Full wwPDB EM Validation Report (i)

Aug 27, 2026 – 03:26 am BST

PDB ID	:	8B6G / pdb_00008b6g
EMDB ID	:	EMD-15866
Title	:	Cryo-EM structure of succinate dehydrogenase complex (complex-II) in respiratory supercomplex of Tetrahymena thermophila
Authors	:	Muhleip, A.; Kock Flygaard, R.; Baradaran, R.; Amunts, A.
Deposited on	:	2022-09-27
Resolution	:	3.00 Å(reported)

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

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

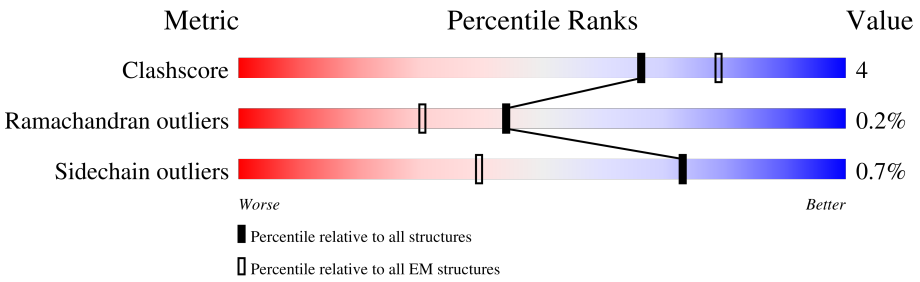
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

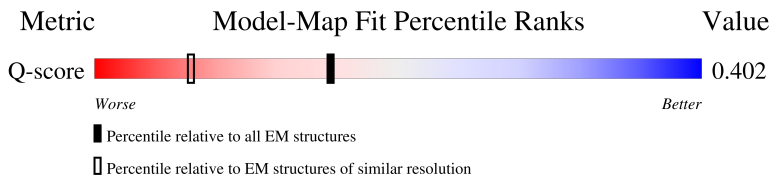
1 Overall quality at a glance (i)

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	CH	195	5% 50% 6% 44%
2	CM	76	• 88% 9% •
3	CL	89	10% 88% 11% •
4	CA	636	9% 82% 12% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	CI	114	18% 92% 8%
6	CB	312	80% 11% 9%
7	CF	296	8% 67% 7% 26%
8	CG	198	87% 12%
9	CK	93	90% 9%
10	CE	322	9% 86% 12%
11	CJ	103	91% 9%
12	CN	62	19% 85% 15%
13	CC	60	92% 7%
14	CO	43	5% 91% 9%
15	CD	44	95% 5%

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
23	HEC	CE	401	X	-	-	-

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 41412 atoms, of which 20810 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 Diphthamide synthesis protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	CH	110	1700	529	845	147	171	8	0	0

- Molecule 2 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	CM	74	1232	403	603	115	109	2	0	0

- Molecule 3 is a protein called Transposase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	CL	88	1522	499	752	125	144	2	0	0

- Molecule 4 is a protein called Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	CA	599	9198	2907	4574	825	866	26	0	0

- Molecule 5 is a protein called DUF4885 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	CI	114	1805	580	890	153	180	2	0	0

- Molecule 6 is a protein called Succinate dehydrogenase (quinone).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	CB	285	4561	1457	2261	392	430	21	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	CF	218	3598	1171	1786	306	331	4	0	0

- Molecule 8 is a protein called SDHTT3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	CG	196	3247	1072	1593	273	305	4	0	0

- Molecule 9 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	CK	93	1577	530	782	129	134	2	0	0

- Molecule 10 is a protein called NmrA domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	CE	321	5115	1623	2554	449	488	1	0	0

- Molecule 11 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	CJ	103	1663	554	815	140	151	3	0	0

- Molecule 12 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	CN	62	1029	345	515	80	87	2	0	0

- Molecule 13 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	CC	59	976	319	487	86	83	1	0	0

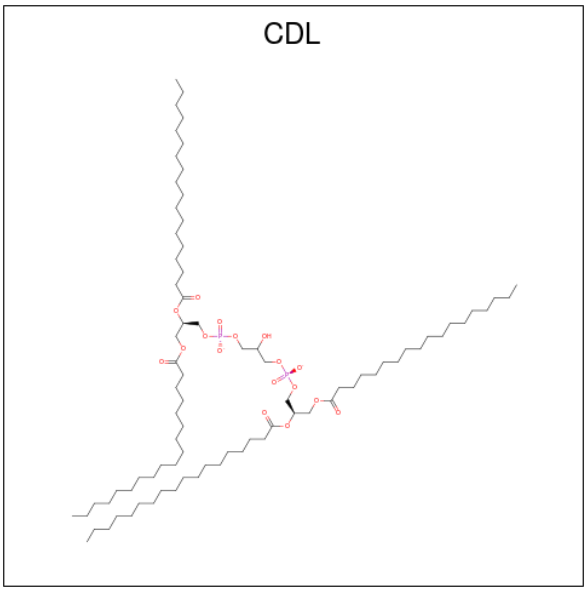
- Molecule 14 is a protein called SDHTT11.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	CO	43	742	245	378	60	57	2	0	0

- Molecule 15 is a protein called SDHD.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	CD	44	807	271	412	61	62	1	0	0

- Molecule 16 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

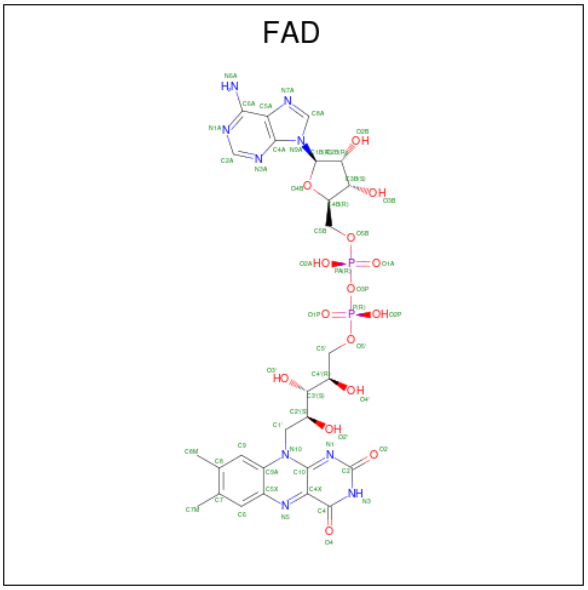


Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
16	CM	1	256	81	156	17	2	0
16	CG	1	256	81	156	17	2	0
16	CG	1	256	81	156	17	2	0
16	CK	1	256	81	156	17	2	0
16	CJ	1	256	81	156	17	2	0
16	CO	1	256	81	156	17	2	0
16	CD	1	256	81	156	17	2	0

- Molecule 17 is CALCIUM ION (CCD ID: CA) (formula: Ca).

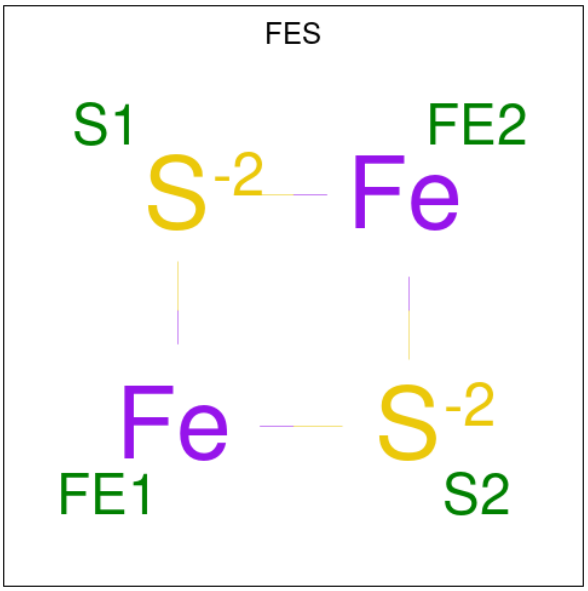
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
17	CA	1	1	1	0
17	CB	1	1	1	0

- Molecule 18 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



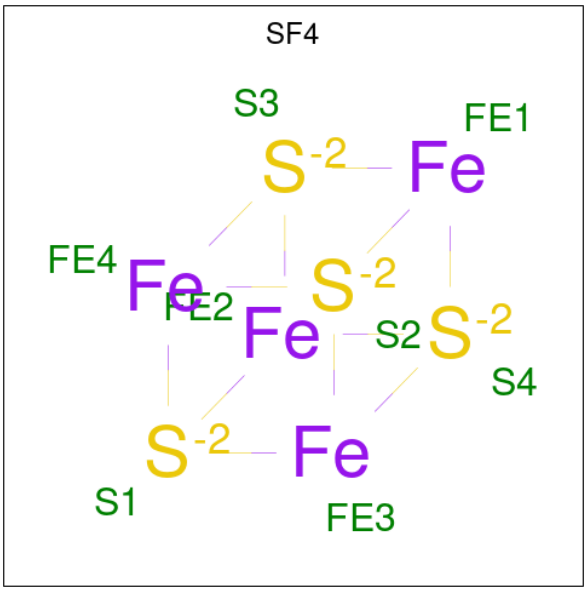
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
18	CA	1	84	27	31	9	15	2	0

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



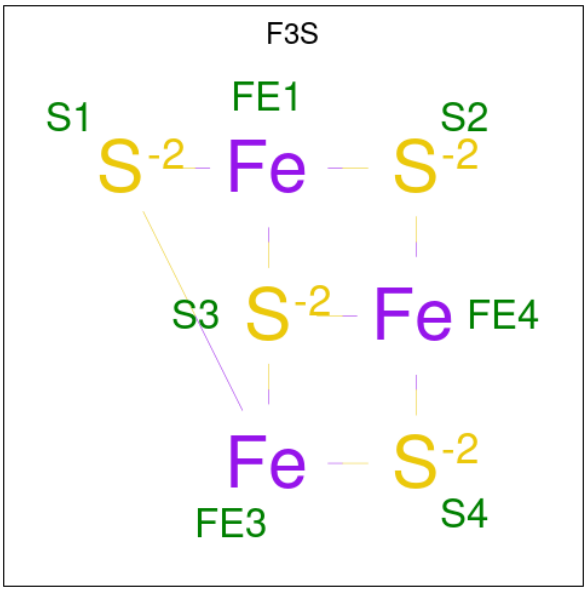
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
19	CB	1	4	2	2	0

- Molecule 20 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



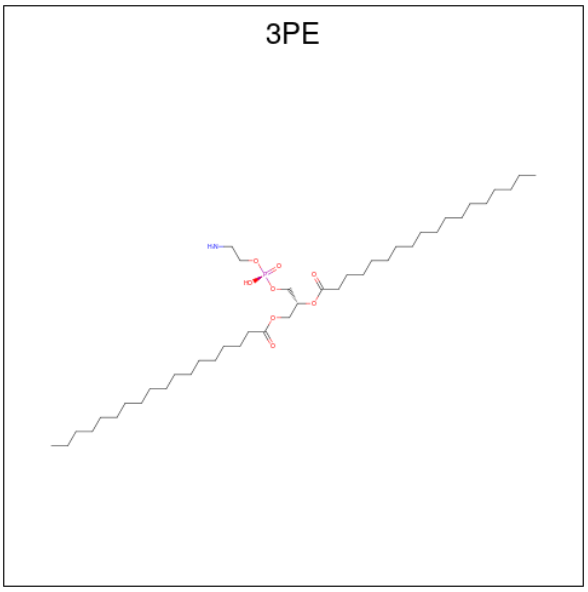
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
20	CB	1	8	4	4	0

- Molecule 21 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
21	CB	1	7	3	4	0

- Molecule 22 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



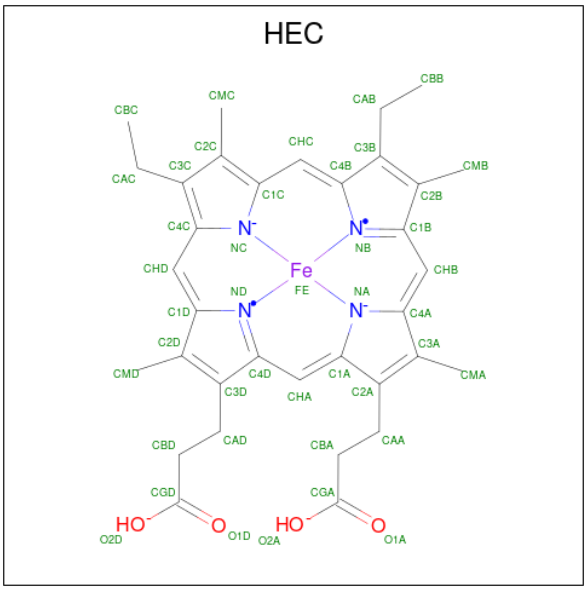
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
22	CK	1	133	41	82	1	8	1	0
22	CC	1	133	41	82	1	8	1	0

Continued on next page...

Continued from previous page...

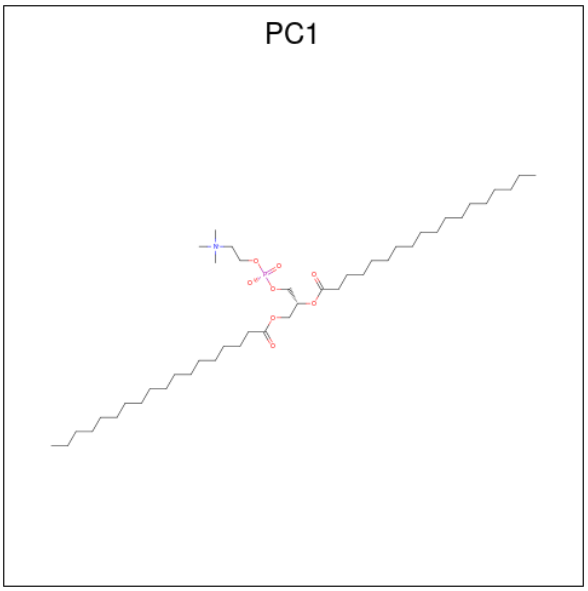
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
22	CD	1	133	41	82	1	8	1	0

- Molecule 23 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



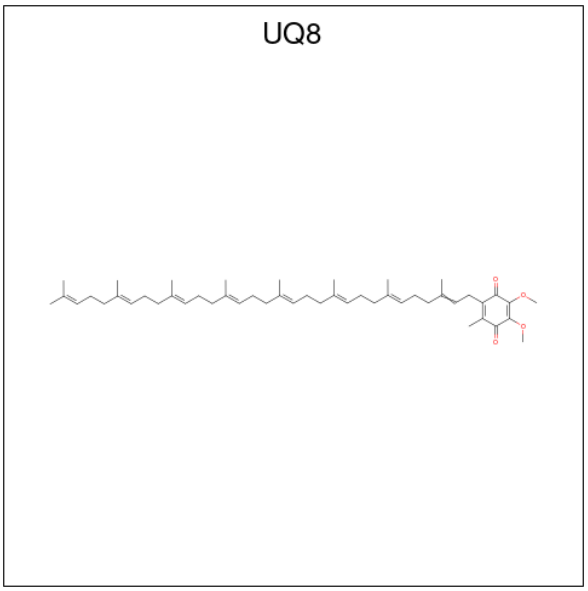
Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
23	CE	1	75	34	1	32	4	4	0

- Molecule 24 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
24	CC	1	142	44	88	1	8	1	0

- Molecule 25 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$) (labeled as "Ligand of Interest" by depositor).



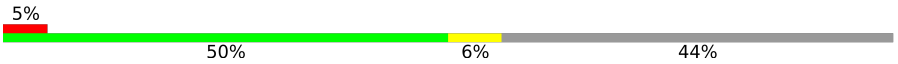
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
25	CC	1	127	49	74	4	0

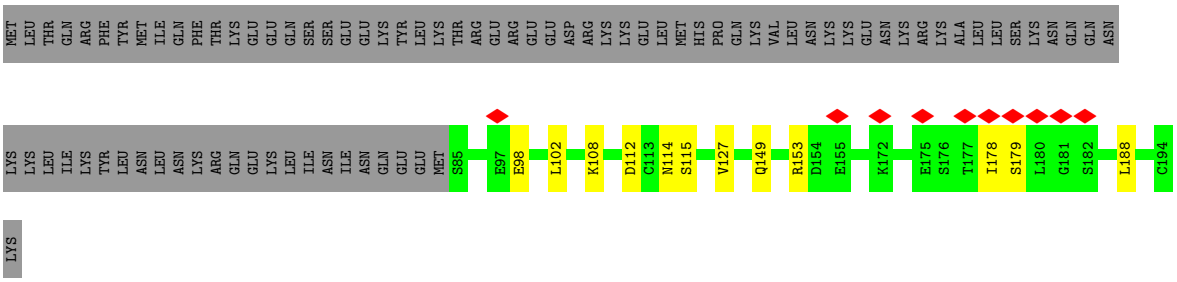
3 Residue-property plots (i)

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: Diphthamide synthesis protein

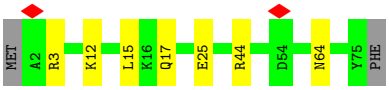
Chain CH:





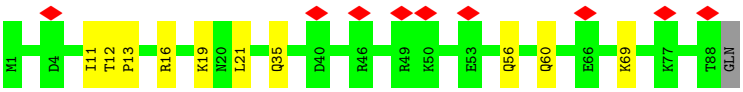
- Molecule 2: Transmembrane protein, putative

Chain CM:



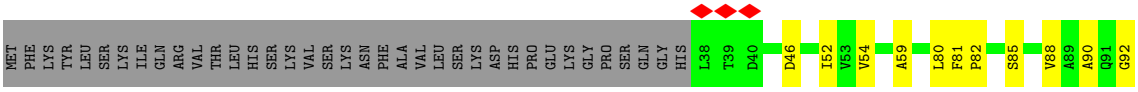
- Molecule 3: Transposase

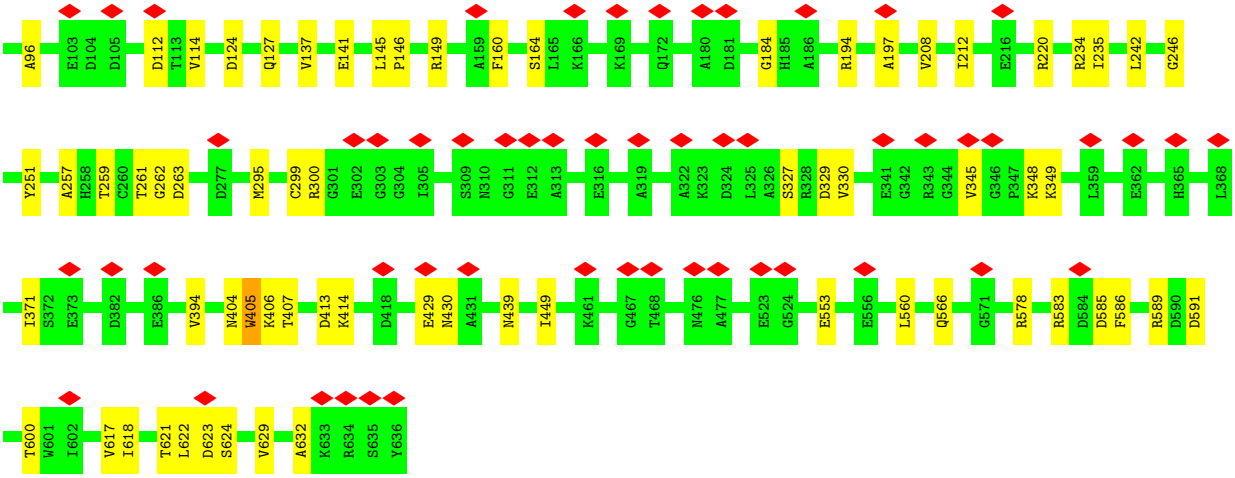
Chain CL:



- Molecule 4: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

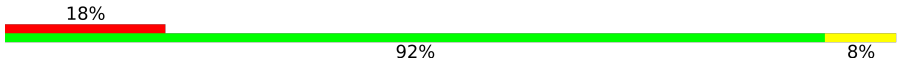
Chain CA:

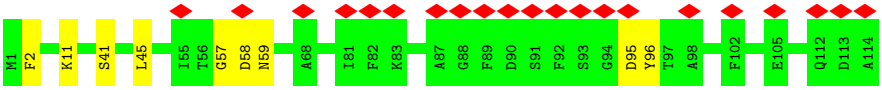




- Molecule 5: DUF4885 domain-containing protein

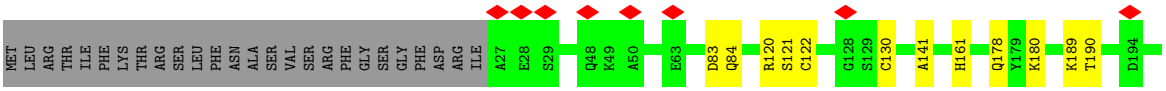
Chain CI:

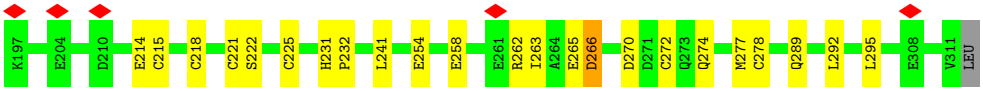




- Molecule 6: Succinate dehydrogenase (quinone)

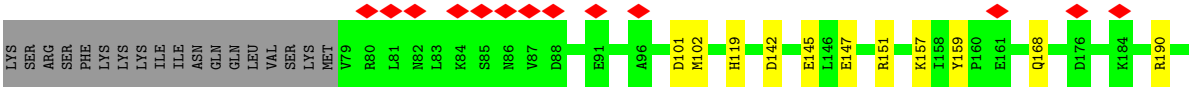
Chain CB:

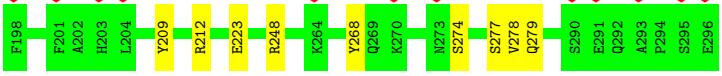




- Molecule 7: Transmembrane protein, putative

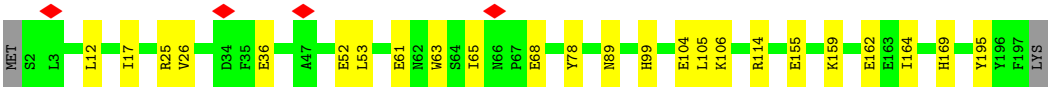
Chain CF:





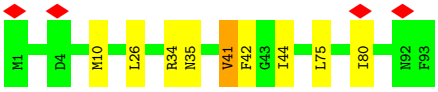
- Molecule 8: SDHTT3

Chain CG:



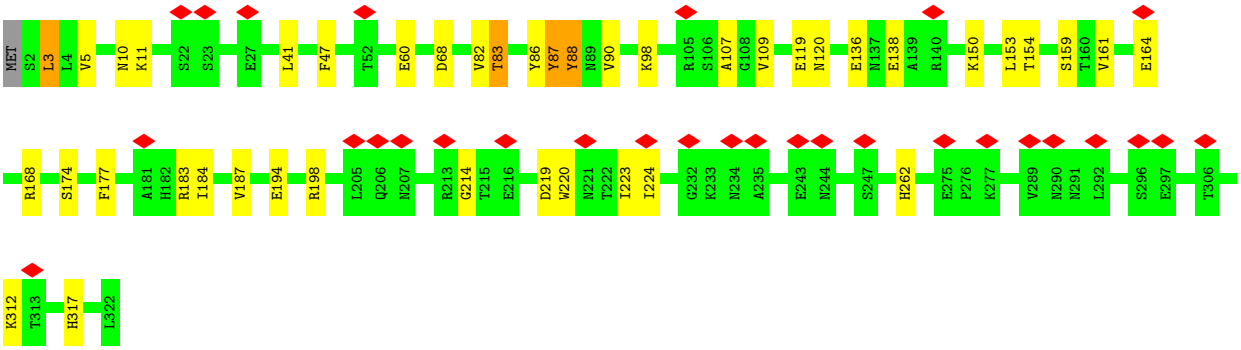
• Molecule 9: Transmembrane protein, putative

Chain CK:



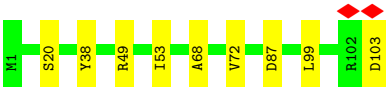
• Molecule 10: NmrA domain-containing protein

Chain CE:



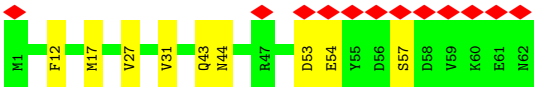
• Molecule 11: Transmembrane protein, putative

Chain CJ:



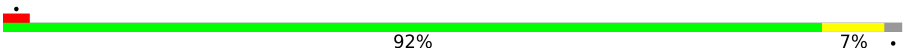
• Molecule 12: Transmembrane protein, putative

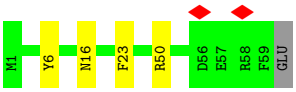
Chain CN:



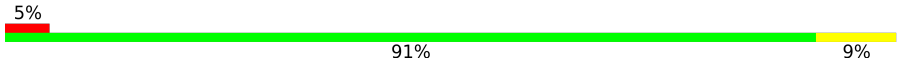
• Molecule 13: Cytochrome b-c1 complex subunit 8

Chain CC:

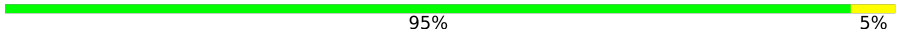




• Molecule 14: SDHTT11

Chain CO: 

- Molecule 15: SDHD

Chain CD: 

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	6.278	Depositor
Minimum map value	-2.240	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.109	Depositor
Recommended contour level	0.8	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: 3PE, UQ8, HEC, FAD, FES, F3S, CDL, PC1, SF4, CA

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	CH	0.18	0/867	0.25	0/1166
2	CM	0.17	0/648	0.23	0/879
3	CL	0.18	0/788	0.24	0/1058
4	CA	0.16	0/4722	0.26	0/6385
5	CI	0.18	0/930	0.25	0/1244
6	CB	0.17	0/2355	0.25	0/3191
7	CF	0.18	0/1857	0.30	0/2512
8	CG	0.18	0/1699	0.27	0/2296
9	CK	0.20	0/821	0.28	0/1112
10	CE	0.17	0/2615	0.29	0/3553
11	CJ	0.18	0/875	0.24	0/1186
12	CN	0.17	0/530	0.28	0/719
13	CC	0.20	0/501	0.26	0/674
14	CO	0.20	0/375	0.24	0/508
15	CD	0.19	0/406	0.26	0/546
All	All	0.17	0/19989	0.27	0/27029

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	CH	855	845	844	9	0
2	CM	629	603	602	6	0
3	CL	770	752	752	7	0
4	CA	4624	4574	4573	48	0
5	CI	915	890	890	7	0
6	CB	2300	2261	2270	22	0
7	CF	1812	1786	1785	16	0
8	CG	1654	1593	1592	17	0
9	CK	795	782	782	11	0
10	CE	2561	2554	2553	24	0
11	CJ	848	815	815	8	0
12	CN	514	515	515	7	0
13	CC	489	487	487	4	0
14	CO	364	378	375	3	0
15	CD	395	412	412	2	0
16	CD	100	156	156	1	0
16	CG	200	312	312	1	0
16	CJ	100	156	156	2	0
16	CK	100	156	156	1	0
16	CM	100	156	156	1	0
16	CO	100	156	156	0	0
17	CA	1	0	0	0	0
17	CB	1	0	0	0	0
18	CA	53	31	29	7	0
19	CB	4	0	0	0	0
20	CB	8	0	0	1	0
21	CB	7	0	0	1	0
22	CC	51	82	82	1	0
22	CD	51	82	82	2	0
22	CK	51	82	82	0	0
23	CE	43	32	31	2	0
24	CC	54	88	88	1	0
25	CC	53	74	74	0	0
All	All	20602	20810	20807	162	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 4.

All (162) 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)
11:CJ:49:ARG:NH1	16:CJ:201:CDL:OB7	2.08	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CA:589:ARG:NH2	4:CA:632:ALA:O	2.12	0.82
16:CG:301:CDL:OB3	11:CJ:38:TYR:OH	1.99	0.80
8:CG:114:ARG:NH1	16:CD:301:CDL:OB4	2.18	0.77
7:CF:277:SER:HB3	9:CK:80:ILE:HD11	1.67	0.77
6:CB:180:LYS:NZ	8:CG:195:TYR:O	2.18	0.76
7:CF:145:GLU:OE1	14:CO:35:LYS:NZ	2.18	0.76
6:CB:130:CYS:SG	6:CB:141:ALA:N	2.62	0.73
4:CA:553:GLU:OE2	6:CB:120:ARG:NH2	2.22	0.72
10:CE:183:ARG:NE	10:CE:219:ASP:OD1	2.24	0.70
9:CK:34:ARG:NH1	9:CK:35:ASN:OD1	2.27	0.68
6:CB:258:GLU:N	6:CB:258:GLU:OE1	2.28	0.66
4:CA:242:LEU:O	4:CA:430:ASN:ND2	2.28	0.66
8:CG:52:GLU:N	8:CG:52:GLU:OE1	2.29	0.64
8:CG:61:GLU:OE2	8:CG:89:ASN:ND2	2.29	0.64
10:CE:154:THR:O	10:CE:159:SER:OG	2.15	0.64
5:CI:57:GLY:O	7:CF:274:SER:OG	2.04	0.64
6:CB:178:GLN:NE2	6:CB:232:PRO:O	2.31	0.64
4:CA:429:GLU:OE1	18:CA:702:FAD:O3'	2.14	0.62
10:CE:168:ARG:NH2	10:CE:174:SER:O	2.33	0.62
8:CG:155:GLU:N	8:CG:155:GLU:OE1	2.34	0.61
4:CA:52:ILE:HD11	4:CA:235:ILE:HG22	1.83	0.60
8:CG:68:GLU:N	8:CG:68:GLU:OE1	2.30	0.60
7:CF:119:HIS:NE2	7:CF:142:ASP:OD2	2.35	0.60
10:CE:312:LYS:O	10:CE:317:HIS:ND1	2.34	0.60
8:CG:36:GLU:OE2	8:CG:106:LYS:NZ	2.34	0.60
10:CE:10:ASN:ND2	10:CE:120:ASN:OD1	2.34	0.59
4:CA:449:ILE:HD11	18:CA:702:FAD:C4'	2.32	0.59
6:CB:189:LYS:N	6:CB:254:GLU:OE1	2.35	0.59
1:CH:153:ARG:NH1	3:CL:19:LYS:O	2.36	0.59
8:CG:17:ILE:HD11	8:CG:78:TYR:HA	1.84	0.59
12:CN:44:ASN:ND2	14:CO:34:TYR:OH	2.37	0.58
4:CA:112:ASP:OD1	4:CA:164:SER:OG	2.21	0.58
1:CH:188:LEU:HD22	5:CI:2:PHE:CD1	2.39	0.58
4:CA:583:ARG:NH2	4:CA:585:ASP:OD2	2.38	0.57
2:CM:64:ASN:ND2	7:CF:168:GLN:OE1	2.34	0.57
4:CA:623:ASP:OD1	4:CA:624:SER:N	2.36	0.57
10:CE:10:ASN:OD1	10:CE:11:LYS:N	2.37	0.57
4:CA:621:THR:OG1	4:CA:623:ASP:O	2.23	0.56
5:CI:58:ASP:OD1	5:CI:59:ASN:ND2	2.38	0.56
6:CB:262:ARG:NH2	8:CG:162:GLU:OE2	2.39	0.56
4:CA:145:LEU:HD12	4:CA:146:PRO:HD2	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CA:406:LYS:O	4:CA:407:THR:OG1	2.15	0.55
6:CB:83:ASP:OD1	6:CB:84:GLN:N	2.39	0.55
4:CA:404:ASN:O	4:CA:405:TRP:HB3	2.07	0.55
4:CA:449:ILE:HD11	18:CA:702:FAD:H4'	1.88	0.55
7:CF:190:ARG:NH2	7:CF:223:GLU:OE2	2.40	0.54
10:CE:3:LEU:HD23	10:CE:5:VAL:HG23	1.88	0.54
5:CI:41:SER:OG	9:CK:75:LEU:HD11	2.08	0.54
3:CL:35:GLN:O	3:CL:69:LYS:NZ	2.24	0.54
10:CE:184:ILE:HD11	10:CE:220:TRP:CD1	2.43	0.54
10:CE:164:GLU:OE2	10:CE:262:HIS:NE2	2.39	0.54
1:CH:108:LYS:NZ	1:CH:112:ASP:OD2	2.36	0.54
12:CN:43:GLN:NE2	12:CN:44:ASN:OD1	2.40	0.54
6:CB:214:GLU:N	6:CB:214:GLU:OE1	2.39	0.53
4:CA:80:LEU:HD11	4:CA:259:THR:HG21	1.91	0.53
4:CA:578:ARG:NH2	4:CA:591:ASP:OD1	2.39	0.52
8:CG:105:LEU:HD12	8:CG:164:ILE:CG2	2.39	0.52
15:CD:35:ILE:HD13	22:CD:302:3PE:H32	1.90	0.52
6:CB:263:ILE:CD1	6:CB:295:LEU:HD22	2.40	0.52
9:CK:41:VAL:HG12	9:CK:42:PHE:N	2.24	0.52
5:CI:95:ASP:OD1	5:CI:96:TYR:N	2.43	0.52
7:CF:268:TYR:CD2	9:CK:75:LEU:HD13	2.45	0.51
4:CA:212:ILE:O	4:CA:220:ARG:N	2.43	0.51
4:CA:257:ALA:HB1	6:CB:121:SER:O	2.10	0.51
4:CA:263:ASP:CG	18:CA:702:FAD:H61A	2.17	0.51
7:CF:101:ASP:OD1	7:CF:159:TYR:OH	2.28	0.51
10:CE:82:VAL:O	10:CE:83:THR:C	2.53	0.51
10:CE:184:ILE:HD13	10:CE:223:ILE:HD12	1.92	0.51
4:CA:59:ALA:N	4:CA:449:ILE:HG23	2.26	0.51
1:CH:149:GLN:NE2	3:CL:21:LEU:O	2.43	0.51
10:CE:177:PHE:CE1	10:CE:224:ILE:HD12	2.46	0.50
8:CG:25:ARG:NH2	10:CE:68:ASP:OD1	2.45	0.50
8:CG:65:ILE:HD12	8:CG:78:TYR:CE2	2.47	0.50
2:CM:44:ARG:NH1	11:CJ:87:ASP:OD1	2.45	0.50
4:CA:251:TYR:CG	4:CA:394:VAL:HG21	2.47	0.50
8:CG:159:LYS:HD2	9:CK:10:MET:HE1	1.92	0.49
6:CB:218:CYS:N	20:CB:1001:SF4:S3	2.80	0.49
6:CB:221:CYS:SG	6:CB:222:SER:N	2.85	0.49
4:CA:261:THR:HA	4:CA:560:LEU:HD21	1.95	0.49
8:CG:26:VAL:HG21	8:CG:53:LEU:HD12	1.95	0.49
10:CE:136:GLU:OE2	10:CE:150:LYS:NZ	2.42	0.49
2:CM:17:GLN:NE2	11:CJ:53:ILE:O	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CA:299:CYS:SG	4:CA:300:ARG:N	2.86	0.48
8:CG:17:ILE:HG21	10:CE:41:LEU:HD21	1.95	0.48
11:CJ:99:LEU:HD23	11:CJ:103:ASP:O	2.13	0.48
1:CH:178:ILE:HG22	1:CH:179:SER:N	2.29	0.48
9:CK:41:VAL:HG13	22:CD:302:3PE:H3F1	1.94	0.48
16:CJ:201:CDL:H801	15:CD:33:THR:HG21	1.94	0.48
4:CA:327:SER:O	4:CA:330:VAL:HG12	2.15	0.47
4:CA:413:ASP:OD1	4:CA:414:LYS:N	2.47	0.47
7:CF:277:SER:CB	9:CK:80:ILE:HD11	2.40	0.47
10:CE:60:GLU:OE1	10:CE:60:GLU:N	2.47	0.47
10:CE:107:ALA:O	10:CE:109:VAL:HG23	2.15	0.47
4:CA:585:ASP:OD1	4:CA:586:PHE:N	2.48	0.47
7:CF:147:GLU:OE2	7:CF:151:ARG:NE	2.48	0.46
5:CI:11:LYS:NZ	12:CN:54:GLU:OE2	2.46	0.46
23:CE:401:HEC:HHC	23:CE:401:HEC:HBB3	1.97	0.46
4:CA:617:VAL:HG12	4:CA:618:ILE:N	2.31	0.46
4:CA:85:SER:O	4:CA:88:VAL:HG12	2.15	0.46
4:CA:246:GLY:O	4:CA:262:GLY:N	2.49	0.45
13:CC:50:ARG:NH2	22:CC:301:3PE:O12	2.48	0.45
2:CM:3:ARG:NH2	6:CB:270:ASP:O	2.49	0.45
4:CA:329:ASP:OD1	4:CA:439:ASN:ND2	2.50	0.45
6:CB:263:ILE:HD11	6:CB:295:LEU:HD22	1.98	0.45
10:CE:194:GLU:OE2	10:CE:198:ARG:NH2	2.50	0.45
12:CN:12:PHE:CE2	12:CN:17:MET:HE2	2.52	0.45
2:CM:25:GLU:HG2	11:CJ:72:VAL:HG21	1.98	0.44
4:CA:141:GLU:OE2	4:CA:149:ARG:NH2	2.50	0.44
12:CN:17:MET:HE1	13:CC:23:PHE:CE2	2.53	0.44
4:CA:92:GLY:N	18:CA:702:FAD:O4	2.50	0.44
3:CL:56:GLN:N	3:CL:60:GLN:OE1	2.47	0.44
4:CA:46:ASP:OD1	4:CA:234:ARG:NE	2.49	0.44
8:CG:104:GLU:HG3	9:CK:26:LEU:HD12	1.98	0.44
10:CE:119:GLU:HB2	10:CE:161:VAL:HG23	1.99	0.43
10:CE:187:VAL:HG22	10:CE:214:GLY:N	2.32	0.43
1:CH:102:LEU:HD23	3:CL:11:ILE:HG23	1.99	0.43
2:CM:12:LYS:HA	2:CM:15:LEU:HD12	2.01	0.43
5:CI:45:LEU:HD21	7:CF:268:TYR:CD2	2.53	0.43
4:CA:404:ASN:OD1	4:CA:405:TRP:N	2.47	0.43
13:CC:6:TYR:OH	24:CC:302:PC1:O12	2.35	0.43
6:CB:277:MET:SD	13:CC:16:ASN:ND2	2.86	0.43
12:CN:27:VAL:O	12:CN:31:VAL:HG22	2.19	0.43
12:CN:53:ASP:OD2	12:CN:57:SER:OG	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CH:98:GLU:OE2	3:CL:16:ARG:NH2	2.52	0.43
1:CH:114:ASN:OD1	1:CH:115:SER:N	2.52	0.43
7:CF:209:TYR:HA	7:CF:212:ARG:HG2	2.01	0.43
6:CB:241:LEU:HB2	6:CB:292:LEU:HD21	2.01	0.42
4:CA:566:GLN:OE1	4:CA:600:THR:OG1	2.26	0.42
4:CA:145:LEU:HD12	4:CA:146:PRO:CD	2.49	0.42
6:CB:265:GLU:O	6:CB:266:ASP:C	2.62	0.42
14:CO:3:LEU:N	14:CO:4:PRO:CD	2.82	0.42
4:CA:124:ASP:N	4:CA:124:ASP:OD1	2.52	0.42
7:CF:279:GLN:OE1	7:CF:279:GLN:N	2.51	0.42
16:CK:102:CDL:OA5	11:CJ:20:SER:OG	2.36	0.42
4:CA:114:VAL:HG11	4:CA:629:VAL:HB	2.02	0.42
4:CA:90:ALA:O	4:CA:184:GLY:N	2.48	0.42
4:CA:263:ASP:CB	18:CA:702:FAD:H61A	2.33	0.42
7:CF:278:VAL:HG21	9:CK:75:LEU:HD12	2.02	0.42
11:CJ:68:ALA:O	11:CJ:72:VAL:HG23	2.20	0.42
4:CA:194:ARG:O	4:CA:197:ALA:HB3	2.19	0.41
18:CA:702:FAD:H9	18:CA:702:FAD:H1'1	1.87	0.41
4:CA:127:GLN:OE1	4:CA:622:LEU:N	2.52	0.41
10:CE:87:TYR:O	10:CE:88:TYR:HB2	2.19	0.41
16:CM:201:CDL:H671	9:CK:44:ILE:HD12	2.01	0.41
10:CE:86:TYR:HB2	10:CE:90:VAL:HG11	2.01	0.41
6:CB:274:GLN:OE1	6:CB:289:GLN:NE2	2.54	0.41
6:CB:278:CYS:N	21:CB:1002:F3S:S4	2.93	0.41
6:CB:120:ARG:O	6:CB:120:ARG:CG	2.69	0.41
4:CA:54:VAL:HG13	4:CA:208:VAL:HG21	2.02	0.41
4:CA:81:PHE:O	4:CA:82:PRO:C	2.63	0.41
4:CA:96:ALA:CB	4:CA:137:VAL:HG21	2.51	0.41
4:CA:96:ALA:HB2	4:CA:137:VAL:HG21	2.02	0.41
4:CA:295:MET:SD	4:CA:371:ILE:HD11	2.60	0.41
3:CL:12:THR:N	3:CL:13:PRO:CD	2.84	0.41
10:CE:262:HIS:NE2	23:CE:401:HEC:O2A	2.53	0.41
1:CH:127:VAL:HG23	7:CF:102:MET:HE2	2.02	0.40
4:CA:348:LYS:O	4:CA:349:LYS:C	2.64	0.40
6:CB:190:THR:N	6:CB:254:GLU:OE1	2.54	0.40
8:CG:12:LEU:HD21	8:CG:63:TRP:CE3	2.56	0.40
7:CF:157:LYS:O	7:CF:248:ARG:NH2	2.48	0.40
10:CE:98:LYS:NZ	10:CE:138:GLU:OE1	2.48	0.40

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	CH	108/195 (55%)	104 (96%)	4 (4%)	0	100	100
2	CM	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
3	CL	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
4	CA	597/636 (94%)	581 (97%)	15 (2%)	1 (0%)	43	76
5	CI	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
6	CB	283/312 (91%)	272 (96%)	10 (4%)	1 (0%)	30	65
7	CF	216/296 (73%)	208 (96%)	8 (4%)	0	100	100
8	CG	194/198 (98%)	190 (98%)	4 (2%)	0	100	100
9	CK	91/93 (98%)	88 (97%)	3 (3%)	0	100	100
10	CE	319/322 (99%)	293 (92%)	23 (7%)	3 (1%)	14	48
11	CJ	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
12	CN	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
13	CC	57/60 (95%)	57 (100%)	0	0	100	100
14	CO	41/43 (95%)	41 (100%)	0	0	100	100
15	CD	42/44 (96%)	42 (100%)	0	0	100	100
All	All	2379/2643 (90%)	2296 (96%)	78 (3%)	5 (0%)	44	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	CA	405	TRP
10	CE	83	THR
10	CE	153	LEU
6	CB	266	ASP
10	CE	88	TYR

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	CH	100/184 (54%)	100 (100%)	0	100	100
2	CM	65/67 (97%)	65 (100%)	0	100	100
3	CL	82/83 (99%)	82 (100%)	0	100	100
4	CA	481/515 (93%)	479 (100%)	2 (0%)	84	90
5	CI	97/97 (100%)	97 (100%)	0	100	100
6	CB	259/283 (92%)	253 (98%)	6 (2%)	44	74
7	CF	194/268 (72%)	194 (100%)	0	100	100
8	CG	179/181 (99%)	177 (99%)	2 (1%)	65	83
9	CK	85/85 (100%)	84 (99%)	1 (1%)	63	82
10	CE	286/287 (100%)	283 (99%)	3 (1%)	68	84
11	CJ	86/86 (100%)	86 (100%)	0	100	100
12	CN	56/56 (100%)	56 (100%)	0	100	100
13	CC	50/51 (98%)	50 (100%)	0	100	100
14	CO	38/38 (100%)	38 (100%)	0	100	100
15	CD	43/43 (100%)	43 (100%)	0	100	100
All	All	2101/2324 (90%)	2087 (99%)	14 (1%)	73	86

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	CA	160	PHE
4	CA	345	VAL
6	CB	122	CYS
6	CB	161	HIS
6	CB	215	CYS
6	CB	225	CYS
6	CB	231	HIS
6	CB	272	CYS
8	CG	99	HIS
8	CG	169	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	CK	41	VAL
10	CE	3	LEU
10	CE	47	PHE
10	CE	87	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	CH	105	HIS
3	CL	76	GLN
4	CA	157	GLN
4	CA	282	GLN
4	CA	365	HIS
4	CA	439	ASN
6	CB	56	HIS
6	CB	70	GLN
6	CB	205	GLN
6	CB	257	GLN
9	CK	51	ASN
10	CE	114	ASN
10	CE	238	ASN
10	CE	265	ASN
11	CJ	25	ASN
12	CN	43	GLN
12	CN	44	ASN
15	CD	25	ASN
15	CD	29	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
25	UQ8	CC	303	-	53,53,53	0.52	0	64,67,67	0.79	4 (6%)
16	CDL	CM	201	-	99,99,99	0.29	0	105,111,111	0.26	0
16	CDL	CG	301	-	99,99,99	0.30	0	105,111,111	0.26	0
22	3PE	CD	302	-	50,50,50	0.27	0	53,55,55	0.20	0
23	HEC	CE	401	10	50,50,50	1.71	5 (10%)	68,82,82	1.35	6 (8%)
20	SF4	CB	1001	-	0,12,12	-	-	-		
16	CDL	CG	302	-	99,99,99	0.30	0	105,111,111	0.25	0
22	3PE	CC	301	-	50,50,50	0.27	0	53,55,55	0.21	0
16	CDL	CO	101	-	99,99,99	0.29	0	105,111,111	0.27	0
16	CDL	CJ	201	-	99,99,99	0.30	0	105,111,111	0.26	0
18	FAD	CA	702	4	56,58,58	0.37	0	81,89,89	0.46	1 (1%)
19	FES	CB	1000	-	0,4,4	-	-	-		
22	3PE	CK	101	-	50,50,50	0.27	0	53,55,55	0.21	0
21	F3S	CB	1002	-	0,9,9	-	-	-		
24	PC1	CC	302	-	53,53,53	0.29	0	59,61,61	0.28	0
16	CDL	CK	102	-	99,99,99	0.29	0	105,111,111	0.26	0
16	CDL	CD	301	-	99,99,99	0.30	0	105,111,111	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	UQ8	CC	303	-	-	9/51/75/75	0/1/1/1
16	CDL	CM	201	-	-	17/110/110/110	-
16	CDL	CG	301	-	-	23/110/110/110	-
22	3PE	CD	302	-	-	14/54/54/54	-
23	HEC	CE	401	10	1/1/7/7	4/14/54/54	-
20	SF4	CB	1001	-	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CDL	CG	302	-	-	27/110/110/110	-
22	3PE	CC	301	-	-	5/54/54/54	-
16	CDL	CO	101	-	-	20/110/110/110	-
16	CDL	CJ	201	-	-	18/110/110/110	-
18	FAD	CA	702	4	-	12/34/50/50	0/6/6/6
19	FES	CB	1000	-	-	-	0/1/1/1
22	3PE	CK	101	-	-	4/54/54/54	-
21	F3S	CB	1002	-	-	-	0/3/3/3
24	PC1	CC	302	-	-	15/57/57/57	-
16	CDL	CK	102	-	-	31/110/110/110	-
16	CDL	CD	301	-	-	32/110/110/110	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CE	401	HEC	C3D-C2D	7.79	1.53	1.36
23	CE	401	HEC	FE-NB	3.90	2.06	1.94
23	CE	401	HEC	FE-ND	3.68	2.06	1.94
23	CE	401	HEC	FE-NA	2.85	2.04	1.95
23	CE	401	HEC	FE-NC	2.47	2.03	1.95

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	CE	401	HEC	C1D-ND-C4D	5.95	111.22	105.07
18	CA	702	FAD	P-O3P-PA	-3.24	121.72	132.83
25	CC	303	UQ8	C7-C8-C9	3.01	131.81	126.79
25	CC	303	UQ8	C11-C9-C8	-2.74	115.58	121.12
23	CE	401	HEC	C4B-NB-C1B	2.36	107.51	105.07
25	CC	303	UQ8	C17-C18-C19	-2.28	122.17	127.66
23	CE	401	HEC	CAA-CBA-CGA	-2.27	108.72	113.60
25	CC	303	UQ8	C10-C9-C11	2.22	119.00	115.27
23	CE	401	HEC	C4C-NC-C1C	2.18	107.48	105.35
23	CE	401	HEC	CAD-CBD-CGD	-2.10	109.09	113.60
23	CE	401	HEC	C2A-C1A-NA	-2.06	108.32	110.32

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	CE	401	HEC	NA

All (231) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	CM	201	CDL	OB6-CB4-CB6-OB8
16	CG	301	CDL	CA2-OA2-PA1-OA3
16	CG	301	CDL	CA2-OA2-PA1-OA4
16	CG	301	CDL	CB2-OB2-PB2-OB3
16	CG	301	CDL	OB9-CB7-OB8-CB6
16	CG	302	CDL	C11-CA5-OA6-CA4
16	CG	302	CDL	CB2-OB2-PB2-OB4
16	CG	302	CDL	CB3-OB5-PB2-OB2
16	CG	302	CDL	CB3-OB5-PB2-OB3
16	CG	302	CDL	CB3-OB5-PB2-OB4
16	CK	102	CDL	CA3-OA5-PA1-OA2
16	CK	102	CDL	CA3-OA5-PA1-OA3
16	CK	102	CDL	CA4-CA3-OA5-PA1
16	CK	102	CDL	C11-CA5-OA6-CA4
16	CK	102	CDL	CB2-OB2-PB2-OB3
16	CK	102	CDL	CB2-OB2-PB2-OB4
16	CJ	201	CDL	O1-C1-CA2-OA2
16	CJ	201	CDL	CB3-OB5-PB2-OB3
16	CO	101	CDL	OB7-CB5-OB6-CB4
16	CD	301	CDL	CA2-OA2-PA1-OA4
16	CD	301	CDL	CB2-OB2-PB2-OB3
16	CD	301	CDL	CB2-OB2-PB2-OB4
16	CD	301	CDL	CB3-OB5-PB2-OB3
18	CA	702	FAD	C5B-O5B-PA-O2A
18	CA	702	FAD	O4B-C4B-C5B-O5B
18	CA	702	FAD	N10-C1'-C2'-O2'
18	CA	702	FAD	N10-C1'-C2'-C3'
18	CA	702	FAD	C5'-O5'-P-O1P
18	CA	702	FAD	C5'-O5'-P-O2P
18	CA	702	FAD	C5'-O5'-P-O3P
22	CK	101	3PE	C1-O11-P-O14
22	CD	302	3PE	C1-O11-P-O12
24	CC	302	PC1	C1-O11-P-O14
24	CC	302	PC1	O13-C11-C12-N
24	CC	302	PC1	O21-C2-C3-O31
25	CC	303	UQ8	C12-C11-C9-C10
22	CD	302	3PE	O32-C31-O31-C3
22	CD	302	3PE	C32-C31-O31-C3
16	CK	102	CDL	OA9-CA7-OA8-CA6
22	CK	101	3PE	O32-C31-O31-C3
16	CG	302	CDL	OA7-CA5-OA6-CA4
16	CD	301	CDL	CB4-CB6-OB8-CB7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	CG	301	CDL	C71-CB7-OB8-CB6
16	CK	102	CDL	C31-CA7-OA8-CA6
16	CO	101	CDL	C51-CB5-OB6-CB4
25	CC	303	UQ8	C12-C11-C9-C8
16	CM	201	CDL	C71-CB7-OB8-CB6
22	CK	101	3PE	C32-C31-O31-C3
16	CK	102	CDL	OA7-CA5-OA6-CA4
16	CD	301	CDL	OA9-CA7-OA8-CA6
16	CJ	201	CDL	C31-CA7-OA8-CA6
16	CM	201	CDL	OB9-CB7-OB8-CB6
16	CD	301	CDL	C31-CA7-OA8-CA6
16	CK	102	CDL	C1-CB2-OB2-PB2
16	CJ	201	CDL	OA9-CA7-OA8-CA6
16	CG	302	CDL	C31-CA7-OA8-CA6
16	CO	101	CDL	C31-CA7-OA8-CA6
16	CG	302	CDL	C51-CB5-OB6-CB4
16	CG	302	CDL	OA9-CA7-OA8-CA6
24	CC	302	PC1	C32-C31-O31-C3
18	CA	702	FAD	C3B-C4B-C5B-O5B
16	CO	101	CDL	OA9-CA7-OA8-CA6
24	CC	302	PC1	O32-C31-O31-C3
16	CG	301	CDL	CA2-OA2-PA1-OA5
16	CG	301	CDL	CB2-OB2-PB2-OB5
16	CK	102	CDL	CB2-OB2-PB2-OB5
16	CO	101	CDL	CA3-OA5-PA1-OA2
16	CO	101	CDL	CB2-OB2-PB2-OB5
16	CD	301	CDL	CA2-OA2-PA1-OA5
16	CD	301	CDL	CA3-OA5-PA1-OA2
16	CD	301	CDL	CB2-OB2-PB2-OB5
24	CC	302	PC1	C1-O11-P-O13
16	CJ	201	CDL	CB2-C1-CA2-OA2
16	CG	302	CDL	OB7-CB5-OB6-CB4
22	CD	302	3PE	C22-C21-O21-C2
22	CD	302	3PE	O22-C21-O21-C2
22	CD	302	3PE	C27-C28-C29-C2A
16	CO	101	CDL	C11-C12-C13-C14
22	CC	301	3PE	O13-C11-C12-N
16	CK	102	CDL	C61-C62-C63-C64
16	CJ	201	CDL	C76-C77-C78-C79
16	CK	102	CDL	C39-C40-C41-C42
16	CK	102	CDL	C51-CB5-OB6-CB4
16	CG	302	CDL	C78-C79-C80-C81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	CK	102	CDL	OB7-CB5-OB6-CB4
16	CG	302	CDL	C14-C15-C16-C17
16	CG	302	CDL	C20-C21-C22-C23
16	CG	301	CDL	C63-C64-C65-C66
16	CO	101	CDL	C58-C59-C60-C61
16	CG	302	CDL	C72-C73-C74-C75
16	CD	301	CDL	C72-C73-C74-C75
16	CJ	201	CDL	C51-CB5-OB6-CB4
16	CD	301	CDL	C61-C62-C63-C64
16	CJ	201	CDL	C79-C80-C81-C82
16	CJ	201	CDL	OB7-CB5-OB6-CB4
16	CM	201	CDL	C13-C14-C15-C16
25	CC	303	UQ8	C15-C14-C16-C17
22	CD	302	3PE	C32-C33-C34-C35
16	CO	101	CDL	C36-C37-C38-C39
16	CD	301	CDL	C51-CB5-OB6-CB4
16	CG	302	CDL	CB2-OB2-PB2-OB5
16	CD	301	CDL	OA5-CA3-CA4-CA6
16	CO	101	CDL	C52-C53-C54-C55
16	CG	302	CDL	C42-C43-C44-C45
16	CK	102	CDL	O1-C1-CA2-OA2
16	CM	201	CDL	CB3-CB4-CB6-OB8
25	CC	303	UQ8	C1-C6-C7-C8
16	CK	102	CDL	C51-C52-C53-C54
16	CK	102	CDL	C71-CB7-OB8-CB6
25	CC	303	UQ8	C5-C6-C7-C8
16	CK	102	CDL	CA3-CA4-OA6-CA5
16	CD	301	CDL	CB3-CB4-OB6-CB5
16	CK	102	CDL	OA5-CA3-CA4-OA6
16	CG	301	CDL	OB6-CB4-CB6-OB8
16	CJ	201	CDL	C81-C82-C83-C84
16	CD	301	CDL	C71-CB7-OB8-CB6
16	CG	301	CDL	OA5-CA3-CA4-CA6
25	CC	303	UQ8	C39-C41-C42-C43
25	CC	303	UQ8	C14-C16-C17-C18
16	CD	301	CDL	OB7-CB5-OB6-CB4
24	CC	302	PC1	C22-C21-O21-C2
16	CD	301	CDL	CA5-C11-C12-C13
16	CG	302	CDL	C1-CB2-OB2-PB2
16	CD	301	CDL	C1-CB2-OB2-PB2
16	CM	201	CDL	CA3-CA4-CA6-OA8
16	CK	102	CDL	CA3-CA4-CA6-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	CC	301	3PE	C1-C2-C3-O31
24	CC	302	PC1	C1-C2-C3-O31
16	CK	102	CDL	OB9-CB7-OB8-CB6
16	CG	302	CDL	CA2-OA2-PA1-OA5
16	CJ	201	CDL	C14-C15-C16-C17
22	CD	302	3PE	C2C-C2D-C2E-C2F
16	CK	102	CDL	OB5-CB3-CB4-OB6
16	CG	302	CDL	C71-CB7-OB8-CB6
16	CK	102	CDL	OA6-CA4-CA6-OA8
16	CD	301	CDL	OB6-CB4-CB6-OB8
16	CK	102	CDL	CB2-C1-CA2-OA2
24	CC	302	PC1	O22-C21-O21-C2
16	CG	301	CDL	C1-CB2-OB2-PB2
16	CO	101	CDL	C11-CA5-OA6-CA4
16	CD	301	CDL	OB9-CB7-OB8-CB6
24	CC	302	PC1	C35-C36-C37-C38
16	CK	102	CDL	OB5-CB3-CB4-CB6
16	CK	102	CDL	O1-C1-CB2-OB2
16	CD	301	CDL	C37-C38-C39-C40
16	CO	101	CDL	OA7-CA5-OA6-CA4
16	CG	301	CDL	C53-C54-C55-C56
16	CO	101	CDL	CB6-CB4-OB6-CB5
24	CC	302	PC1	C1-C2-O21-C21
25	CC	303	UQ8	C13-C14-C16-C17
16	CD	301	CDL	CB3-CB4-CB6-OB8
18	CA	702	FAD	C5B-O5B-PA-O3P
16	CG	302	CDL	OB9-CB7-OB8-CB6
16	CJ	201	CDL	CB3-OB5-PB2-OB2
16	CG	302	CDL	CB4-CB3-OB5-PB2
22	CD	302	3PE	C2-C1-O11-P
24	CC	302	PC1	C2-C1-O11-P
16	CG	301	CDL	CB2-OB2-PB2-OB4
16	CJ	201	CDL	CB3-OB5-PB2-OB4
16	CO	101	CDL	CA3-OA5-PA1-OA3
16	CO	101	CDL	CB2-OB2-PB2-OB3
16	CO	101	CDL	CB2-OB2-PB2-OB4
16	CD	301	CDL	CA2-OA2-PA1-OA3
16	CD	301	CDL	CA3-OA5-PA1-OA3
16	CD	301	CDL	CB3-OB5-PB2-OB4
18	CA	702	FAD	C5B-O5B-PA-O1A
22	CD	302	3PE	C1-O11-P-O14
24	CC	302	PC1	C1-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	CK	102	CDL	OA5-CA3-CA4-CA6
16	CG	301	CDL	C54-C55-C56-C57
22	CC	301	3PE	C12-C11-O13-P
16	CK	102	CDL	C12-C13-C14-C15
23	CE	401	HEC	C2B-C3B-CAB-CBB
23	CE	401	HEC	C2C-C3C-CAC-CBC
16	CG	301	CDL	OA5-CA3-CA4-OA6
16	CD	301	CDL	OA5-CA3-CA4-OA6
16	CG	302	CDL	C52-C53-C54-C55
16	CG	301	CDL	C71-C72-C73-C74
16	CD	301	CDL	CA3-CA4-CA6-OA8
16	CM	201	CDL	OA6-CA4-CA6-OA8
16	CD	301	CDL	OA6-CA4-CA6-OA8
22	CC	301	3PE	O21-C2-C3-O31
16	CJ	201	CDL	C73-C74-C75-C76
16	CD	301	CDL	C32-C31-CA7-OA8
16	CM	201	CDL	C32-C31-CA7-OA8
16	CO	101	CDL	C12-C13-C14-C15
16	CG	302	CDL	CB6-CB4-OB6-CB5
16	CO	101	CDL	CA6-CA4-OA6-CA5
16	CG	301	CDL	OA7-CA5-OA6-CA4
16	CD	301	CDL	OA7-CA5-OA6-CA4
16	CM	201	CDL	CA3-OA5-PA1-OA2
16	CM	201	CDL	CB2-OB2-PB2-OB5
16	CJ	201	CDL	CA2-OA2-PA1-OA5
16	CO	101	CDL	CB3-OB5-PB2-OB2
16	CJ	201	CDL	CB5-C51-C52-C53
24	CC	302	PC1	C3D-C3E-C3F-C3G
16	CG	301	CDL	C32-C33-C34-C35
16	CM	201	CDL	C1-CB2-OB2-PB2
22	CD	302	3PE	C21-C22-C23-C24
22	CK	101	3PE	C11-O13-P-O11
16	CM	201	CDL	OA5-CA3-CA4-OA6
16	CM	201	CDL	OA5-CA3-CA4-CA6
16	CD	301	CDL	C11-CA5-OA6-CA4
16	CG	301	CDL	C58-C59-C60-C61
16	CG	302	CDL	C12-C13-C14-C15
16	CG	301	CDL	C11-CA5-OA6-CA4
24	CC	302	PC1	O31-C31-C32-C33
16	CK	102	CDL	C19-C20-C21-C22
25	CC	303	UQ8	C9-C11-C12-C13
18	CA	702	FAD	C2'-C3'-C4'-O4'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	CM	201	CDL	OB7-CB5-OB6-CB4
16	CM	201	CDL	C43-C44-C45-C46
16	CJ	201	CDL	C32-C31-CA7-OA8
23	CE	401	HEC	CAD-CBD-CGD-O2D
16	CG	301	CDL	CB3-CB4-CB6-OB8
22	CD	302	3PE	C33-C34-C35-C36
16	CG	301	CDL	C32-C31-CA7-OA8
23	CE	401	HEC	CAD-CBD-CGD-O1D
16	CM	201	CDL	C51-CB5-OB6-CB4
16	CJ	201	CDL	C32-C31-CA7-OA9
16	CG	301	CDL	C32-C31-CA7-OA9
16	CG	302	CDL	C73-C74-C75-C76
22	CD	302	3PE	C37-C38-C39-C3A
16	CG	302	CDL	CA2-OA2-PA1-OA3
16	CG	302	CDL	CB2-OB2-PB2-OB3
16	CO	101	CDL	CB3-OB5-PB2-OB3
22	CD	302	3PE	C11-O13-P-O14
16	CK	102	CDL	C18-C19-C20-C21
22	CC	301	3PE	O31-C31-C32-C33
16	CM	201	CDL	C40-C41-C42-C43
18	CA	702	FAD	O3'-C3'-C4'-C5'

There are no ring outliers.

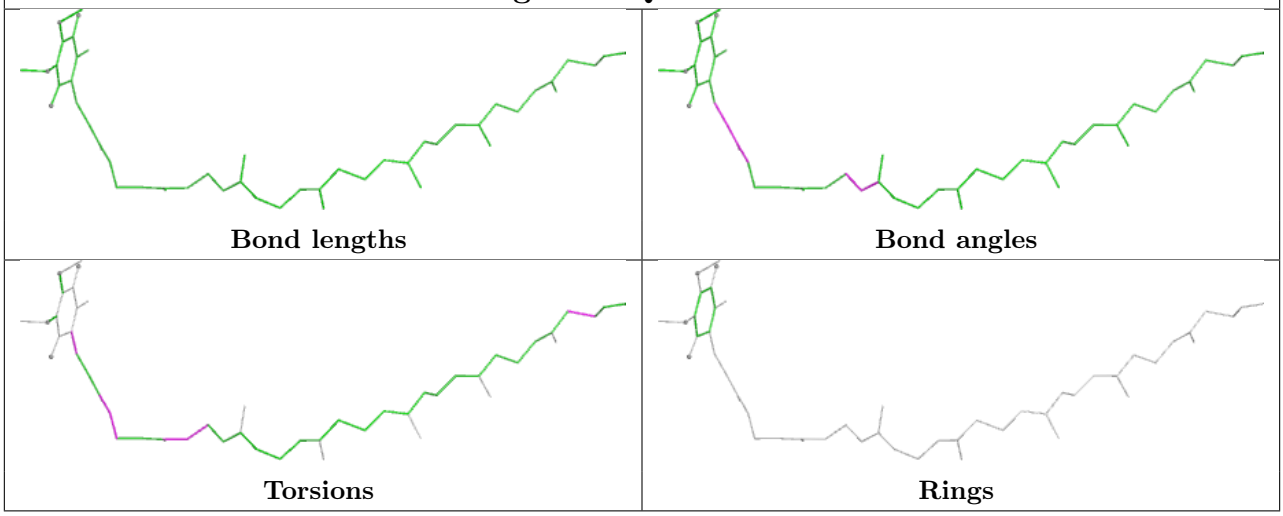
12 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	CM	201	CDL	1	0
16	CG	301	CDL	1	0
22	CD	302	3PE	2	0
23	CE	401	HEC	2	0
20	CB	1001	SF4	1	0
22	CC	301	3PE	1	0
16	CJ	201	CDL	2	0
18	CA	702	FAD	7	0
21	CB	1002	F3S	1	0
24	CC	302	PC1	1	0
16	CK	102	CDL	1	0
16	CD	301	CDL	1	0

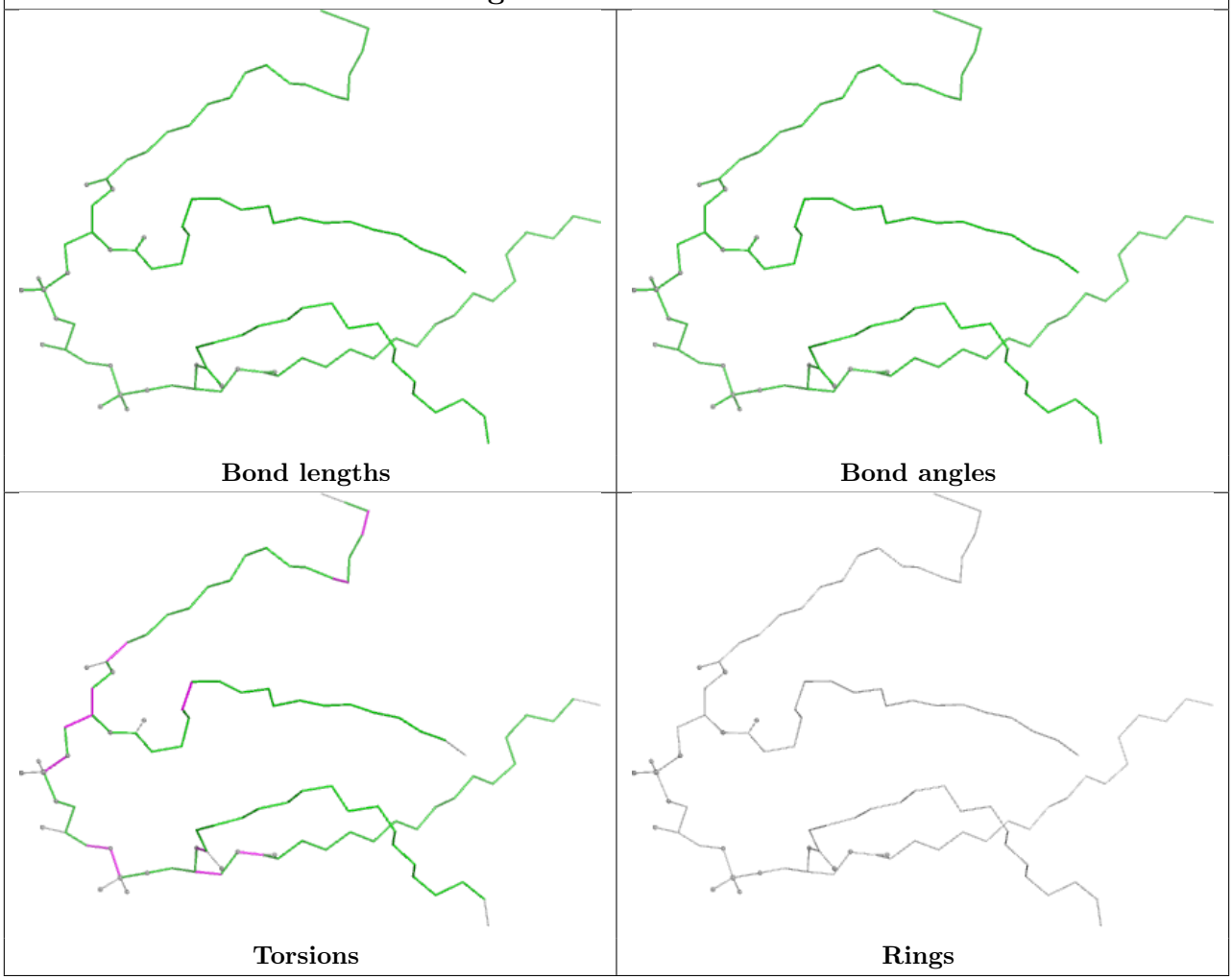
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

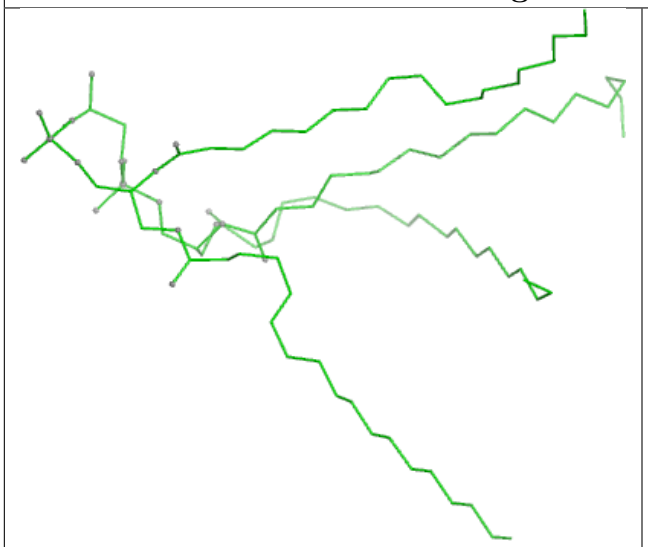
Ligand UQ8 CC 303



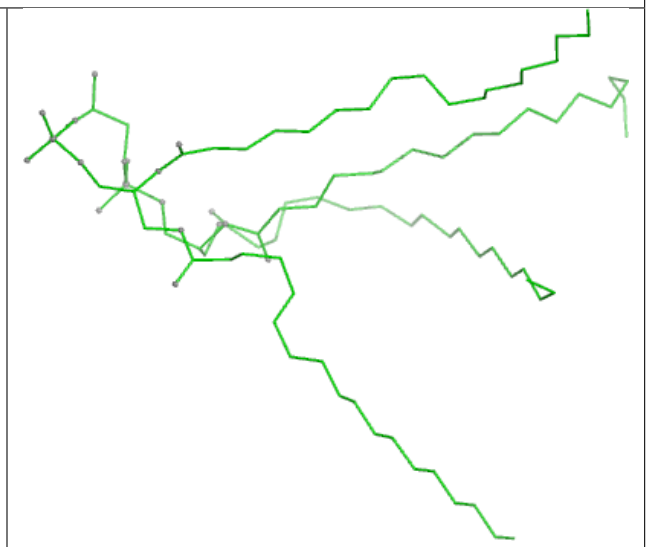
Ligand CDL CM 201



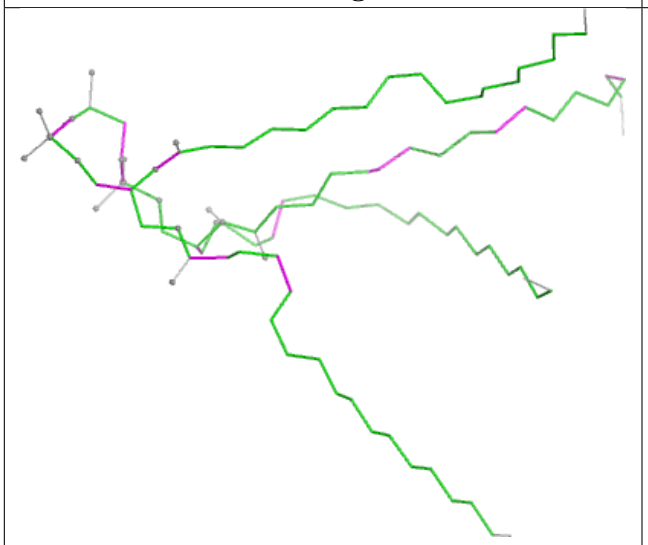
Ligand CDL CG 301



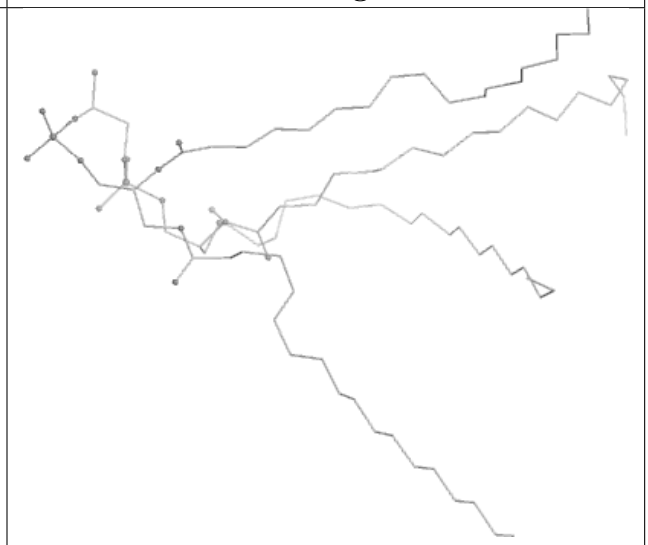
Bond lengths



Bond angles

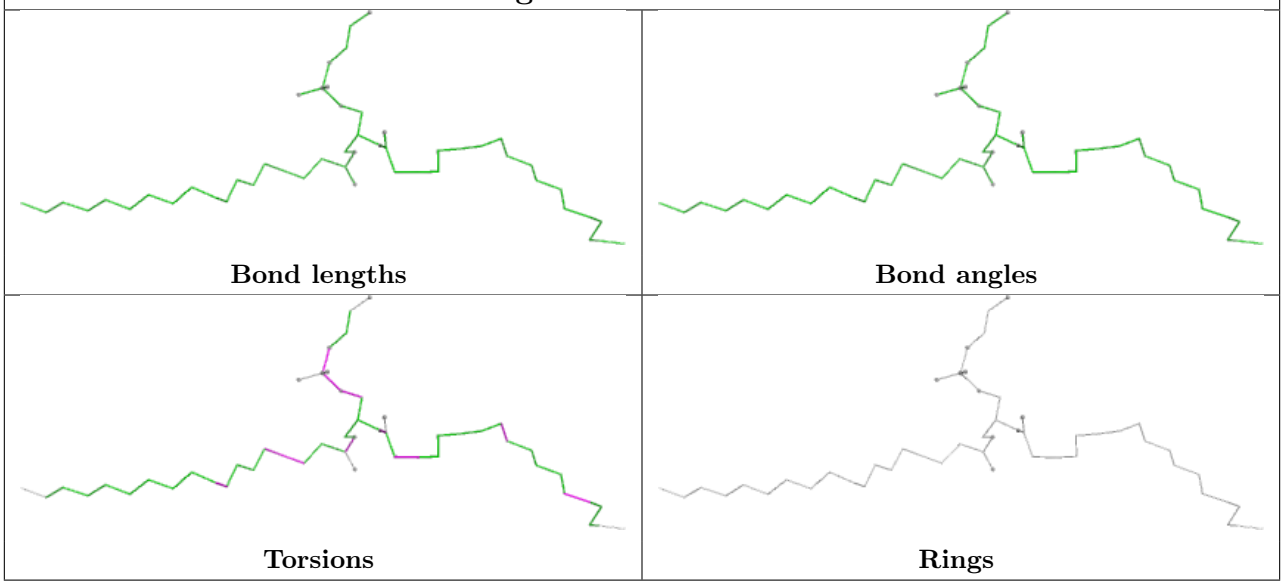


Torsions

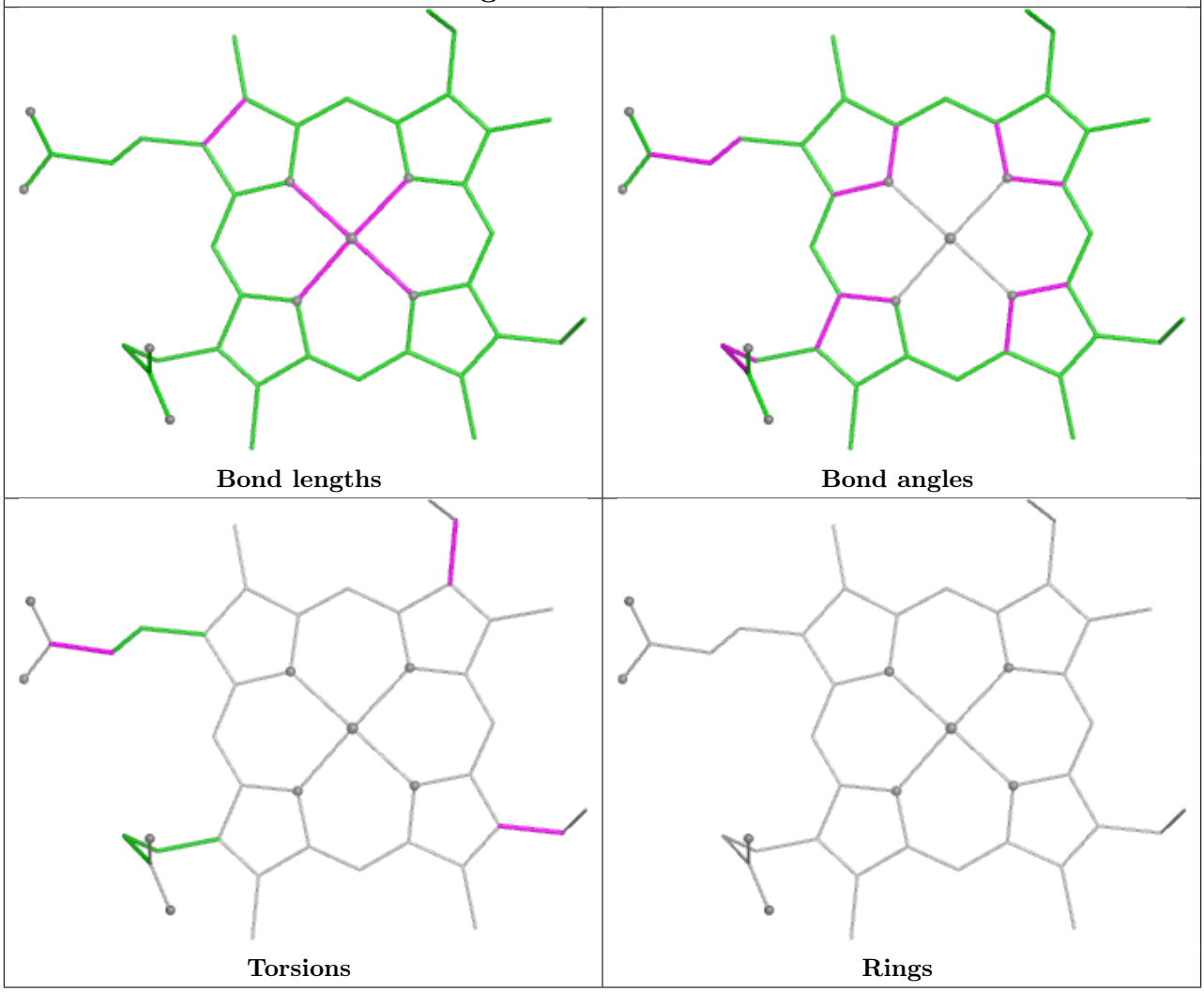


Rings

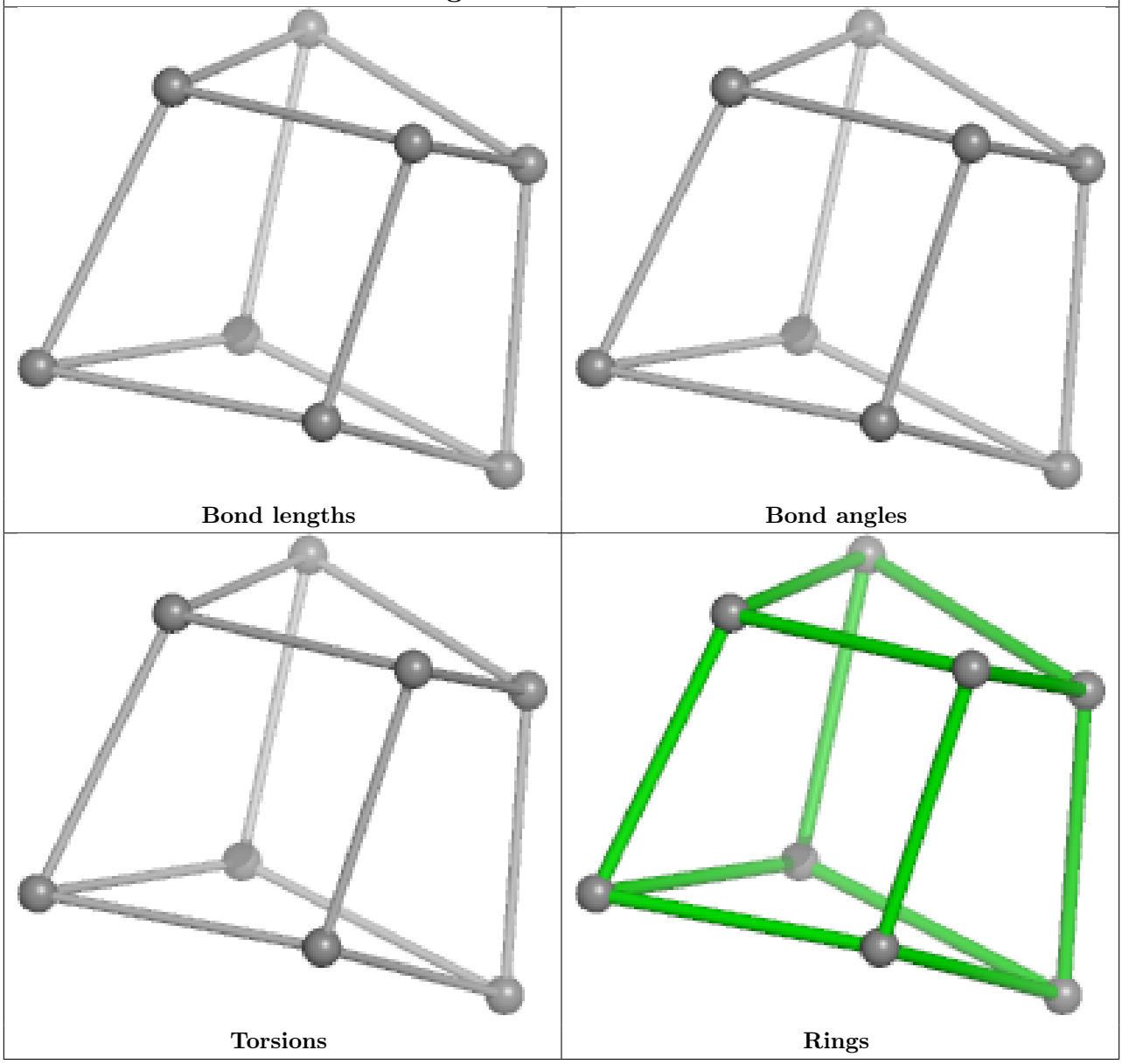
Ligand 3PE CD 302



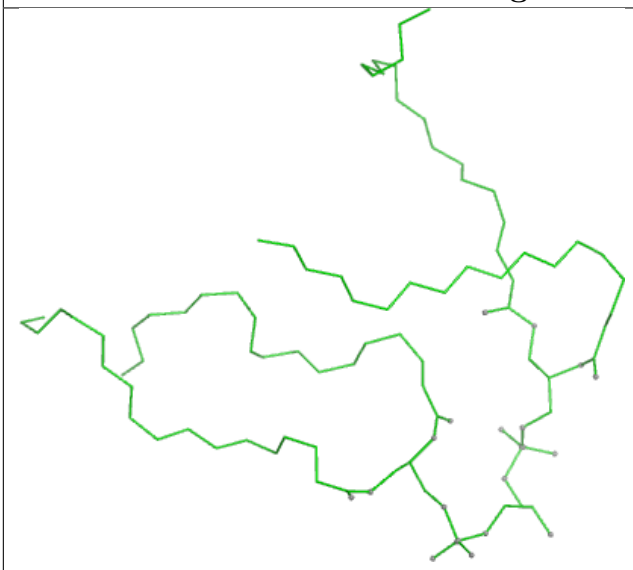
Ligand HEC CE 401



Ligand SF4 CB 1001

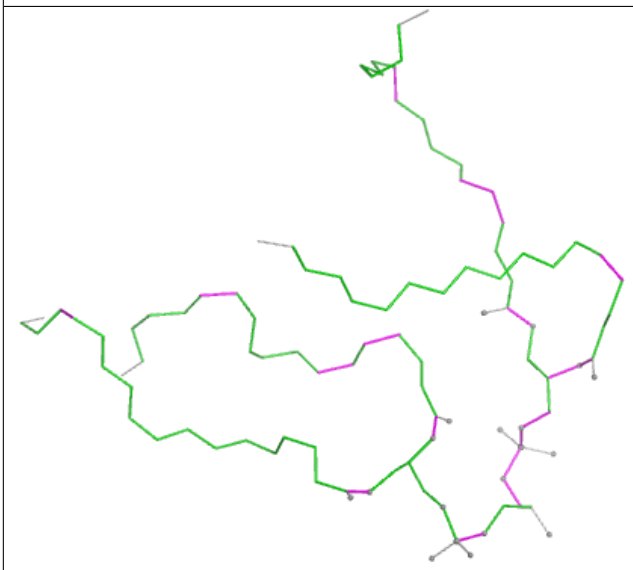


Ligand CDL CG 302



Bond lengths

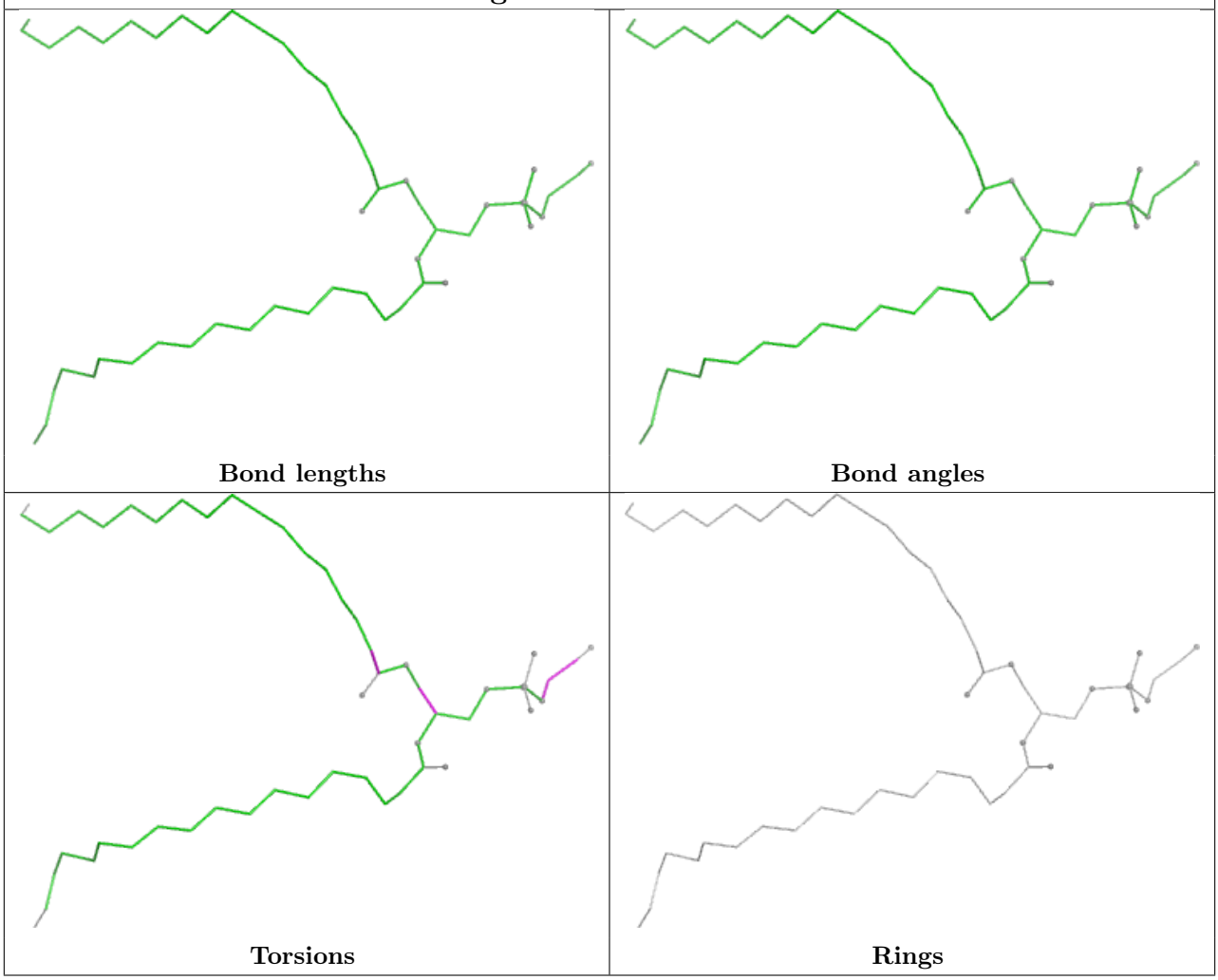
Bond angles



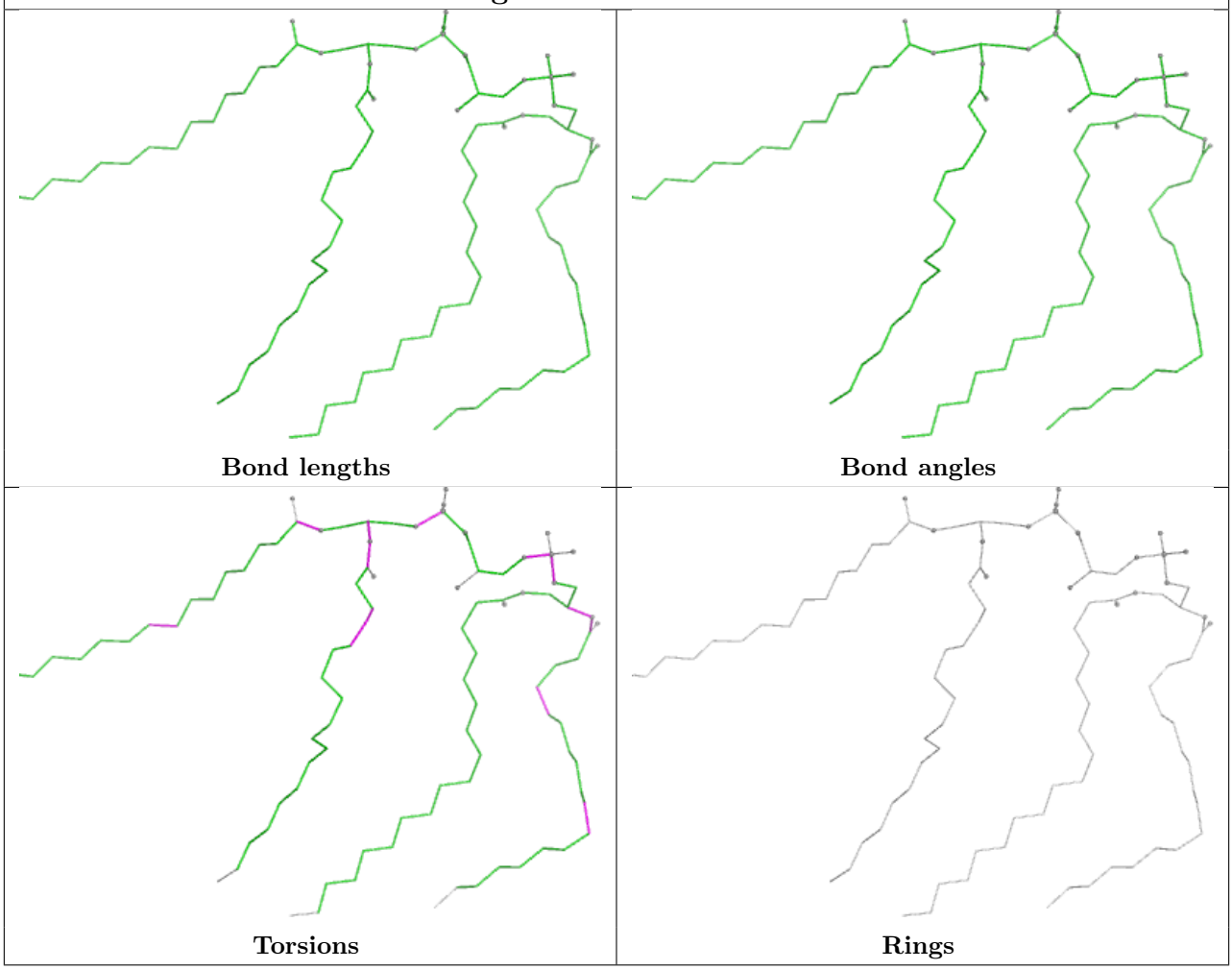
Torsions

Rings

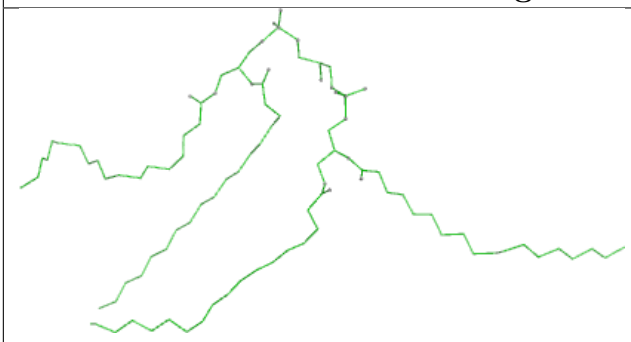
Ligand 3PE CC 301



Ligand CDL CO 101

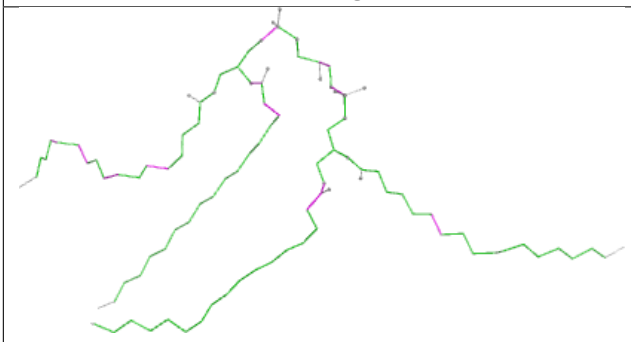


Ligand CDL CJ 201

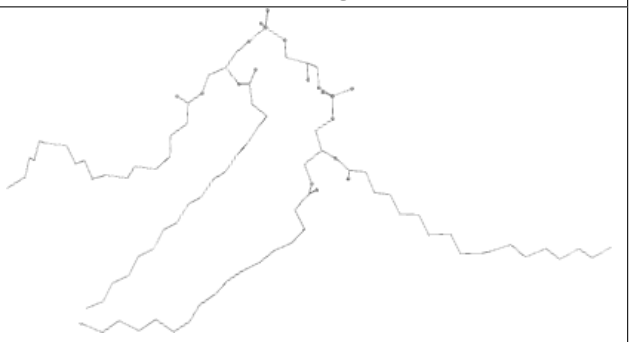


Bond lengths

Bond angles

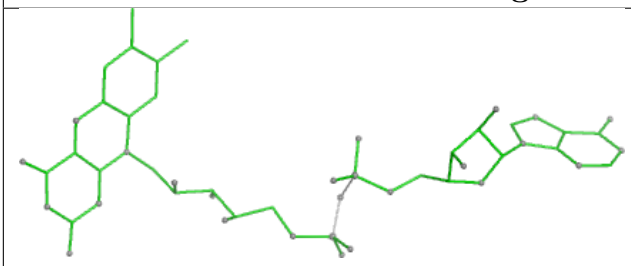


Torsions

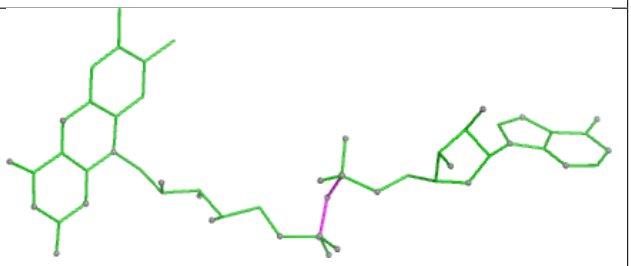


Rings

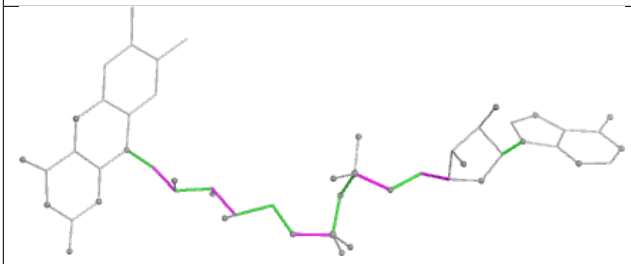
Ligand FAD CA 702



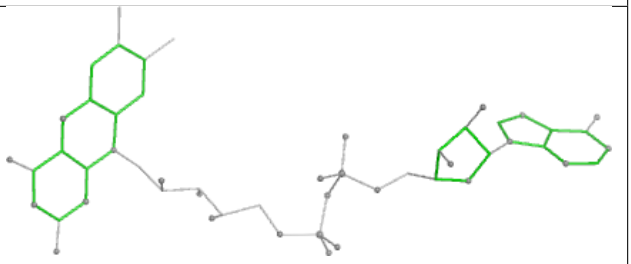
Bond lengths



Bond angles

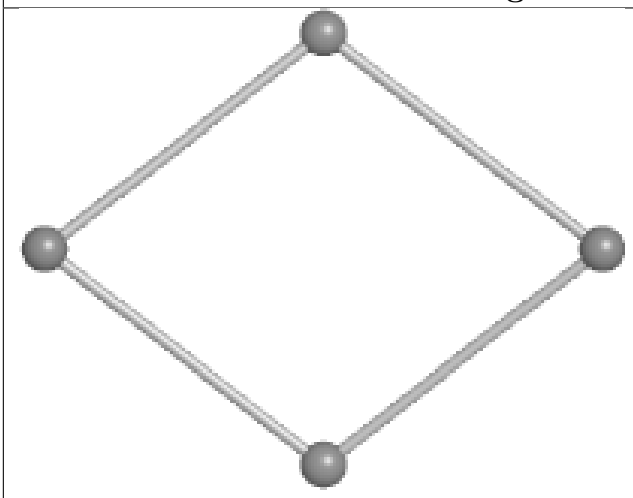


Torsions

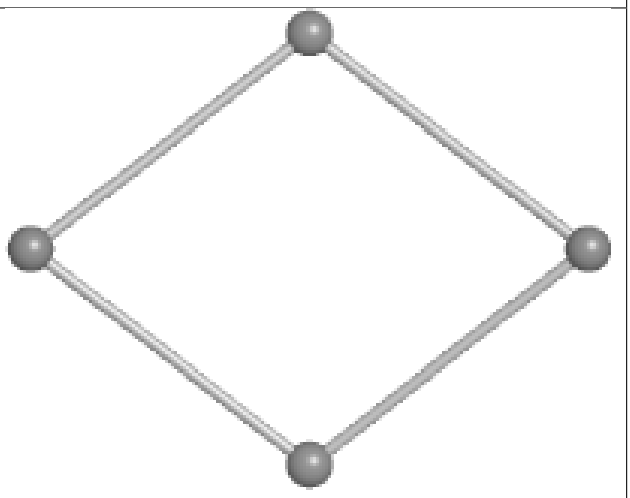


Rings

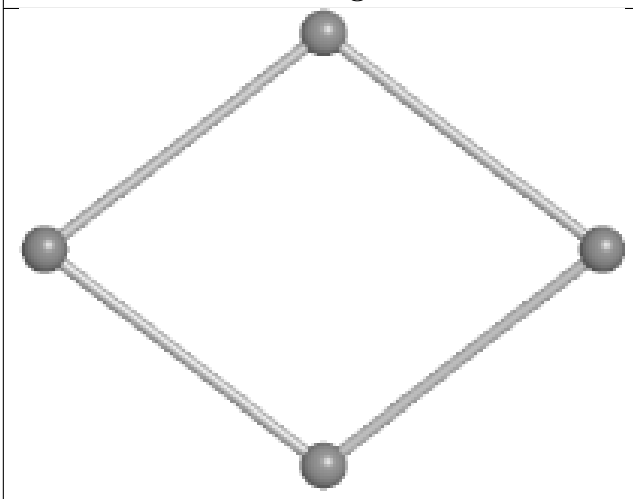
Ligand FES CB 1000



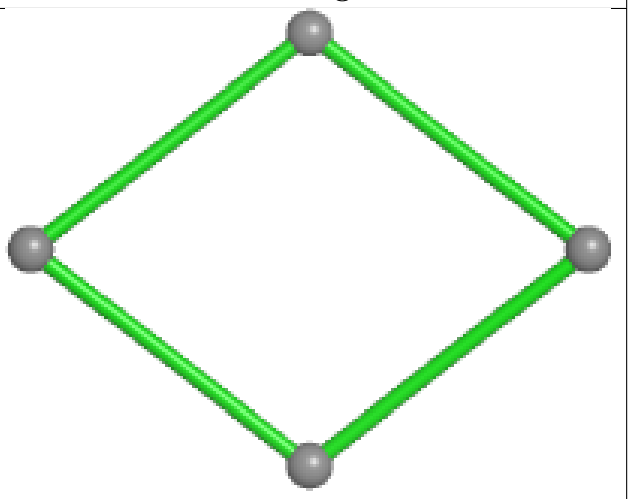
Bond lengths



Bond angles

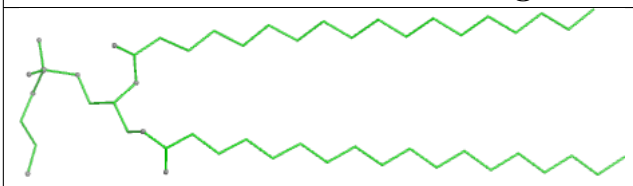


Torsions

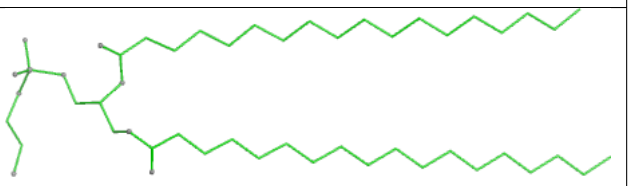


Rings

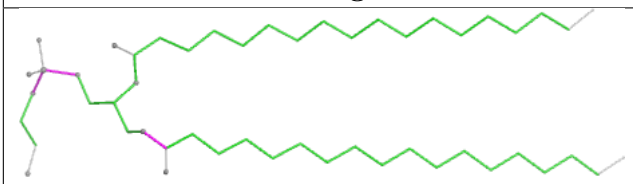
Ligand 3PE CK 101



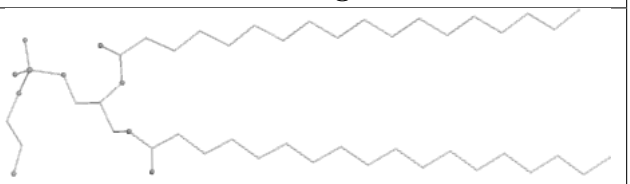
Bond lengths



Bond angles

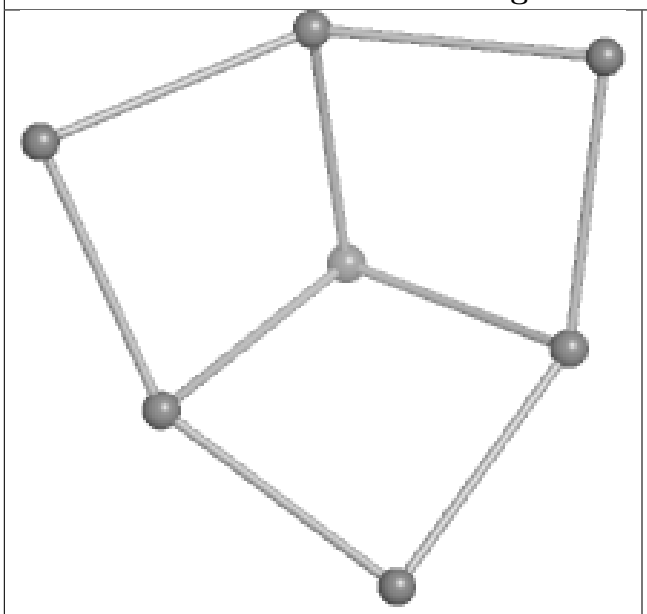


Torsions

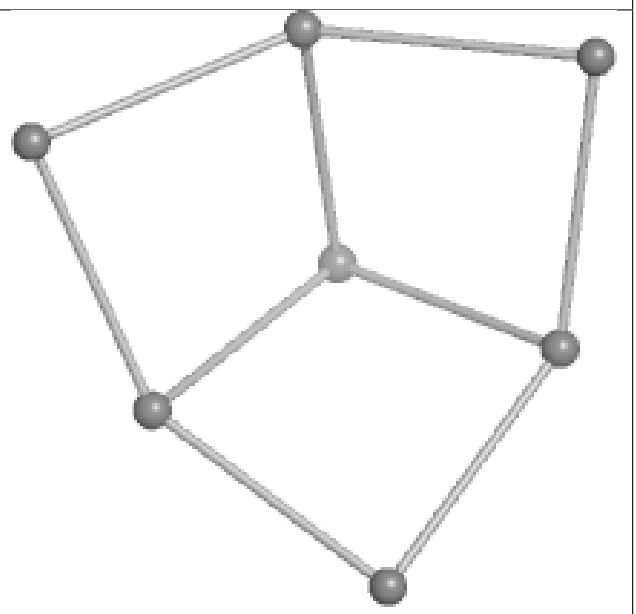


Rings

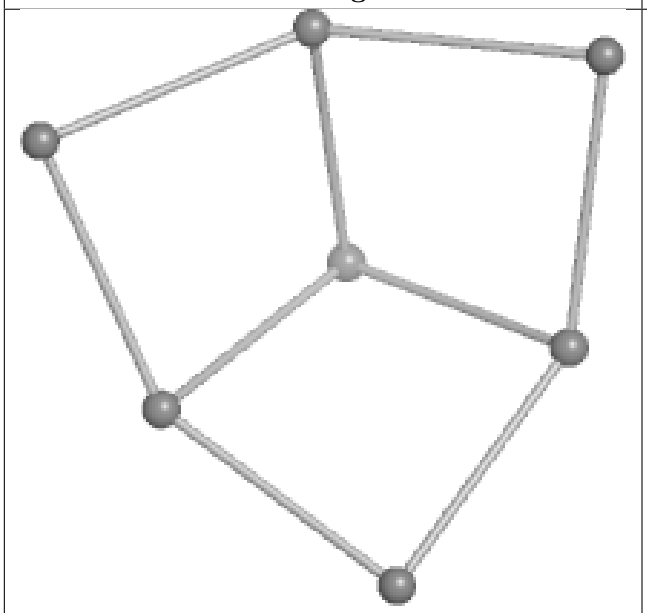
Ligand F3S CB 1002



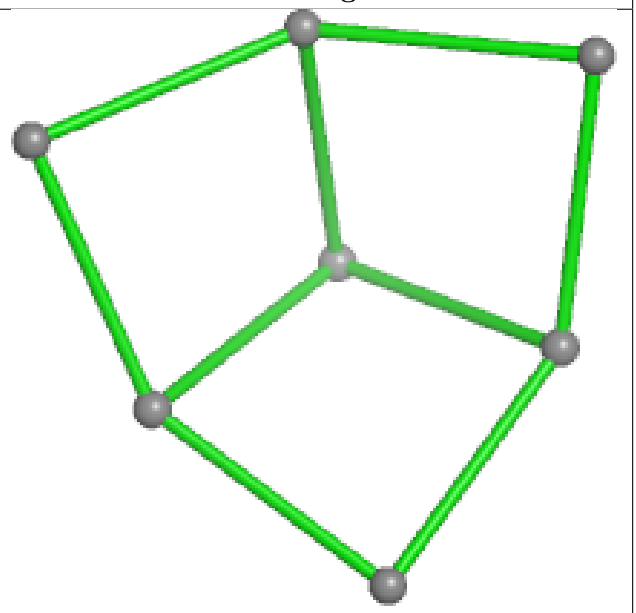
Bond lengths



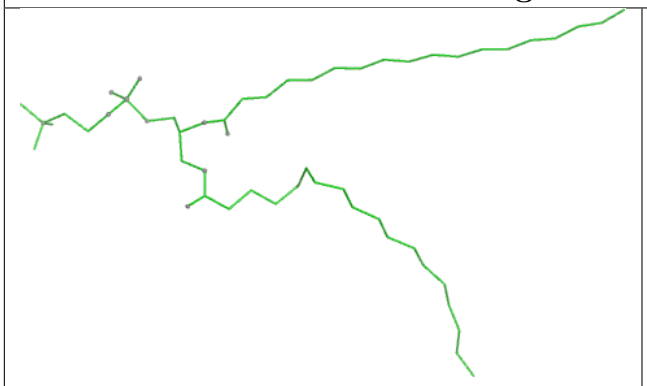
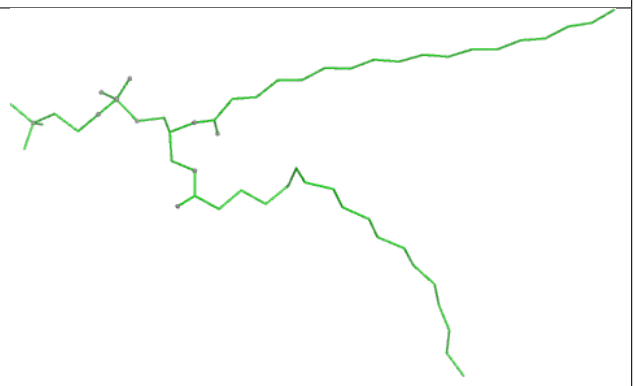
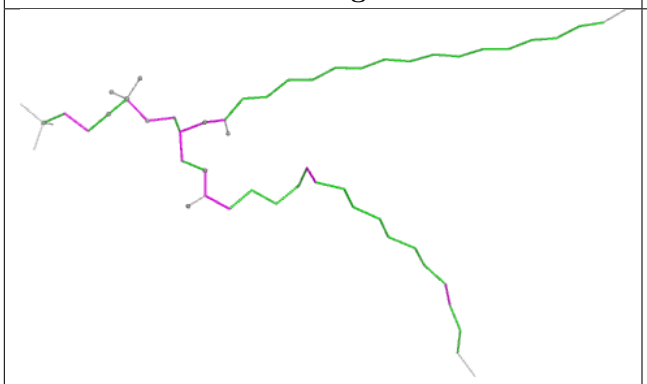
Bond angles



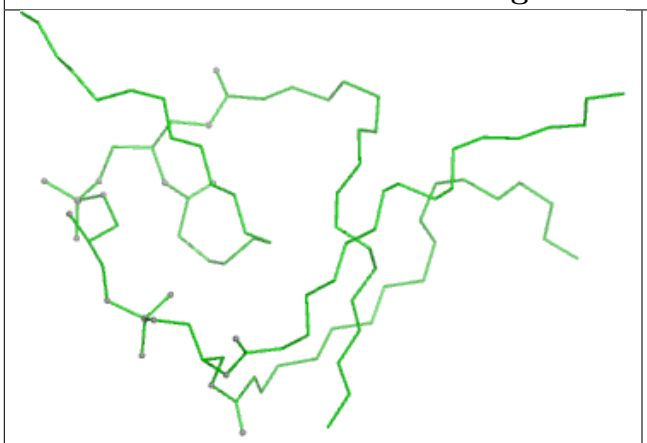
Torsions



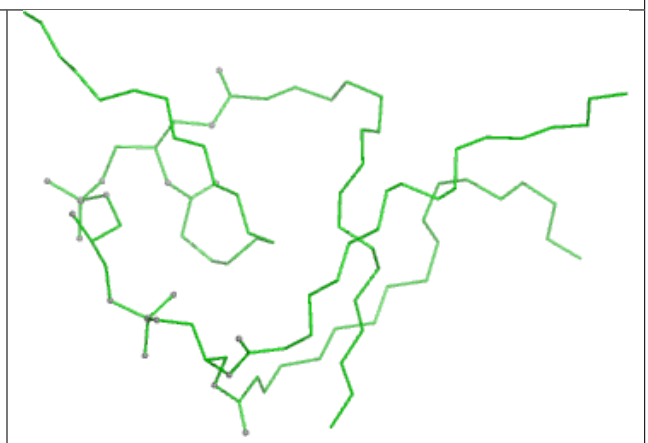
Rings

Ligand PC1 CC 302	
 **Bond lengths**	 **Bond angles**
 **Torsions**	**Rings**

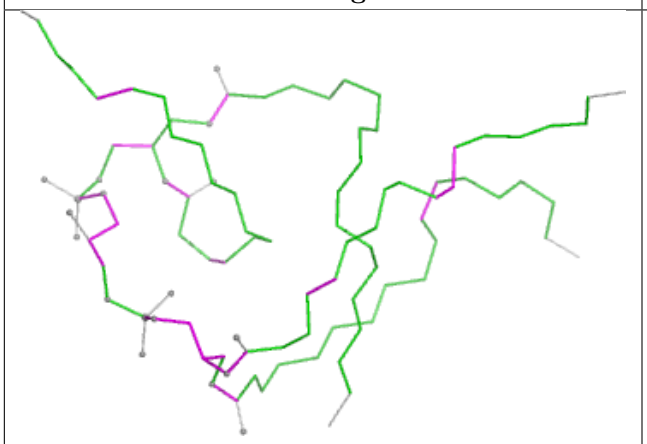
Ligand CDL CK 102



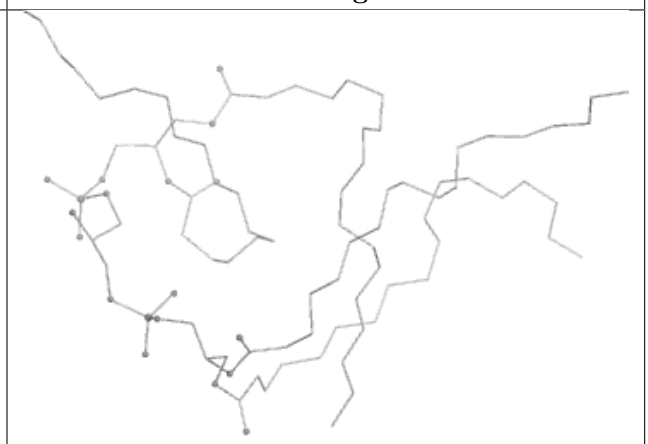
Bond lengths



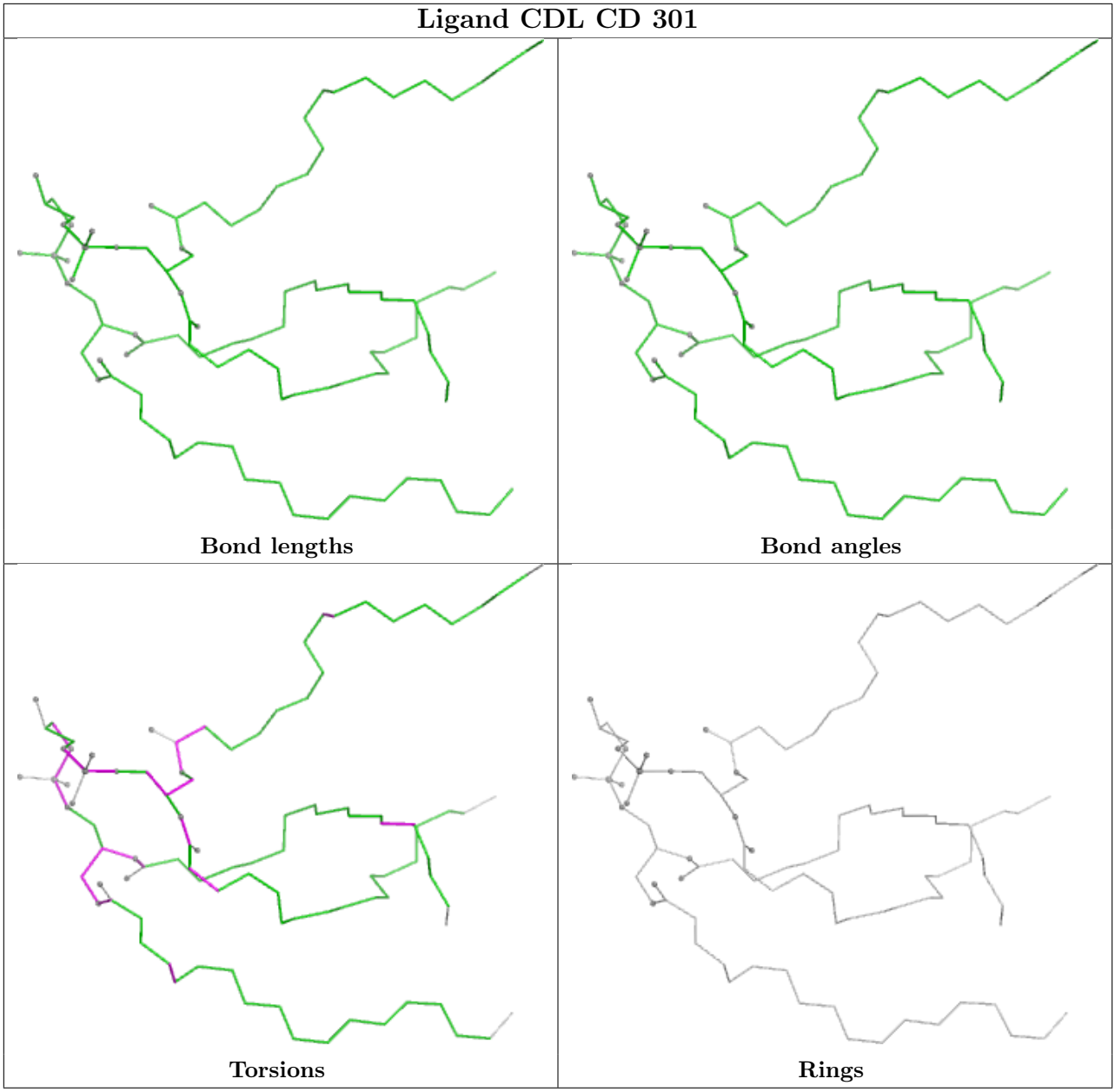
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

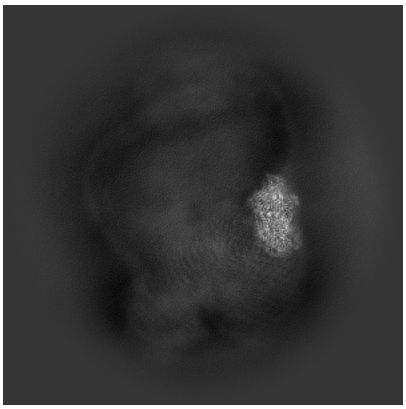
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-15866. These allow visual inspection of the internal detail of the map and identification of artifacts.

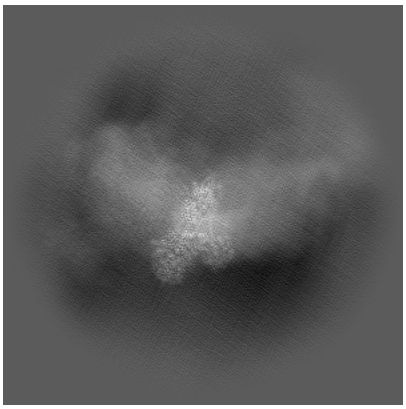
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

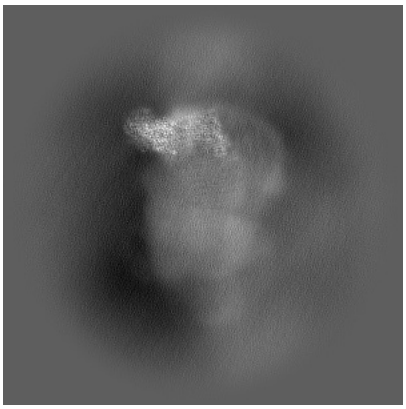
6.1.1 Primary map



X

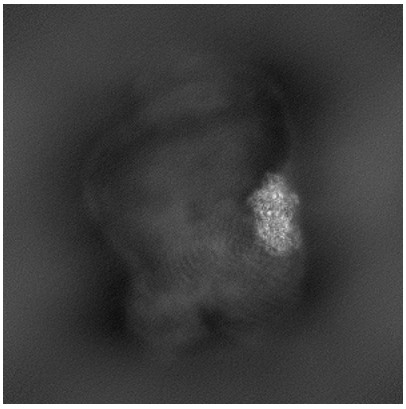


Y

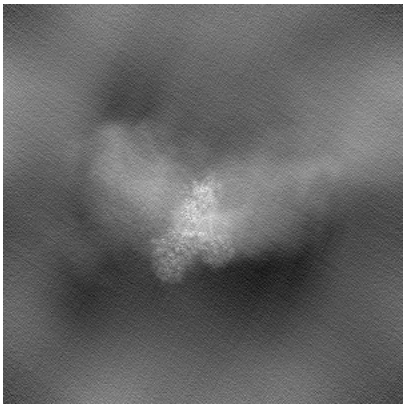


Z

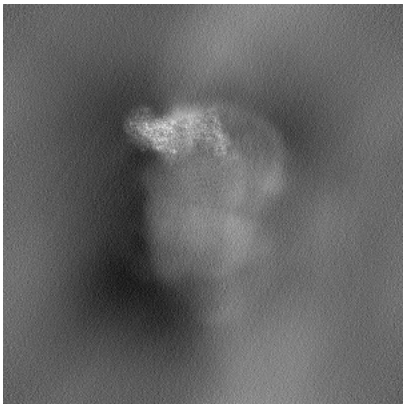
6.1.2 Raw map



X



Y

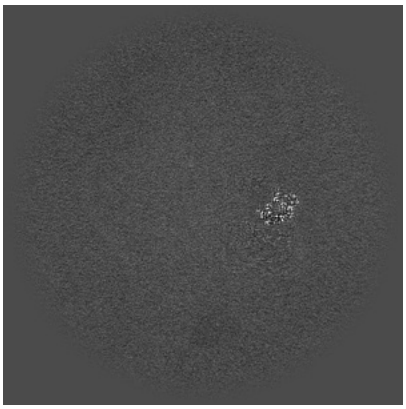


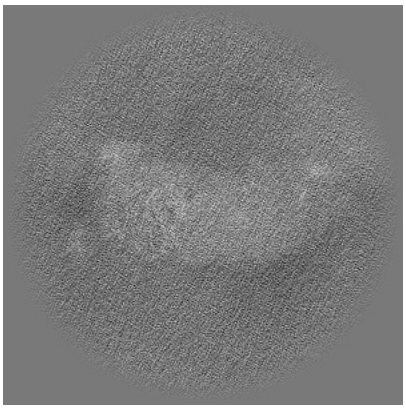
Z

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

6.2 Central slices (i)

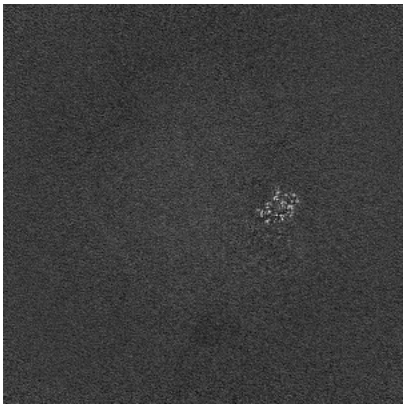
6.2.1 Primary map

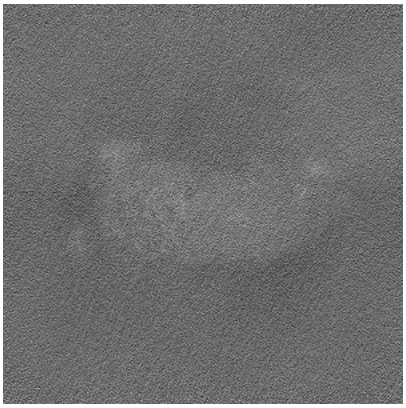

X Index: 240


Y Index: 240

Z Index: 240

6.2.2 Raw map


X Index: 240

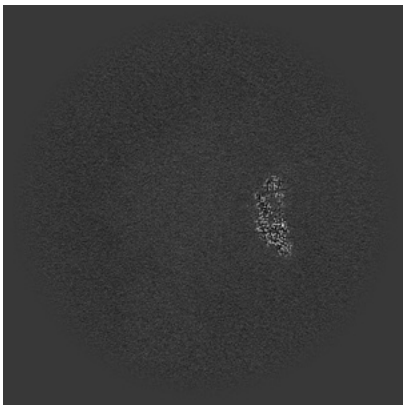

Y Index: 240

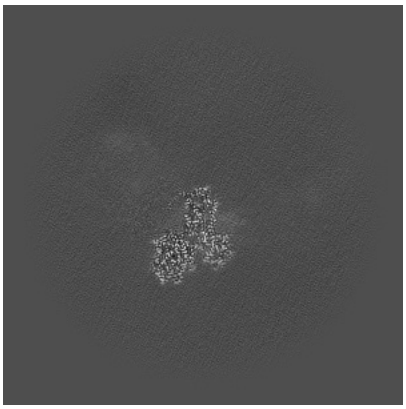
Z Index: 240

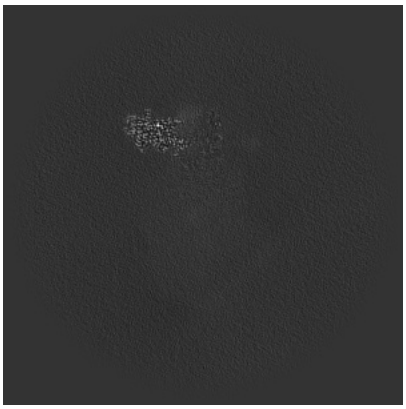
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

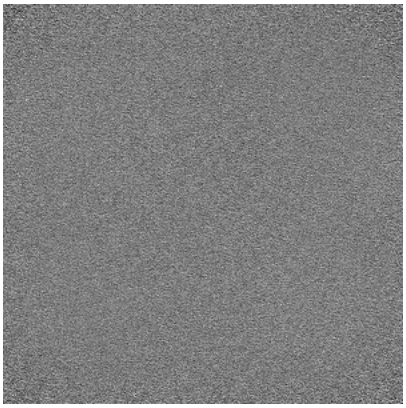
6.3.1 Primary map

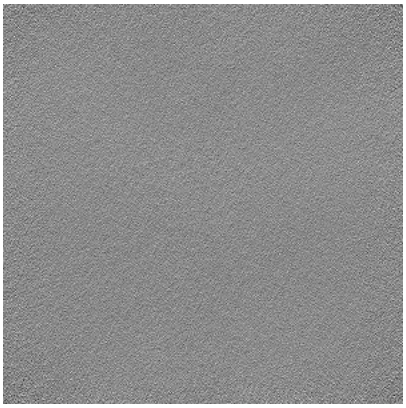

X Index: 193

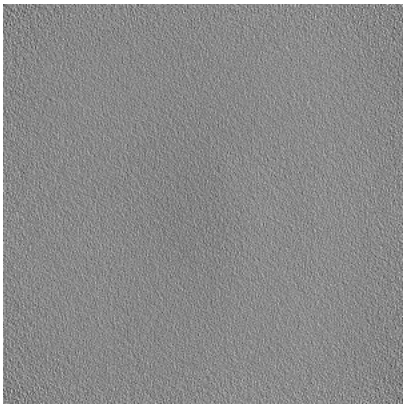

Y Index: 331


Z Index: 210

6.3.2 Raw map


X Index: 0

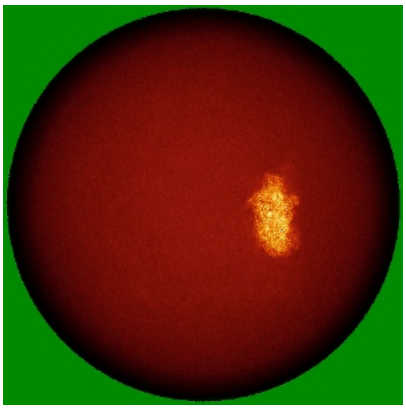

Y Index: 0

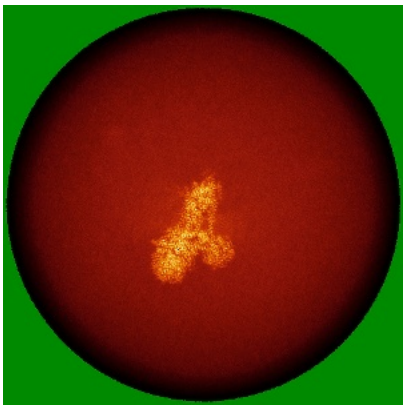

Z Index: 0

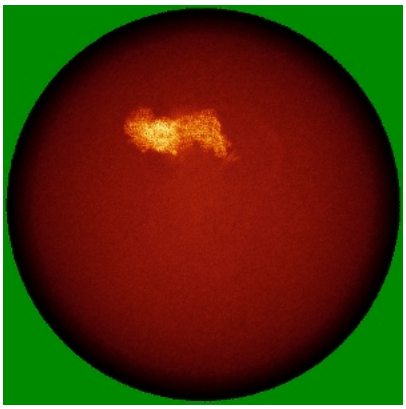
The images above show the largest variance slices of the map in three orthogonal directions.

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

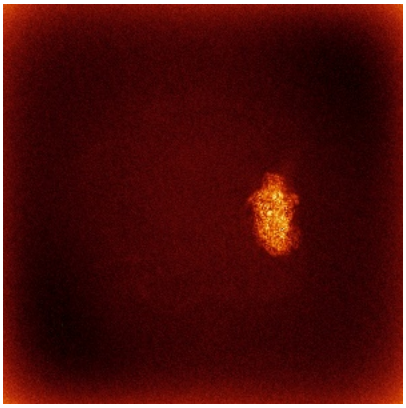
6.4.1 Primary map

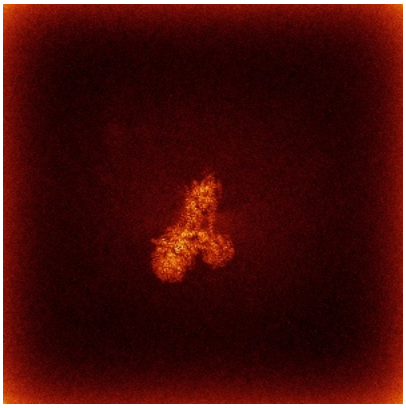

X

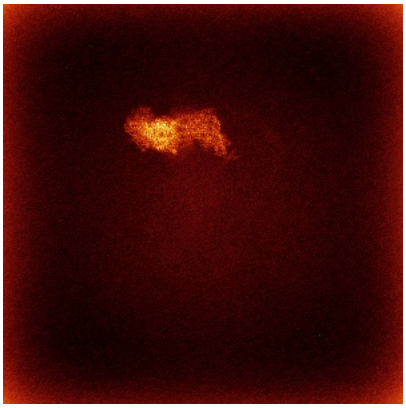

Y


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

6.5.2 Raw map

X Y Z

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

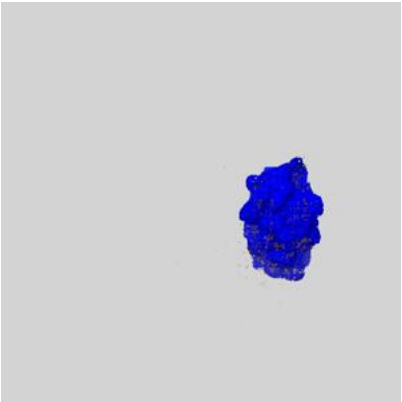
6.6 Mask visualisation (i)

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

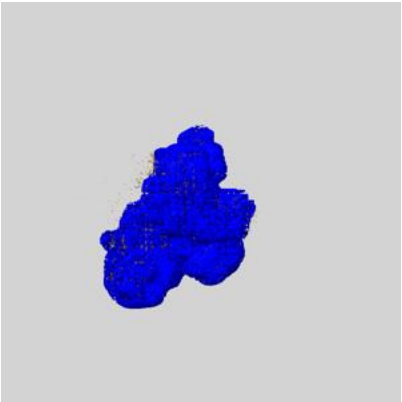
A mask typically either:

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

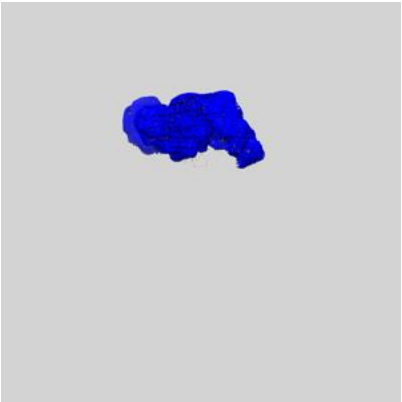
6.6.1 emd_15866_msk_1.map (i)



X



Y

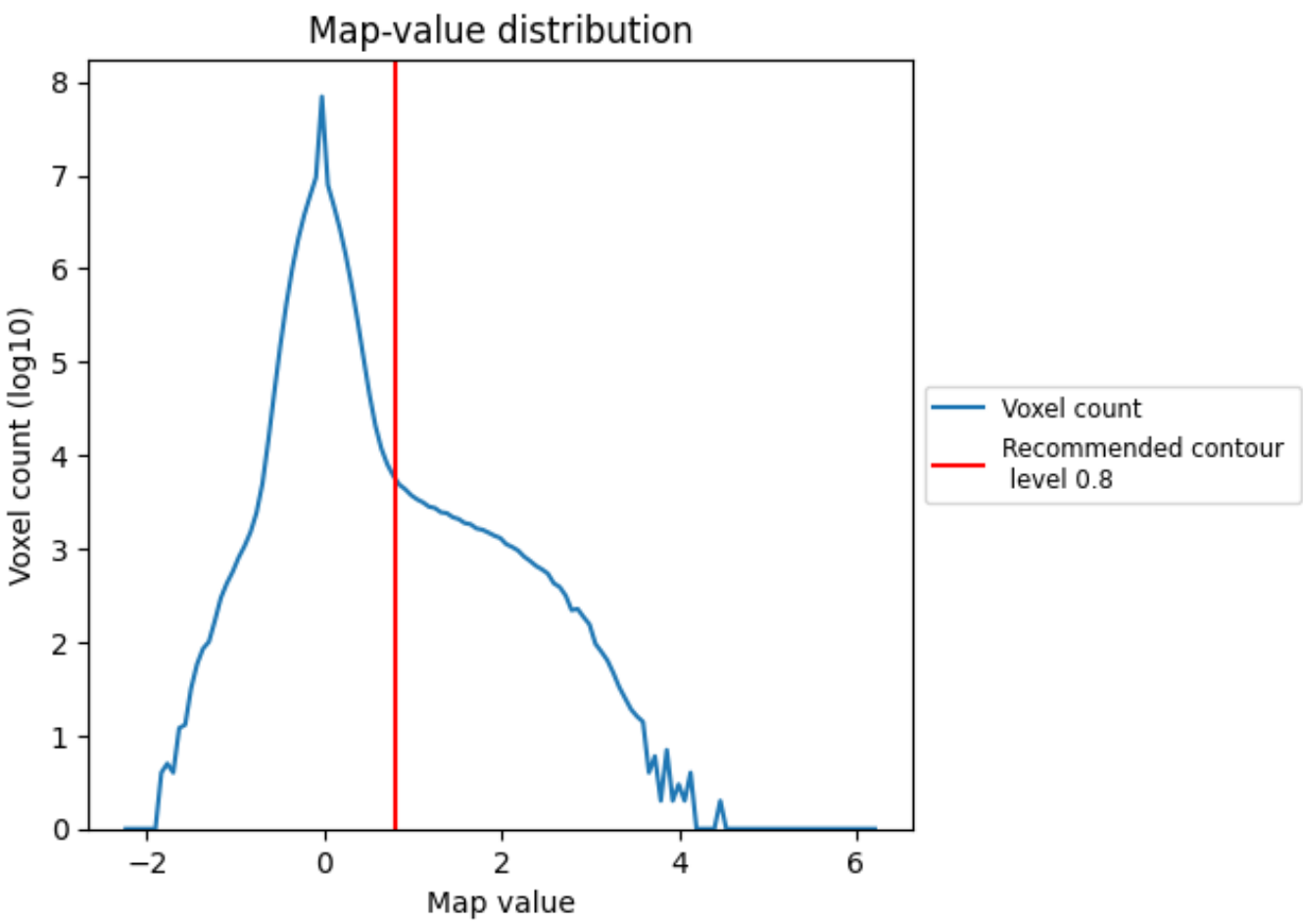


Z

7 Map analysis (i)

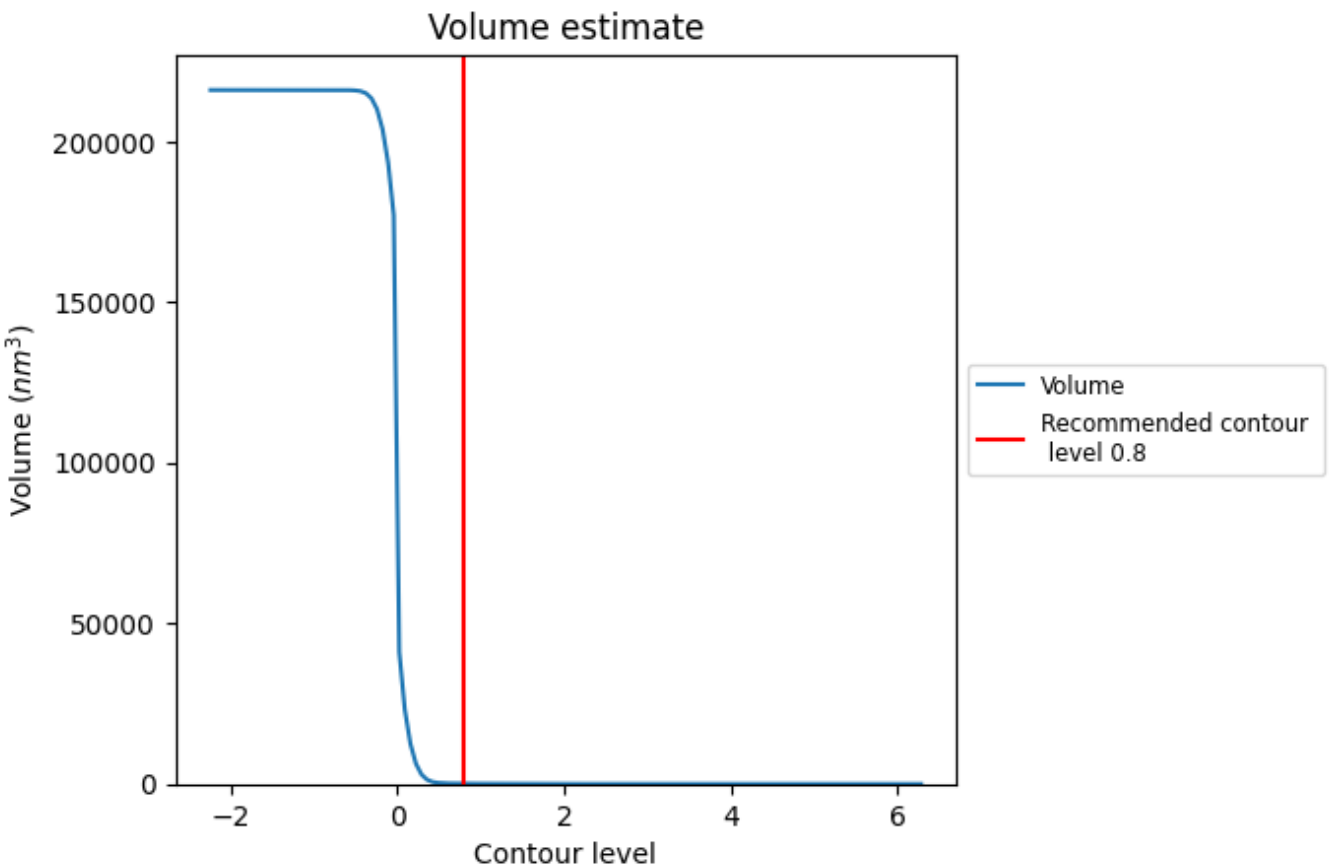
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

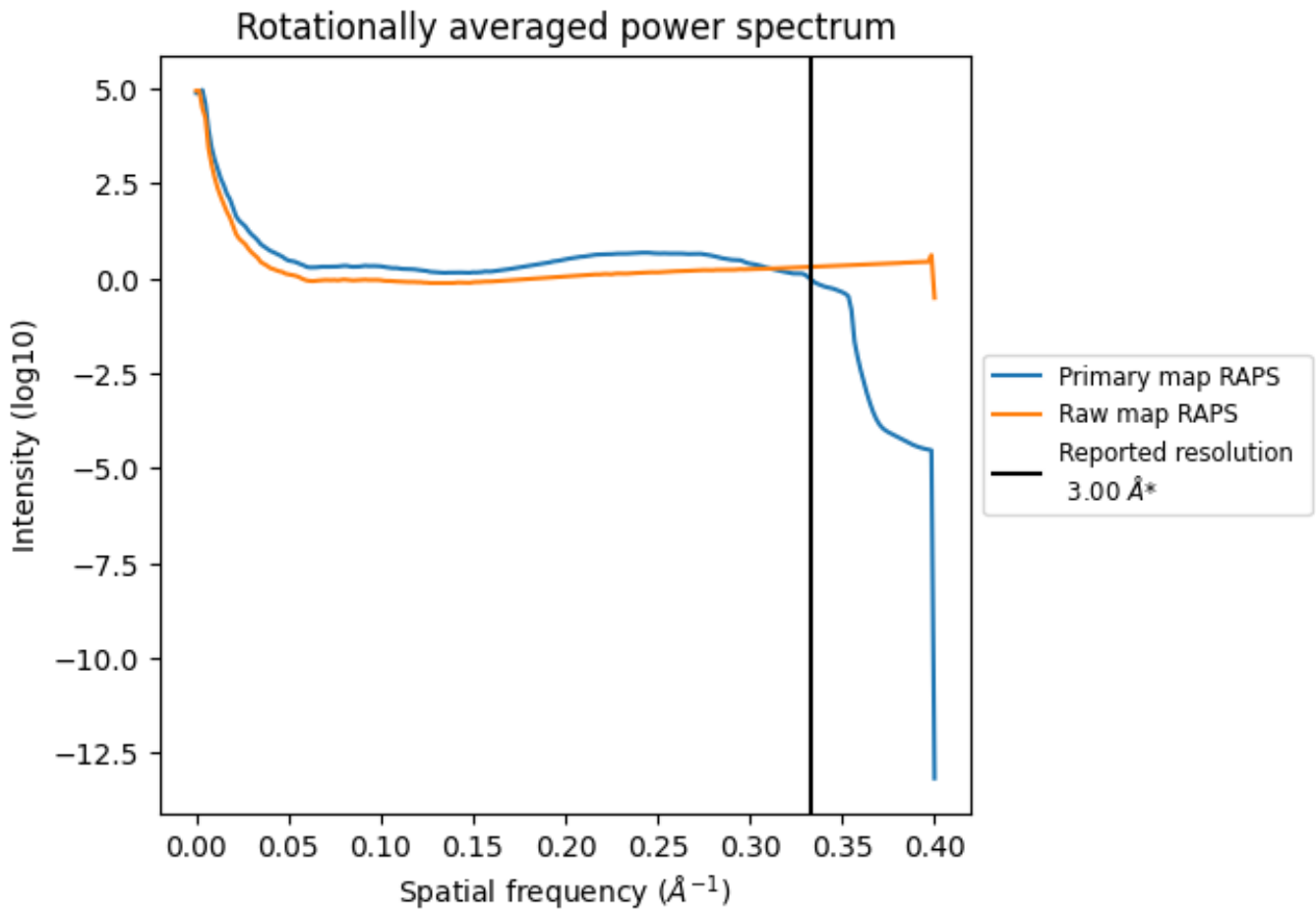
7.2 Volume estimate (i)



The volume at the recommended contour level is 114 nm^3; this corresponds to an approximate mass of 103 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)

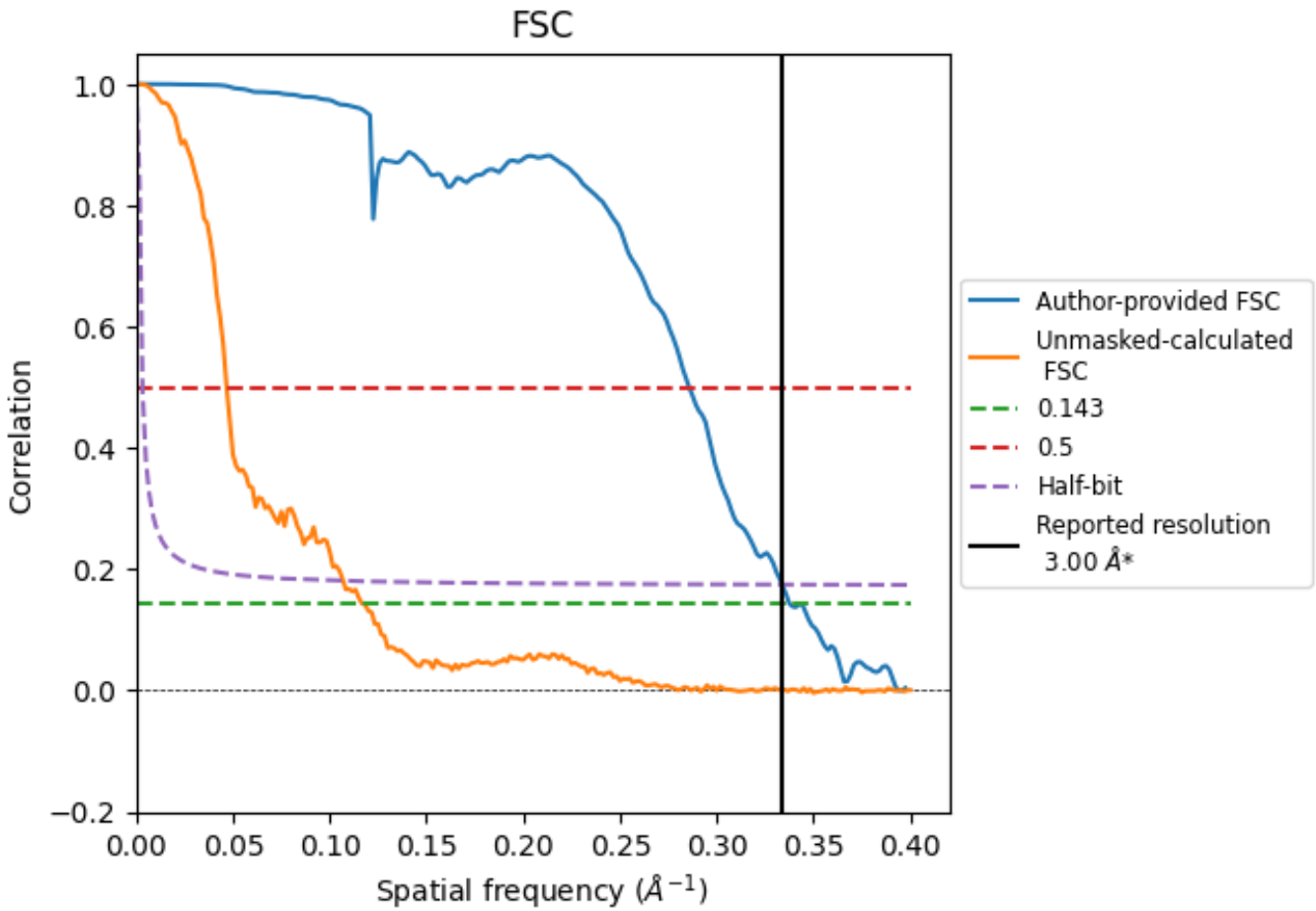


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

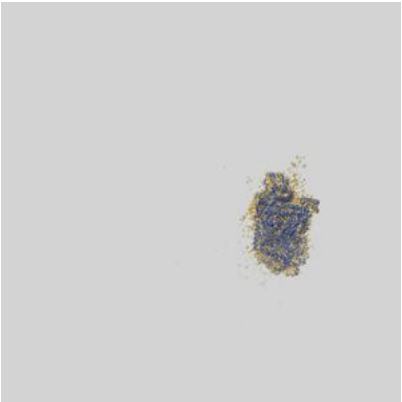
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.96	3.50	3.00
Unmasked-calculated*	8.57	21.41	9.35

*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 8.57 differs from the reported value 3.0 by more than 10 %

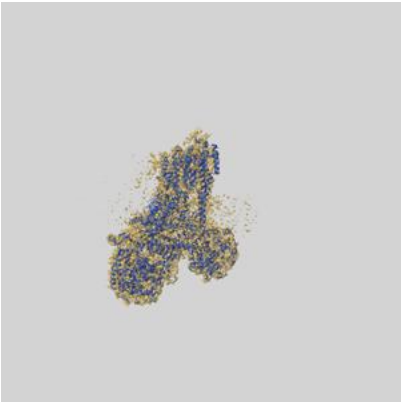
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-15866 and PDB model 8B6G. Per-residue inclusion information can be found in section 3 on page 12.

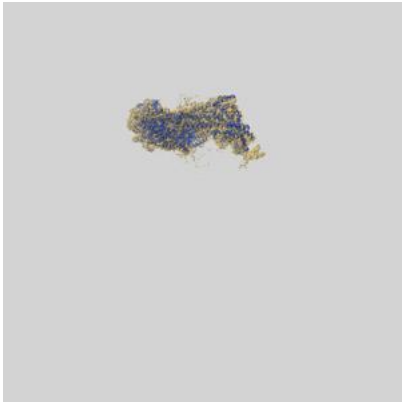
9.1 Map-model overlay (i)



X



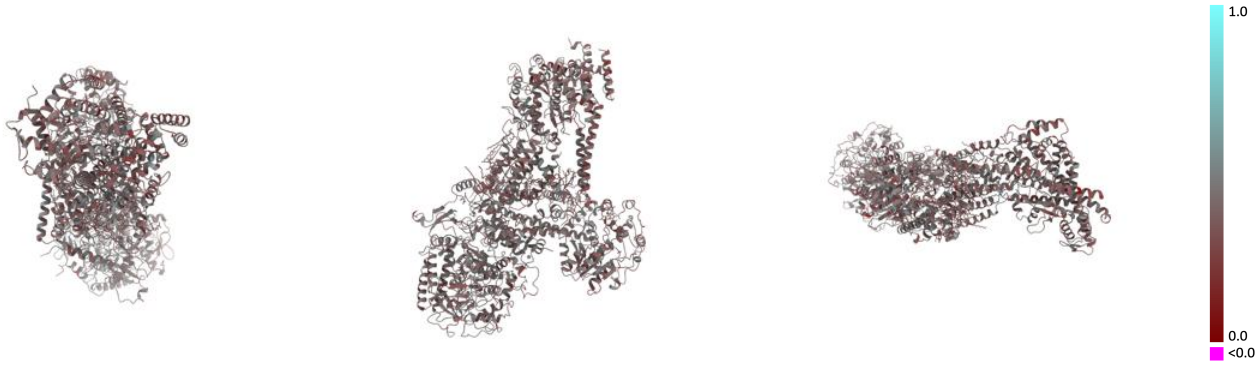
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

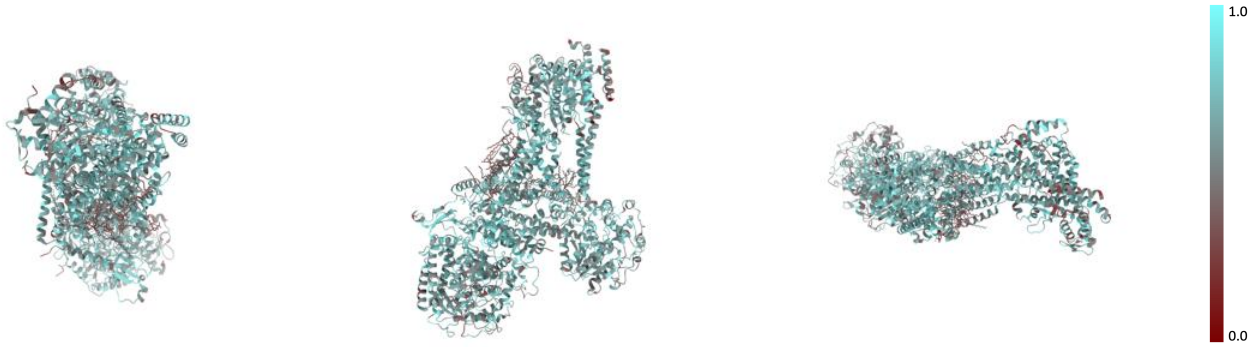
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

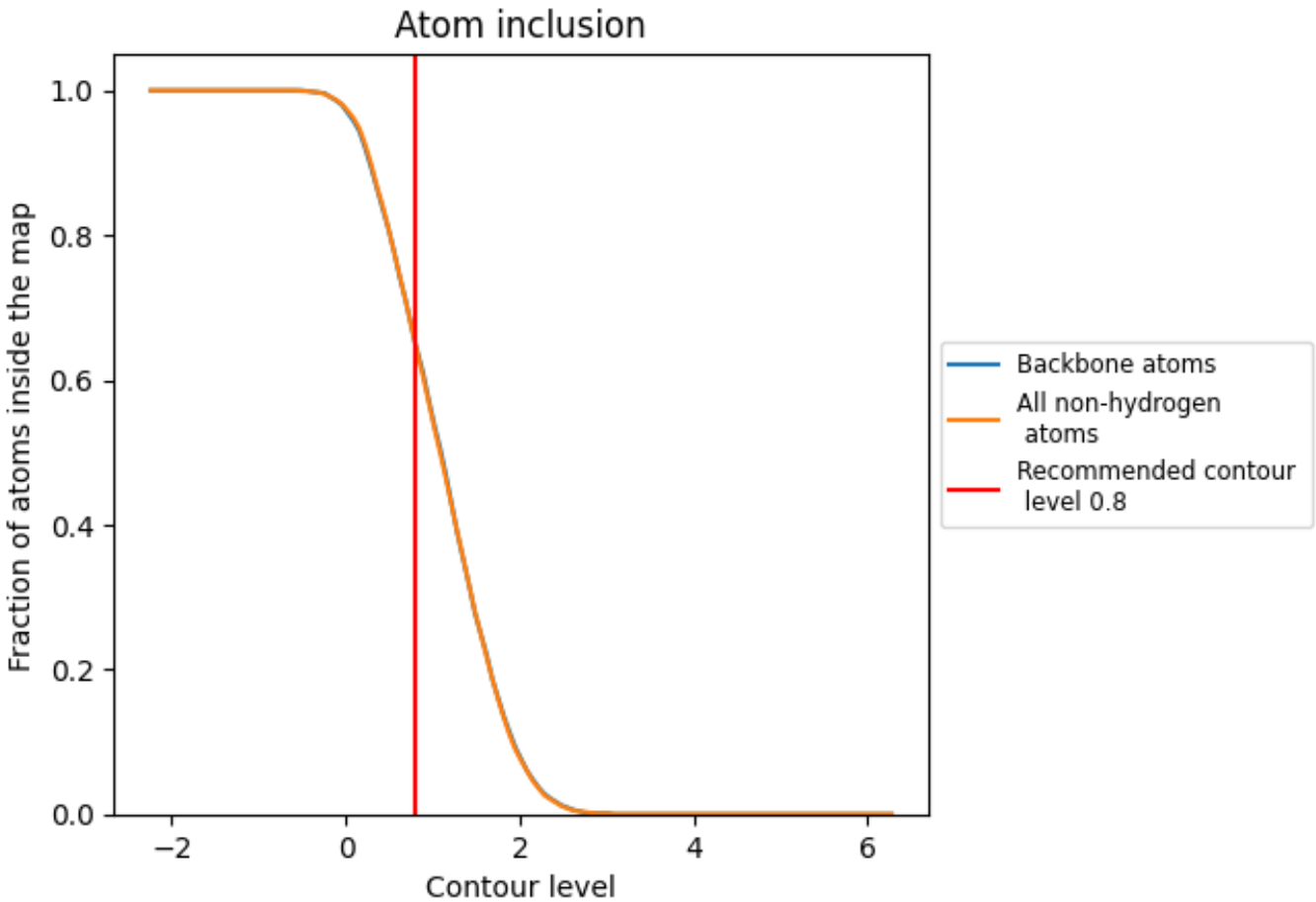
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6500	0.4020
CA	0.6540	0.4150
CB	0.7150	0.4140
CC	0.6250	0.4050
CD	0.6390	0.3790
CE	0.6420	0.3920
CF	0.6350	0.4080
CG	0.6770	0.4080
CH	0.6430	0.3620
CI	0.6070	0.3840
CJ	0.6690	0.3930
CK	0.6530	0.3860
CL	0.6570	0.4000
CM	0.6930	0.3980
CN	0.6220	0.3890
CO	0.6330	0.4080