Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 01:25 pm BST

PDB ID	:	8RBQ / pdb_00008rbq
EMDB ID	:	EMD-19034
Title	:	Cryo-EM structure of the NADH:ferredoxin oxidoreductase RNF from Azotobacter vinelandii, dithionite reduced
Authors	:	Zhang, L.; Einsle, O.
Deposited on	:	2023-12-04
Resolution	:	3.32 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 ⓘ symbol.

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

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

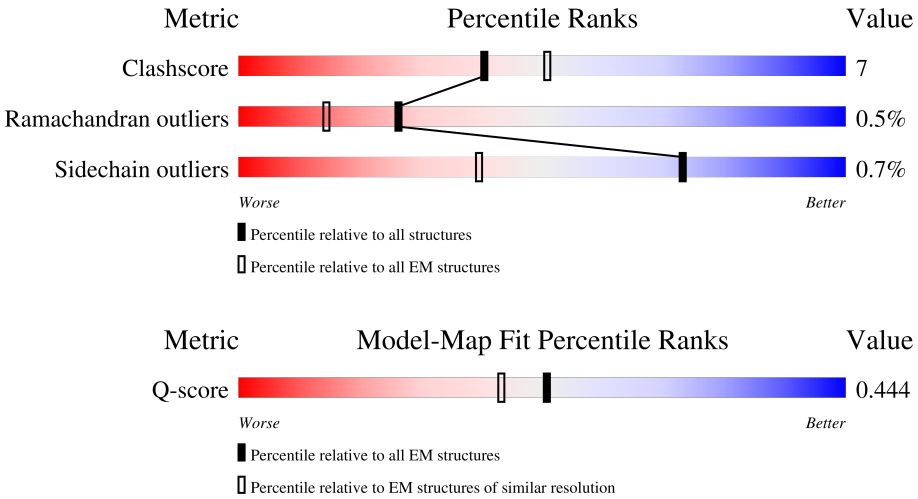
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.32 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	14518 (2.82 - 3.82)

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	190	79% 18%
2	C	496	84% 12%
3	E	238	82% 7% 11%
4	G	229	17% 57% 25% 15%

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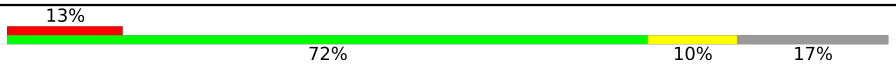
Mol	Chain	Length	Quality of chain
5	H	86	
6	B	174	
7	D	366	

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
10	FMN	G	301	X	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 12140 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 Ion-translocating oxidoreductase complex subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	189	1394	933	220	232	9	0	0

- Molecule 2 is a protein called Ion-translocating oxidoreductase complex subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	477	3523	2220	627	654	22	0	0

- Molecule 3 is a protein called Ion-translocating oxidoreductase complex subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	213	1601	1042	270	276	13	0	0

- Molecule 4 is a protein called Ion-translocating oxidoreductase complex subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	194	1478	937	258	277	6	0	0

- Molecule 5 is a protein called Protein RnfH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	71	548	346	94	104	4	0	0

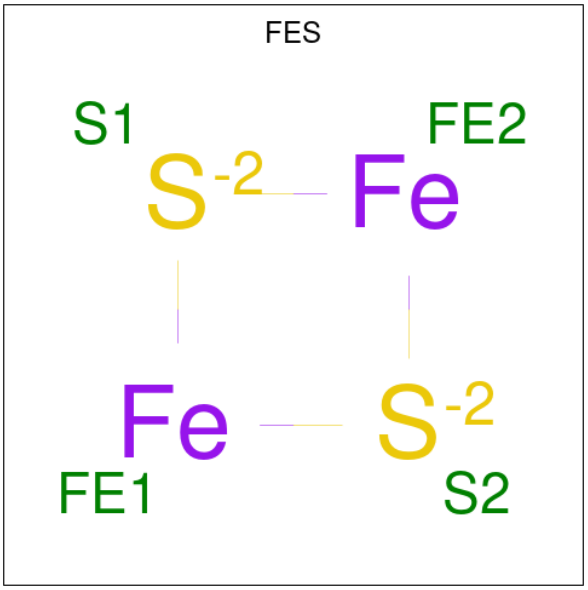
- Molecule 6 is a protein called Ion-translocating oxidoreductase complex subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	112	807	502	142	151	12	0	0

- Molecule 7 is a protein called Ion-translocating oxidoreductase complex subunit D.

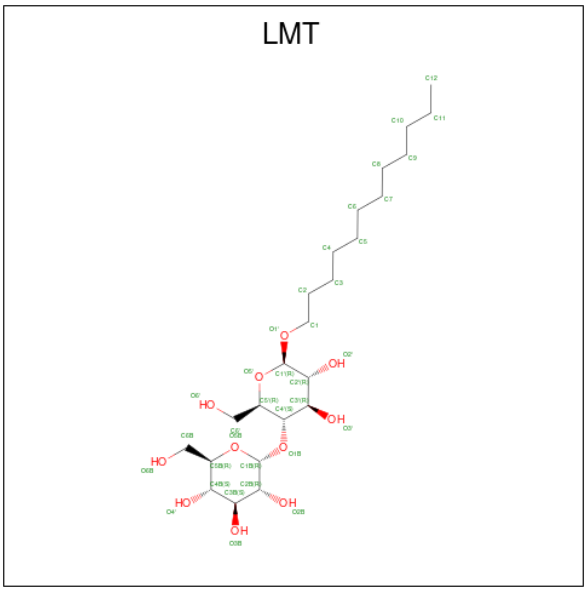
Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	305	Total	C	N	O	S	0	0
			2320	1541	387	380	12		

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



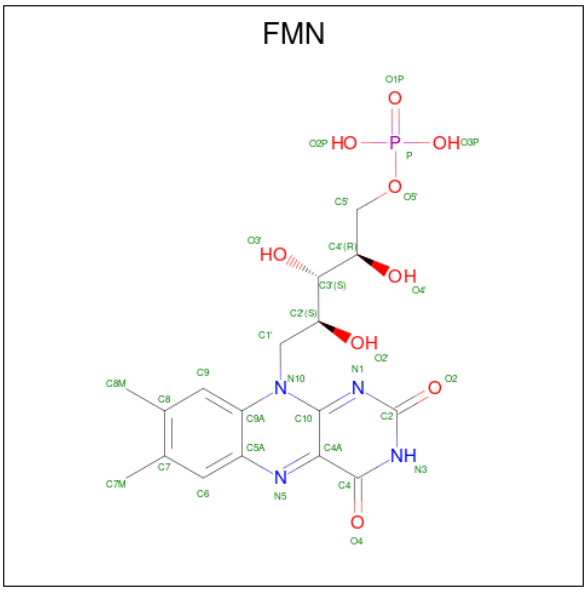
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	Fe	S	0
			4	2	2	

- Molecule 9 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



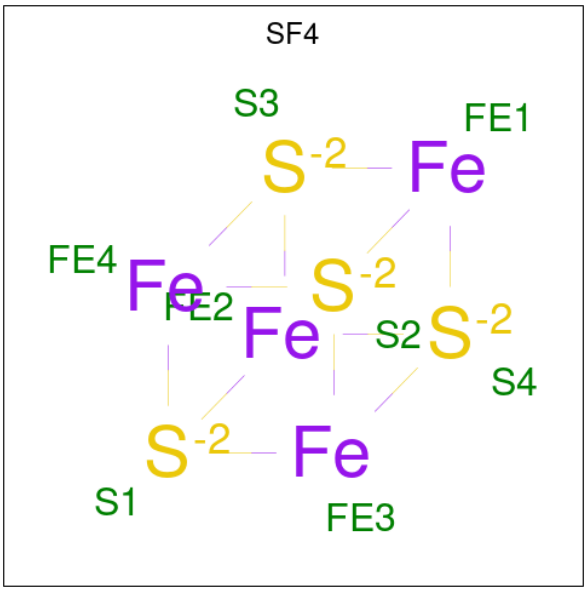
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			35	24	11	
9	E	1	Total	C	O	0
			35	24	11	
9	D	1	Total	C	O	0
			35	24	11	
9	D	1	Total	C	O	0
			35	24	11	
9	D	1	Total	C	O	0
			35	24	11	
9	D	1	Total	C	O	0
			35	24	11	
9	D	1	Total	C	O	0
			35	24	11	

- Molecule 10 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total	C	N	O	P	0
			31	17	4	9	1	
10	G	1	Total	C	N	O	P	0
			30	17	4	8	1	

- Molecule 11 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
11	C	1	Total	Fe	S	0
			8	4	4	

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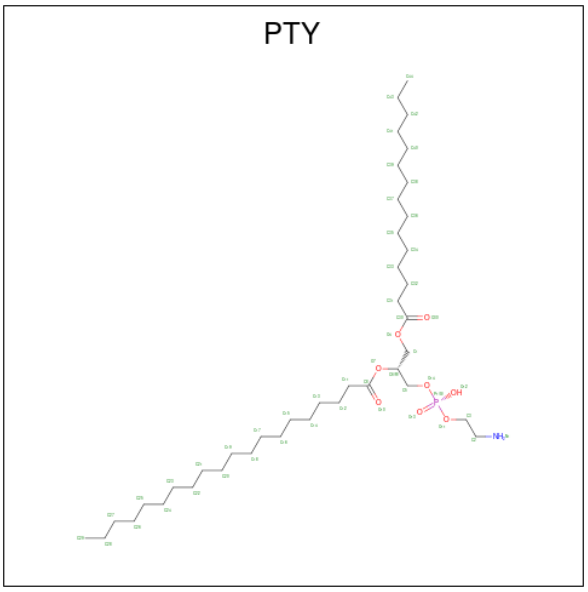
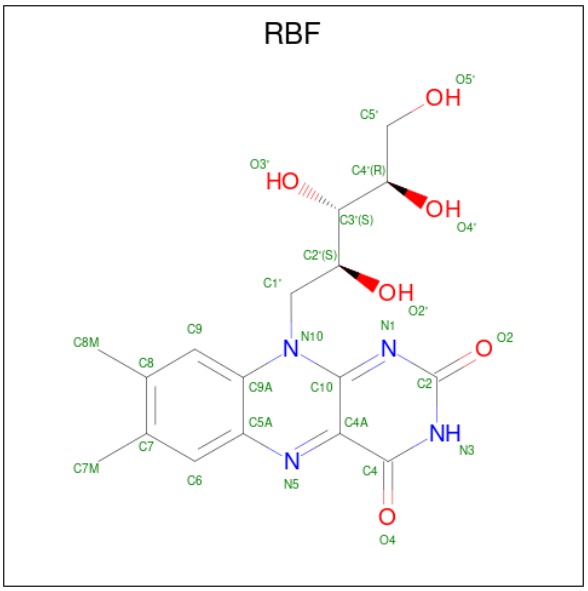
Mol	Chain	Residues	Atoms			AltConf
11	C	1	Total	Fe	S	0
			8	4	4	
11	B	1	Total	Fe	S	0
			8	4	4	
11	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 12 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
12	D	1	Total	C	N	O	P	0
			50	40	1	8	1	
12	D	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 13 is RIBOFLAVIN (CCD ID: RBF) (formula: $C_{17}H_{20}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
13	D	1	Total	C	N	O	0
			27	17	4	6	

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: Ion-translocating oxidoreductase complex subunit A

Chain A:

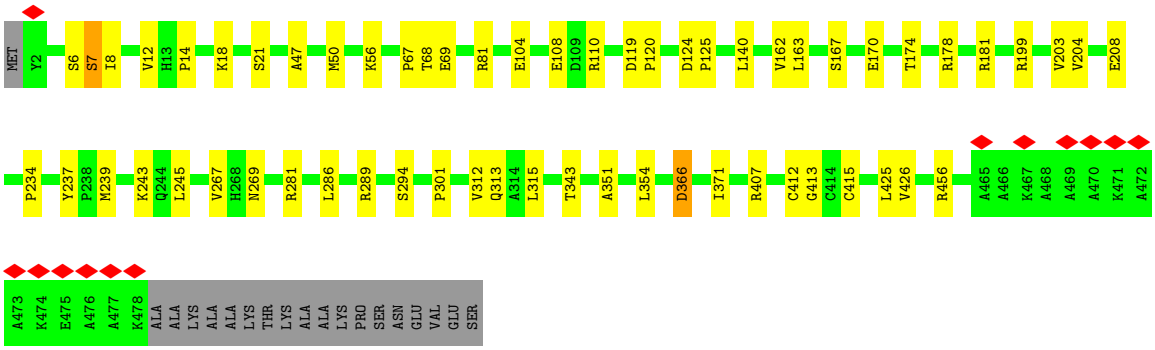




• Molecule 2: Ion-translocating oxidoreductase complex subunit C

Chain C:

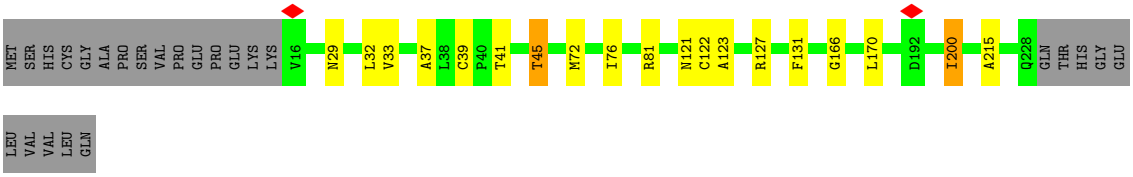




• Molecule 3: Ion-translocating oxidoreductase complex subunit E

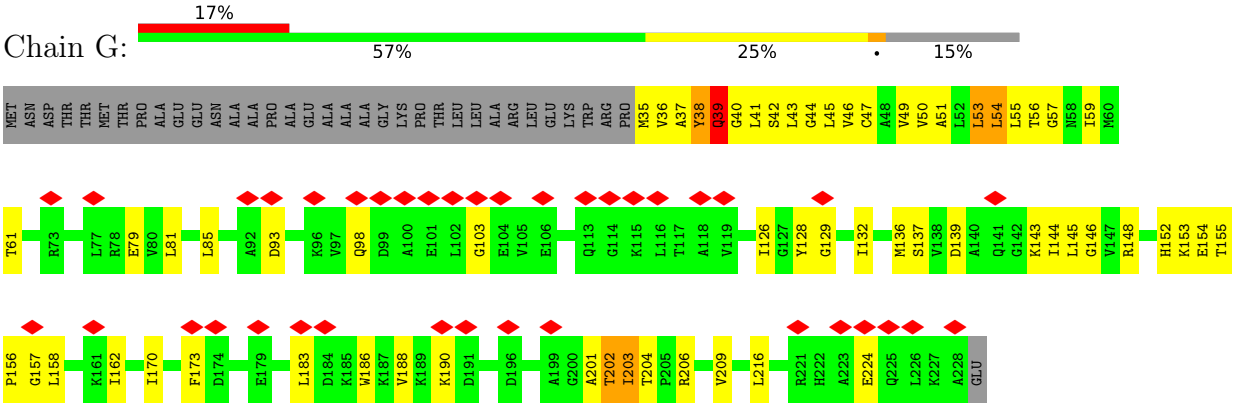
Chain E:





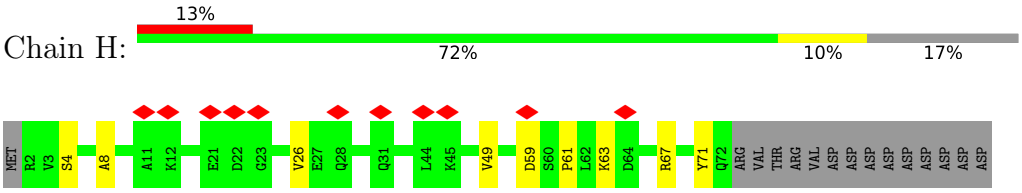
• Molecule 4: Ion-translocating oxidoreductase complex subunit G

Chain G:



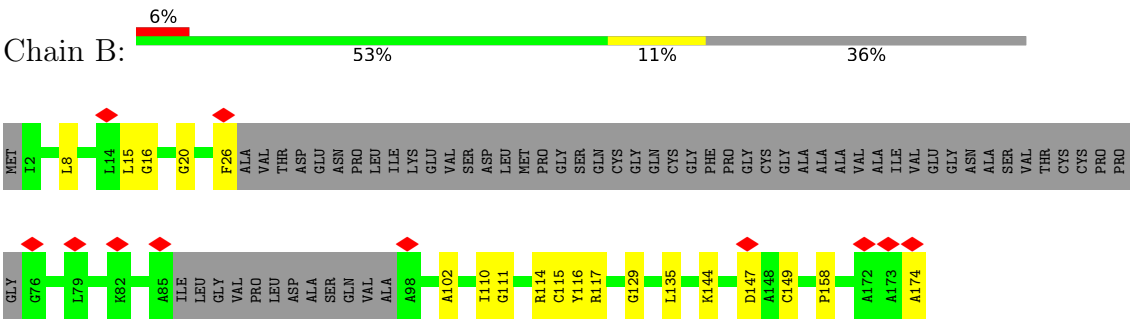
• Molecule 5: Protein RnfH

Chain H:



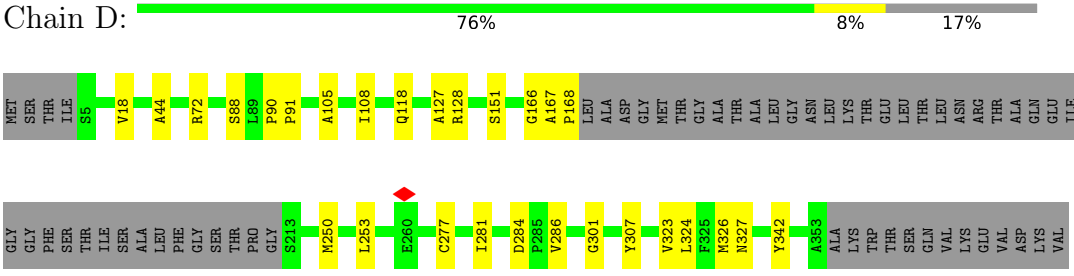
• Molecule 6: Ion-translocating oxidoreductase complex subunit B

Chain B:



• Molecule 7: Ion-translocating oxidoreductase complex subunit D

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	165903	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 ($e^-/Å^2$)	37	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.792	Depositor
Minimum map value	-0.174	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	229.59999, 229.59999, 229.59999	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	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: PTY, RBF, SF4, LMT, FMN, FES

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	0.47	1/1423 (0.1%)	0.97	13/1936 (0.7%)
2	C	0.24	0/3593	0.56	4/4893 (0.1%)
3	E	0.38	1/1632 (0.1%)	0.68	1/2223 (0.0%)
4	G	0.45	0/1499	0.75	3/2027 (0.1%)
5	H	0.28	0/555	0.74	1/746 (0.1%)
6	B	0.34	0/816	0.96	3/1104 (0.3%)
7	D	0.22	0/2389	0.50	0/3271
All	All	0.33	2/11907 (0.0%)	0.69	25/16200 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	G	1	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	39	CYS	N-CA	-5.63	1.42	1.46
1	A	113	CYS	C-N	-5.03	1.26	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	CYS	N-CA-CB	13.06	122.80	110.39
6	B	158	PRO	CA-N-CD	-11.36	96.10	112.00
1	A	25	CYS	CA-C-N	-10.81	107.39	119.28
1	A	25	CYS	C-N-CA	-10.81	107.39	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	61	PRO	CA-N-CD	-9.61	98.55	112.00
6	B	149	CYS	N-CA-CB	-9.06	96.92	110.32
1	A	24	LEU	CA-C-N	-7.41	111.60	119.83
1	A	24	LEU	C-N-CA	-7.41	111.60	119.83
2	C	204	VAL	CB-CA-C	6.34	121.69	111.29
4	G	54	LEU	N-CA-C	6.30	119.98	112.93
3	E	72	MET	CA-CB-CG	6.21	126.51	114.10
1	A	25	CYS	CA-CB-SG	6.09	128.41	114.40
4	G	39	GLN	N-CA-C	-6.07	104.45	112.34
2	C	204	VAL	CA-CB-CG1	5.95	120.51	110.40
4	G	53	LEU	N-CA-C	-5.61	105.70	112.54
6	B	110	ILE	N-CA-C	-5.52	106.93	112.17
1	A	25	CYS	CB-CA-C	-5.34	105.19	113.57
1	A	93	LYS	CA-C-N	5.25	131.57	121.54
1	A	93	LYS	C-N-CA	5.25	131.57	121.54
2	C	119	ASP	CA-CB-CG	5.25	117.85	112.60
2	C	119	ASP	CB-CA-C	5.18	120.37	110.17
1	A	111	THR	CA-C-N	5.16	131.39	121.54
1	A	111	THR	C-N-CA	5.16	131.39	121.54
1	A	106	LEU	CA-CB-CG	5.12	134.23	116.30
1	A	112	ASN	CA-CB-CG	5.00	117.60	112.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	G	202	THR	CB

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	1394	0	1496	25	0
2	C	3523	0	3583	33	0
3	E	1601	0	1680	11	0
4	G	1478	0	1514	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	548	0	566	5	0
6	B	807	0	809	16	0
7	D	2320	0	2396	22	0
8	A	4	0	0	1	0
9	A	35	0	46	4	0
9	D	175	0	228	8	0
9	E	35	0	45	2	0
10	C	31	0	19	0	0
10	G	30	0	19	10	0
11	B	16	0	0	1	0
11	C	16	0	0	0	0
12	D	100	0	158	6	0
13	D	27	0	20	2	0
All	All	12140	0	12579	172	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.

All (172) 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)
4:G:155:THR:HG21	10:G:301:FMN:H6	1.38	1.01
4:G:201:ALA:HA	10:G:301:FMN:H5'2	1.44	1.00
4:G:36:VAL:HG13	6:B:20:GLY:HA3	1.53	0.90
7:D:108:ILE:HD11	12:D:403:PTY:H202	1.65	0.77
4:G:201:ALA:CA	10:G:301:FMN:H5'2	2.16	0.76
4:G:39:GLN:C	4:G:39:GLN:HE21	1.99	0.71
4:G:155:THR:HG21	10:G:301:FMN:C6	2.18	0.70
4:G:201:ALA:HA	10:G:301:FMN:C5'	2.21	0.69
4:G:40:GLY:O	4:G:41:LEU:C	2.39	0.66
4:G:203:ILE:O	4:G:206:ARG:N	2.28	0.65
4:G:36:VAL:O	4:G:39:GLN:HG3	1.98	0.64
3:E:127:ARG:HH21	3:E:131:PHE:HB2	1.65	0.62
4:G:36:VAL:HA	4:G:39:GLN:HG2	1.82	0.62
9:E:301:LMT:H82	12:D:403:PTY:H241	1.82	0.60
1:A:89:MET:HA	1:A:92:ARG:HG3	1.86	0.58
4:G:203:ILE:HB	10:G:301:FMN:O2	2.04	0.58
1:A:72:ARG:C	1:A:74:LEU:H	2.12	0.57
7:D:277:CYS:HA	7:D:281:ILE:HB	1.85	0.57
4:G:51:ALA:HB2	6:B:8:LEU:HD13	1.87	0.57
4:G:46:VAL:O	4:G:50:VAL:HG23	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:156:PRO:O	4:G:158:LEU:N	2.37	0.57
3:E:122:CYS:O	3:E:123:ALA:C	2.44	0.56
4:G:40:GLY:O	4:G:43:LEU:N	2.39	0.56
4:G:203:ILE:O	4:G:204:THR:C	2.49	0.56
4:G:41:LEU:O	4:G:44:GLY:N	2.38	0.56
3:E:166:GLY:HA3	3:E:200:ILE:HD13	1.88	0.56
9:A:201:LMT:H41	9:D:401:LMT:H81	1.88	0.55
7:D:250:MET:HE3	9:D:402:LMT:H82	1.87	0.55
4:G:42:SER:OG	4:G:43:LEU:N	2.39	0.55
7:D:284:ASP:OD1	13:D:404:RBF:O2'	2.24	0.55
2:C:18:LYS:NZ	2:C:170:GLU:O	2.39	0.55
4:G:156:PRO:C	4:G:158:LEU:H	2.15	0.55
5:H:59:ASP:OD1	5:H:59:ASP:N	2.40	0.54
7:D:88:SER:O	7:D:128:ARG:NH1	2.40	0.54
3:E:215:ALA:HB2	12:D:403:PTY:H352	1.89	0.54
7:D:250:MET:HE2	7:D:307:TYR:HD2	1.72	0.54
1:A:30:VAL:HG11	1:A:40:LEU:HD22	1.90	0.54
6:B:174:ALA:OXT	7:D:72:ARG:NH2	2.41	0.54
7:D:253:LEU:HD11	9:D:402:LMT:H81	1.90	0.53
2:C:140:LEU:HD21	2:C:286:LEU:HD21	1.90	0.53
1:A:72:ARG:O	1:A:74:LEU:N	2.42	0.53
4:G:144:ILE:HD11	4:G:216:LEU:HD11	1.90	0.53
4:G:128:TYR:HB3	4:G:154:GLU:OE1	2.09	0.53
1:A:91:ILE:HD11	1:A:98:LEU:HG	1.90	0.53
1:A:82:GLY:HA3	6:B:15:LEU:HD13	1.90	0.52
2:C:456:ARG:NH2	6:B:116:TYR:O	2.42	0.52
8:A:200:FES:S2	3:E:37:ALA:HA	2.50	0.52
2:C:289:ARG:NH1	2:C:351:ALA:O	2.43	0.52
2:C:234:PRO:HD2	2:C:239:MET:HE3	1.90	0.52
2:C:163:LEU:HD23	2:C:267:VAL:HG22	1.92	0.52
2:C:313:GLN:HB2	2:C:343:THR:HB	1.92	0.52
1:A:127:HIS:HD2	1:A:131:MET:HG3	1.75	0.51
2:C:366:ASP:OD1	2:C:366:ASP:N	2.42	0.51
4:G:47:CYS:SG	6:B:8:LEU:HD22	2.51	0.51
3:E:76:ILE:HD11	3:E:81:ARG:HA	1.93	0.50
4:G:38:TYR:C	4:G:40:GLY:N	2.63	0.50
4:G:190:LYS:HE2	10:G:301:FMN:O1P	2.11	0.50
4:G:139:ASP:OD1	4:G:143:LYS:N	2.44	0.50
4:G:42:SER:O	4:G:43:LEU:C	2.55	0.50
7:D:44:ALA:HB1	9:D:407:LMT:H112	1.94	0.50
2:C:162:VAL:HB	2:C:203:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:125:PRO:HG3	2:C:199:ARG:HH12	1.78	0.49
9:A:201:LMT:H32	9:D:401:LMT:H31	1.95	0.49
9:E:301:LMT:H6'2	7:D:166:GLY:HA3	1.94	0.49
2:C:237:TYR:OH	2:C:412:CYS:O	2.30	0.49
10:G:301:FMN:N1	10:G:301:FMN:O4'	2.43	0.49
2:C:56:LYS:HE2	2:C:81:ARG:HD3	1.95	0.49
2:C:12:VAL:HG23	2:C:14:PRO:HD3	1.94	0.49
2:C:108:GLU:OE1	2:C:110:ARG:NH1	2.46	0.48
2:C:167:SER:HB2	2:C:208:GLU:HG3	1.95	0.48
6:B:115:CYS:N	11:B:202:SF4:S1	2.87	0.48
2:C:120:PRO:HG3	2:C:281:ARG:HD3	1.94	0.48
7:D:105:ALA:HB2	7:D:127:ALA:HB2	1.95	0.48
4:G:36:VAL:HA	4:G:39:GLN:CG	2.43	0.48
9:A:201:LMT:H6'2	4:G:126:ILE:HG12	1.95	0.47
2:C:21:SER:OG	2:C:174:THR:OG1	2.29	0.47
1:A:70:PHE:CD1	1:A:71:ILE:HG13	2.49	0.47
1:A:111:THR:O	1:A:113:CYS:N	2.44	0.47
4:G:49:VAL:O	4:G:53:LEU:HG	2.14	0.47
4:G:156:PRO:C	4:G:158:LEU:N	2.72	0.47
4:G:41:LEU:O	4:G:42:SER:C	2.56	0.47
1:A:70:PHE:HZ	4:G:55:LEU:HD23	1.80	0.47
2:C:47:ALA:HA	2:C:67:PRO:HD3	1.96	0.47
2:C:312:VAL:HG13	2:C:354:LEU:HD11	1.96	0.47
4:G:45:LEU:C	4:G:45:LEU:HD23	2.40	0.47
6:B:144:LYS:HA	6:B:144:LYS:HD3	1.72	0.47
9:D:405:LMT:H3B	9:D:406:LMT:H2'	1.97	0.47
2:C:243:LYS:O	7:D:342:TYR:OH	2.32	0.46
3:E:29:ASN:H	3:E:33:VAL:HB	1.81	0.46
1:A:16:VAL:HG22	1:A:22:LEU:HB2	1.98	0.46
1:A:111:THR:C	1:A:113:CYS:H	2.21	0.46
3:E:29:ASN:HB3	3:E:32:LEU:HB2	1.98	0.46
4:G:202:THR:N	10:G:301:FMN:H5'2	2.31	0.46
2:C:178:ARG:HH11	2:C:181:ARG:HH11	1.63	0.46
5:H:8:ALA:HB3	5:H:71:TYR:HB3	1.97	0.45
9:D:401:LMT:H1B	9:D:401:LMT:H3'	1.50	0.45
4:G:38:TYR:O	4:G:39:GLN:C	2.58	0.45
1:A:125:GLU:HB2	1:A:127:HIS:CE1	2.52	0.45
4:G:137:SER:O	4:G:137:SER:OG	2.32	0.45
4:G:36:VAL:O	4:G:37:ALA:C	2.59	0.45
2:C:413:GLY:HA2	2:C:426:VAL:HG21	1.98	0.45
4:G:39:GLN:NE2	6:B:16:GLY:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:57:GLY:O	4:G:61:THR:OG1	2.32	0.45
1:A:161:ASN:H	7:D:118:GLN:HG2	1.81	0.45
4:G:132:ILE:HG12	4:G:152:HIS:HB2	1.98	0.45
5:H:26:VAL:HG11	5:H:49:VAL:HG21	1.99	0.45
7:D:323:VAL:O	7:D:327:ASN:ND2	2.50	0.45
1:A:91:ILE:HG23	1:A:99:TYR:HD1	1.81	0.44
6:B:102:ALA:HB3	6:B:135:LEU:HD13	1.98	0.44
2:C:81:ARG:NH2	2:C:104:GLU:OE2	2.50	0.44
4:G:183:LEU:HA	4:G:186:TRP:HD1	1.82	0.44
1:A:47:VAL:HG21	1:A:84:VAL:HG22	2.00	0.44
4:G:35:MET:HG3	4:G:37:ALA:HB3	1.97	0.44
4:G:188:VAL:HG21	4:G:202:THR:HG23	1.98	0.44
12:D:408:PTY:H312	12:D:408:PTY:H341	1.87	0.44
3:E:41:THR:O	3:E:45:THR:OG1	2.26	0.44
7:D:151:SER:O	7:D:151:SER:OG	2.33	0.44
4:G:36:VAL:CG1	6:B:20:GLY:HA3	2.35	0.44
4:G:144:ILE:HG22	4:G:146:GLY:H	1.82	0.44
4:G:46:VAL:O	4:G:47:CYS:C	2.60	0.43
6:B:114:ARG:HA	6:B:117:ARG:HB2	1.99	0.43
5:H:4:SER:O	5:H:67:ARG:HA	2.18	0.43
6:B:111:GLY:HA3	6:B:129:GLY:HA2	2.00	0.43
2:C:289:ARG:HE	2:C:289:ARG:HB2	1.70	0.43
4:G:79:GLU:HG3	4:G:148:ARG:HE	1.84	0.43
1:A:72:ARG:C	1:A:74:LEU:N	2.76	0.43
7:D:324:LEU:HA	7:D:327:ASN:HD22	1.84	0.43
1:A:68:ILE:HD12	1:A:71:ILE:HD12	2.00	0.43
12:D:408:PTY:H311	12:D:408:PTY:H121	2.00	0.43
12:D:403:PTY:H443	12:D:403:PTY:H412	1.88	0.43
3:E:121:ASN:O	3:E:122:CYS:C	2.58	0.42
5:H:63:LYS:HB2	5:H:63:LYS:HE2	1.84	0.42
1:A:25:CYS:O	1:A:26:PRO:C	2.54	0.42
4:G:155:THR:OG1	4:G:158:LEU:HD23	2.20	0.42
7:D:301:GLY:HA3	7:D:326:MET:HE3	2.01	0.42
1:A:27:PHE:HD1	1:A:147:MET:HG3	1.84	0.42
4:G:152:HIS:HD2	4:G:154:GLU:HG2	1.84	0.42
2:C:294:SER:HA	2:C:301:PRO:HB3	2.00	0.42
9:D:405:LMT:H12	9:D:405:LMT:H2'	1.88	0.42
2:C:124:ASP:N	2:C:124:ASP:OD1	2.51	0.42
4:G:98:GLN:HA	4:G:103:GLY:O	2.19	0.42
9:A:201:LMT:H4B	4:G:126:ILE:HG12	2.00	0.42
2:C:140:LEU:O	2:C:269:ASN:ND2	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:323:VAL:HG12	7:D:327:ASN:HD21	1.85	0.42
1:A:57:LEU:O	1:A:61:TYR:HB2	2.20	0.41
7:D:167:ALA:HA	7:D:168:PRO:HD3	1.91	0.41
1:A:93:LYS:HB2	6:B:26:PHE:HB2	2.01	0.41
7:D:286:VAL:HG21	13:D:404:RBF:HC52	2.01	0.41
2:C:407:ARG:H	2:C:407:ARG:HG3	1.60	0.41
4:G:45:LEU:O	4:G:49:VAL:HG23	2.20	0.41
4:G:56:THR:O	4:G:59:ILE:HG13	2.21	0.41
1:A:11:VAL:HG12	1:A:12:LEU:HG	2.02	0.41
4:G:81:LEU:HD22	4:G:85:LEU:HD12	2.03	0.41
4:G:93:ASP:OD1	4:G:93:ASP:N	2.49	0.41
4:G:173:PHE:HZ	4:G:209:VAL:HG22	1.85	0.41
2:C:415:CYS:HB3	2:C:425:LEU:HD13	2.02	0.41
6:B:147:ASP:OD1	6:B:147:ASP:N	2.53	0.41
7:D:90:PRO:HA	7:D:91:PRO:HD3	1.89	0.41
1:A:70:PHE:CE1	4:G:54:LEU:O	2.74	0.41
2:C:68:THR:OG1	2:C:69:GLU:N	2.53	0.41
2:C:371:ILE:HD13	7:D:18:VAL:HG13	2.03	0.41
4:G:129:GLY:O	4:G:153:LYS:HD3	2.19	0.41
6:B:15:LEU:HD23	6:B:15:LEU:HA	1.96	0.41
4:G:139:ASP:HB3	4:G:145:LEU:HD11	2.03	0.41
4:G:162:ILE:H	4:G:162:ILE:HG12	1.68	0.41
4:G:201:ALA:C	10:G:301:FMN:H5'2	2.45	0.41
2:C:163:LEU:HD21	2:C:245:LEU:HD23	2.03	0.40
4:G:170:ILE:HD12	4:G:170:ILE:HA	1.92	0.40
3:E:170:LEU:HD23	3:E:170:LEU:HA	1.84	0.40
4:G:136:MET:N	4:G:136:MET:SD	2.94	0.40
1:A:59:GLU:HA	1:A:63:LEU:HB2	2.04	0.40
2:C:6:SER:OG	2:C:7:SER:N	2.55	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	A	187/190 (98%)	172 (92%)	12 (6%)	3 (2%)	7 32
2	C	475/496 (96%)	448 (94%)	25 (5%)	2 (0%)	30 60
3	E	211/238 (89%)	194 (92%)	17 (8%)	0	100 100
4	G	192/229 (84%)	178 (93%)	11 (6%)	3 (2%)	7 32
5	H	69/86 (80%)	68 (99%)	1 (1%)	0	100 100
6	B	106/174 (61%)	96 (91%)	10 (9%)	0	100 100
7	D	301/366 (82%)	294 (98%)	7 (2%)	0	100 100
All	All	1541/1779 (87%)	1450 (94%)	83 (5%)	8 (0%)	26 56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ILE
1	A	94	ALA
1	A	112	ASN
2	C	8	ILE
4	G	157	GLY
4	G	224	GLU
2	C	7	SER
4	G	203	ILE

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	148/149 (99%)	148 (100%)	0	100 100
2	C	367/380 (97%)	364 (99%)	3 (1%)	73 78
3	E	171/194 (88%)	169 (99%)	2 (1%)	63 74
4	G	156/183 (85%)	153 (98%)	3 (2%)	50 68
5	H	63/78 (81%)	63 (100%)	0	100 100
6	B	83/129 (64%)	83 (100%)	0	100 100
7	D	238/286 (83%)	238 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1226/1399 (88%)	1218 (99%)	8 (1%)	73 79

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	50	MET
2	C	315	LEU
2	C	366	ASP
3	E	45	THR
3	E	200	ILE
4	G	38	TYR
4	G	39	GLN
4	G	202	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
2	C	196	HIS
4	G	89	ASN
4	G	152	HIS
7	D	111	GLN
7	D	327	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

17 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	$\#\|Z\|>2$
11	SF4	C	502	2	0,12,12	-	-	-		
11	SF4	B	201	6	0,12,12	-	-	-		
13	RBF	D	404	-	29,29,29	1.11	1 (3%)	41,43,43	1.13	3 (7%)
10	FMN	G	301	4	29,32,33	0.25	0	40,47,50	0.22	0
12	PTY	D	403	-	49,49,49	0.90	2 (4%)	52,54,54	1.15	4 (7%)
9	LMT	E	301	-	36,36,36	1.14	5 (13%)	47,47,47	1.07	3 (6%)
12	PTY	D	408	-	49,49,49	0.47	0	52,54,54	0.42	0
9	LMT	A	201	-	36,36,36	1.17	5 (13%)	47,47,47	1.23	5 (10%)
9	LMT	D	401	-	36,36,36	1.22	6 (16%)	47,47,47	1.30	6 (12%)
11	SF4	C	501	2	0,12,12	-	-	-		
9	LMT	D	407	-	36,36,36	1.23	6 (16%)	47,47,47	1.13	4 (8%)
11	SF4	B	202	6	0,12,12	-	-	-		
8	FES	A	200	3,1	0,4,4	-	-	-		
9	LMT	D	406	-	36,36,36	1.18	5 (13%)	47,47,47	0.95	1 (2%)
9	LMT	D	402	-	36,36,36	1.18	5 (13%)	47,47,47	0.97	1 (2%)
9	LMT	D	405	-	36,36,36	1.17	5 (13%)	47,47,47	1.06	3 (6%)
10	FMN	C	500	-	33,33,33	1.93	7 (21%)	48,50,50	1.20	5 (10%)

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
11	SF4	C	502	2	-	-	0/6/5/5
13	RBF	D	404	-	-	12/14/14/14	0/3/3/3
11	SF4	B	201	6	-	-	0/6/5/5
10	FMN	G	301	4	2/2/4/4	9/15/17/18	0/3/3/3
12	PTY	D	403	-	-	8/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	LMT	E	301	-	-	6/21/61/61	0/2/2/2
12	PTY	D	408	-	-	14/53/53/53	-
9	LMT	A	201	-	-	11/21/61/61	0/2/2/2
9	LMT	D	401	-	-	5/21/61/61	0/2/2/2
11	SF4	C	501	2	-	-	0/6/5/5
9	LMT	D	407	-	-	2/21/61/61	0/2/2/2
11	SF4	B	202	6	-	-	0/6/5/5
8	FES	A	200	3,1	-	-	0/1/1/1
9	LMT	D	406	-	-	4/21/61/61	0/2/2/2
9	LMT	D	402	-	-	7/21/61/61	0/2/2/2
9	LMT	D	405	-	-	9/21/61/61	0/2/2/2
10	FMN	C	500	-	-	10/18/18/18	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	500	FMN	P-O5'	7.00	1.82	1.60
10	C	500	FMN	C5'-C4'	4.29	1.57	1.51
12	D	403	PTY	O4-C30	3.99	1.45	1.33
12	D	403	PTY	O7-C8	3.99	1.45	1.34
9	D	406	LMT	O3'-C3'	-2.67	1.36	1.43
9	E	301	LMT	O3'-C3'	-2.65	1.36	1.43
9	D	405	LMT	O3'-C3'	-2.63	1.36	1.43
10	C	500	FMN	O5'-C5'	-2.60	1.34	1.44
9	D	401	LMT	O3'-C3'	-2.58	1.36	1.43
9	D	402	LMT	O3'-C3'	-2.57	1.36	1.43
9	D	407	LMT	O3'-C3'	-2.54	1.37	1.43
9	D	406	LMT	O2'-C2'	-2.54	1.37	1.43
9	A	201	LMT	O3'-C3'	-2.54	1.37	1.43
9	D	405	LMT	O2'-C2'	-2.53	1.37	1.43
9	D	407	LMT	O2B-C2B	-2.42	1.37	1.43
9	E	301	LMT	O2B-C2B	-2.38	1.37	1.43
9	D	402	LMT	O2'-C2'	-2.35	1.37	1.43
9	D	402	LMT	O2B-C2B	-2.35	1.37	1.43
10	C	500	FMN	C2-N3	2.34	1.44	1.39
10	C	500	FMN	C1'-C2'	2.34	1.56	1.52
9	D	406	LMT	O2B-C2B	-2.33	1.37	1.43
9	D	407	LMT	O3B-C3B	-2.32	1.37	1.43
9	D	405	LMT	O2B-C2B	-2.31	1.37	1.43
9	D	402	LMT	O3B-C3B	-2.31	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	201	LMT	O3B-C3B	-2.29	1.37	1.43
9	E	301	LMT	O3B-C3B	-2.27	1.37	1.43
9	D	405	LMT	O3B-C3B	-2.27	1.37	1.43
9	A	201	LMT	O2B-C2B	-2.27	1.37	1.43
9	D	406	LMT	O3B-C3B	-2.27	1.37	1.43
9	D	401	LMT	O3B-C3B	-2.26	1.37	1.43
9	D	401	LMT	O2B-C2B	-2.21	1.37	1.43
13	D	404	RBF	C2-N1	2.19	1.42	1.36
9	E	301	LMT	O2'-C2'	-2.19	1.37	1.43
9	D	401	LMT	C3'-C2'	2.19	1.57	1.52
9	D	401	LMT	O2'-C2'	-2.19	1.37	1.43
9	D	406	LMT	O4'-C4B	-2.16	1.37	1.43
10	C	500	FMN	C2-N1	2.11	1.41	1.36
9	D	402	LMT	O4'-C4B	-2.11	1.38	1.43
9	D	407	LMT	C3'-C2'	2.10	1.57	1.52
9	D	405	LMT	O4'-C4B	-2.10	1.38	1.43
9	D	407	LMT	O2'-C2'	-2.10	1.38	1.43
9	D	401	LMT	O4'-C4B	-2.09	1.38	1.43
9	E	301	LMT	O4'-C4B	-2.09	1.38	1.43
10	C	500	FMN	C6-C7	-2.07	1.36	1.39
9	D	407	LMT	O4'-C4B	-2.04	1.38	1.43
9	A	201	LMT	O4'-C4B	-2.01	1.38	1.43
9	A	201	LMT	O2'-C2'	-2.01	1.38	1.43

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	403	PTY	O7-C8-C11	4.37	120.91	111.50
13	D	404	RBF	C5'-C4'-C3'	-4.23	103.24	112.41
13	D	404	RBF	O5'-C5'-C4'	-3.82	102.74	111.07
9	D	401	LMT	O5B-C5B-C4B	3.41	115.88	109.69
9	D	401	LMT	C2'-C3'-C4'	3.20	116.99	109.68
9	D	407	LMT	C2'-C3'-C4'	3.04	116.63	109.68
12	D	403	PTY	C6-O7-C8	-2.98	110.46	117.79
9	D	407	LMT	O5'-C1'-C2'	2.86	116.40	110.35
10	C	500	FMN	O5'-P-O1P	-2.85	98.47	106.47
10	C	500	FMN	C5'-C4'-C3'	-2.81	106.78	112.20
9	A	201	LMT	C1'-O5'-C5'	2.80	119.18	113.69
9	E	301	LMT	C3'-C4'-C5'	-2.76	104.60	110.93
12	D	403	PTY	O4-C30-C31	2.75	120.54	111.91
9	D	405	LMT	O1'-C1'-C2'	2.66	112.46	108.30
10	C	500	FMN	O2P-P-O5'	-2.64	99.70	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	401	LMT	O1B-C4'-C3'	2.64	114.29	107.28
10	C	500	FMN	O3P-P-O2P	2.58	117.51	107.64
10	C	500	FMN	O3P-P-O5'	-2.53	99.99	106.73
9	A	201	LMT	C1B-O1B-C4'	2.47	124.09	117.96
9	D	406	LMT	C3'-C4'-C5'	-2.47	105.27	110.93
9	D	401	LMT	C1B-O5B-C5B	2.46	118.51	113.69
9	A	201	LMT	C2'-C3'-C4'	2.45	115.28	109.68
9	A	201	LMT	O5B-C5B-C4B	2.42	114.09	109.69
9	A	201	LMT	O5'-C1'-C2'	2.35	115.33	110.35
9	D	407	LMT	C1'-C2'-C3'	2.29	114.77	110.00
9	D	402	LMT	C1'-O5'-C5'	-2.25	109.27	113.69
9	D	401	LMT	C1'-O5'-C5'	-2.22	109.33	113.69
9	E	301	LMT	O5'-C1'-O1'	-2.17	104.83	109.97
9	D	405	LMT	C1-O1'-C1'	2.12	117.36	113.84
13	D	404	RBF	O3'-C3'-C2'	-2.11	103.71	108.81
9	D	407	LMT	O5B-C5B-C4B	2.09	113.49	109.69
9	E	301	LMT	C3B-C4B-C5B	-2.06	106.56	110.24
9	D	401	LMT	C4B-C3B-C2B	2.05	114.40	110.82
12	D	403	PTY	O4-C30-O30	-2.04	118.45	123.59
9	D	405	LMT	C1'-O5'-C5'	-2.00	109.76	113.69

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	G	301	FMN	C2'
10	G	301	FMN	C4'

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	201	LMT	C2'-C1'-O1'-C1
9	A	201	LMT	O5'-C1'-O1'-C1
9	A	201	LMT	C2-C1-O1'-C1'
9	E	301	LMT	C2'-C1'-O1'-C1
9	E	301	LMT	O5'-C1'-O1'-C1
9	D	402	LMT	C2-C1-O1'-C1'
9	D	406	LMT	O5'-C1'-O1'-C1
10	C	500	FMN	N10-C1'-C2'-O2'
10	C	500	FMN	N10-C1'-C2'-C3'
10	C	500	FMN	C1'-C2'-C3'-C4'
10	C	500	FMN	O3'-C3'-C4'-C5'
10	G	301	FMN	N10-C1'-C2'-O2'

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Mol	Chain	Res	Type	Atoms
10	G	301	FMN	N10-C1'-C2'-C3'
10	G	301	FMN	C1'-C2'-C3'-O3'
10	G	301	FMN	C1'-C2'-C3'-C4'
10	G	301	FMN	O2'-C2'-C3'-O3'
10	G	301	FMN	O2'-C2'-C3'-C4'
10	G	301	FMN	C3'-C4'-C5'-O5'
10	G	301	FMN	O4'-C4'-C5'-O5'
12	D	403	PTY	C3-O11-P1-O13
12	D	403	PTY	C5-O14-P1-O12
12	D	408	PTY	N1-C2-C3-O11
12	D	408	PTY	C3-O11-P1-O13
13	D	404	RBF	N10-C1'-C2'-O2'
13	D	404	RBF	N10-C1'-C2'-C3'
13	D	404	RBF	C1'-C2'-C3'-O3'
13	D	404	RBF	C1'-C2'-C3'-C4'
13	D	404	RBF	C2'-C3'-C4'-C5'
13	D	404	RBF	O3'-C3'-C4'-O4'
13	D	404	RBF	O3'-C3'-C4'-C5'
13	D	404	RBF	O4'-C4'-C5'-O5'
9	D	401	LMT	C3'-C4'-O1B-C1B
13	D	404	RBF	C3'-C4'-C5'-O5'
9	A	201	LMT	O5B-C5B-C6B-O6B
9	D	405	LMT	O5'-C5'-C6'-O6'
10	C	500	FMN	O3'-C3'-C4'-O4'
9	D	402	LMT	O5'-C5'-C6'-O6'
9	A	201	LMT	C4B-C5B-C6B-O6B
9	D	401	LMT	C2'-C1'-O1'-C1
9	A	201	LMT	C4'-C5'-C6'-O6'
12	D	403	PTY	C31-C30-O4-C1
13	D	404	RBF	C2'-C3'-C4'-O4'
9	A	201	LMT	C5'-C4'-O1B-C1B
9	D	402	LMT	C4'-C5'-C6'-O6'
10	C	500	FMN	C2'-C3'-C4'-C5'
12	D	403	PTY	O30-C30-O4-C1
12	D	403	PTY	C5-O14-P1-O11
10	C	500	FMN	C2'-C3'-C4'-O4'
9	D	402	LMT	C3-C4-C5-C6
9	D	407	LMT	C2-C1-O1'-C1'
9	A	201	LMT	C3'-C4'-O1B-C1B
9	D	402	LMT	C6-C7-C8-C9
12	D	408	PTY	C35-C36-C37-C38
12	D	408	PTY	O10-C8-O7-C6

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Mol	Chain	Res	Type	Atoms
9	D	401	LMT	C2-C3-C4-C5
9	D	405	LMT	C4'-C5'-C6'-O6'
12	D	408	PTY	C11-C8-O7-C6
9	A	201	LMT	C4-C5-C6-C7
9	D	402	LMT	O1'-C1-C2-C3
9	E	301	LMT	O5'-C5'-C6'-O6'
9	D	406	LMT	O5'-C5'-C6'-O6'
9	A	201	LMT	O5'-C5'-C6'-O6'
9	D	405	LMT	C2'-C1'-O1'-C1
9	D	405	LMT	C3'-C4'-O1B-C1B
12	D	403	PTY	C8-C11-C12-C13
9	D	407	LMT	C3-C4-C5-C6
9	E	301	LMT	C2-C1-O1'-C1'
9	D	406	LMT	C2-C1-O1'-C1'
9	D	405	LMT	O1'-C1-C2-C3
9	E	301	LMT	C5-C6-C7-C8
12	D	408	PTY	C36-C37-C38-C39
10	C	500	FMN	O2'-C2'-C3'-C4'
9	D	401	LMT	O5'-C1'-O1'-C1
9	D	405	LMT	C5'-C4'-O1B-C1B
12	D	408	PTY	C3-O11-P1-O14
9	D	405	LMT	C3-C4-C5-C6
9	D	405	LMT	C4B-C5B-C6B-O6B
9	E	301	LMT	C4B-C5B-C6B-O6B
13	D	404	RBF	O2'-C2'-C3'-C4'
12	D	408	PTY	C24-C25-C26-C27
12	D	408	PTY	C31-C30-O4-C1
10	C	500	FMN	O2'-C2'-C3'-O3'
12	D	408	PTY	O30-C30-O4-C1
10	G	301	FMN	C4'-C5'-O5'-P
9	D	402	LMT	C9-C10-C11-C12
9	A	201	LMT	C9-C10-C11-C12
9	D	401	LMT	O1'-C1-C2-C3
12	D	408	PTY	C22-C23-C24-C25
12	D	408	PTY	C12-C11-C8-O7
9	D	405	LMT	C1-C2-C3-C4
9	D	406	LMT	C5-C6-C7-C8
12	D	408	PTY	O14-C5-C6-C1
12	D	408	PTY	C12-C11-C8-O10
13	D	404	RBF	O2'-C2'-C3'-O3'
12	D	403	PTY	C3-O11-P1-O12
12	D	403	PTY	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
10	C	500	FMN	C1'-C2'-C3'-O3'

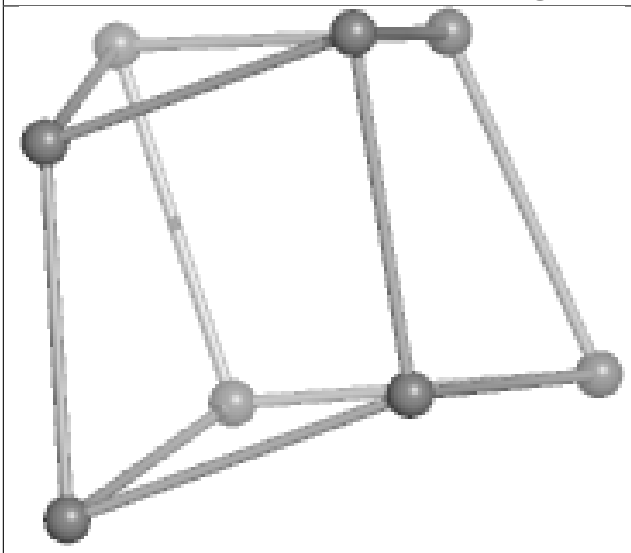
There are no ring outliers.

13 monomers are involved in 31 short contacts:

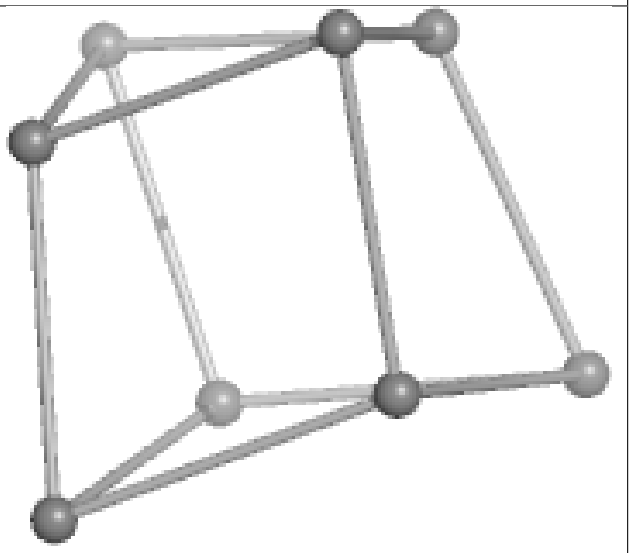
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	404	RBF	2	0
10	G	301	FMN	10	0
12	D	403	PTY	4	0
9	E	301	LMT	2	0
12	D	408	PTY	2	0
9	A	201	LMT	4	0
9	D	401	LMT	3	0
9	D	407	LMT	1	0
11	B	202	SF4	1	0
8	A	200	FES	1	0
9	D	406	LMT	1	0
9	D	402	LMT	2	0
9	D	405	LMT	2	0

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.

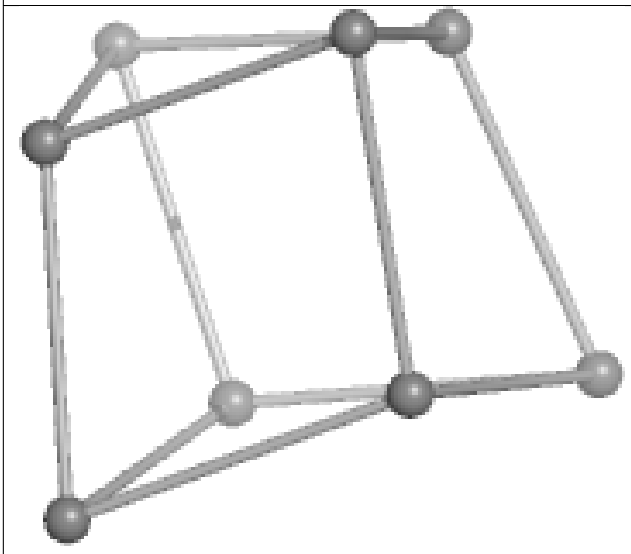
Ligand SF4 C 502



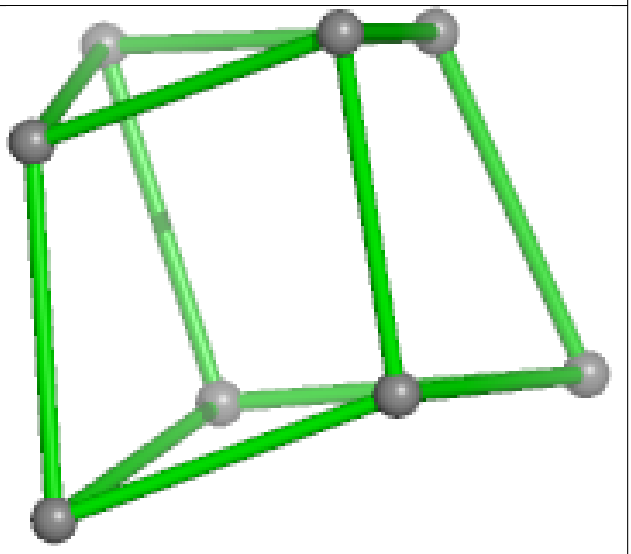
Bond lengths



Bond angles

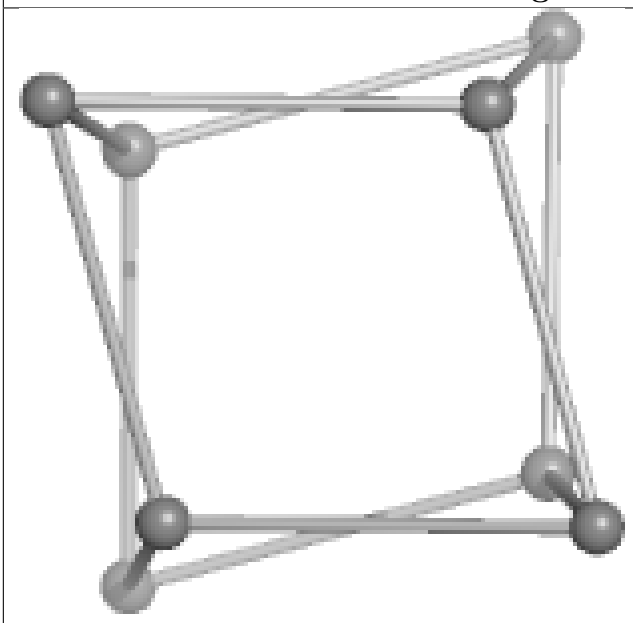


Torsions

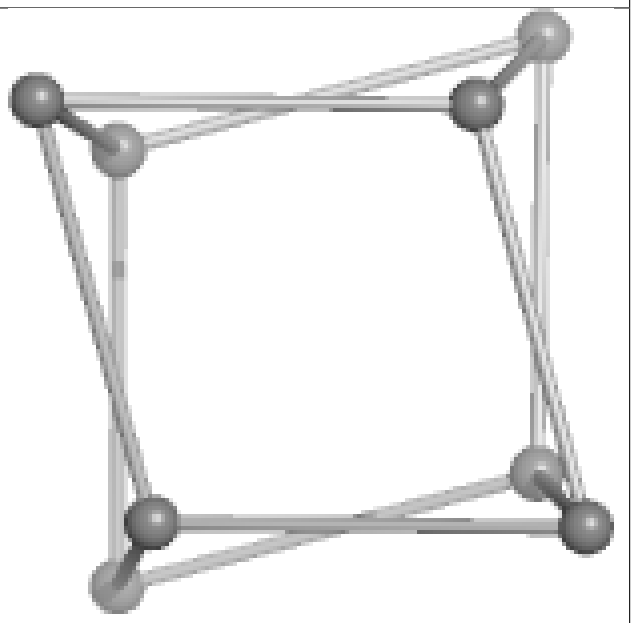


Rings

Ligand SF4 B 201



Bond lengths



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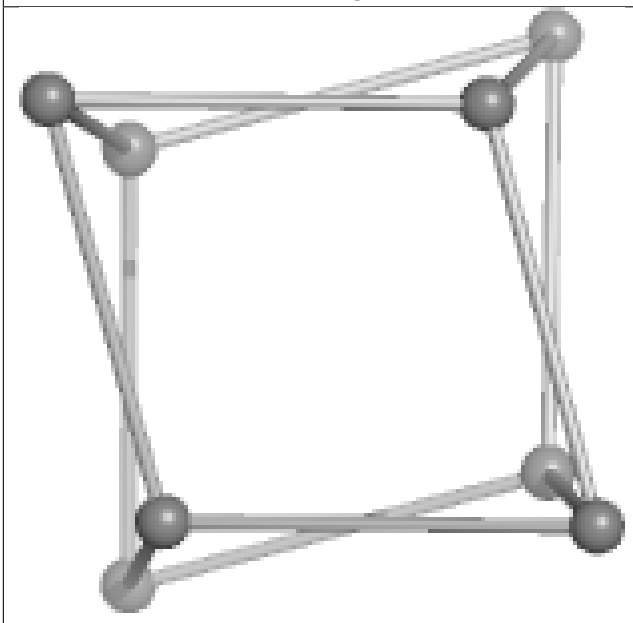

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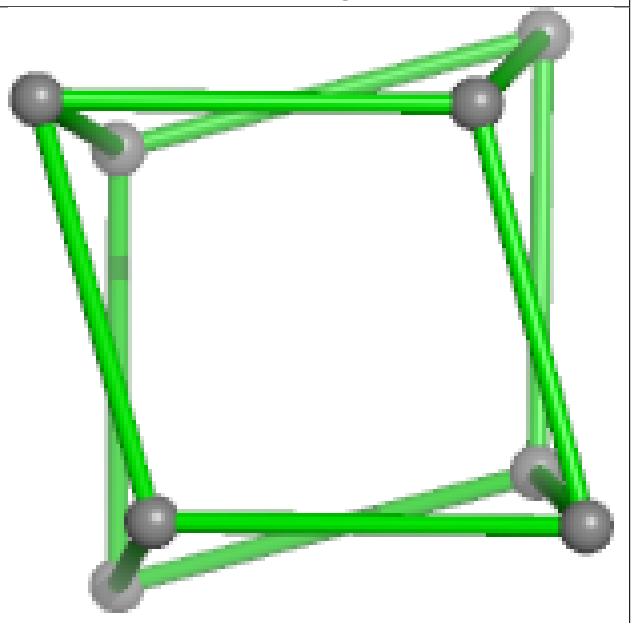
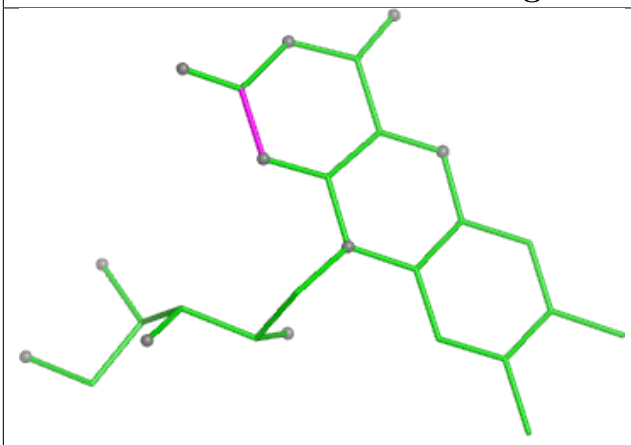
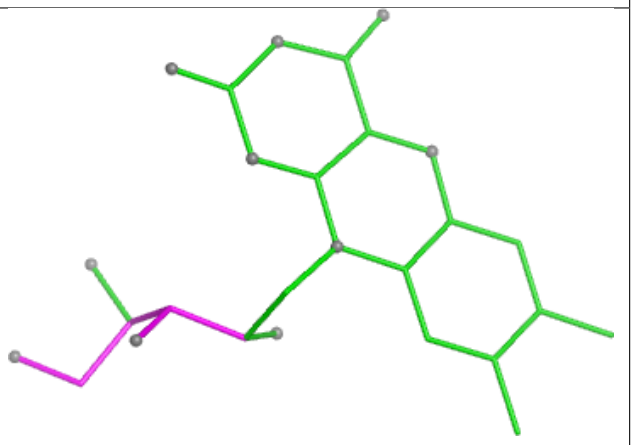


Rings

Ligand RBF D 404



Bond lengths



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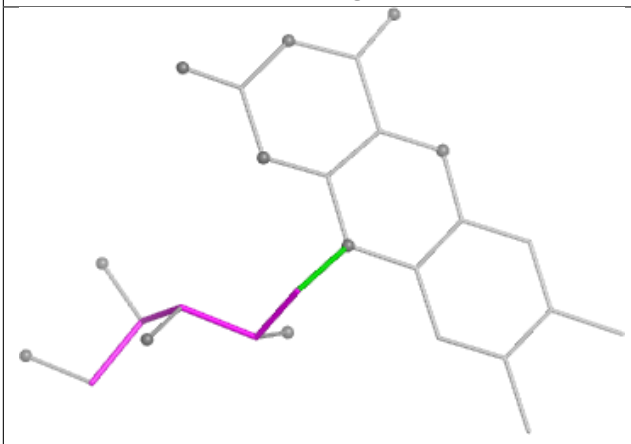

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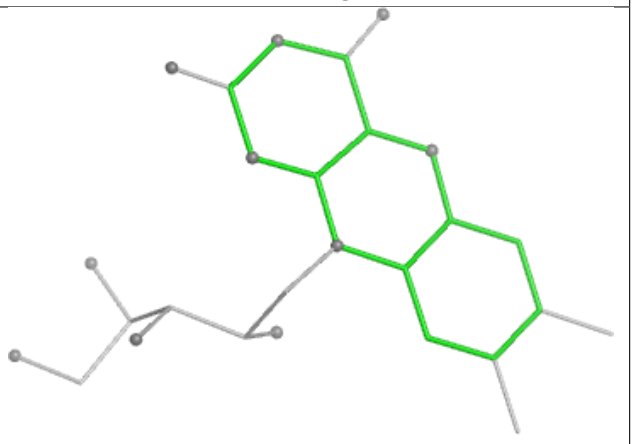
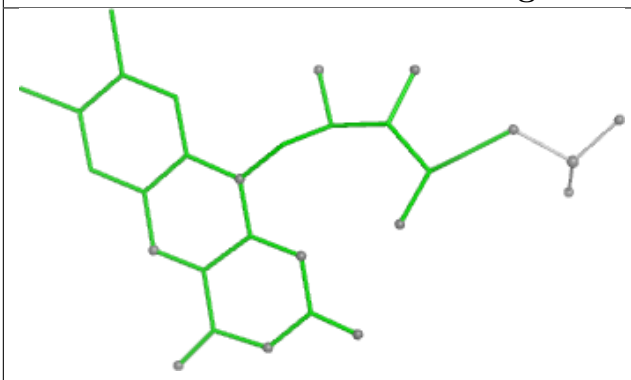


Rings

Ligand FMN G 301



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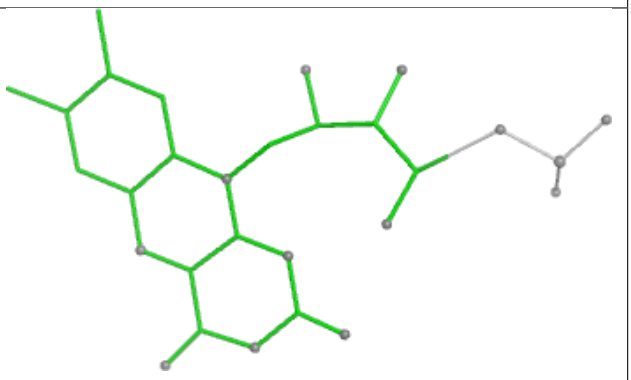
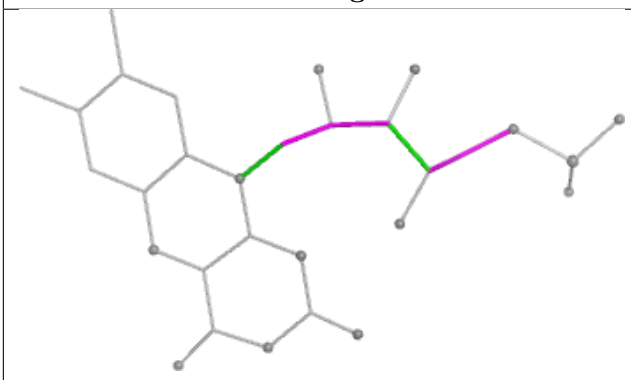


Bond angles



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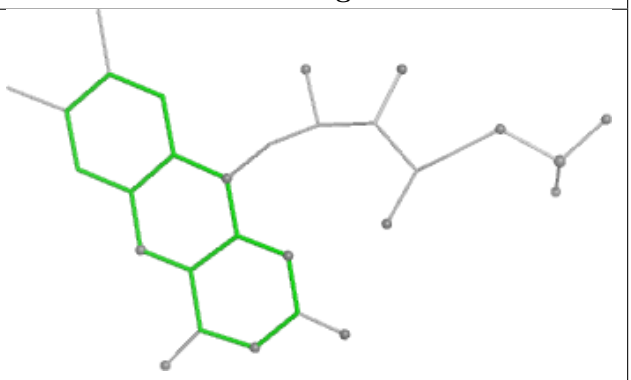
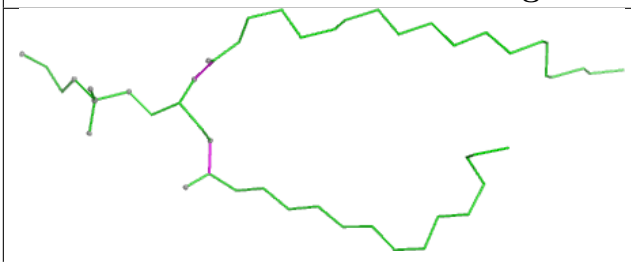


Rings

Ligand PTY D 403



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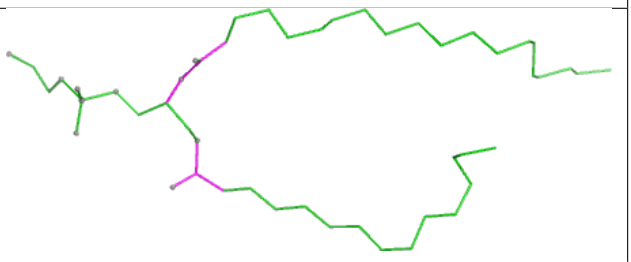
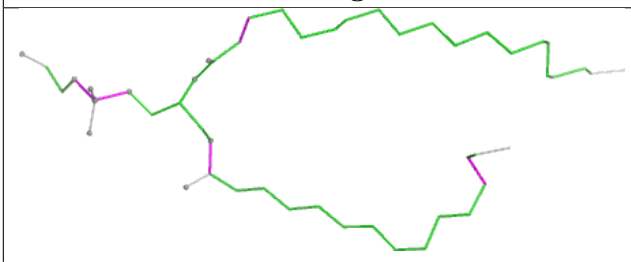


Bond angles



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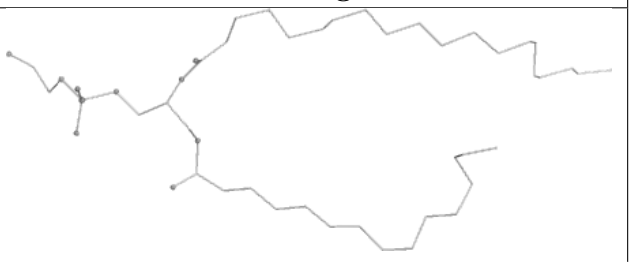
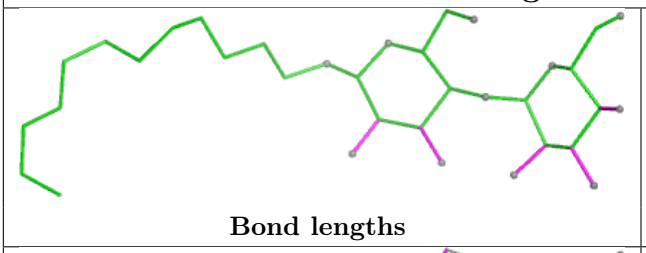


Rings

Ligand LMT E 301



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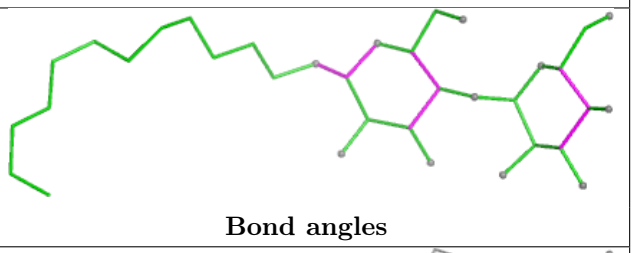
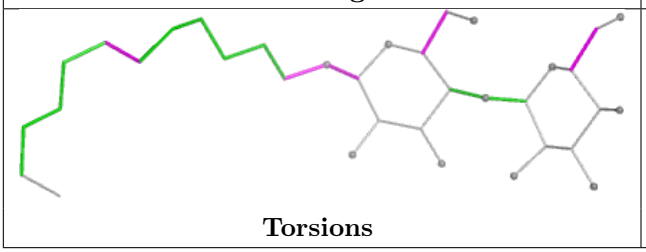


Bond angles



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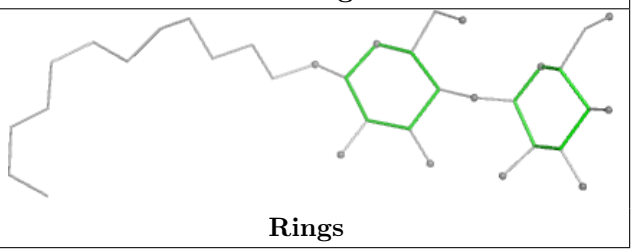
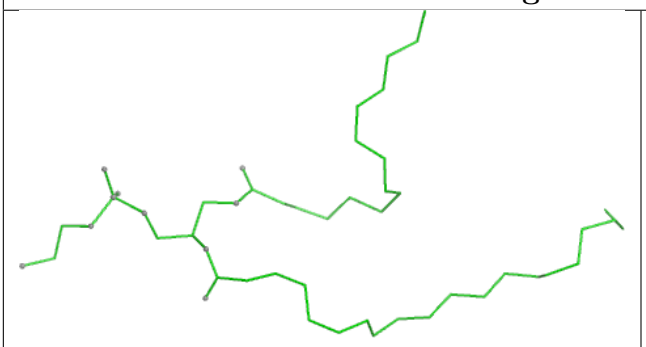


Rings

Ligand PTY D 408



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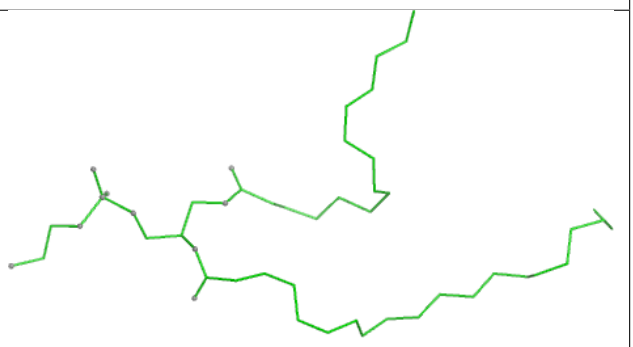
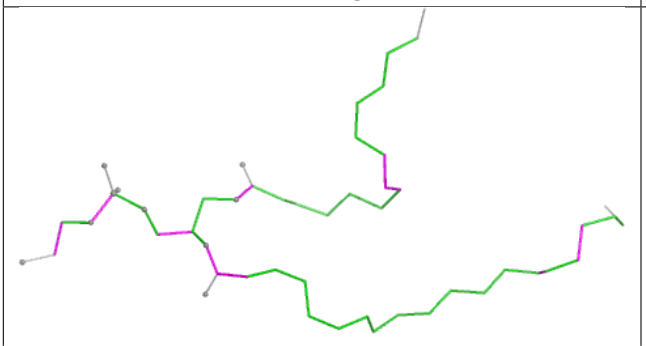
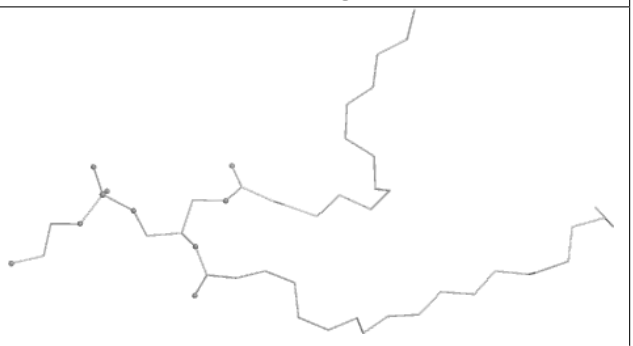


Bond angles

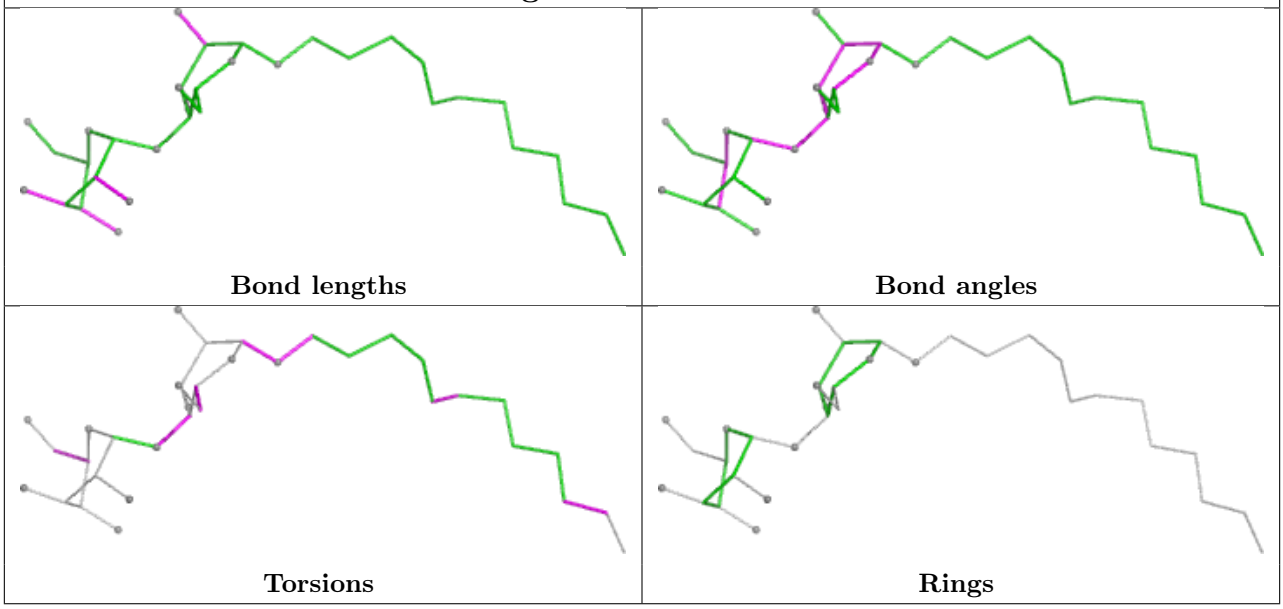


Torsions

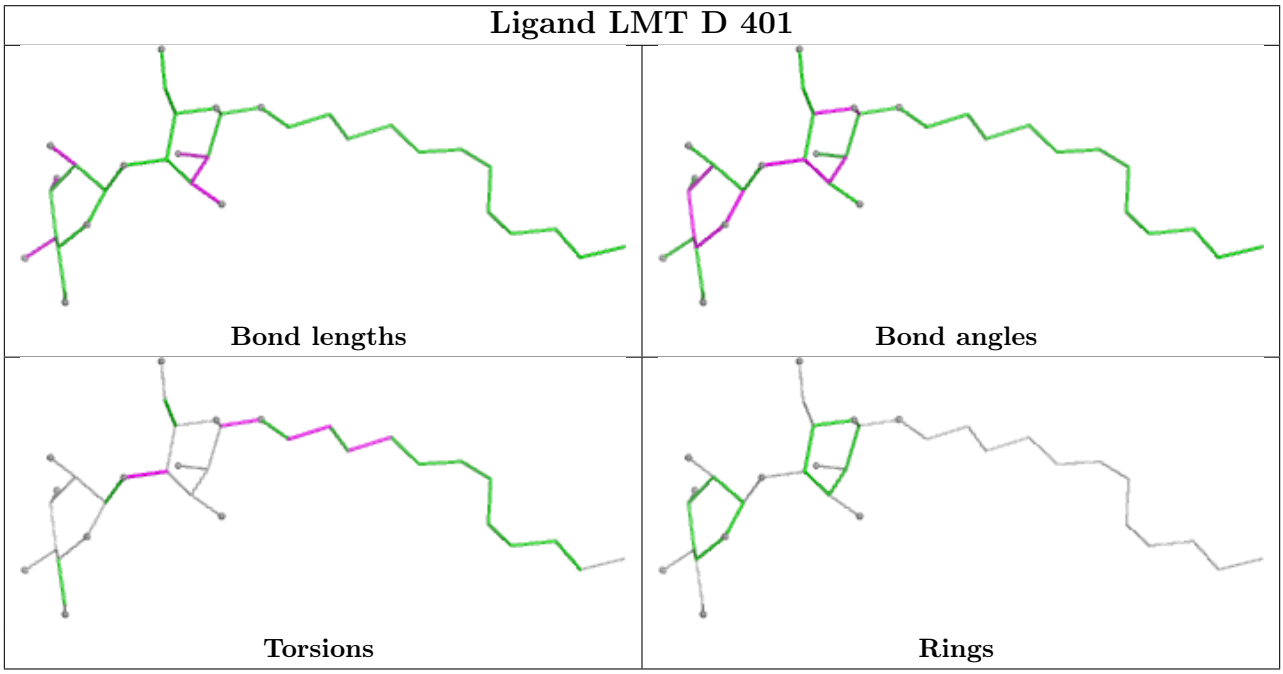


Rings

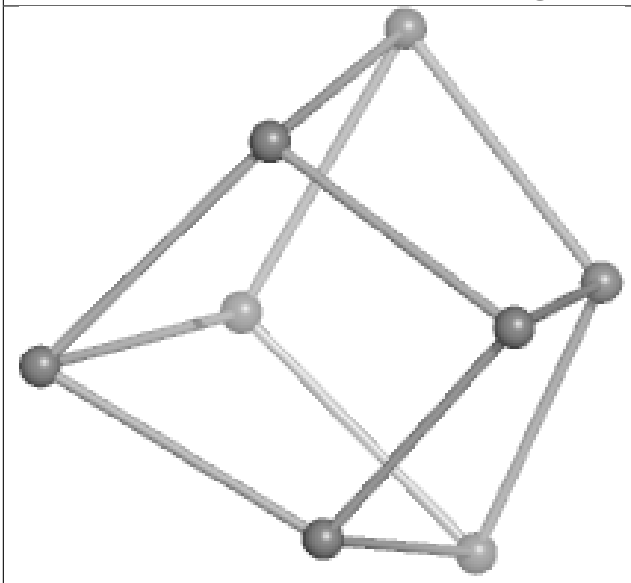
Ligand LMT A 201



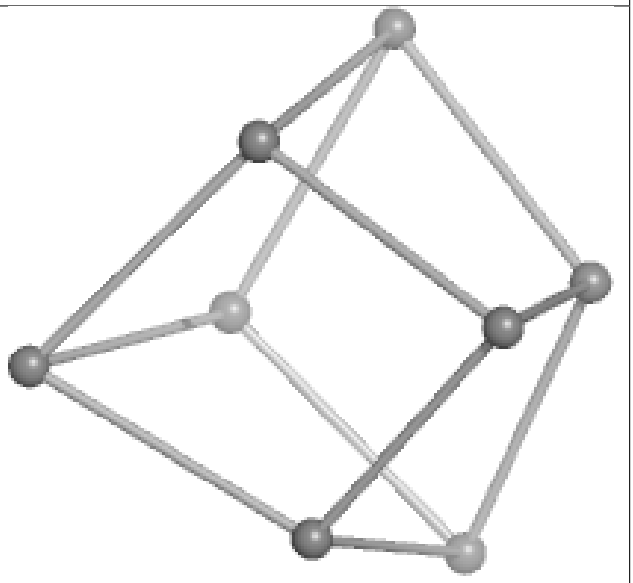
Ligand LMT D 401



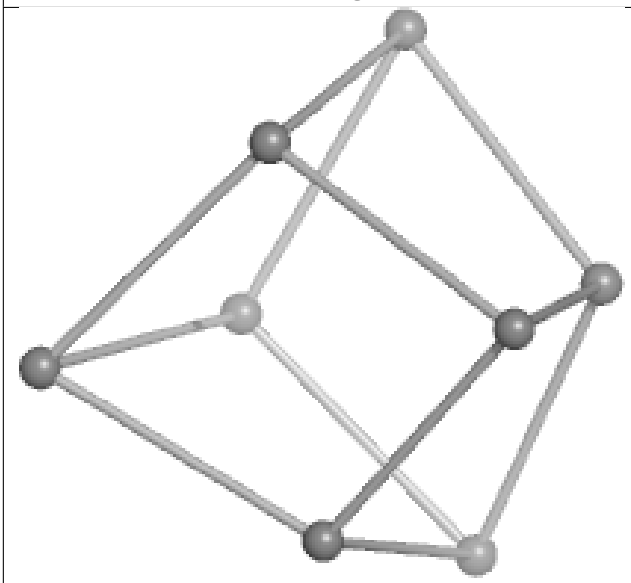
Ligand SF4 C 501



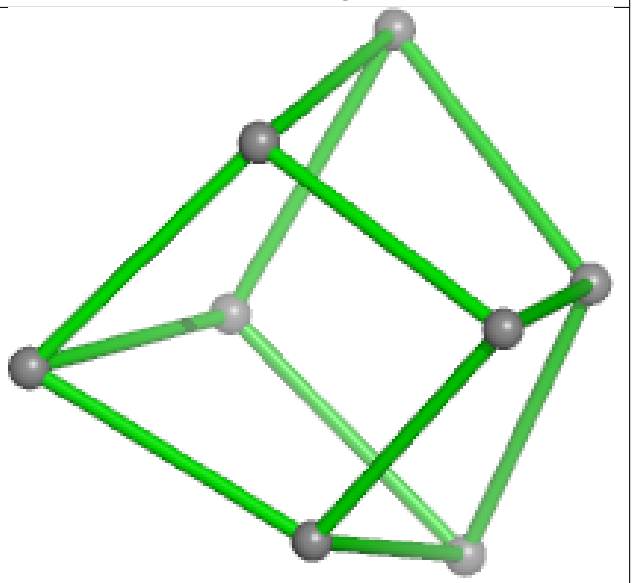
Bond lengths



Bond angles

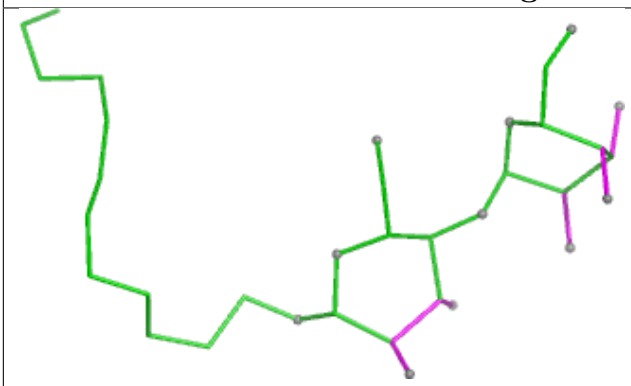


Torsions

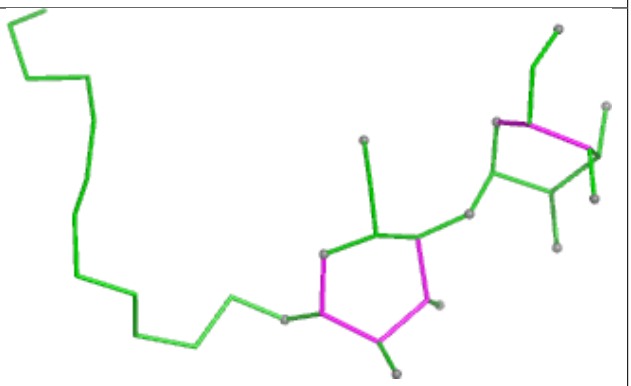


Rings

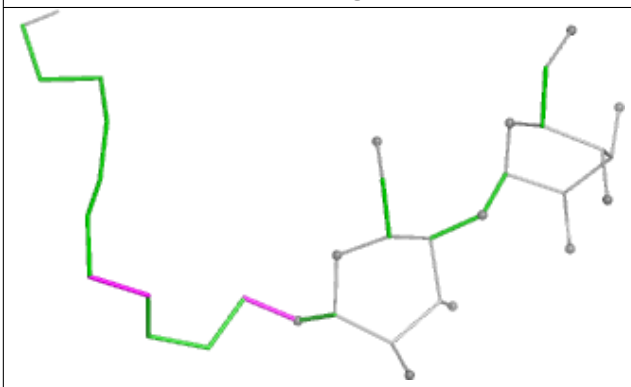
Ligand LMT D 407



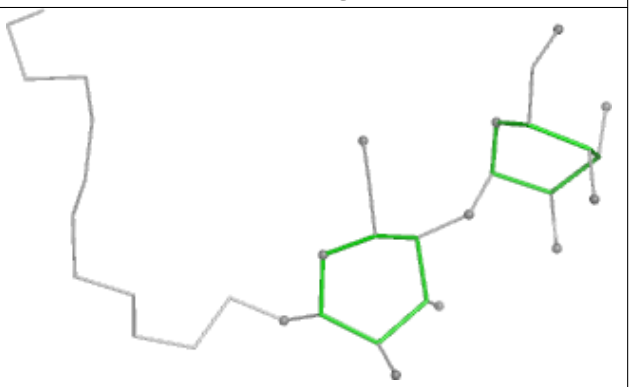
Bond lengths



Bond angles

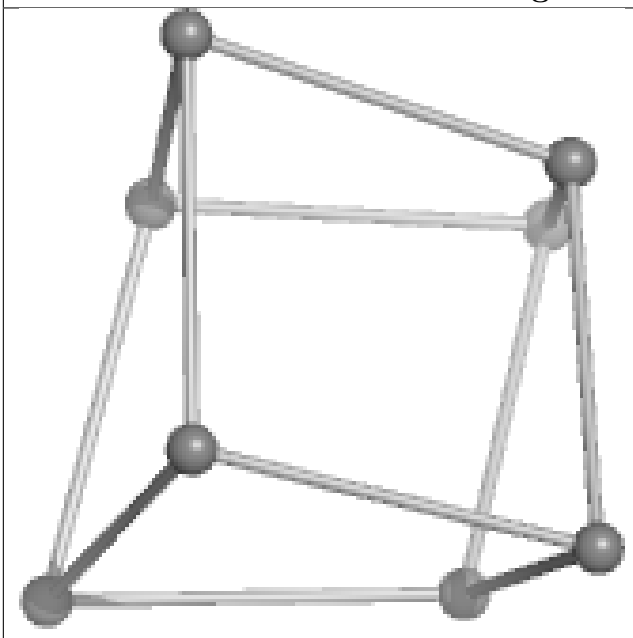


Torsions

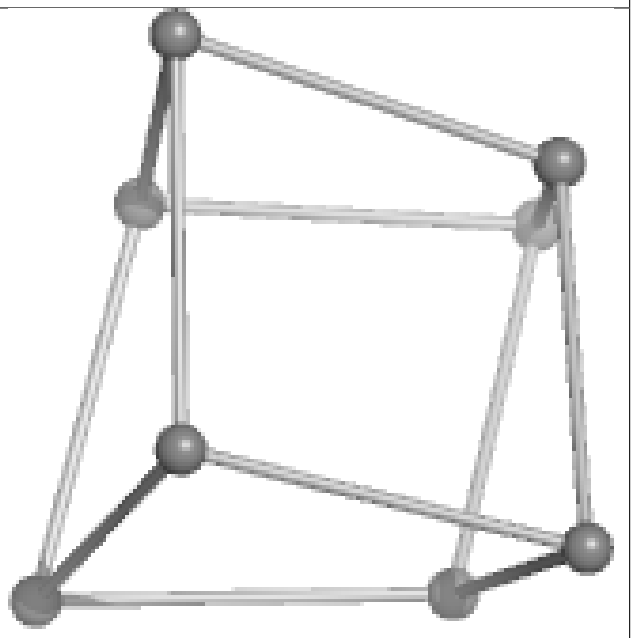


Rings

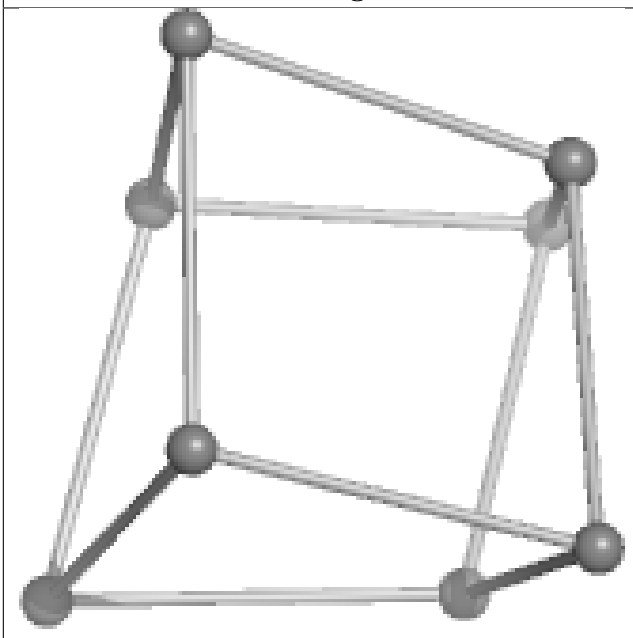
Ligand SF4 B 202



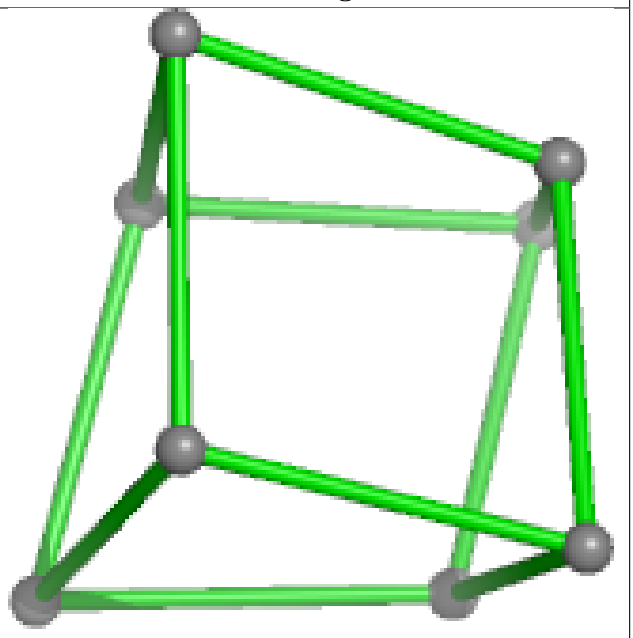
Bond lengths



Bond angles

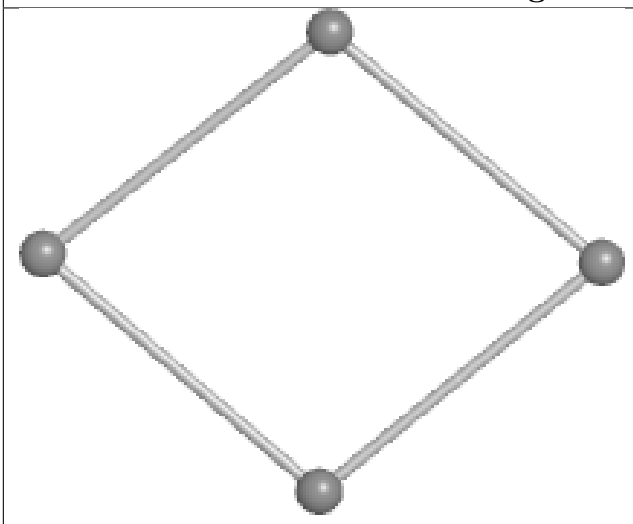


Torsions

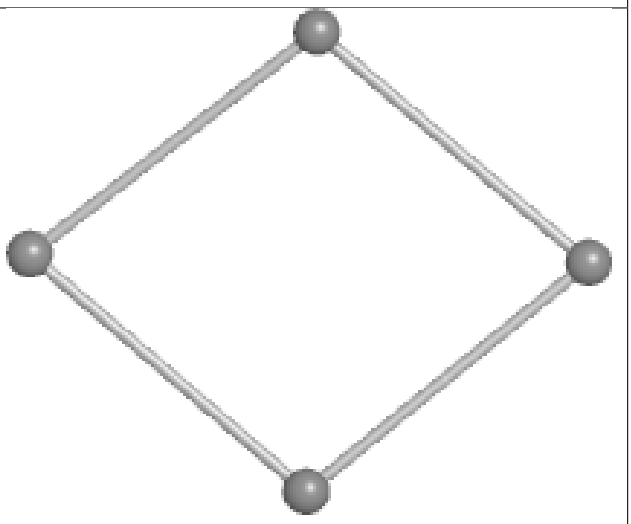


Rings

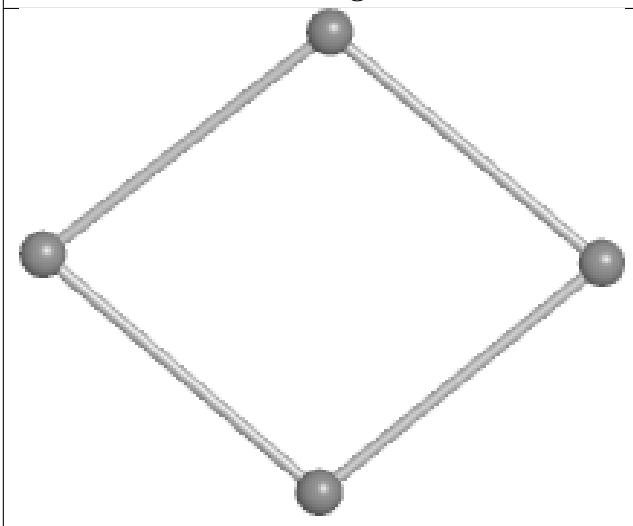
Ligand FES A 200



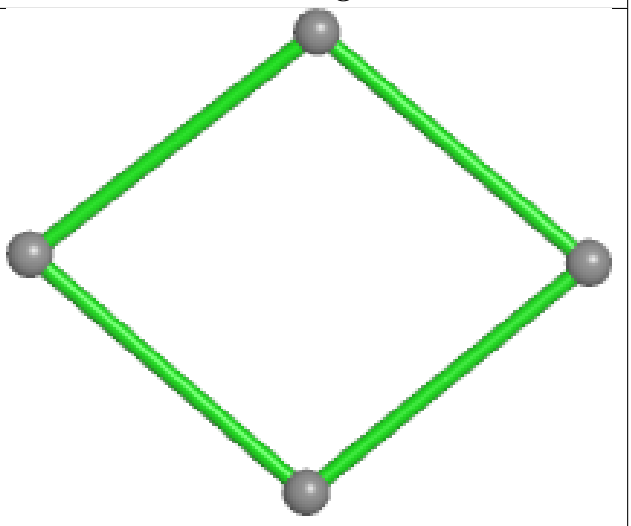
Bond lengths



Bond angles

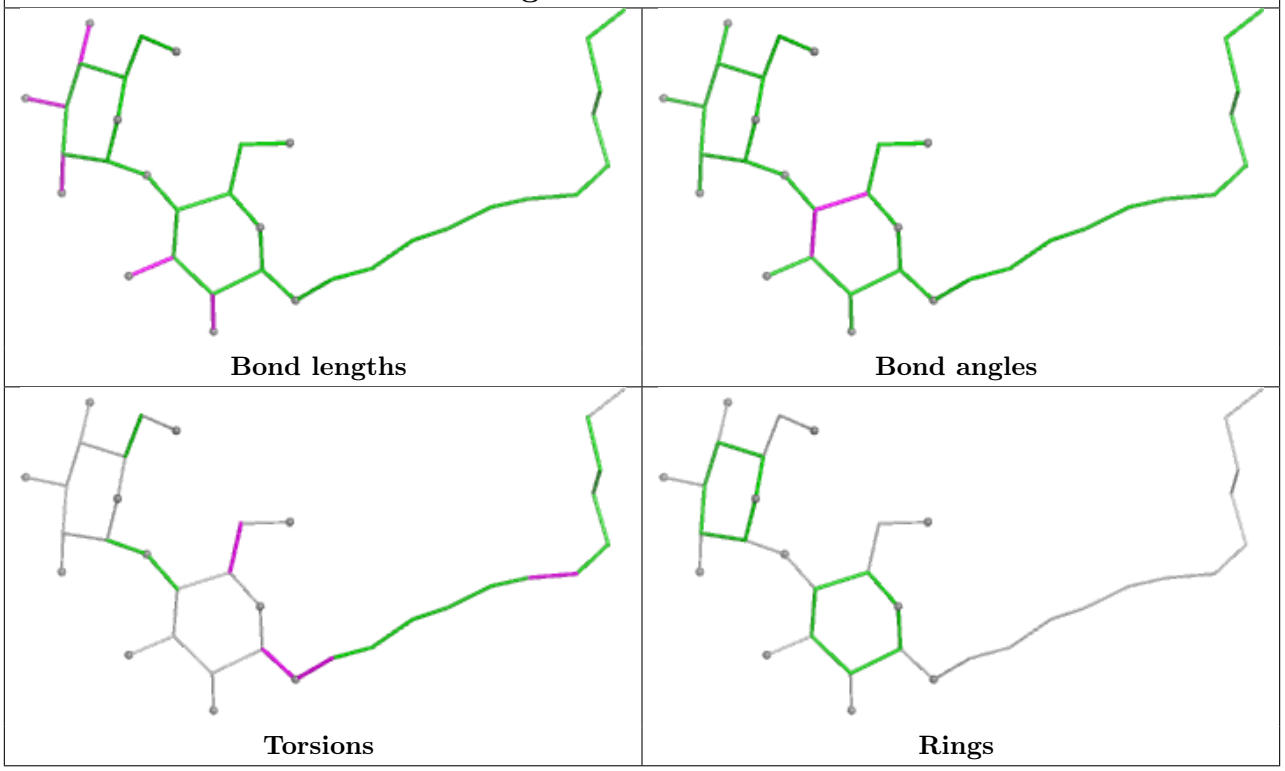


Torsions

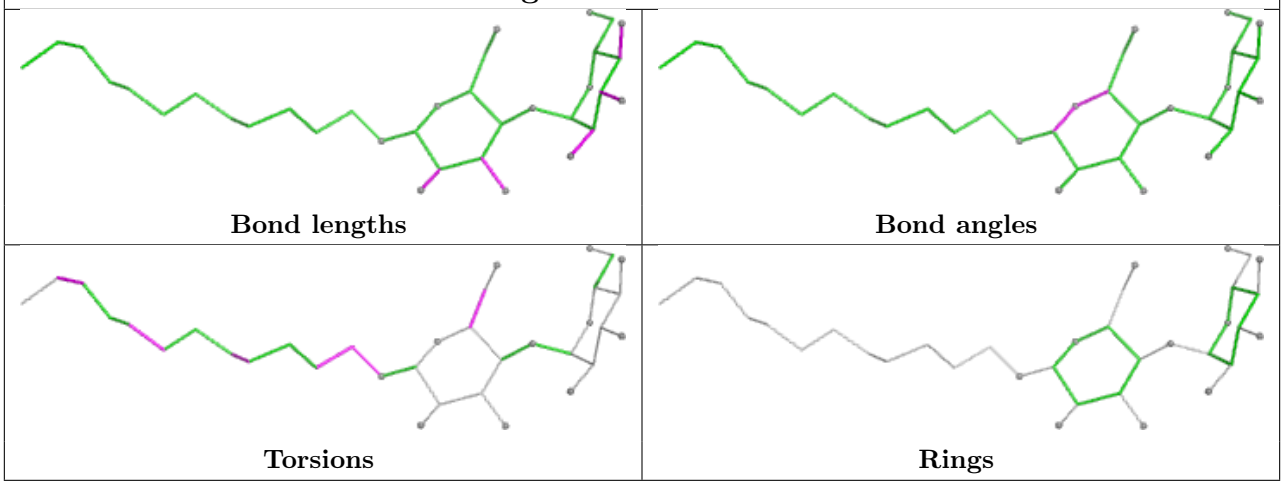


Rings

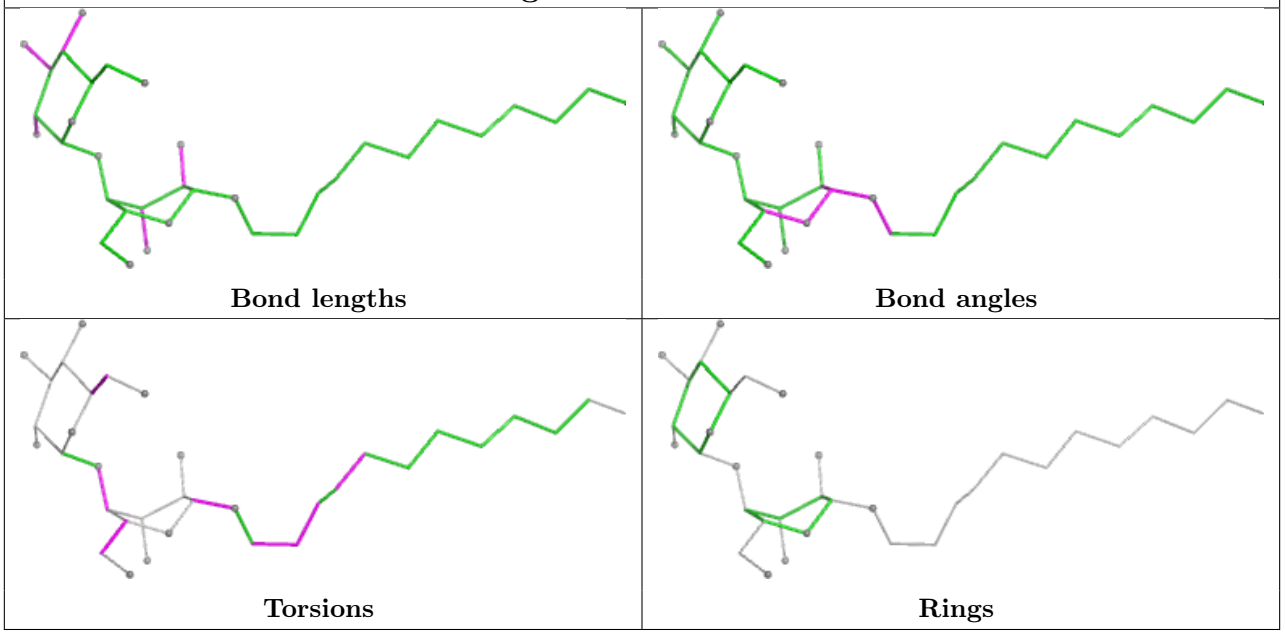
Ligand LMT D 406



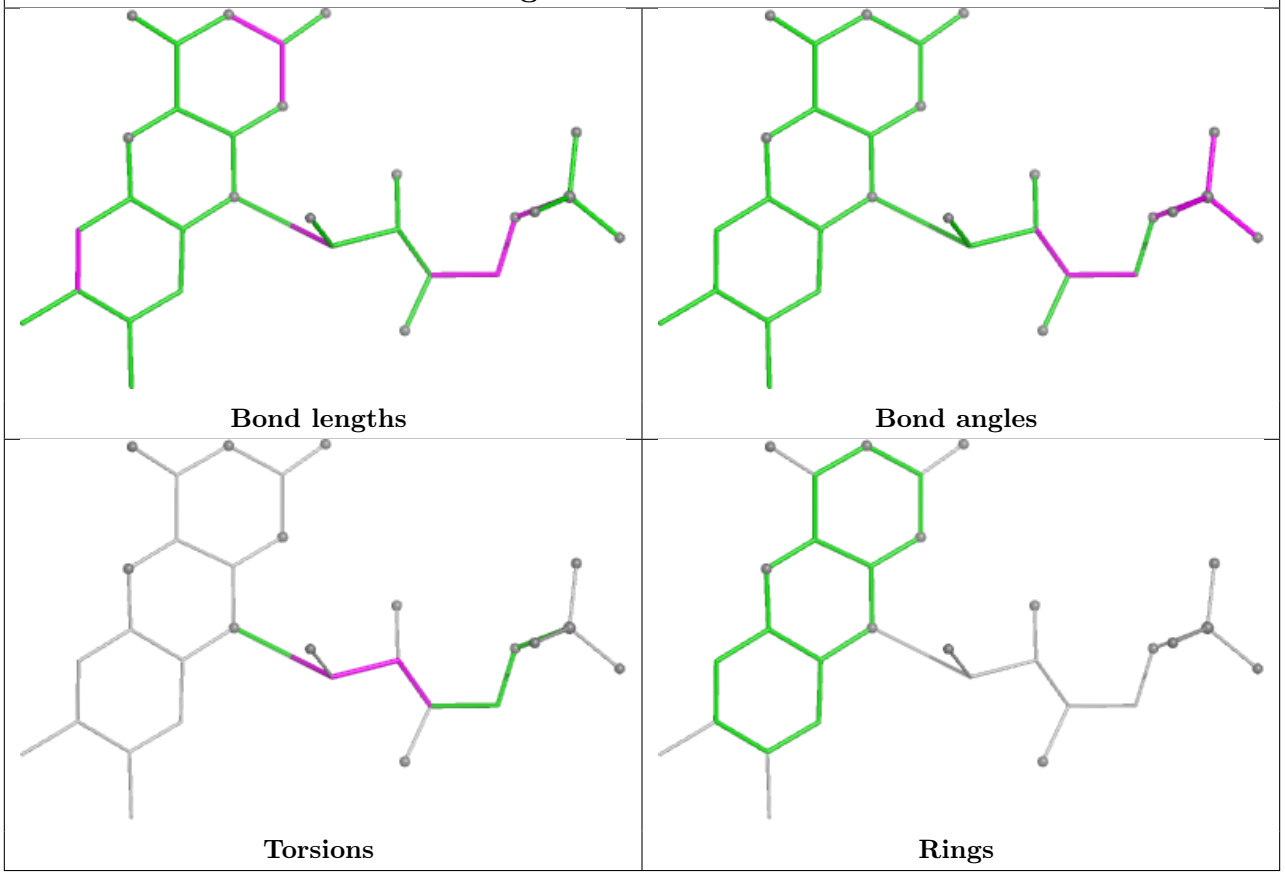
Ligand LMT D 402



Ligand LMT D 405



Ligand FMN C 500



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.

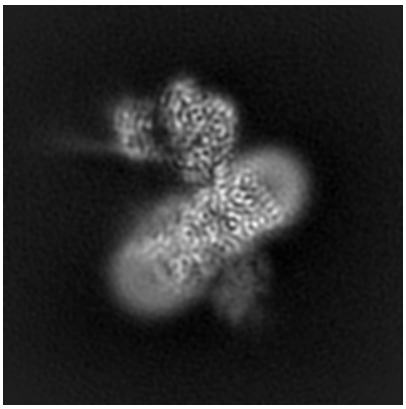
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19034. These allow visual inspection of the internal detail of the map and identification of artifacts.

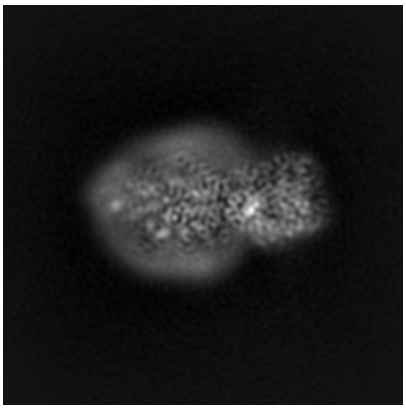
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

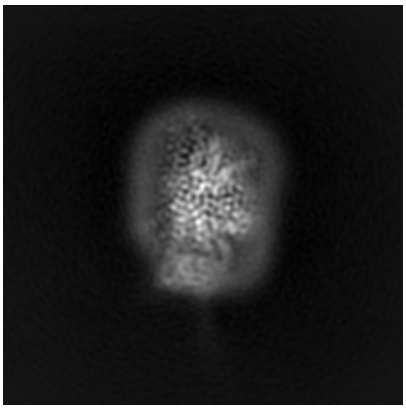
6.1.1 Primary map



X

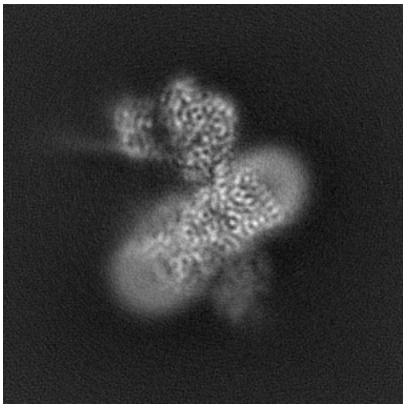


Y

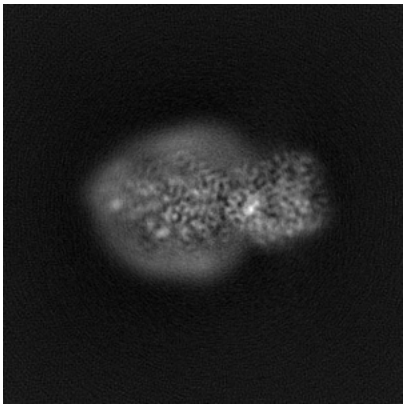


Z

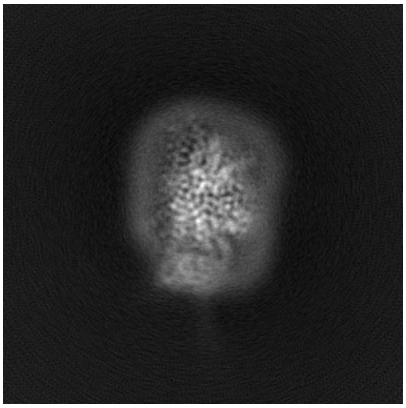
6.1.2 Raw map



X



Y

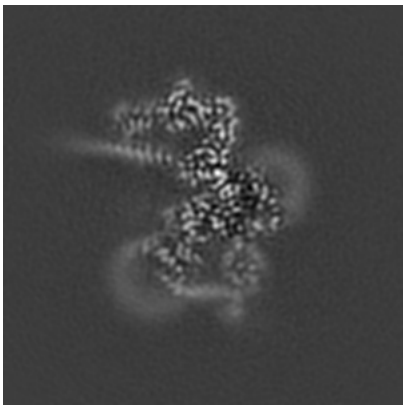


Z

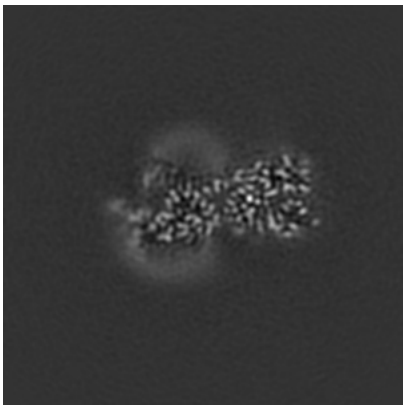
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

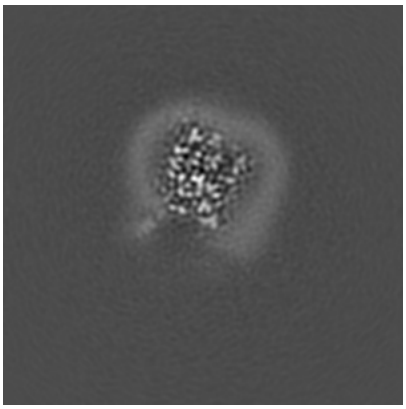
6.2.1 Primary map



X Index: 140

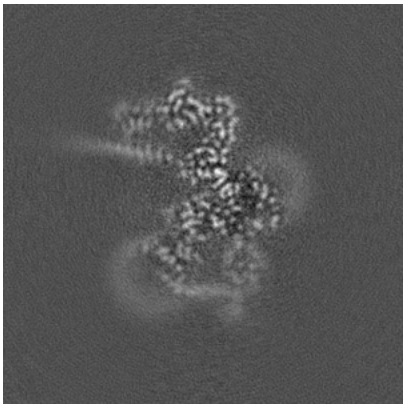


Y Index: 140

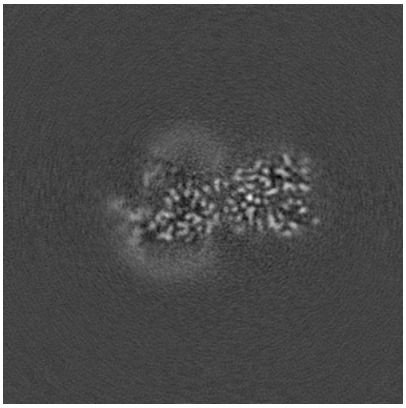


Z Index: 140

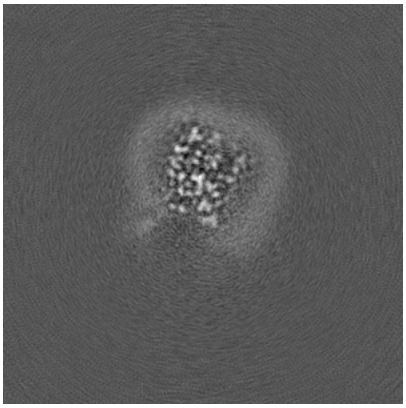
6.2.2 Raw map



X Index: 140



Y Index: 140

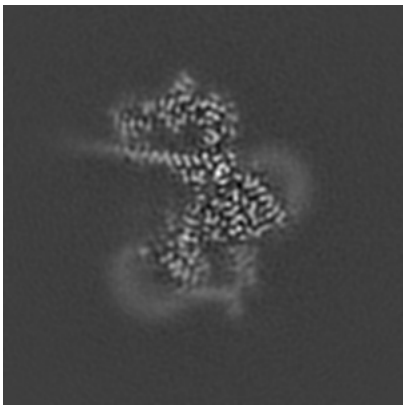


Z Index: 140

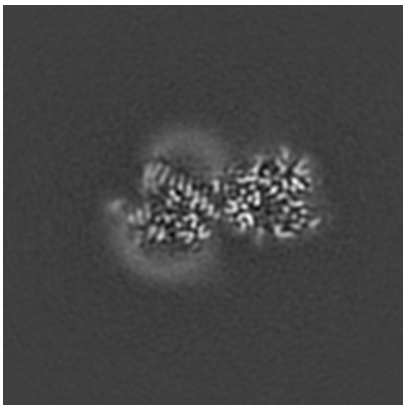
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

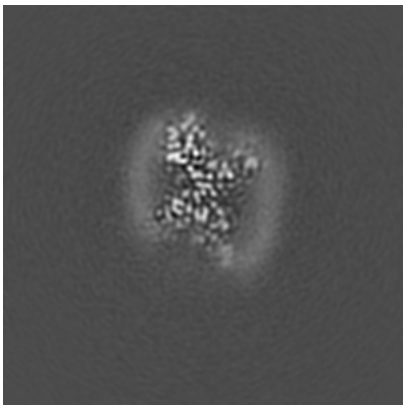
6.3.1 Primary map



X Index: 136

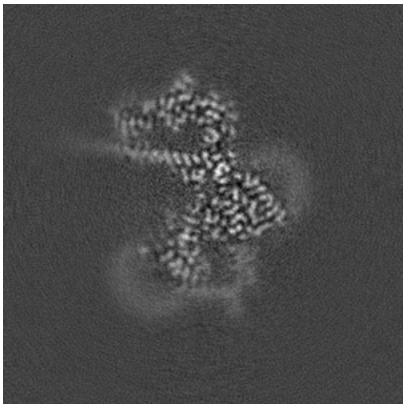


Y Index: 138

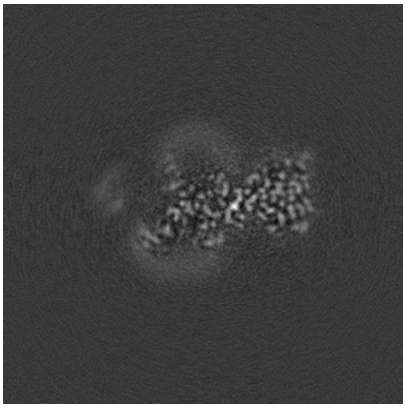


Z Index: 127

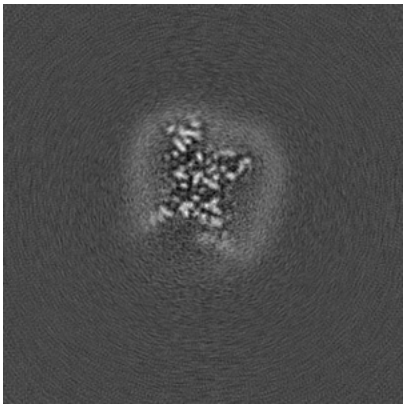
6.3.2 Raw map



X Index: 136



Y Index: 149

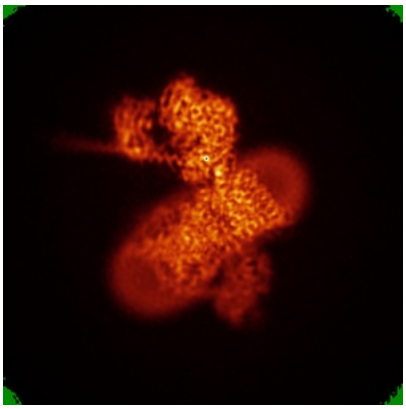


Z Index: 134

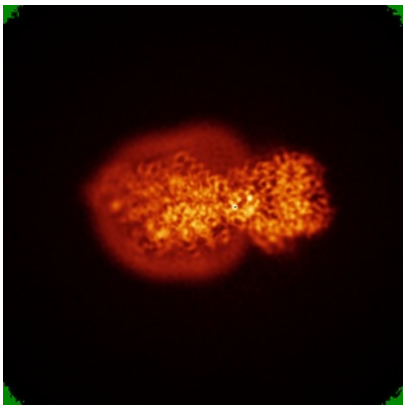
The images above show the largest variance slices of the map in three orthogonal directions.

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

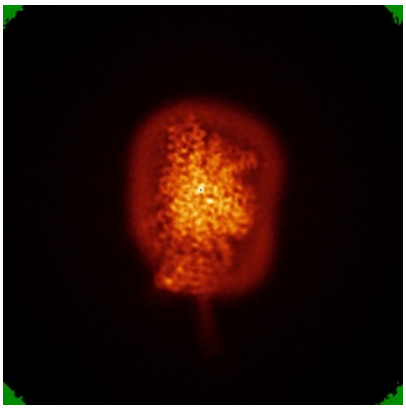
6.4.1 Primary map



X

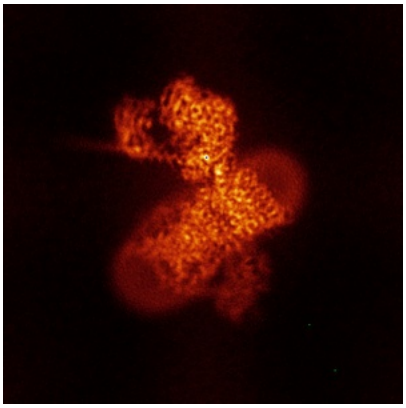


Y



Z

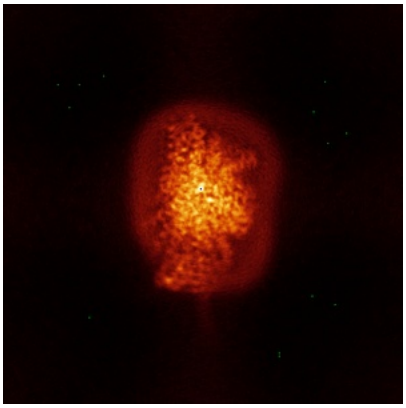
6.4.2 Raw map



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 0.07. 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.

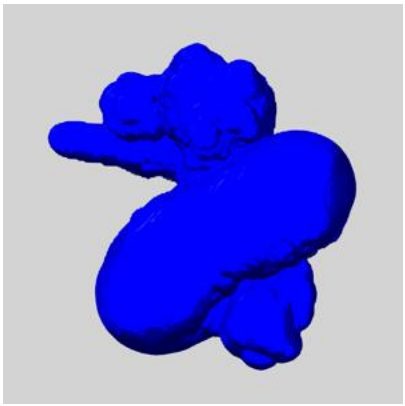
6.6 Mask visualisation (i)

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

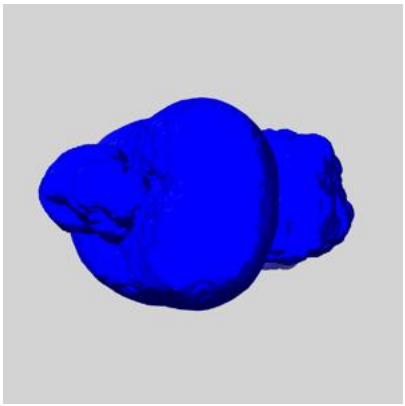
A mask typically either:

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

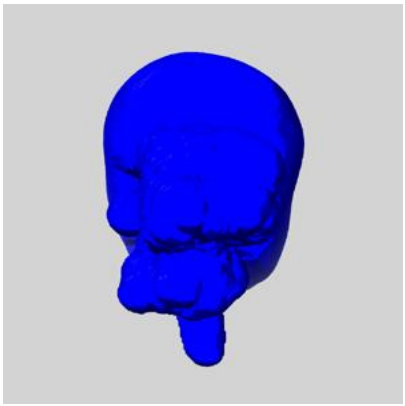
6.6.1 emd_19034_msk_1.map (i)



X



Y

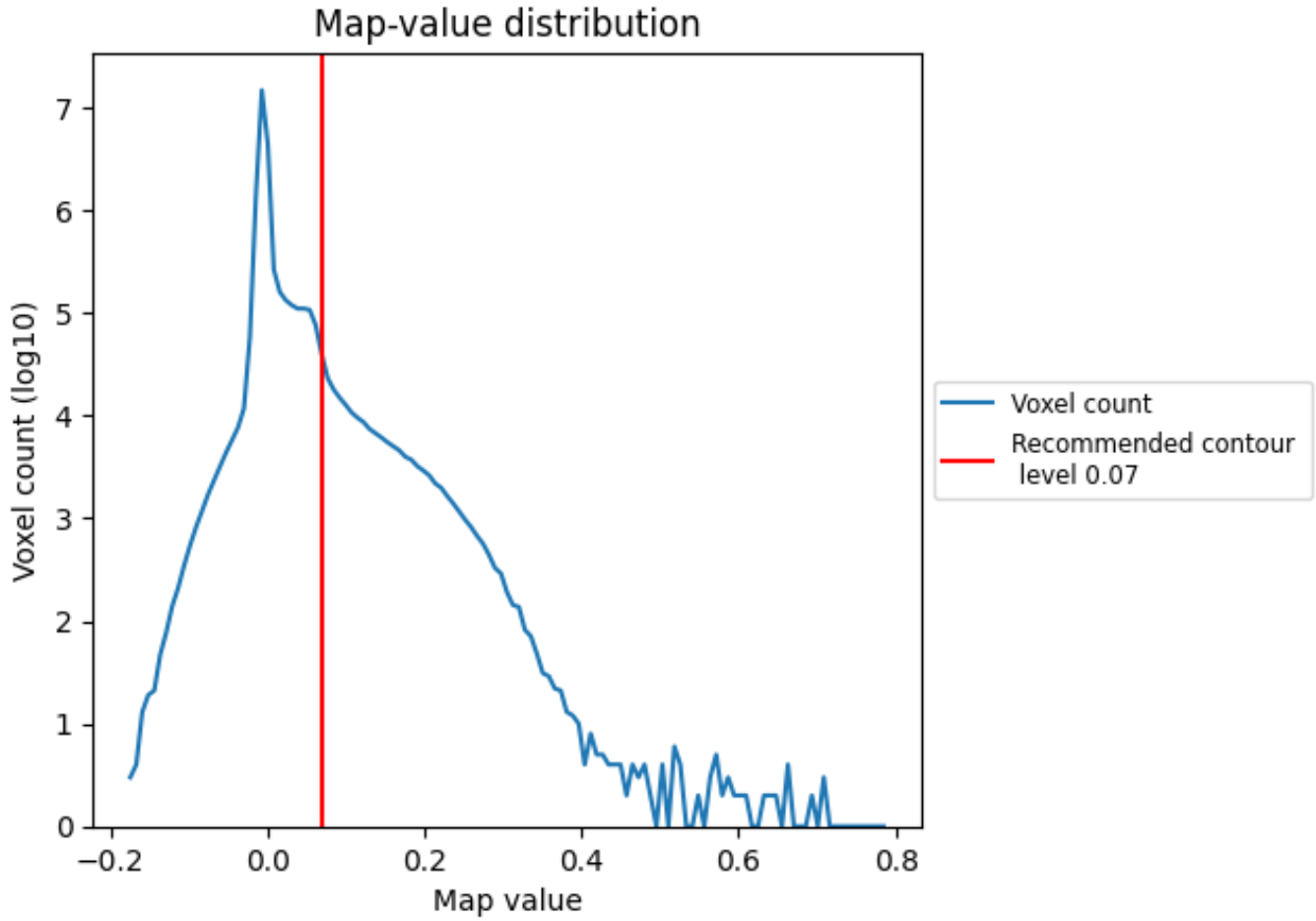


Z

7 Map analysis

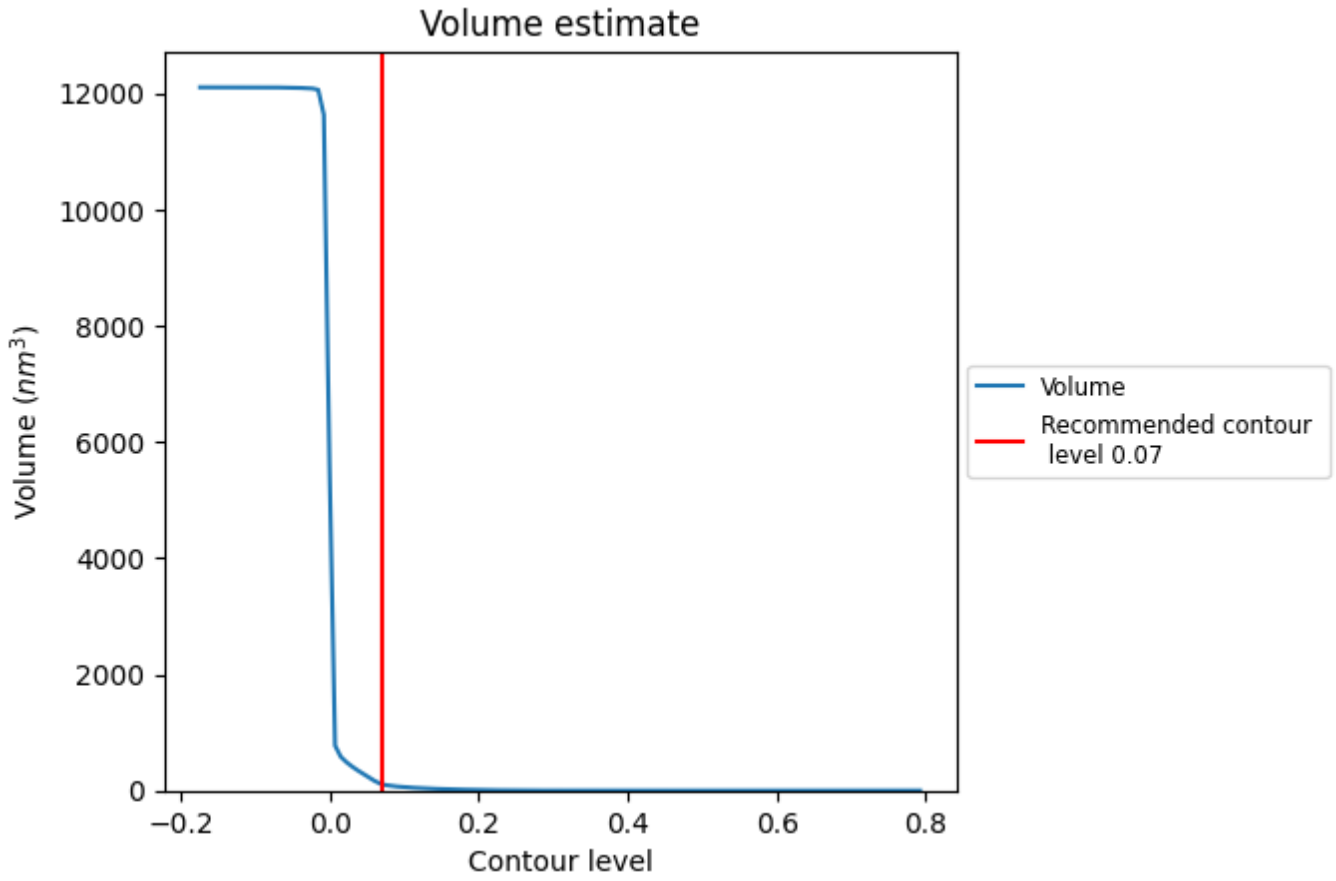
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

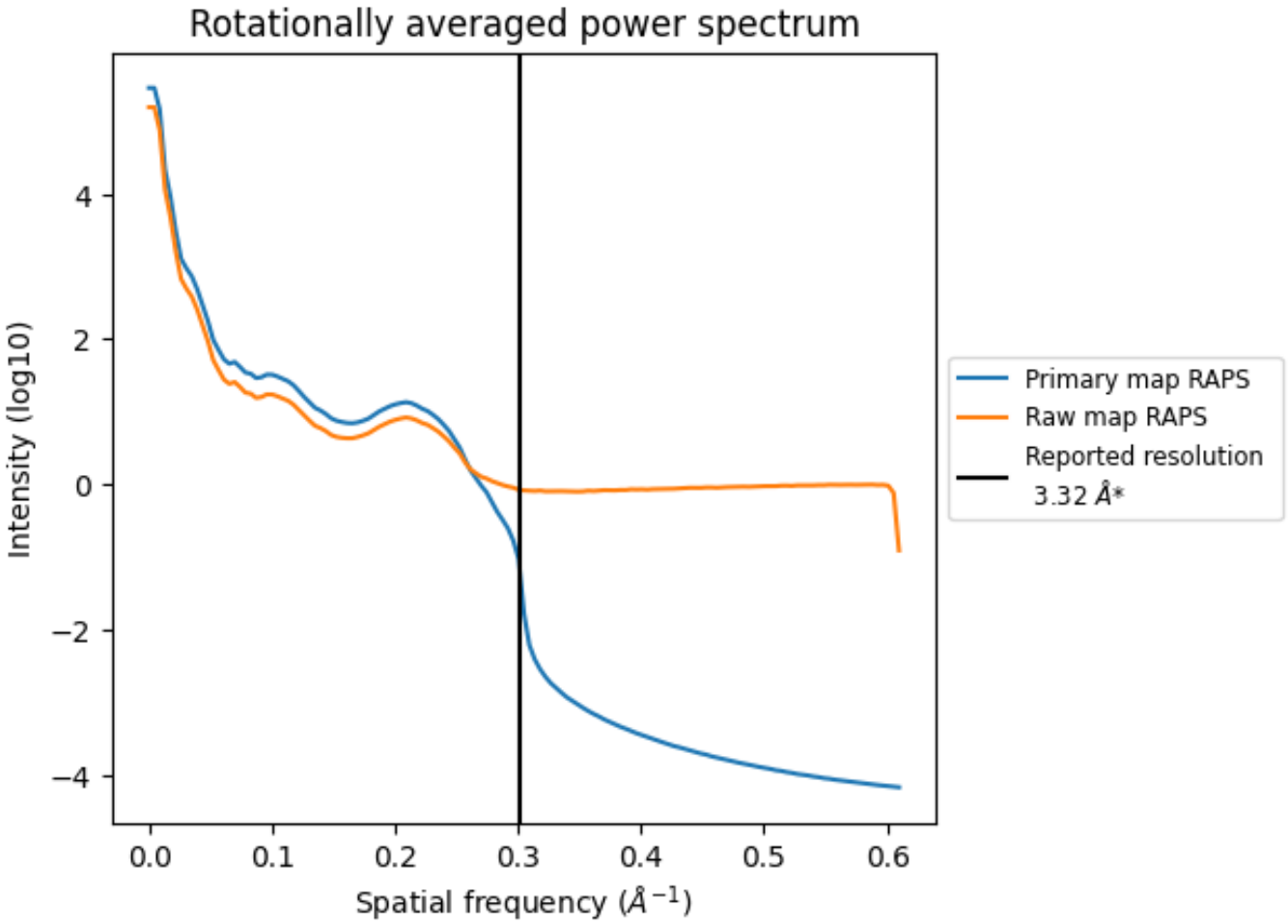
7.2 Volume estimate



The volume at the recommended contour level is 111 nm^3; this corresponds to an approximate mass of 101 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)

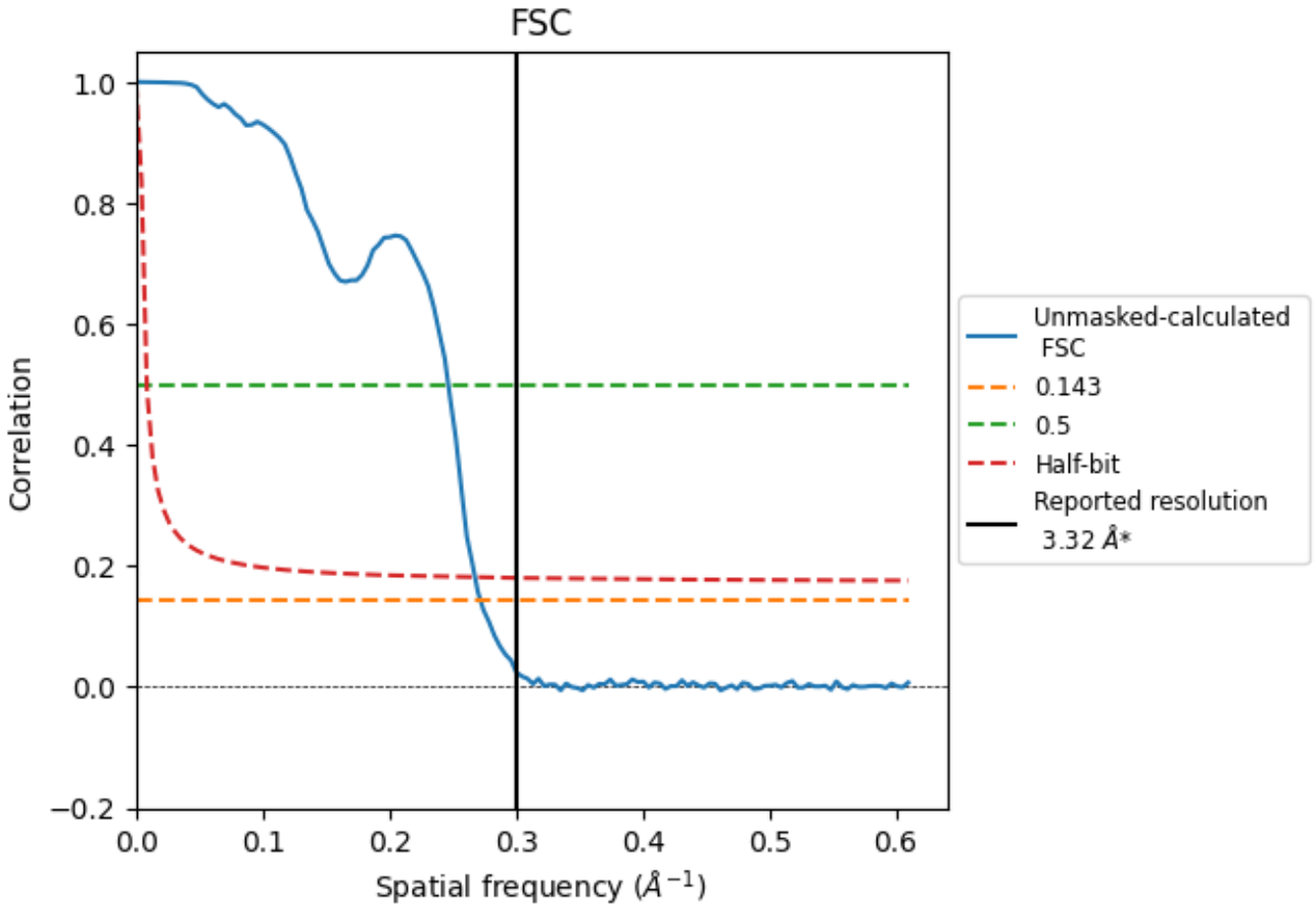


*Reported resolution corresponds to spatial frequency of 0.301 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.301 Å^{-1}

8.2 Resolution estimates (i)

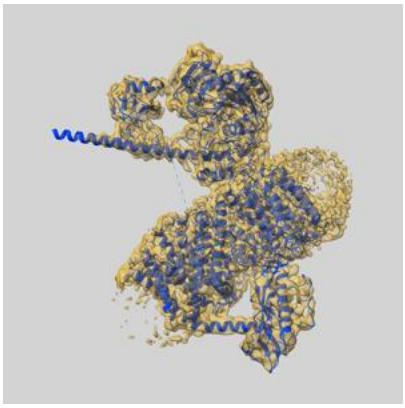
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.32	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.68	4.06	3.73

*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 3.68 differs from the reported value 3.32 by more than 10 %

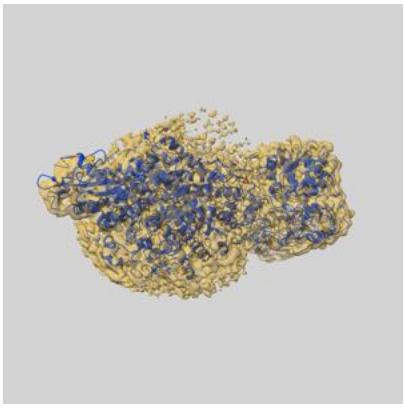
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19034 and PDB model 8RBQ. Per-residue inclusion information can be found in section 3 on page 10.

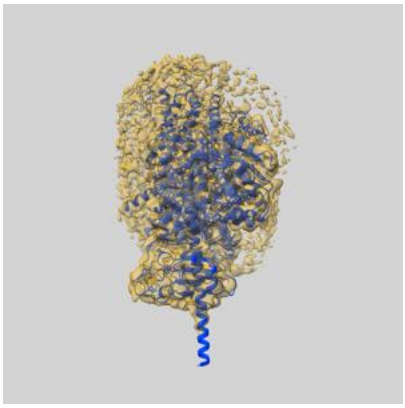
9.1 Map-model overlay



X



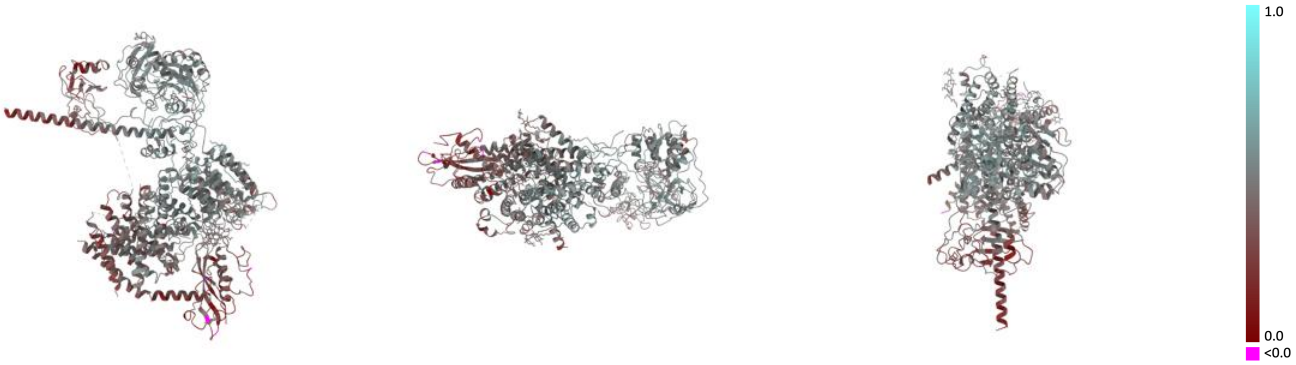
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

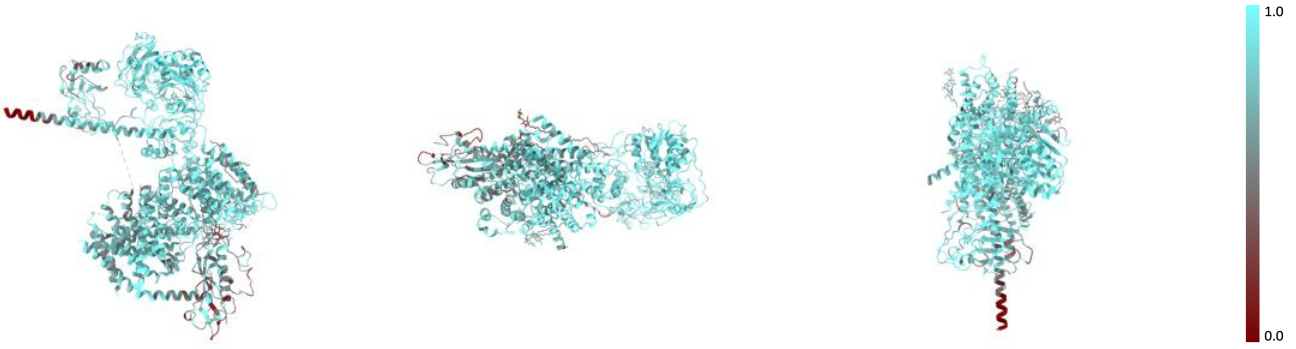
9.2 Q-score mapped to coordinate model



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.

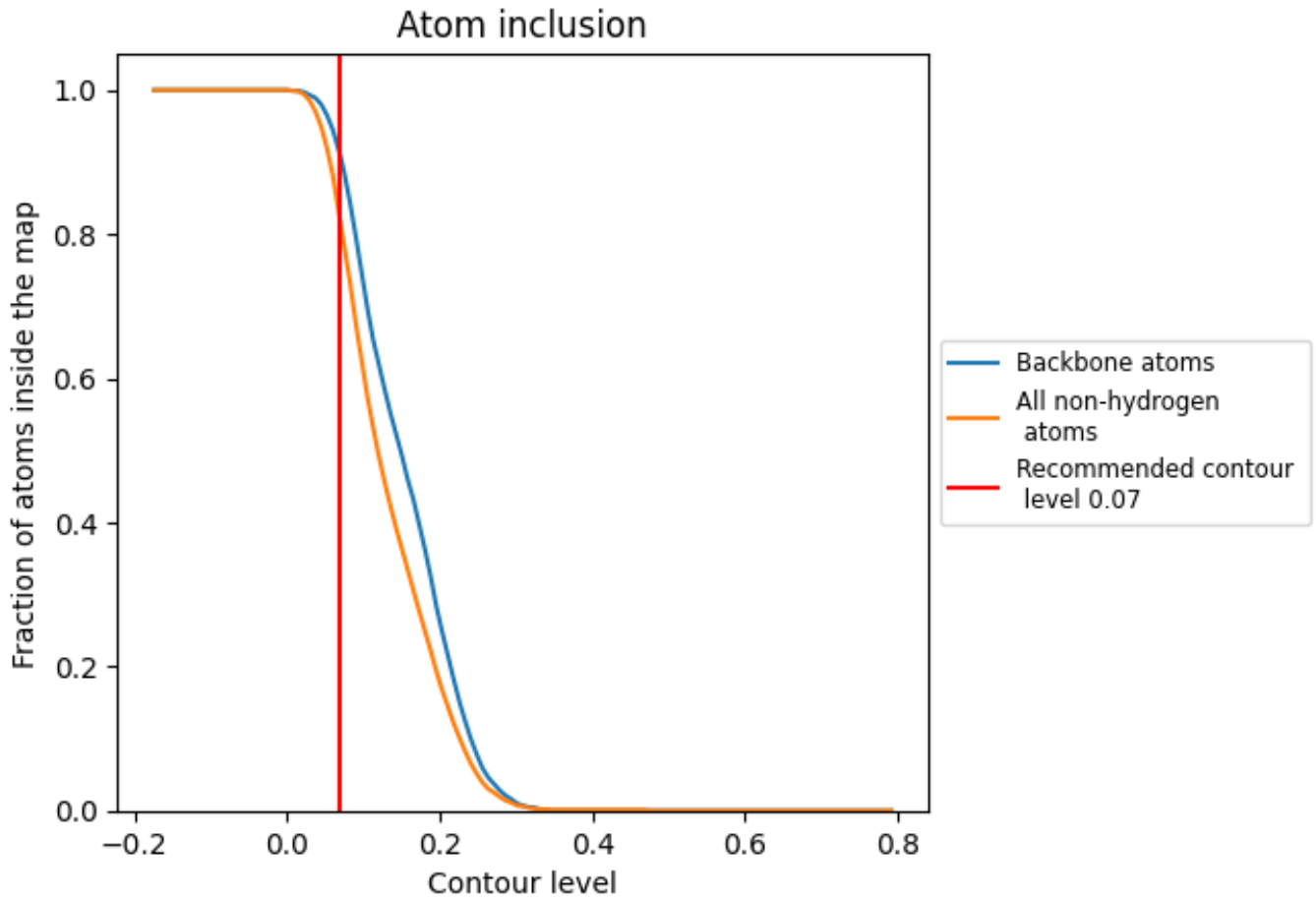
9.3 Atom inclusion mapped to coordinate model



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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 82% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8160	0.4440
A	0.8330	0.4540
B	0.7560	0.3620
C	0.8850	0.4950
D	0.8590	0.5030
E	0.8380	0.4340
G	0.6250	0.3060
H	0.6810	0.3310

