Full wwPDB EM Validation Report ⓘ

Sep 9, 2026 – 07:00 am BST

PDB ID	:	8RVV / pdb_00008rvv
EMDB ID	:	EMD-19534
Title	:	CryoEM structure of the Elp-Hdr complex of Methanothermobacter marburgensis state 2, dimer (composite structure)
Authors	:	San Segundo-Acosta, P.; Murphy, B.J.
Deposited on	:	2024-02-15
Resolution	:	2.20 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:

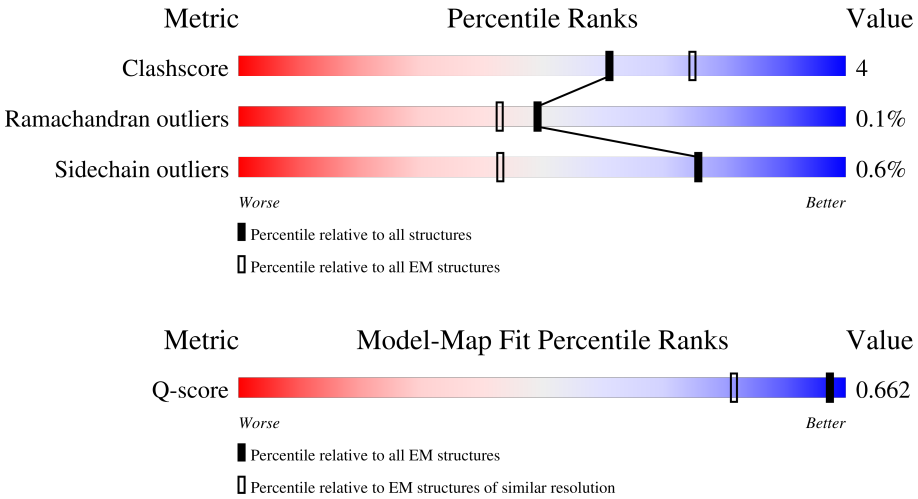
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

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

The reported resolution of this entry is 2.20 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	3184 (1.71 - 2.70)

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	643	94% 6%
2	B	284	5% 93% 7%
3	C	183	92% 8%
4	D	339	15% 87% 13%

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Mol	Chain	Length	Quality of chain
5	E	380	86% 14%
6	F	129	91% 9%

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
7	SF4	A	703	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 30454 atoms, of which 14912 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	643	9782	3096	4872	818	948	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	284	4367	1389	2168	364	424	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	183	2846	890	1429	252	264	11	0	0

- Molecule 4 is a protein called Formate dehydrogenase, alpha subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	339	5094	1632	2515	437	495	15	0	0

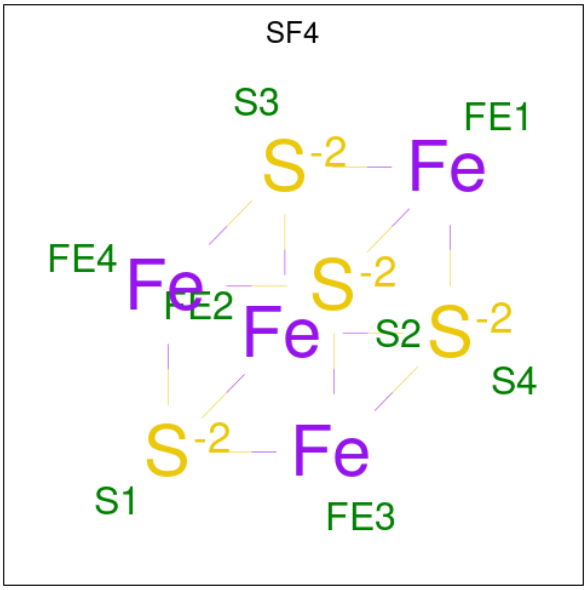
- Molecule 5 is a protein called Formate dehydrogenase, beta subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	380	5928	1882	2908	515	591	32	0	0

- Molecule 6 is a protein called Methyl viologen-reducing hydrogenase, subunit D-related protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	129	Total	C	H	N	O	S	0	0
			2026	663	989	179	185	10		

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



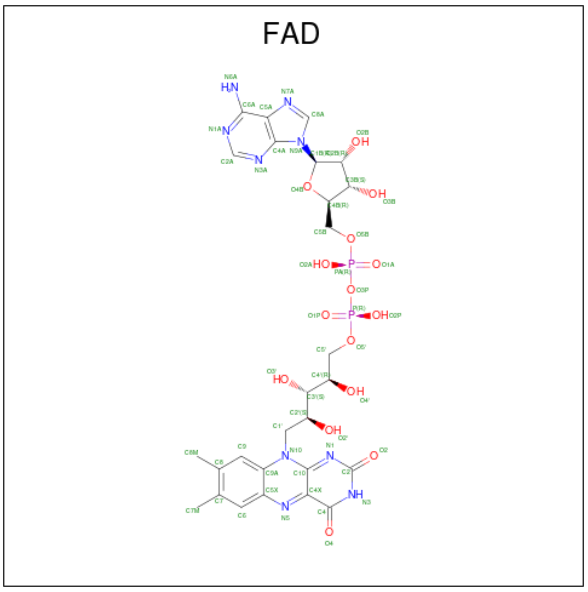
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	
7	C	1	Total	Fe	S	0
			8	4	4	
7	C	1	Total	Fe	S	0
			8	4	4	
7	D	1	Total	Fe	S	0
			8	4	4	
7	E	1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

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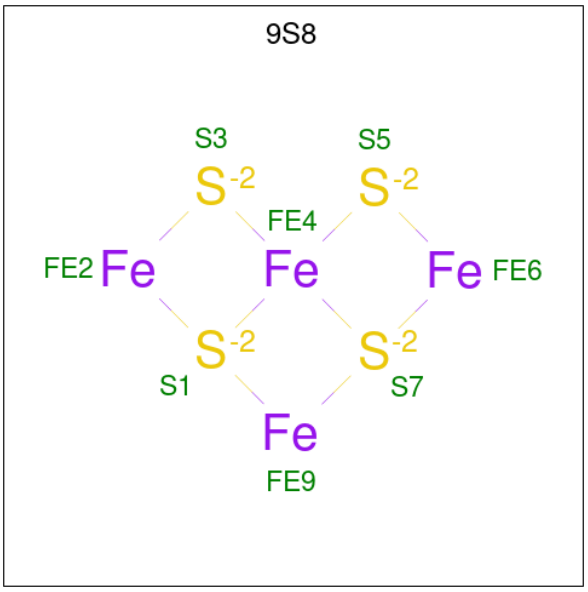
Mol	Chain	Residues	Atoms	AltConf
7	E	1	Total Fe S 8 4 4	0
7	E	1	Total Fe S 8 4 4	0
7	E	1	Total Fe S 8 4 4	0

- 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).



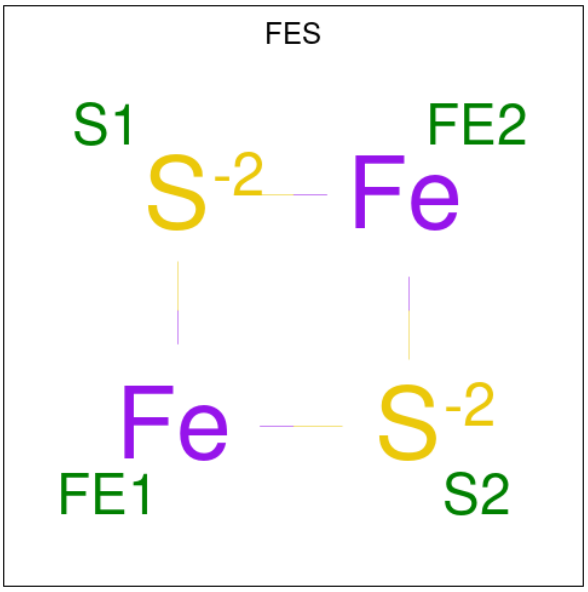
Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C H N O P 84 27 31 9 15 2	0

- 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
			Total	Fe	S	
9	B	1	8	4	4	0
			Total	Fe	S	
9	B	1	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
			Total	Fe	S	
10	F	1	4	2	2	0

- Molecule 11 is water.

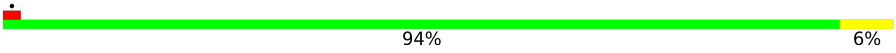
Mol	Chain	Residues	Atoms	AltConf
11	A	49	Total O 49 49	0
11	B	21	Total O 21 21	0
11	C	9	Total O 9 9	0
11	D	37	Total O 37 37	0
11	E	63	Total O 63 63	0
11	F	24	Total O 24 24	0

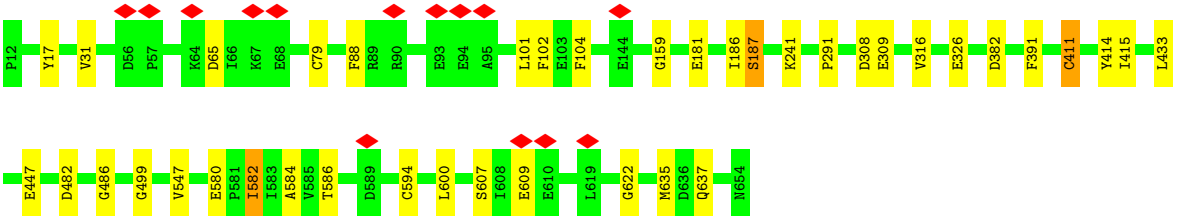
3 Residue-property plots (i)

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

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

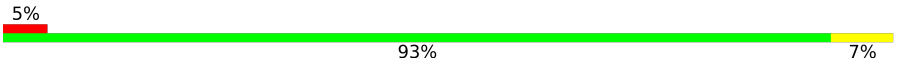
Chain A:

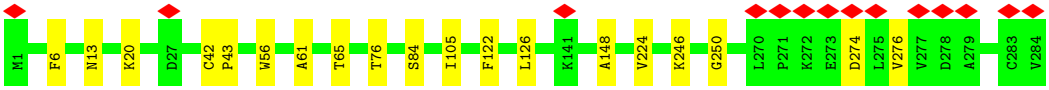




• Molecule 2: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit B

Chain B:

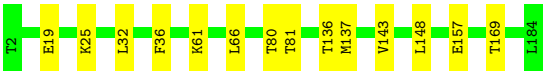




• Molecule 3: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit C

Chain C:

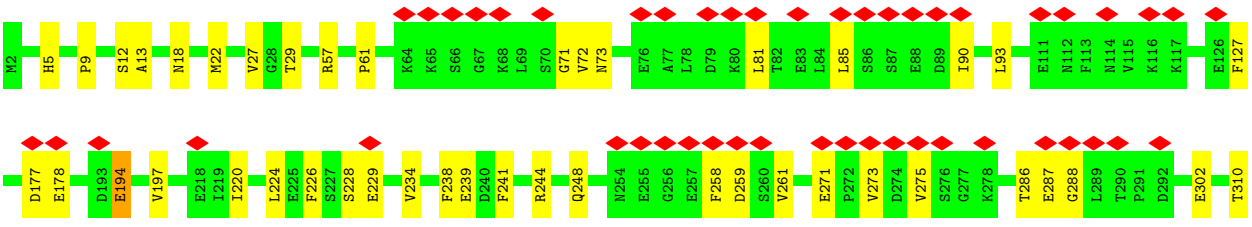


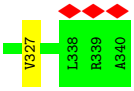


• Molecule 4: Formate dehydrogenase, alpha subunit

Chain D:





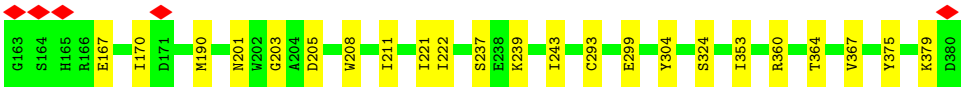


• Molecule 5: Formate dehydrogenase, beta subunit

Chain E:



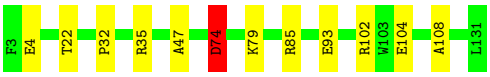




• Molecule 6: Methyl viologen-reducing hydrogenase, subunit D-related protein

Chain F:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	234858	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 ($e^-/Å^2$)	65	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	46.015	Depositor
Minimum map value	-23.199	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.855	Depositor
Recommended contour level	4.6	Depositor
Map size (Å)	374.976, 374.976, 374.976	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	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, SF4, 9S8, 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	0.17	0/4999	0.35	1/6764 (0.0%)
2	B	0.15	0/2236	0.29	0/3016
3	C	0.15	0/1442	0.30	0/1944
4	D	0.18	1/2632 (0.0%)	0.34	0/3580
5	E	0.16	0/3076	0.35	0/4144
6	F	0.18	0/1066	0.36	1/1434 (0.1%)
All	All	0.17	1/15451 (0.0%)	0.33	2/20882 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	61	PRO	N-CD	-5.34	1.40	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	101	LEU	N-CA-C	-5.18	106.81	113.02
6	F	74	ASP	N-CA-CB	-5.12	108.33	114.17

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	4910	4872	4872	30	0
2	B	2199	2168	2168	13	0
3	C	1417	1429	1429	11	0
4	D	2579	2515	2514	32	0
5	E	3020	2908	2908	50	0
6	F	1037	989	989	11	0
7	A	48	0	0	2	0
7	C	16	0	0	0	0
7	D	8	0	0	0	0
7	E	32	0	0	0	0
8	A	53	31	31	0	0
9	B	16	0	0	0	0
10	F	4	0	0	0	0
11	A	49	0	0	1	0
11	B	21	0	0	0	0
11	C	9	0	0	0	0
11	D	37	0	0	3	0
11	E	63	0	0	8	0
11	F	24	0	0	0	0
All	All	15542	14912	14911	134	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (134) 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)
1:A:635:MET:HG2	7:A:703:SF4:S1	1.85	1.15
5:E:4:LEU:HD11	5:E:211:ILE:HB	1.48	0.95
5:E:4:LEU:CD1	5:E:211:ILE:HB	2.00	0.91
5:E:78:ASP:OD1	11:E:501:HOH:O	1.93	0.86
5:E:4:LEU:HD11	5:E:211:ILE:CG1	2.06	0.85
5:E:4:LEU:HD11	5:E:211:ILE:CB	2.07	0.84
1:A:635:MET:CG	7:A:703:SF4:S1	2.66	0.82
5:E:203:GLY:O	11:E:502:HOH:O	1.98	0.81
5:E:75:MET:O	11:E:501:HOH:O	2.02	0.77
5:E:153:ARG:NH1	5:E:167:GLU:OE2	2.18	0.76
5:E:293:CYS:O	11:E:503:HOH:O	2.04	0.76
5:E:4:LEU:HD11	5:E:211:ILE:HD12	1.69	0.75
4:D:13:ALA:O	11:D:501:HOH:O	2.03	0.74
4:D:12:SER:HB2	4:D:310:THR:HG23	1.69	0.74
5:E:205:ASP:O	11:E:504:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:VAL:HG22	3:C:143:VAL:HG11	1.72	0.71
1:A:308:ASP:OD1	1:A:316:VAL:CG1	2.39	0.70
5:E:4:LEU:HD11	5:E:211:ILE:CD1	2.22	0.70
5:E:8:ALA:O	5:E:14:GLN:NE2	2.25	0.70
5:E:4:LEU:CG	5:E:211:ILE:HB	2.23	0.68
5:E:299:GLU:OE2	5:E:304:TYR:OH	2.11	0.67
1:A:291:PRO:O	11:A:801:HOH:O	2.12	0.66
2:B:61:ALA:O	2:B:65:THR:HG23	1.95	0.65
3:C:157:GLU:OE2	3:C:157:GLU:N	2.22	0.65
5:E:116:TYR:HD2	5:E:221:ILE:HD11	1.62	0.64
1:A:308:ASP:OD1	1:A:316:VAL:HG11	1.97	0.64
4:D:85:LEU:HD22	4:D:90:ILE:HD13	1.83	0.60
1:A:586:THR:OG1	1:A:635:MET:SD	2.52	0.59
4:D:127:PHE:HZ	4:D:228:SER:HG	1.51	0.58
5:E:208:TRP:O	11:E:504:HOH:O	2.17	0.58
2:B:13:ASN:C	3:C:136:THR:HG21	2.29	0.58
4:D:248:GLN:NE2	11:D:503:HOH:O	2.33	0.57
5:E:4:LEU:C	5:E:4:LEU:HD12	2.30	0.57
5:E:4:LEU:HG	5:E:211:ILE:HB	1.86	0.57
3:C:137:MET:HE3	3:C:148:LEU:HD21	1.87	0.56
5:E:190:MET:N	5:E:190:MET:SD	2.79	0.55
5:E:364:THR:HG23	5:E:367:VAL:HB	1.88	0.55
2:B:148:ALA:HB2	2:B:224:VAL:HG11	1.88	0.54
6:F:102:ARG:NE	6:F:104:GLU:OE2	2.40	0.54
6:F:32:PRO:O	6:F:35:ARG:NH1	2.41	0.54
4:D:57:ARG:NH2	4:D:302:GLU:OE1	2.39	0.54
5:E:10:ASP:OD1	5:E:11:GLU:N	2.39	0.54
2:B:20:LYS:NZ	2:B:274:ASP:OD1	2.41	0.53
5:E:379:LYS:NZ	6:F:74:ASP:OD2	2.38	0.53
5:E:237:SER:N	11:E:510:HOH:O	2.40	0.53
5:E:4:LEU:CD2	5:E:222:ILE:HD12	2.39	0.53
4:D:261:VAL:HG12	4:D:275:VAL:HG13	1.90	0.53
4:D:127:PHE:CZ	4:D:228:SER:OG	2.62	0.52
5:E:4:LEU:HD13	5:E:6:ALA:HB2	1.91	0.52
3:C:137:MET:HE3	3:C:148:LEU:CD2	2.39	0.52
4:D:238:PHE:H	4:D:310:THR:HG21	1.75	0.51
5:E:4:LEU:CD1	5:E:211:ILE:CB	2.78	0.51
5:E:84:LEU:HB3	5:E:89:LEU:HD11	1.93	0.51
5:E:154:GLY:O	5:E:170:ILE:HG22	2.10	0.51
4:D:194:GLU:O	4:D:197:VAL:HG12	2.10	0.50
2:B:276:VAL:CG2	3:C:143:VAL:HG11	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:139:TYR:OH	5:E:156:PHE:O	2.28	0.50
6:F:22:THR:OG1	6:F:108:ALA:O	2.29	0.50
4:D:244:ARG:NH1	4:D:310:THR:O	2.44	0.50
1:A:308:ASP:OD1	1:A:316:VAL:HB	2.11	0.50
4:D:127:PHE:CE1	4:D:228:SER:OG	2.65	0.50
4:D:71:GLY:O	4:D:72:VAL:HG23	2.11	0.49
1:A:391:PHE:HB2	1:A:433:LEU:HD22	1.93	0.49
5:E:144:ASP:O	5:E:145:ASP:HB2	2.12	0.49
5:E:159:GLU:OE2	5:E:160:LEU:O	2.30	0.49
3:C:80:THR:O	3:C:81:THR:OG1	2.24	0.48
1:A:17:TYR:OH	1:A:65:ASP:OD2	2.24	0.48
2:B:42:CYS:N	2:B:43:PRO:HA	2.28	0.48
4:D:224:LEU:CD2	4:D:234:VAL:HG11	2.44	0.48
4:D:238:PHE:CD2	4:D:310:THR:HG22	2.49	0.48
2:B:6:PHE:HB3	2:B:76:THR:HG22	1.96	0.48
1:A:584:ALA:HB1	1:A:635:MET:HE3	1.95	0.48
5:E:4:LEU:HD21	5:E:222:ILE:HD12	1.95	0.48
4:D:72:VAL:HG12	4:D:73:ASN:O	2.14	0.47
5:E:4:LEU:CD1	5:E:211:ILE:CG1	2.88	0.47
5:E:379:LYS:NZ	6:F:74:ASP:O	2.43	0.47
1:A:547:VAL:HG12	1:A:547:VAL:O	2.15	0.47
1:A:186:ILE:O	1:A:187:SER:CB	2.63	0.46
2:B:105:ILE:HD13	3:C:169:THR:HG22	1.97	0.46
5:E:379:LYS:HZ1	6:F:74:ASP:CG	2.22	0.46
1:A:31:VAL:HG12	1:A:31:VAL:O	2.15	0.46
4:D:259:ASP:OD1	4:D:259:ASP:C	2.58	0.46
3:C:61:LYS:HG2	3:C:66:LEU:HD12	1.98	0.46
5:E:147:VAL:HG22	5:E:159:GLU:O	2.15	0.46
4:D:81:LEU:O	4:D:85:LEU:HG	2.16	0.46
4:D:12:SER:HA	4:D:241:PHE:HA	1.98	0.45
4:D:9:PRO:O	11:D:502:HOH:O	2.21	0.45
4:D:226:PHE:O	4:D:229:GLU:O	2.35	0.45
1:A:415:ILE:HD11	1:A:499:GLY:HA3	1.98	0.45
2:B:122:PHE:CZ	2:B:126:LEU:HD11	2.52	0.45
4:D:287:GLU:O	4:D:288:GLY:C	2.60	0.45
5:E:360:ARG:HD3	6:F:85:ARG:HH21	1.82	0.45
1:A:600:LEU:HD22	6:F:79:LYS:HD2	1.98	0.45
1:A:159:GLY:N	1:A:181:GLU:OE1	2.48	0.45
1:A:580:GLU:HG2	1:A:582:ILE:HG12	1.99	0.44
5:E:121:ASN:ND2	11:E:516:HOH:O	2.50	0.44
4:D:271:GLU:O	4:D:273:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ASP:OD1	1:A:316:VAL:CB	2.65	0.44
1:A:382:ASP:OD1	1:A:382:ASP:N	2.51	0.44
1:A:447:GLU:OE1	1:A:447:GLU:N	2.43	0.44
6:F:4:GLU:OE2	6:F:4:GLU:HA	2.18	0.43
1:A:607:SER:OG	1:A:609:GLU:OE1	2.37	0.43
5:E:16:LYS:HG2	5:E:66:CYS:HB2	2.00	0.43
4:D:238:PHE:H	4:D:310:THR:CG2	2.31	0.43
5:E:19:CYS:SG	5:E:201:ASN:HB3	2.58	0.43
5:E:144:ASP:O	5:E:145:ASP:CB	2.66	0.42
3:C:19:GLU:CD	3:C:19:GLU:H	2.27	0.42
5:E:324:SER:HB2	6:F:47:ALA:HB3	2.02	0.42
1:A:600:LEU:HD21	5:E:375:TYR:HA	2.01	0.42
4:D:22:MET:HB2	4:D:27:VAL:HG11	2.01	0.42
5:E:93:VAL:O	5:E:119:GLY:HA2	2.19	0.42
1:A:594:CYS:HA	5:E:107:ARG:O	2.20	0.42
5:E:353:ILE:HD11	6:F:93:GLU:HG3	2.01	0.42
4:D:239:GLU:OE1	4:D:239:GLU:N	2.53	0.42
1:A:411:CYS:HA	1:A:414:TYR:CE2	2.55	0.41
4:D:5:HIS:ND1	4:D:18:ASN:OD1	2.40	0.41
4:D:93:LEU:HD11	4:D:258:PHE:CE2	2.54	0.41
4:D:178:GLU:OE1	4:D:178:GLU:N	2.53	0.41
1:A:622:GLY:O	1:A:637:GLN:NE2	2.53	0.41
3:C:25:LYS:HE3	3:C:32:LEU:HD11	2.01	0.41
4:D:286:THR:O	4:D:287:GLU:C	2.63	0.41
2:B:42:CYS:SG	2:B:43:PRO:C	3.03	0.41
4:D:177:ASP:O	4:D:177:ASP:OD2	2.38	0.41
4:D:220:ILE:O	4:D:224:LEU:HG	2.21	0.41
1:A:88:PHE:CB	1:A:102:PHE:CZ	3.03	0.41
5:E:8:ALA:HB2	5:E:25:ALA:HB2	2.02	0.41
1:A:414:TYR:CD1	1:A:414:TYR:C	2.98	0.41
1:A:79:CYS:O	1:A:104:PHE:CE1	2.74	0.41
2:B:246:LYS:O	2:B:250:GLY:HA2	2.21	0.41
1:A:241:LYS:HG3	1:A:326:GLU:HG2	2.03	0.41
5:E:4:LEU:HD21	5:E:222:ILE:CD1	2.51	0.41
1:A:482:ASP:O	1:A:486:GLY:N	2.54	0.40
2:B:56:TRP:NE1	2:B:84:SER:OG	2.51	0.40
5:E:239:LYS:O	5:E:243:ILE:HG13	2.21	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	641/643 (100%)	621 (97%)	19 (3%)	1 (0%)	43 51
2	B	282/284 (99%)	279 (99%)	3 (1%)	0	100 100
3	C	181/183 (99%)	179 (99%)	2 (1%)	0	100 100
4	D	337/339 (99%)	325 (96%)	12 (4%)	0	100 100
5	E	378/380 (100%)	366 (97%)	12 (3%)	0	100 100
6	F	127/129 (98%)	125 (98%)	2 (2%)	0	100 100
All	All	1946/1958 (99%)	1895 (97%)	50 (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	533/533 (100%)	530 (99%)	3 (1%)	78 89
2	B	240/240 (100%)	240 (100%)	0	100 100
3	C	153/153 (100%)	152 (99%)	1 (1%)	76 87
4	D	277/290 (96%)	274 (99%)	3 (1%)	65 79
5	E	328/329 (100%)	326 (99%)	2 (1%)	78 89
6	F	107/107 (100%)	106 (99%)	1 (1%)	70 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1638/1652 (99%)	1628 (99%)	10 (1%)	76 89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	GLU
1	A	411	CYS
1	A	582	ILE
3	C	36	PHE
4	D	29	THR
4	D	194	GLU
4	D	327	VAL
5	E	1	MET
5	E	151	ILE
6	F	74	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	471	ASN
1	A	612	HIS
1	A	654	ASN
3	C	173	GLN
4	D	202	GLN
4	D	203	GLN
4	D	230	ASN
5	E	70	HIS
5	E	185	GLN
5	E	249	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 (i)

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	$\#\|Z\| > 2$
7	SF4	E	402	5	0,12,12	-	-	-		
7	SF4	A	704	1	0,12,12	-	-	-		
7	SF4	C	201	3	0,12,12	-	-	-		
7	SF4	A	703	1	0,12,12	-	-	-		
7	SF4	C	202	3	0,12,12	-	-	-		
7	SF4	D	401	4	0,12,12	-	-	-		
8	FAD	A	707	-	56,58,58	0.55	0	81,89,89	0.66	1 (1%)
7	SF4	A	702	1	0,12,12	-	-	-		
7	SF4	E	401	5	0,12,12	-	-	-		
7	SF4	E	404	5	0,12,12	-	-	-		
7	SF4	E	403	5	0,12,12	-	-	-		
7	SF4	A	705	1	0,12,12	-	-	-		
9	9S8	B	401	2	2,10,10	5.08	2 (100%)	-		
7	SF4	A	706	1	0,12,12	-	-	-		
7	SF4	A	701	1	0,12,12	-	-	-		
10	FES	F	201	6	0,4,4	-	-	-		
9	9S8	B	400	2	2,10,10	5.66	2 (100%)	-		

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	E	402	5	-	-	0/6/5/5
7	SF4	A	704	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	C	201	3	-	-	0/6/5/5
7	SF4	A	703	1	-	-	0/6/5/5
7	SF4	C	202	3	-	-	0/6/5/5
7	SF4	D	401	4	-	-	0/6/5/5
8	FAD	A	707	-	-	1/34/50/50	0/6/6/6
7	SF4	A	702	1	-	-	0/6/5/5
7	SF4	E	401	5	-	-	0/6/5/5
7	SF4	E	404	5	-	-	0/6/5/5
7	SF4	E	403	5	-	-	0/6/5/5
7	SF4	A	705	1	-	-	0/6/5/5
9	9S8	B	401	2	-	-	0/3/3/3
7	SF4	A	706	1	-	-	0/6/5/5
7	SF4	A	701	1	-	-	0/6/5/5
10	FES	F	201	6	-	-	0/1/1/1
9	9S8	B	400	2	-	-	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	400	9S8	S3-FE4	-7.17	2.08	2.24
9	B	401	9S8	S3-FE4	-6.77	2.08	2.24
9	B	400	9S8	S5-FE4	-3.55	2.16	2.24
9	B	401	9S8	S5-FE4	-2.39	2.19	2.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	707	FAD	C4-N3-C2	-2.03	121.89	125.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	707	FAD	O4B-C4B-C5B-O5B

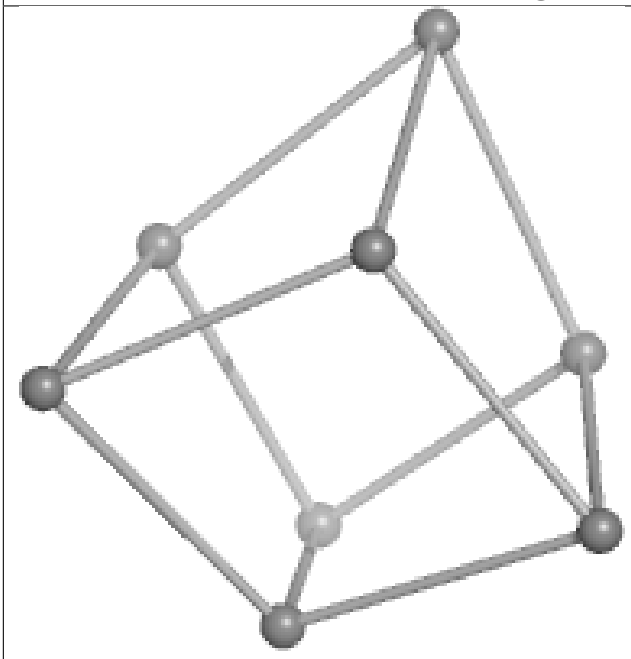
There are no ring outliers.

1 monomer is involved in 2 short contacts:

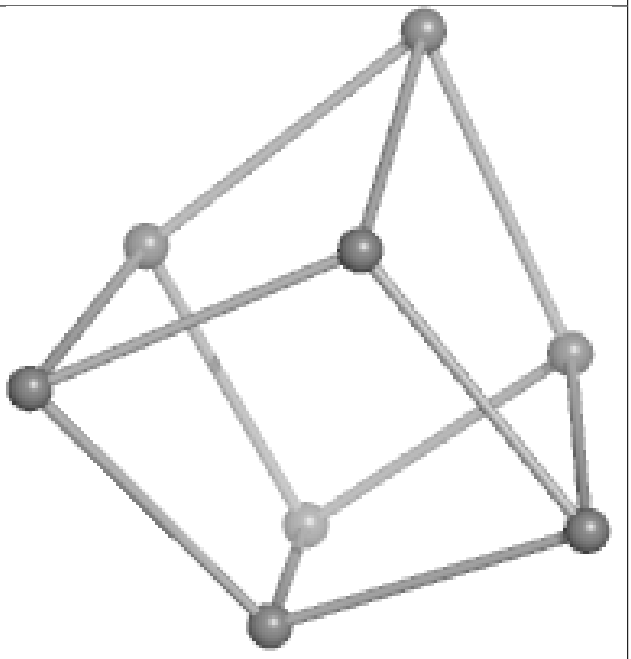
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	703	SF4	2	0

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.

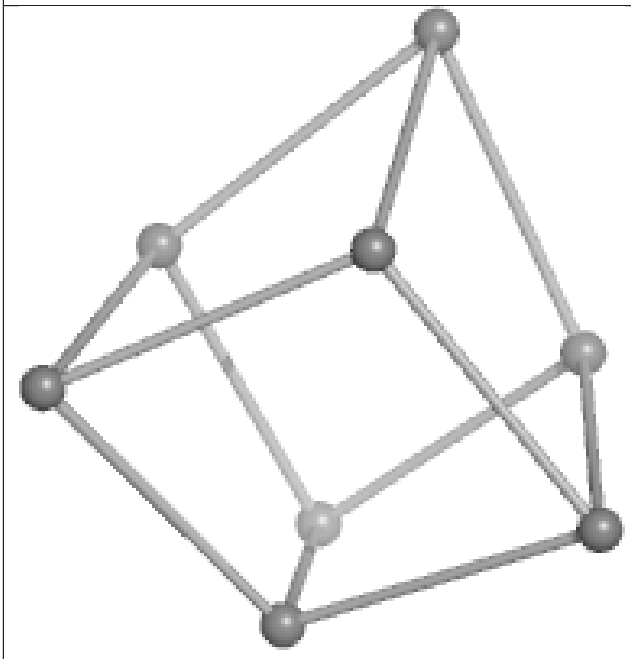
Ligand SF4 E 402



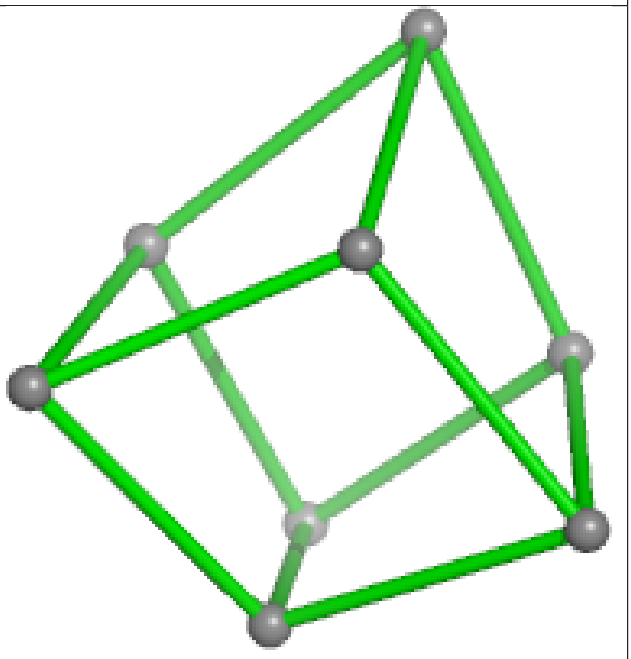
Bond lengths



Bond angles

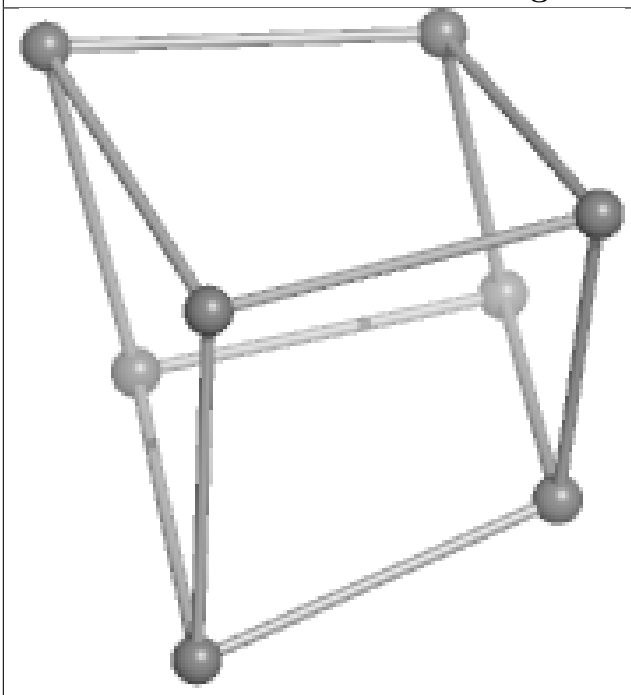


Torsions

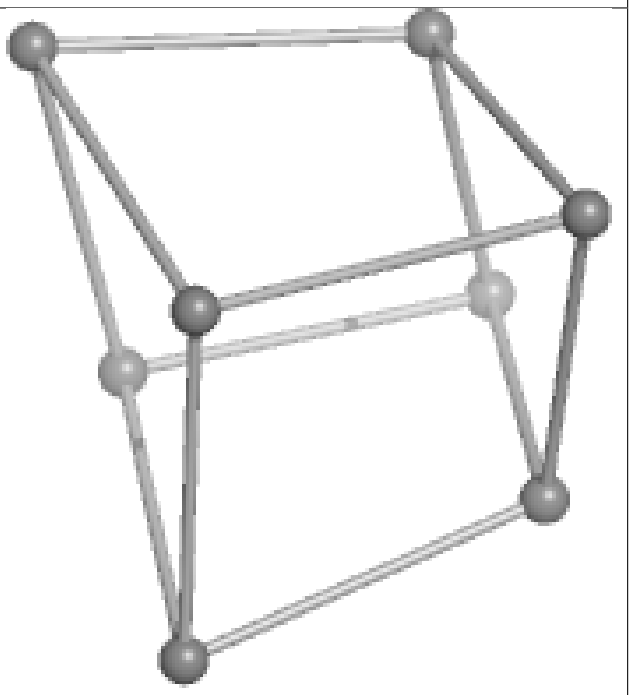


Rings

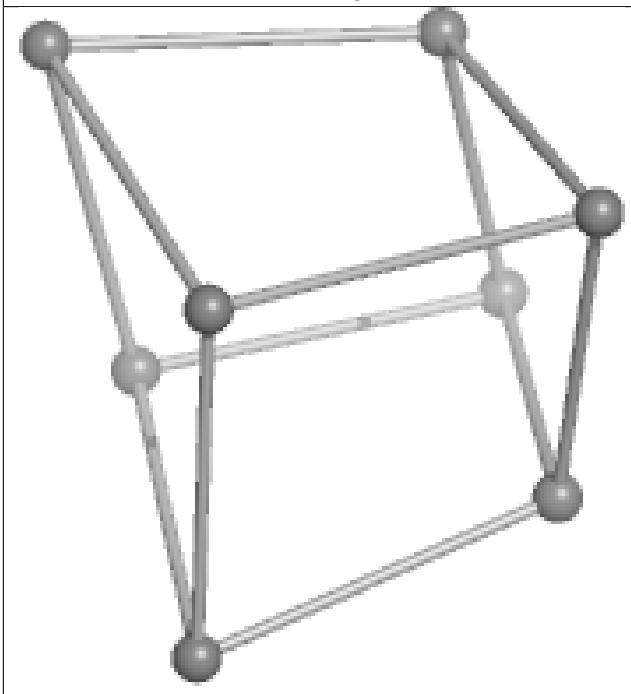
Ligand SF4 A 704



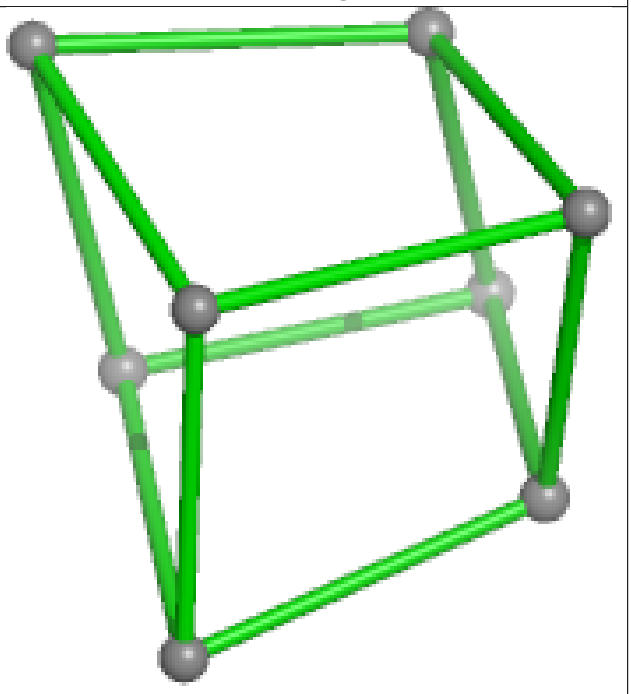
Bond lengths



Bond angles

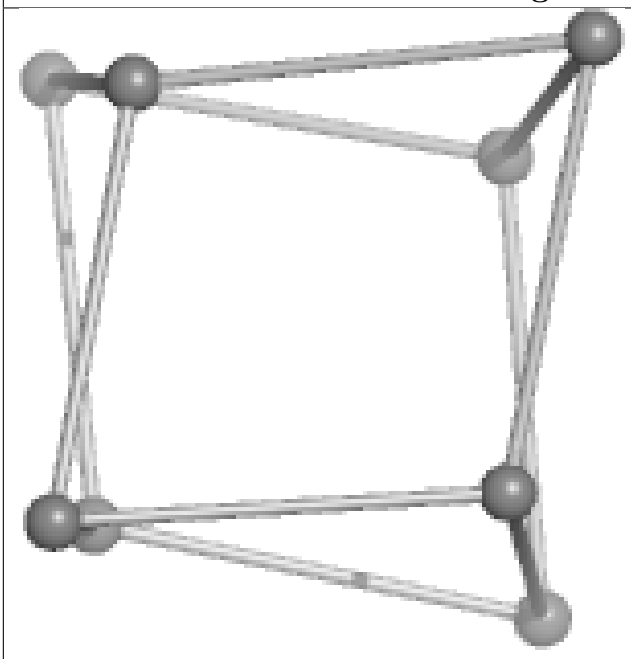


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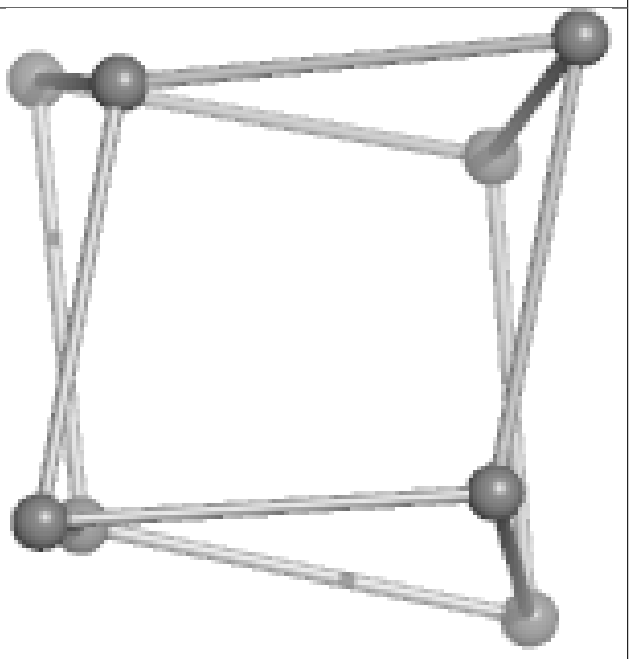


Rings

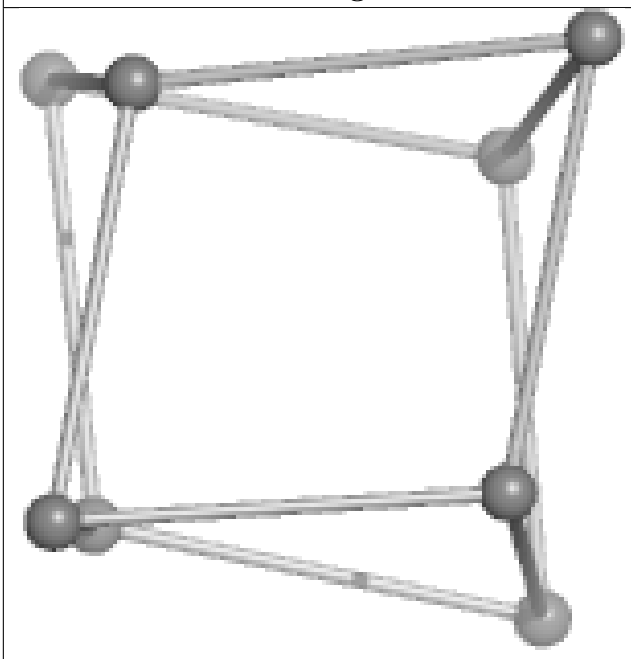
Ligand SF4 C 201



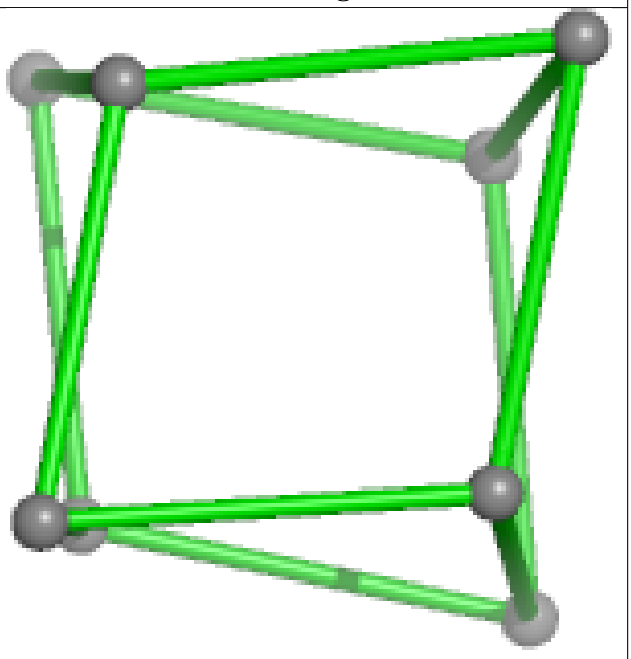
Bond lengths



Bond angles

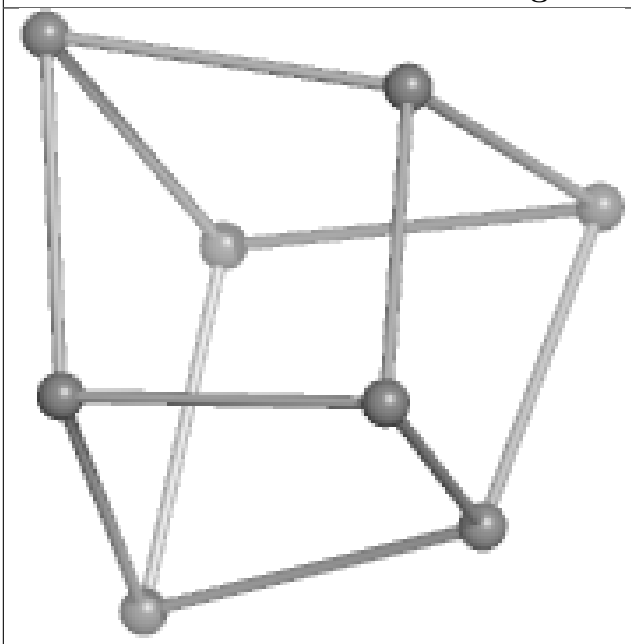


Torsions

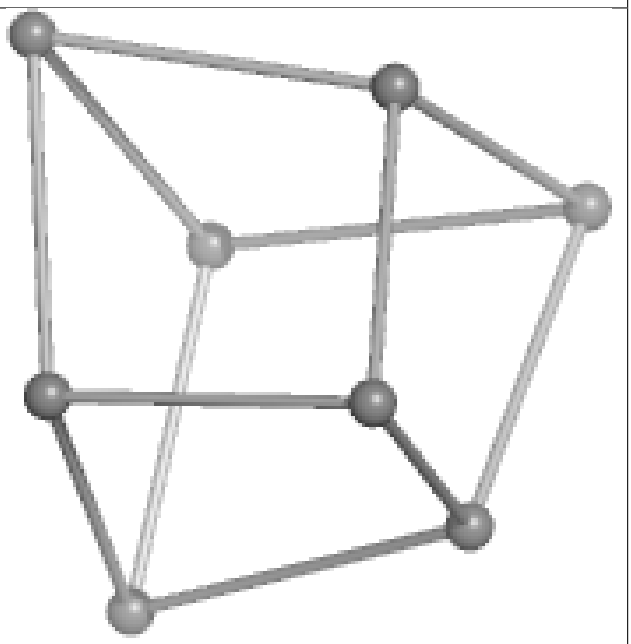


Rings

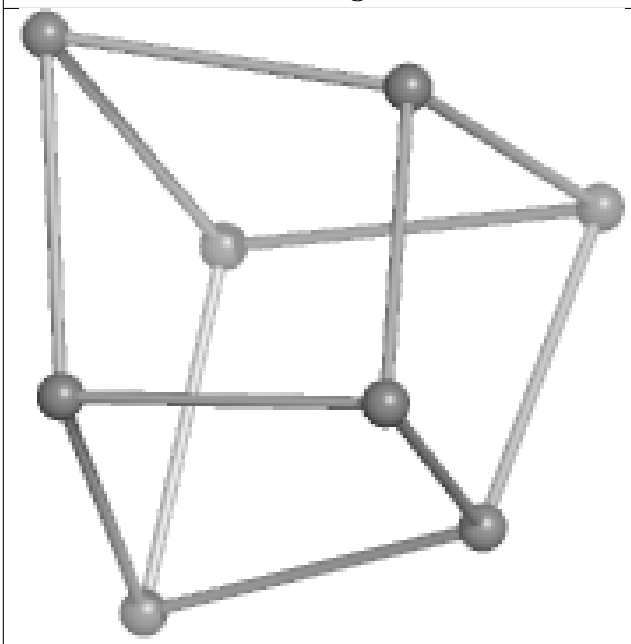
Ligand SF4 A 703



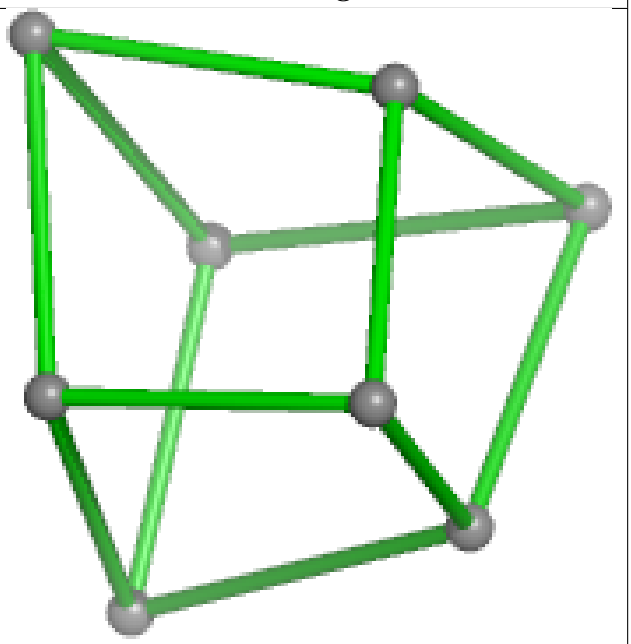
Bond lengths



Bond angles

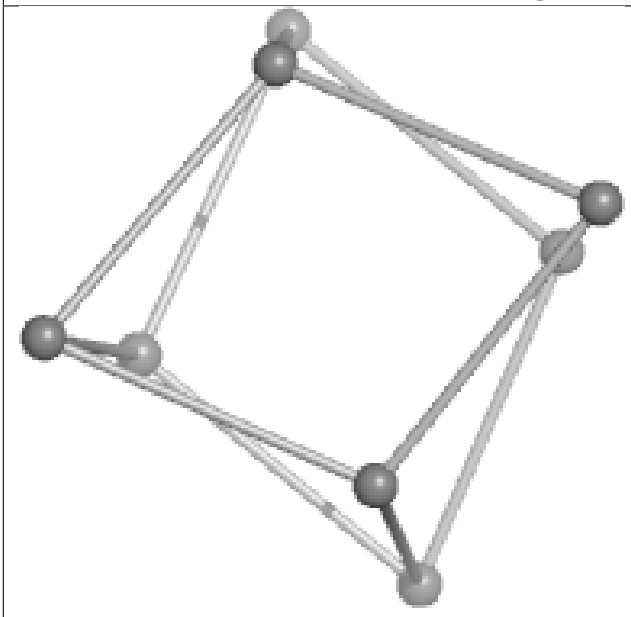


Torsions

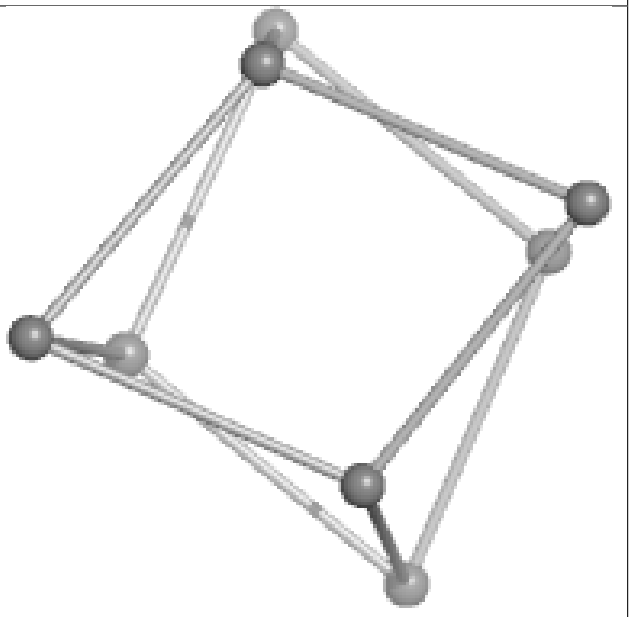


Rings

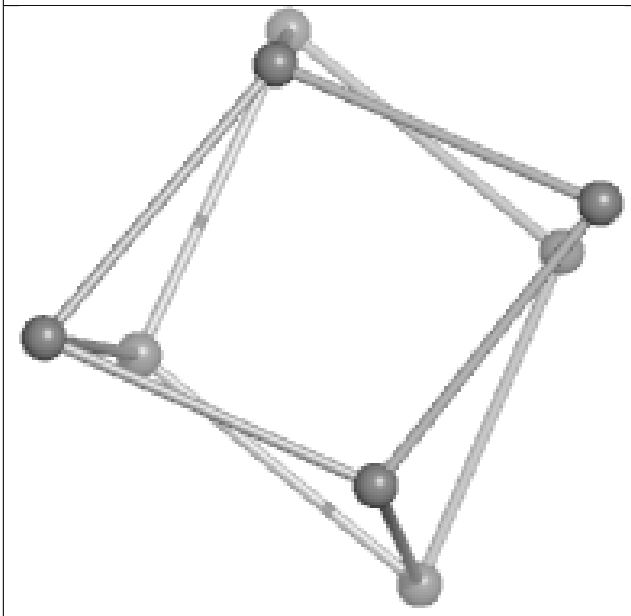
Ligand SF4 C 202



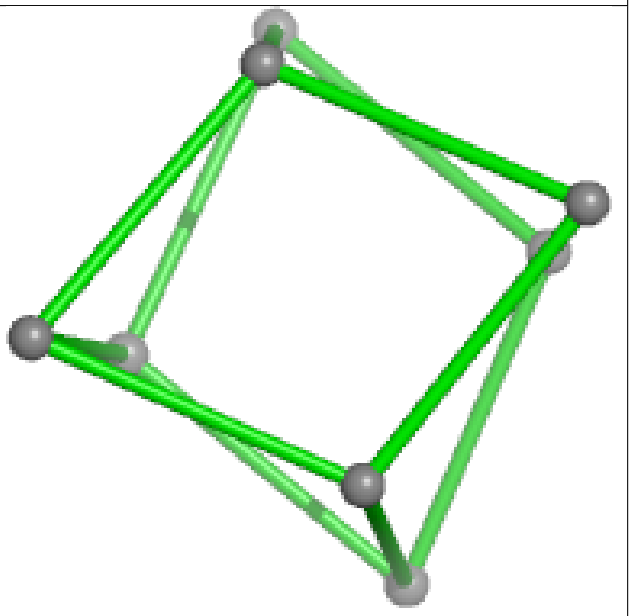
Bond lengths



Bond angles

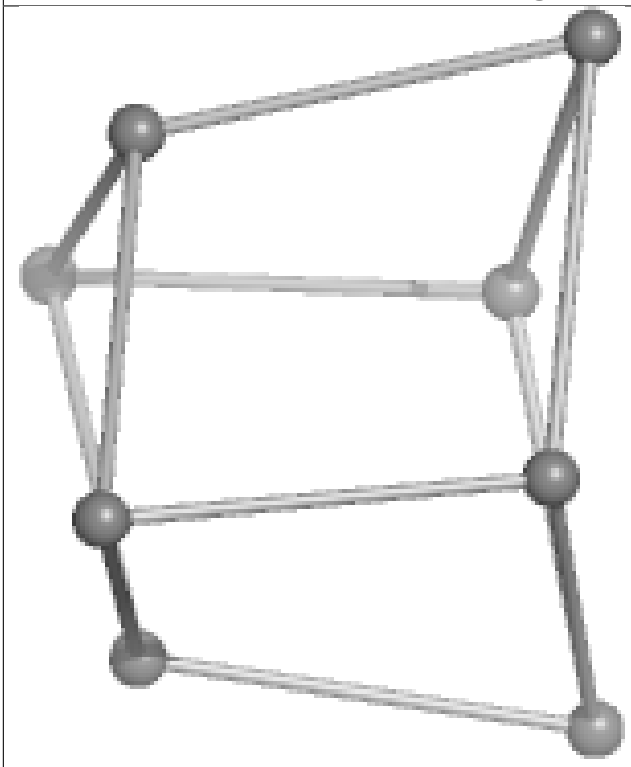


Torsions

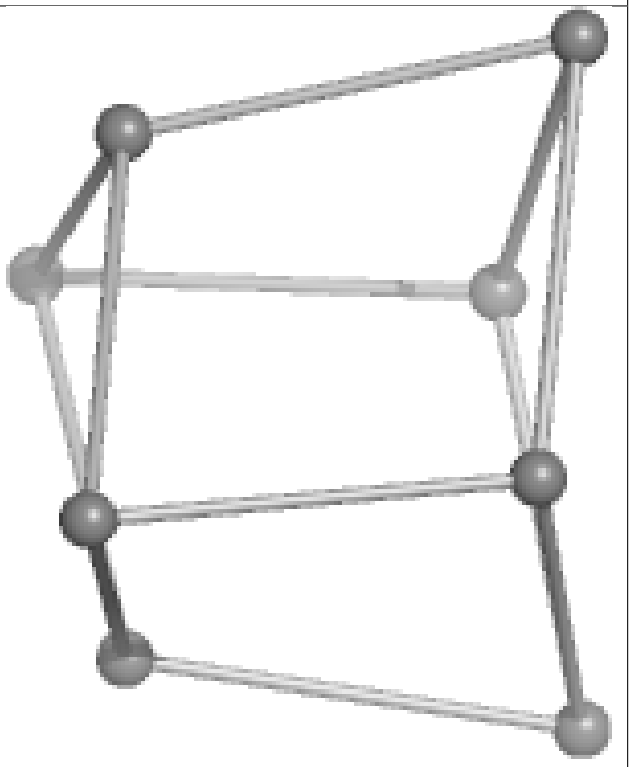


Rings

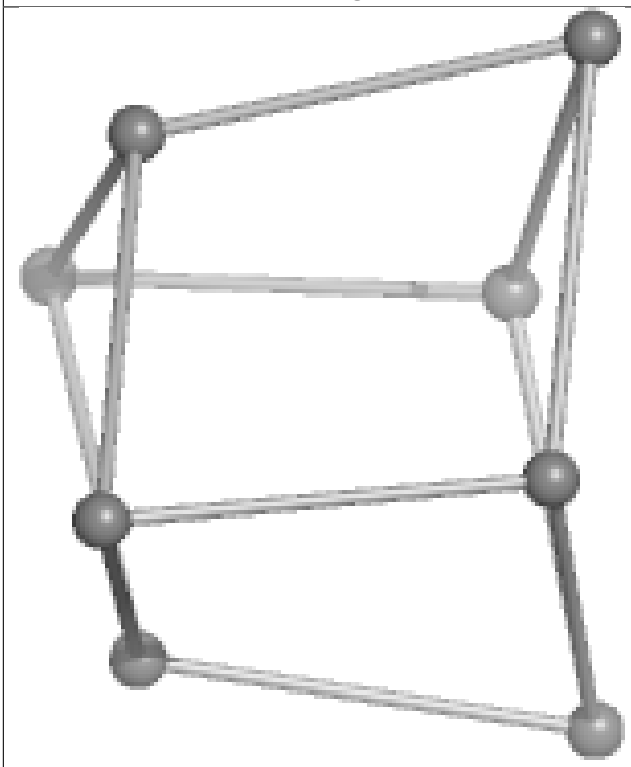
Ligand SF4 D 401



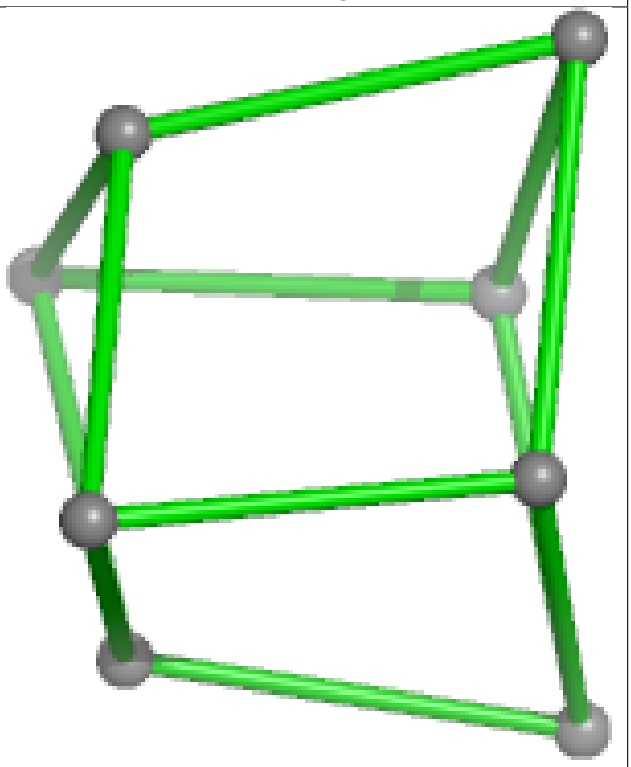
Bond lengths



Bond angles

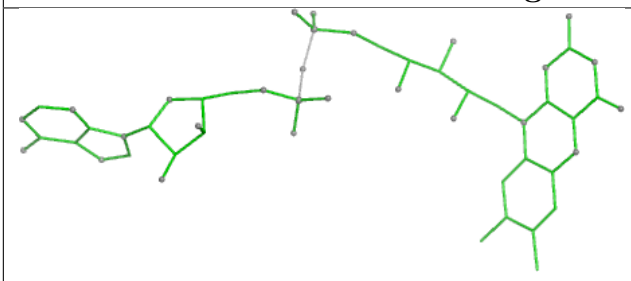


Torsions

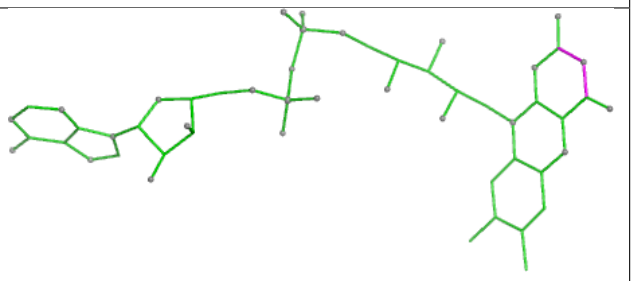


Rings

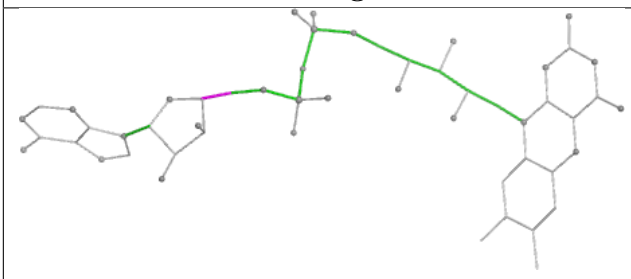
Ligand FAD A 707



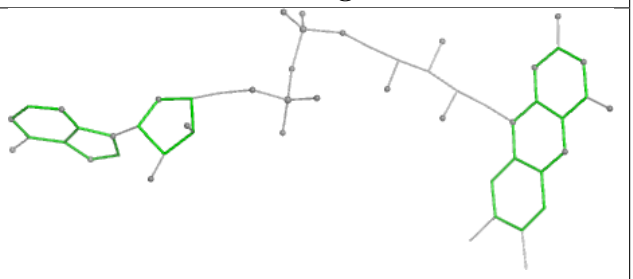
Bond lengths



Bond angles

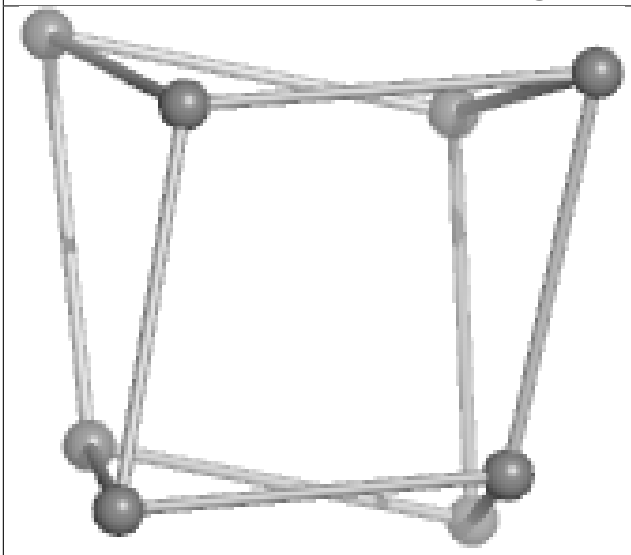


Torsions

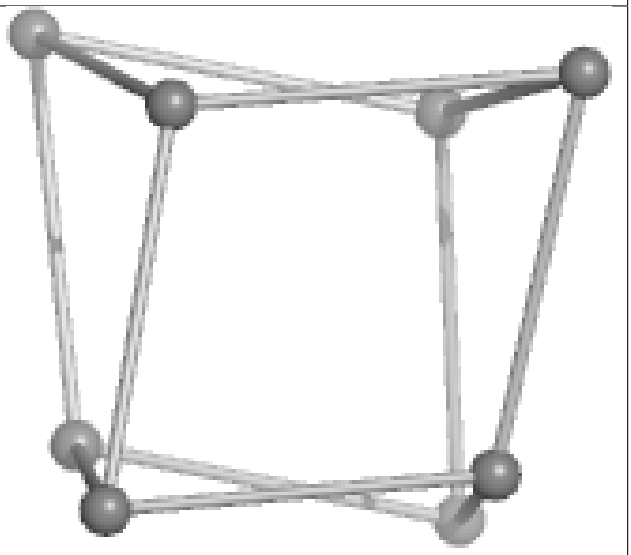


Rings

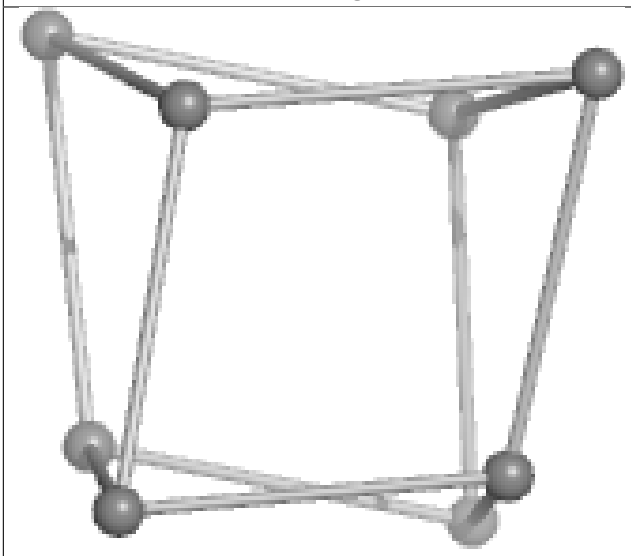
Ligand SF4 A 702



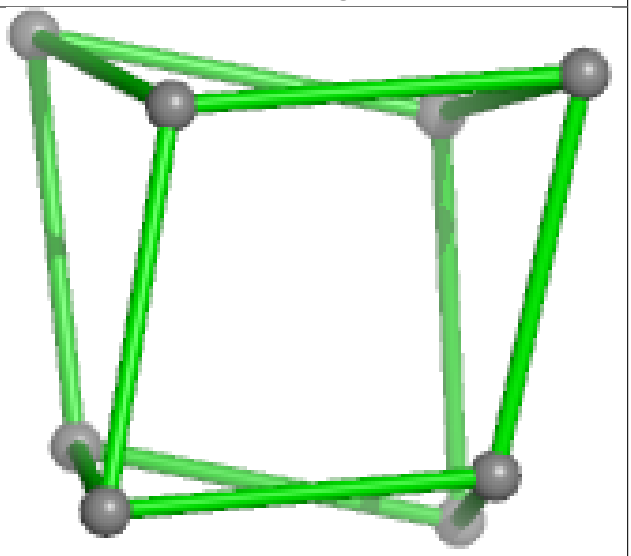
Bond lengths



Bond angles

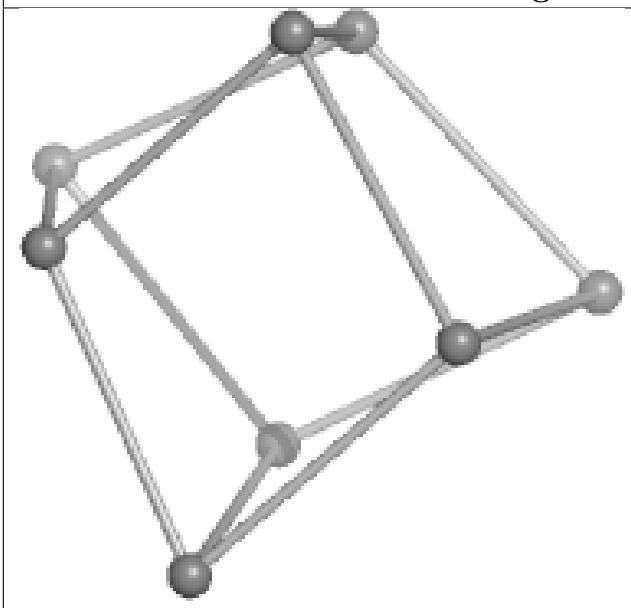


Torsions

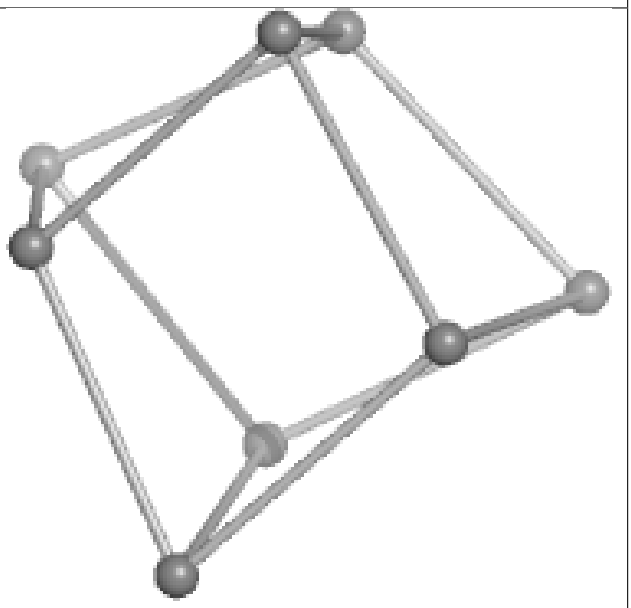


Rings

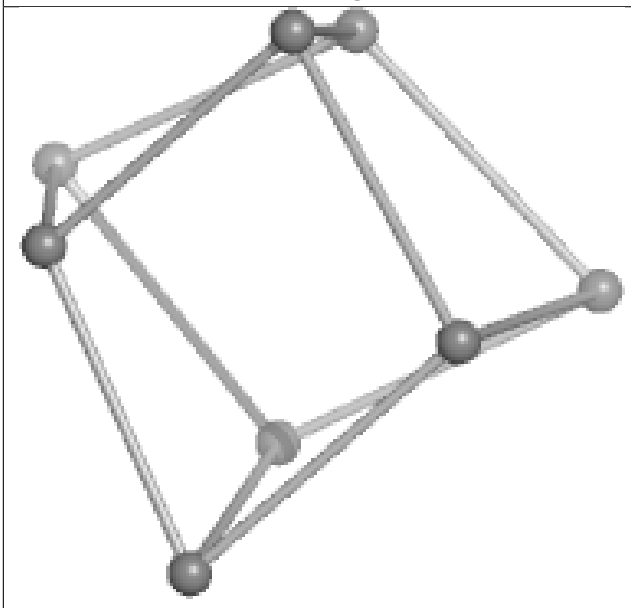
Ligand SF4 E 401



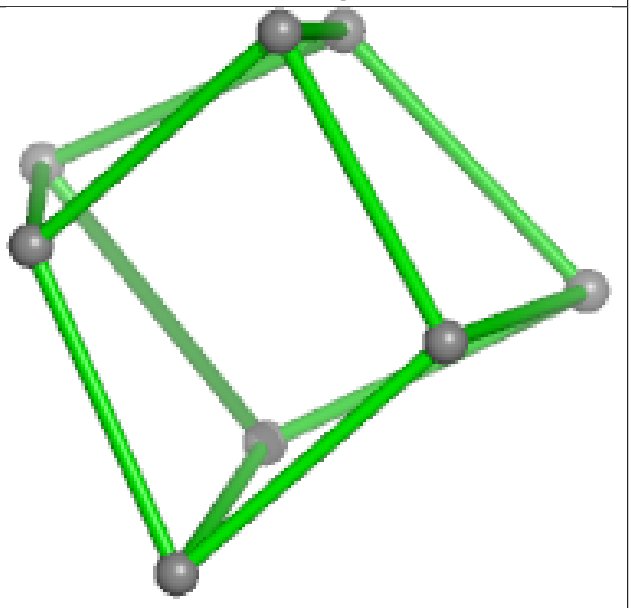
Bond lengths



Bond angles

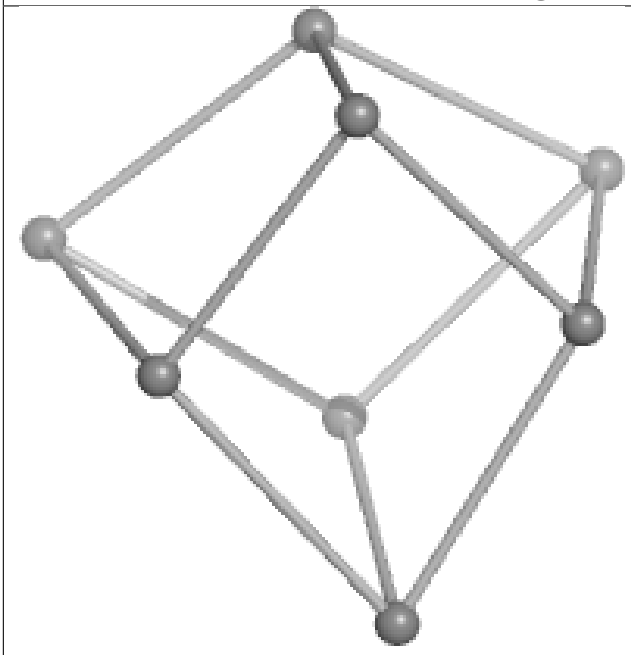


Torsions

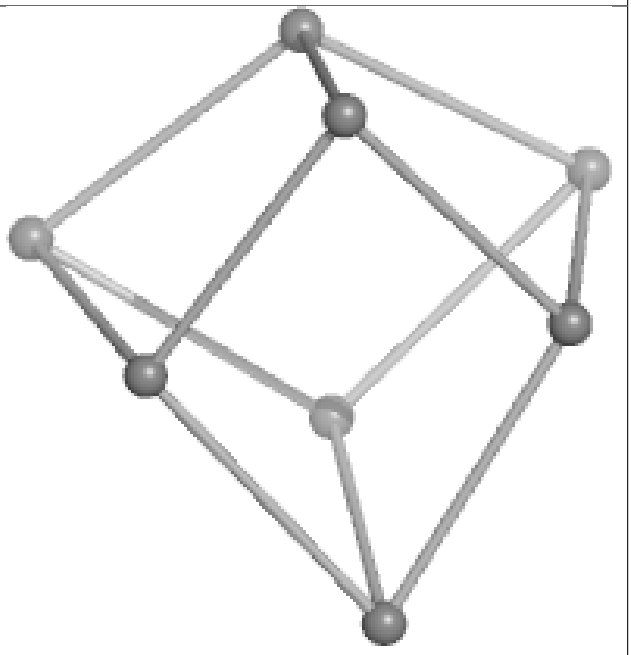


Rings

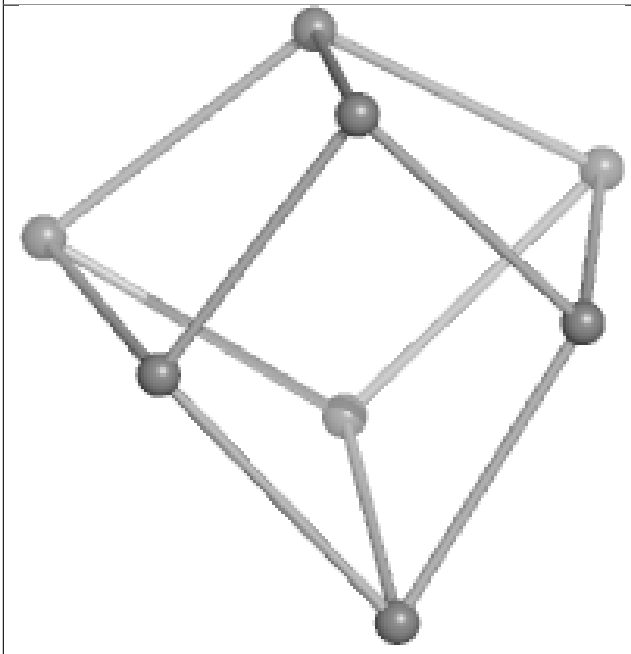
Ligand SF4 E 404



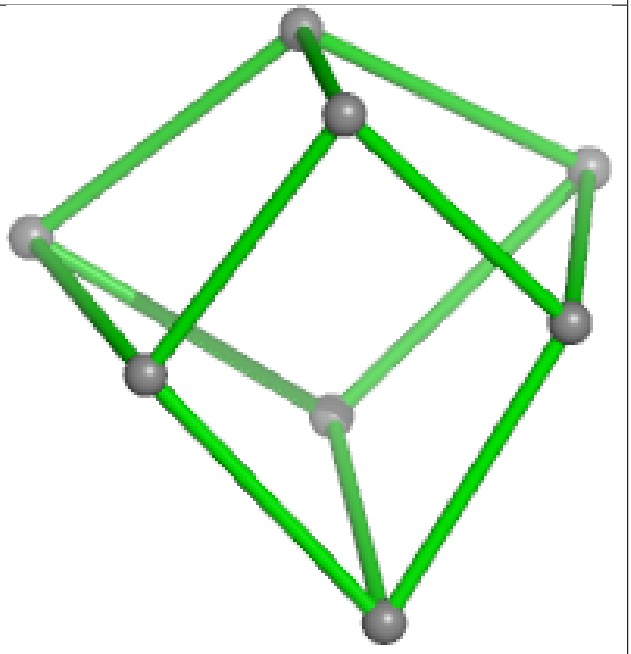
Bond lengths



Bond angles

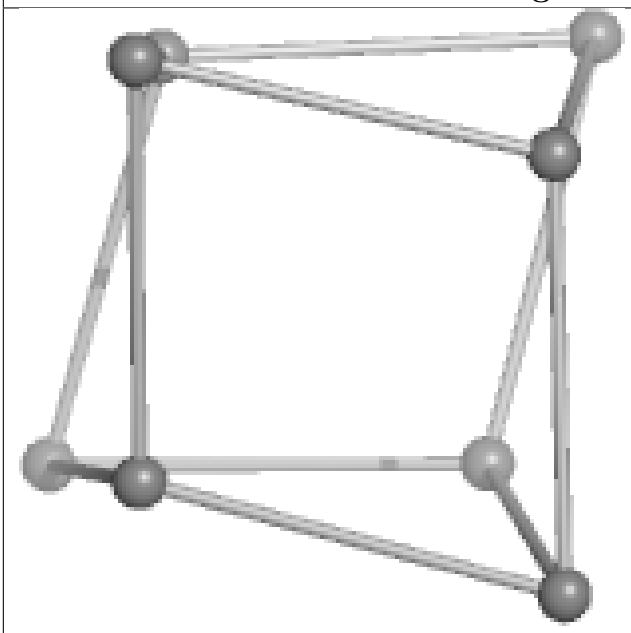


Torsions

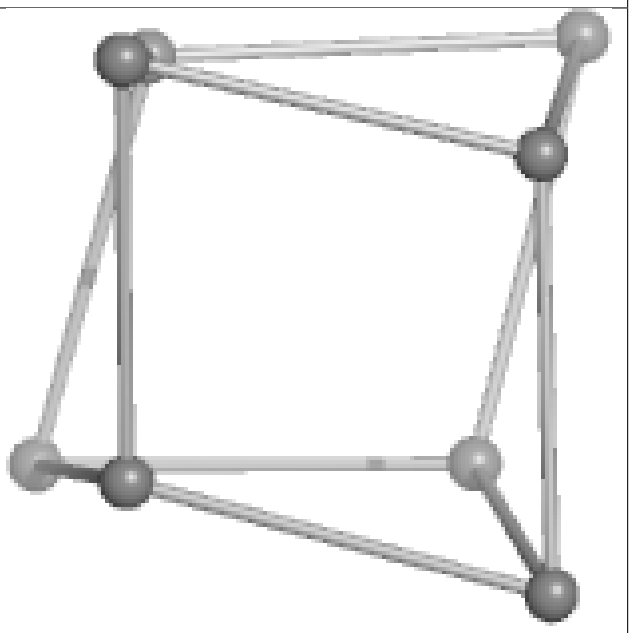


Rings

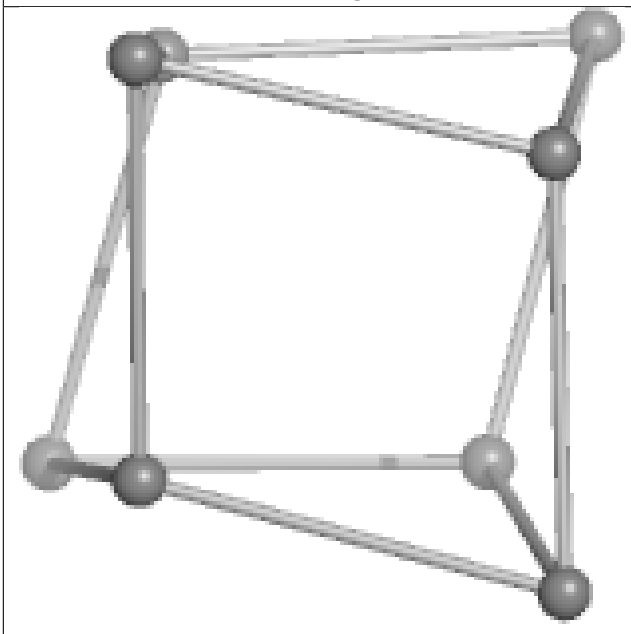
Ligand SF4 E 403



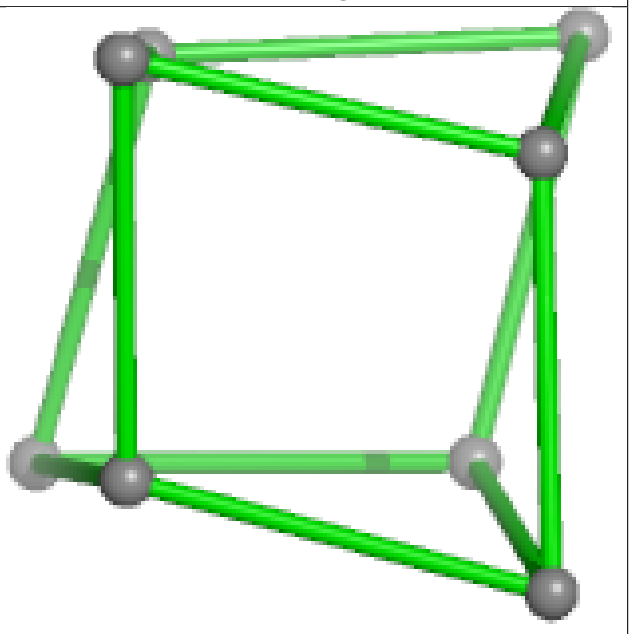
Bond lengths



Bond angles

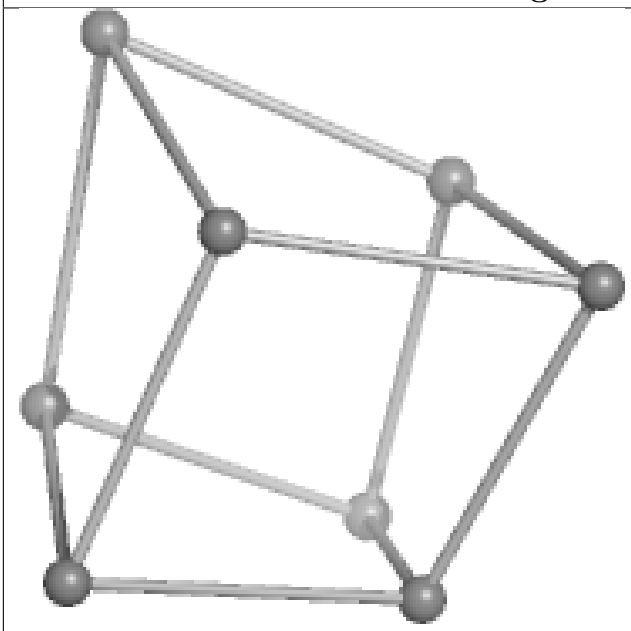


Torsions

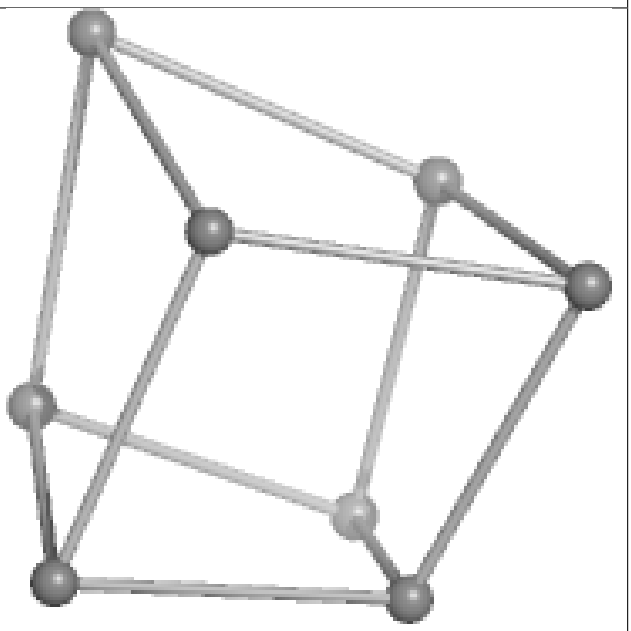


Rings

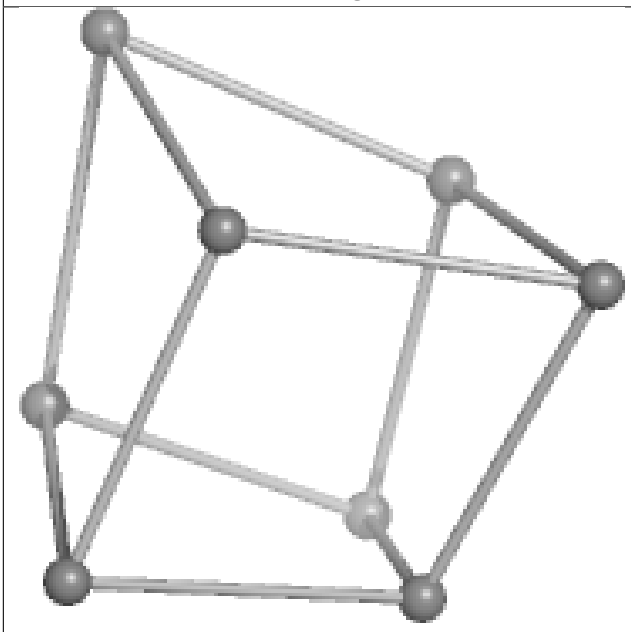
Ligand SF4 A 705



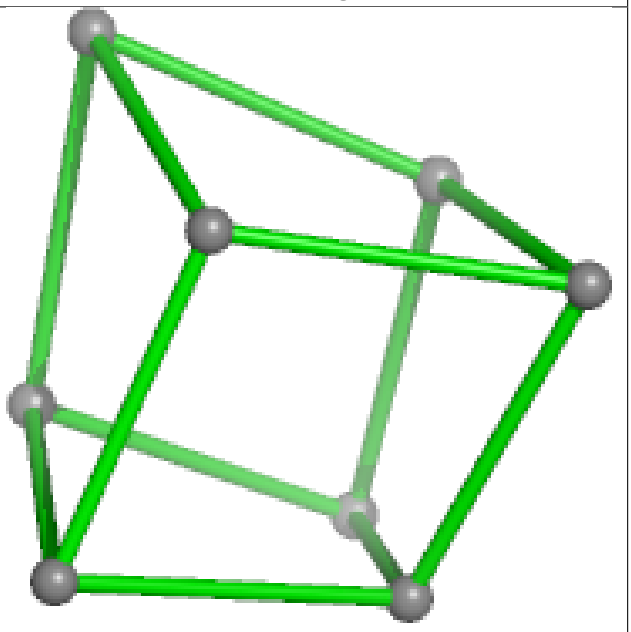
Bond lengths



Bond angles

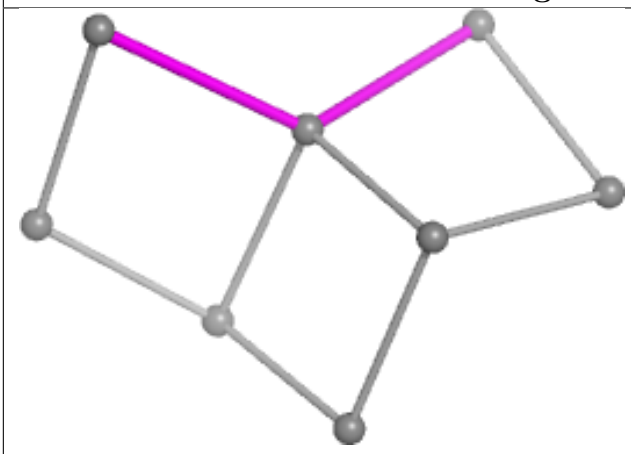


Torsions

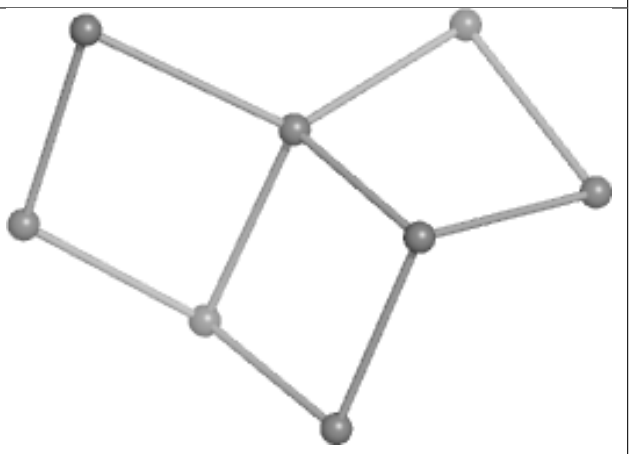


Rings

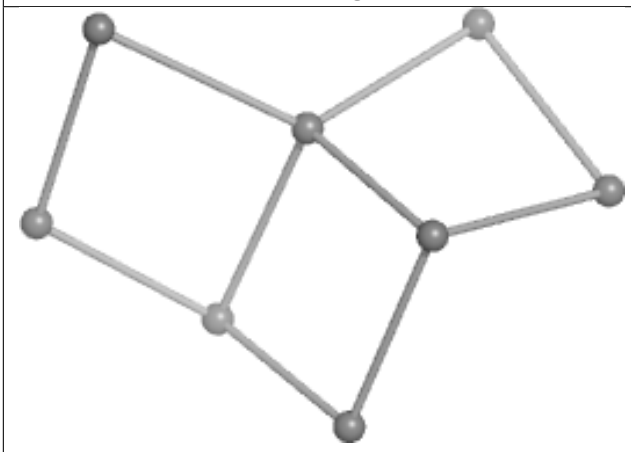
Ligand 9S8 B 401



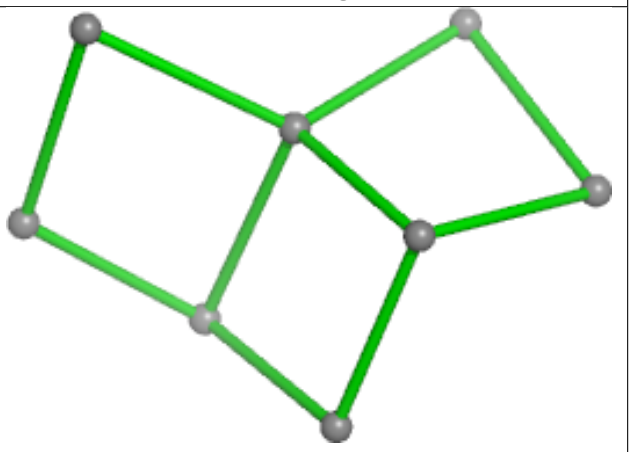
Bond lengths



Bond angles

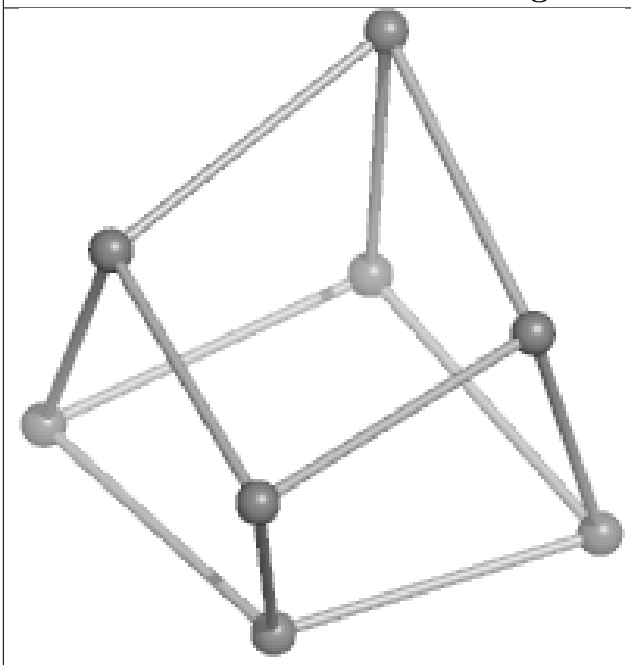


Torsions

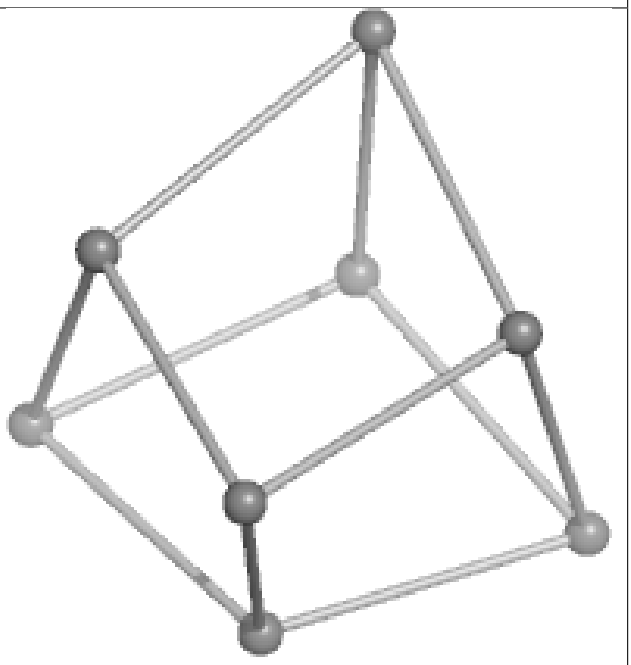


Rings

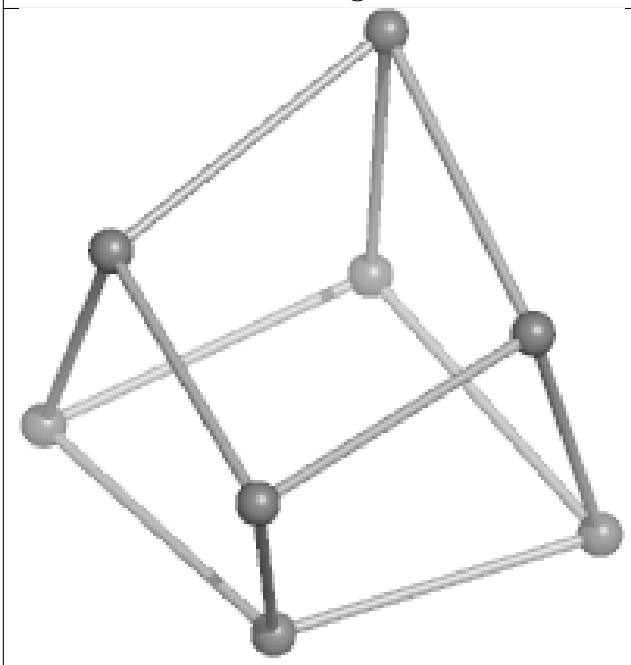
Ligand SF4 A 706



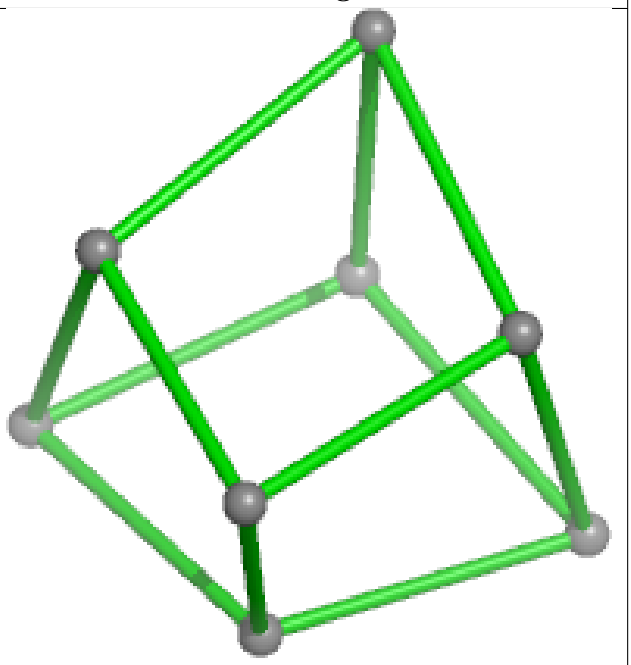
Bond lengths



Bond angles

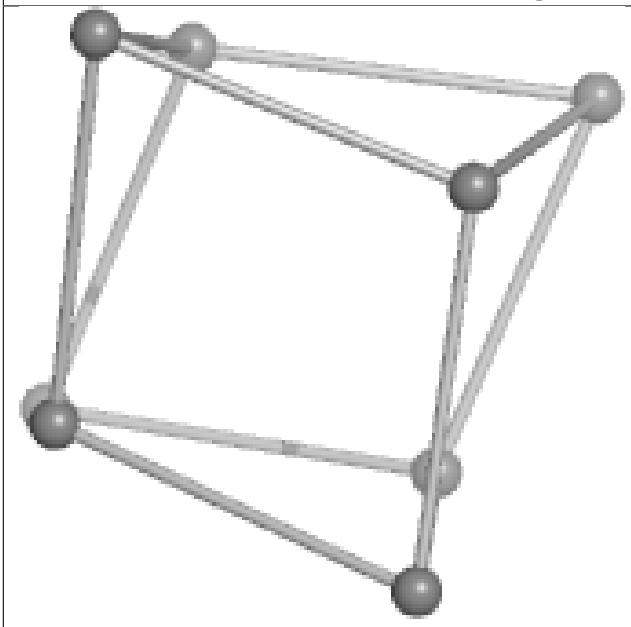


Torsions

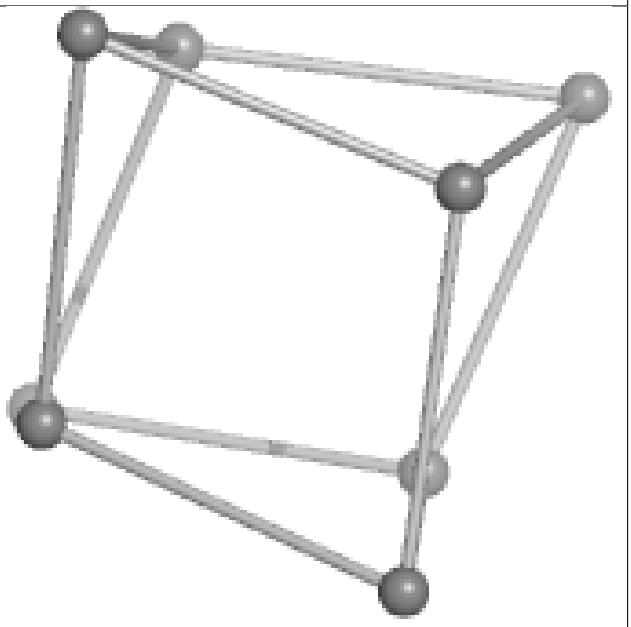


Rings

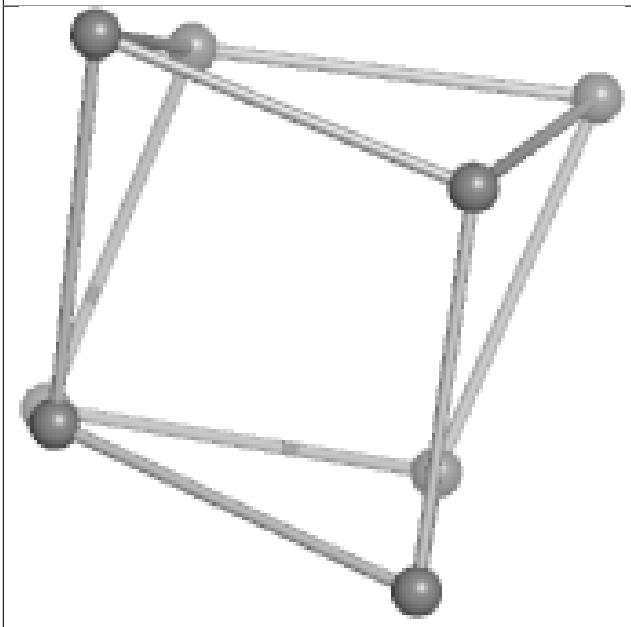
Ligand SF4 A 701



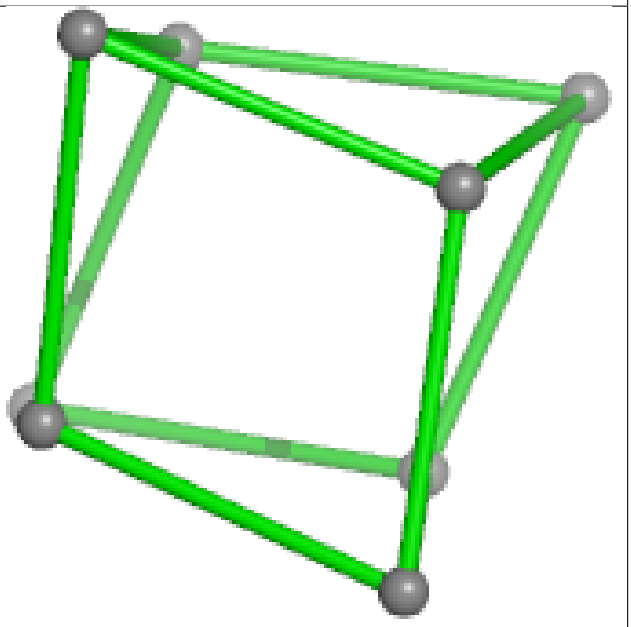
Bond lengths



Bond angles

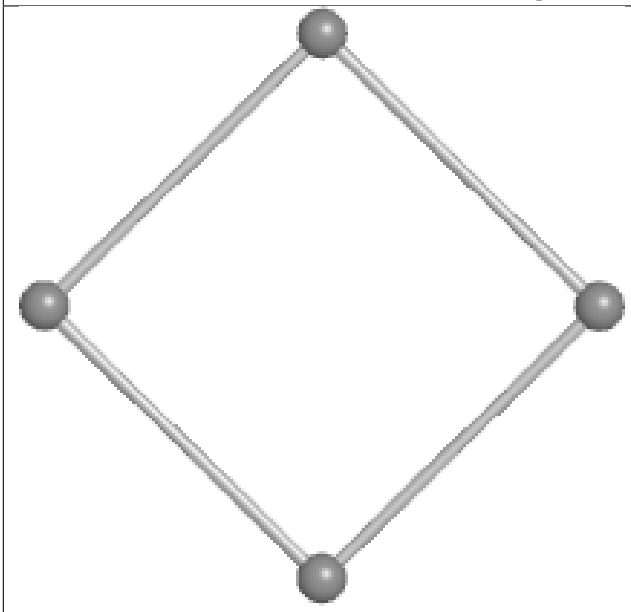


Torsions

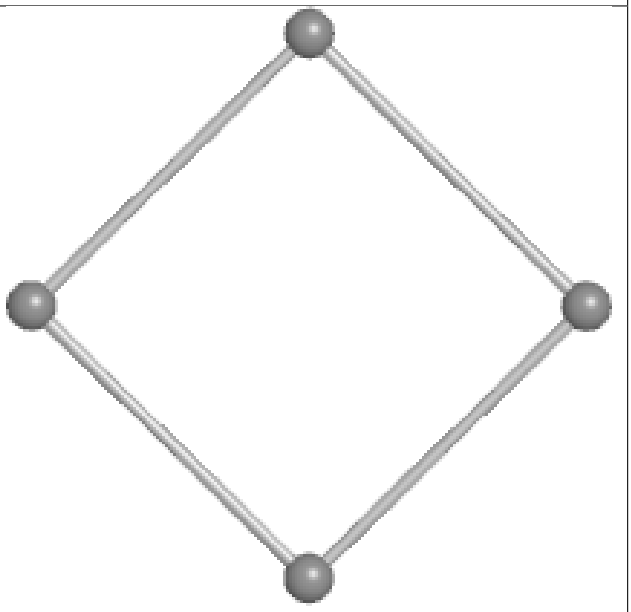


Rings

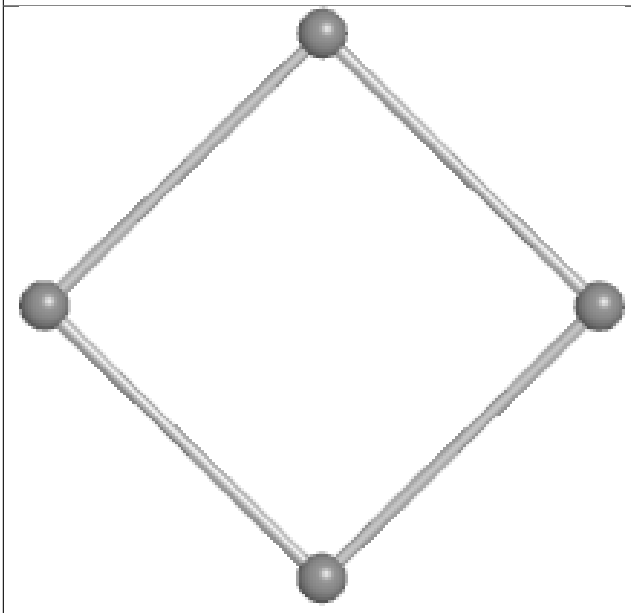
Ligand FES F 201



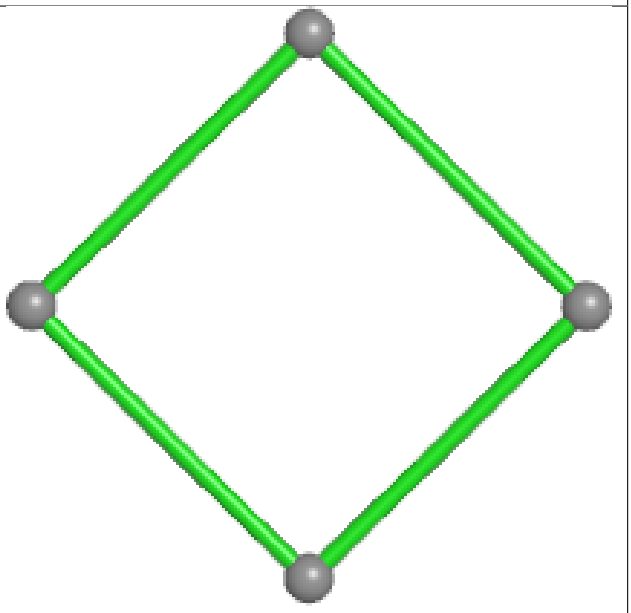
Bond lengths



Bond angles

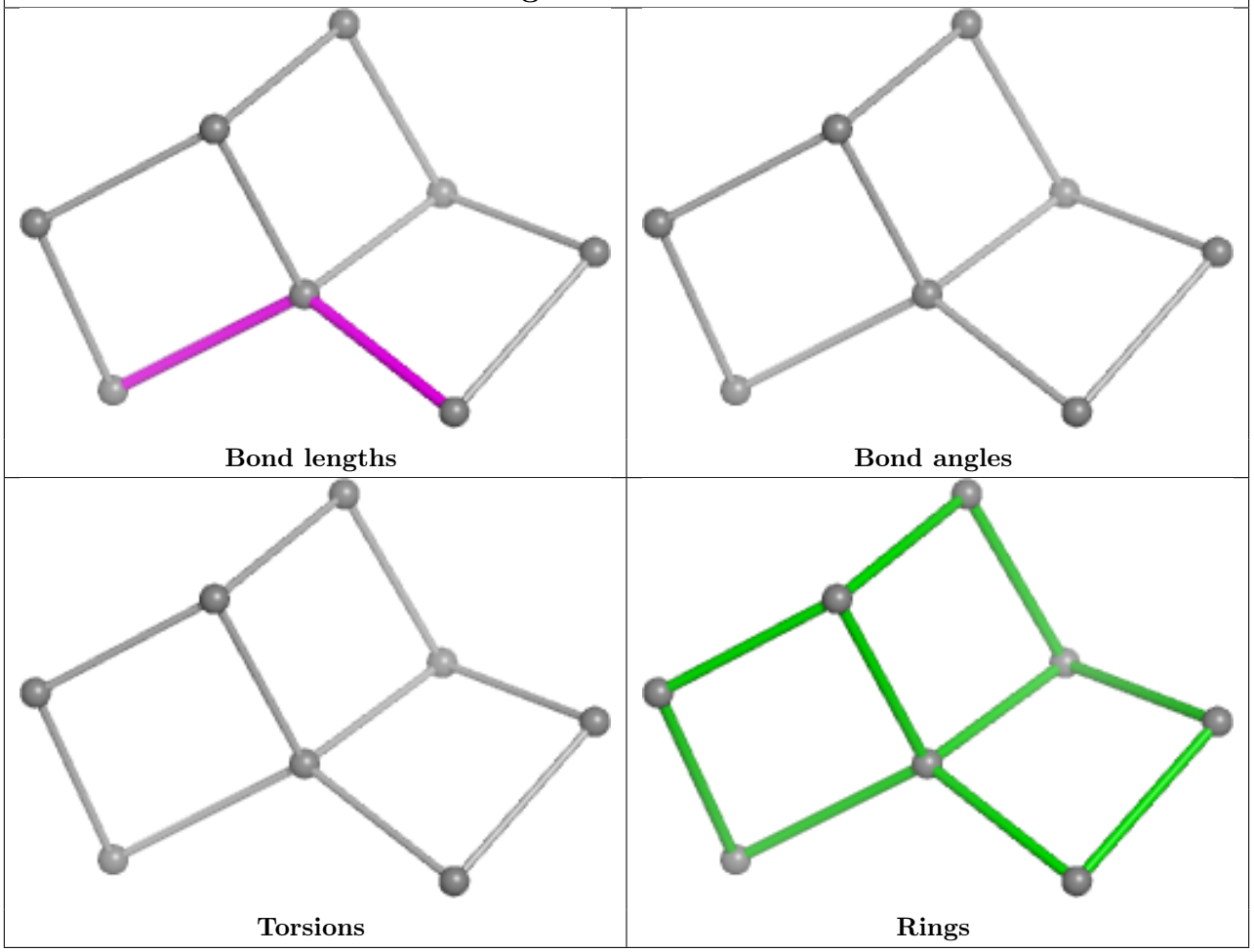


Torsions



Rings

Ligand 9S8 B 400



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.

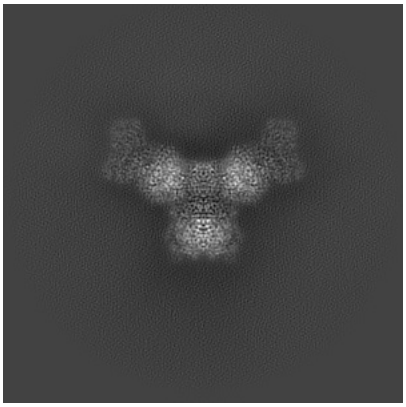
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19534. These allow visual inspection of the internal detail of the map and identification of artifacts.

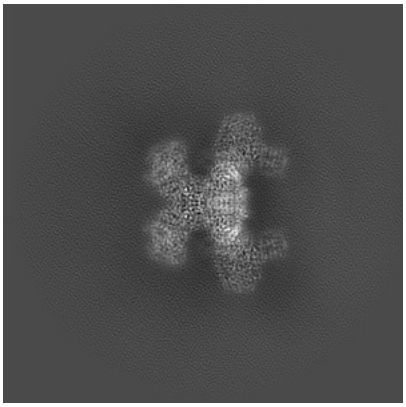
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

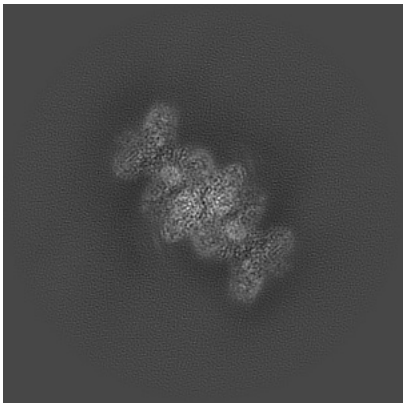
6.1.1 Primary map



X



Y

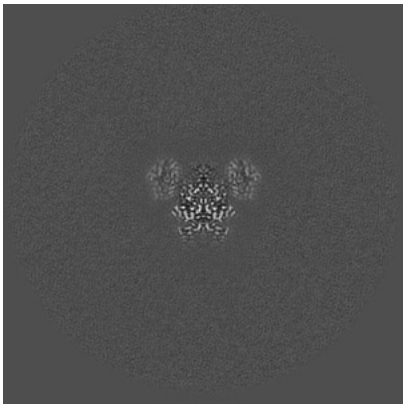


Z

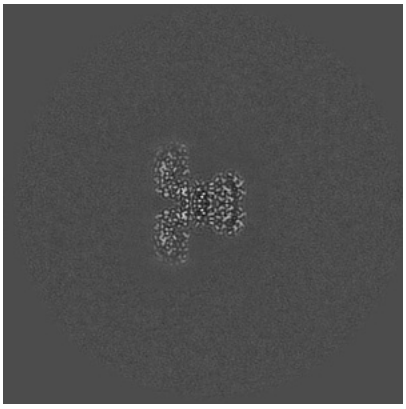
The images above show the map projected in three orthogonal directions.

6.2 Central slices

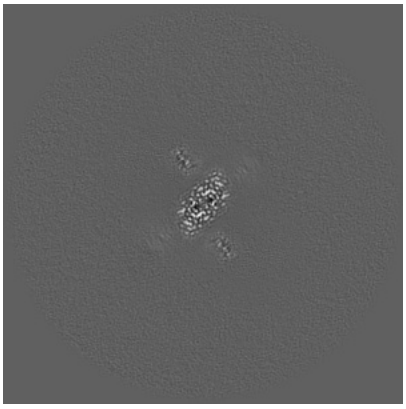
6.2.1 Primary map



X Index: 224



Y Index: 224

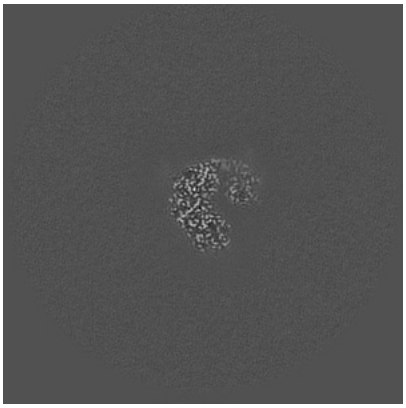


Z Index: 224

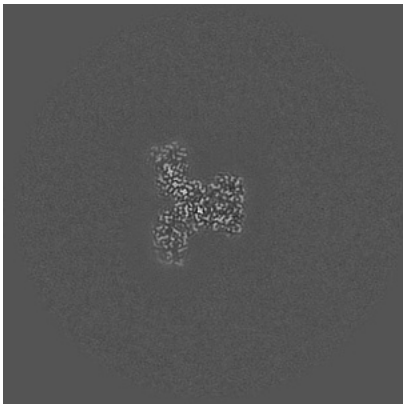
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

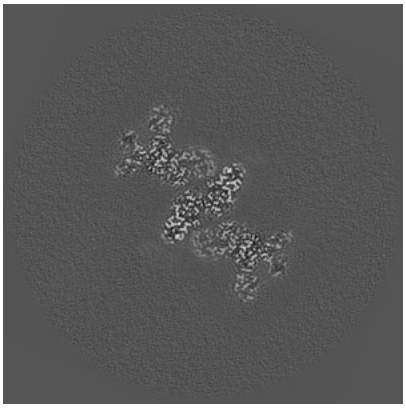
6.3.1 Primary map



X Index: 208



Y Index: 219

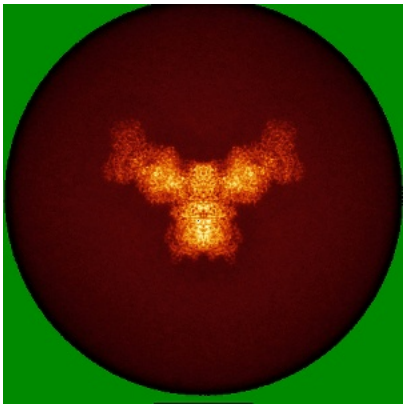


Z Index: 252

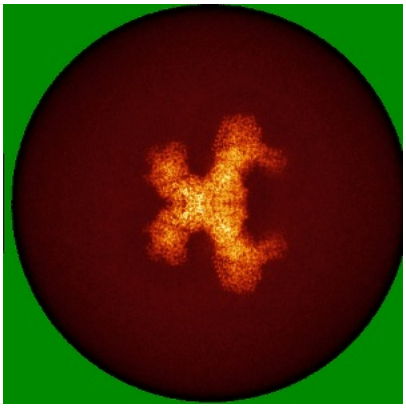
The images above show the largest variance slices of the map in three orthogonal directions.

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

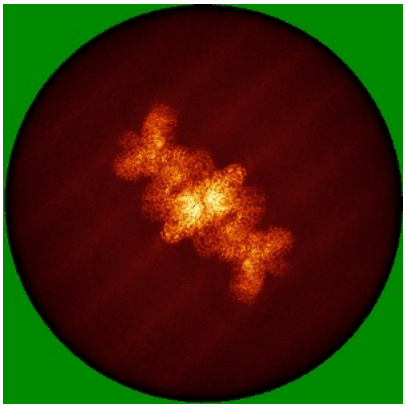
6.4.1 Primary map



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

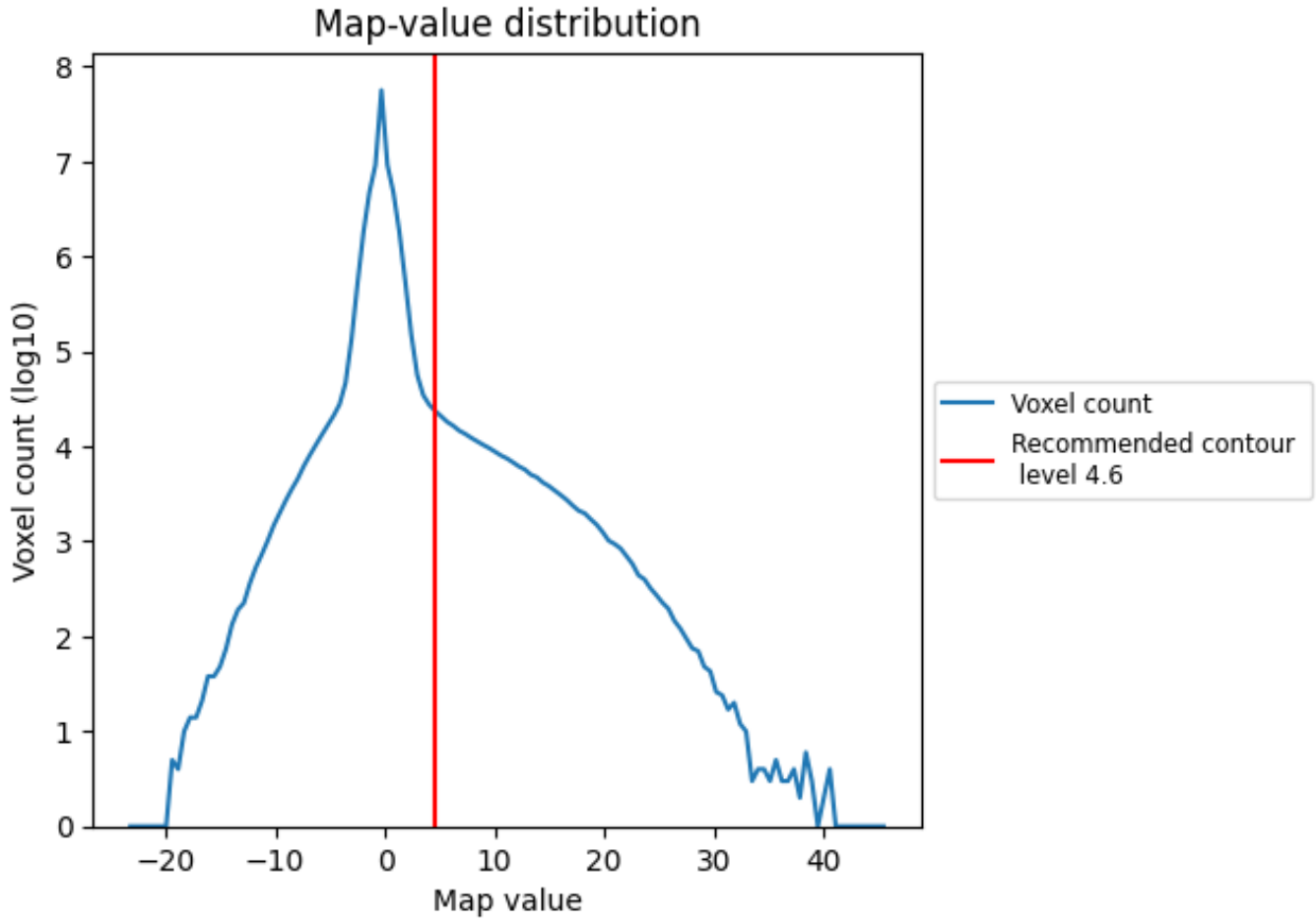
6.6 Mask visualisation (i)

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

7 Map analysis

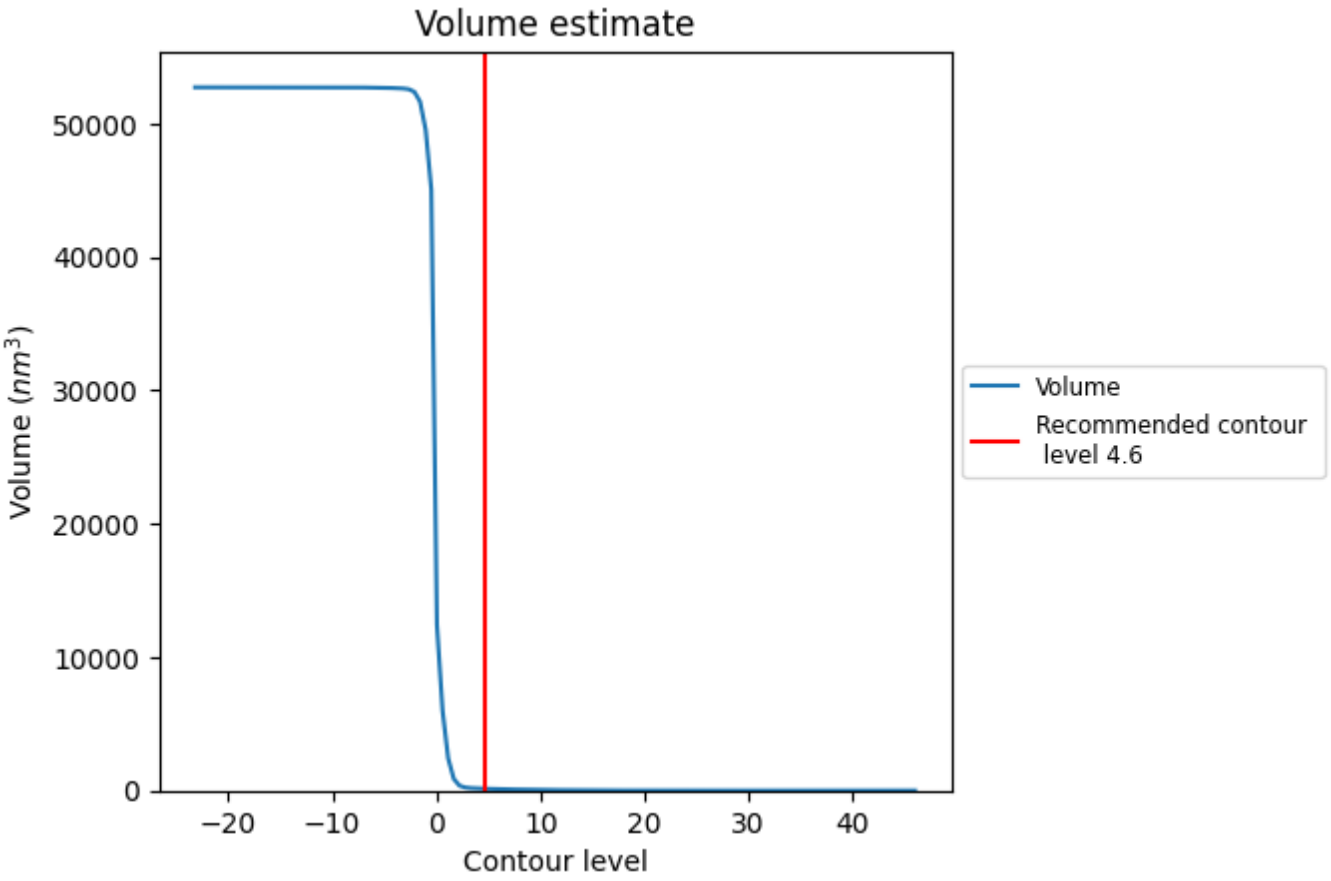
This section contains the results of statistical analysis of the map.

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.

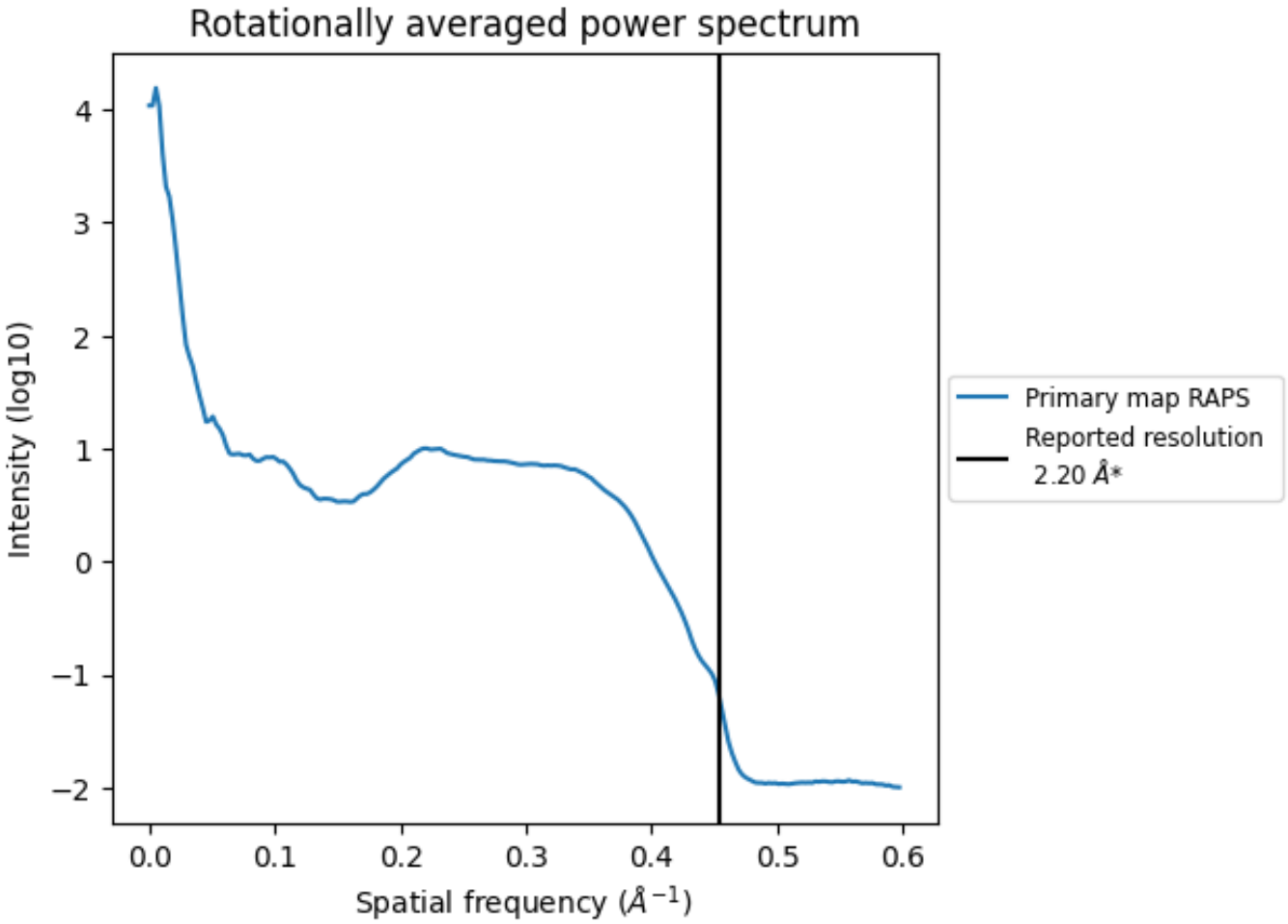
7.2 Volume estimate



The volume at the recommended contour level is 140 nm^3; this corresponds to an approximate mass of 127 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 0.455 Å^{-1}

8 Fourier-Shell correlation

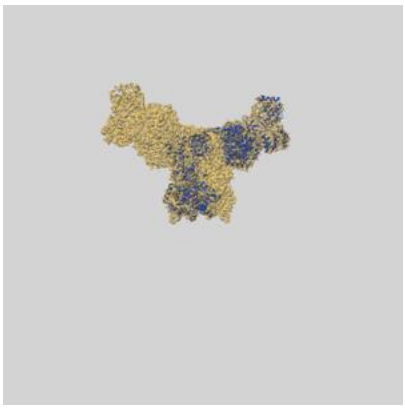
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

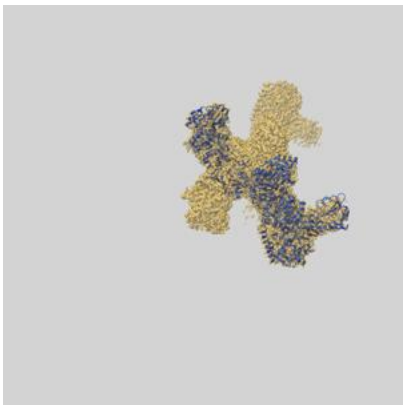
This section contains information regarding the fit between EMDB map EMD-19534 and PDB model 8RVV. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

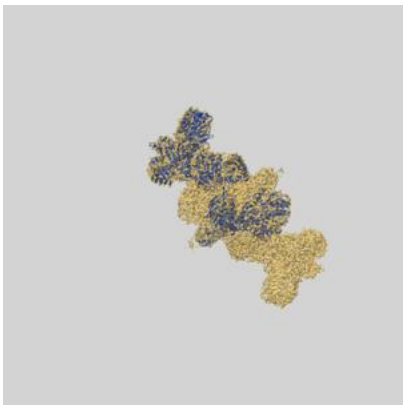
9.1.1 Map-model overlay



X

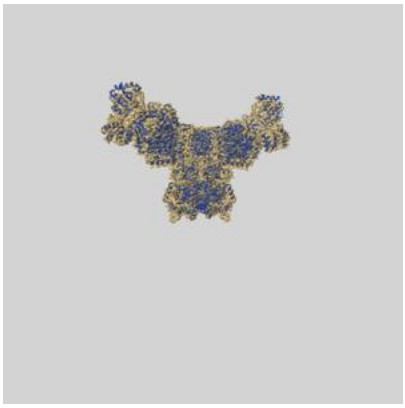


Y

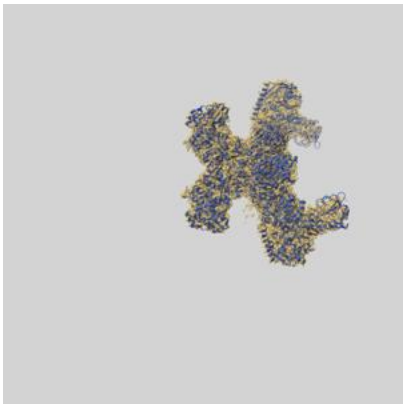


Z

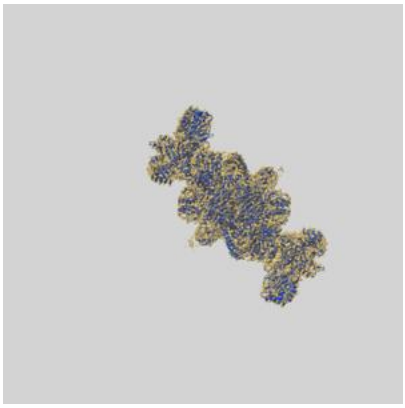
9.1.2 Map-model assembly overlay



X



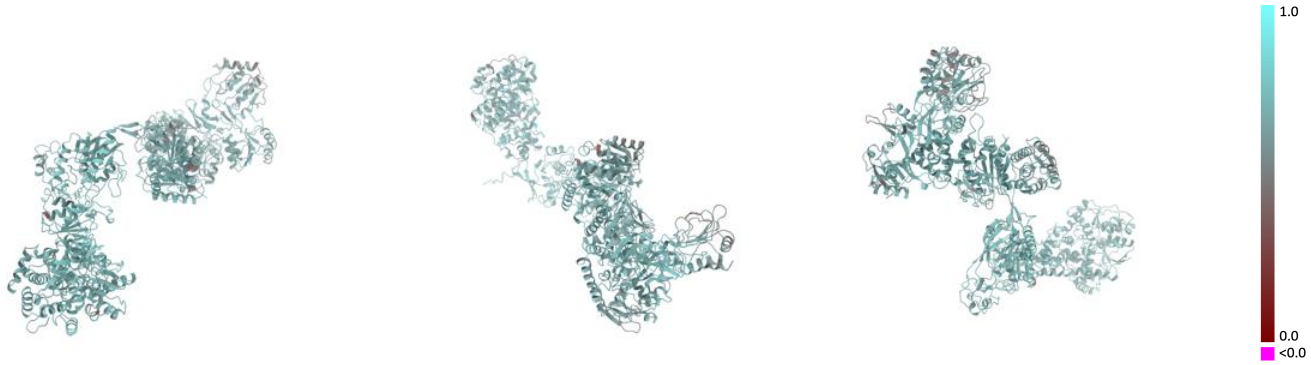
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.6 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.

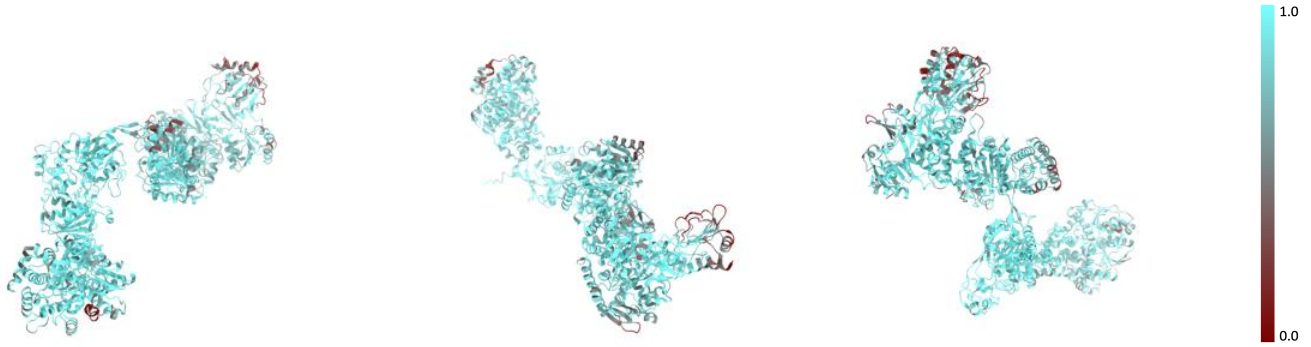
9.2 Q-score mapped to coordinate model (i)



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.

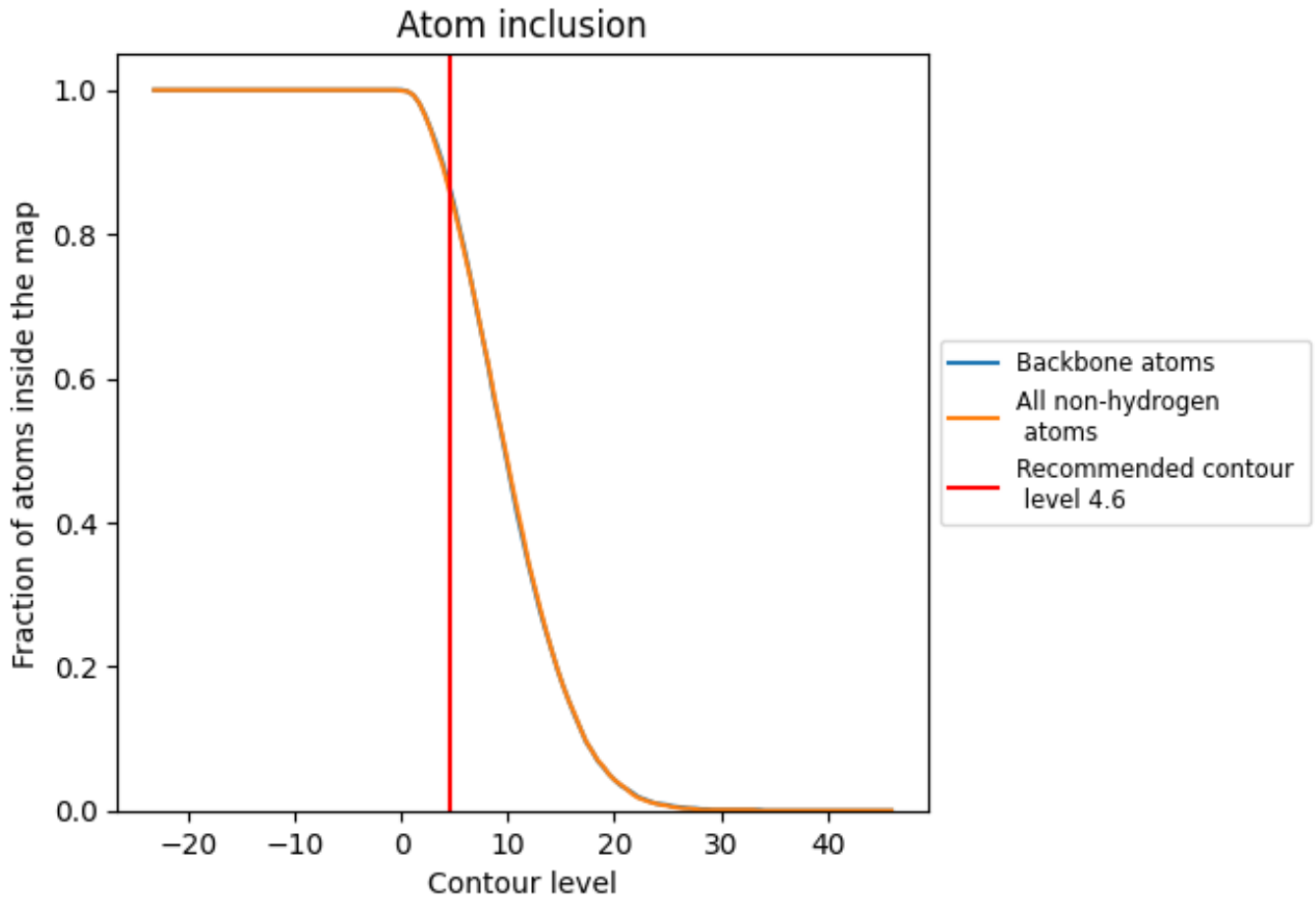
9.3 Atom inclusion mapped to coordinate model (i)



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 (4.6).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (4.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8560	0.6620
A	0.8980	0.6650
B	0.8520	0.6690
C	0.9030	0.6810
D	0.7620	0.6330
E	0.8480	0.6580
F	0.9520	0.6960

