wwPDB EM Validation Summary Report (i)

Aug 29, 2026 – 07:43 am BST

PDB ID	:	9T1S / pdb_00009t1s
EMDB ID	:	EMD-55451
Title	:	Heterodisulfide-Hydrogenase-Formate Dehydrogenase dimer
Authors	:	Paul, S.; Schuller, J.M.
Deposited on	:	2025-10-22
Resolution	:	4.00 Å(reported)

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

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

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

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

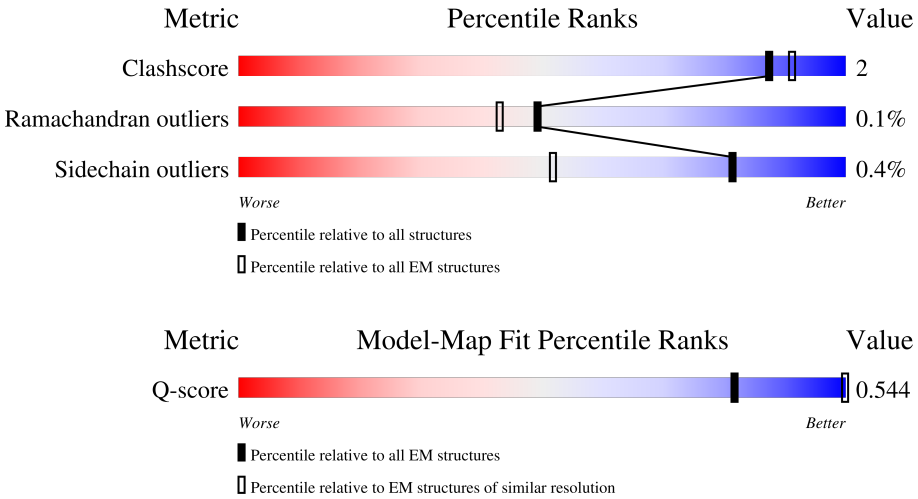
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	658	94% 6%
1	B	658	95% 5%
2	C	293	98%
2	D	293	95% 5%

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Mol	Chain	Length	Quality of chain
3	E	184	96%
3	F	184	95% 5%
4	G	418	95% 5%
5	H	288	96%
6	I	134	94% 6%
6	J	134	88% 12%
7	K	27	89% 11%
8	L	674	93% 7%
9	M	383	94% 6%

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
13	FCO	G	419	-	-	X	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 33539 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CoB–CoM heterodisulfide reductase iron-sulfur subunit A.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	658	Total	C	N	O	S	Se	0	0
			4970	3126	834	957	52	1		
1	B	658	Total	C	N	O	S	Se	0	0
			4970	3126	834	957	52	1		

- Molecule 2 is a protein called Heterodisulfide reductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	293	Total	C	N	O	S	0	0
			2236	1420	373	419	24		
2	D	293	Total	C	N	O	S	0	0
			2236	1420	373	419	24		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	144	ALA	ASN	conflict	UNP A0A7J9NT94
D	144	ALA	ASN	conflict	UNP A0A7J9NT94

- Molecule 3 is a protein called H(2)/formate:CoB-CoM heterodisulfide,ferredoxin reductase subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	184	Total	C	N	O	S	0	0
			1426	892	252	268	14		
3	F	184	Total	C	N	O	S	0	0
			1426	892	252	268	14		

- Molecule 4 is a protein called Coenzyme F420-reducing hydrogenase, alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	418	Total	C	N	O	S	0	0
			3207	2033	553	604	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	288	Total	C	N	O	S	0	0
			2149	1360	354	416	19		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	I	134	Total	C	N	O	S	Se	0	0
			1018	647	173	187	9	2		
6	J	134	Total	C	N	O	S	Se	0	0
			1018	647	173	187	9	2		

- Molecule 7 is a protein called F420 non-reducing hydrogenase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	K	27	Total	C	N	O	S	Se	0	0
			211	134	34	39	3	1		

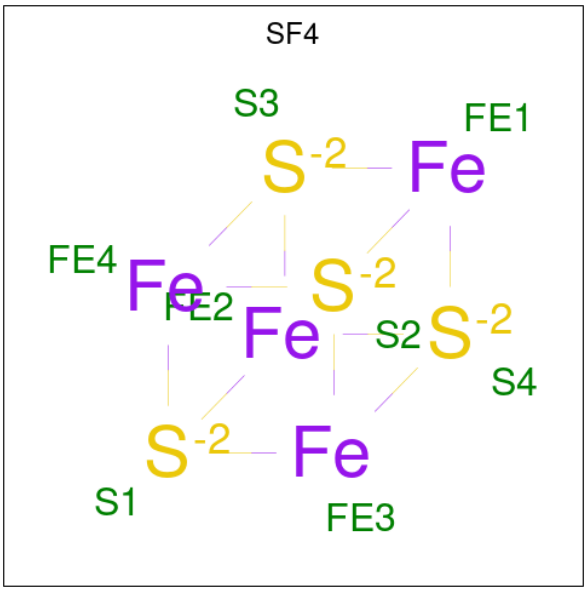
- Molecule 8 is a protein called formate dehydrogenase (coenzyme F420).

Mol	Chain	Residues	Atoms						AltConf	Trace
8	L	674	Total	C	N	O	S	Se	0	0
			5202	3280	886	997	38	1		

- Molecule 9 is a protein called formate dehydrogenase (coenzyme F420).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	383	Total	C	N	O	S	0	0
			2976	1879	500	563	34		

- Molecule 10 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total Fe S 8 4 4	0
10	A	1	Total Fe S 8 4 4	0
10	A	1	Total Fe S 8 4 4	0
10	A	1	Total Fe S 8 4 4	0
10	A	1	Total Fe S 8 4 4	0
10	A	1	Total Fe S 8 4 4	0
10	B	1	Total Fe S 8 4 4	0
10	B	1	Total Fe S 8 4 4	0
10	B	1	Total Fe S 8 4 4	0
10	B	1	Total Fe S 8 4 4	0
10	B	1	Total Fe S 8 4 4	0
10	B	1	Total Fe S 8 4 4	0
10	E	1	Total Fe S 8 4 4	0
10	E	1	Total Fe S 8 4 4	0

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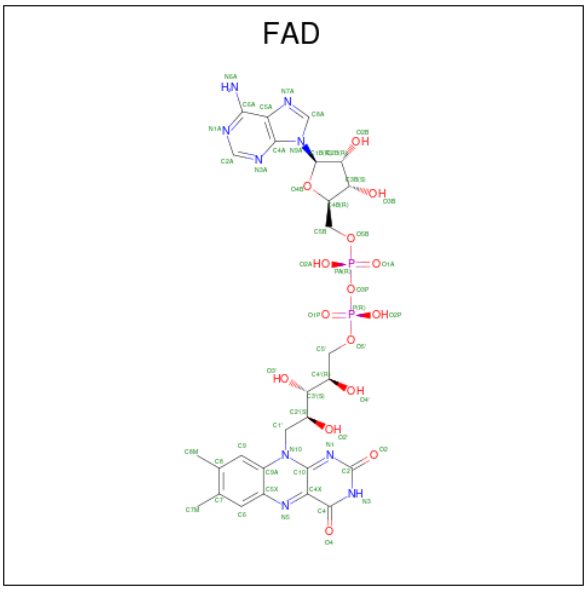
Mol	Chain	Residues	Atoms	AltConf
10	F	1	Total Fe S 8 4 4	0
10	F	1	Total Fe S 8 4 4	0
10	H	1	Total Fe S 8 4 4	0
10	H	1	Total Fe S 8 4 4	0
10	H	1	Total Fe S 8 4 4	0
10	L	1	Total Fe S 8 4 4	0
10	M	1	Total Fe S 8 4 4	0
10	M	1	Total Fe S 8 4 4	0
10	M	1	Total Fe S 8 4 4	0
10	M	1	Total Fe S 8 4 4	0

- Molecule 11 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
11	A	1	Total C N O P 53 27 9 15 2	0

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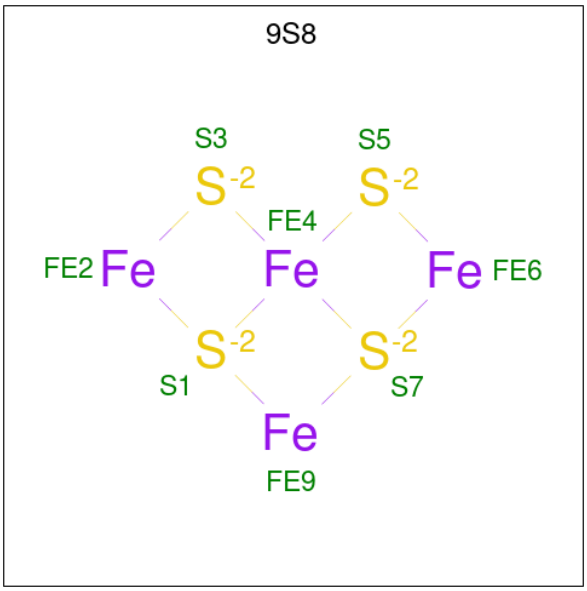
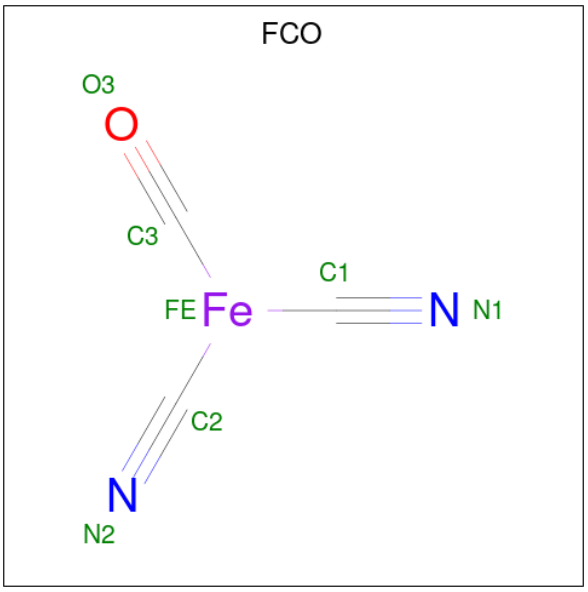
Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	N	O	P	0
			53	27	9	15	2	
11	M	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 12 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
12	C	1	Total	Fe	S		0
			8	4	4		
12	C	1	Total	Fe	S		0
			8	4	4		
12	D	1	Total	Fe	S		0
			8	4	4		
12	D	1	Total	Fe	S		0
			8	4	4		

- Molecule 13 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: C_3FeN_2O) (labeled as "Ligand of Interest" by depositor).

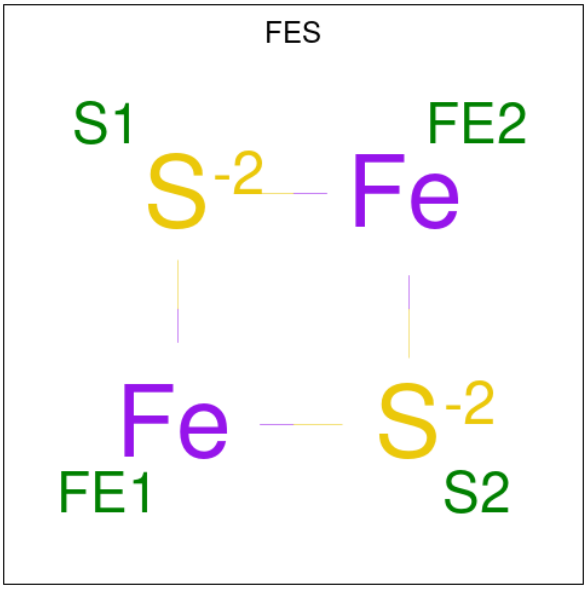


Mol	Chain	Residues	Atoms					AltConf
13	G	1	Total	C	Fe	N	O	0
			7	3	1	2	1	

- Molecule 14 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
14	G	1	Total	Ni	0
			1	1	

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

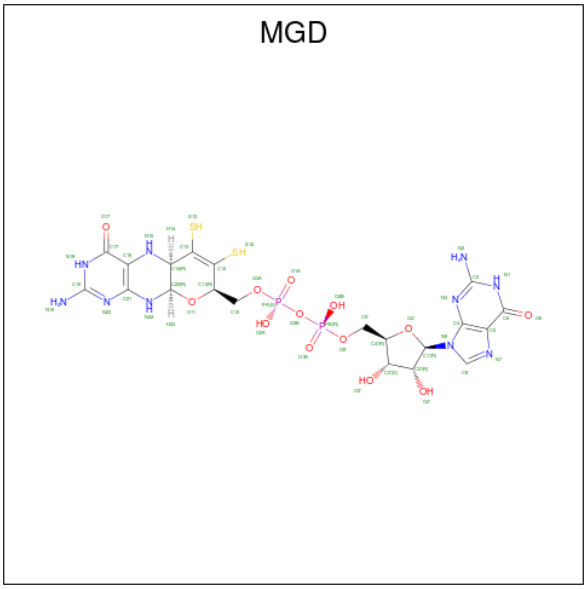


Mol	Chain	Residues	Atoms	AltConf
15	I	1	Total Fe S 4 2 2	0
15	J	1	Total Fe S 4 2 2	0

- Molecule 16 is TUNGSTEN ION (CCD ID: W) (formula: W) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
16	L	1	Total W 1 1	0

- Molecule 17 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).



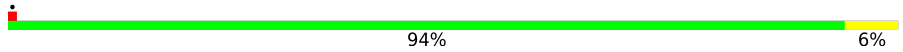
Mol	Chain	Residues	Atoms	AltConf
17	L	1	Total C N O P S 47 20 10 13 2 2	0
17	L	1	Total C N O P S 47 20 10 13 2 2	0

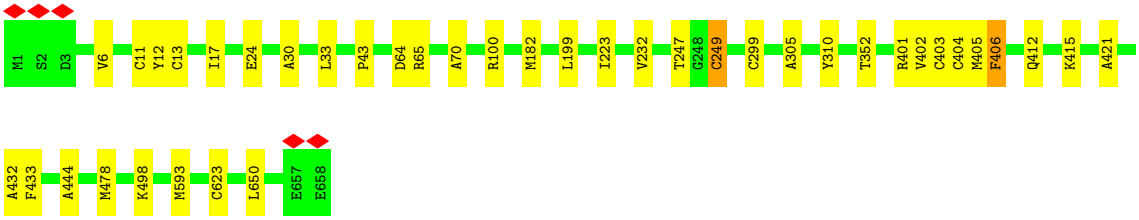
3 Residue-property plots (i)

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: CoB–CoM heterodisulfide reductase iron-sulfur subunit A

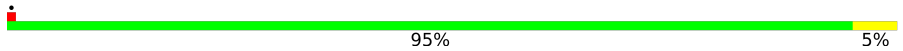
Chain A:

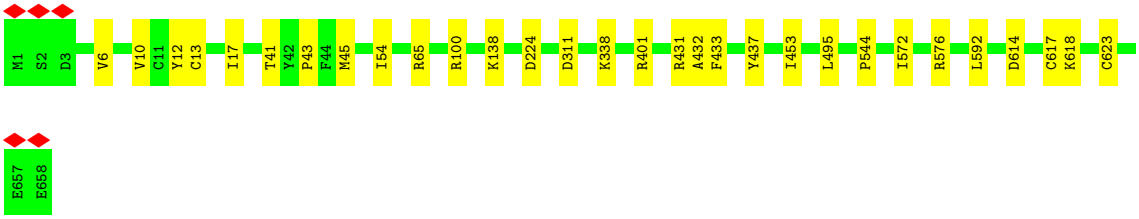




• Molecule 1: CoB–CoM heterodisulfide reductase iron-sulfur subunit A

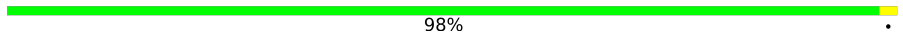
Chain B:





• Molecule 2: Heterodisulfide reductase subunit B

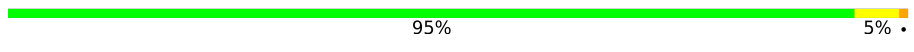
Chain C:





• Molecule 2: Heterodisulfide reductase subunit B

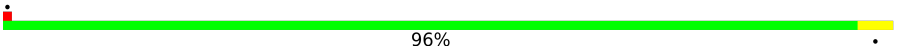
Chain D:





• Molecule 3: H(2)/formate:CoB-CoM heterodisulfide,ferredoxin reductase subunit C2

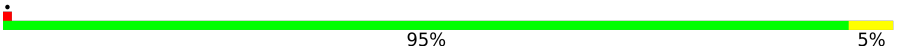
Chain E:

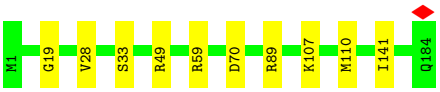




• Molecule 3: H(2)/formate:CoB-CoM heterodisulfide,ferredoxin reductase subunit C2

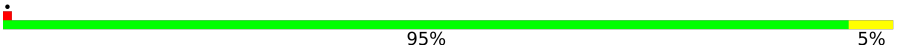
Chain F:

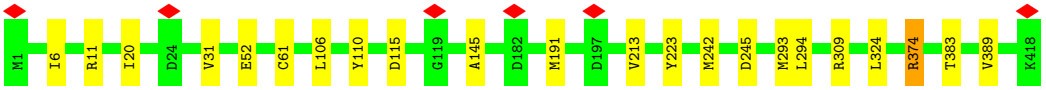




• Molecule 4: Coenzyme F420-reducing hydrogenase, alpha subunit

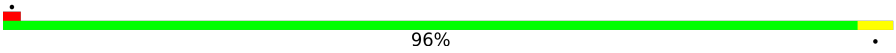
Chain G:

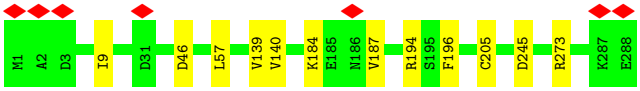




• Molecule 5: F420-non-reducing hydrogenase small subunit

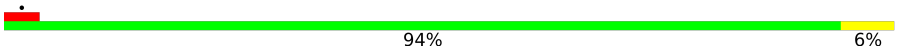
Chain H:

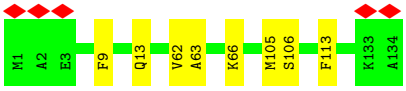




• Molecule 6: F420-non-reducing hydrogenase subunit delta

Chain I:

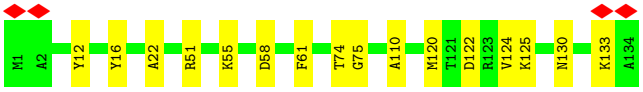




• Molecule 6: F420-non-reducing hydrogenase subunit delta

Chain J:

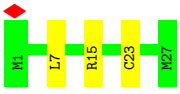




• Molecule 7: F420 non-reducing hydrogenase subunit

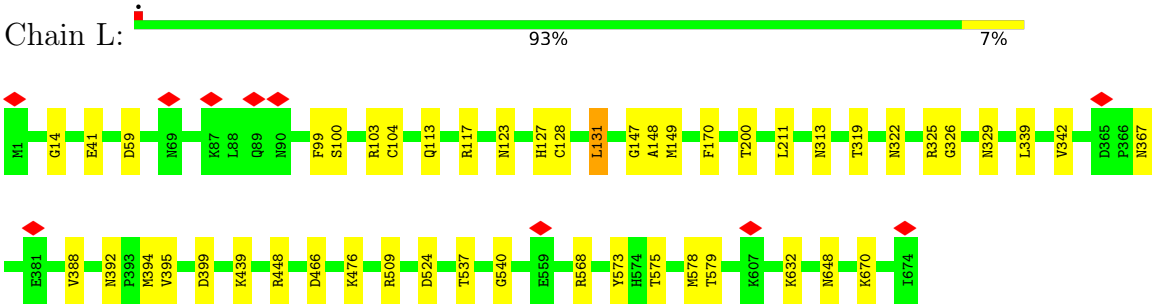
Chain K:





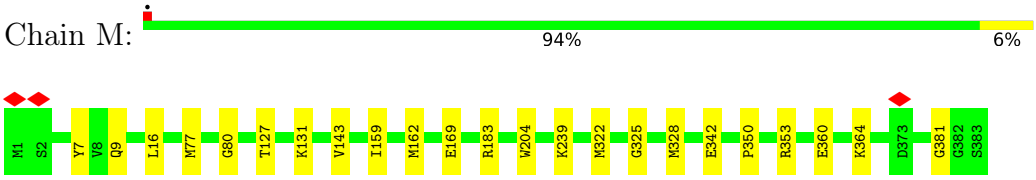
• Molecule 8: formate dehydrogenase (coenzyme F420)

Chain L:



• Molecule 9: formate dehydrogenase (coenzyme F420)

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110231	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)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.805	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.174	Depositor
Map size (Å)	760.0, 760.0, 760.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality

5.1 Standard geometry

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

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	0/5052	0.40	0/6830
1	B	0.17	0/5052	0.38	0/6830
2	C	0.17	0/2277	0.38	0/3073
2	D	0.17	0/2277	0.40	2/3073 (0.1%)
3	E	0.15	0/1447	0.35	0/1944
3	F	0.16	0/1447	0.36	0/1944
4	G	0.18	0/3275	0.39	0/4435
5	H	0.16	0/2192	0.37	0/2982
6	I	0.14	0/1023	0.34	0/1367
6	J	0.18	0/1023	0.46	0/1367
7	K	0.16	0/207	0.41	0/278
8	L	0.14	0/5302	0.35	0/7190
9	M	0.16	0/3035	0.36	0/4090
All	All	0.16	0/33609	0.38	2/45403 (0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	42	CYS	CA-C-N	5.37	139.90	127.00
2	D	42	CYS	C-N-CA	5.37	139.90	127.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	374	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4970	0	4902	23	0
1	B	4970	0	4902	22	0
2	C	2236	0	2240	5	0
2	D	2236	0	2240	10	0
3	E	1426	0	1460	5	0
3	F	1426	0	1460	7	0
4	G	3207	0	3219	14	0
5	H	2149	0	2155	9	0
6	I	1018	0	1010	4	0
6	J	1018	0	1009	9	0
7	K	211	0	207	3	0
8	L	5202	0	5146	27	0
9	M	2976	0	2960	13	0
10	A	48	0	0	2	0
10	B	48	0	0	2	0
10	E	16	0	0	0	0
10	F	16	0	0	0	0
10	H	24	0	0	0	0
10	L	8	0	0	0	0
10	M	32	0	0	0	0
11	A	53	0	31	1	0
11	B	53	0	31	0	0
11	M	53	0	31	0	0
12	C	16	0	0	0	0
12	D	16	0	0	0	0
13	G	7	0	0	2	0
14	G	1	0	0	1	0
15	I	4	0	0	0	0
15	J	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	L	1	0	0	0	0
17	L	94	0	44	1	0
All	All	33539	0	33047	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 2.

The worst 5 of 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)
13:G:419:FCO:C3	14:G:420:NI:NI	1.49	0.86
1:B:13:CYS:HB2	10:B:701:SF4:S4	2.31	0.71
1:A:433:PHE:HB2	1:B:401:ARG:HG3	1.79	0.65
1:A:623:CYS:HB3	10:A:703:SF4:S1	2.36	0.65
1:B:592:LEU:HD11	5:H:187:VAL:HB	1.79	0.62

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	655/658 (100%)	627 (96%)	26 (4%)	2 (0%)	36 70
1	B	655/658 (100%)	633 (97%)	22 (3%)	0	100 100
2	C	291/293 (99%)	278 (96%)	13 (4%)	0	100 100
2	D	291/293 (99%)	275 (94%)	16 (6%)	0	100 100
3	E	182/184 (99%)	178 (98%)	4 (2%)	0	100 100
3	F	182/184 (99%)	178 (98%)	4 (2%)	0	100 100
4	G	416/418 (100%)	401 (96%)	15 (4%)	0	100 100
5	H	286/288 (99%)	273 (96%)	13 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	I	130/134 (97%)	127 (98%)	2 (2%)	1 (1%)	16 52
6	J	130/134 (97%)	122 (94%)	8 (6%)	0	100 100
7	K	24/27 (89%)	23 (96%)	1 (4%)	0	100 100
8	L	671/674 (100%)	646 (96%)	25 (4%)	0	100 100
9	M	381/383 (100%)	366 (96%)	14 (4%)	1 (0%)	36 70
All	All	4294/4328 (99%)	4127 (96%)	163 (4%)	4 (0%)	49 81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	ALA
6	I	13	GLN
9	M	204	TRP
1	A	249	CYS

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	525/525 (100%)	519 (99%)	6 (1%)	65 74
1	B	525/525 (100%)	525 (100%)	0	100 100
2	C	239/239 (100%)	239 (100%)	0	100 100
2	D	239/239 (100%)	236 (99%)	3 (1%)	61 72
3	E	155/155 (100%)	155 (100%)	0	100 100
3	F	155/155 (100%)	155 (100%)	0	100 100
4	G	341/341 (100%)	340 (100%)	1 (0%)	86 85
5	H	236/236 (100%)	236 (100%)	0	100 100
6	I	100/100 (100%)	100 (100%)	0	100 100
6	J	100/100 (100%)	100 (100%)	0	100 100
7	K	22/22 (100%)	22 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	L	569/569 (100%)	566 (100%)	3 (0%)	81 82
9	M	324/324 (100%)	324 (100%)	0	100 100
All	All	3530/3530 (100%)	3517 (100%)	13 (0%)	81 84

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	192	MET
2	D	230	VAL
8	L	399	ASP
8	L	128	CYS
8	L	131	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
8	L	7	HIS
8	L	331	GLN
9	M	123	ASN
8	L	353	HIS
2	D	254	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 2 are monoatomic - leaving 36 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	$\#\|Z\| > 2$
17	MGD	L	704	16	45,52,52	0.69	0	54,81,81	1.05	3 (5%)
10	SF4	M	403	9	0,12,12	-	-	-		
10	SF4	A	707	1	0,12,12	-	-	-		
10	SF4	F	201	3	0,12,12	-	-	-		
11	FAD	B	704	-	56,58,58	0.35	0	81,89,89	0.36	0
10	SF4	B	706	1	0,12,12	-	-	-		
10	SF4	L	701	8	0,12,12	-	-	-		
10	SF4	M	401	9	0,12,12	-	-	-		
10	SF4	E	202	3	0,12,12	-	-	-		
10	SF4	B	703	1	0,12,12	-	-	-		
11	FAD	A	704	-	56,58,58	0.35	0	81,89,89	0.33	0
10	SF4	A	706	1	0,12,12	-	-	-		
17	MGD	L	703	16	45,52,52	0.67	0	54,81,81	1.01	4 (7%)
12	9S8	D	301	2	2,10,10	1.33	0	-		
10	SF4	H	301	5	0,12,12	-	-	-		
10	SF4	A	703	1	0,12,12	-	-	-		
10	SF4	B	707	1	0,12,12	-	-	-		
13	FCO	G	419	14,7	1,6,6	2.86	1 (100%)	-		
15	FES	I	201	6	0,4,4	-	-	-		
10	SF4	M	404	9	0,12,12	-	-	-		
10	SF4	H	303	5	0,12,12	-	-	-		
10	SF4	B	705	1	0,12,12	-	-	-		
12	9S8	D	302	2	2,10,10	1.25	0	-		
10	SF4	A	701	1	0,12,12	-	-	-		
10	SF4	A	705	1	0,12,12	-	-	-		
10	SF4	H	302	5	0,12,12	-	-	-		
11	FAD	M	405	-	56,58,58	0.34	0	81,89,89	0.38	1 (1%)
10	SF4	M	402	9	0,12,12	-	-	-		
10	SF4	B	702	1	0,12,12	-	-	-		
12	9S8	C	302	2	2,10,10	1.26	0	-		
10	SF4	F	202	3	0,12,12	-	-	-		
12	9S8	C	301	2	2,10,10	1.29	0	-		
10	SF4	A	702	1	0,12,12	-	-	-		
10	SF4	E	201	3	0,12,12	-	-	-		
15	FES	J	201	6	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	SF4	B	701	1	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MGD	L	704	16	-	4/22/66/66	0/6/6/6
10	SF4	M	403	9	-	-	0/6/5/5
10	SF4	A	707	1	-	-	0/6/5/5
10	SF4	F	201	3	-	-	0/6/5/5
11	FAD	B	704	-	-	15/34/50/50	0/6/6/6
10	SF4	B	706	1	-	-	0/6/5/5
10	SF4	L	701	8	-	-	0/6/5/5
10	SF4	M	401	9	-	-	0/6/5/5
10	SF4	E	202	3	-	-	0/6/5/5
10	SF4	B	703	1	-	-	0/6/5/5
11	FAD	A	704	-	-	15/34/50/50	0/6/6/6
10	SF4	A	706	1	-	-	0/6/5/5
17	MGD	L	703	16	-	7/22/66/66	0/6/6/6
12	9S8	D	301	2	-	-	0/3/3/3
10	SF4	H	301	5	-	-	0/6/5/5
10	SF4	A	703	1	-	-	0/6/5/5
10	SF4	B	707	1	-	-	0/6/5/5
15	FES	I	201	6	-	-	0/1/1/1
10	SF4	M	404	9	-	-	0/6/5/5
10	SF4	H	303	5	-	-	0/6/5/5
10	SF4	B	705	1	-	-	0/6/5/5
12	9S8	D	302	2	-	-	0/3/3/3
10	SF4	A	701	1	-	-	0/6/5/5
10	SF4	A	705	1	-	-	0/6/5/5
10	SF4	H	302	5	-	-	0/6/5/5
11	FAD	M	405	-	-	10/34/50/50	0/6/6/6
10	SF4	M	402	9	-	-	0/6/5/5
10	SF4	B	702	1	-	-	0/6/5/5
12	9S8	C	302	2	-	-	0/3/3/3
10	SF4	F	202	3	-	-	0/6/5/5
12	9S8	C	301	2	-	-	0/3/3/3
10	SF4	A	702	1	-	-	0/6/5/5
10	SF4	E	201	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FES	J	201	6	-	-	0/1/1/1
10	SF4	B	701	1	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	419	FCO	O3-C3	2.86	1.19	1.16

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	L	703	MGD	C19-N20-C21	3.23	119.25	113.43
17	L	704	MGD	C19-N20-C21	3.12	119.06	113.43
17	L	704	MGD	C3'-C2'-C1'	-2.53	96.62	101.43
17	L	703	MGD	PA-O3B-PB	-2.34	124.79	132.83
17	L	703	MGD	O11-C23-N22	2.19	110.82	108.57

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	704	FAD	C3B-C4B-C5B-O5B
11	A	704	FAD	N10-C1'-C2'-O2'
11	A	704	FAD	N10-C1'-C2'-C3'
11	A	704	FAD	C1'-C2'-C3'-O3'
11	A	704	FAD	C1'-C2'-C3'-C4'

There are no ring outliers.

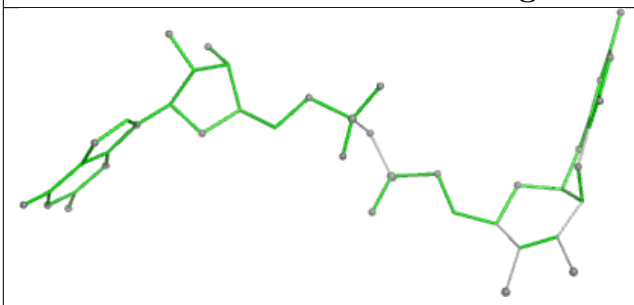
7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	703	SF4	1	0
11	A	704	FAD	1	0
17	L	703	MGD	1	0
10	A	703	SF4	1	0
13	G	419	FCO	2	0
10	A	701	SF4	1	0
10	B	701	SF4	1	0

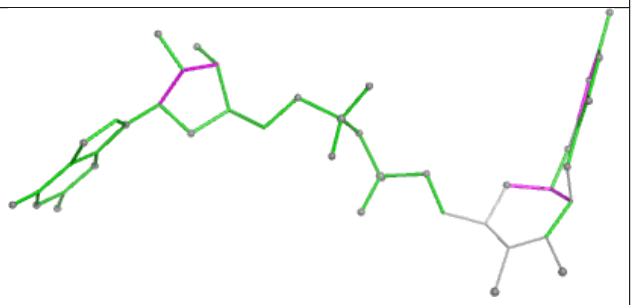
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

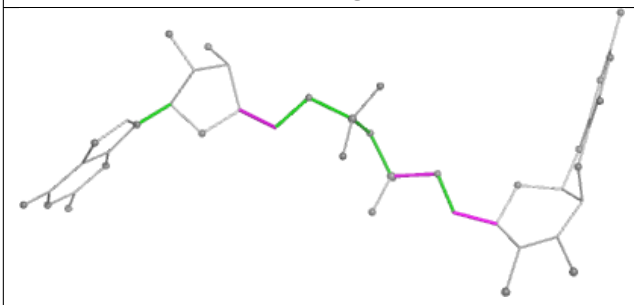
Ligand MGD L 704



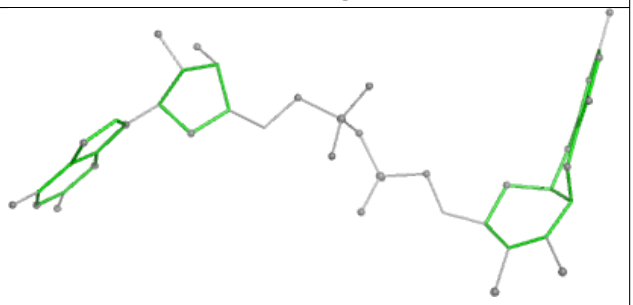
Bond lengths



Bond angles

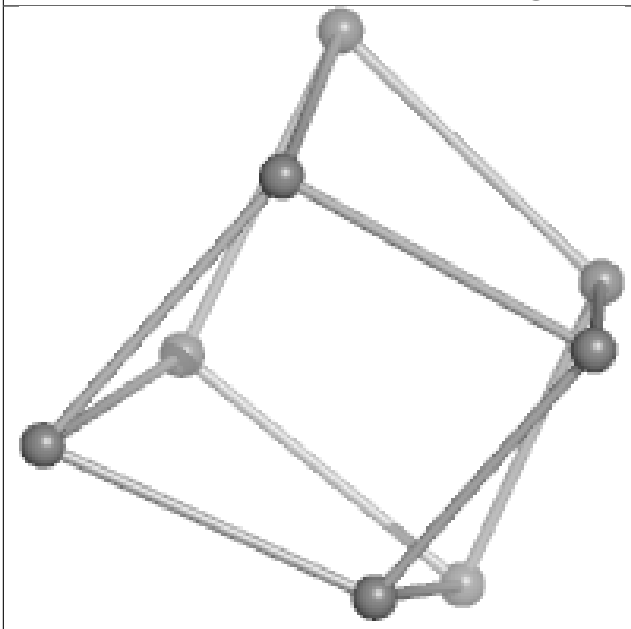


Torsions



Rings

Ligand SF4 M 403



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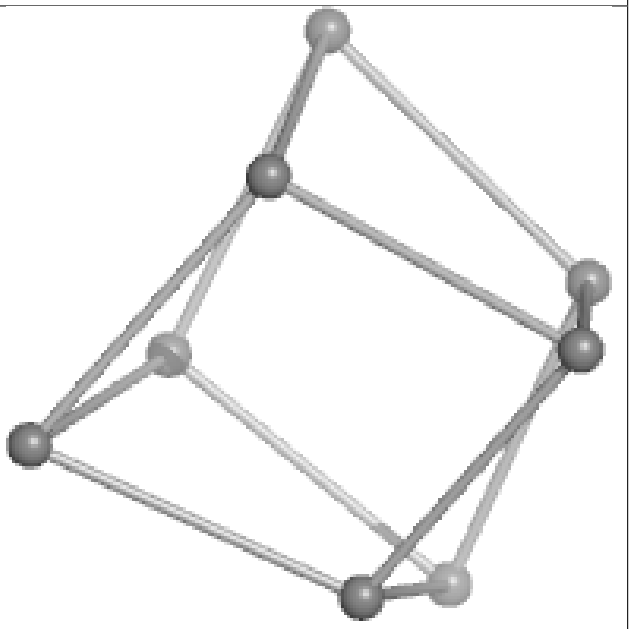

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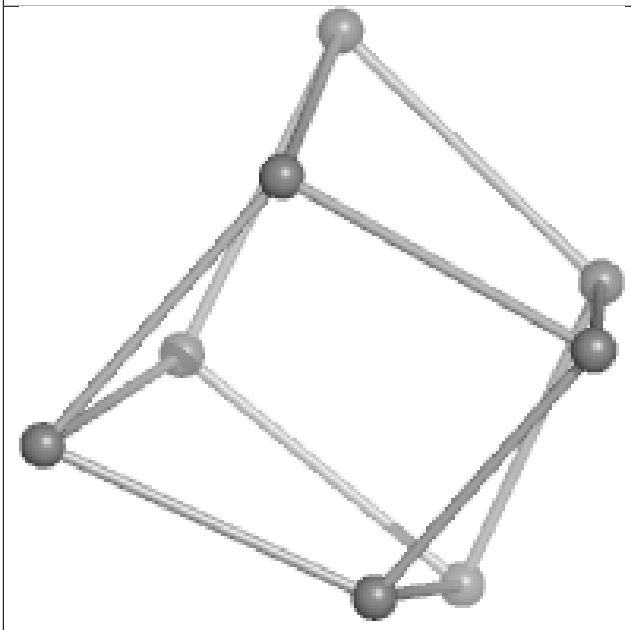

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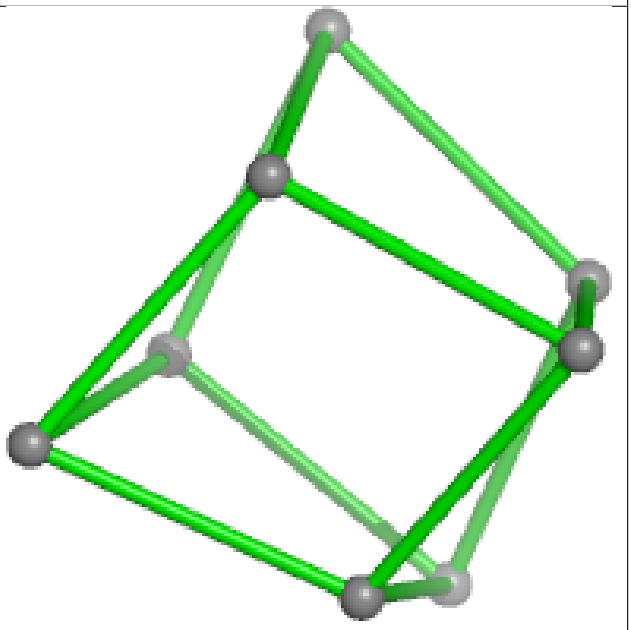
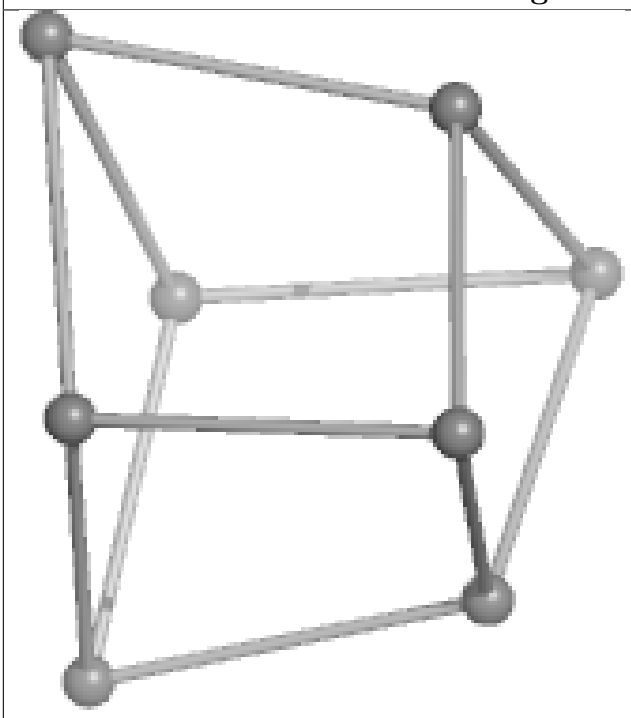
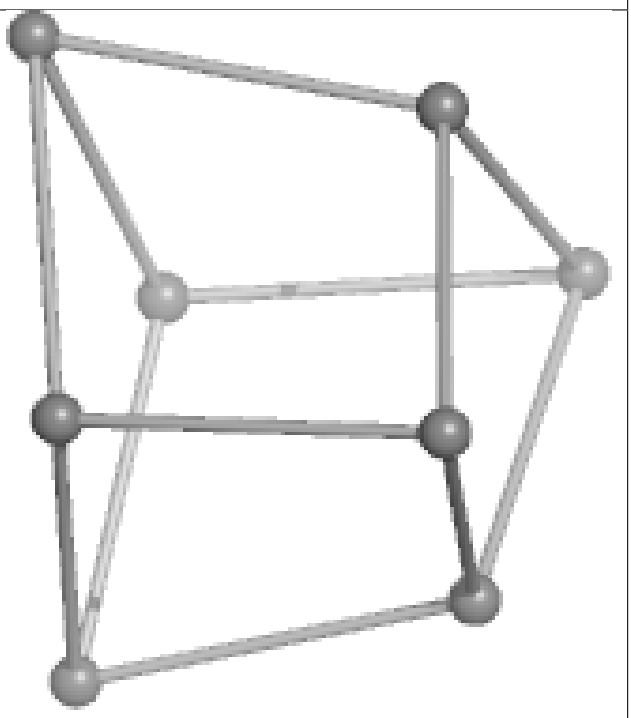


Rings

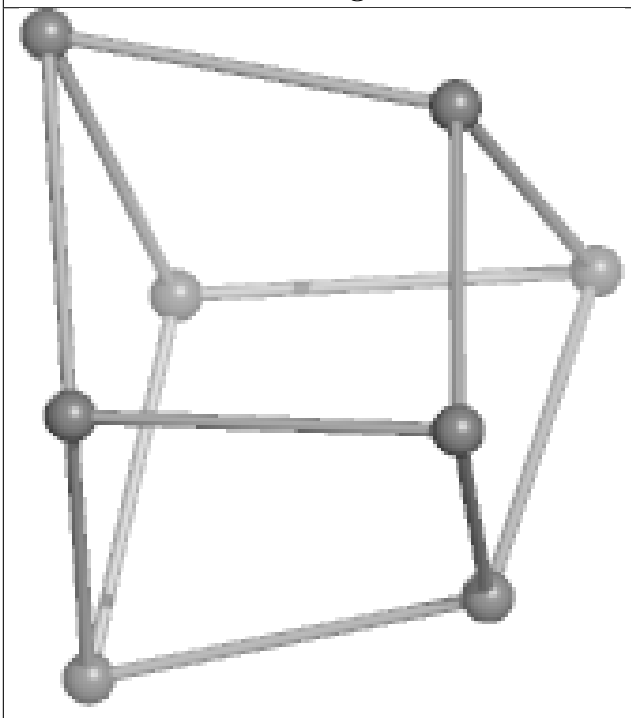
Ligand SF4 A 707



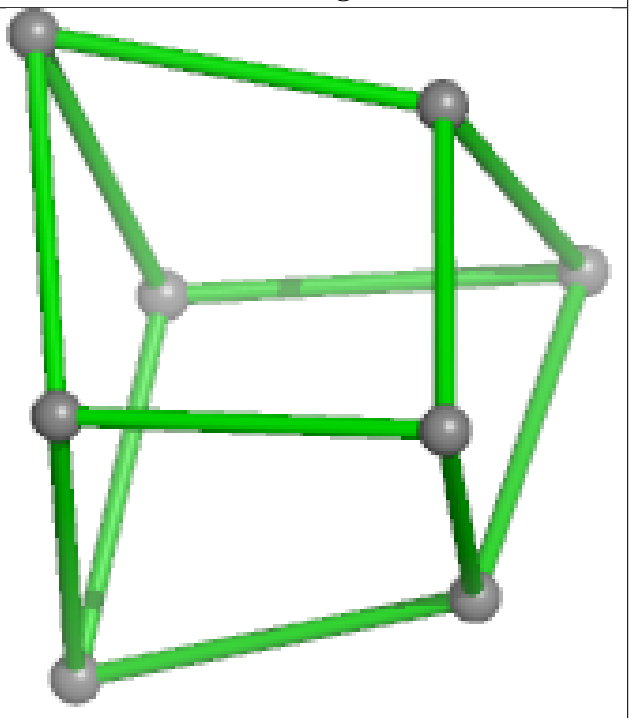
Bond lengths



Bond angles

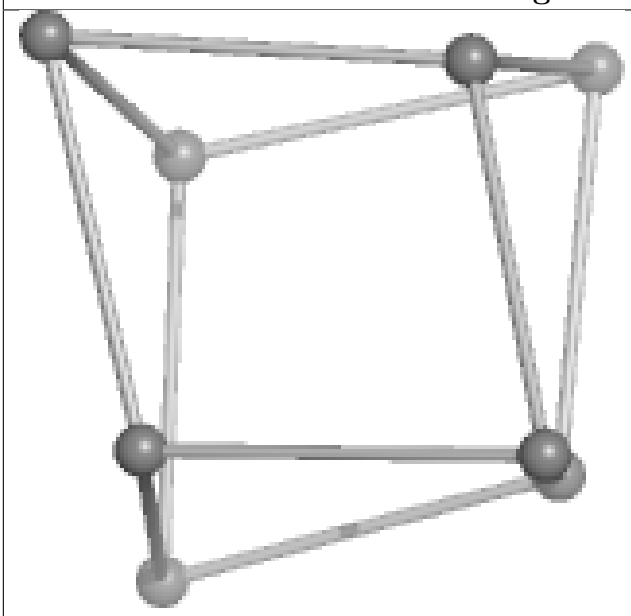


Torsions

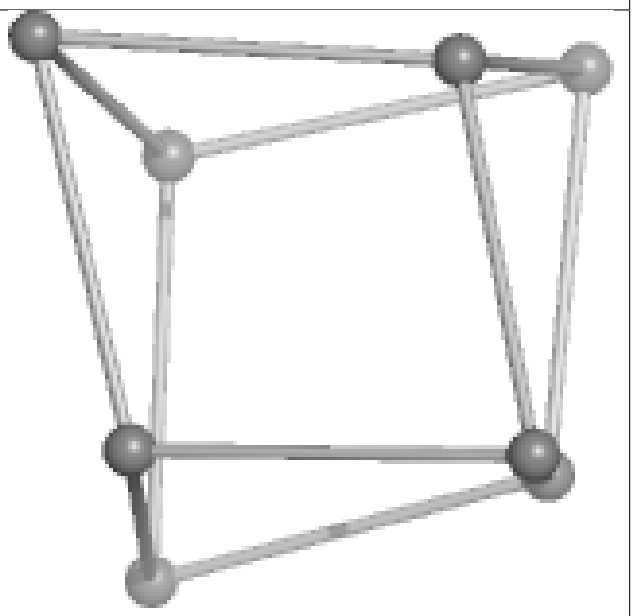


Rings

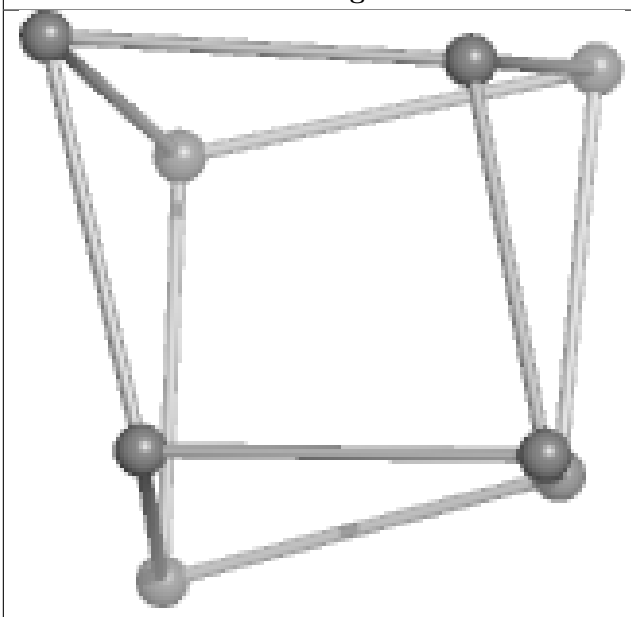
Ligand SF4 F 201



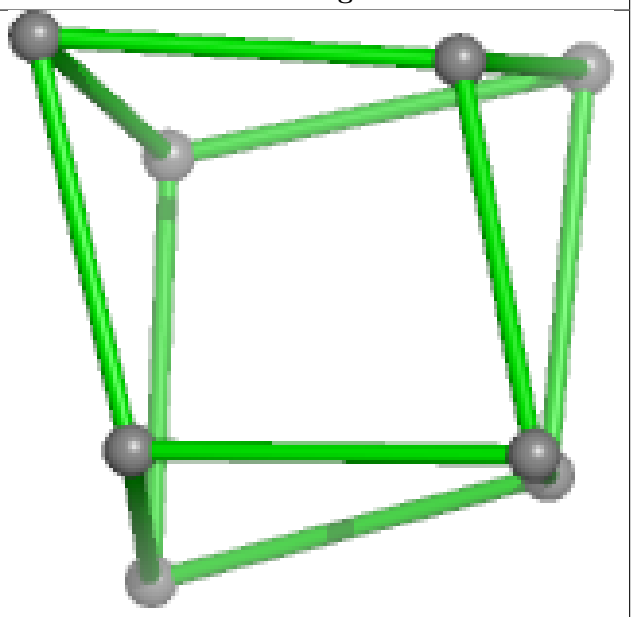
Bond lengths



Bond angles

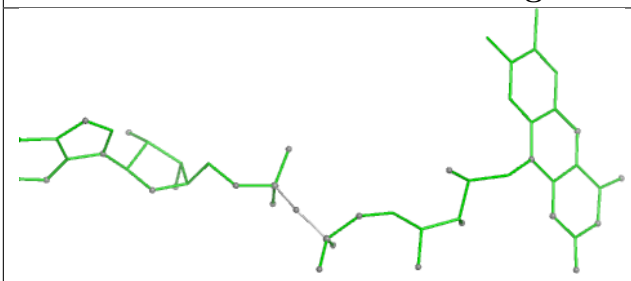


Torsions

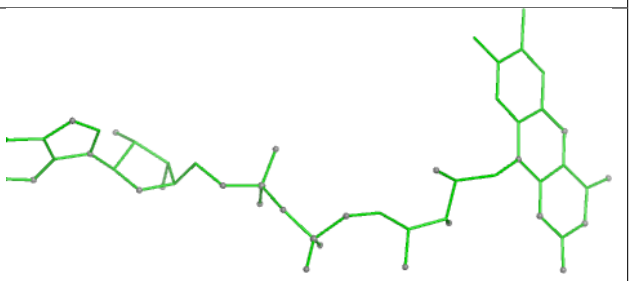


Rings

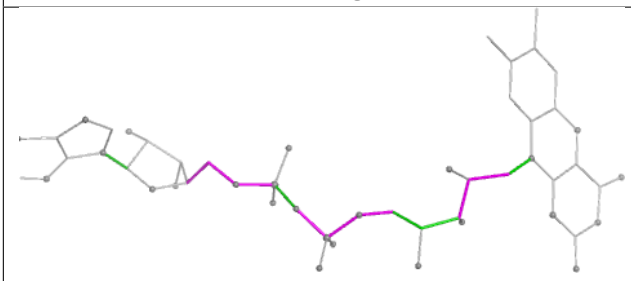
Ligand FAD B 704



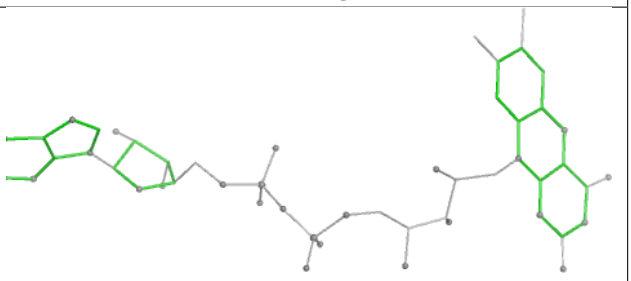
Bond lengths



Bond angles

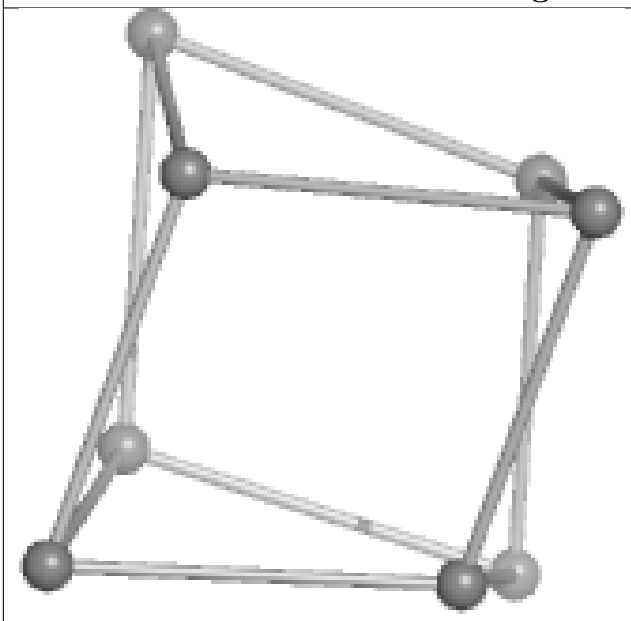


Torsions



Rings

Ligand SF4 B 706



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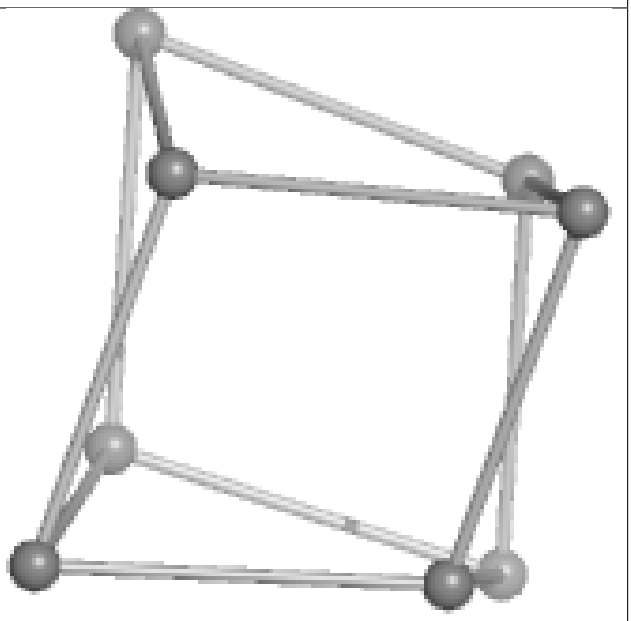
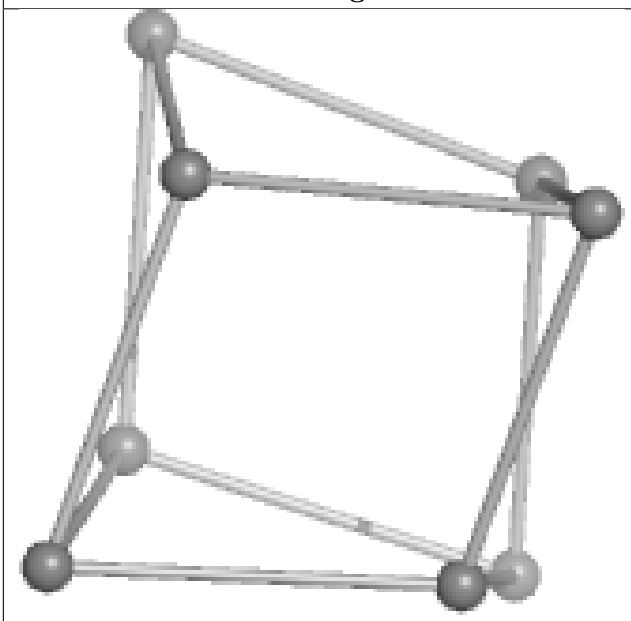


Bond angles



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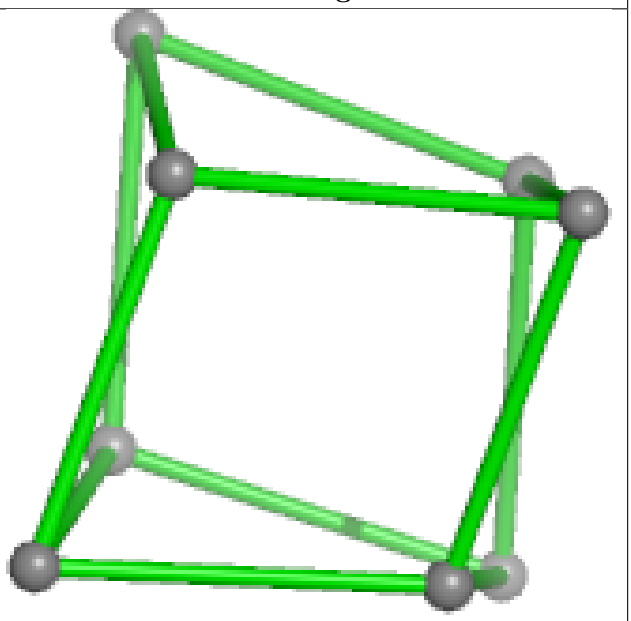
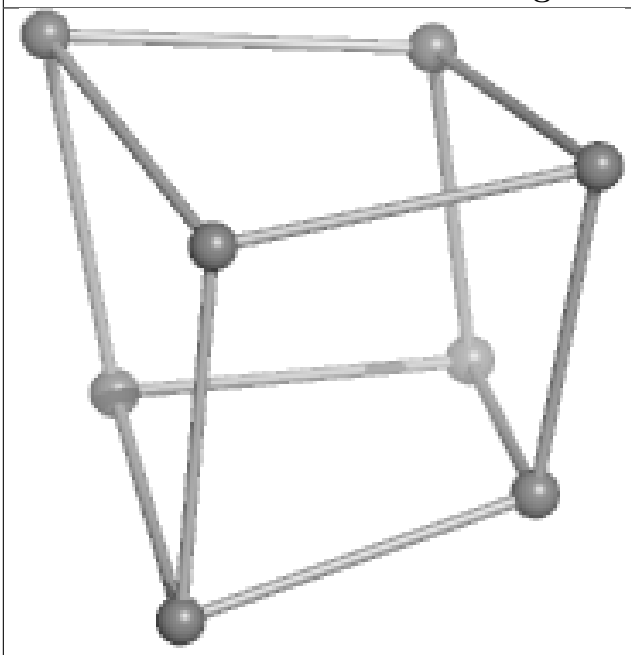


Rings

Ligand SF4 L 701



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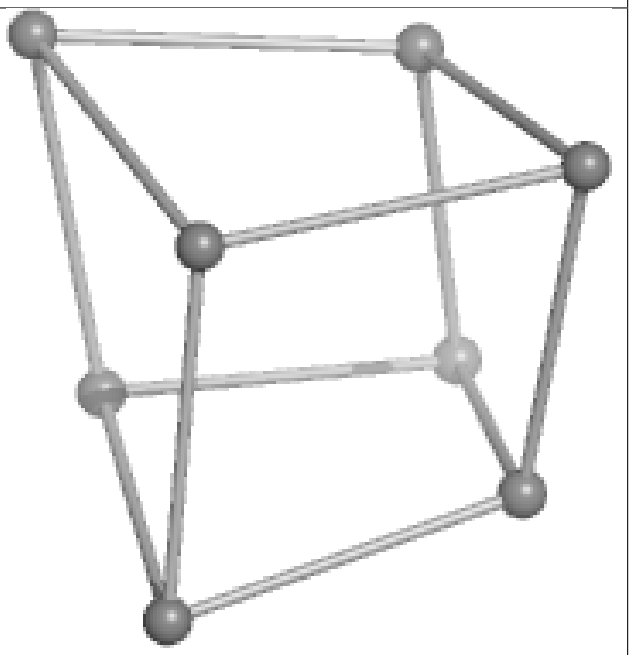

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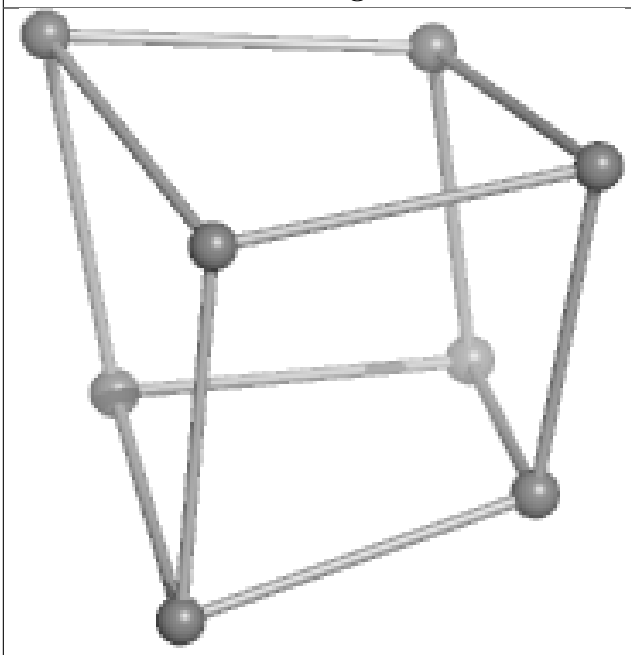

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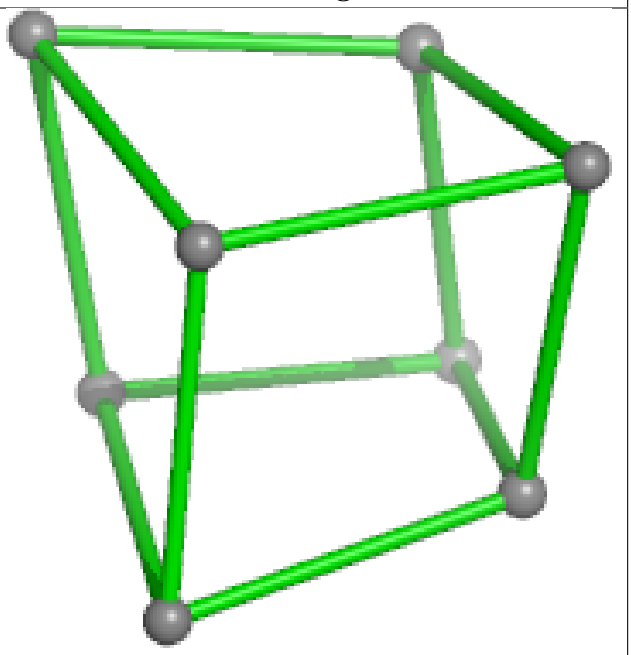
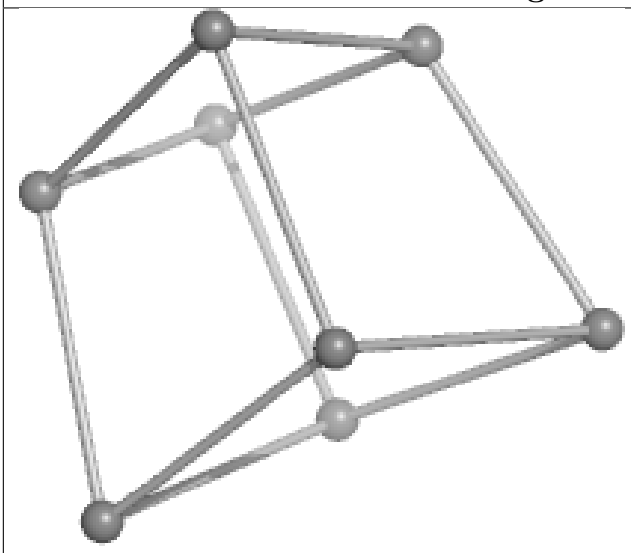


Rings

Ligand SF4 M 401



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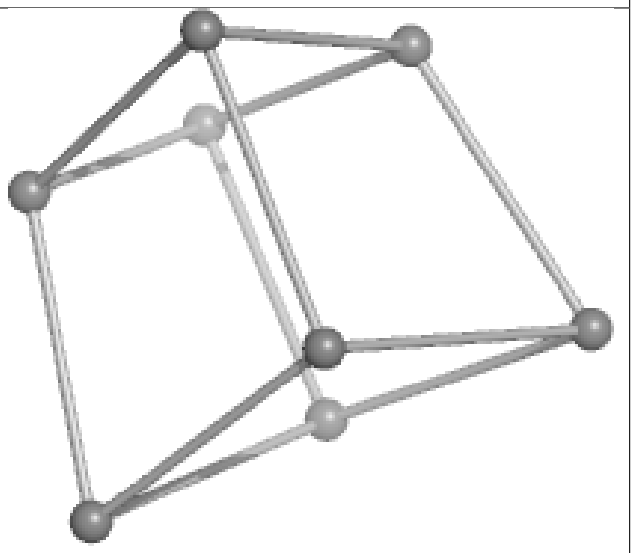
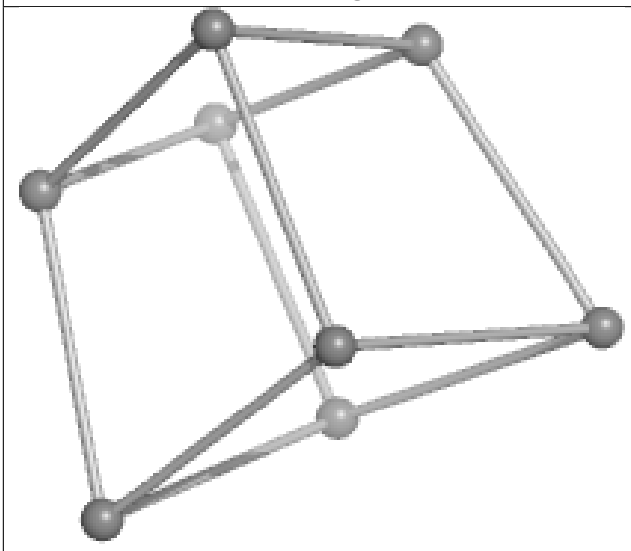


Bond angles



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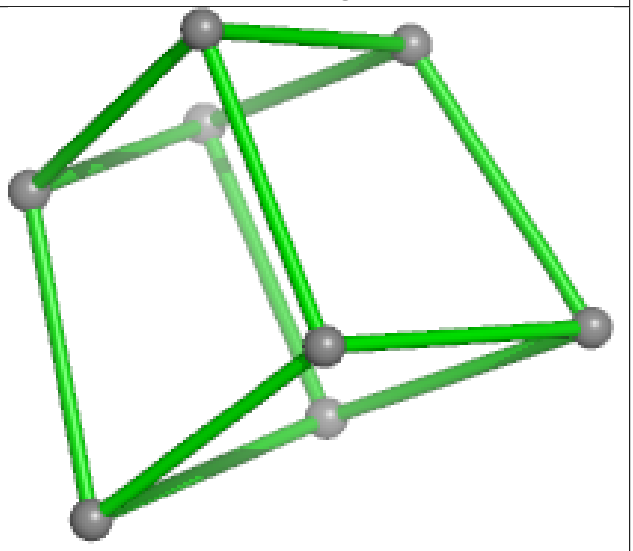
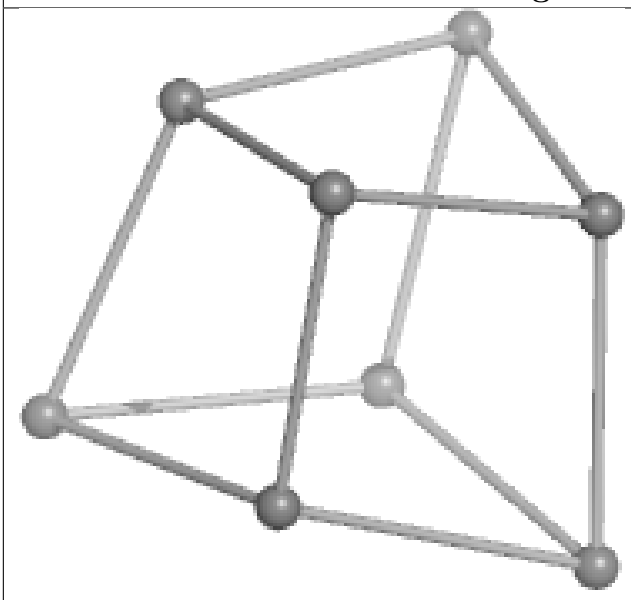


Rings

Ligand SF4 E 202



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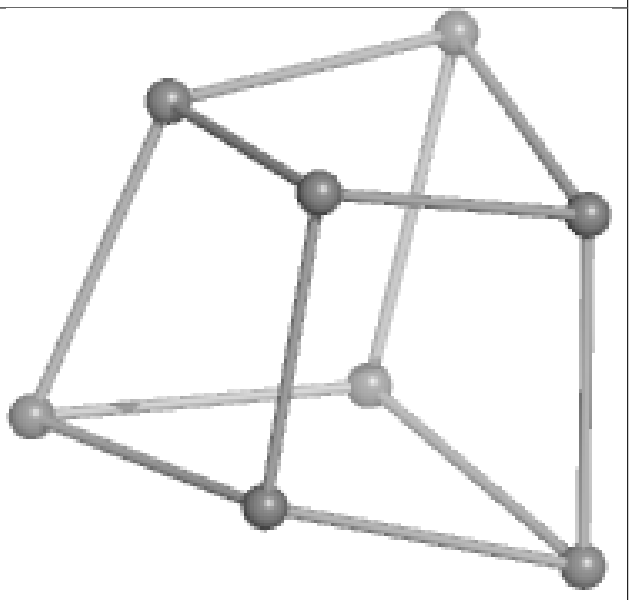
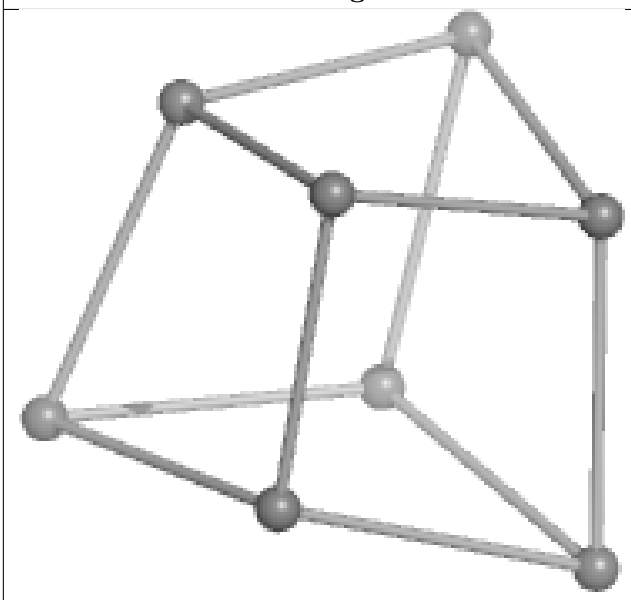


Bond angles



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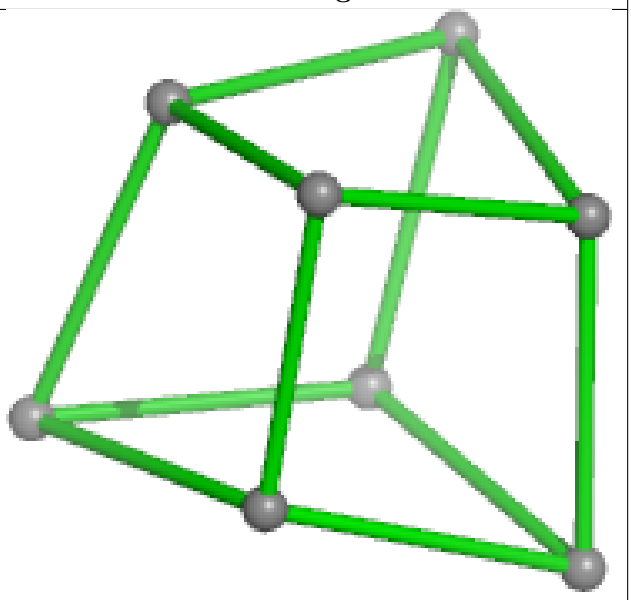
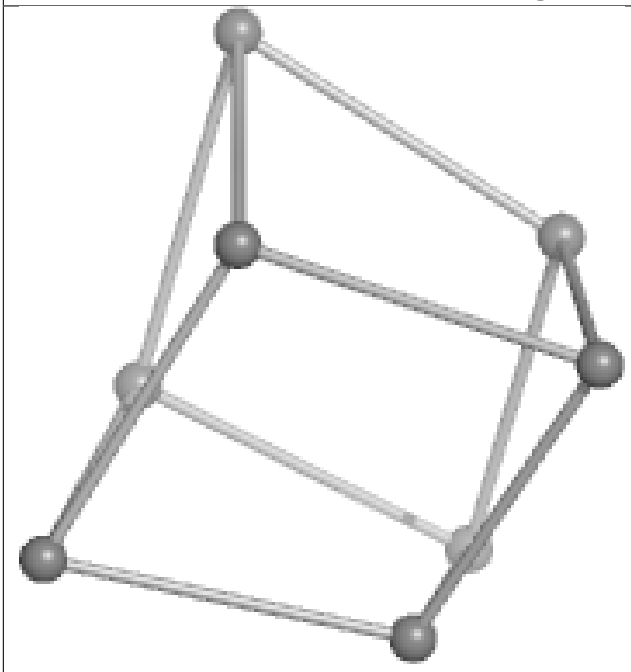


Rings

Ligand SF4 B 703



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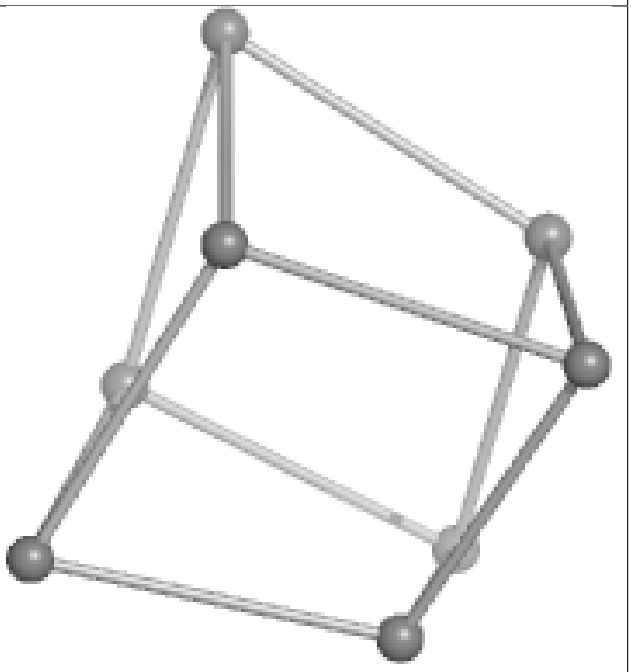
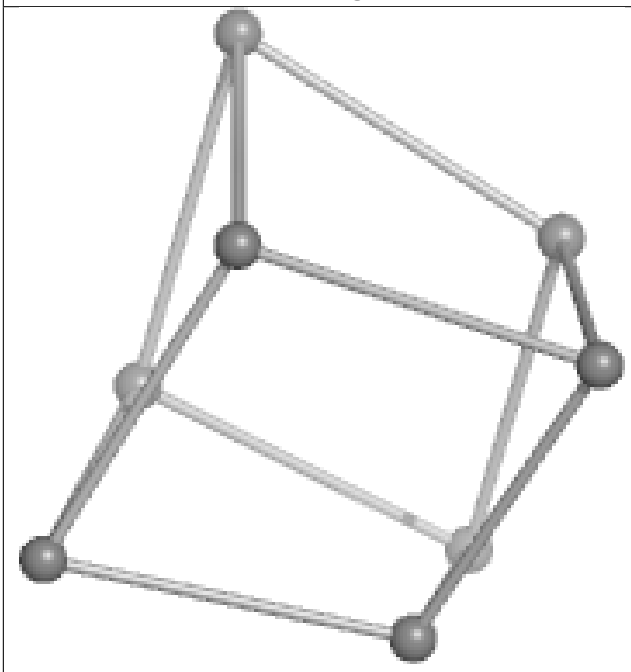


Bond angles



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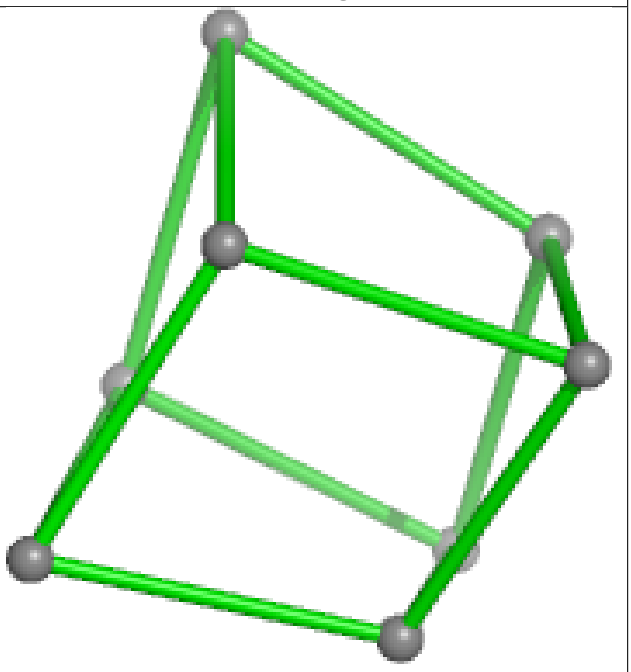
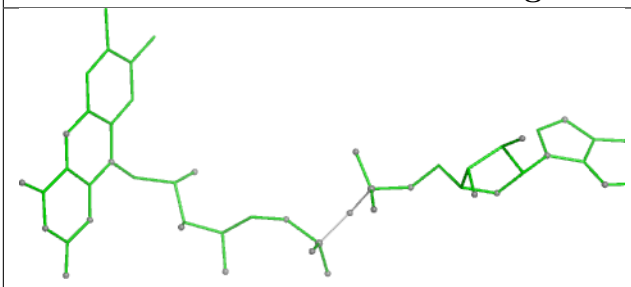


Rings

Ligand FAD A 704



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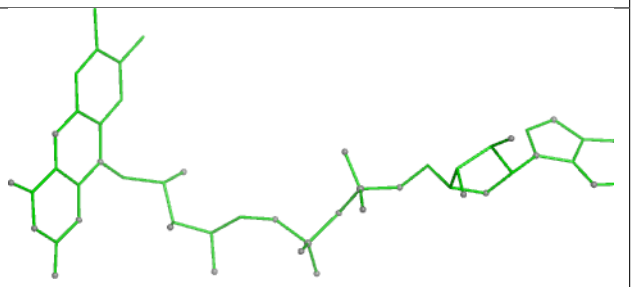
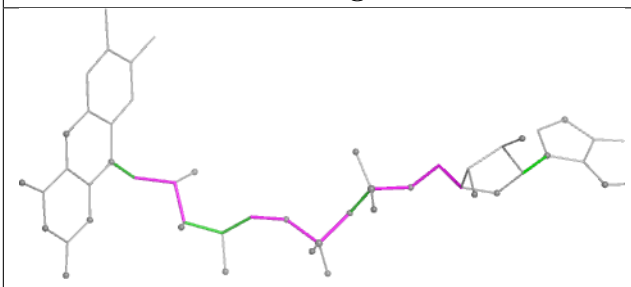


Bond angles



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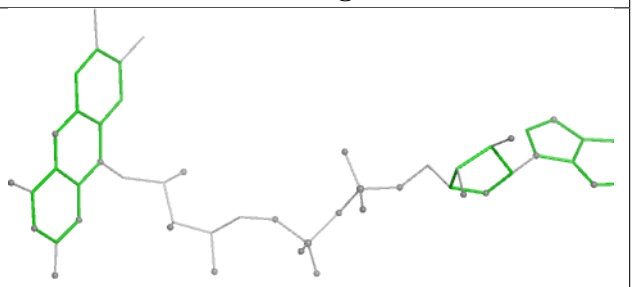
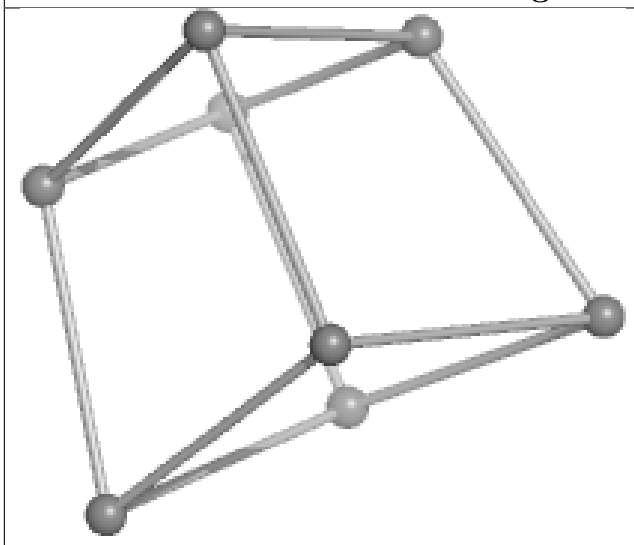


Rings

Ligand SF4 A 706



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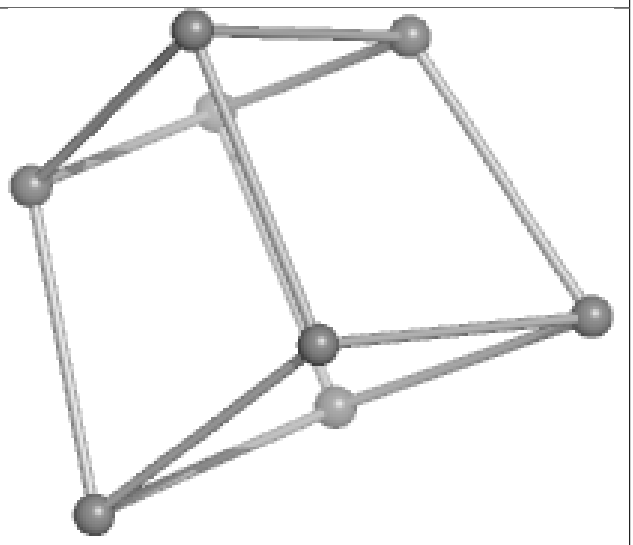

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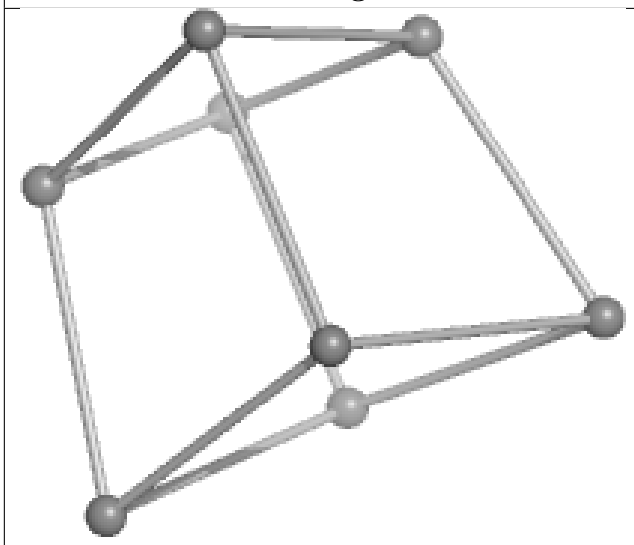

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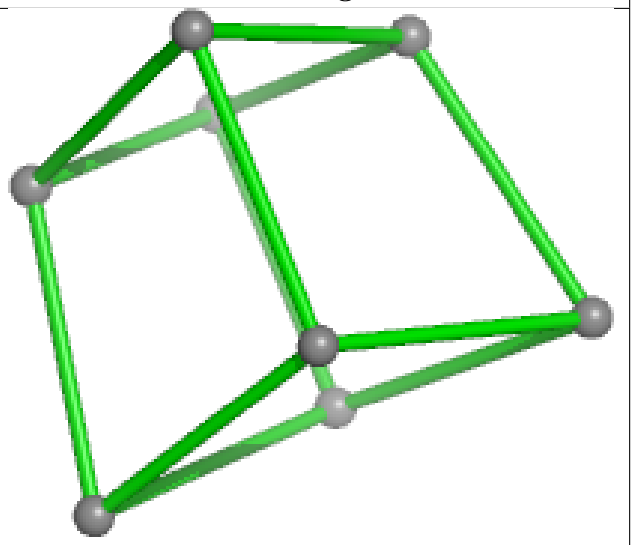
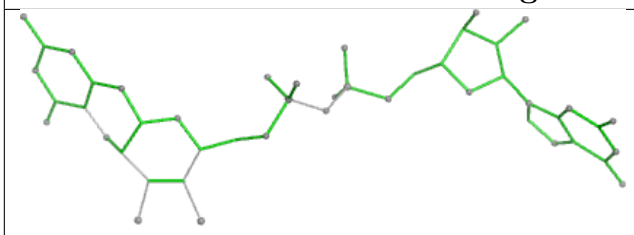


Rings

Ligand MGD L 703



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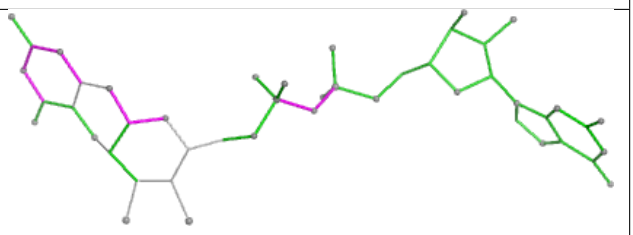
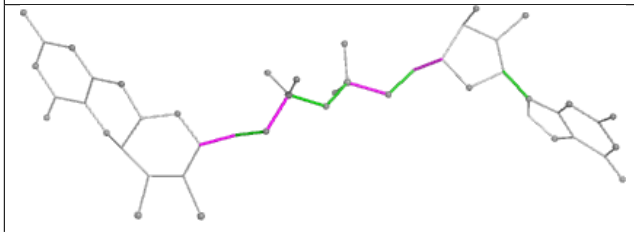


Bond angles



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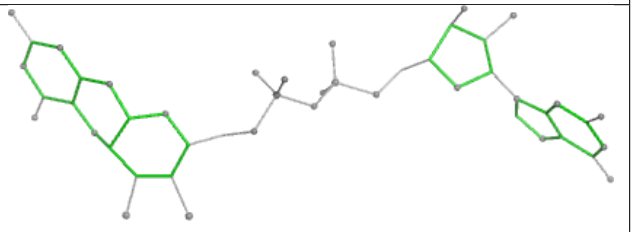
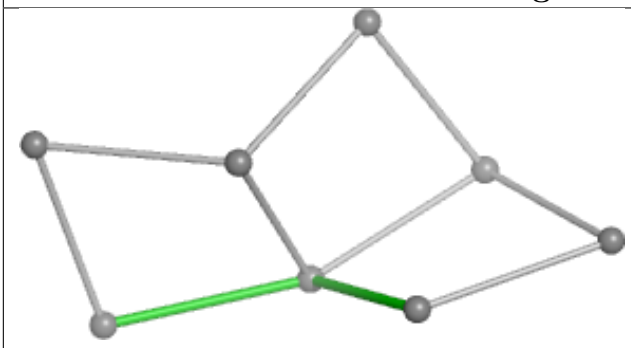


Rings

Ligand 9S8 D 301



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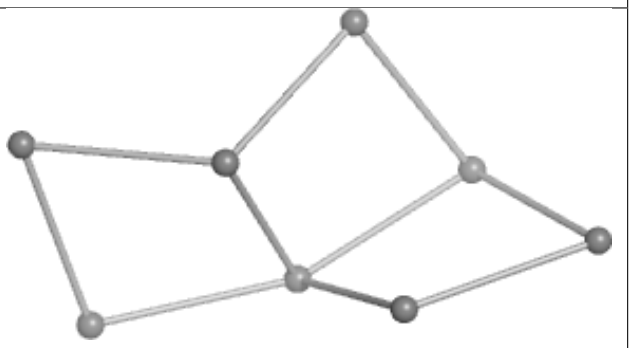
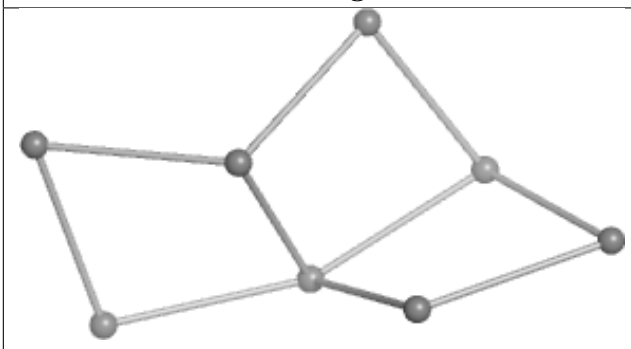


Bond angles



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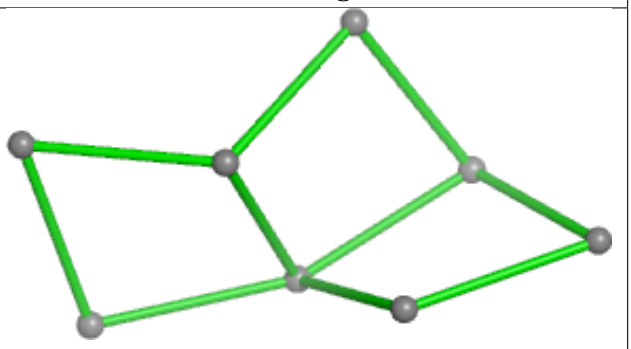
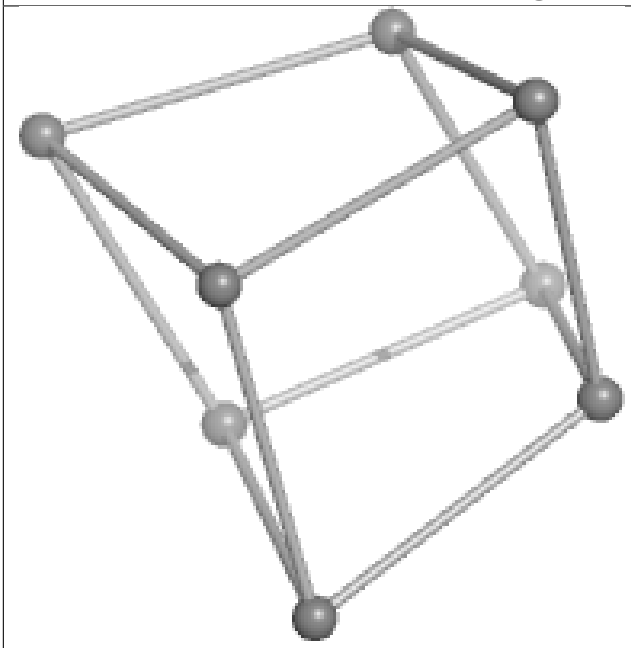


Rings

Ligand SF4 H 301



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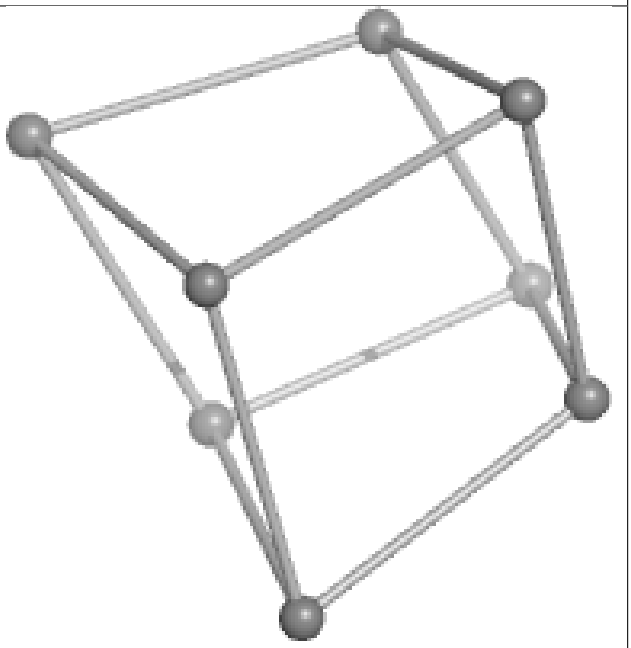
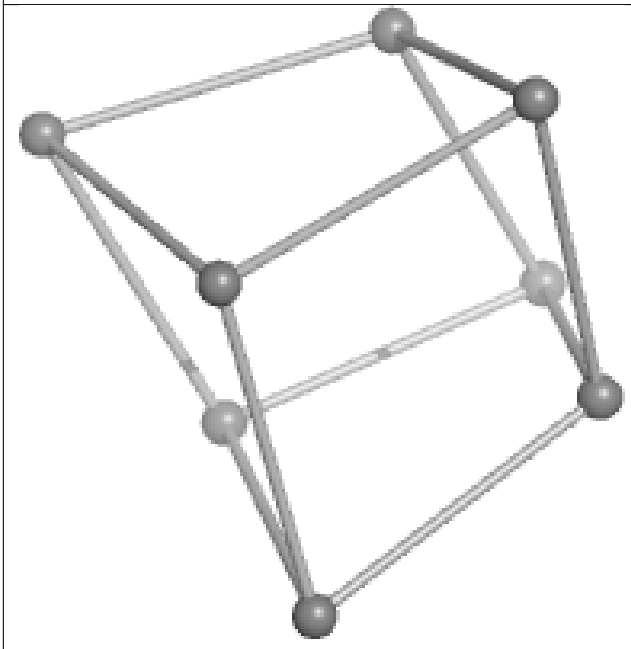


Bond angles



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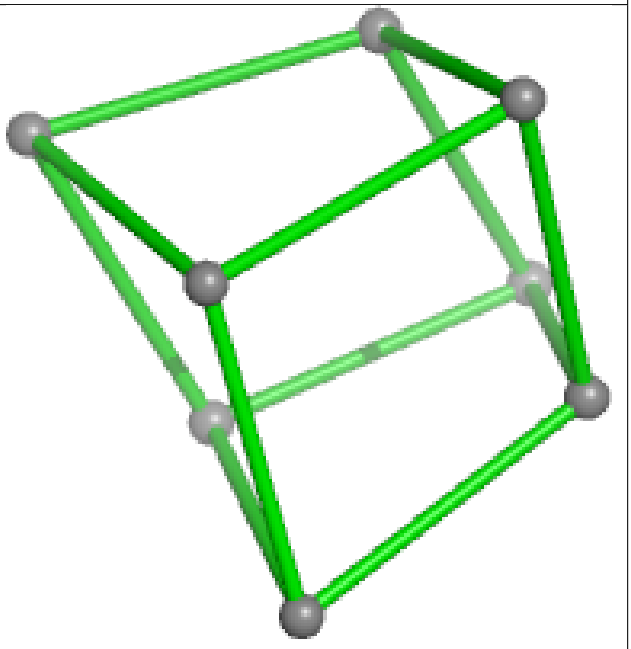
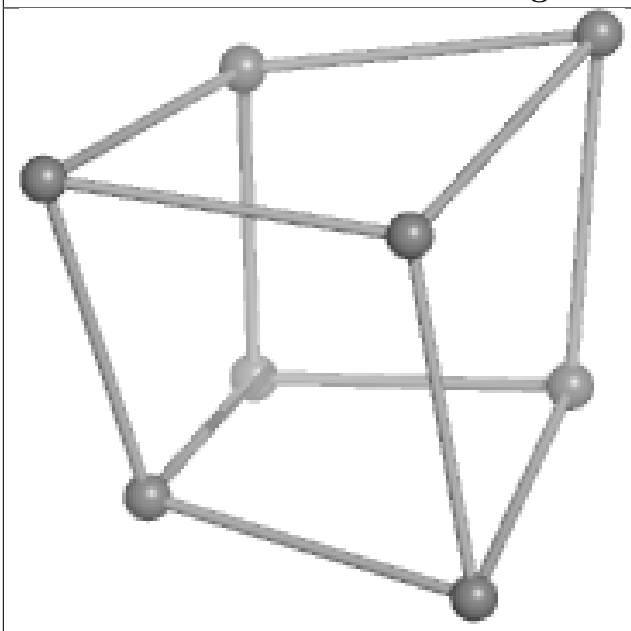


Rings

Ligand SF4 A 703



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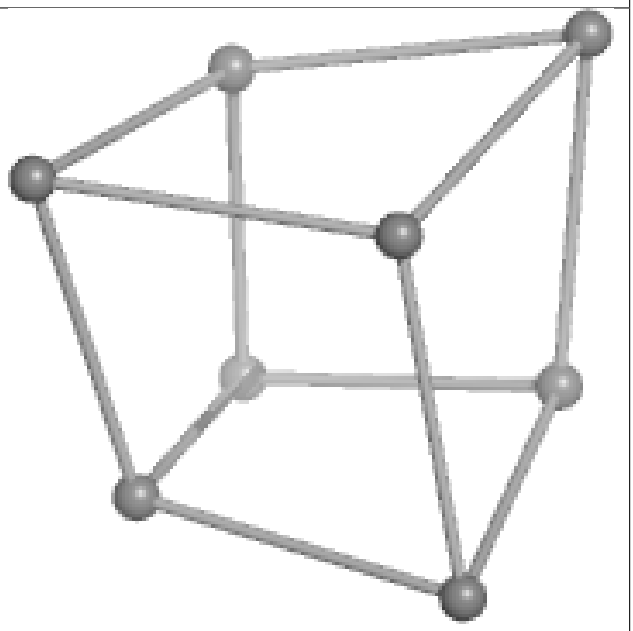
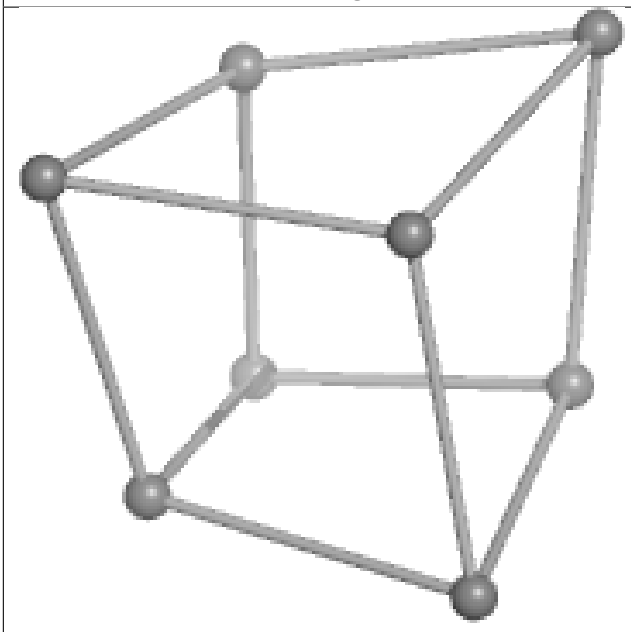


Bond angles



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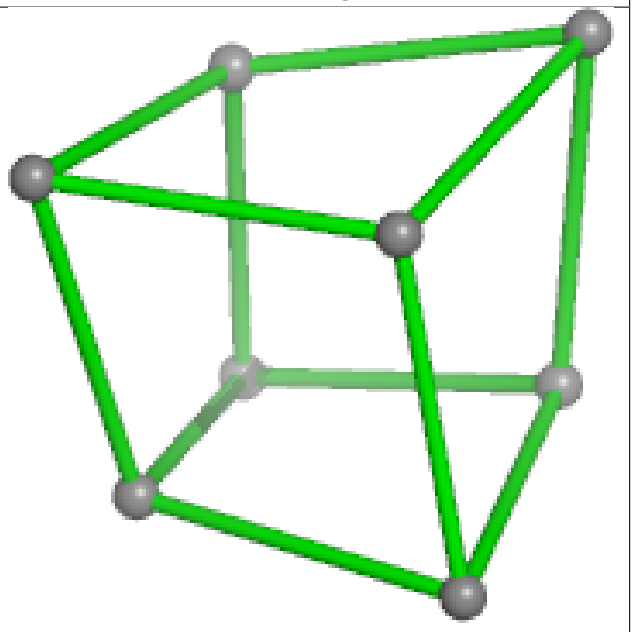
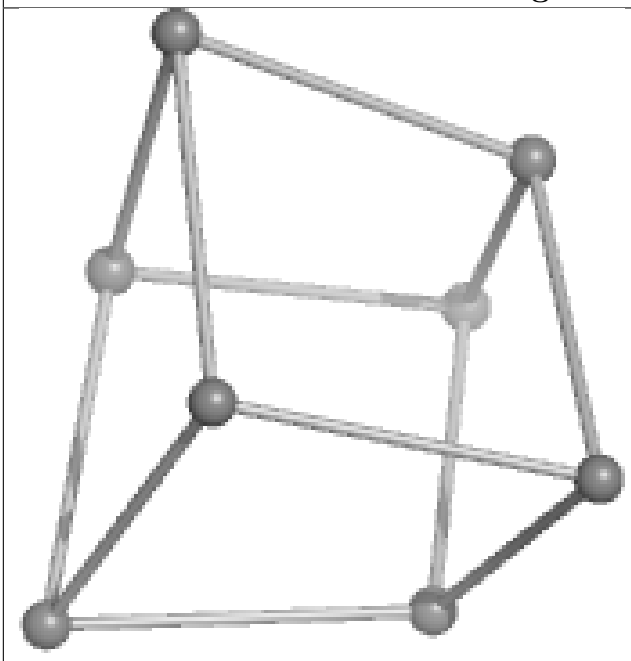


Rings

Ligand SF4 B 707



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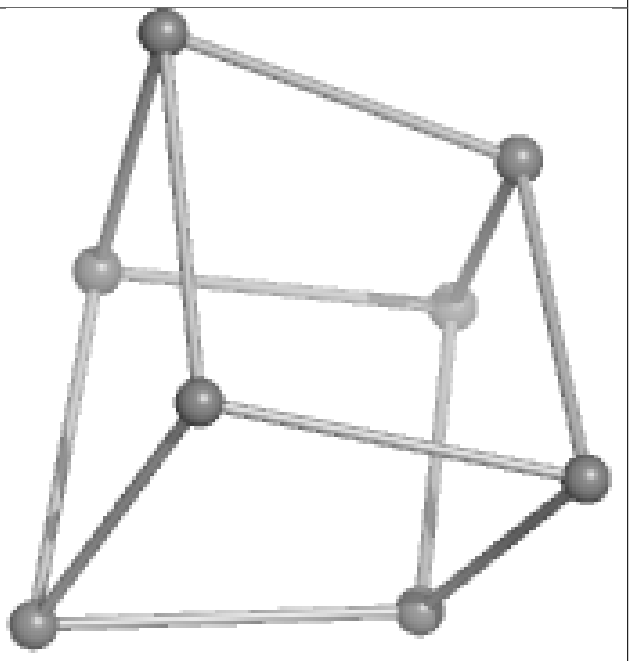
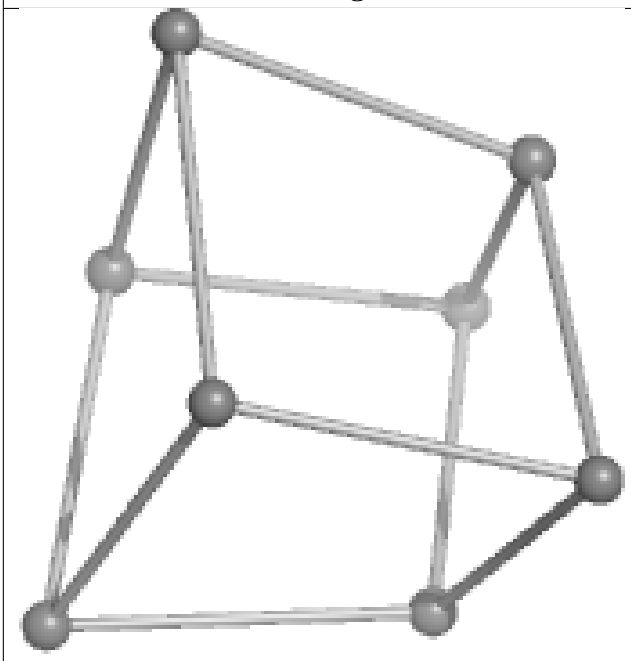


Bond angles



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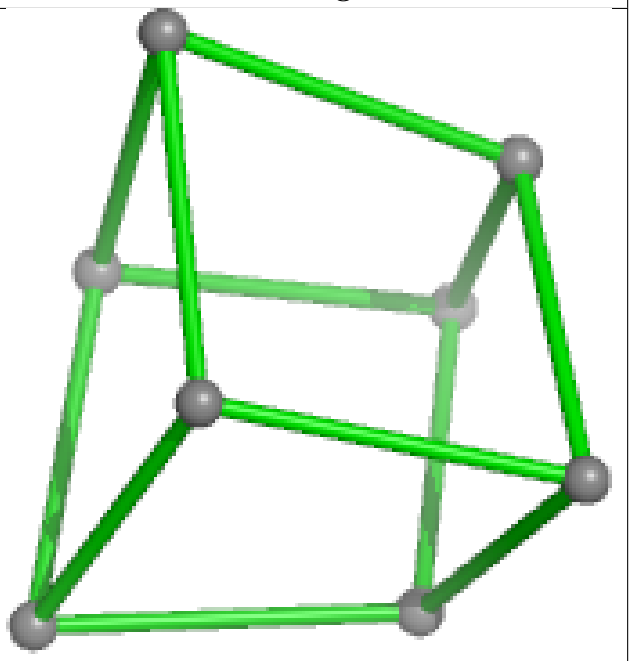
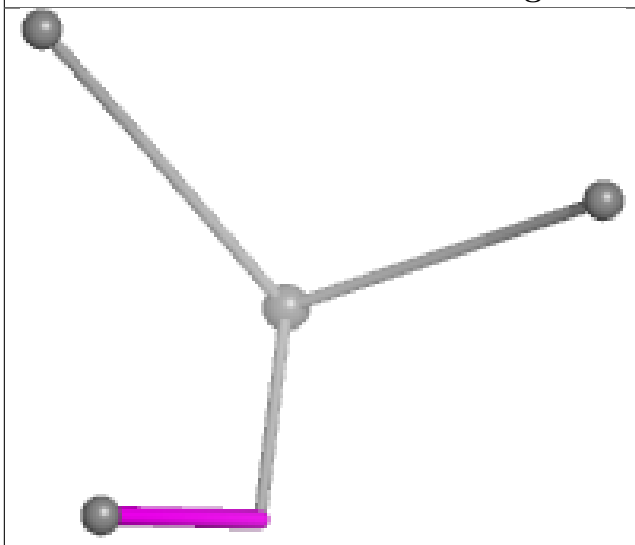
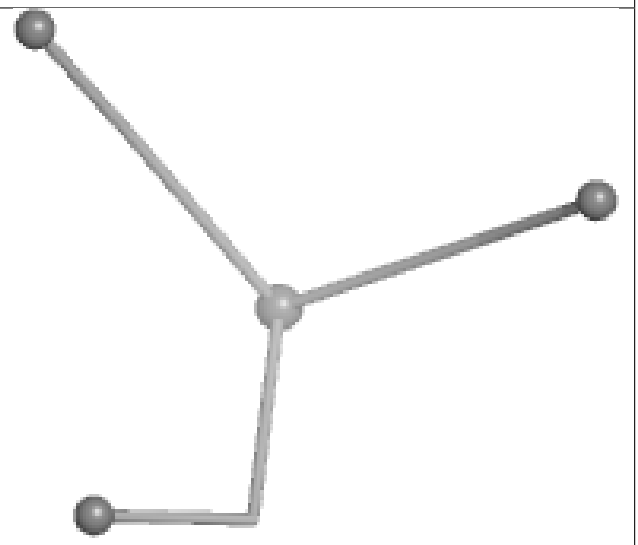


Rings

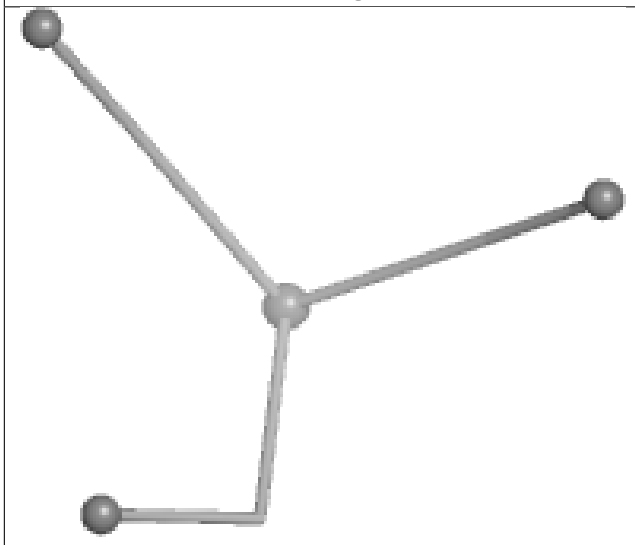
Ligand FCO G 419



Bond lengths



Bond angles



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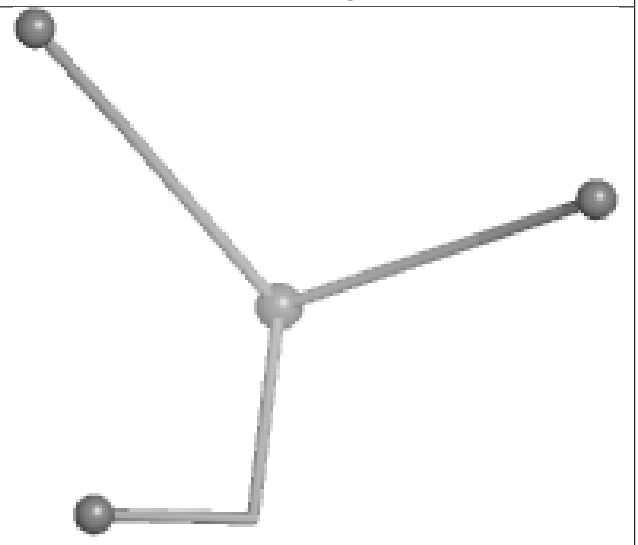
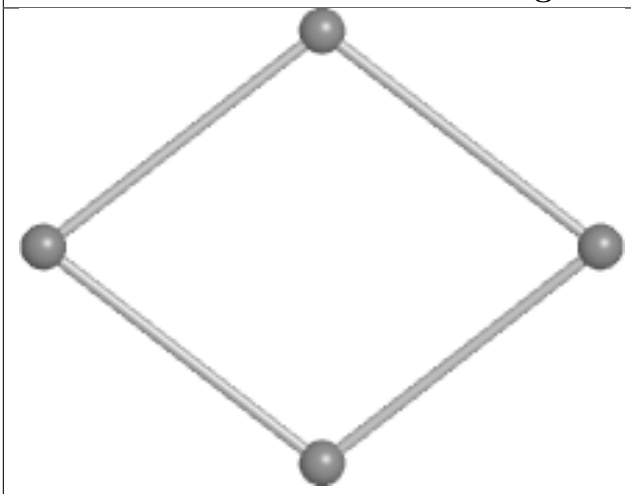
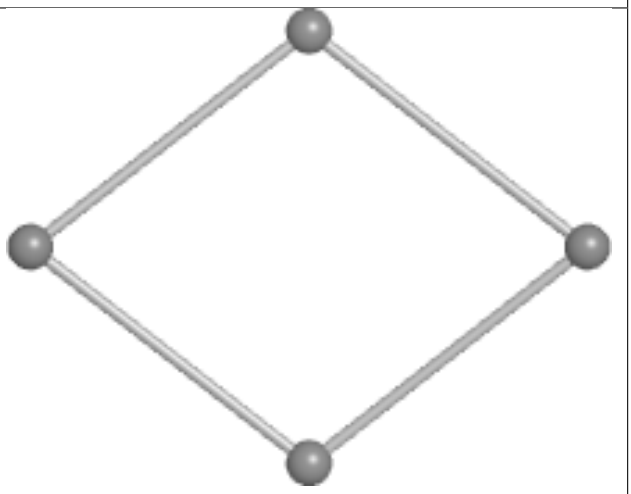


Rings

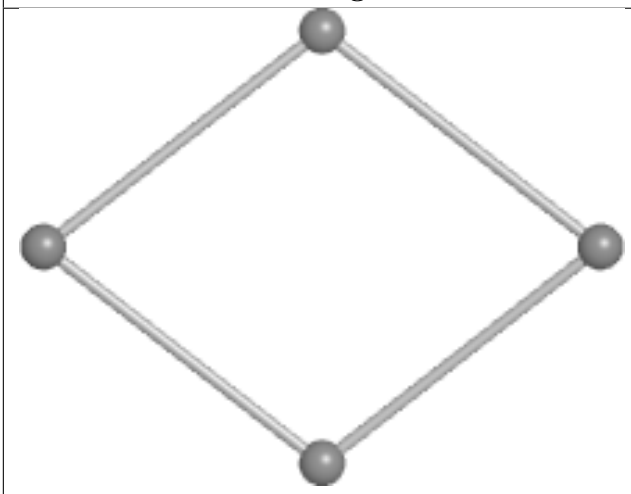
Ligand FES I 201



Bond lengths



Bond angles



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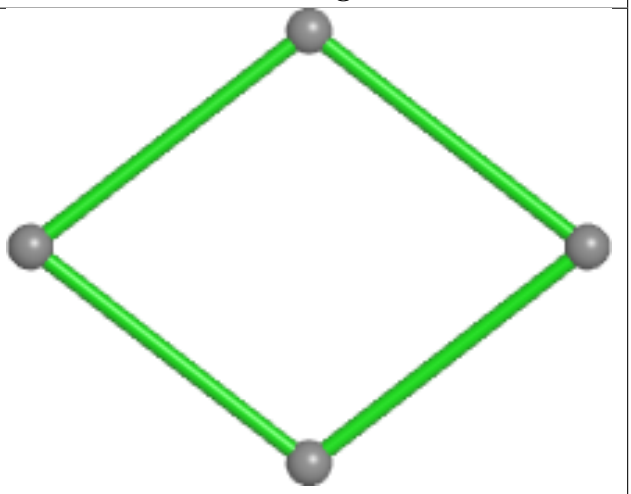
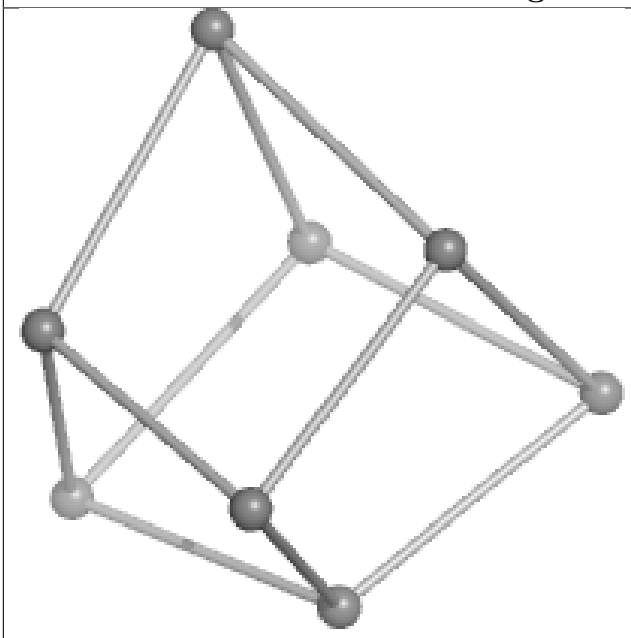
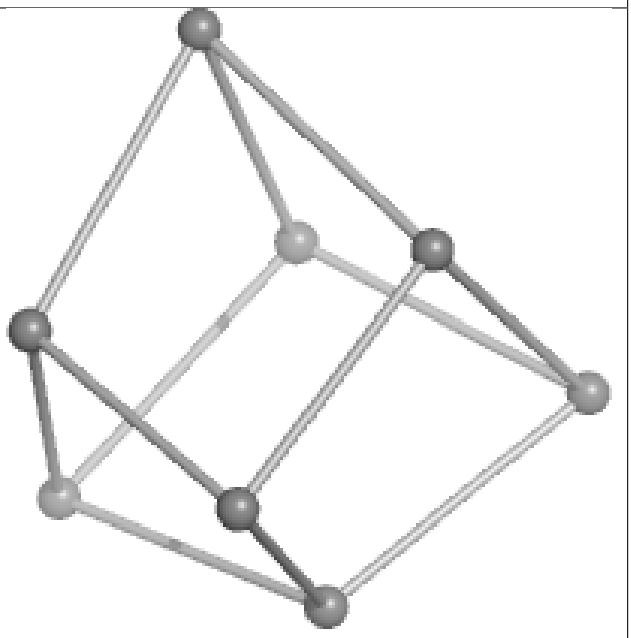


Rings

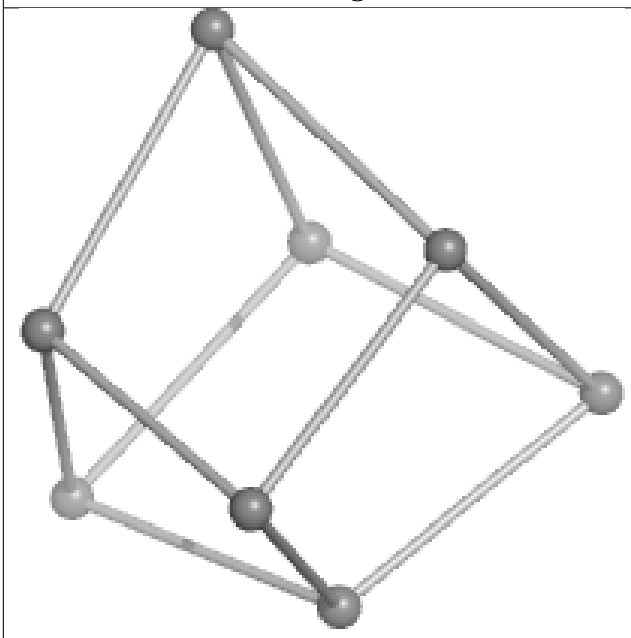
Ligand SF4 M 404



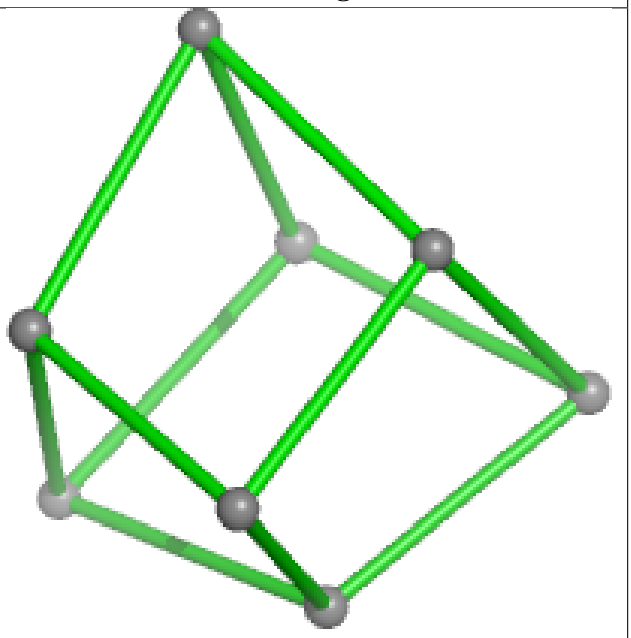
Bond lengths



Bond angles

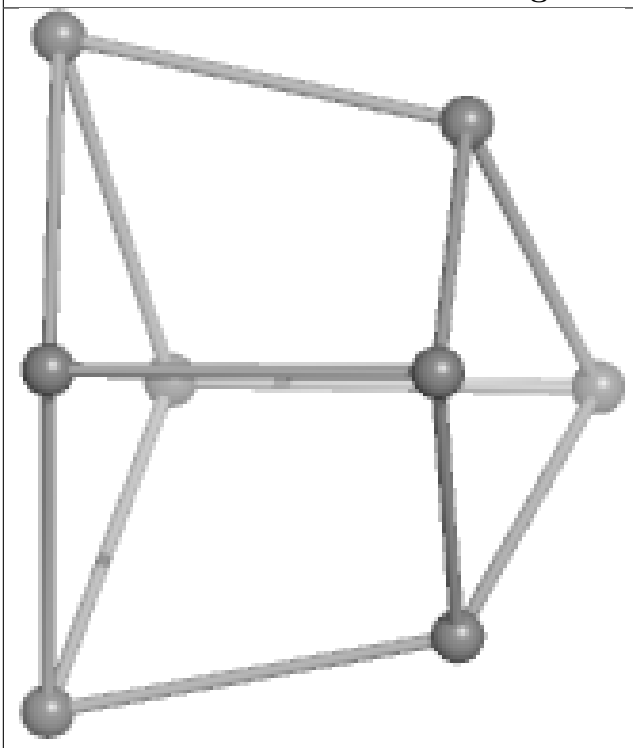


Torsions



Rings

Ligand SF4 H 303



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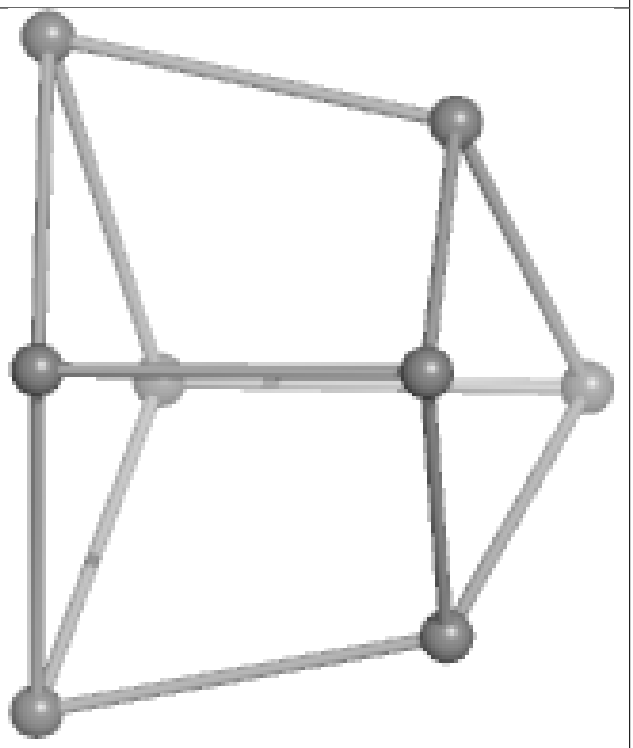

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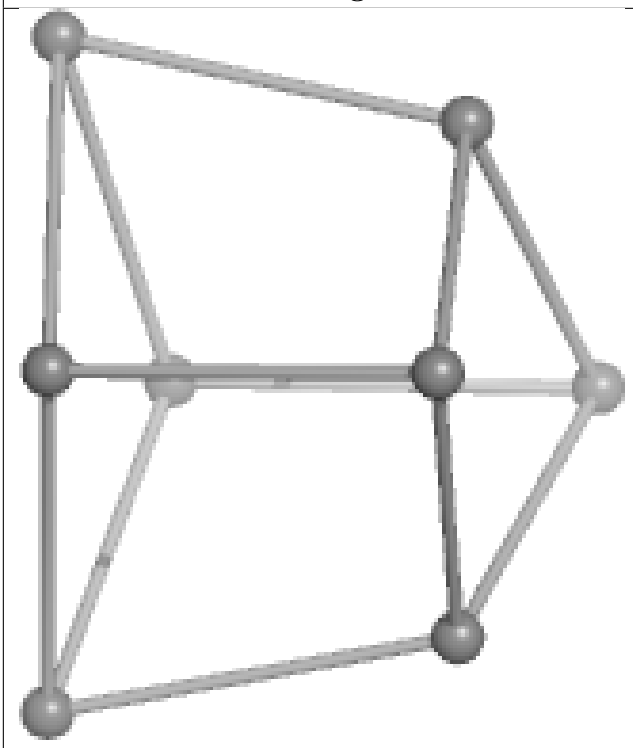

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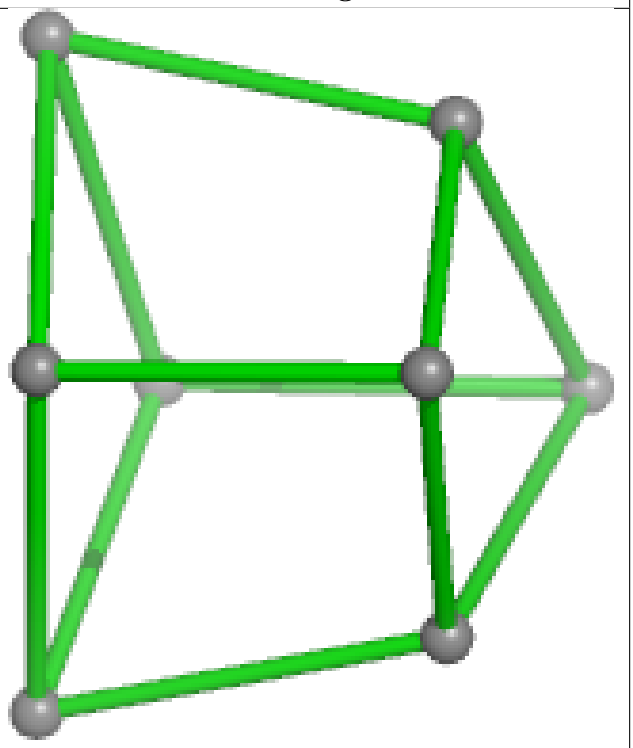
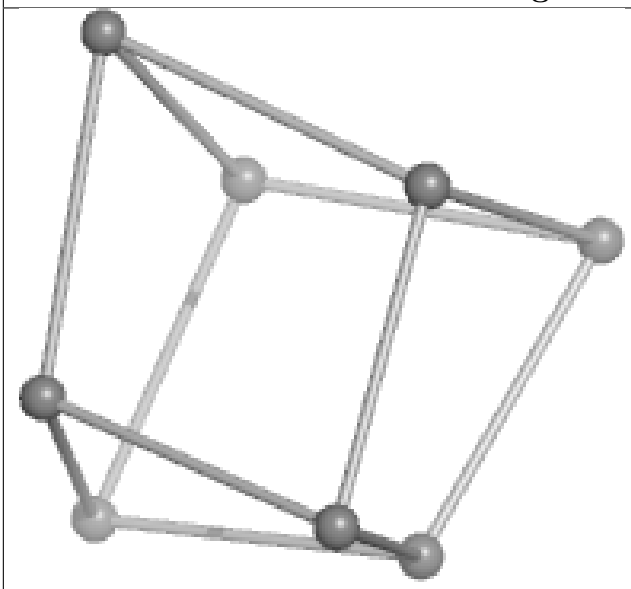


Rings

Ligand SF4 B 705



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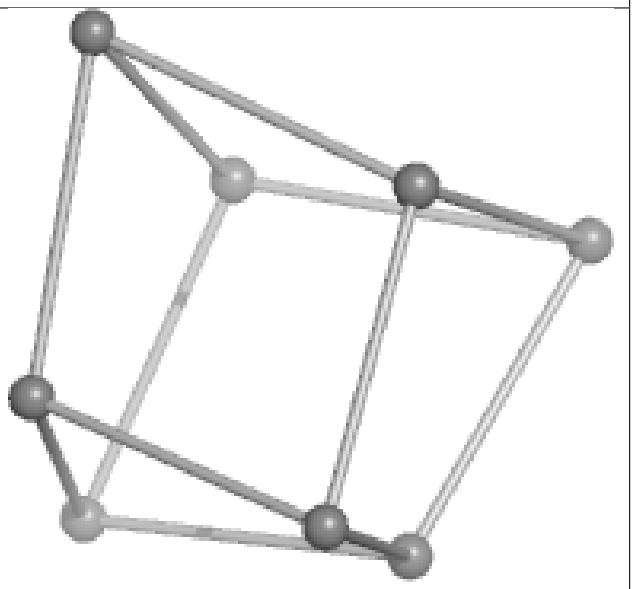
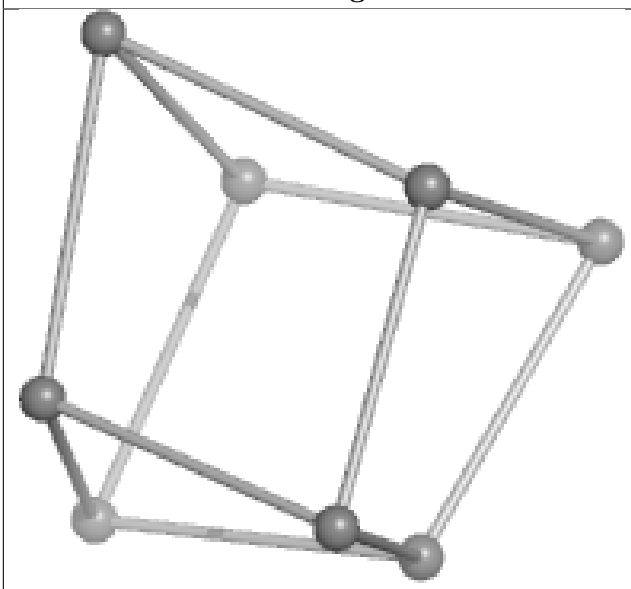


Bond angles



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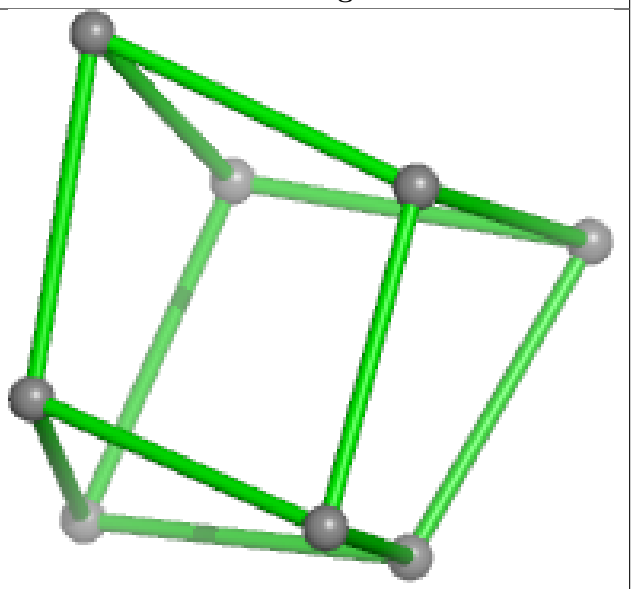
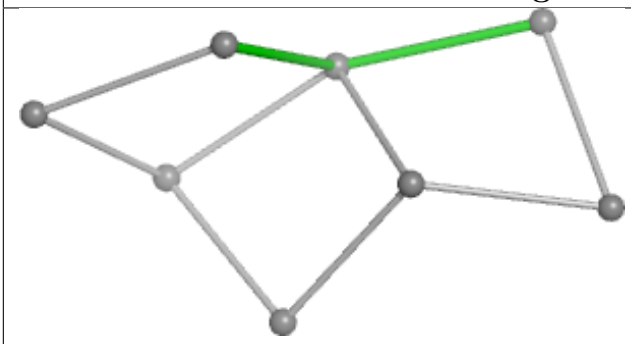


Rings

Ligand 9S8 D 302



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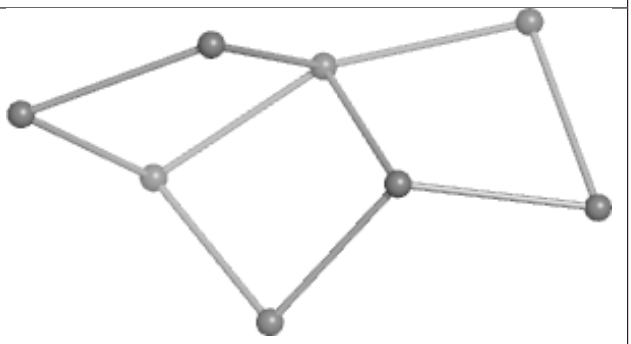
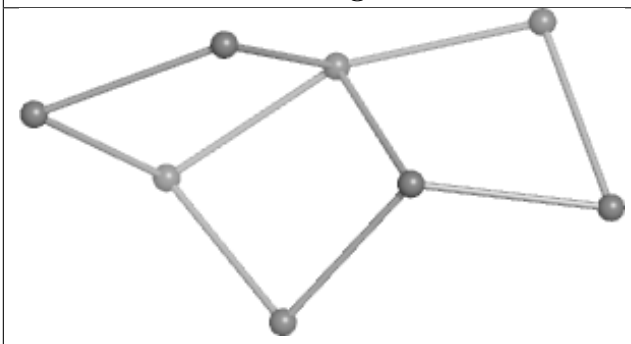


Bond angles



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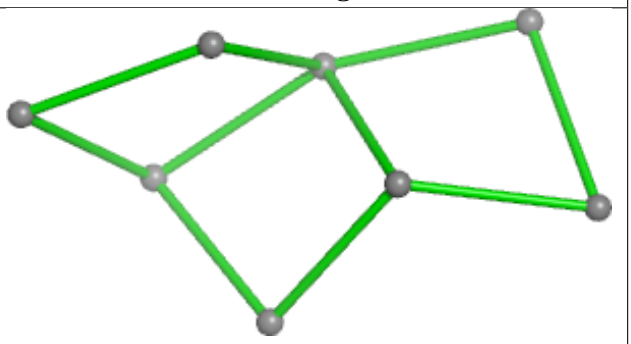
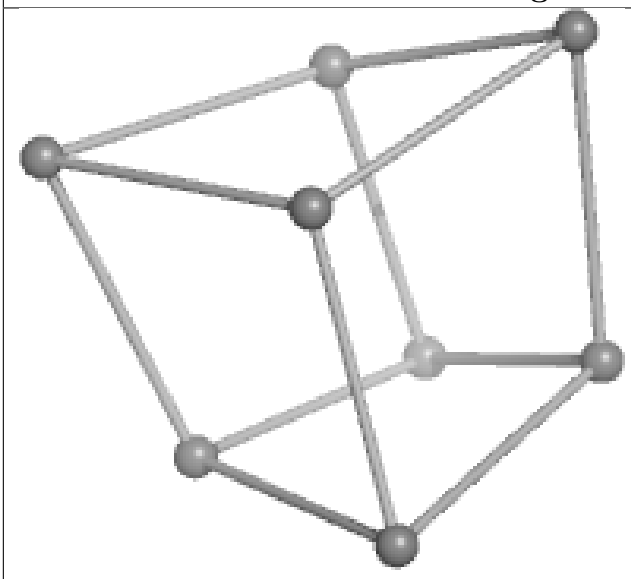


Rings

Ligand SF4 A 701



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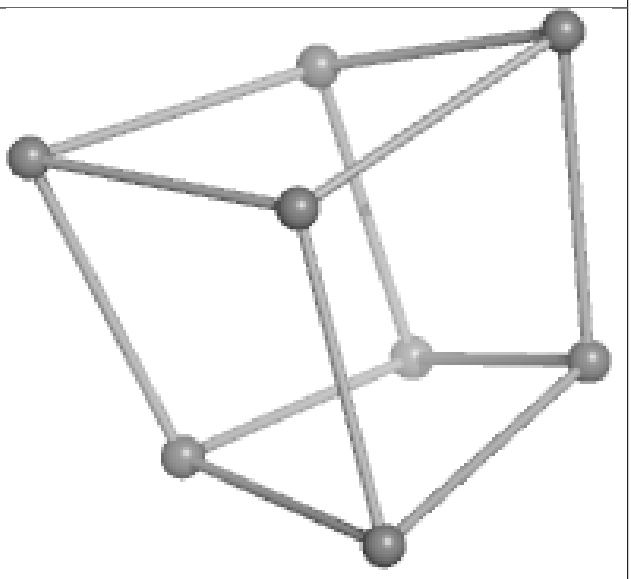
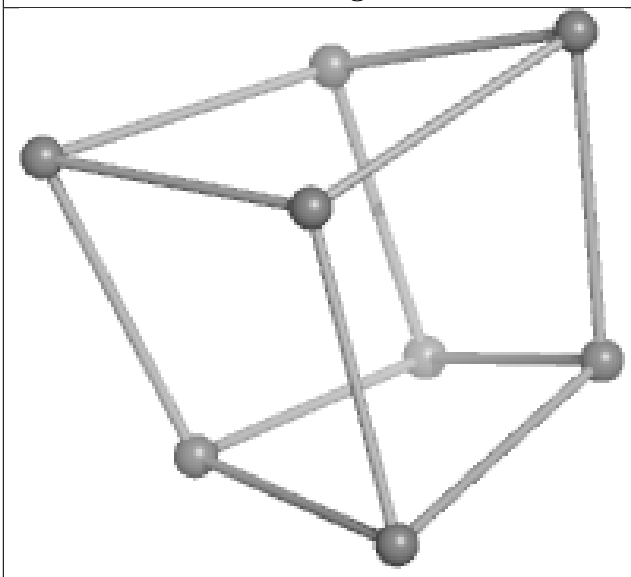


Bond angles



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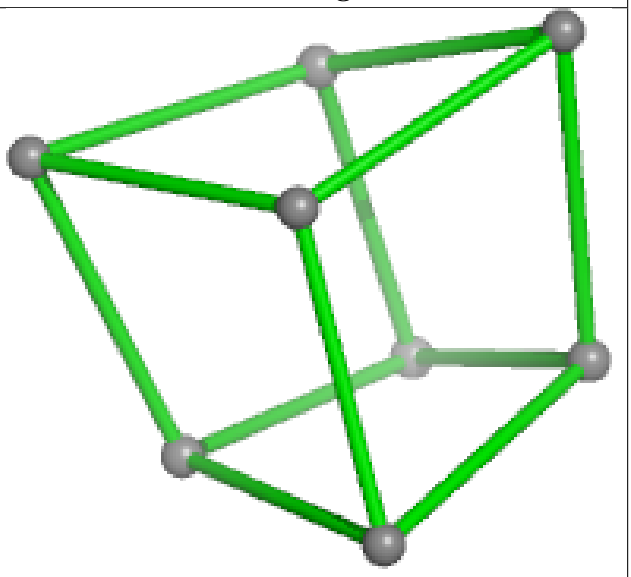
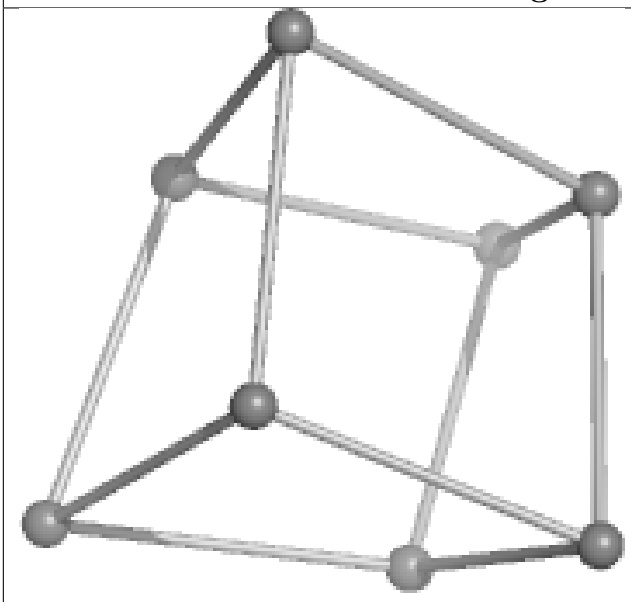


Rings

Ligand SF4 A 705



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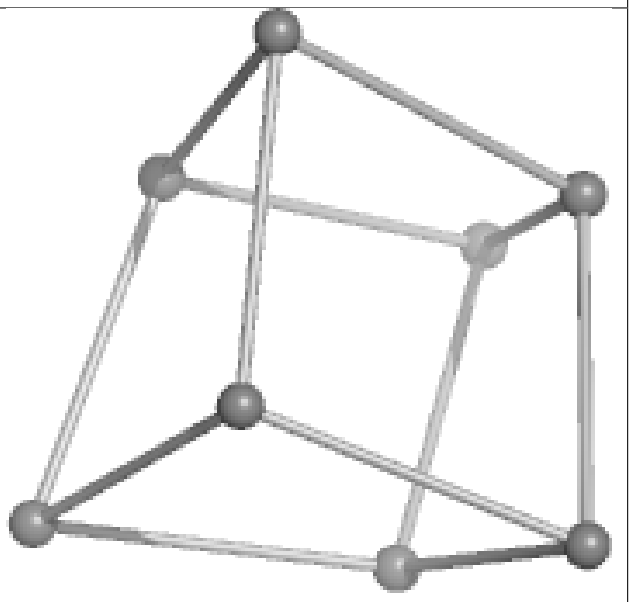

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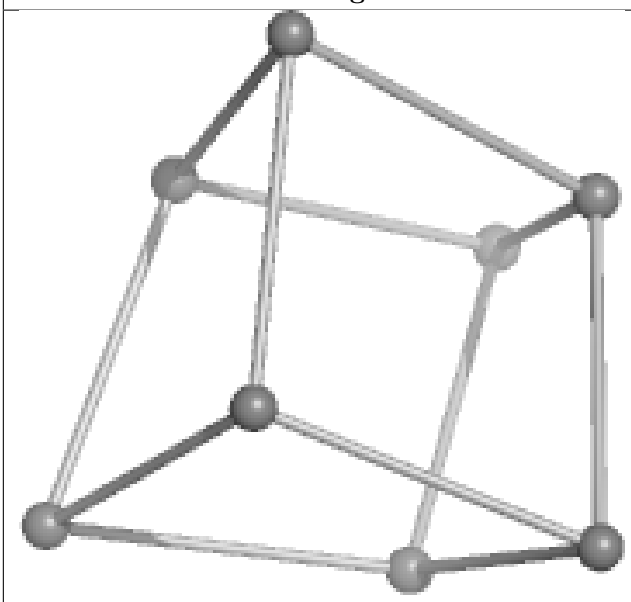

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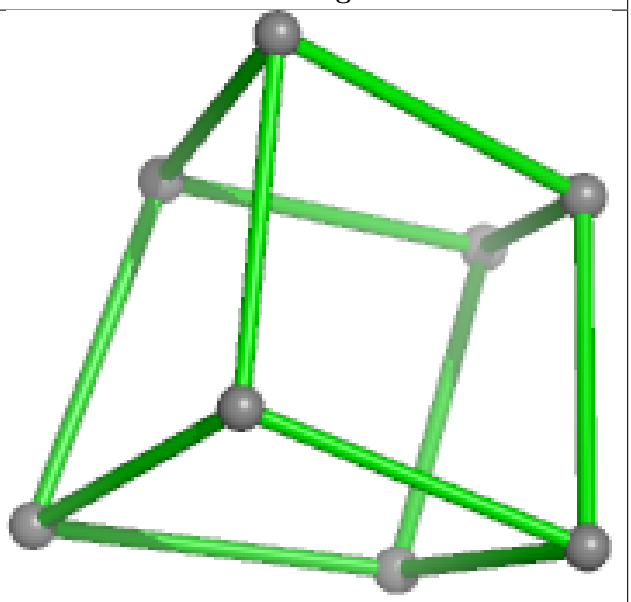
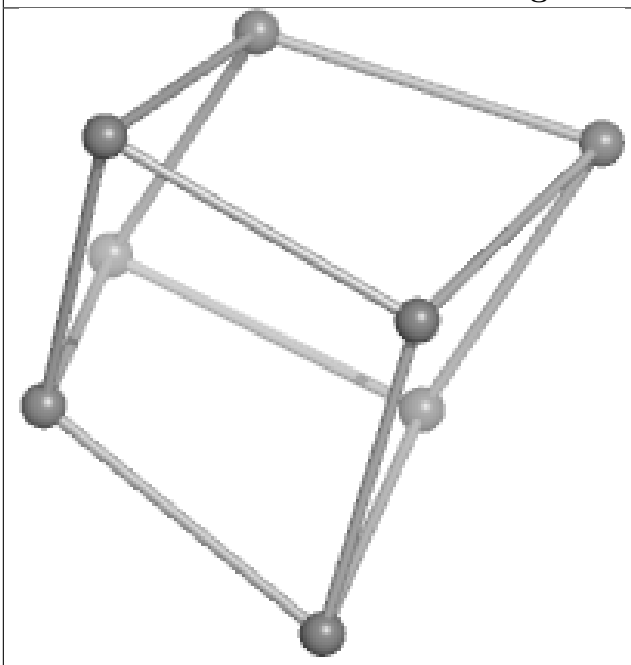


Rings

Ligand SF4 H 302



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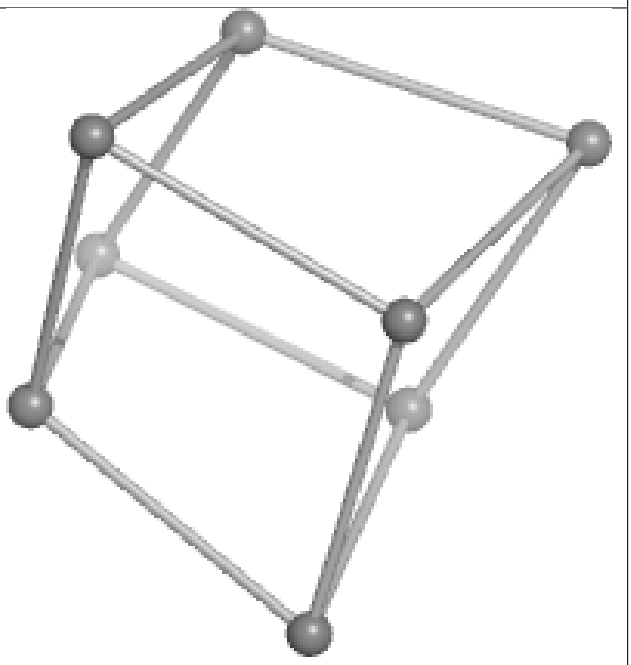
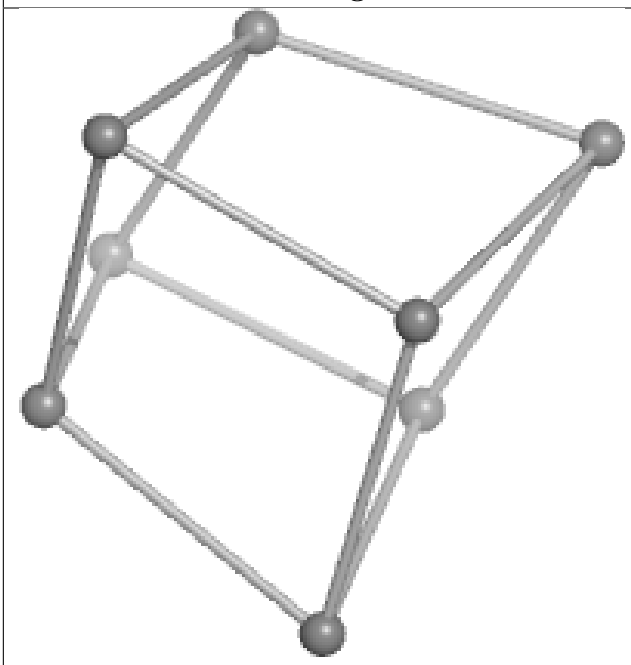


Bond angles



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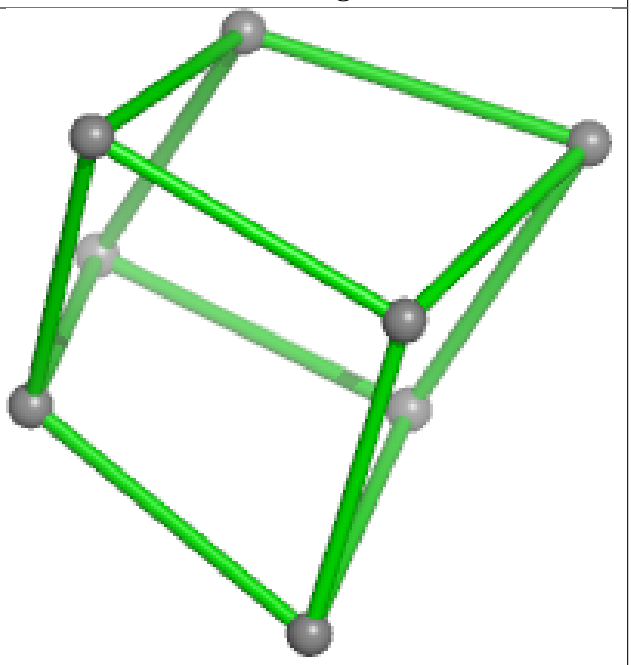
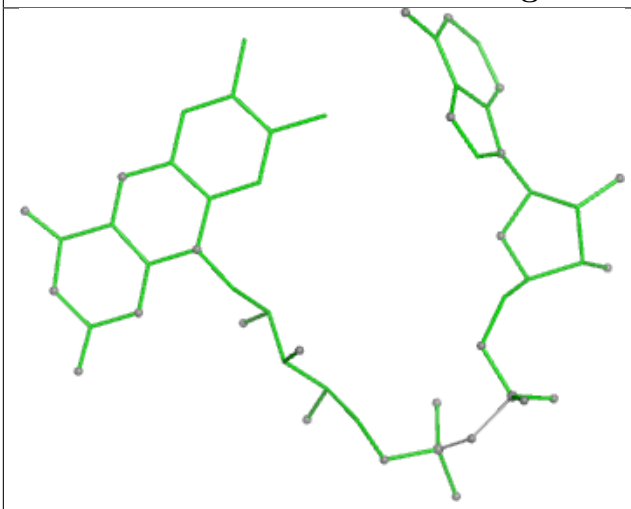


Rings

Ligand FAD M 405



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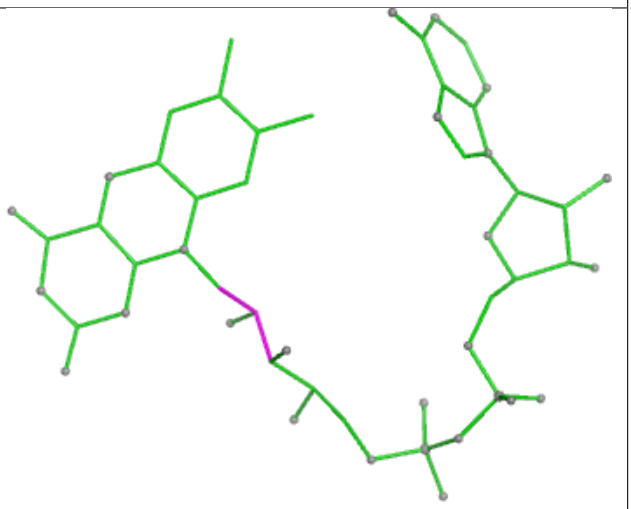
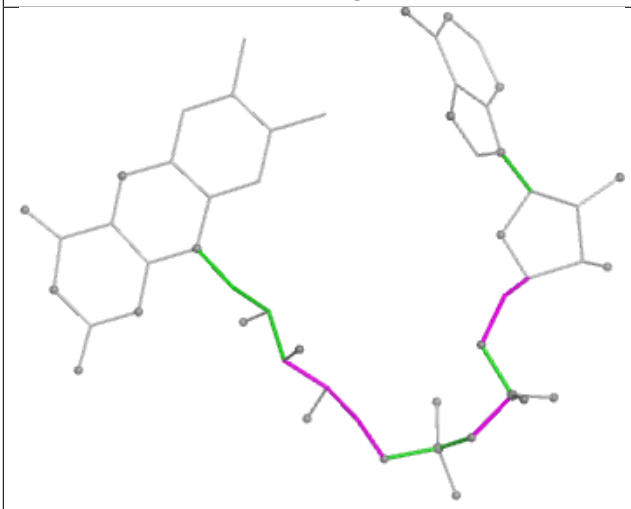


Bond angles



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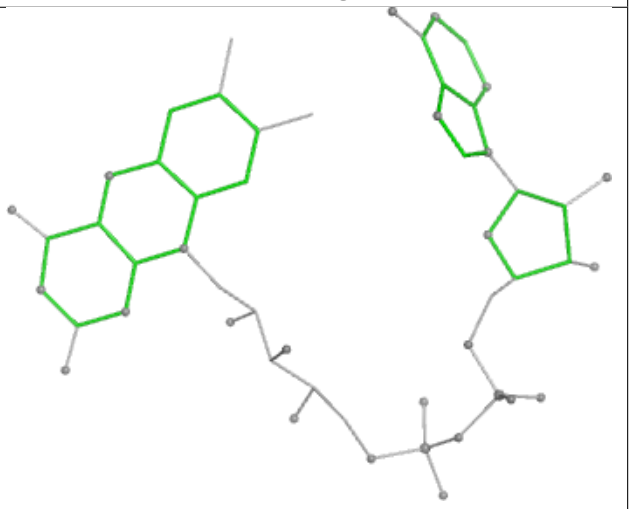
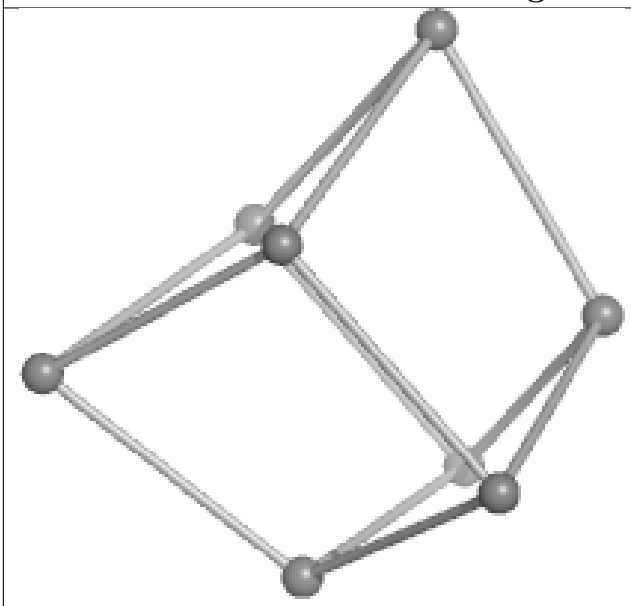


Rings

Ligand SF4 M 402



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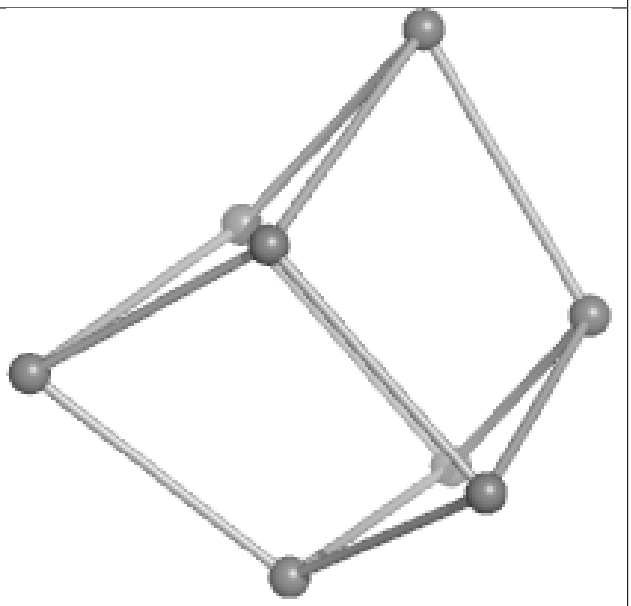
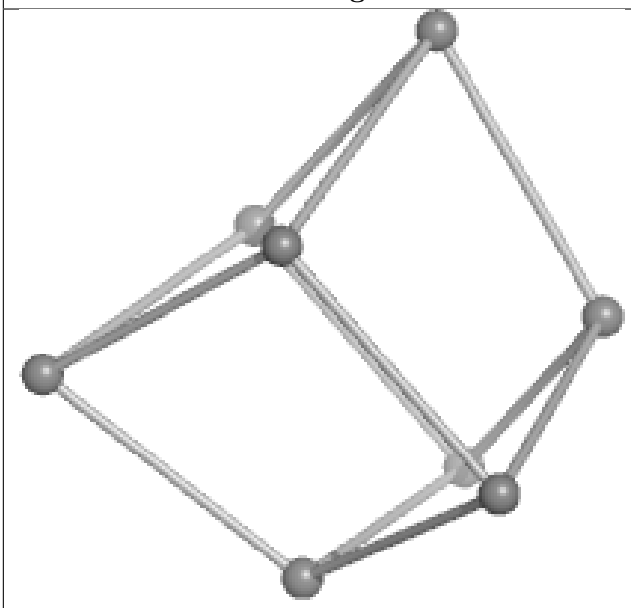


Bond angles



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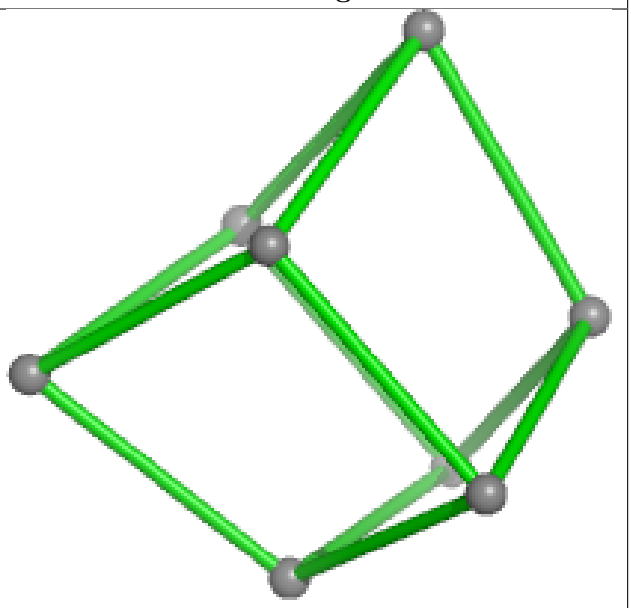
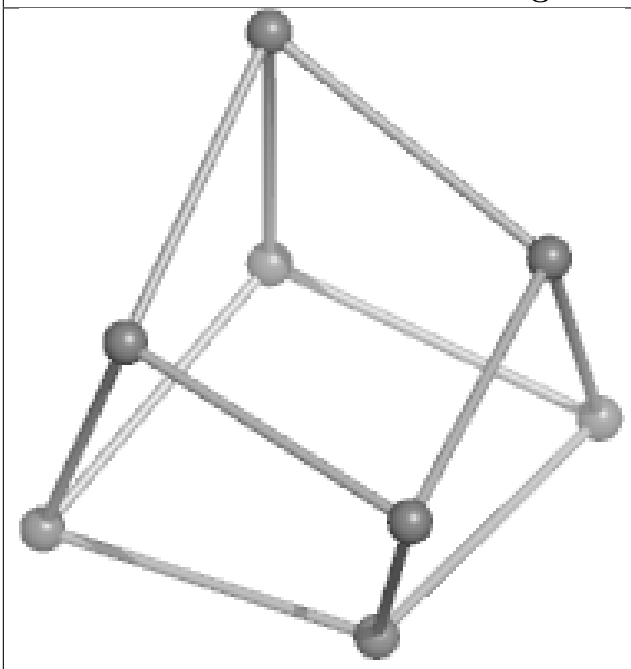


Rings

Ligand SF4 B 702



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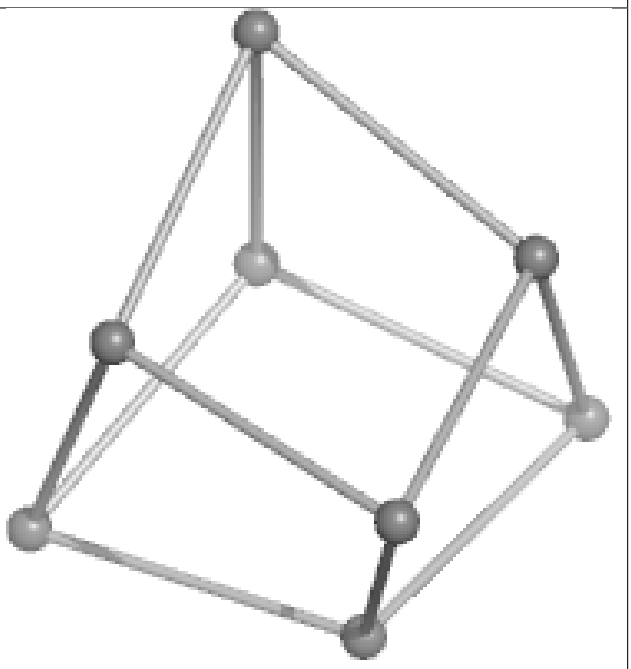

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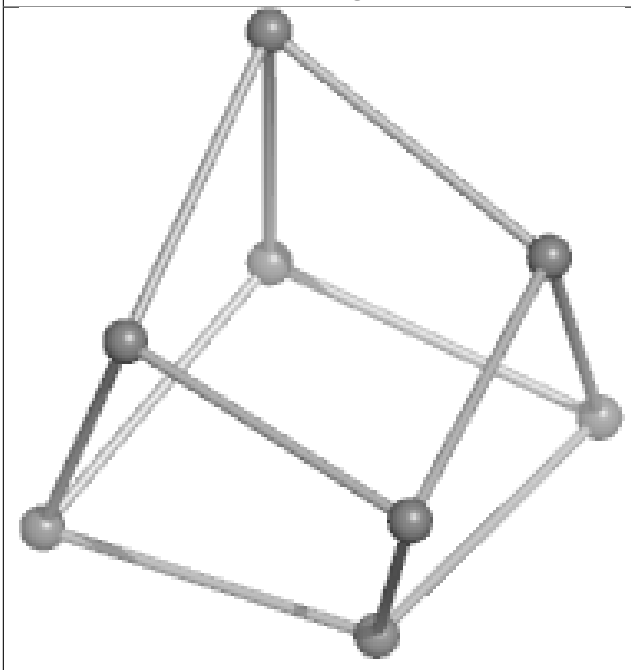

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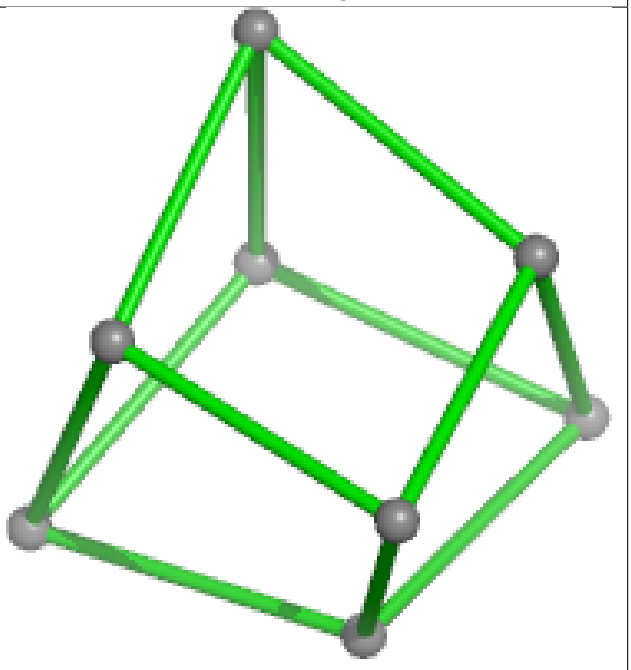
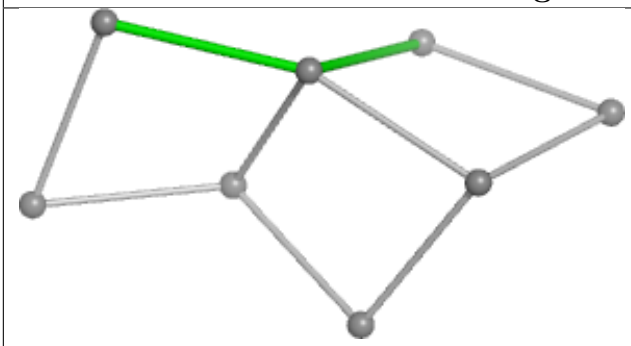


Rings

Ligand 9S8 C 302



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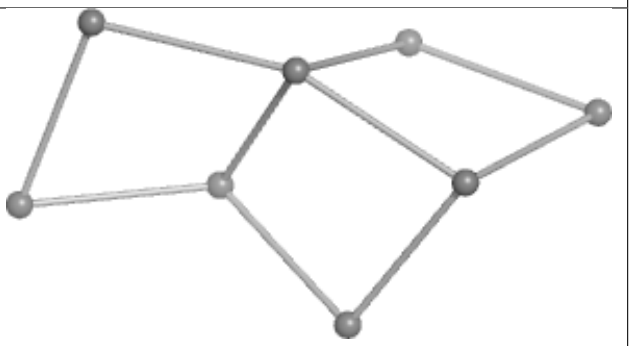
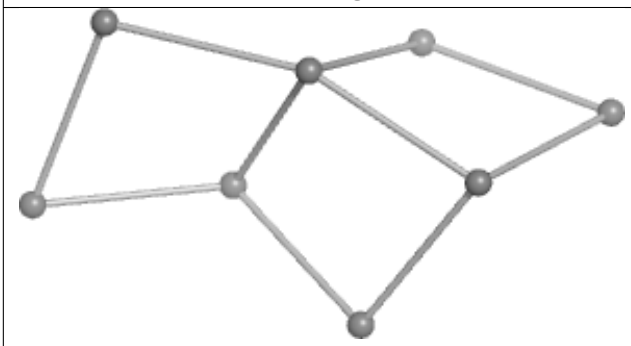


Bond angles



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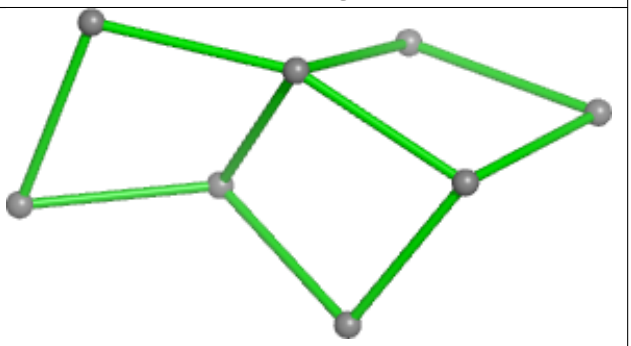
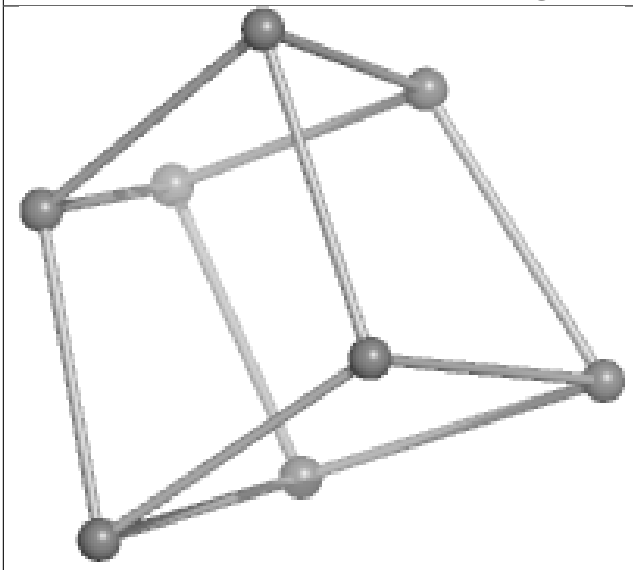


Rings

Ligand SF4 F 202



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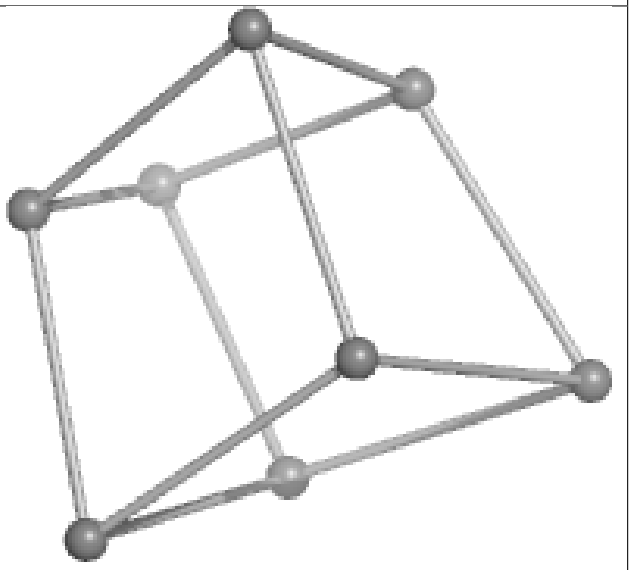
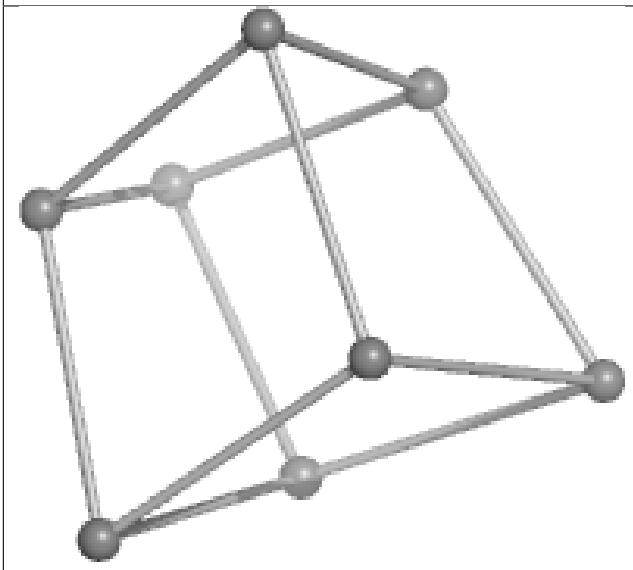


Bond angles



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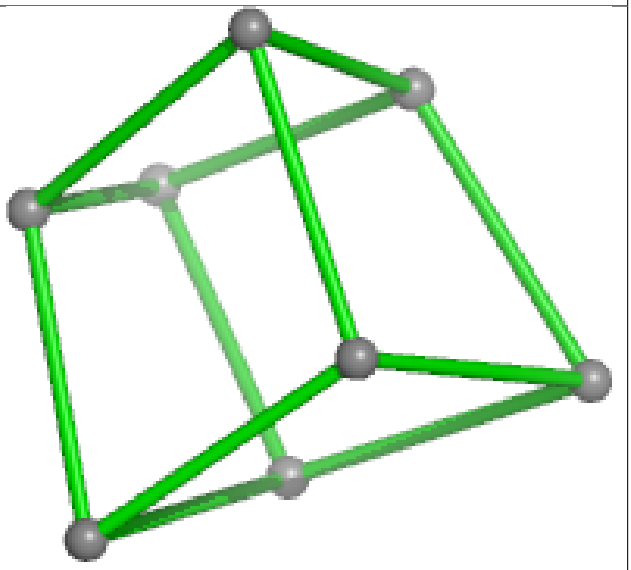
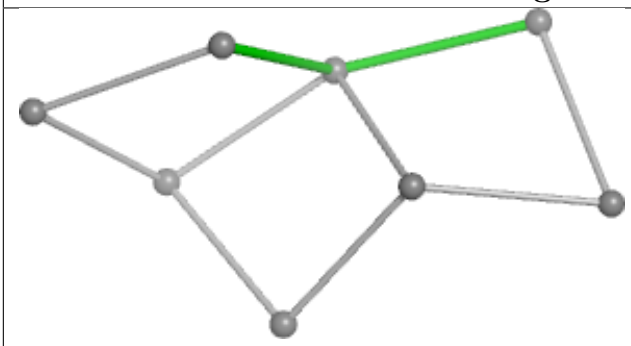


Rings

Ligand 9S8 C 301



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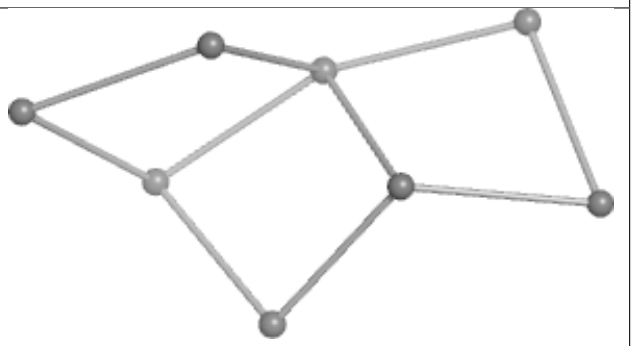
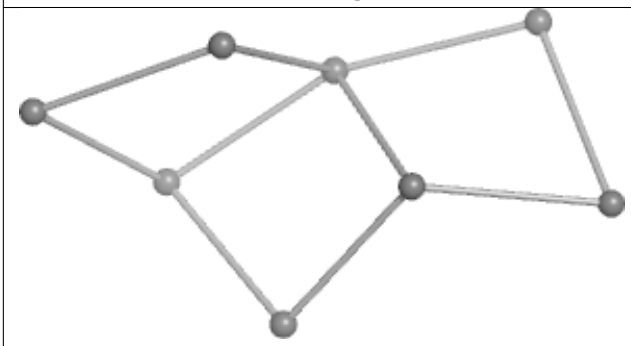


Bond angles



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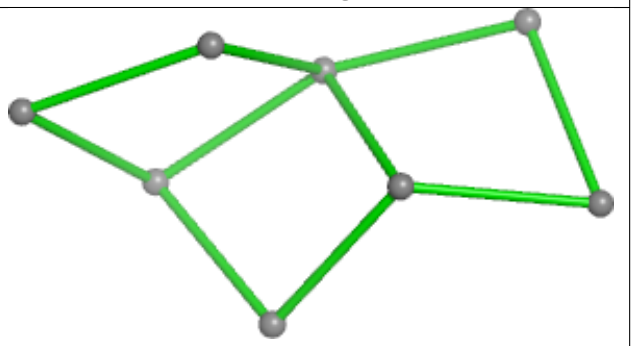
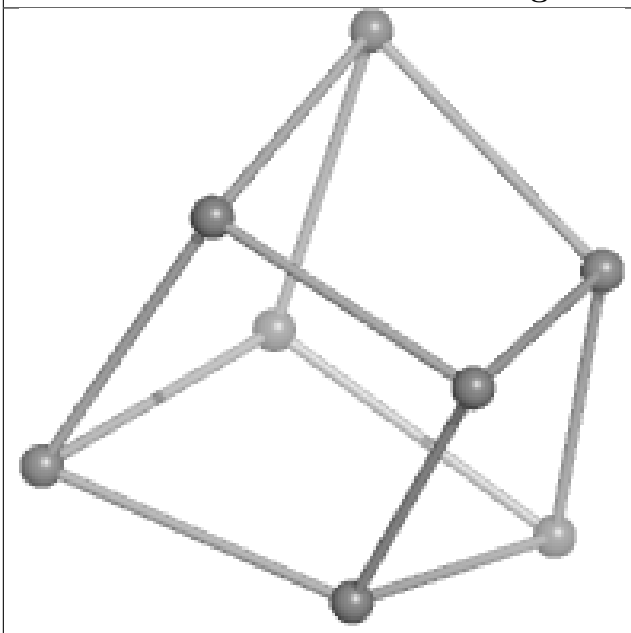
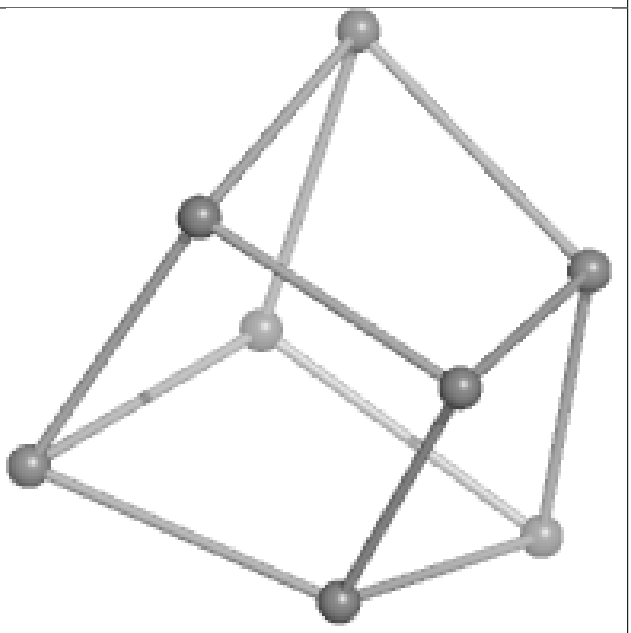


Rings

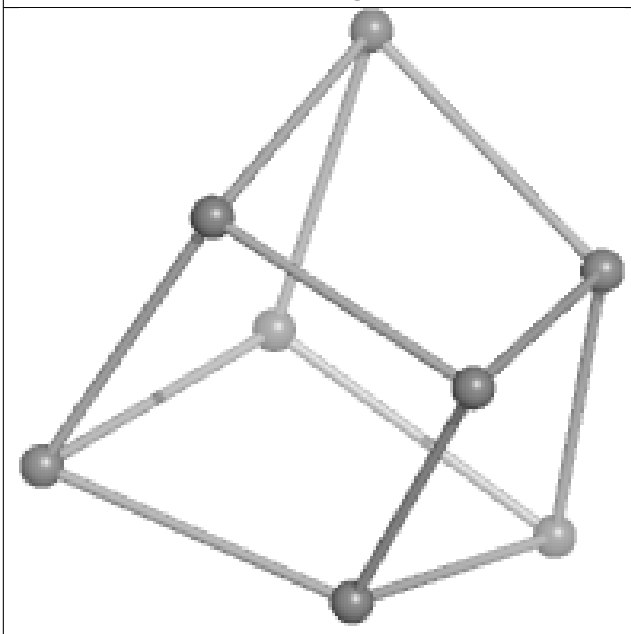
Ligand SF4 A 702



Bond lengths



Bond angles



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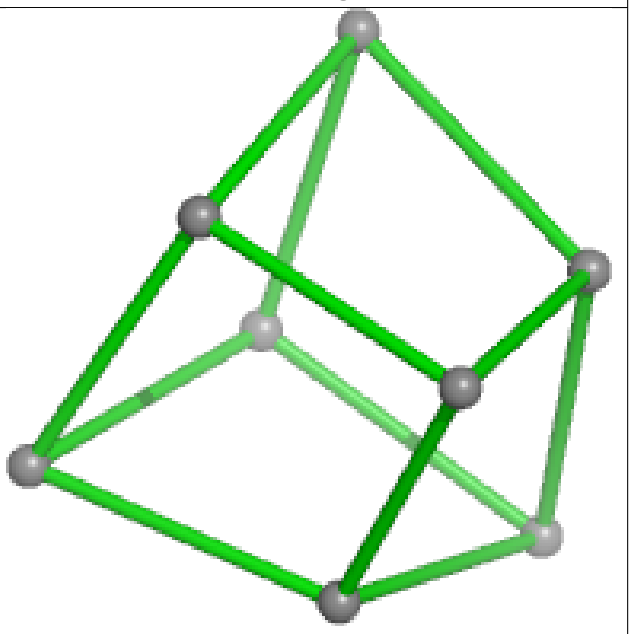
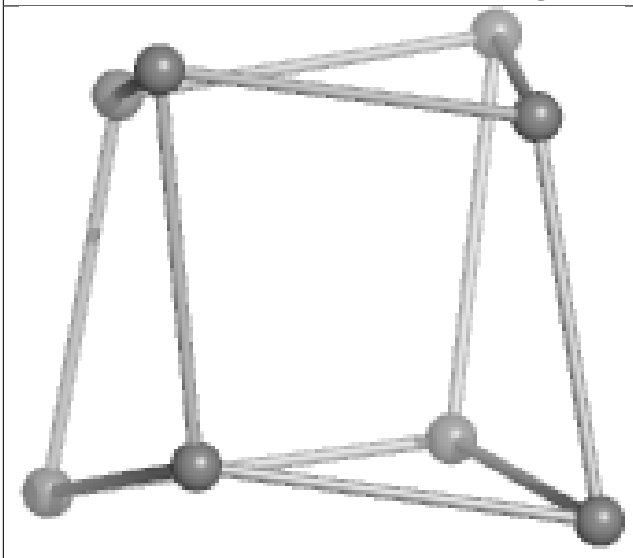
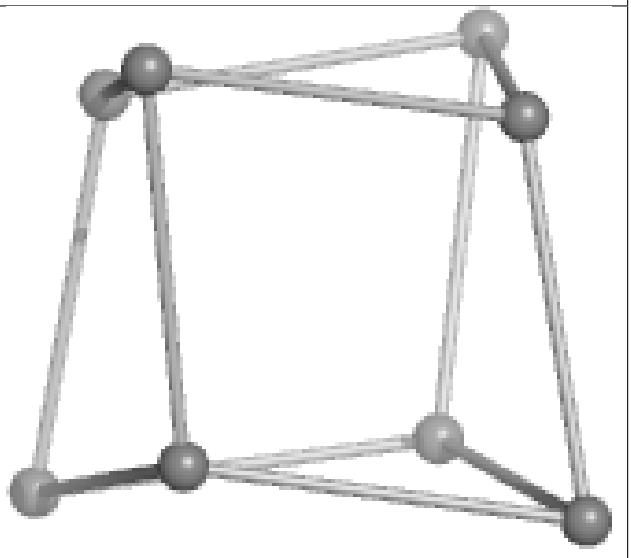


Rings

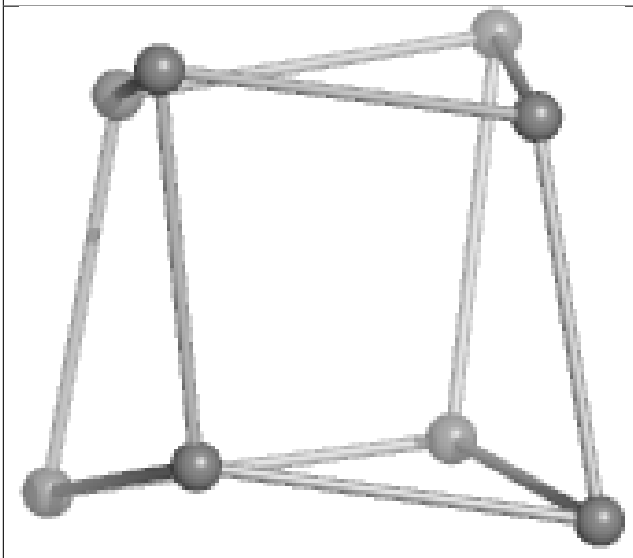
Ligand SF4 E 201



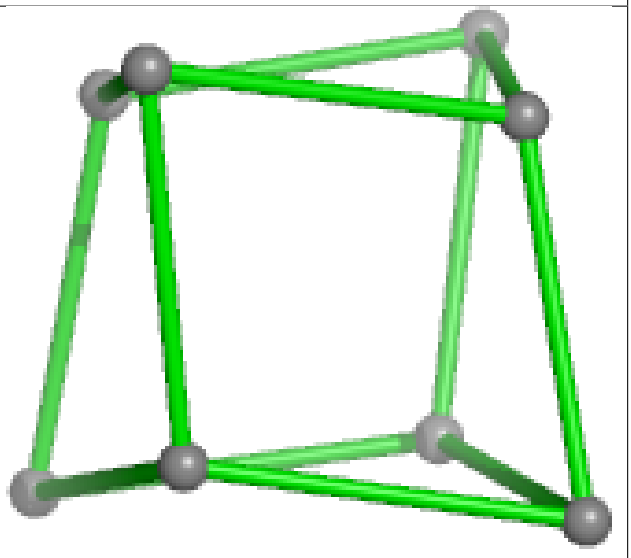
Bond lengths



Bond angles

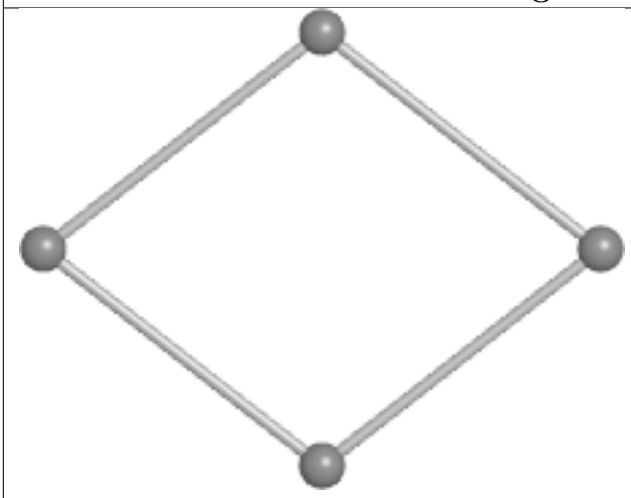


Torsions

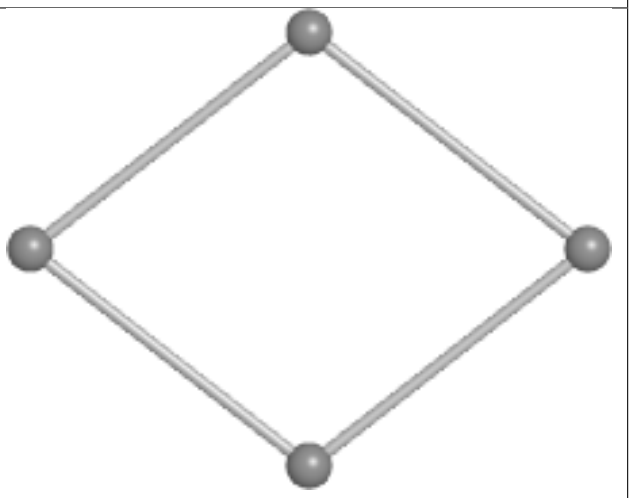


Rings

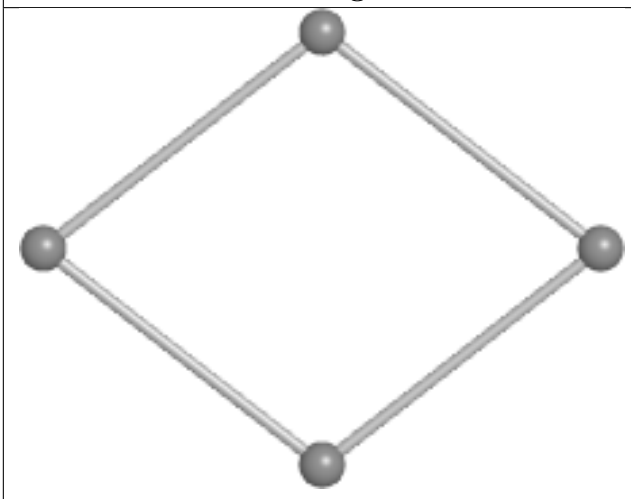
Ligand FES J 201



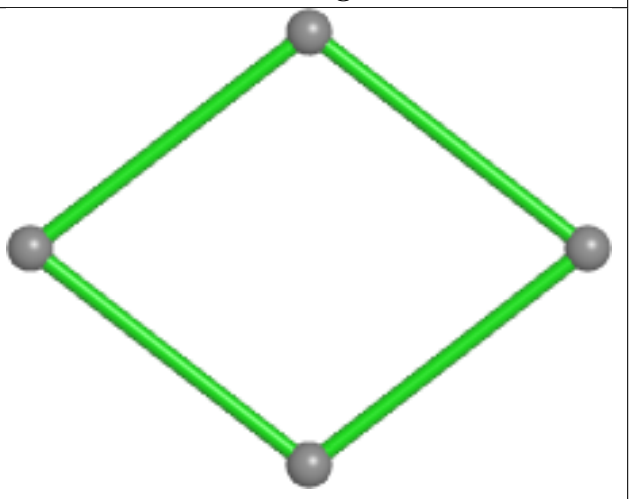
Bond lengths



Bond angles

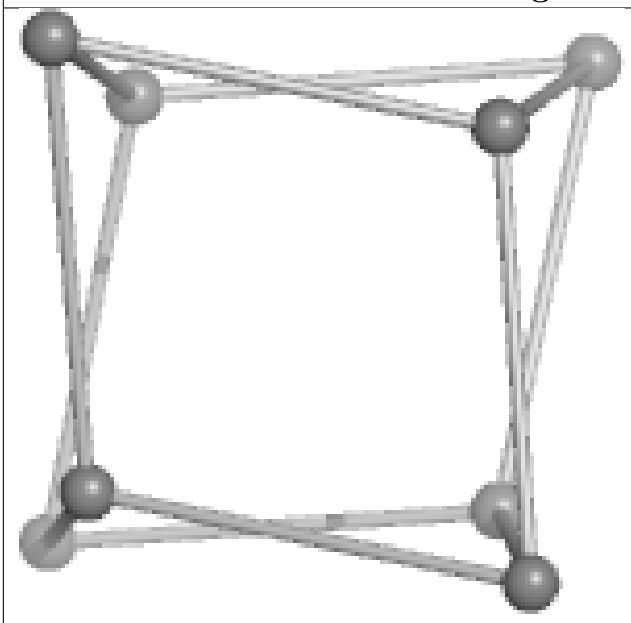


Torsions

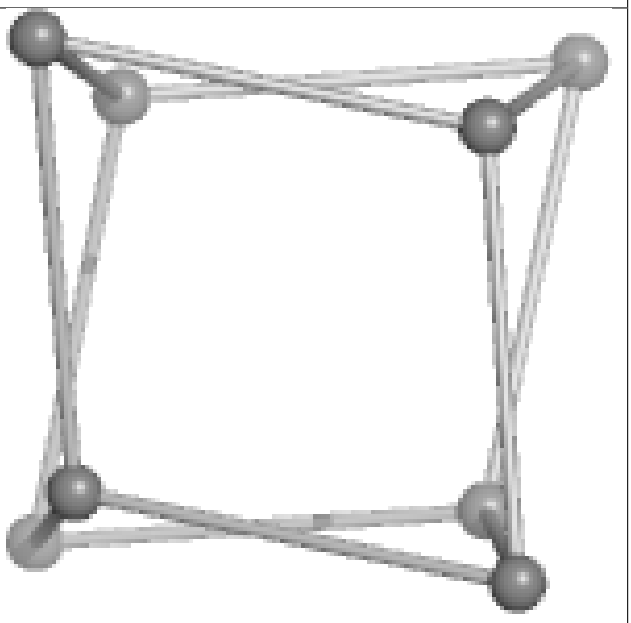


Rings

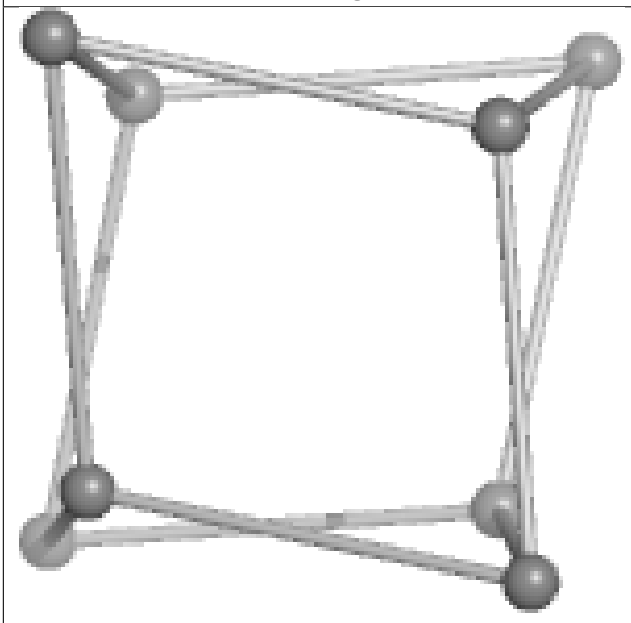
Ligand SF4 B 701



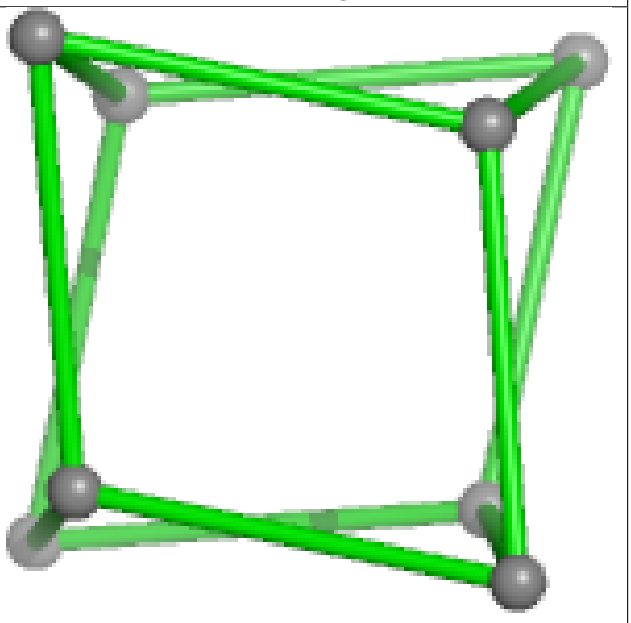
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

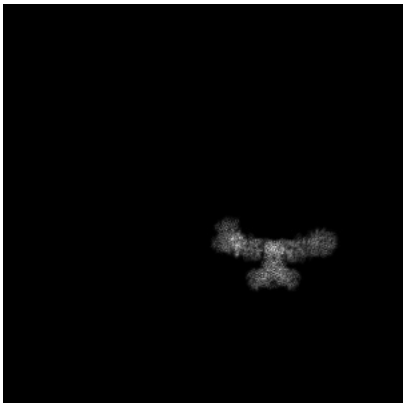
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55451. These allow visual inspection of the internal detail of the map and identification of artifacts.

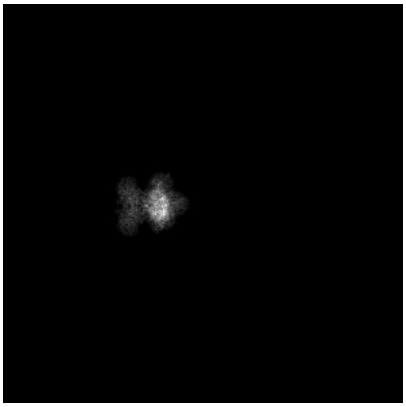
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

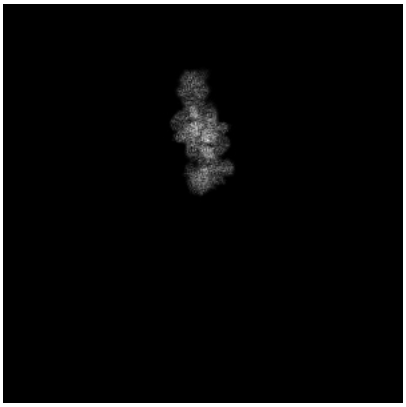
6.1.1 Primary map



X



Y

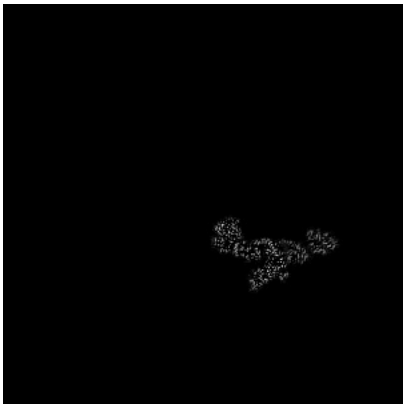


Z

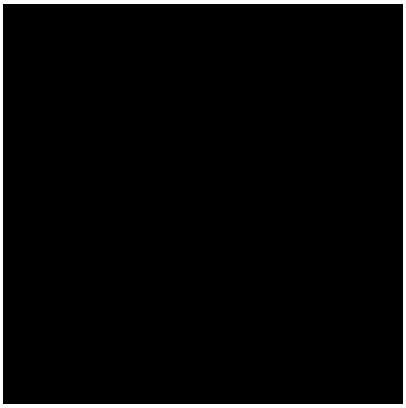
The images above show the map projected in three orthogonal directions.

6.2 Central slices

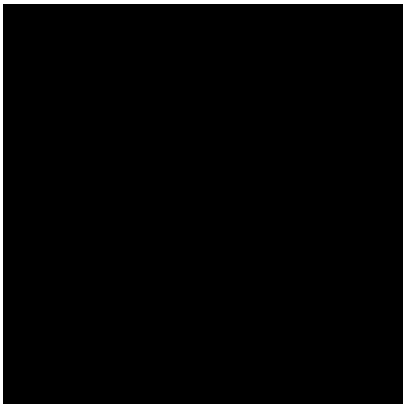
6.2.1 Primary map



X Index: 400



Y Index: 400

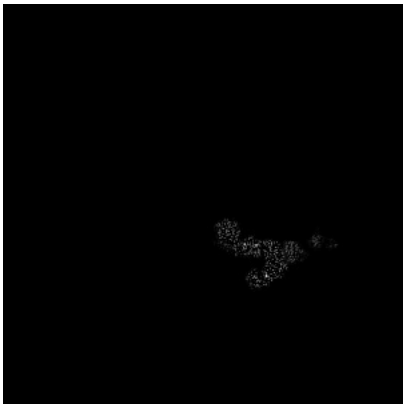


Z Index: 400

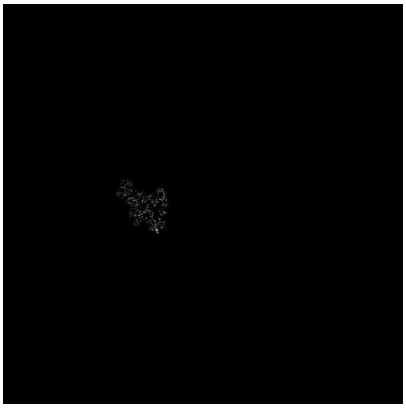
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

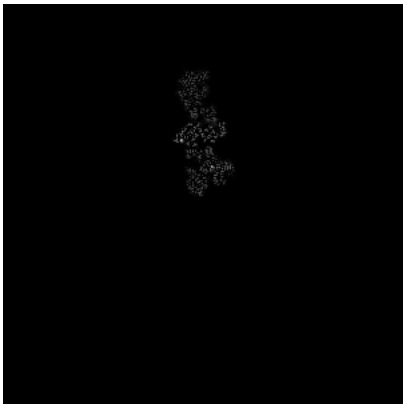
6.3.1 Primary map



X Index: 409



Y Index: 533

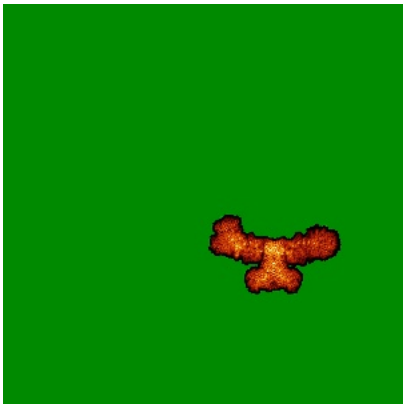


Z Index: 314

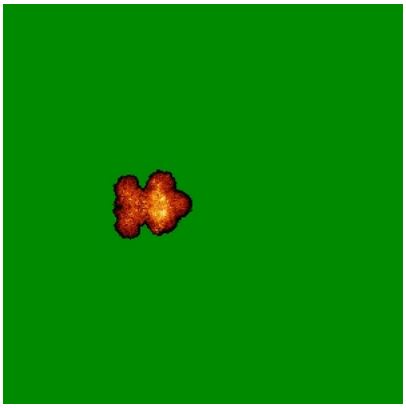
The images above show the largest variance slices of the map in three orthogonal directions.

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

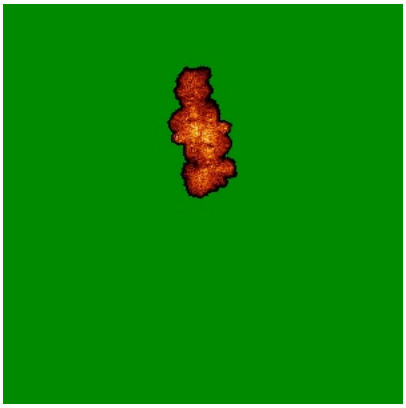
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.174. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

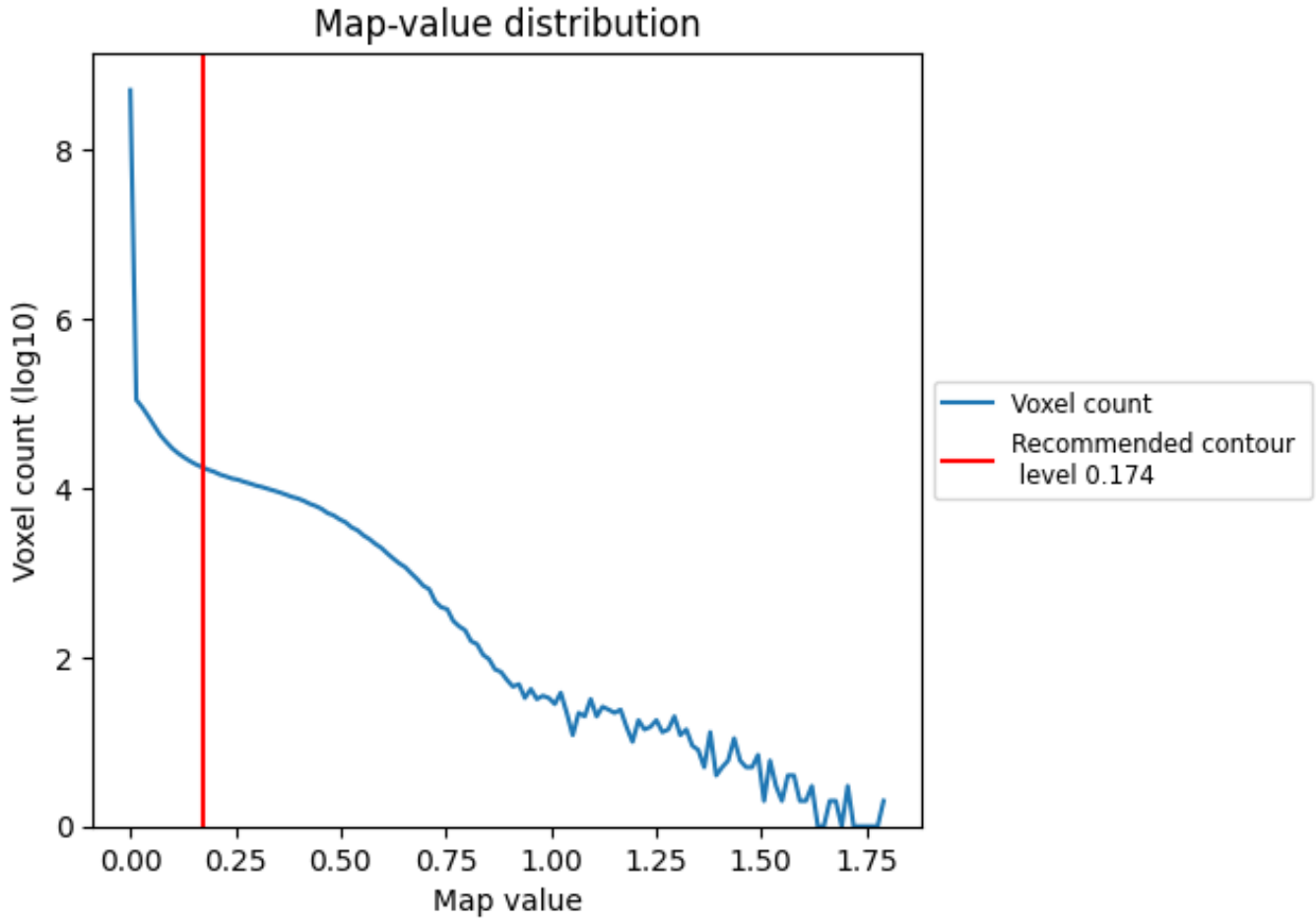
6.6 Mask visualisation (i)

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

7 Map analysis

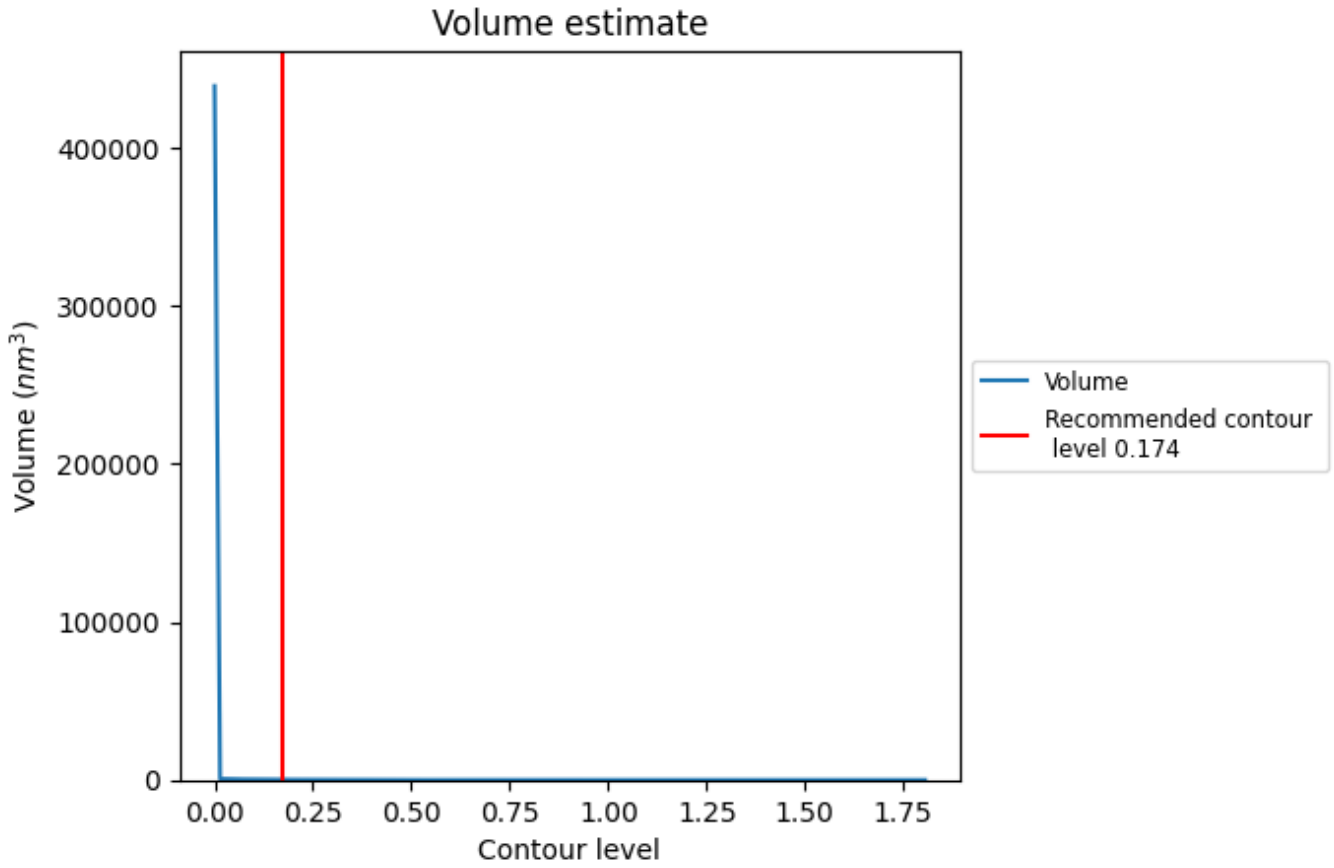
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

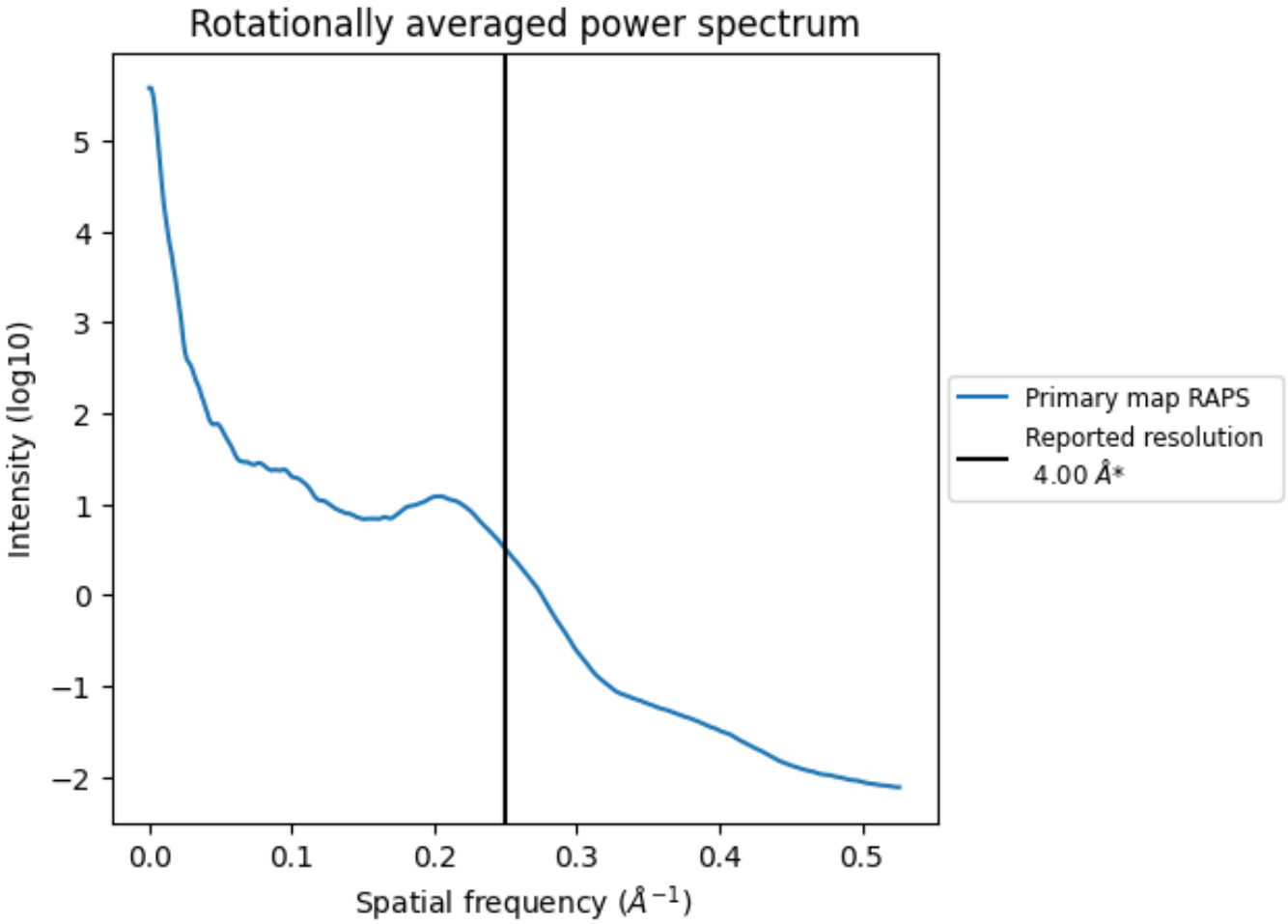
7.2 Volume estimate (i)



The volume at the recommended contour level is 230 nm^3; this corresponds to an approximate mass of 207 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 0.250 Å^{-1}

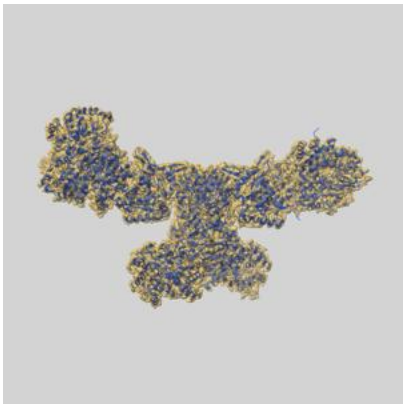
8 Fourier-Shell correlation (i)

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

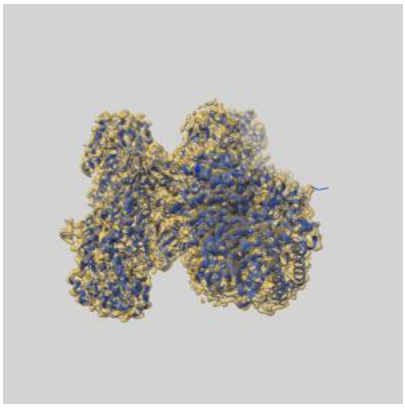
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55451 and PDB model 9T1S. Per-residue inclusion information can be found in section 3 on page 11.

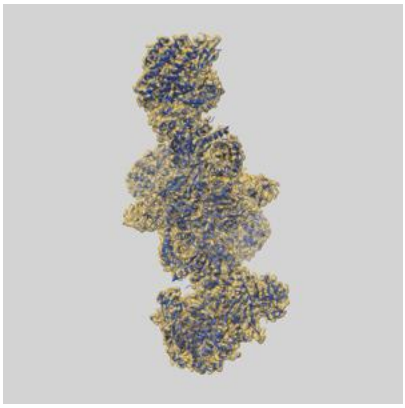
9.1 Map-model overlay



X



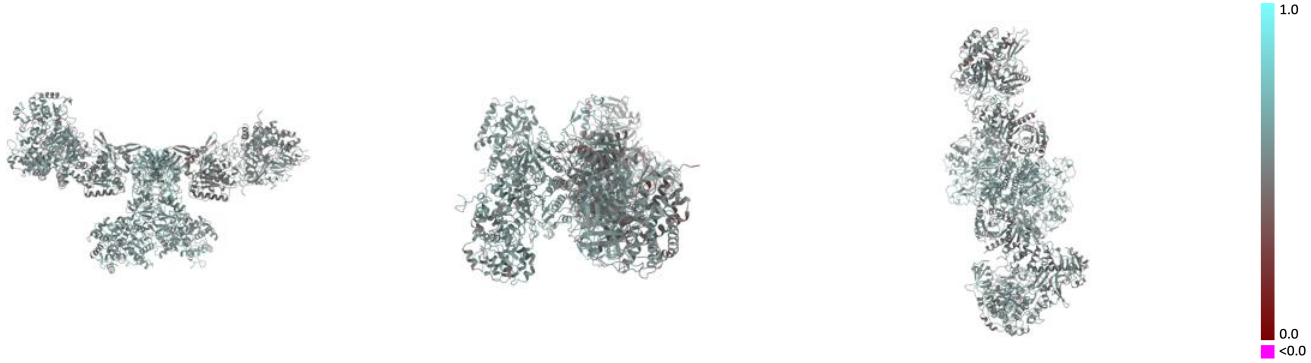
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.174 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

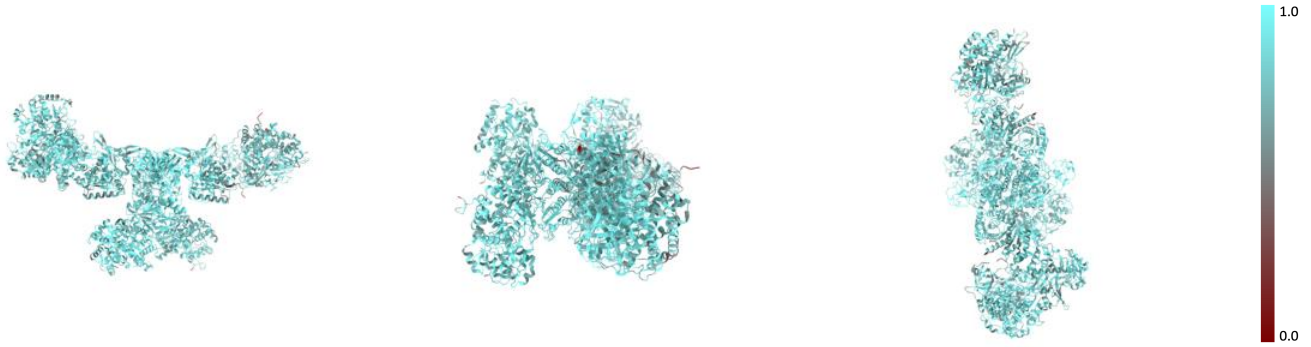
9.2 Q-score mapped to coordinate model



X Y Z

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

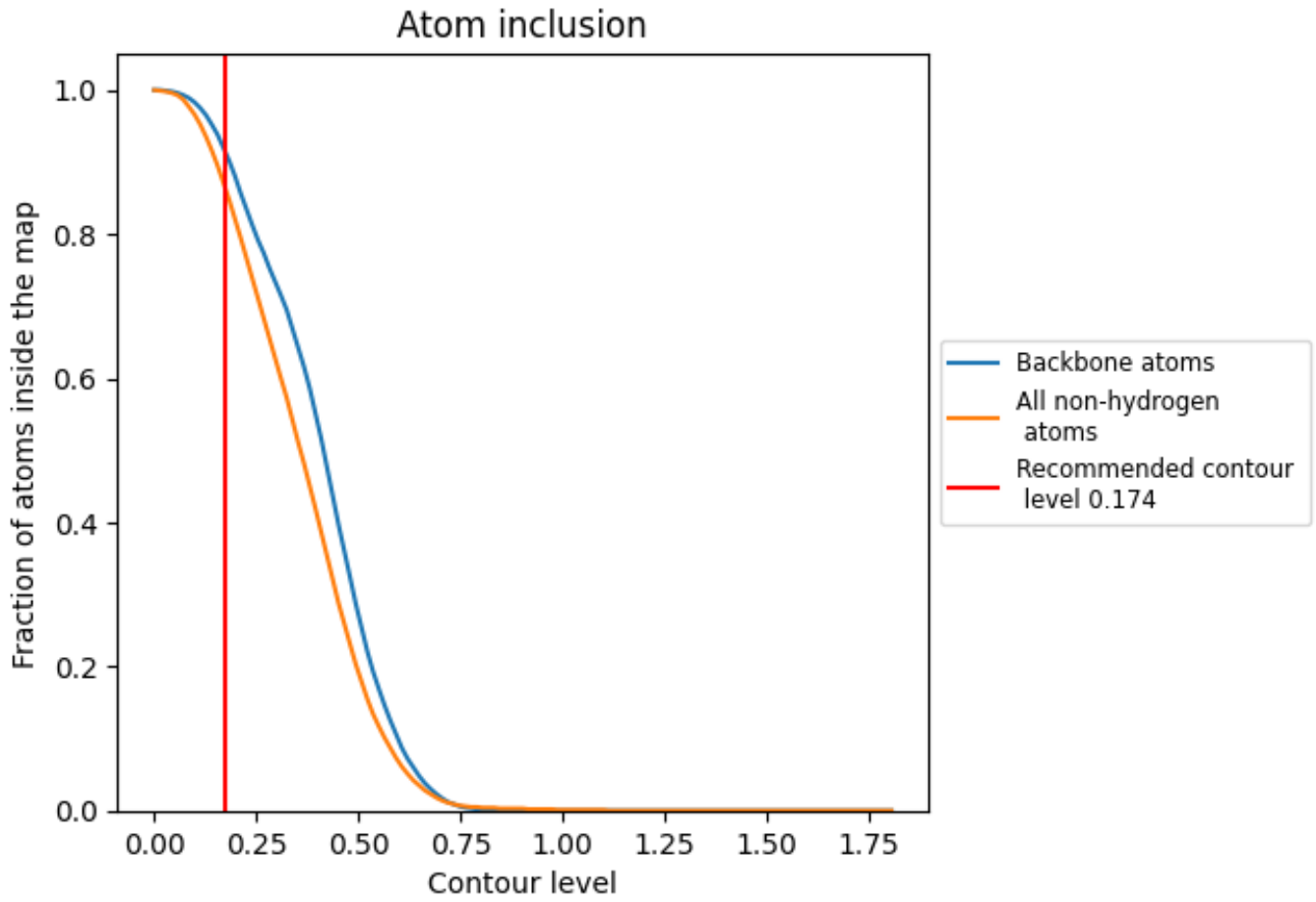
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.174).

9.4 Atom inclusion (i)



At the recommended contour level, 91% 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 (0.174) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8640	0.5440
A	0.9040	0.5620
B	0.9040	0.5540
C	0.8780	0.5630
D	0.8910	0.5700
E	0.8710	0.5620
F	0.8840	0.5680
G	0.8170	0.5200
H	0.8010	0.5120
I	0.8230	0.4960
J	0.8290	0.5220
K	0.7340	0.4750
L	0.8440	0.5430
M	0.8460	0.5260

