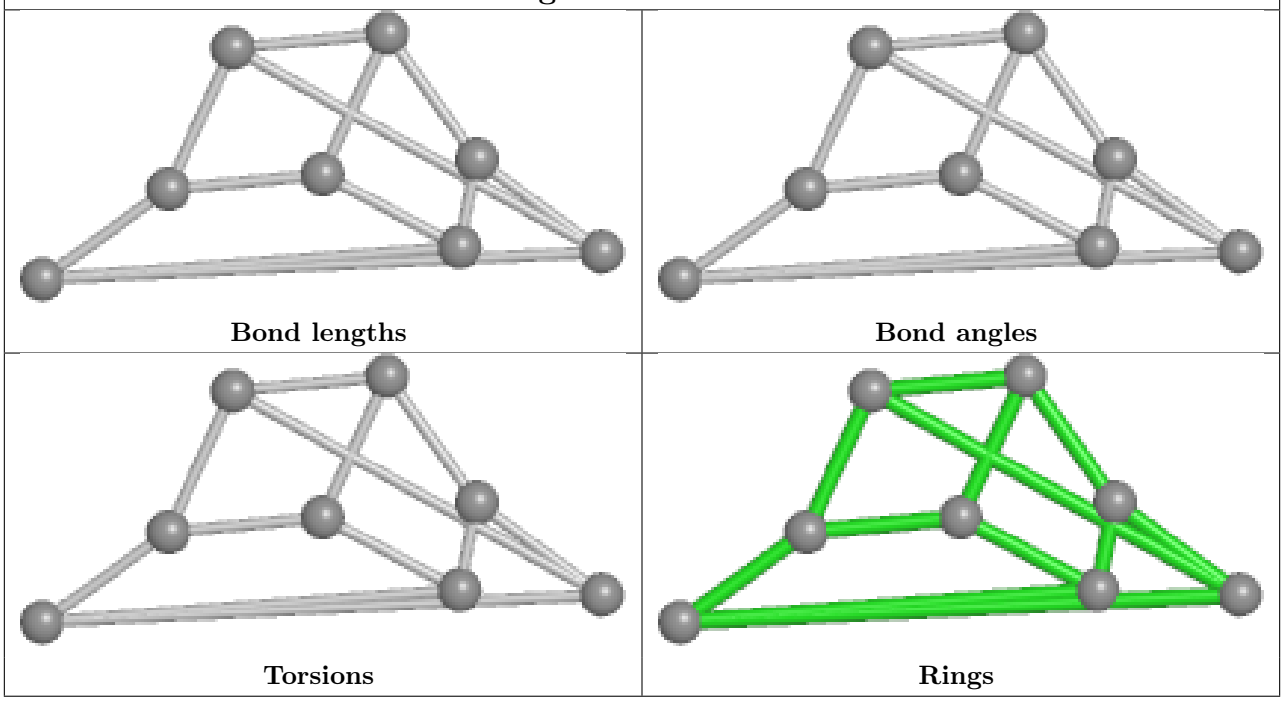
Ligand DGD A 401



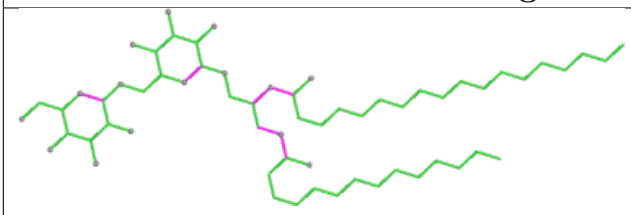
Ligand LHG C 202



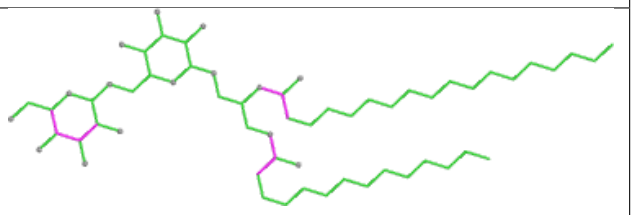
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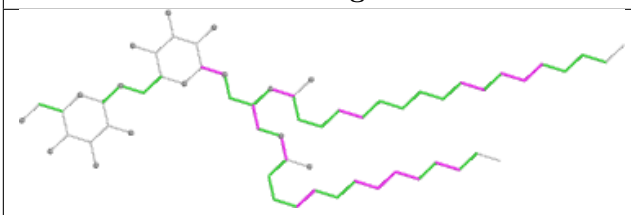
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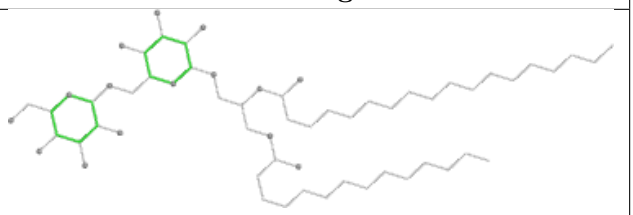
Bond lengths



Bond angles

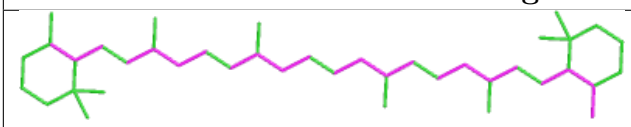


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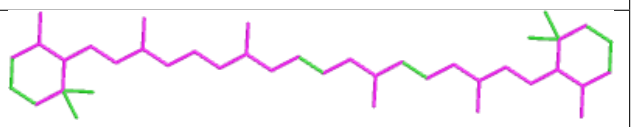


Rings

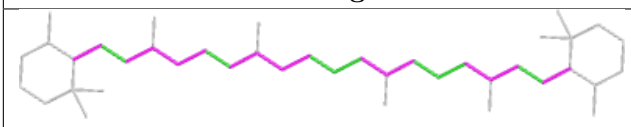
Ligand BCR D 603



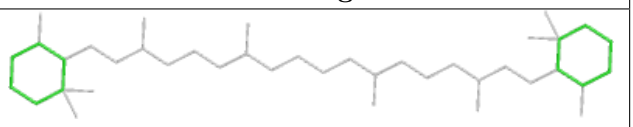
Bond lengths



Bond angles

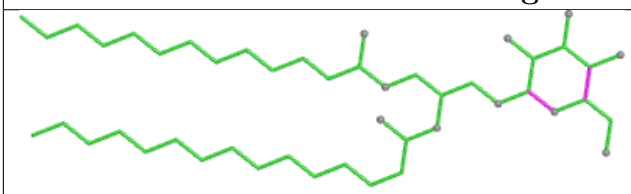


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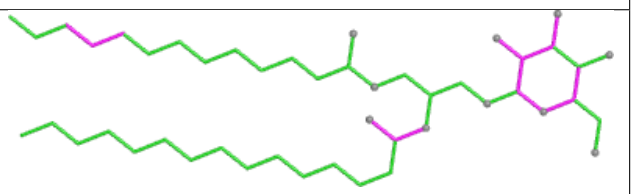


Rings

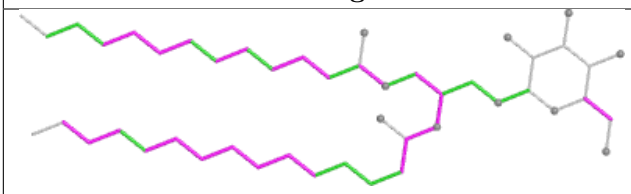
Ligand LMG F 701



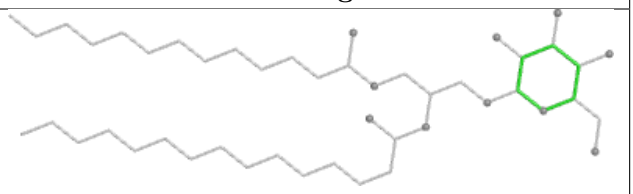
Bond lengths



Bond angles

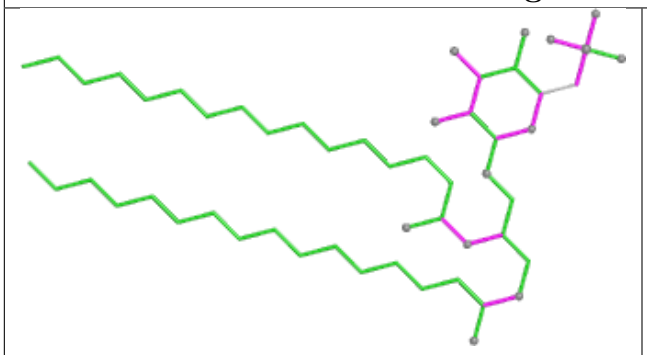


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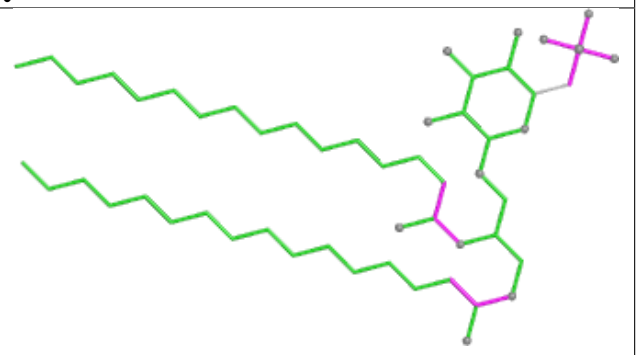


Rings

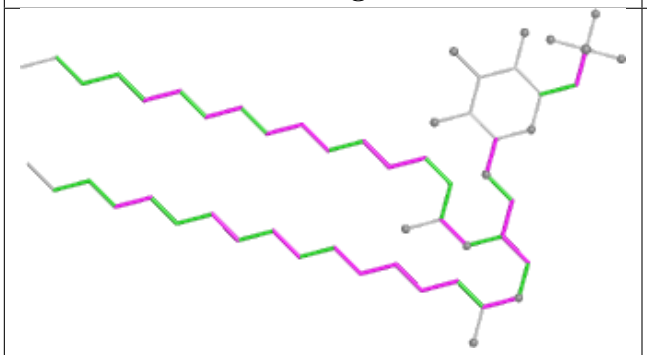
Ligand SQD D 601



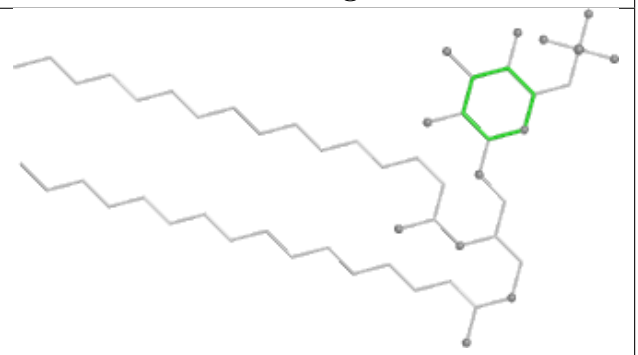
Bond lengths



Bond angles

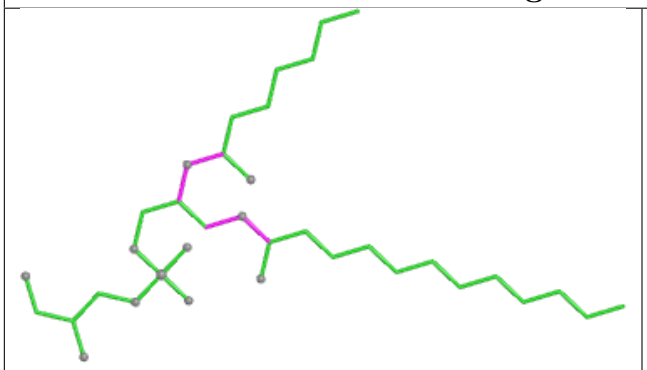


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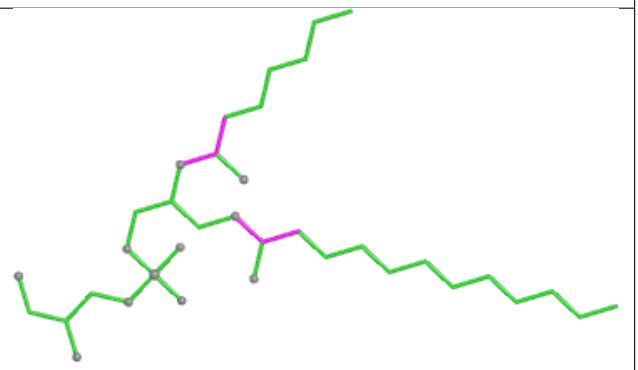


Rings

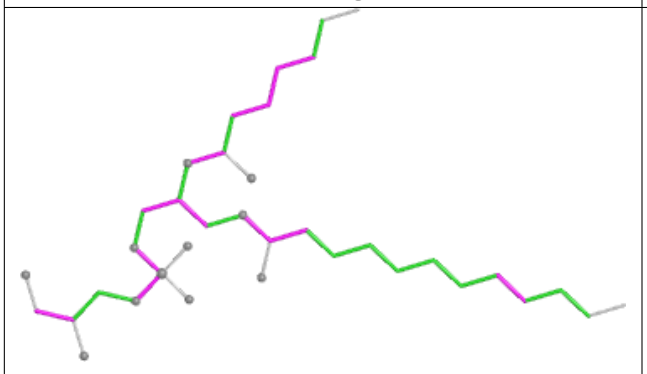
Ligand LHG F 704



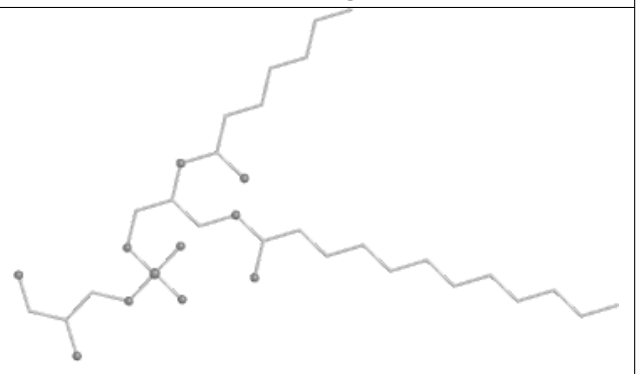
Bond lengths



Bond angles

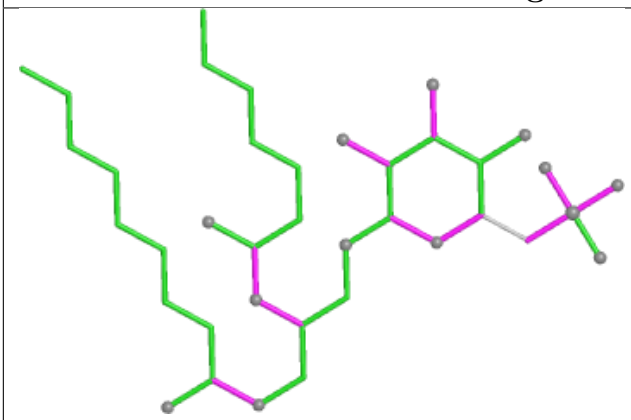


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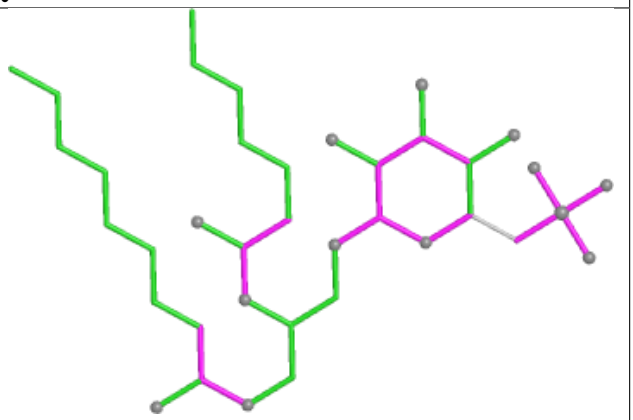


Rings

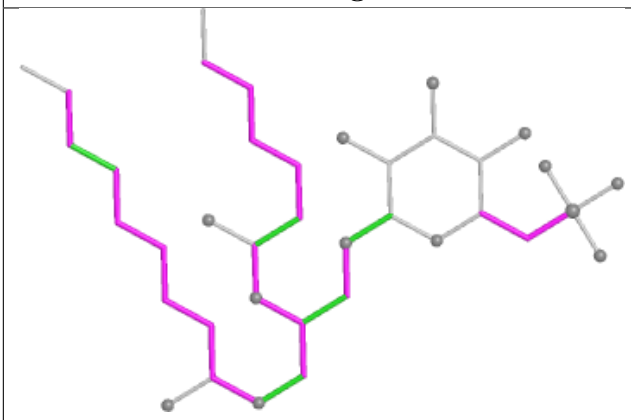
Ligand SQD L 101



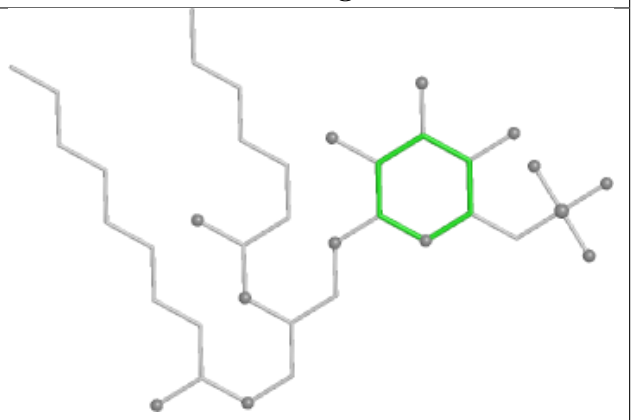
Bond lengths



Bond angles

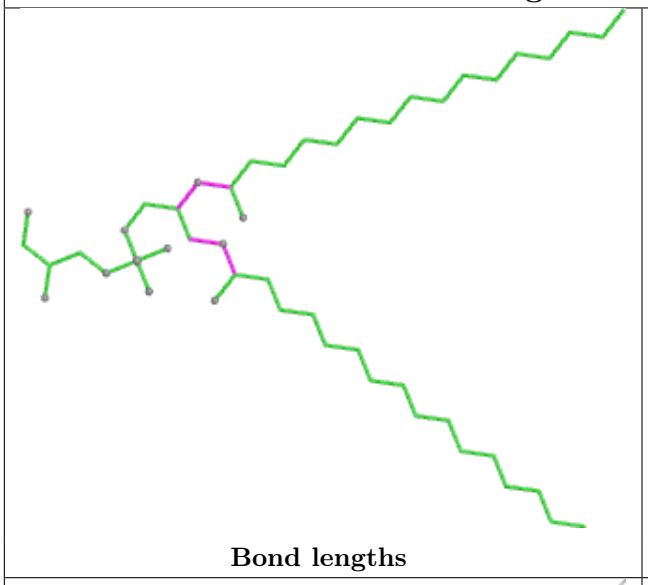


Torsions

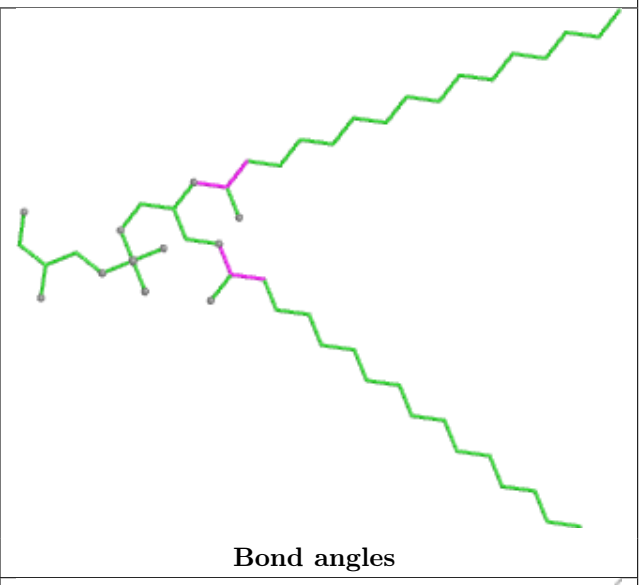


Rings

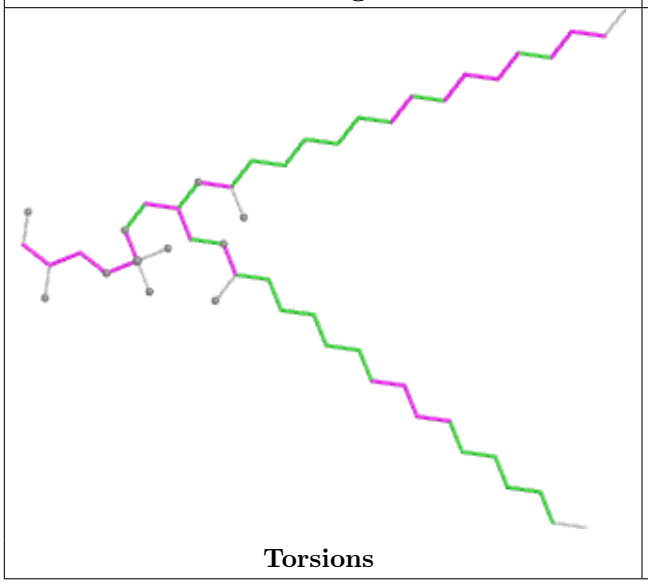
Ligand LHG F 702



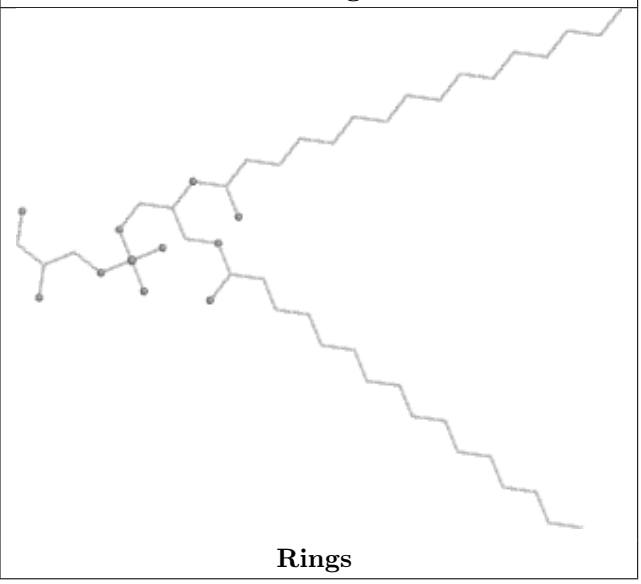
Bond lengths



Bond angles

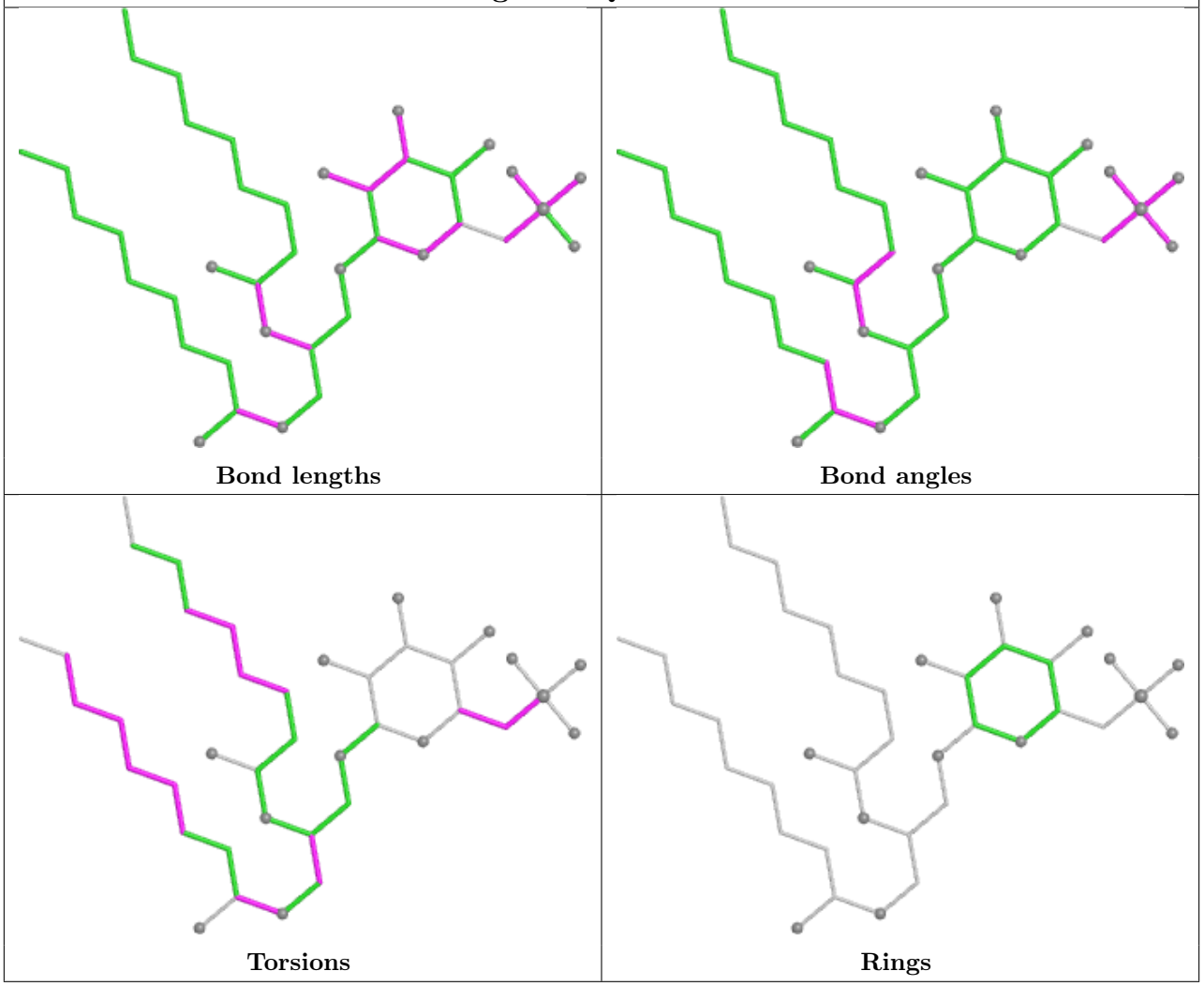


Torsions



Rings

Ligand SQD C 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

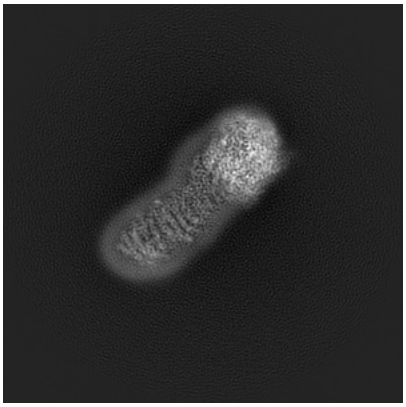
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9989. These allow visual inspection of the internal detail of the map and identification of artifacts.

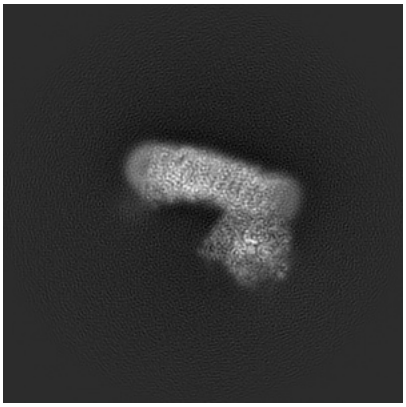
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

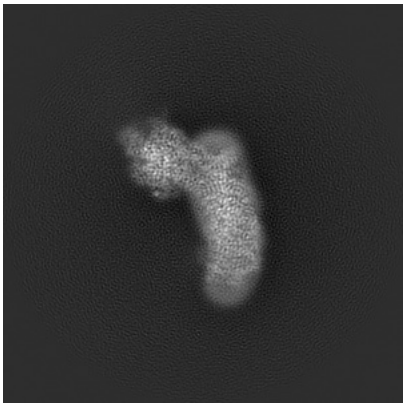
6.1.1 Primary map



X



Y

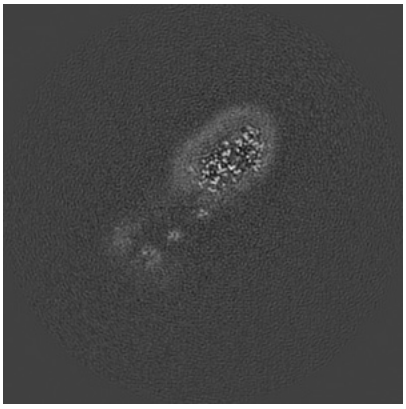


Z

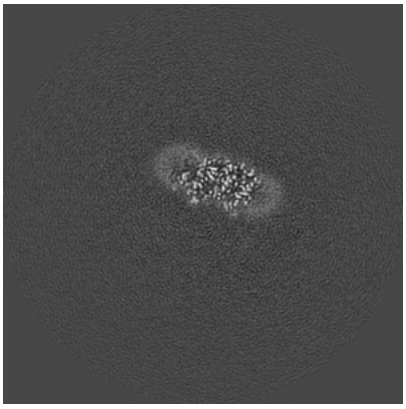
The images above show the map projected in three orthogonal directions.

6.2 Central slices

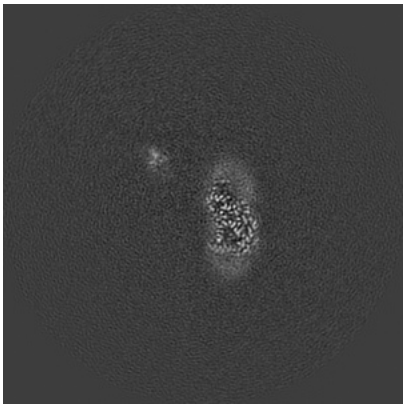
6.2.1 Primary map



X Index: 200



Y Index: 200

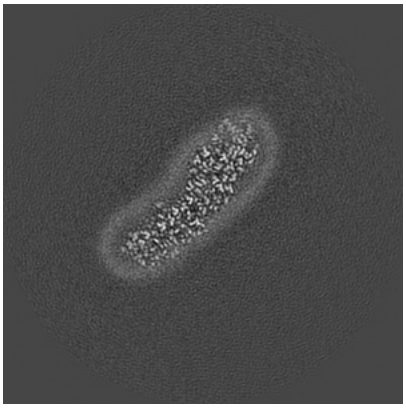


Z Index: 200

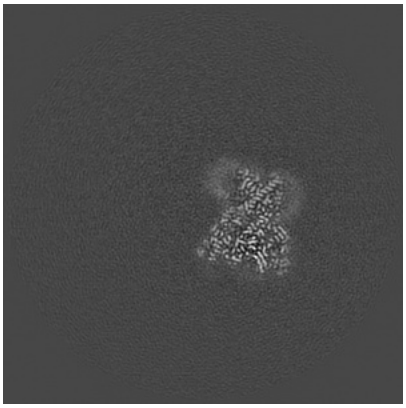
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

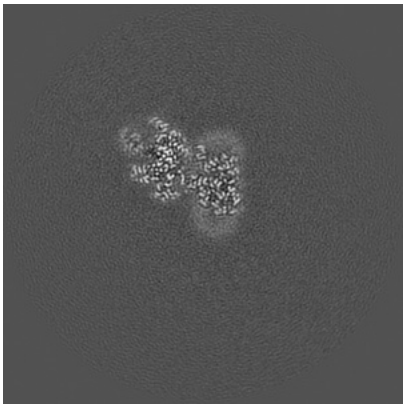
6.3.1 Primary map



X Index: 221



Y Index: 246

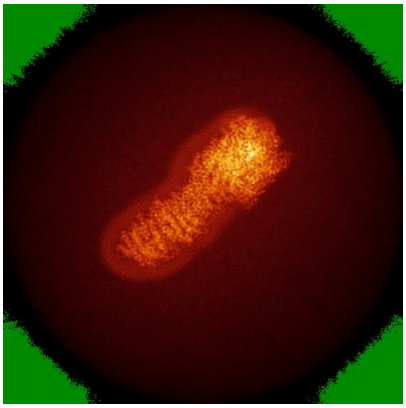


Z Index: 242

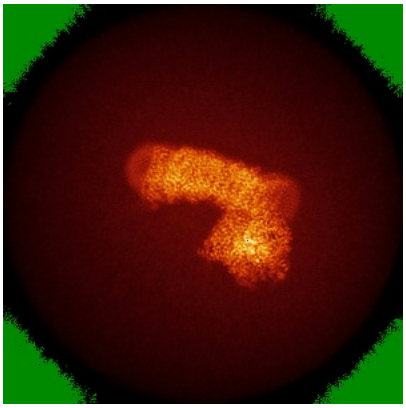
The images above show the largest variance slices of the map in three orthogonal directions.

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

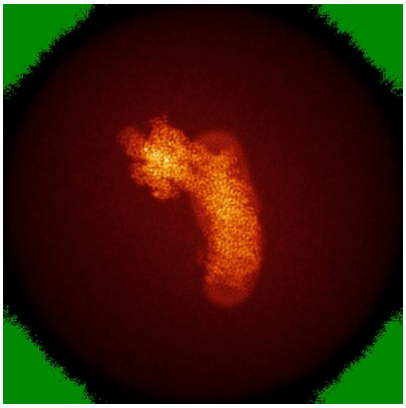
6.4.1 Primary map



X



Y

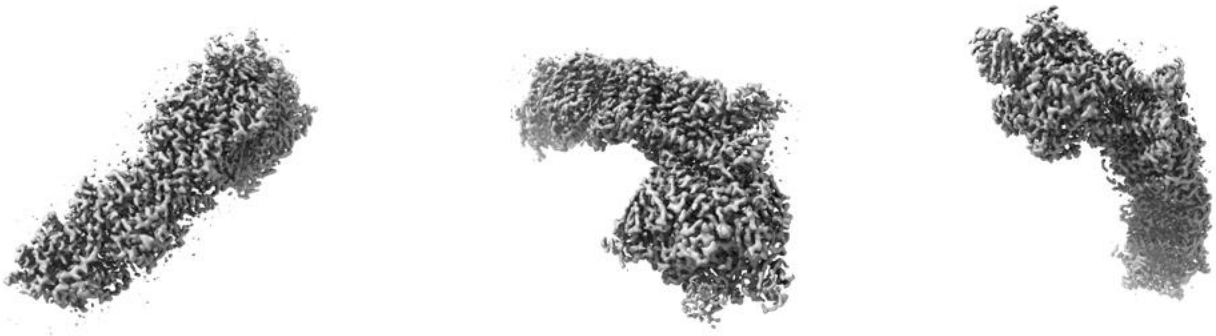


Z

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

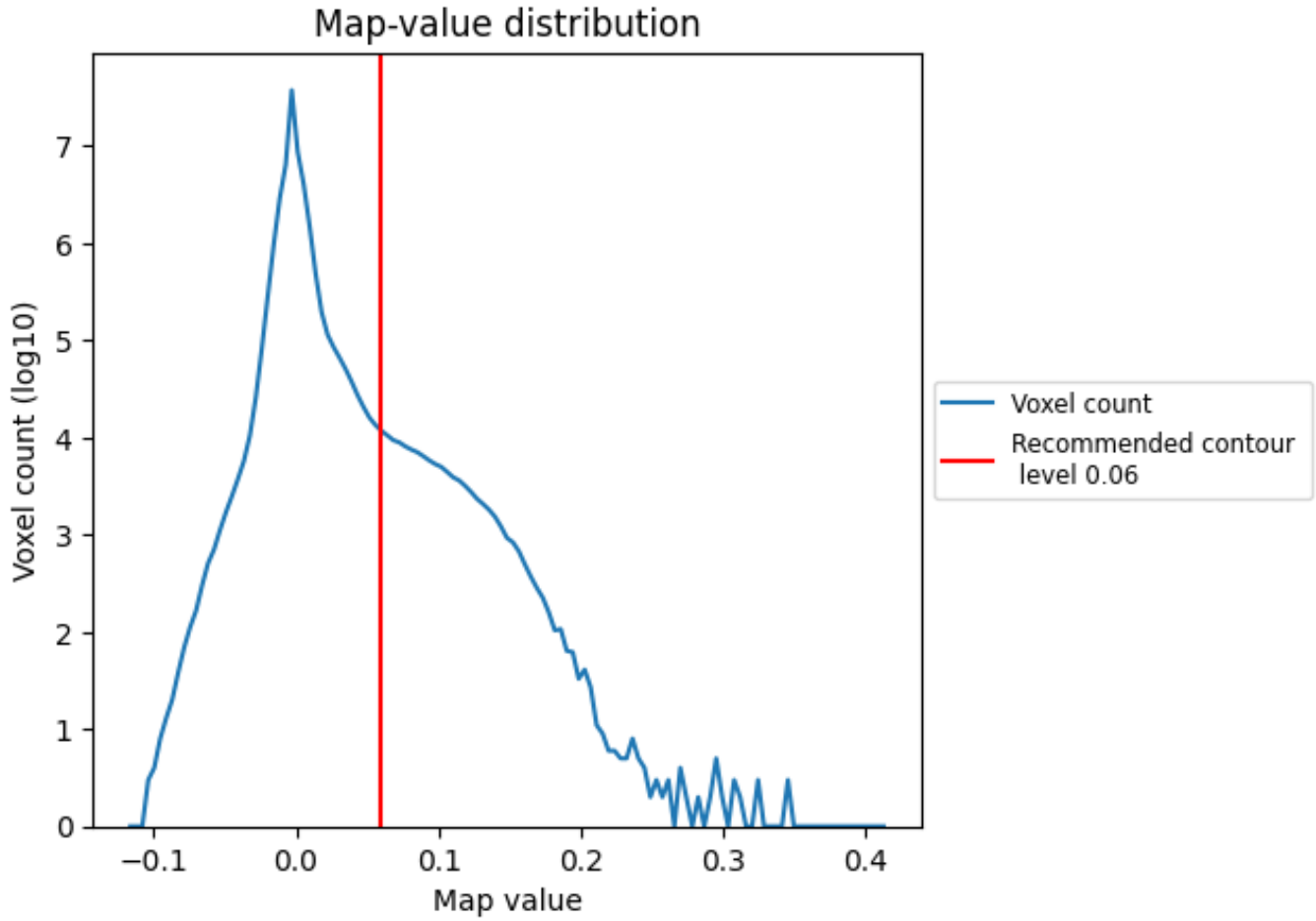
6.6 Mask visualisation (i)

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

7 Map analysis

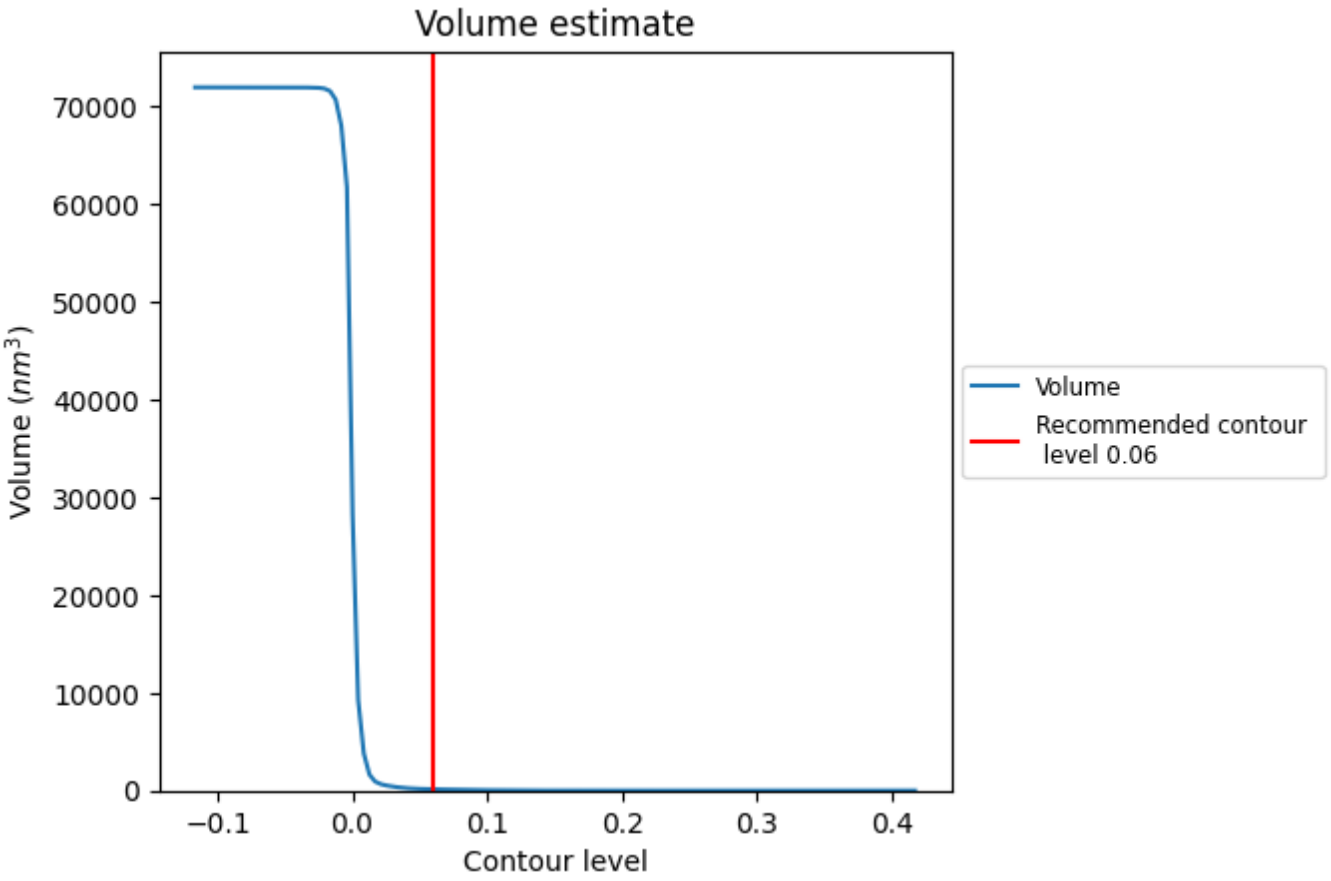
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

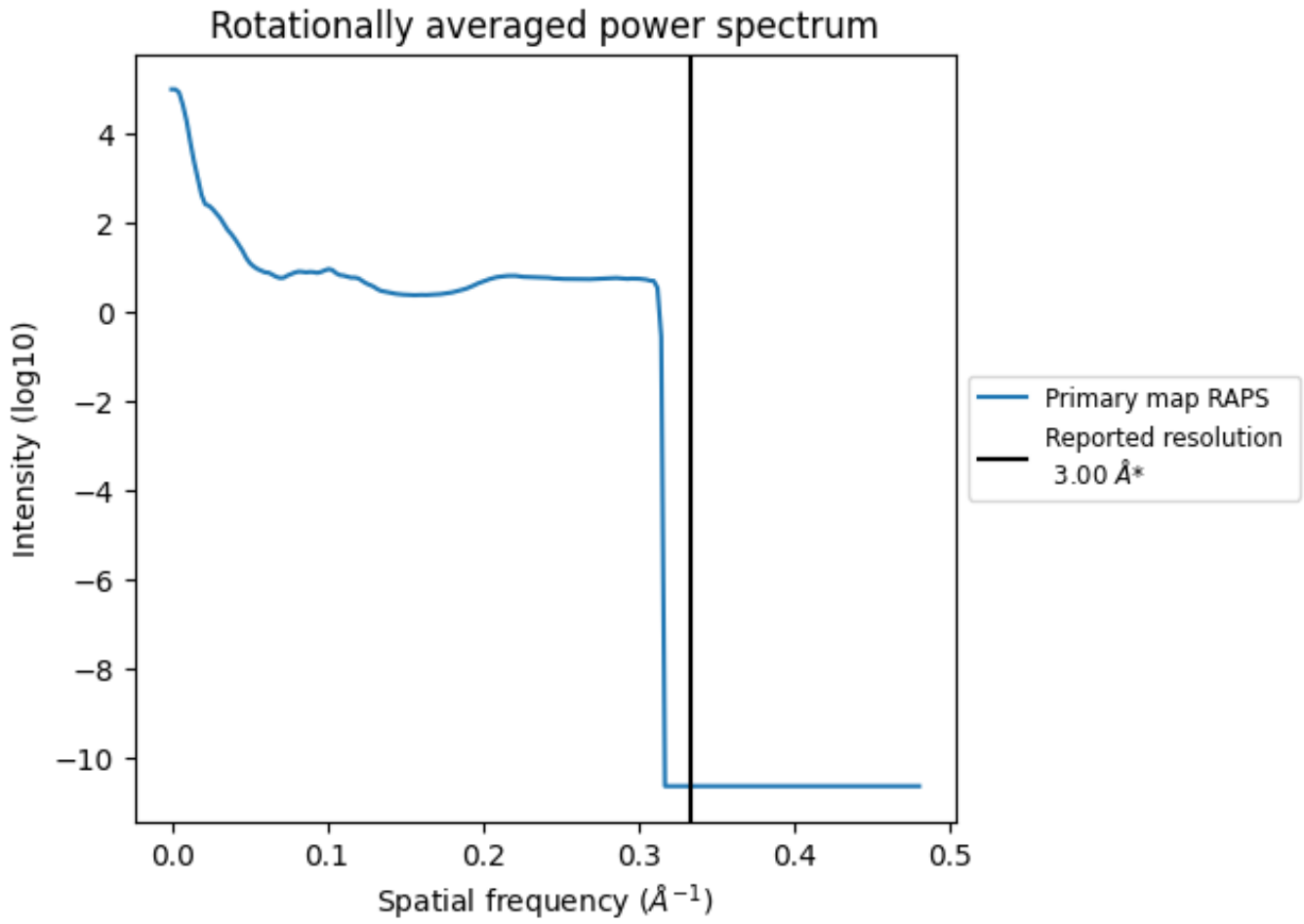
7.2 Volume estimate (i)



The volume at the recommended contour level is 132 nm^3; this corresponds to an approximate mass of 120 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 0.333 Å^{-1}

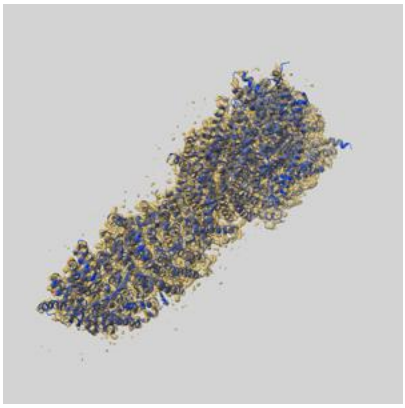
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

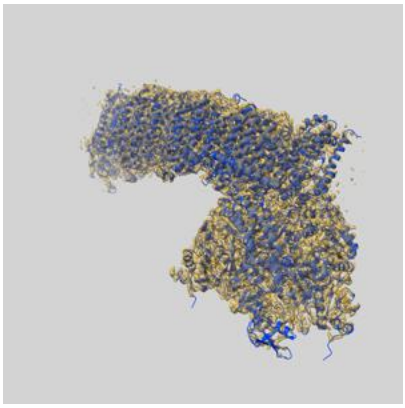
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9989 and PDB model 6KHI. Per-residue inclusion information can be found in section 3 on page 12.

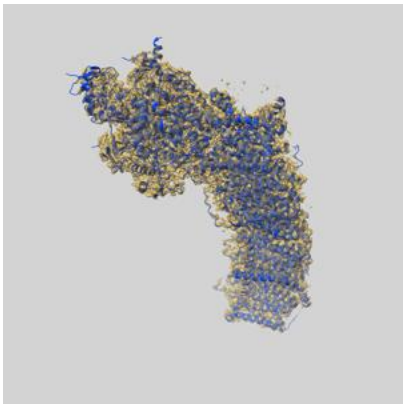
9.1 Map-model overlay



X



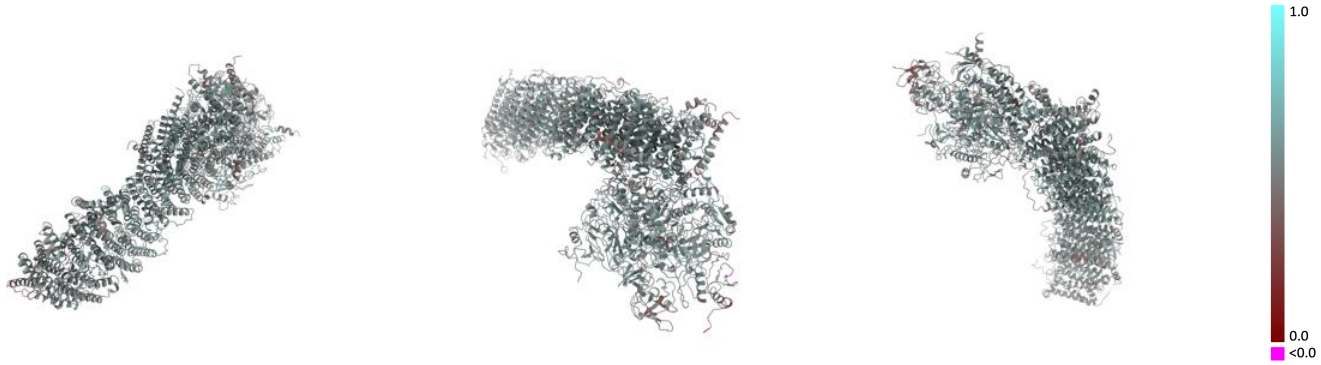
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

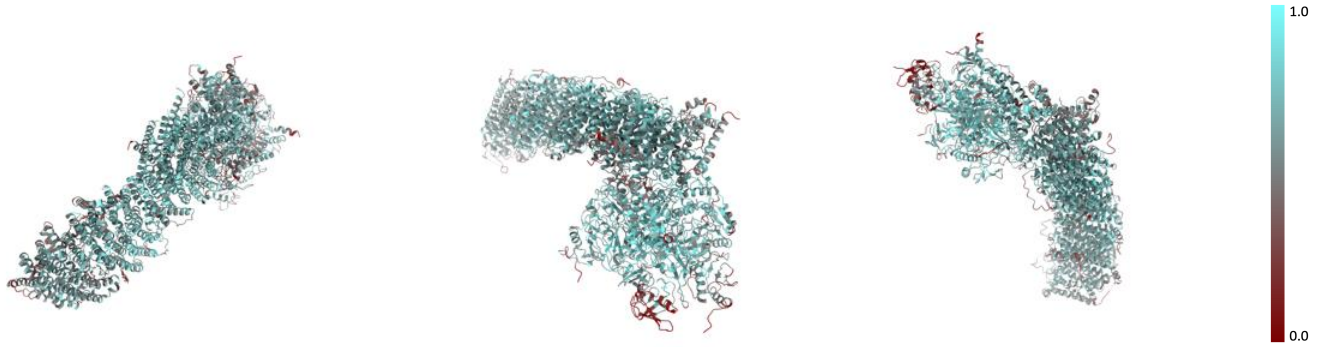
9.2 Q-score mapped to coordinate model



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.

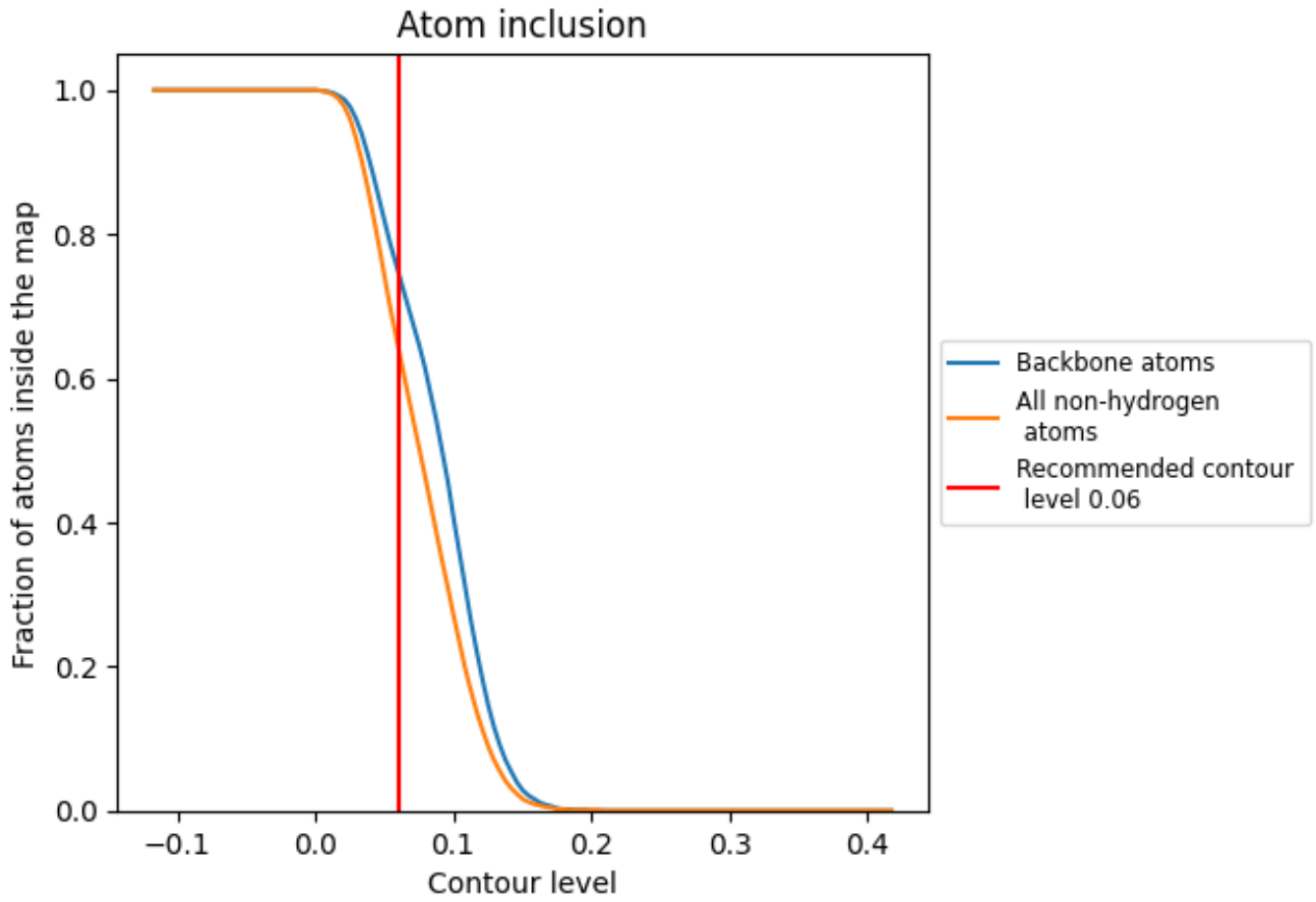
9.3 Atom inclusion mapped to coordinate model



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 64% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6450	0.5250
1	0.2890	0.4610
A	0.6410	0.5260
B	0.6920	0.5410
C	0.6360	0.5270
D	0.6890	0.5390
E	0.6890	0.5400
F	0.5890	0.5040
G	0.6340	0.5320
H	0.6850	0.5330
I	0.6710	0.5260
J	0.6840	0.5260
K	0.7160	0.5400
L	0.5840	0.5040
M	0.6970	0.5330
N	0.6970	0.5370
O	0.6710	0.5540
P	0.6810	0.5310
Q	0.4480	0.4860
S	0.6140	0.5260
V	0.4640	0.4610

