Full wwPDB EM Validation Report

Sep 24, 2026 – 08:20 am BST

PDB ID	:	9SW2 / pdb_00009sw2
EMDB ID	:	EMD-55295
Title	:	Structure of the MvhAGD-HdrABC dimer of M. marburgensis under state 2 substate a (composite structure)
Authors	:	San Segundo-Acosta, P.; Murphy, B.J.
Deposited on	:	2025-10-04
Resolution	:	2.19 Å(reported)
Based on initial model	:	.

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 (1)) were used in the production of this report:

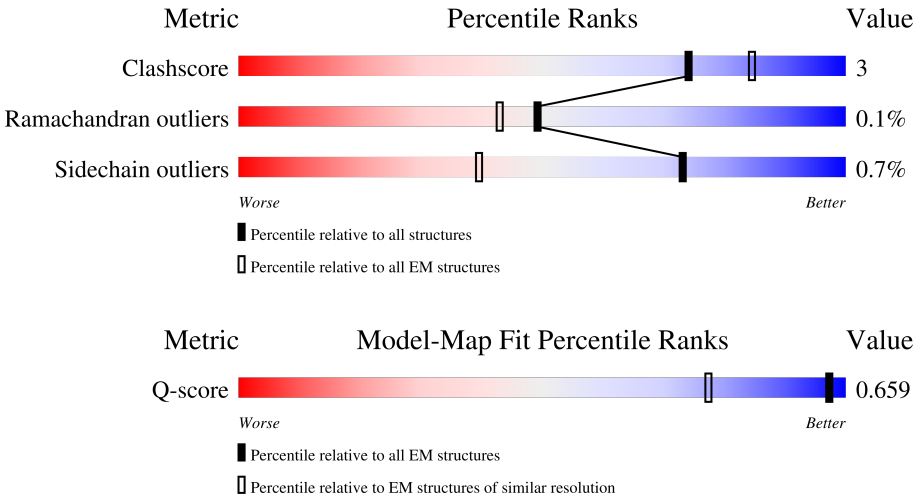
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.19 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.



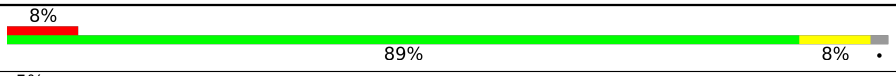
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2745 (1.70 - 2.69)

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	659	93% 5%
2	B	302	12% 85% 11%
3	C	185	10% 96%
4	D	141	85% 11%

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Mol	Chain	Length	Quality of chain
5	E	308	
6	F	472	

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 30994 atoms, of which 15238 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 H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit A.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	647	9830	3114	4890	822	956	48	0	0

- Molecule 2 is a protein called H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit B.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	291	4405	1422	2152	372	437	22	0	0

- Molecule 3 is a protein called H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit C.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	184	2854	893	1432	253	265	11	0	0

- Molecule 4 is a protein called F420-non-reducing hydrogenase iron-sulfur subunit D.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	136	2139	675	1063	198	191	12	0	0

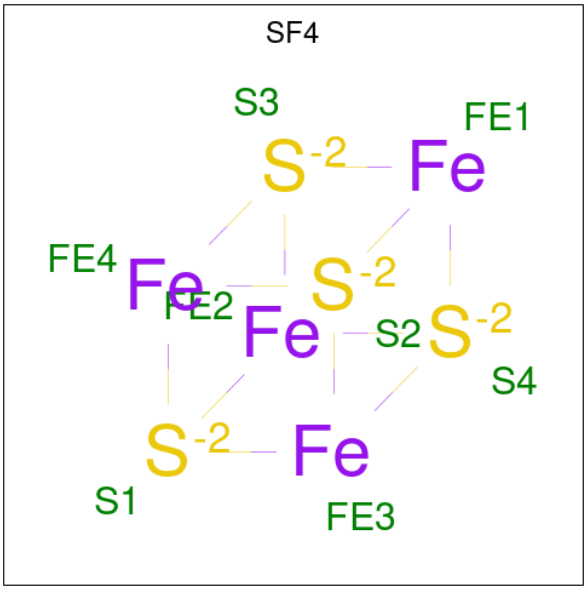
- Molecule 5 is a protein called F420-non-reducing hydrogenase subunit G.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	301	4555	1462	2250	365	458	20	0	0

- Molecule 6 is a protein called F420-non-reducing hydrogenase subunit A.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	444	Total	C	H	N	O	S	0	0
			6916	2222	3419	599	658	18		

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



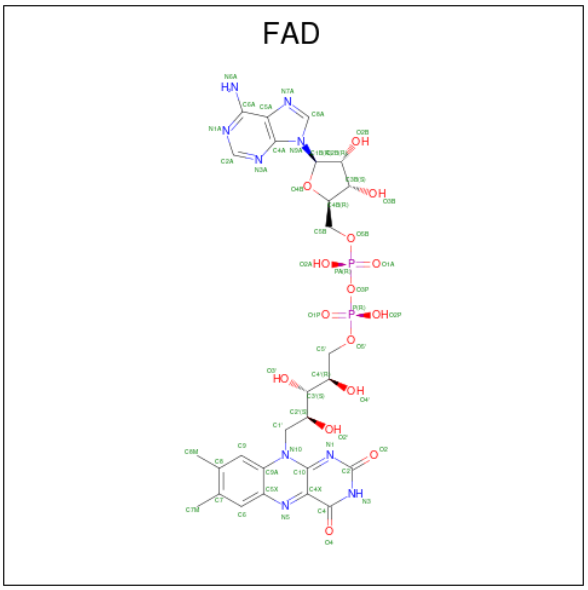
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	Fe	S		0
			8	4	4		
7	A	1	Total	Fe	S		0
			8	4	4		
7	A	1	Total	Fe	S		0
			8	4	4		
7	A	1	Total	Fe	S		0
			8	4	4		
7	A	1	Total	Fe	S		0
			8	4	4		
7	A	1	Total	Fe	S		0
			8	4	4		
7	C	1	Total	Fe	S		0
			8	4	4		
7	C	1	Total	Fe	S		0
			8	4	4		
7	E	1	Total	Fe	S		0
			8	4	4		
7	E	1	Total	Fe	S		0
			8	4	4		

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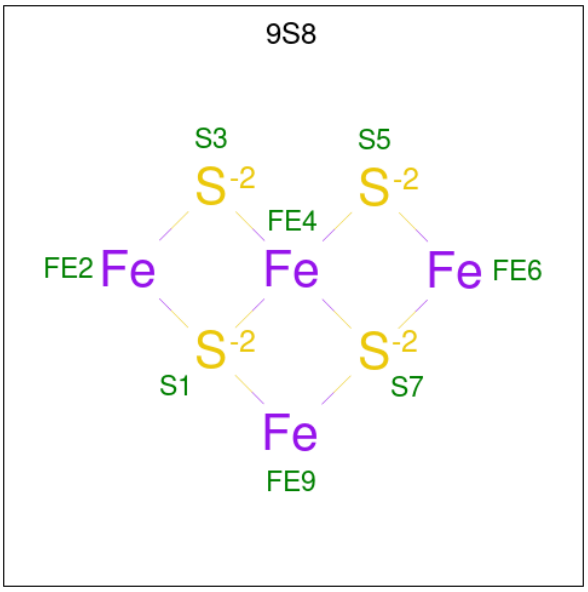
Mol	Chain	Residues	Atoms			AltConf
7	E	1	Total	Fe	S	0
			8	4	4	

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



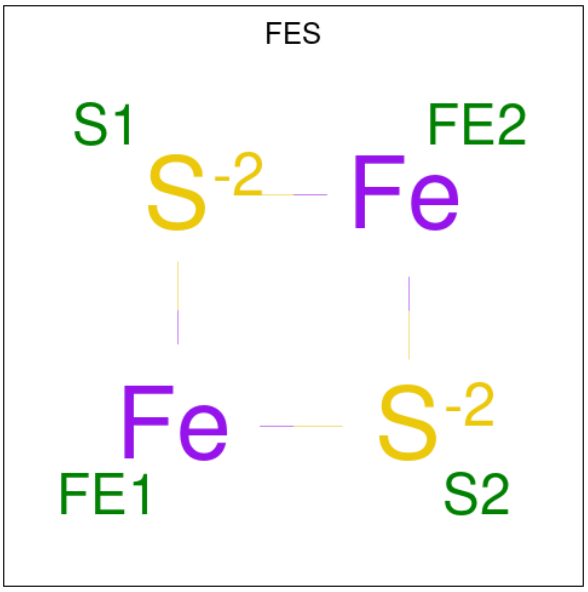
Mol	Chain	Residues	Atoms						AltConf
8	A	1	Total	C	H	N	O	P	0
			84	27	31	9	15	2	

- Molecule 9 is Non-cubane [4Fe-4S]-cluster (CCD ID: 9S8) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



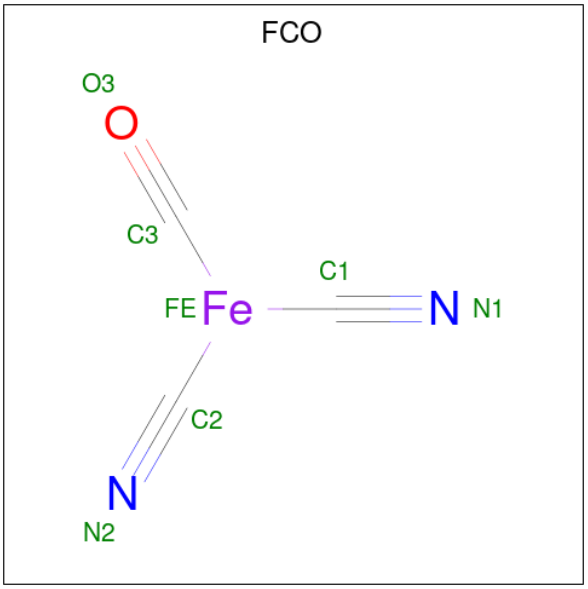
Mol	Chain	Residues	Atoms	AltConf
9	B	1	Total Fe S 8 4 4	0
9	B	1	Total Fe S 8 4 4	0

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 11 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: C_3FeN_2O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
11	F	1	Total	C	Fe	H	N	O	0
			8	3	1	1	2	1	

- Molecule 12 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	F	1	Total	Ni	0
			1	1	

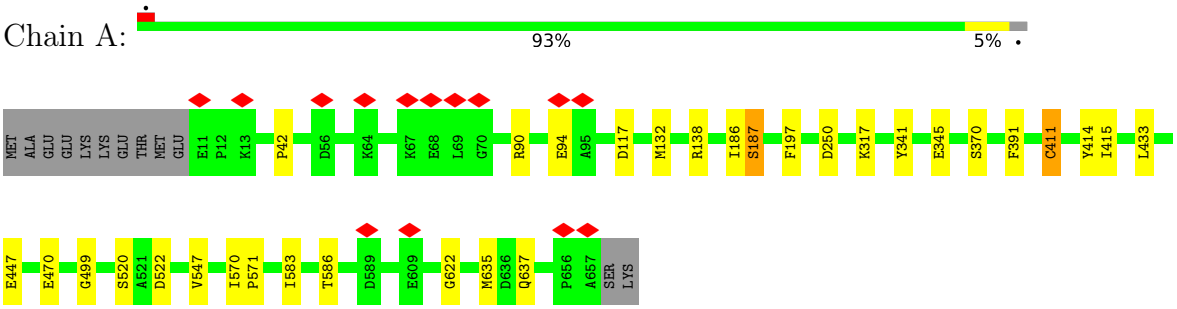
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	A	47	Total	O	0
			47	47	
13	B	8	Total	O	0
			8	8	
13	C	2	Total	O	0
			2	2	
13	D	1	Total	O	0
			1	1	
13	E	16	Total	O	0
			16	16	
13	F	20	Total	O	0
			20	20	

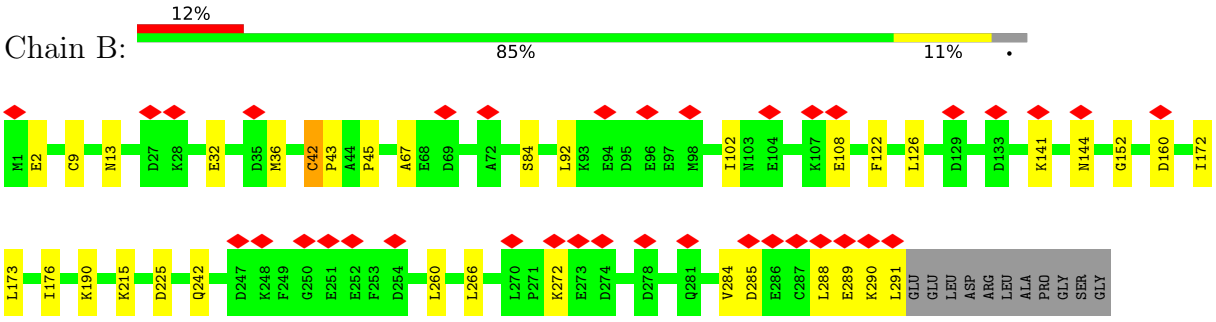
3 Residue-property plots (i)

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.

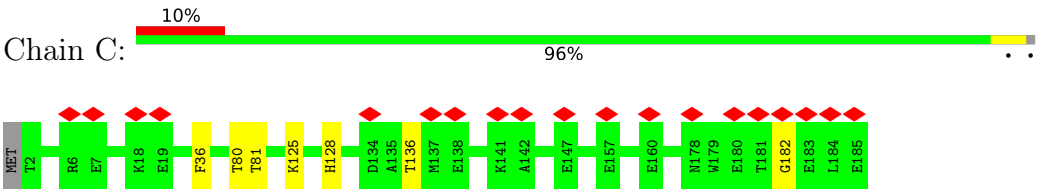
• Molecule 1: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit A



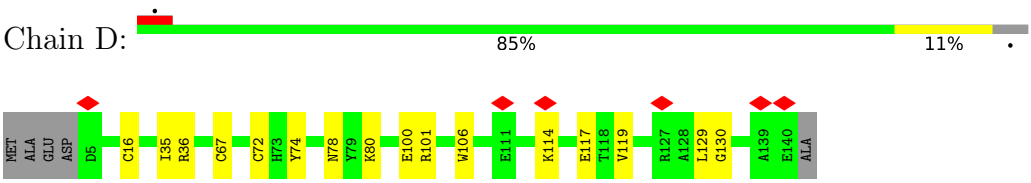
• Molecule 2: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit B



• Molecule 3: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit C

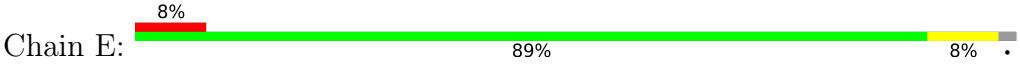


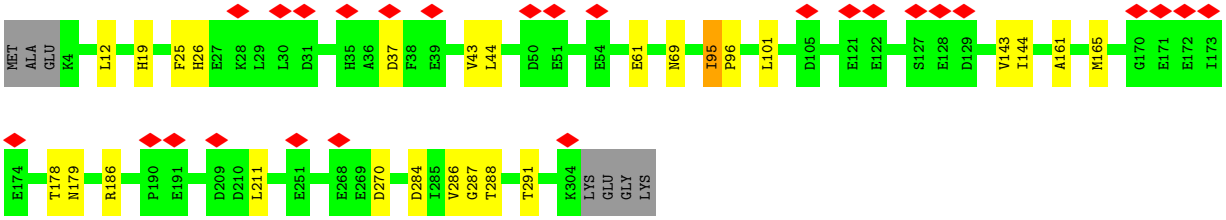
• Molecule 4: F420-non-reducing hydrogenase iron-sulfur subunit D



• Molecule 5: F420-non-reducing hydrogenase subunit G

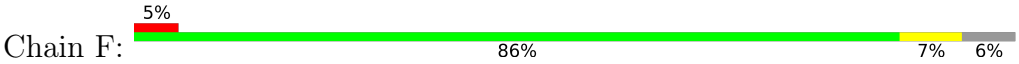
Chain E:

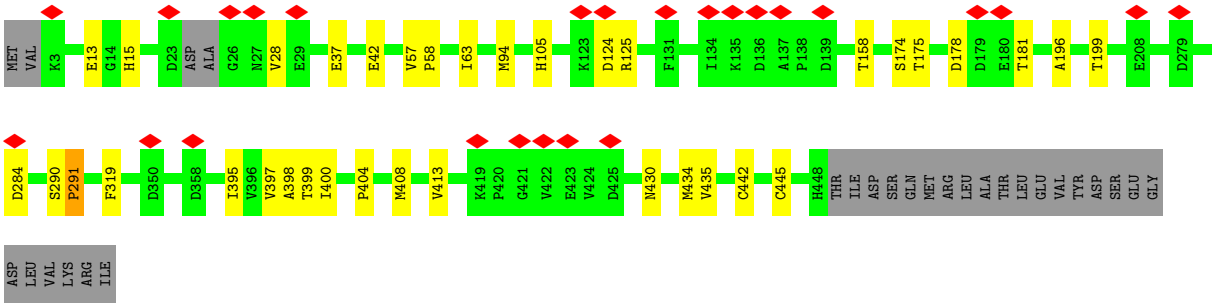




• Molecule 6: F420-non-reducing hydrogenase subunit A

Chain F:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14332	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	46.596	Depositor
Minimum map value	-23.251	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.820	Depositor
Recommended contour level	5.47	Depositor
Map size (Å)	401.1, 401.1, 401.1	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835625, 0.835625, 0.835625	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, FES, 9S8, SF4, NI, FCO

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	0.18	0/5030	0.30	0/6808
2	B	0.18	0/2290	0.38	0/3089
3	C	0.14	0/1447	0.24	0/1951
4	D	0.15	0/1098	0.30	0/1474
5	E	0.13	0/2352	0.29	0/3195
6	F	0.19	1/3576 (0.0%)	0.35	0/4849
All	All	0.17	1/15793 (0.0%)	0.32	0/21366

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	291	PRO	C-O	-5.08	1.17	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4940	4890	4895	25	0
2	B	2253	2152	2217	22	0
3	C	1422	1432	1431	4	0
4	D	1076	1063	1062	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	2305	2250	2258	16	0
6	F	3497	3419	3434	22	0
7	A	48	0	0	0	0
7	C	16	0	0	0	0
7	E	24	0	0	0	0
8	A	53	31	31	5	0
9	B	16	0	0	0	0
10	D	4	0	0	0	0
11	F	7	1	0	1	0
12	F	1	0	0	0	0
13	A	47	0	0	1	0
13	B	8	0	0	1	0
13	C	2	0	0	0	0
13	D	1	0	0	0	0
13	E	16	0	0	1	0
13	F	20	0	0	2	0
All	All	15756	15238	15328	98	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (98) 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:D:72:CYS:SG	4:D:74:TYR:O	2.38	0.81
1:A:520:SER:OG	1:A:522:ASP:OD1	2.04	0.75
1:A:470:GLU:OE2	13:A:801:HOH:O	2.03	0.75
2:B:108:GLU:N	2:B:108:GLU:OE1	2.18	0.75
4:D:106:TRP:O	4:D:114:LYS:NZ	2.21	0.74
6:F:290:SER:HB2	6:F:291:PRO:CD	2.19	0.71
6:F:158:THR:O	6:F:175:THR:HG21	1.90	0.71
6:F:290:SER:HB2	6:F:291:PRO:HD3	1.70	0.71
6:F:15:HIS:ND1	6:F:37:GLU:OE1	2.20	0.70
2:B:152:GLY:O	13:B:501:HOH:O	2.09	0.69
2:B:190:LYS:O	2:B:215:LYS:NZ	2.26	0.68
2:B:2:GLU:OE1	2:B:2:GLU:N	2.26	0.68
5:E:165:MET:HE3	5:E:165:MET:HA	1.74	0.68
6:F:397:VAL:O	6:F:400:ILE:HG22	1.96	0.66
1:A:197:PHE:CE2	8:A:704:FAD:C4	2.78	0.66
5:E:19:HIS:ND1	5:E:61:GLU:OE1	2.30	0.65
6:F:395:ILE:O	13:F:601:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:TYR:OH	1:A:345:GLU:OE2	2.11	0.62
4:D:101:ARG:NH2	4:D:130:GLY:O	2.32	0.62
2:B:160:ASP:O	2:B:160:ASP:OD1	2.18	0.61
2:B:141:LYS:NZ	2:B:266:LEU:O	2.33	0.60
4:D:100:GLU:HG2	4:D:129:LEU:HD21	1.82	0.60
6:F:42:GLU:OE2	13:F:601:HOH:O	2.15	0.60
2:B:285:ASP:O	2:B:289:GLU:HG2	2.04	0.57
6:F:397:VAL:HG11	6:F:445:CYS:HB3	1.85	0.57
1:A:42:PRO:O	1:A:138:ARG:NH1	2.38	0.56
2:B:225:ASP:OD2	2:B:290:LYS:NZ	2.38	0.56
6:F:178:ASP:OD1	6:F:181:THR:OG1	2.20	0.55
6:F:94:MET:CE	6:F:175:THR:HG23	2.37	0.55
2:B:32:GLU:OE2	2:B:32:GLU:HA	2.07	0.54
6:F:397:VAL:HG12	6:F:398:ALA:H	1.73	0.54
2:B:36:MET:HE3	2:B:67:ALA:HB2	1.90	0.54
1:A:415:ILE:HD11	1:A:499:GLY:HA3	1.89	0.54
1:A:132:MET:HE1	4:D:36:ARG:HB3	1.88	0.54
5:E:37:ASP:OD1	5:E:37:ASP:N	2.39	0.53
2:B:45:PRO:HD3	2:B:84:SER:OG	2.08	0.53
5:E:143:VAL:HG12	5:E:144:ILE:HG23	1.90	0.53
6:F:430:ASN:O	6:F:434:MET:HG3	2.09	0.53
5:E:178:THR:HG22	5:E:179:ASN:N	2.25	0.52
6:F:290:SER:CB	6:F:291:PRO:CD	2.86	0.52
6:F:284:ASP:OD1	6:F:284:ASP:C	2.54	0.51
5:E:43:VAL:HG13	5:E:44:LEU:HG	1.92	0.50
5:E:101:LEU:HD21	5:E:286:VAL:HG11	1.93	0.50
1:A:586:THR:OG1	1:A:635:MET:SD	2.66	0.49
5:E:69:ASN:ND2	13:E:501:HOH:O	2.39	0.49
1:A:583:ILE:HD12	1:A:583:ILE:O	2.13	0.48
5:E:186:ARG:NH1	5:E:211:LEU:O	2.44	0.48
1:A:197:PHE:CD2	8:A:704:FAD:O4	2.67	0.47
2:B:9:CYS:SG	3:C:128:HIS:ND1	2.82	0.47
1:A:447:GLU:OE1	1:A:447:GLU:N	2.43	0.47
1:A:622:GLY:O	1:A:637:GLN:NE2	2.47	0.47
6:F:13:GLU:HG3	6:F:63:ILE:HD12	1.96	0.47
1:A:370:SER:O	1:A:370:SER:OG	2.24	0.47
2:B:42:CYS:N	2:B:43:PRO:HA	2.30	0.47
1:A:186:ILE:O	1:A:187:SER:CB	2.62	0.47
3:C:80:THR:O	3:C:81:THR:OG1	2.24	0.46
4:D:80:LYS:NZ	5:E:270:ASP:OD2	2.48	0.46
6:F:404:PRO:O	6:F:408:MET:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:O	1:A:94:GLU:HG3	2.15	0.46
1:A:117:ASP:OD1	1:A:117:ASP:N	2.48	0.46
1:A:197:PHE:CD2	8:A:704:FAD:C4	2.99	0.46
2:B:290:LYS:O	2:B:291:LEU:HB2	2.17	0.45
5:E:12:LEU:O	5:E:69:ASN:ND2	2.50	0.45
4:D:16:CYS:HB2	4:D:67:CYS:SG	2.57	0.45
4:D:117:GLU:OE2	4:D:117:GLU:HA	2.18	0.44
4:D:101:ARG:NH1	4:D:129:LEU:HD23	2.32	0.44
1:A:414:TYR:CD1	1:A:414:TYR:C	2.96	0.44
1:A:197:PHE:CE2	8:A:704:FAD:C4X	3.01	0.44
1:A:547:VAL:HG12	1:A:547:VAL:O	2.17	0.44
5:E:95:ILE:N	5:E:96:PRO:CD	2.81	0.44
5:E:287:GLY:O	5:E:291:THR:OG1	2.34	0.43
6:F:57:VAL:N	6:F:58:PRO:CD	2.81	0.43
5:E:161:ALA:O	5:E:165:MET:HG2	2.17	0.43
6:F:445:CYS:CB	11:F:473:FCO:C2	2.96	0.43
1:A:570:ILE:HB	1:A:571:PRO:HD3	2.01	0.43
5:E:25:PHE:O	5:E:26:HIS:C	2.61	0.43
2:B:144:ASN:O	2:B:144:ASN:CG	2.61	0.43
1:A:411:CYS:HA	1:A:414:TYR:CE2	2.54	0.43
1:A:583:ILE:HD12	1:A:583:ILE:C	2.44	0.42
4:D:78:ASN:N	4:D:78:ASN:OD1	2.42	0.42
6:F:124:ASP:OD1	6:F:125:ARG:N	2.52	0.42
1:A:250:ASP:OD2	1:A:317:LYS:NZ	2.47	0.42
2:B:13:ASN:C	3:C:136:THR:HG21	2.44	0.42
3:C:125:LYS:NZ	3:C:182:GLY:O	2.46	0.42
4:D:35:ILE:HG21	4:D:119:VAL:HG13	2.02	0.42
2:B:122:PHE:CZ	2:B:126:LEU:HD11	2.55	0.41
2:B:141:LYS:O	2:B:141:LYS:CG	2.68	0.41
2:B:172:ILE:HG23	2:B:173:LEU:N	2.34	0.41
2:B:272:LYS:HD2	2:B:288:LEU:HD12	2.02	0.41
6:F:413:VAL:HG21	6:F:435:VAL:HG21	2.02	0.41
2:B:92:LEU:HD21	2:B:102:ILE:HG13	2.02	0.41
4:D:100:GLU:CG	4:D:129:LEU:HD21	2.50	0.41
1:A:391:PHE:HB2	1:A:433:LEU:HD22	2.02	0.41
8:A:704:FAD:O2'	8:A:704:FAD:O4'	2.38	0.41
2:B:176:ILE:HG21	2:B:260:LEU:HD21	2.03	0.41
5:E:284:ASP:O	5:E:288:THR:OG1	2.29	0.41
6:F:13:GLU:O	6:F:442:CYS:O	2.40	0.40
6:F:196:ALA:HA	6:F:199:THR:HG22	2.03	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	645/659 (98%)	627 (97%)	17 (3%)	1 (0%)	43 51
2	B	289/302 (96%)	282 (98%)	7 (2%)	0	100 100
3	C	182/185 (98%)	180 (99%)	2 (1%)	0	100 100
4	D	134/141 (95%)	133 (99%)	1 (1%)	0	100 100
5	E	299/308 (97%)	289 (97%)	10 (3%)	0	100 100
6	F	440/472 (93%)	420 (96%)	20 (4%)	0	100 100
All	All	1989/2067 (96%)	1931 (97%)	57 (3%)	1 (0%)	49 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	SER

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	536/547 (98%)	535 (100%)	1 (0%)	87 94
2	B	246/255 (96%)	243 (99%)	3 (1%)	63 78
3	C	153/155 (99%)	152 (99%)	1 (1%)	76 87
4	D	112/115 (97%)	112 (100%)	0	100 100
5	E	257/262 (98%)	256 (100%)	1 (0%)	84 92
6	F	371/396 (94%)	366 (99%)	5 (1%)	61 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1675/1730 (97%)	1664 (99%)	11 (1%)	73 87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	411	CYS
2	B	42	CYS
2	B	242	GLN
2	B	284	VAL
3	C	36	PHE
5	E	95	ILE
6	F	28	VAL
6	F	105	HIS
6	F	174	SER
6	F	319	PHE
6	F	399	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	165	GLN
1	A	237	ASN
1	A	471	ASN
1	A	513	GLN
1	A	612	HIS
2	B	90	HIS
2	B	242	GLN
2	B	281	GLN
4	D	34	ASN
5	E	35	HIS
6	F	21	HIS
6	F	215	ASN
6	F	401	GLN
6	F	430	ASN

5.3.3 RNA

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 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	$\#\|Z\| > 2$
7	SF4	A	702	1	0,12,12	-	-	-		
7	SF4	E	402	5	0,12,12	-	-	-		
7	SF4	A	703	1	0,12,12	-	-	-		
7	SF4	A	701	1	0,12,12	-	-	-		
7	SF4	C	202	3	0,12,12	-	-	-		
7	SF4	E	401	5	0,12,12	-	-	-		
11	FCO	F	473	6	1,6,6	3.65	1 (100%)	-		
7	SF4	A	706	1	0,12,12	-	-	-		
9	9S8	B	401	2	2,10,10	1.14	0	-		
7	SF4	A	707	1	0,12,12	-	-	-		
7	SF4	E	403	5	0,12,12	-	-	-		
9	9S8	B	402	2	2,10,10	1.11	0	-		
7	SF4	C	201	3	0,12,12	-	-	-		
8	FAD	A	704	-	56,58,58	0.62	1 (1%)	81,89,89	0.81	2 (2%)
7	SF4	A	705	1	0,12,12	-	-	-		
10	FES	D	201	4	0,4,4	-	-	-		

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
7	SF4	A	702	1	-	-	0/6/5/5
7	SF4	E	402	5	-	-	0/6/5/5
7	SF4	A	703	1	-	-	0/6/5/5
7	SF4	A	701	1	-	-	0/6/5/5
7	SF4	C	202	3	-	-	0/6/5/5
7	SF4	E	401	5	-	-	0/6/5/5
7	SF4	A	706	1	-	-	0/6/5/5
9	9S8	B	401	2	-	-	0/3/3/3
7	SF4	A	707	1	-	-	0/6/5/5
7	SF4	E	403	5	-	-	0/6/5/5
9	9S8	B	402	2	-	-	0/3/3/3
7	SF4	C	201	3	-	-	0/6/5/5
8	FAD	A	704	-	-	2/34/50/50	0/6/6/6
7	SF4	A	705	1	-	-	0/6/5/5
10	FES	D	201	4	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	473	FCO	O3-C3	3.65	1.21	1.16
8	A	704	FAD	C10-N10	2.05	1.41	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	704	FAD	C9-C9A-N10	2.91	125.77	121.84
8	A	704	FAD	C4-N3-C2	-2.29	121.42	125.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	704	FAD	C2B-C1B-N9A-C8A
8	A	704	FAD	O4B-C4B-C5B-O5B

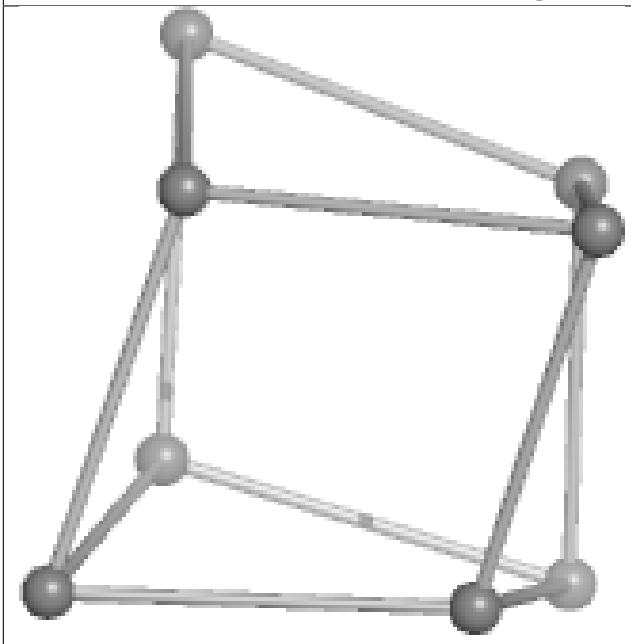
There are no ring outliers.

2 monomers are involved in 6 short contacts:

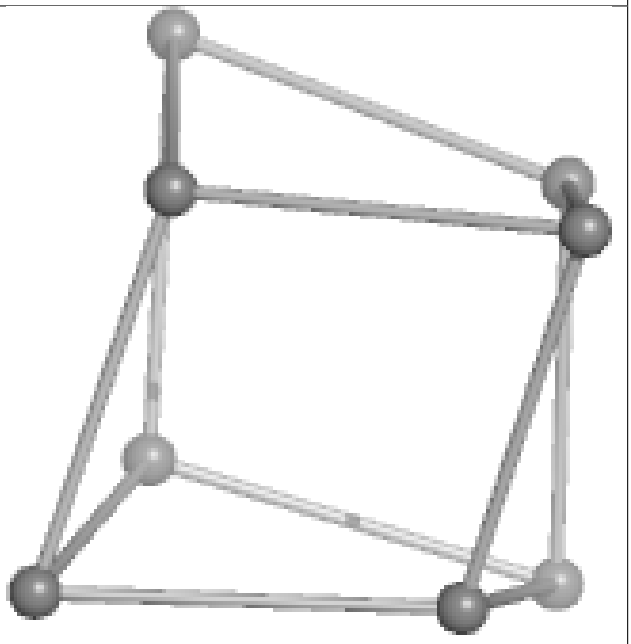
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	473	FCO	1	0
8	A	704	FAD	5	0

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.

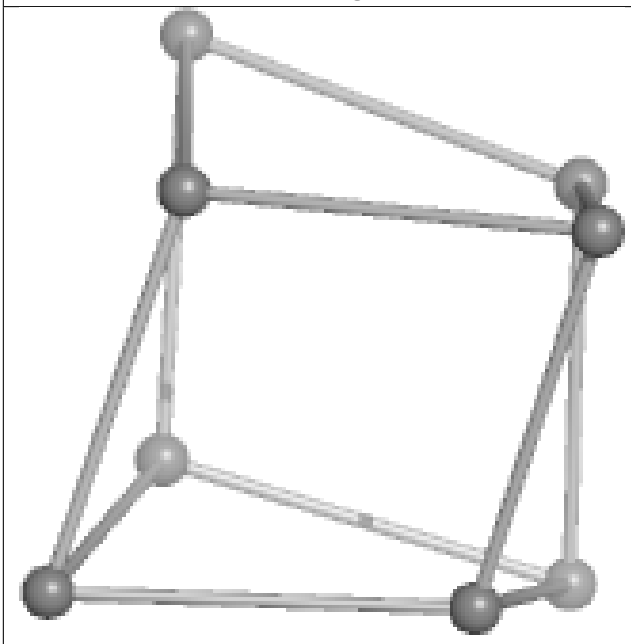
Ligand SF4 A 702



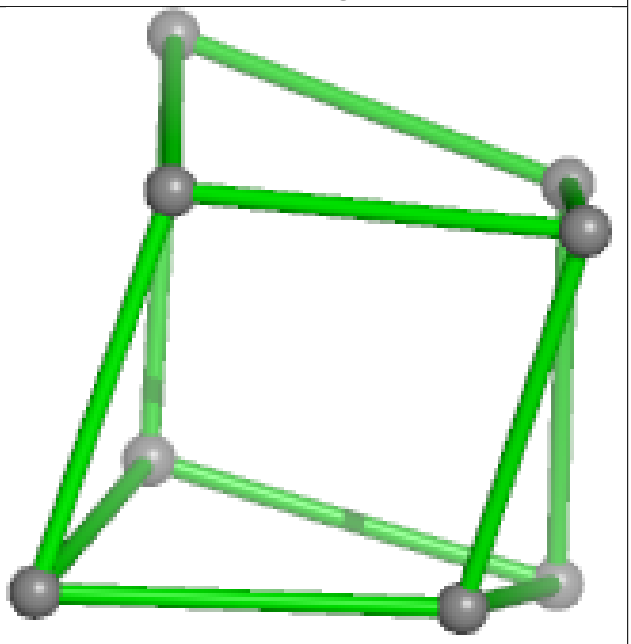
Bond lengths



Bond angles

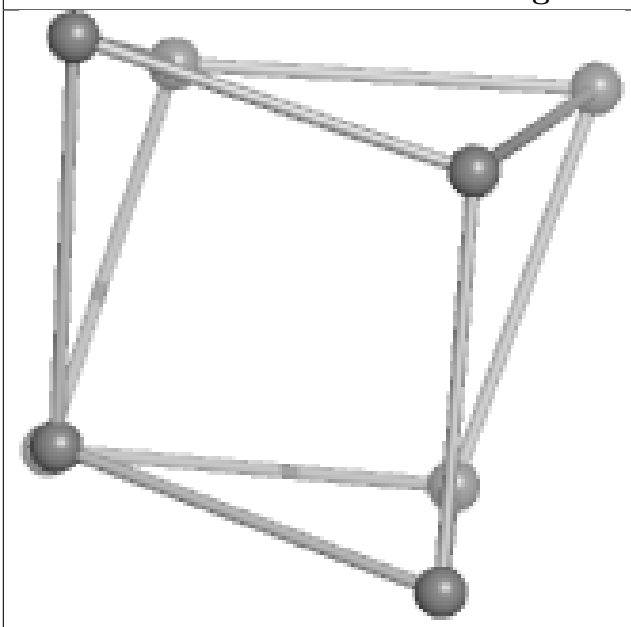


Torsions

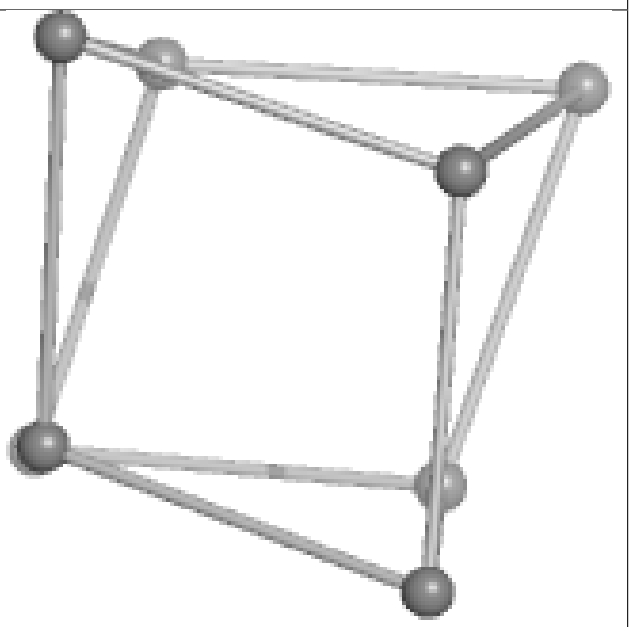


Rings

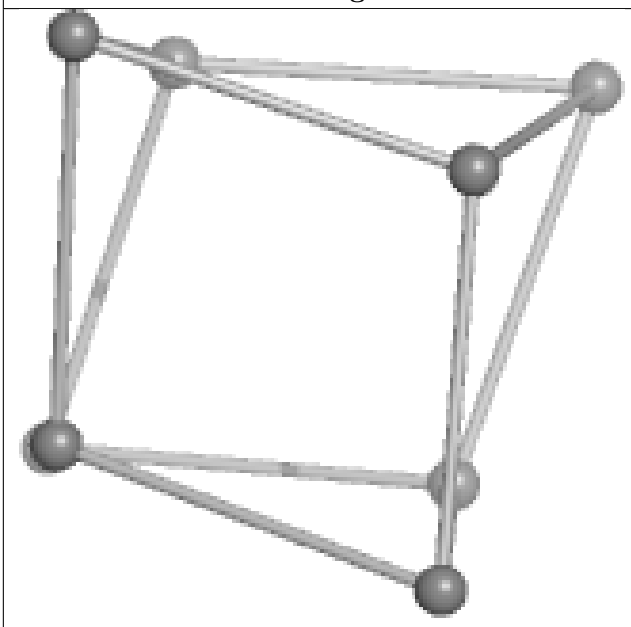
Ligand SF4 E 402



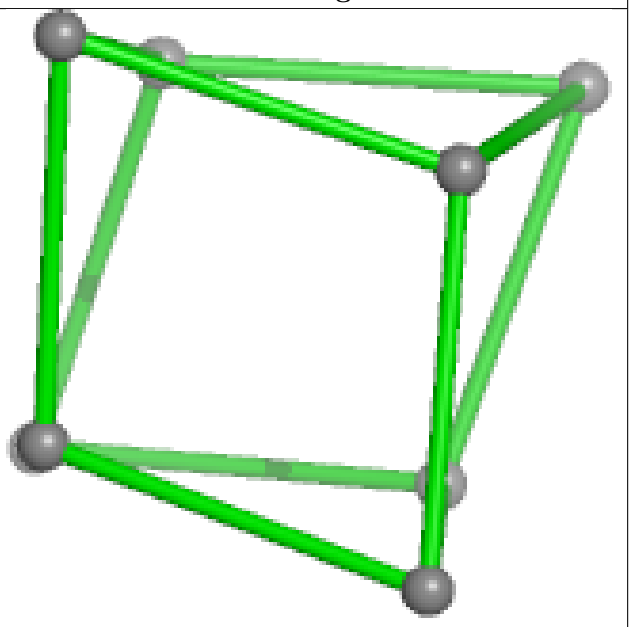
Bond lengths



Bond angles

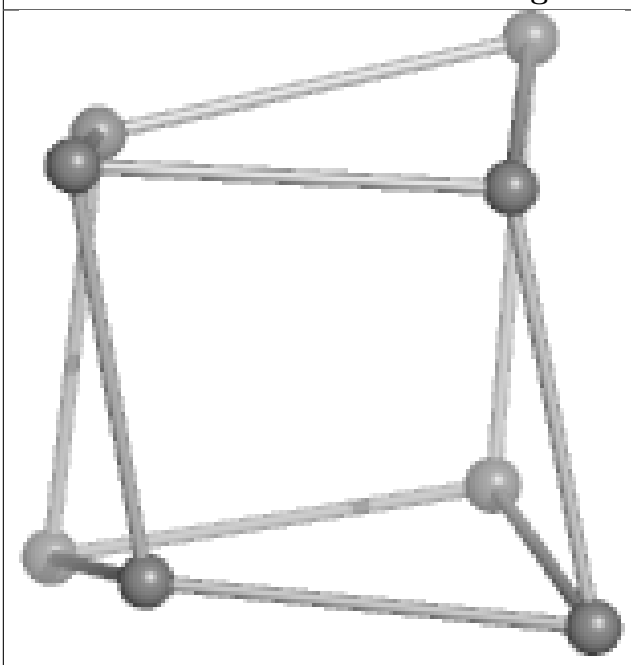


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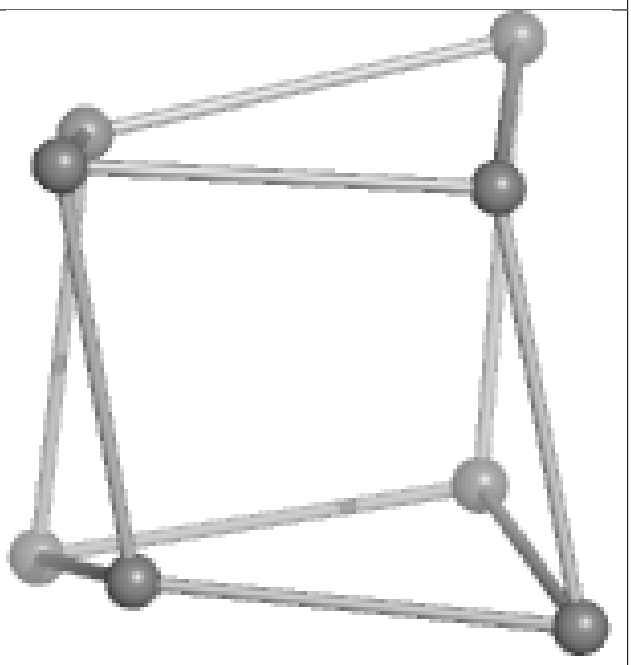


Rings

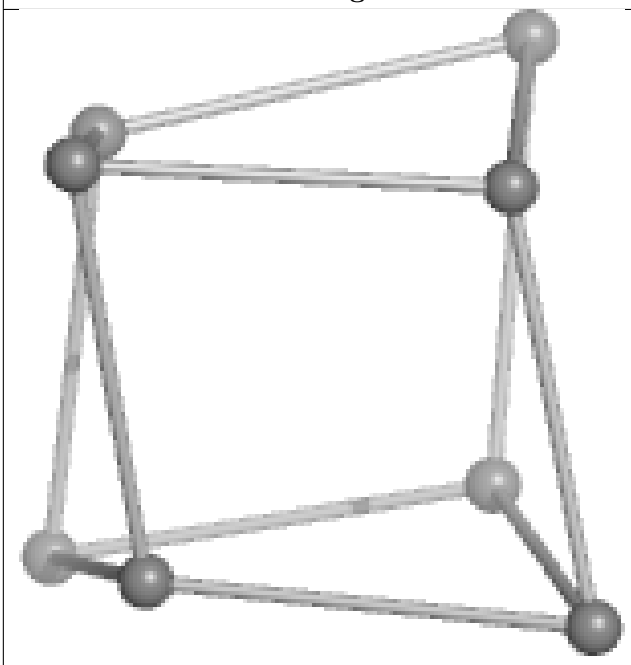
Ligand SF4 A 703



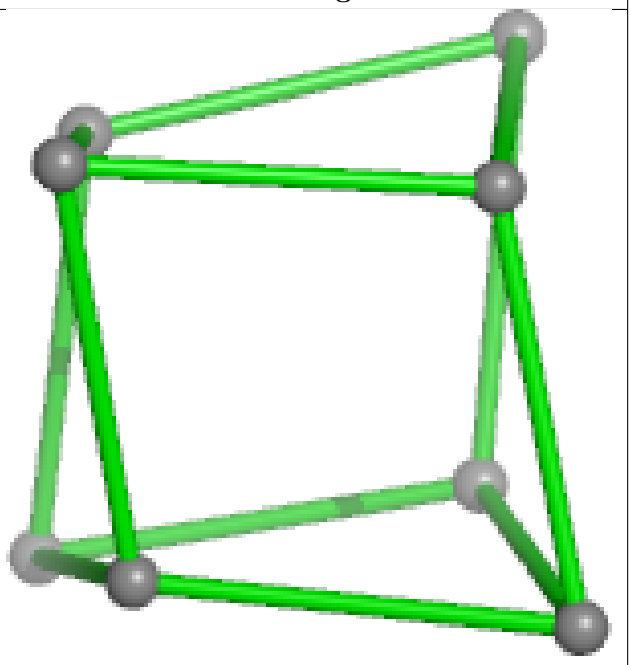
Bond lengths



Bond angles

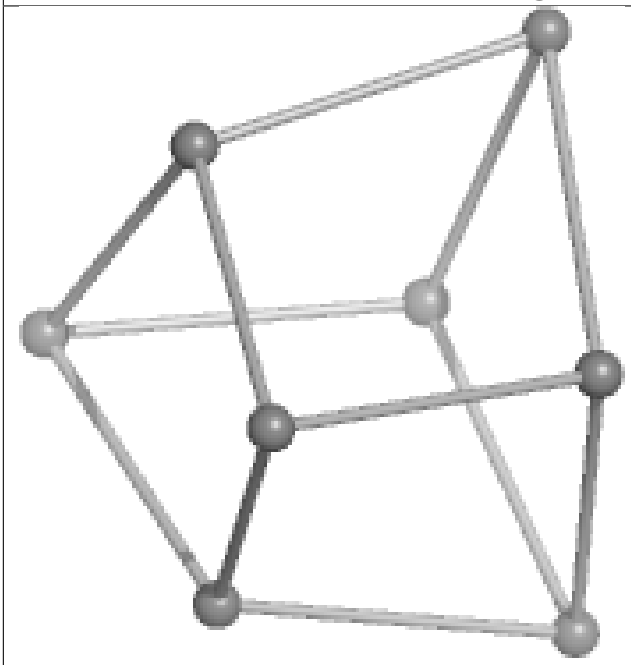


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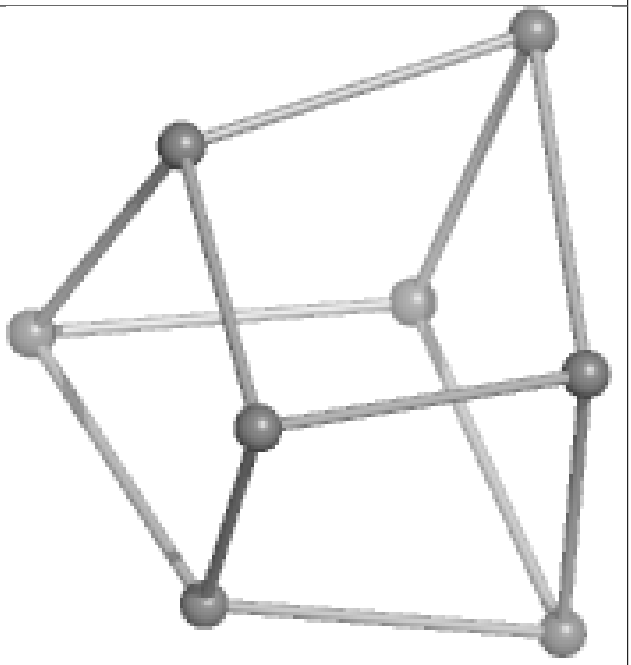


Rings

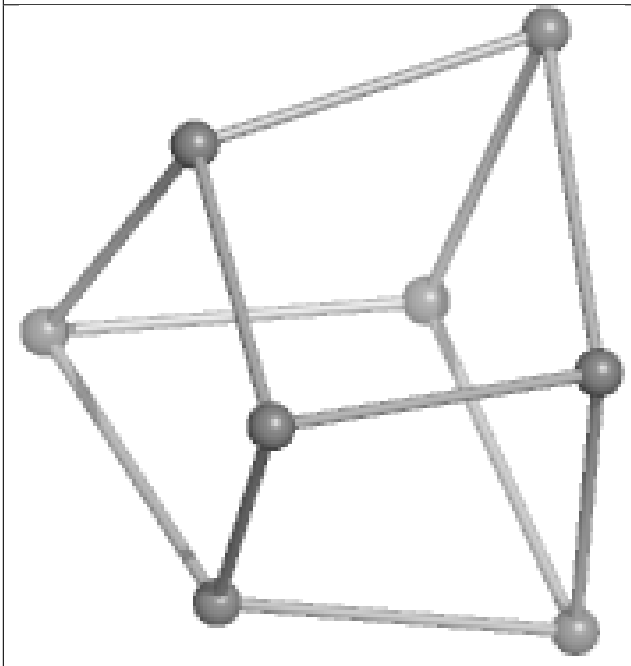
Ligand SF4 A 701



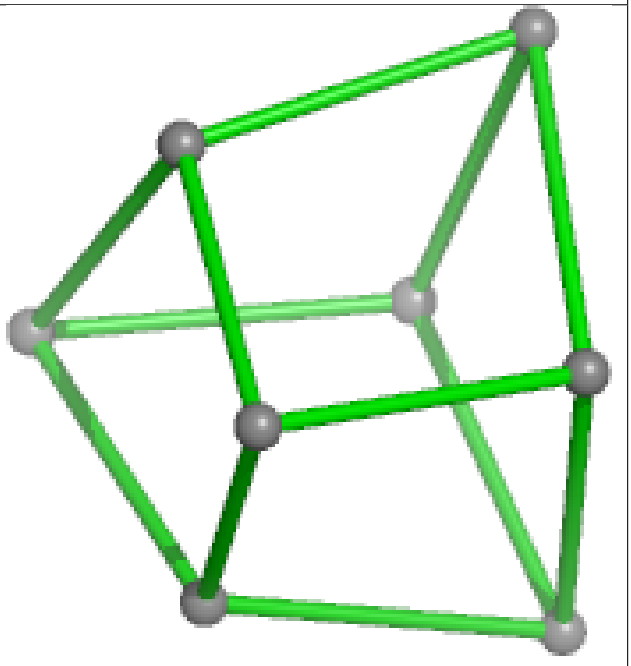
Bond lengths



Bond angles

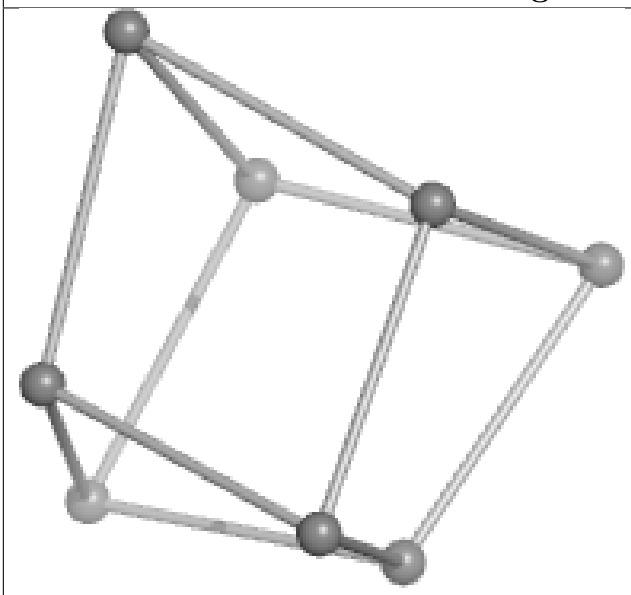


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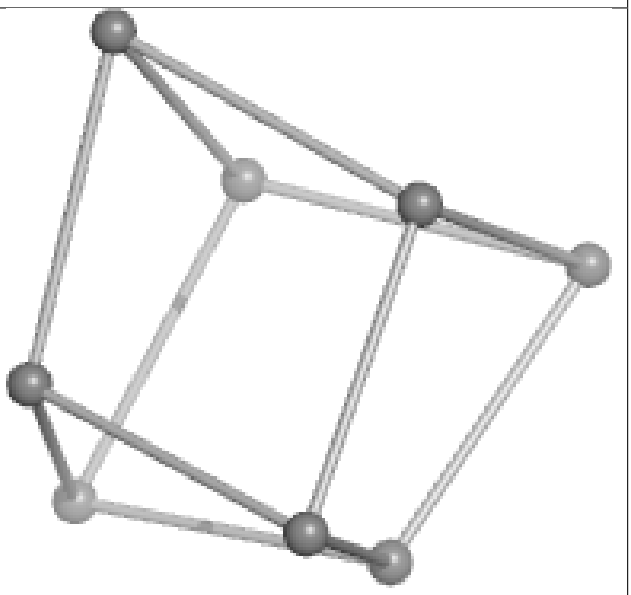


Rings

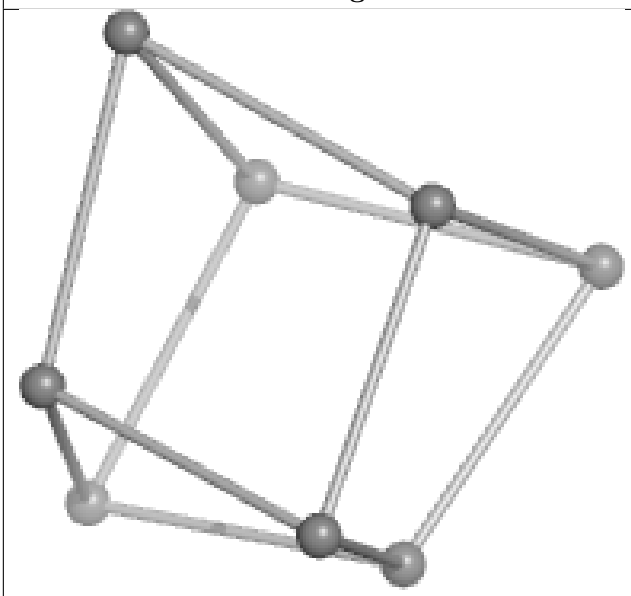
Ligand SF4 C 202



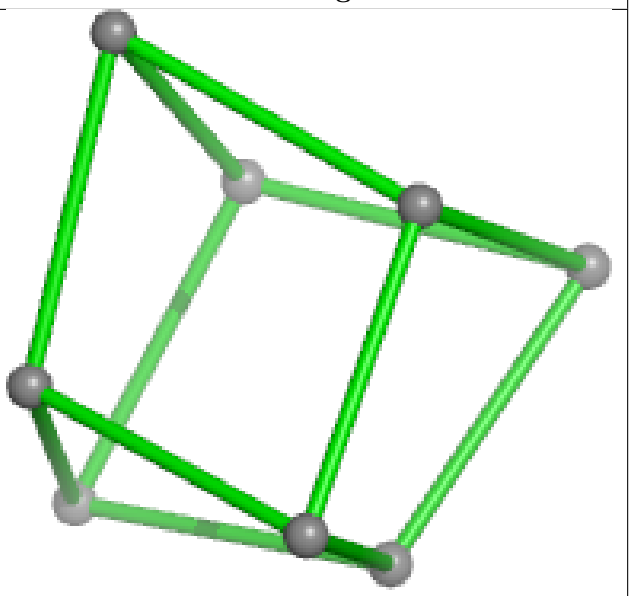
Bond lengths



Bond angles

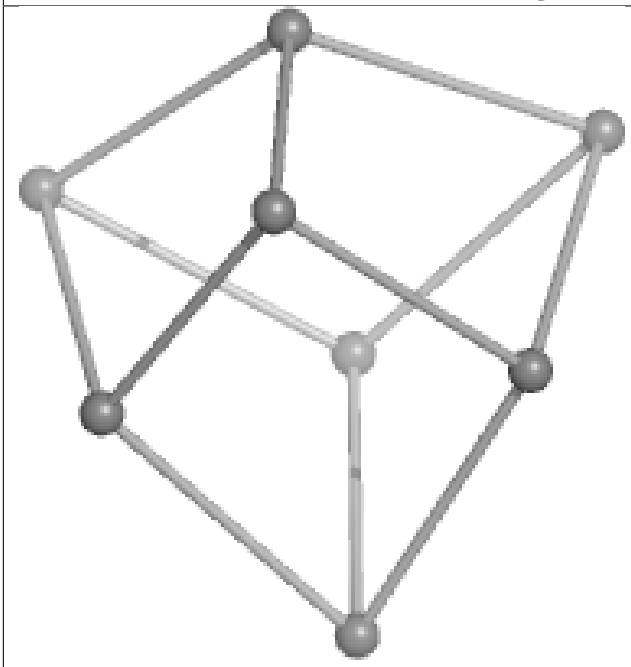


Torsions

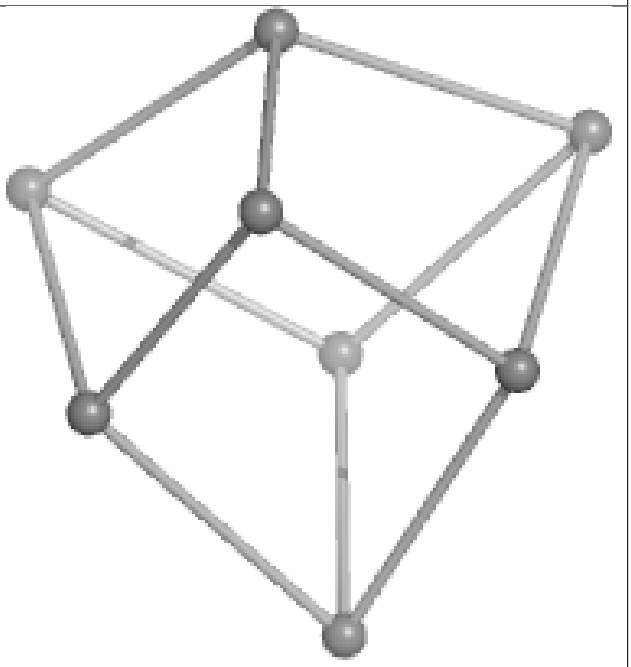


Rings

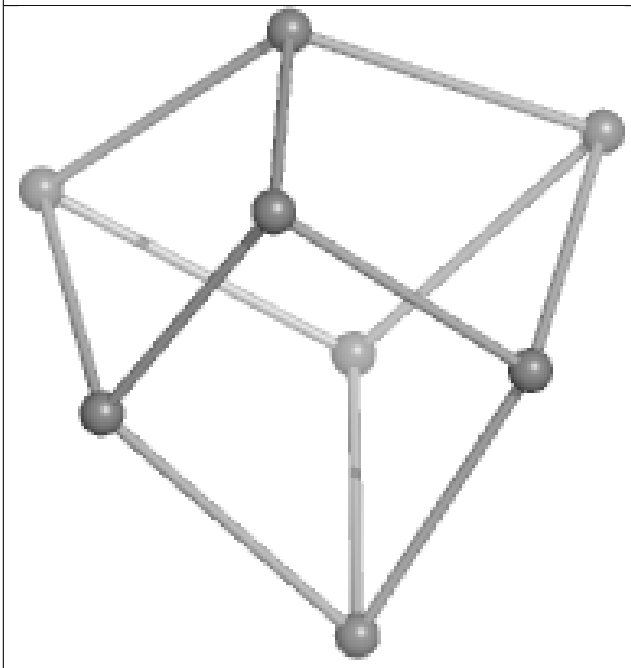
Ligand SF4 E 401



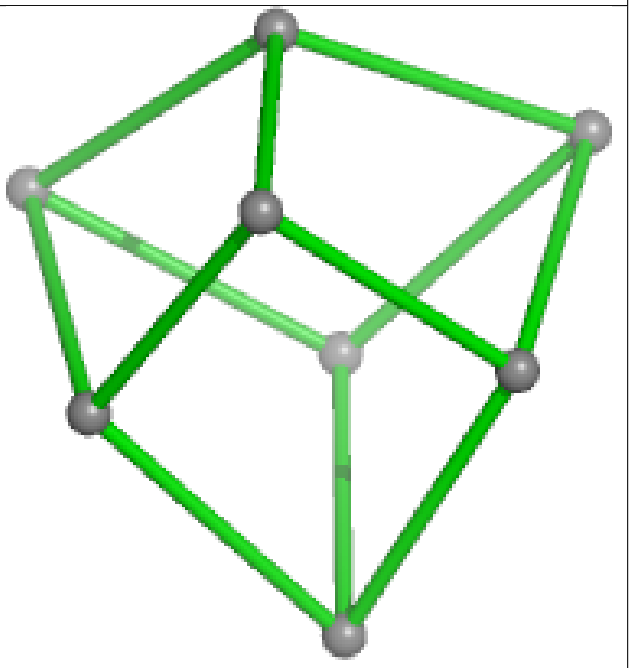
Bond lengths



Bond angles

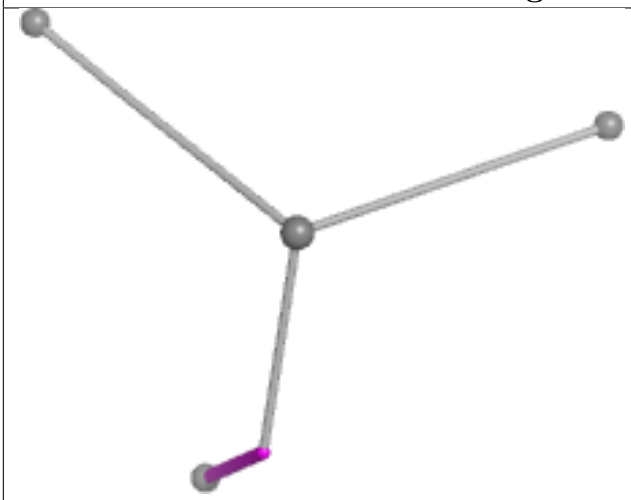


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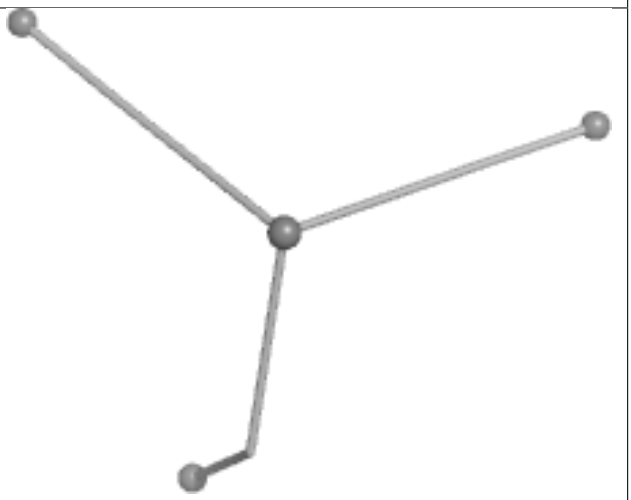


Rings

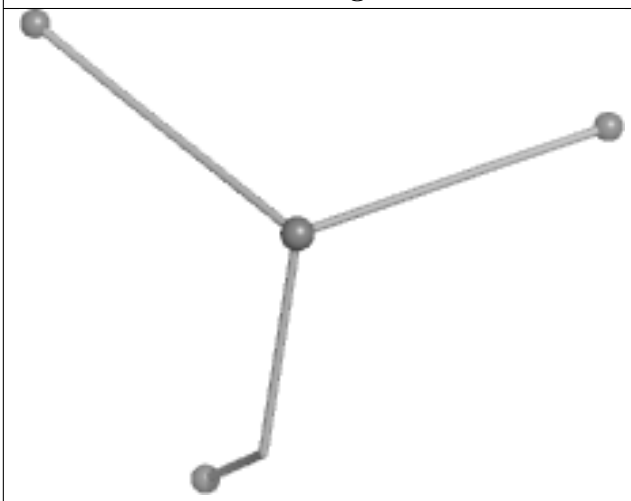
Ligand FCO F 473



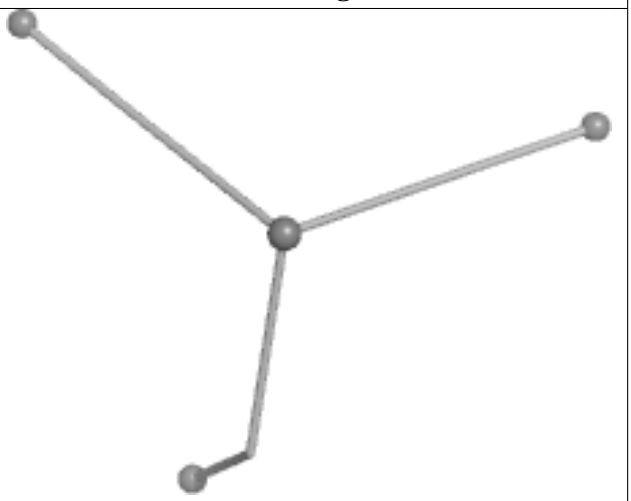
Bond lengths



Bond angles

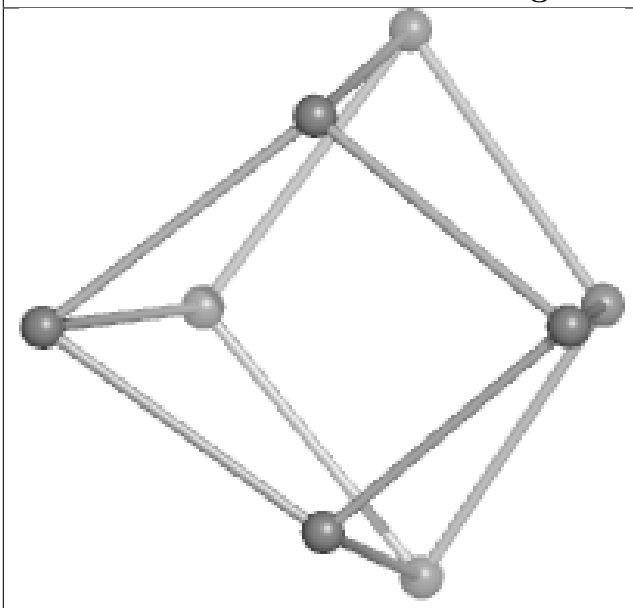


Torsions

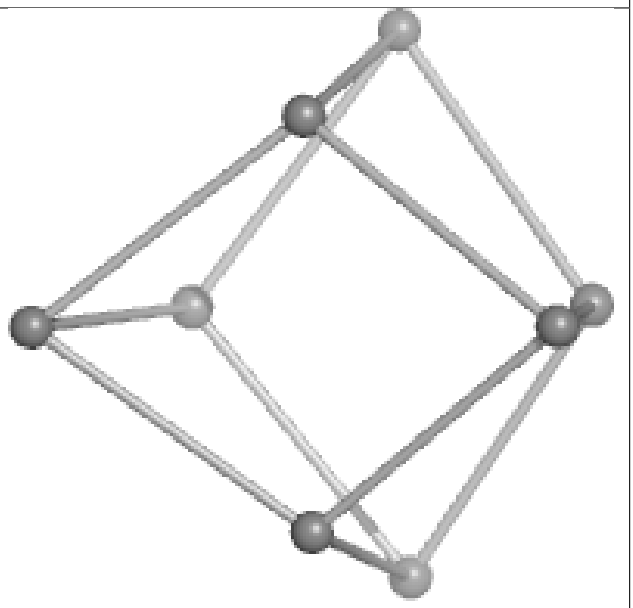


Rings

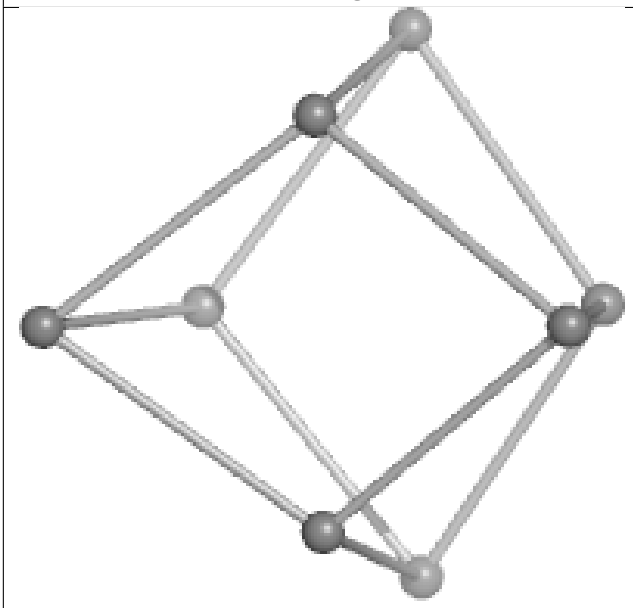
Ligand SF4 A 706



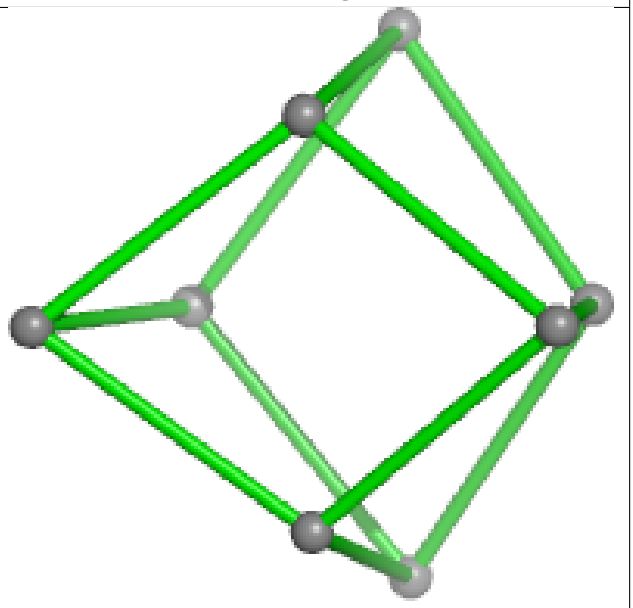
Bond lengths



Bond angles

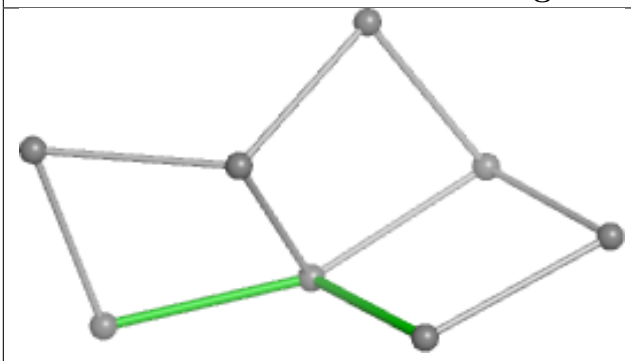


Torsions

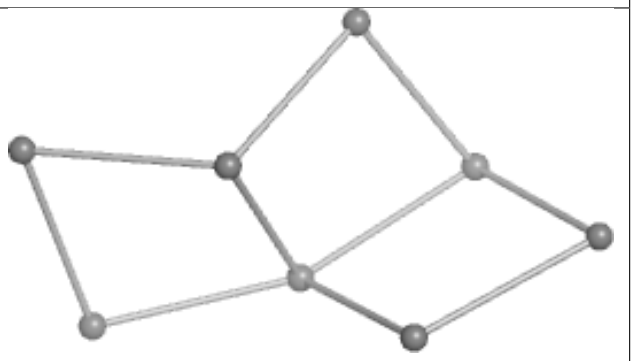


Rings

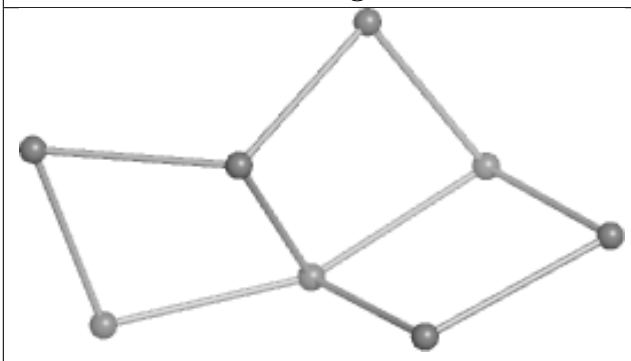
Ligand 9S8 B 401



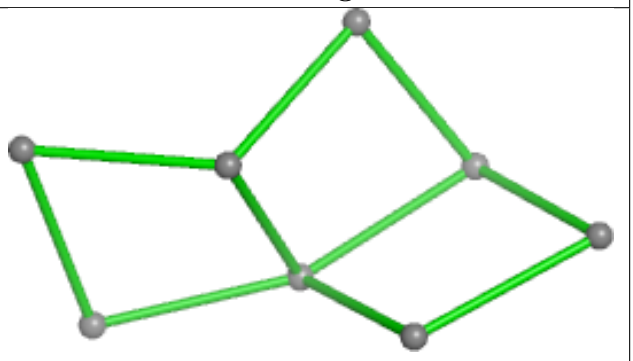
Bond lengths



Bond angles

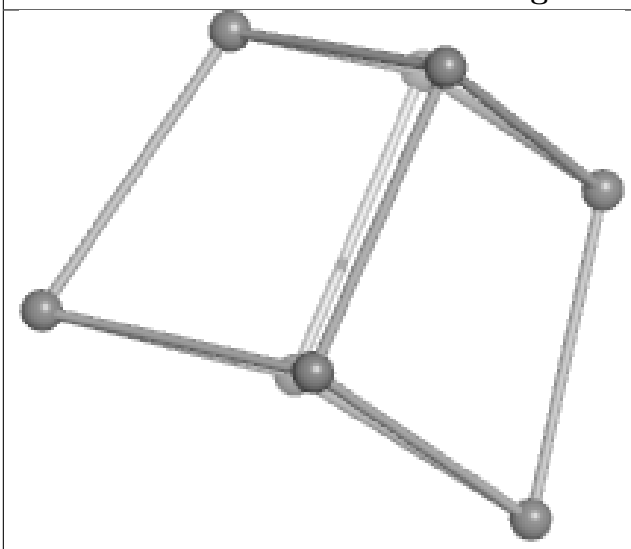


Torsions

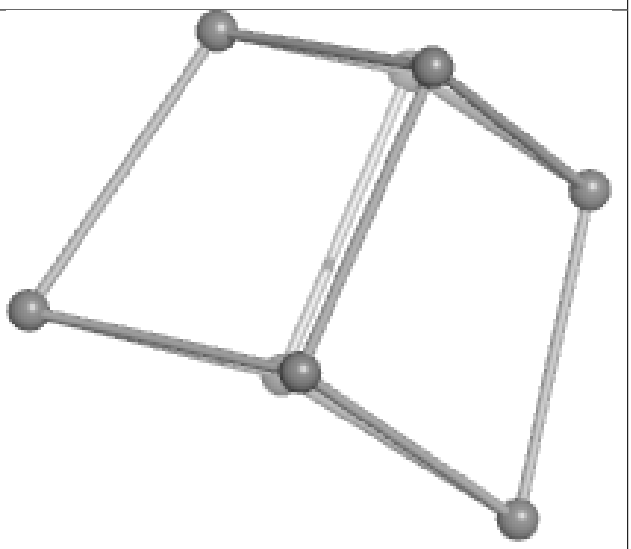


Rings

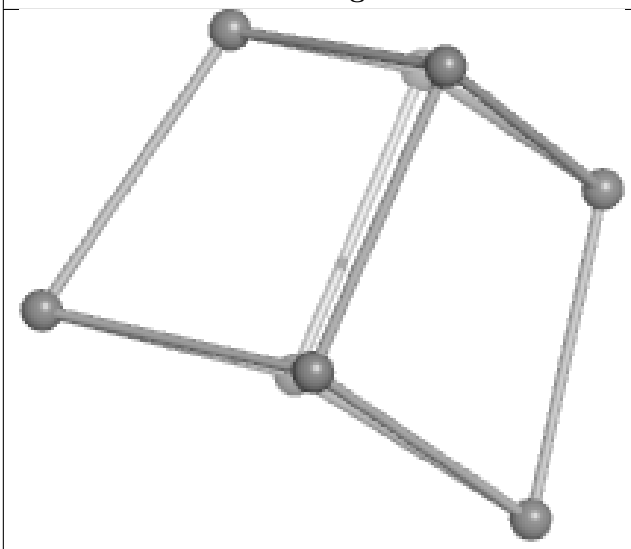
Ligand SF4 A 707



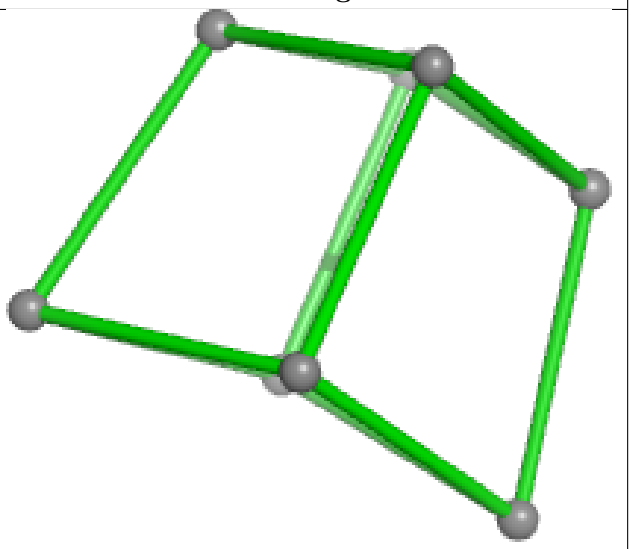
Bond lengths



Bond angles

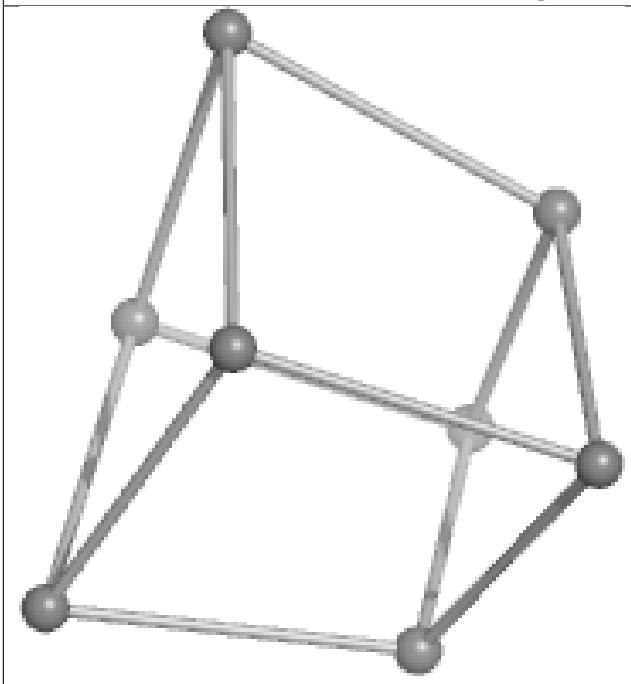


Torsions

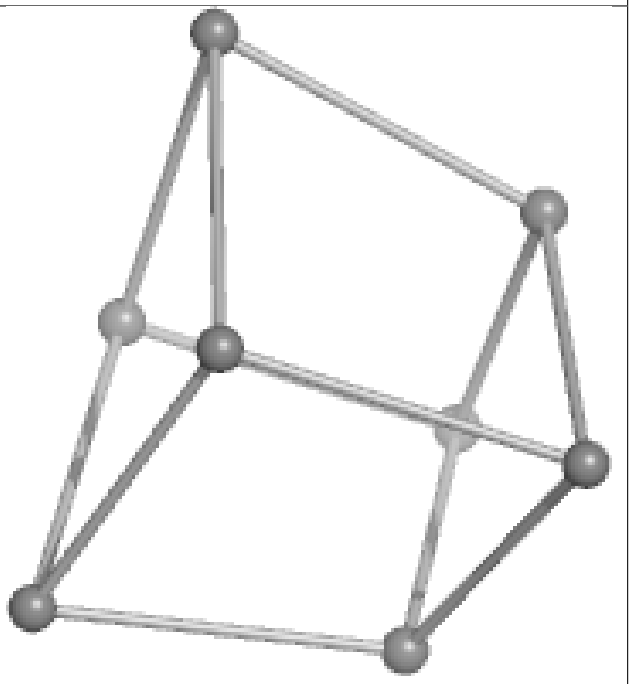


Rings

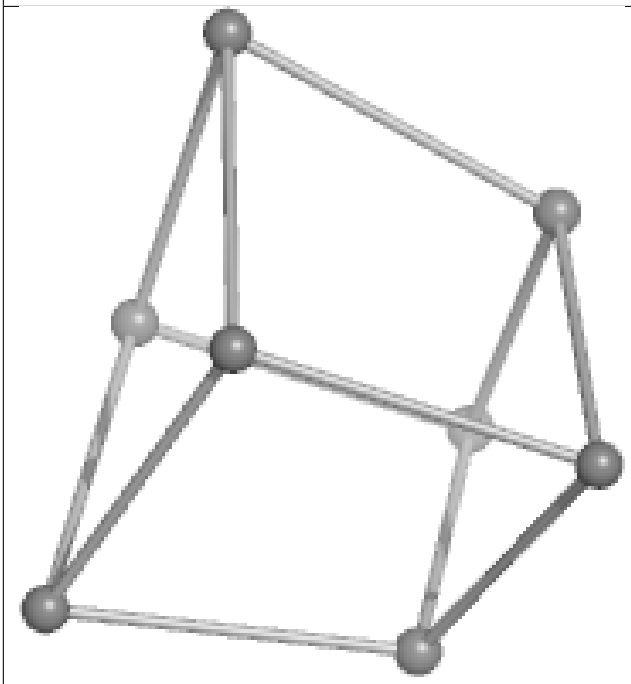
Ligand SF4 E 403



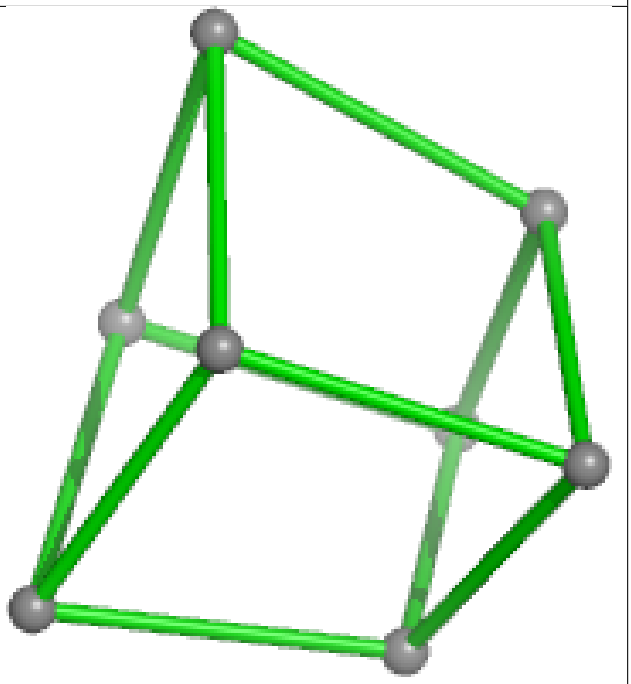
Bond lengths



Bond angles

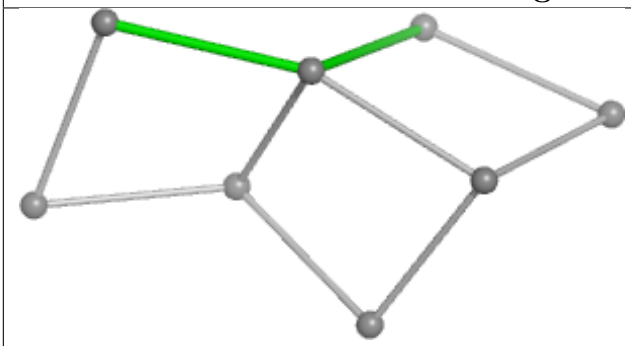


Torsions

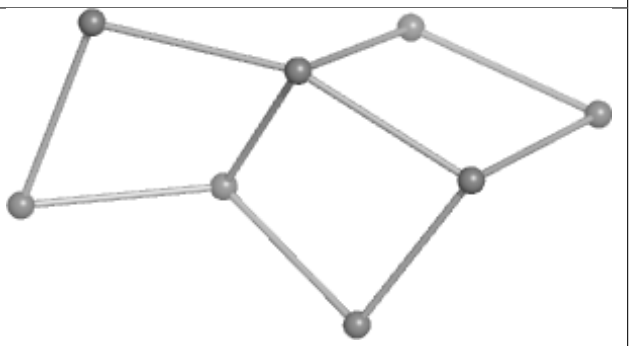


Rings

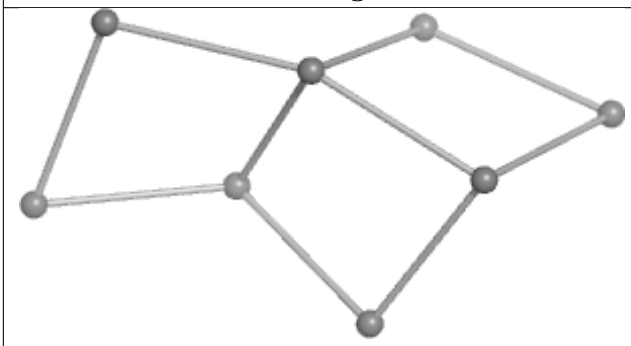
Ligand 9S8 B 402



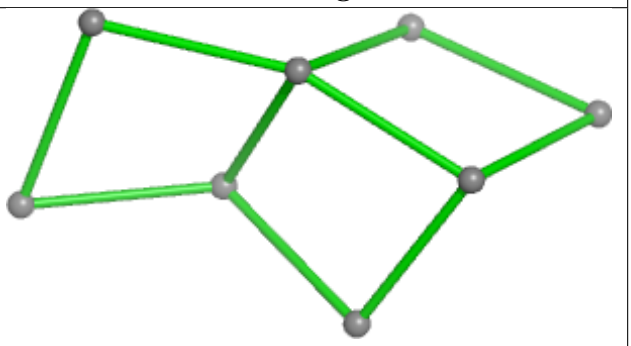
Bond lengths



Bond angles

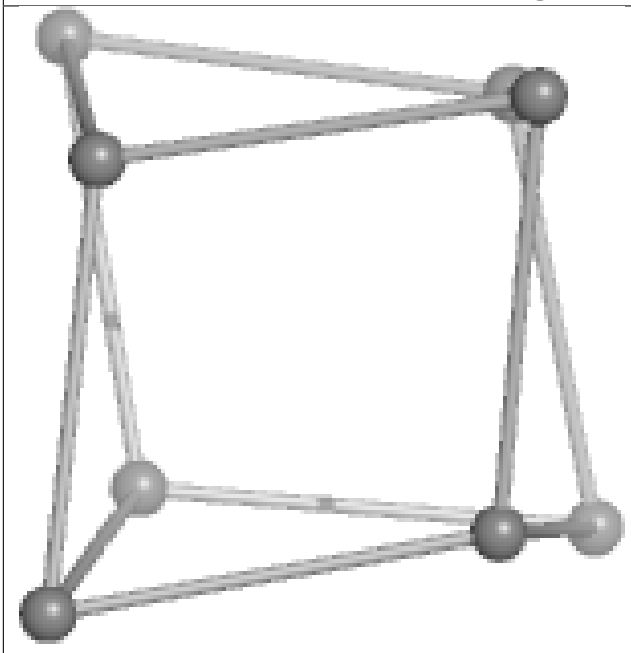


Torsions

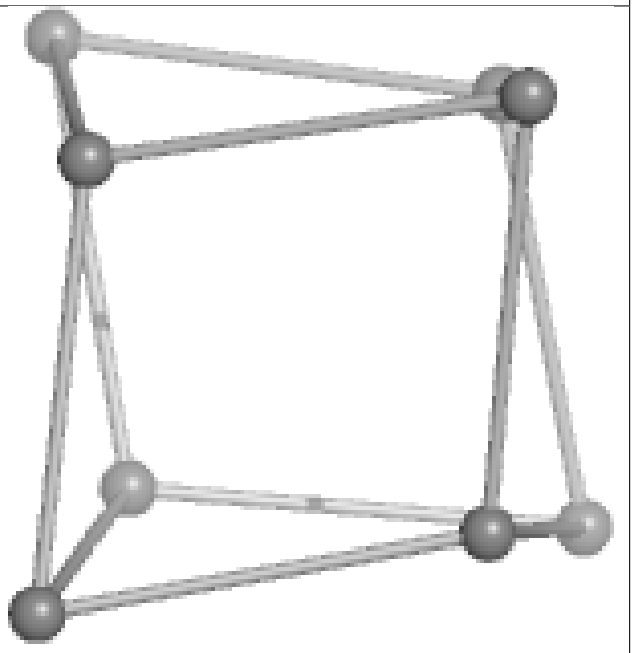


Rings

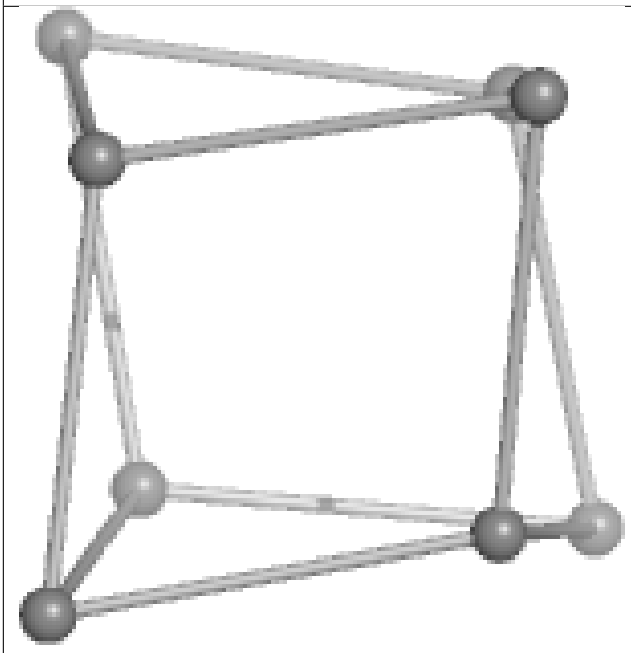
Ligand SF4 C 201



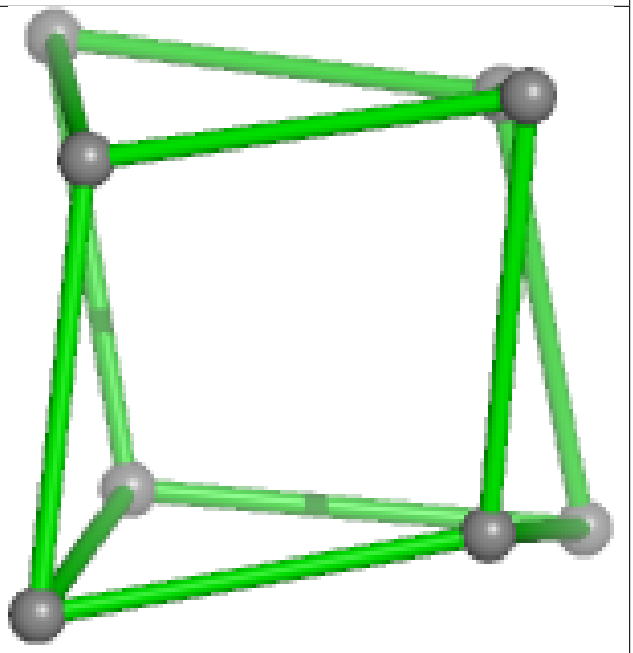
Bond lengths



Bond angles

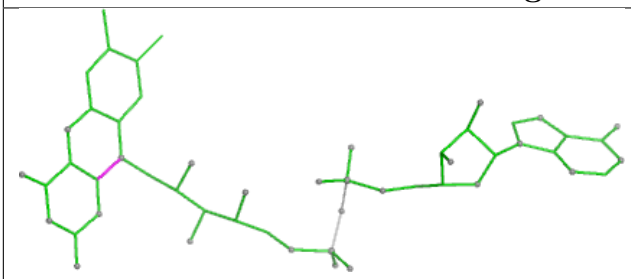


Torsions

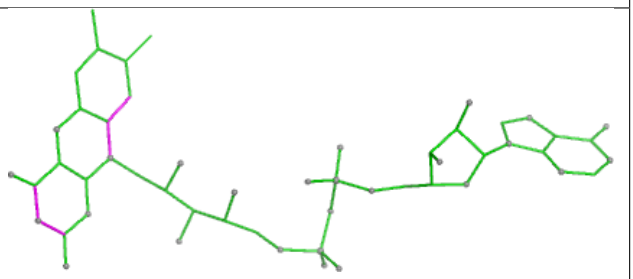


Rings

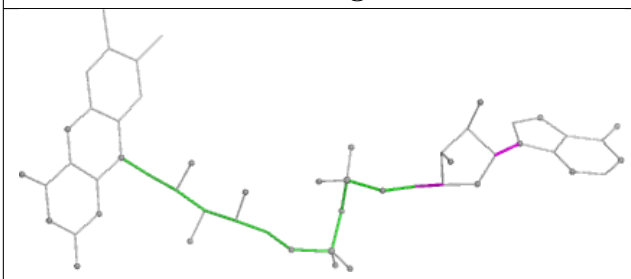
Ligand FAD A 704



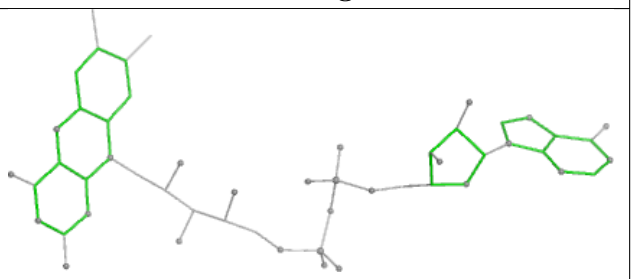
Bond lengths



Bond angles

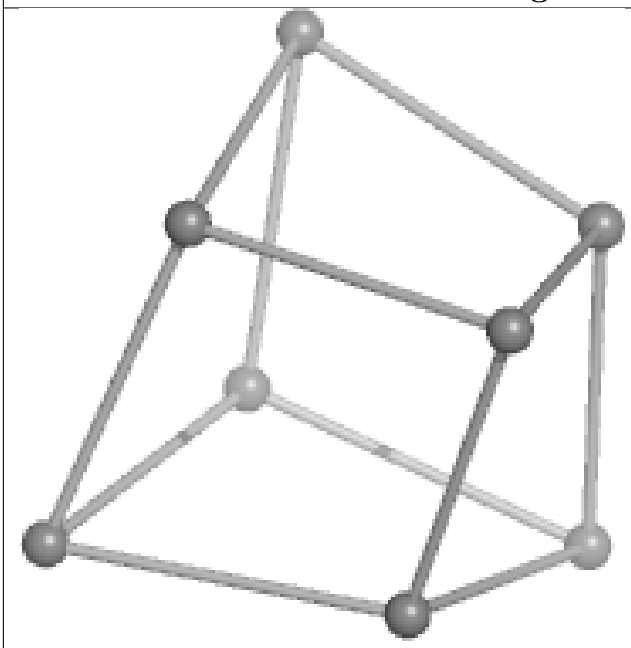


Torsions

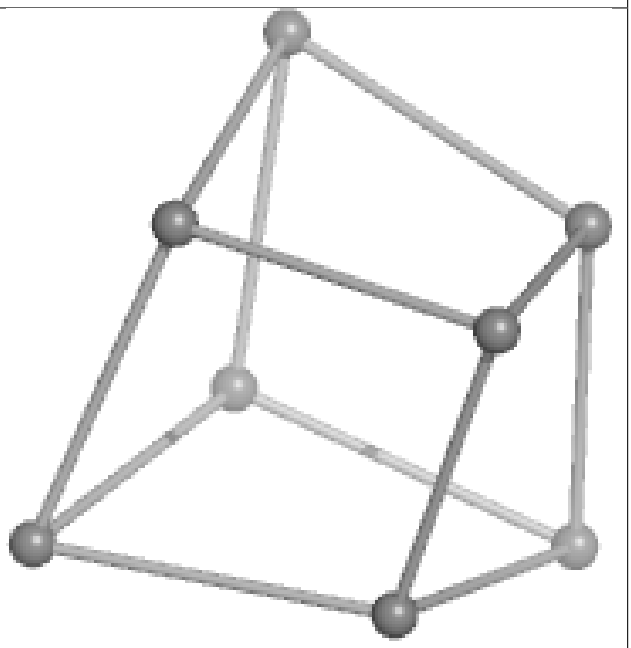


Rings

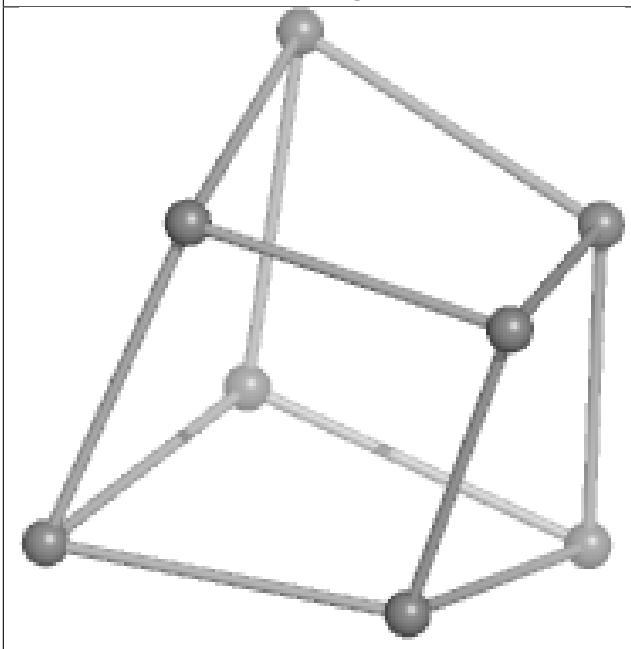
Ligand SF4 A 705



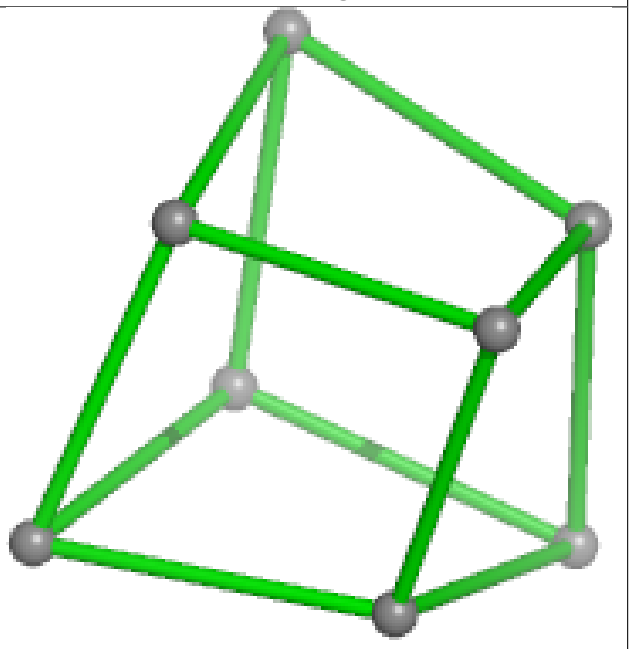
Bond lengths



Bond angles

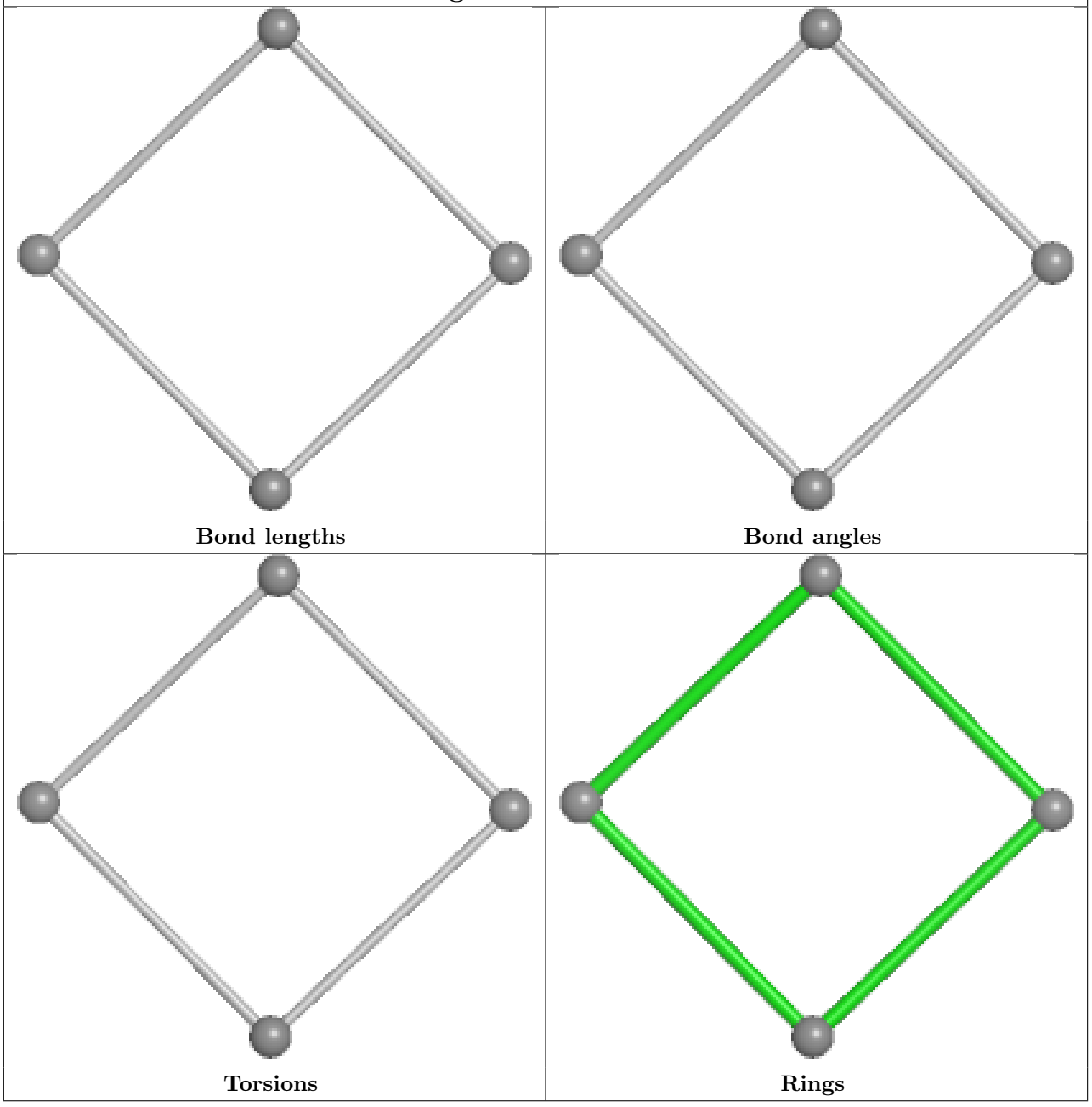


Torsions



Rings

Ligand FES D 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

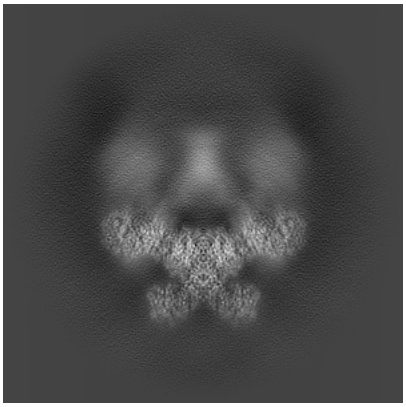
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55295. These allow visual inspection of the internal detail of the map and identification of artifacts.

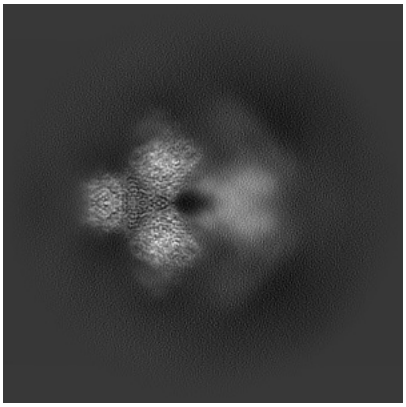
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

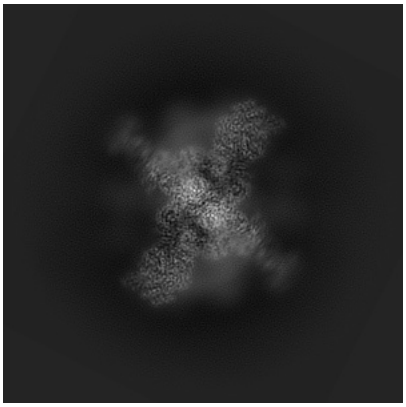
6.1.1 Primary map



X



Y

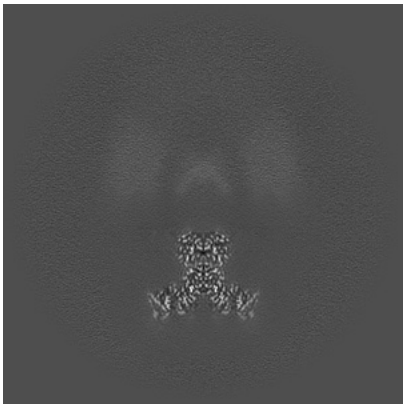


Z

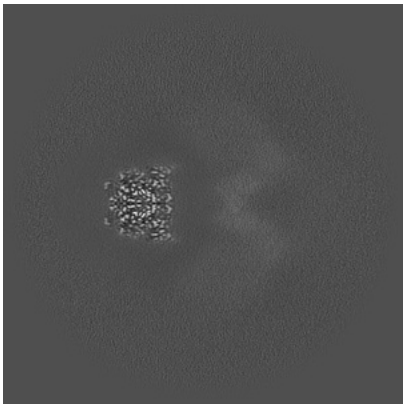
The images above show the map projected in three orthogonal directions.

6.2 Central slices

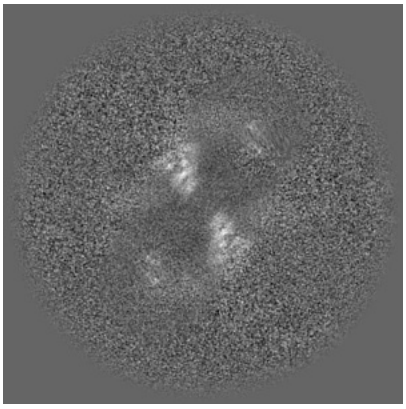
6.2.1 Primary map



X Index: 240



Y Index: 240

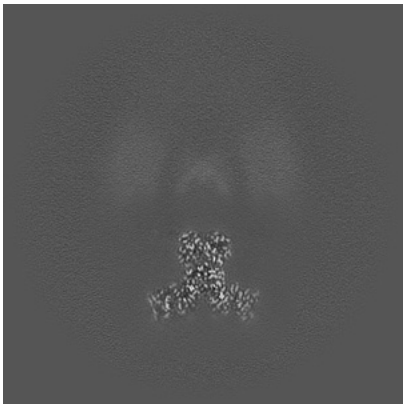


Z Index: 240

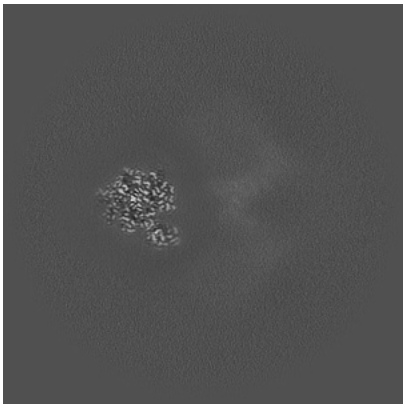
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

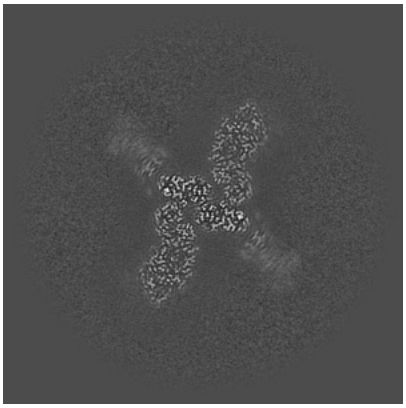
6.3.1 Primary map



X Index: 239



Y Index: 234

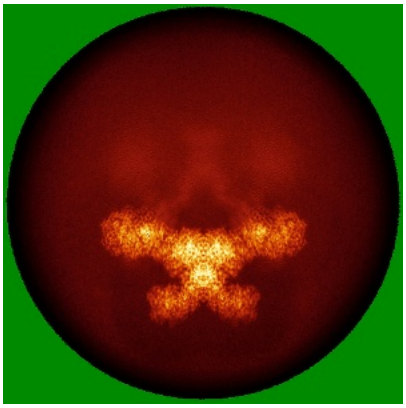


Z Index: 188

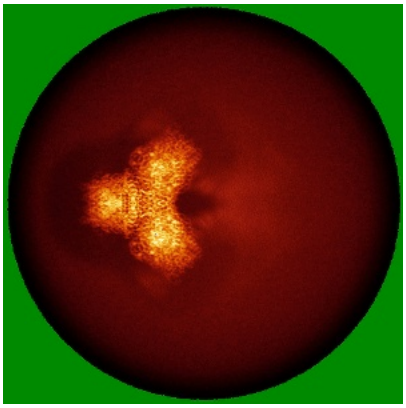
The images above show the largest variance slices of the map in three orthogonal directions.

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

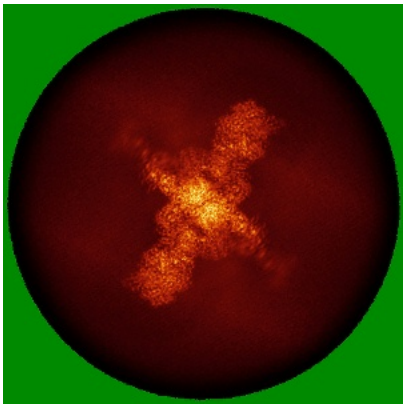
6.4.1 Primary map



X



Y

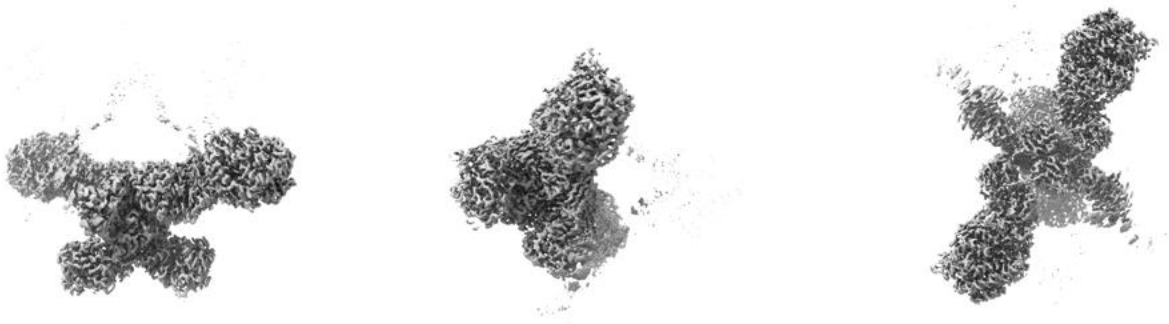


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 5.47. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

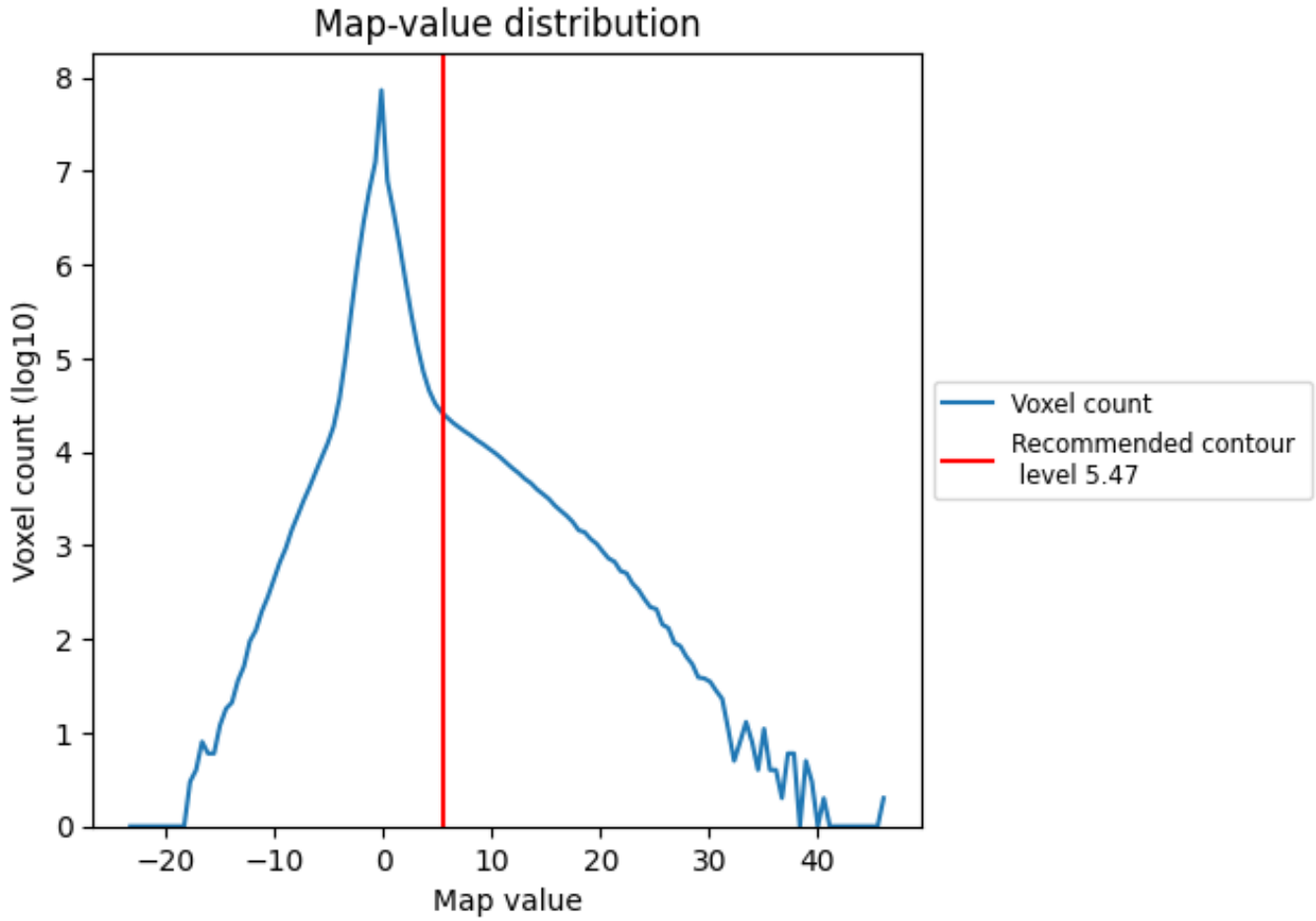
6.6 Mask visualisation (i)

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

7 Map analysis

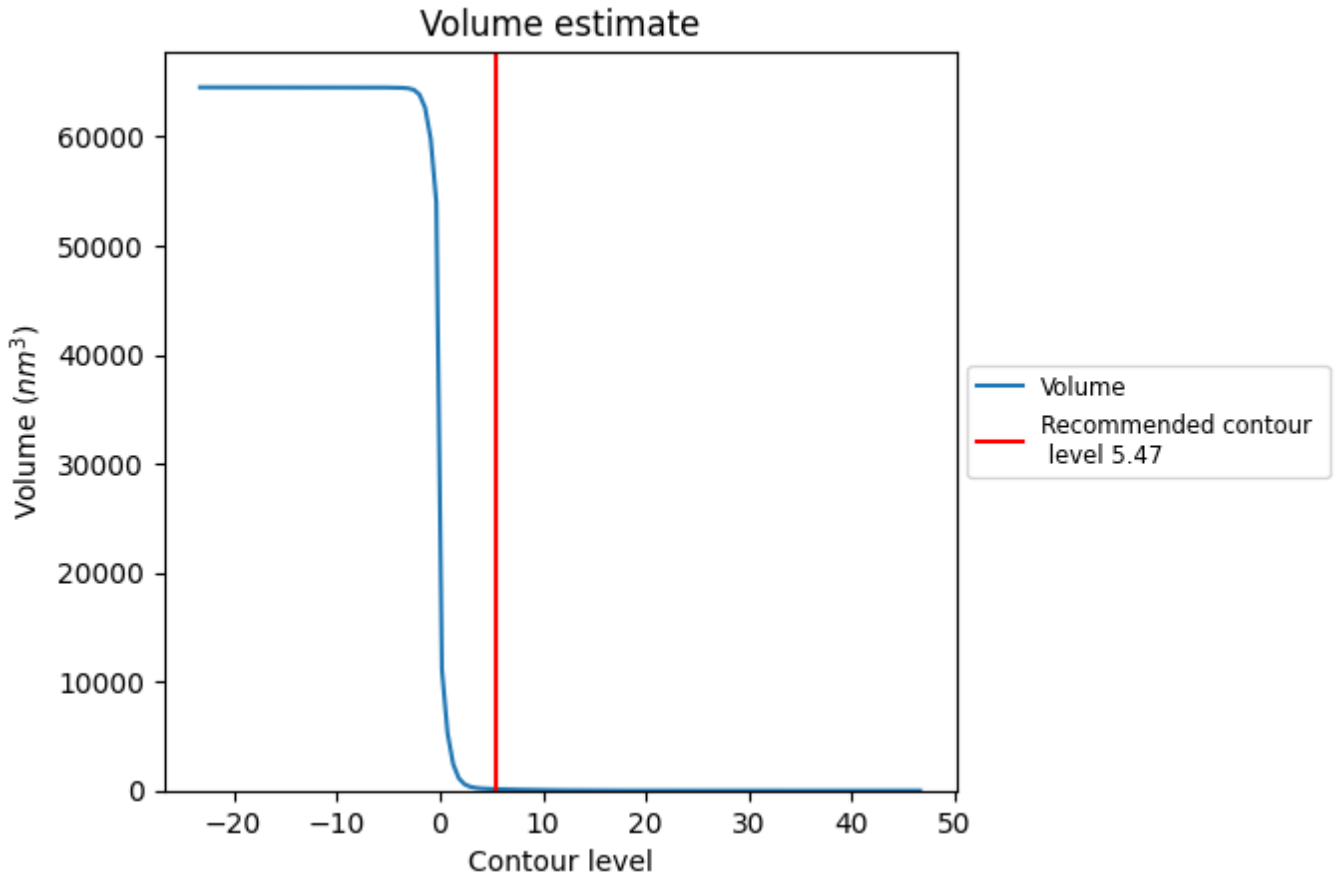
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

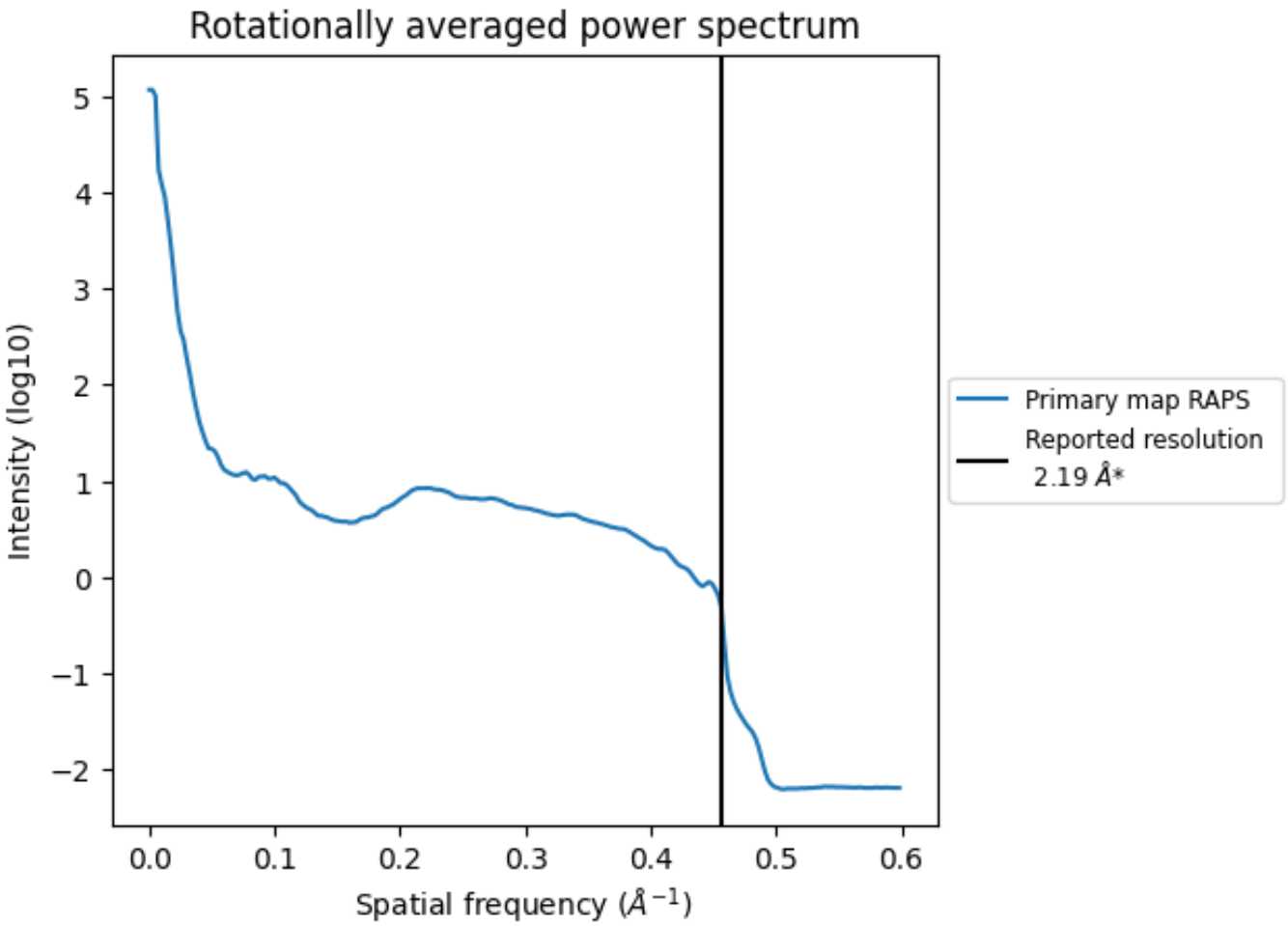
7.2 Volume estimate



The volume at the recommended contour level is 133 nm^3; this corresponds to an approximate mass of 120 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.457 Å^{-1}

8 Fourier-Shell correlation (i)

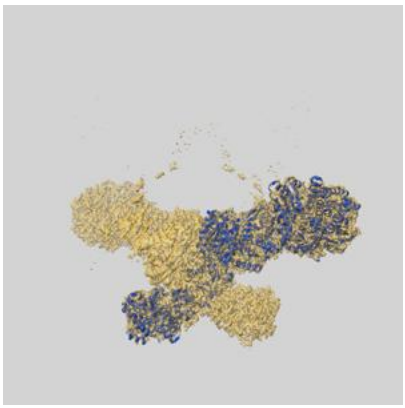
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

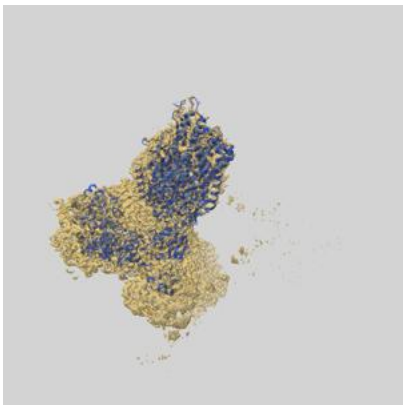
This section contains information regarding the fit between EMDB map EMD-55295 and PDB model 9SW2. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

9.1.1 Map-model overlay



X

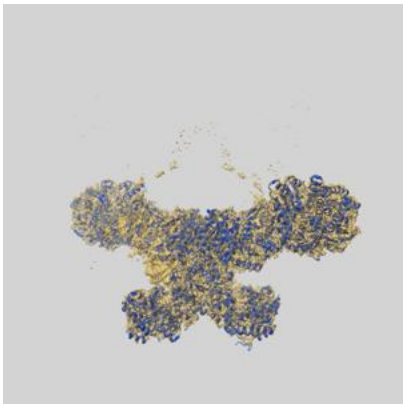


Y

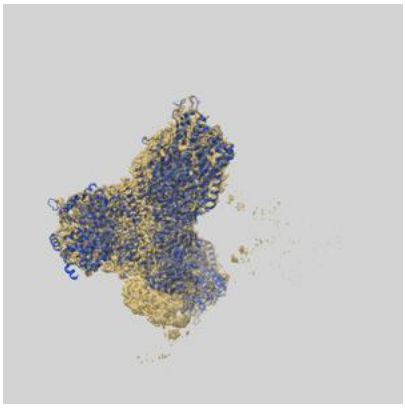


Z

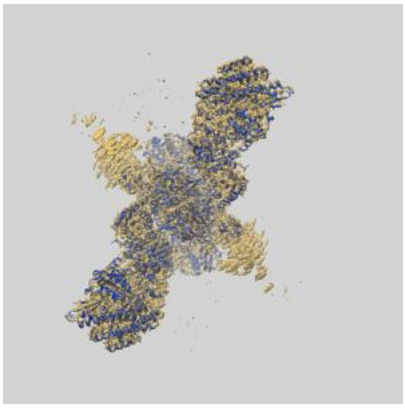
9.1.2 Map-model assembly overlay



X



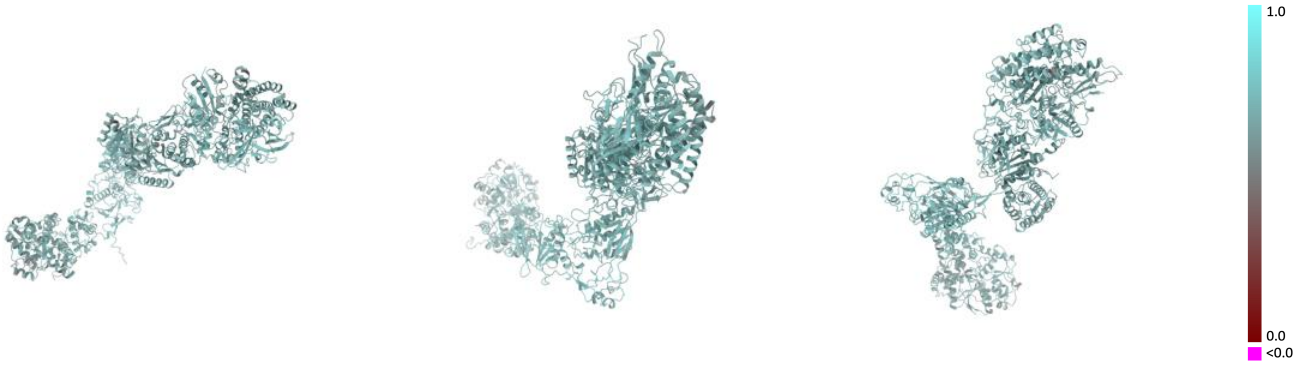
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.47 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.

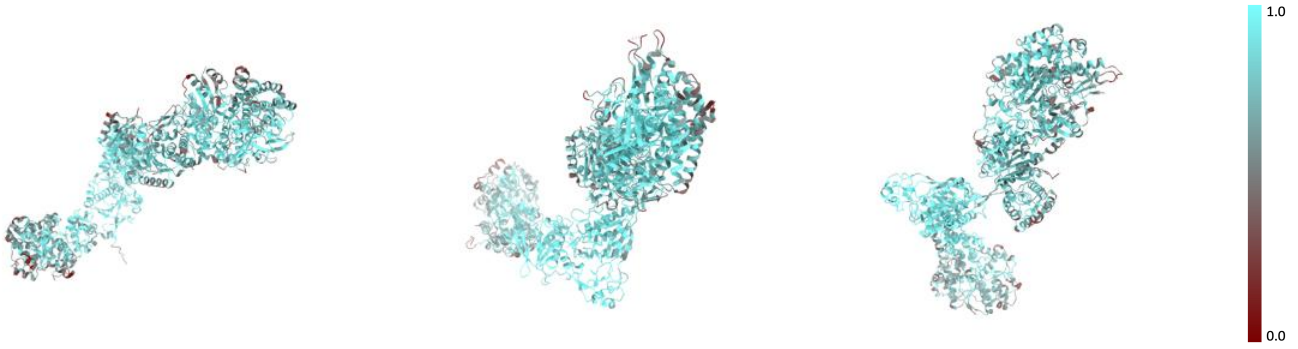
9.2 Q-score mapped to coordinate model (i)



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.

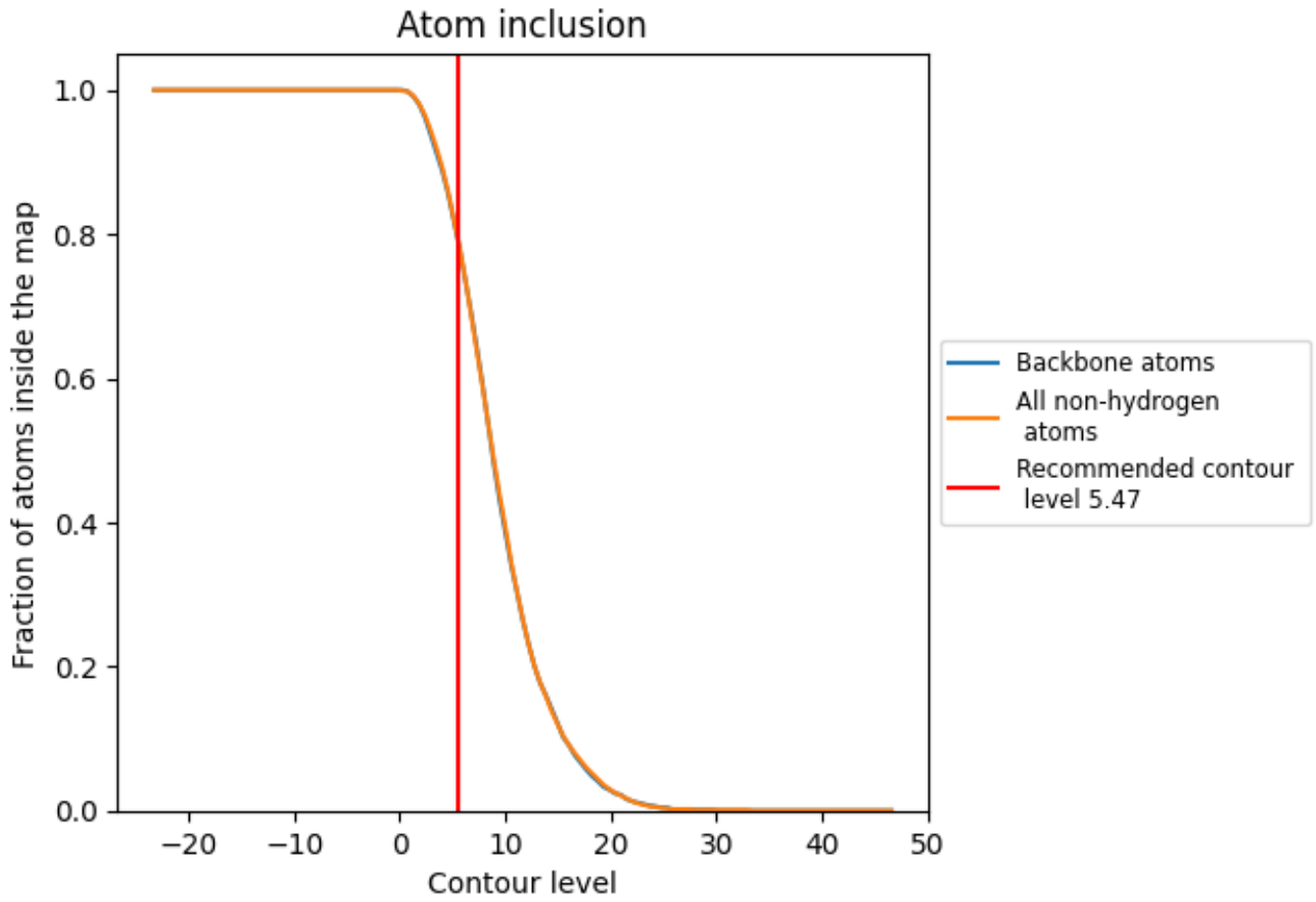
9.3 Atom inclusion mapped to coordinate model (i)



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 (5.47).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (5.47) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7980	0.6590
A	0.8750	0.6730
B	0.7220	0.6340
C	0.7430	0.6490
D	0.7980	0.6540
E	0.7740	0.6630
F	0.8040	0.6590

