Full wwPDB EM Validation Report

Sep 8, 2026 – 06:04 am BST

PDB ID	:	8RVY / pdb_00008rvy
EMDB ID	:	EMD-19538
Title	:	CryoEM structure of the Elp-Hdr complex of Methanothermobacter marburgensis state 1 (composite structure)
Authors	:	San Segundo-Acosta, P.; Murphy, B.J.
Deposited on	:	2024-02-02
Resolution	:	2.36 Å(reported)
Based on initial model	:	.

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

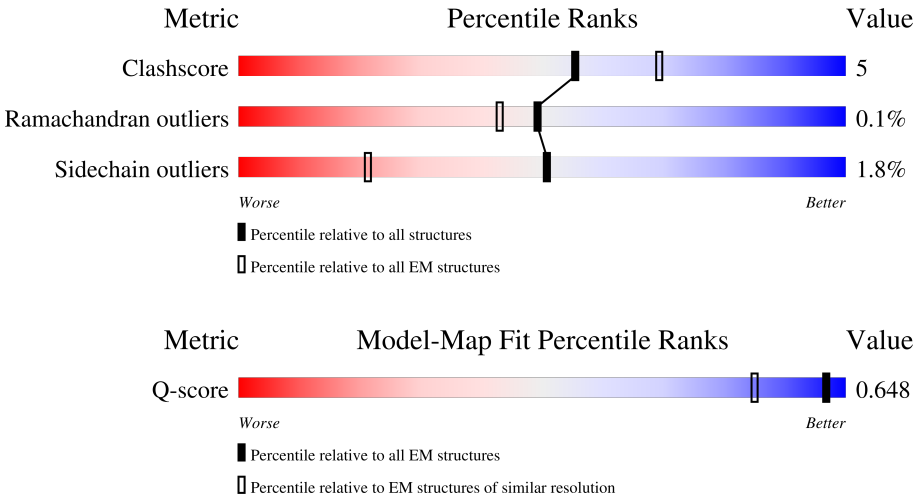
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.36 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.



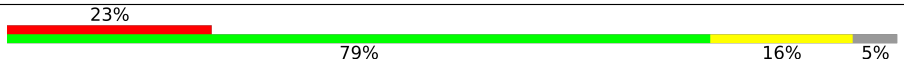
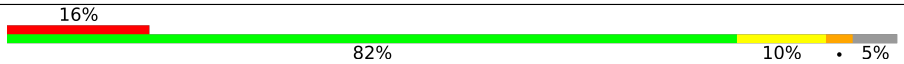
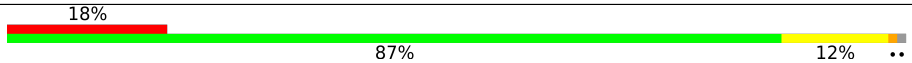
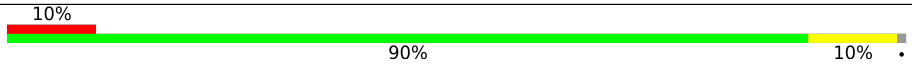
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4686 (1.86 - 2.86)

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

Mol	Chain	Length	Quality of chain
1	A	659	7% 86% 10%
1	a	659	61% 35%
2	E	380	12% 81% 14%
3	D	342	31% 80% 18%

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Mol	Chain	Length	Quality of chain
4	F	136	
5	B	302	
5	b	302	
6	C	185	
6	c	185	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 44212 atoms, of which 21783 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
1	A	644	Total	C	H	N	O	S	0	0
			9794	3101	4875	819	951	48		
1	a	427	Total	C	H	N	O	S	0	0
			6539	2072	3263	537	636	31		

- Molecule 2 is a protein called Formate dehydrogenase, beta subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	380	Total	C	H	N	O	S	0	0
			5883	1882	2863	515	591	32		

- Molecule 3 is a protein called Formate dehydrogenase, alpha subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	335	Total	C	H	N	O	S	0	0
			4993	1608	2459	426	485	15		

- Molecule 4 is a protein called Methyl viologen-reducing hydrogenase, subunit D-related protein.

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

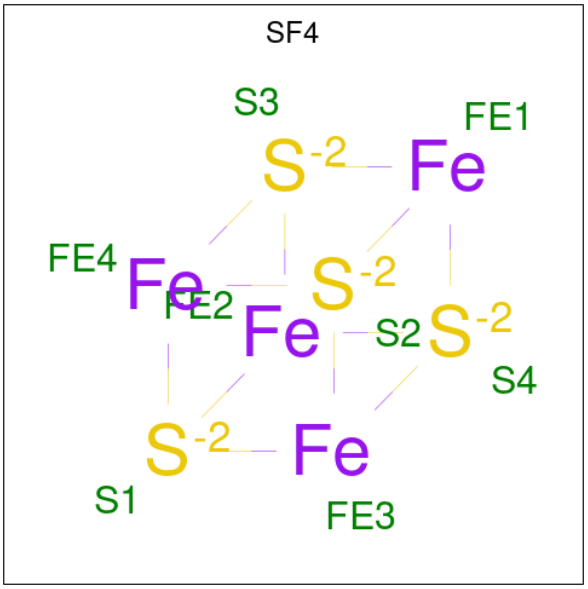
- Molecule 5 is a protein called H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit B.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	b	286	Total	C	H	N	O	S	0	0
			4398	1398	2183	366	428	23		
5	B	288	Total	C	H	N	O	S	0	0
			4411	1404	2188	368	428	23		

- Molecule 6 is a protein called H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit C.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	c	184	Total	C	H	N	O	S	0	0
			2862	895	1436	253	267	11		
6	C	184	Total	C	H	N	O	S	0	0
			2861	895	1435	253	267	11		

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



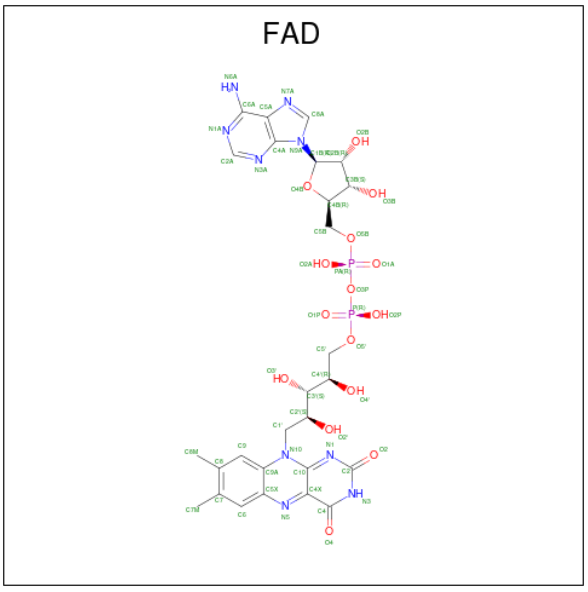
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	Fe	S		0
			8	4	4		
7	A	1	Total	Fe	S		0
			8	4	4		
7	A	1	Total	Fe	S		0
			8	4	4		
7	A	1	Total	Fe	S		0
			8	4	4		
7	A	1	Total	Fe	S		0
			8	4	4		
7	A	1	Total	Fe	S		0
			8	4	4		
7	E	1	Total	Fe	S		0
			8	4	4		
7	E	1	Total	Fe	S		0
			8	4	4		

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Mol	Chain	Residues	Atoms	AltConf
7	E	1	Total Fe S 8 4 4	0
7	E	1	Total Fe S 8 4 4	0
7	D	1	Total Fe S 8 4 4	0
7	c	1	Total Fe S 8 4 4	0
7	c	1	Total Fe S 8 4 4	0
7	C	1	Total Fe S 8 4 4	0
7	C	1	Total Fe S 8 4 4	0
7	a	1	Total Fe S 8 4 4	0
7	a	1	Total Fe S 8 4 4	0
7	a	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).



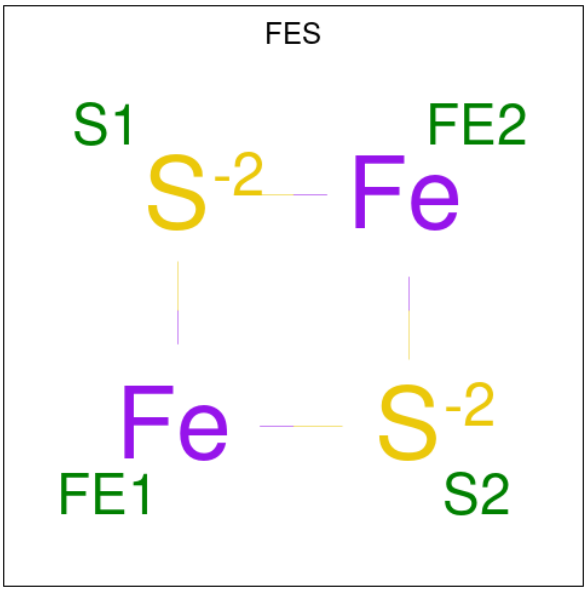
Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C H N O P 84 27 31 9 15 2	0

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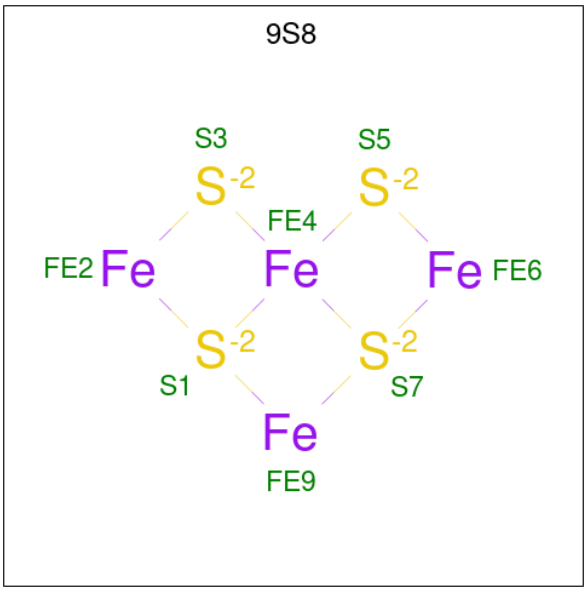
Mol	Chain	Residues	Atoms						AltConf
8	E	1	Total	C	H	N	O	P	0
			84	27	31	9	15	2	
8	a	1	Total	C	H	N	O	P	0
			83	27	30	9	15	2	

- Molecule 9 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
9	F	1	Total	Fe	S		0
			4	2	2		

- Molecule 10 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
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

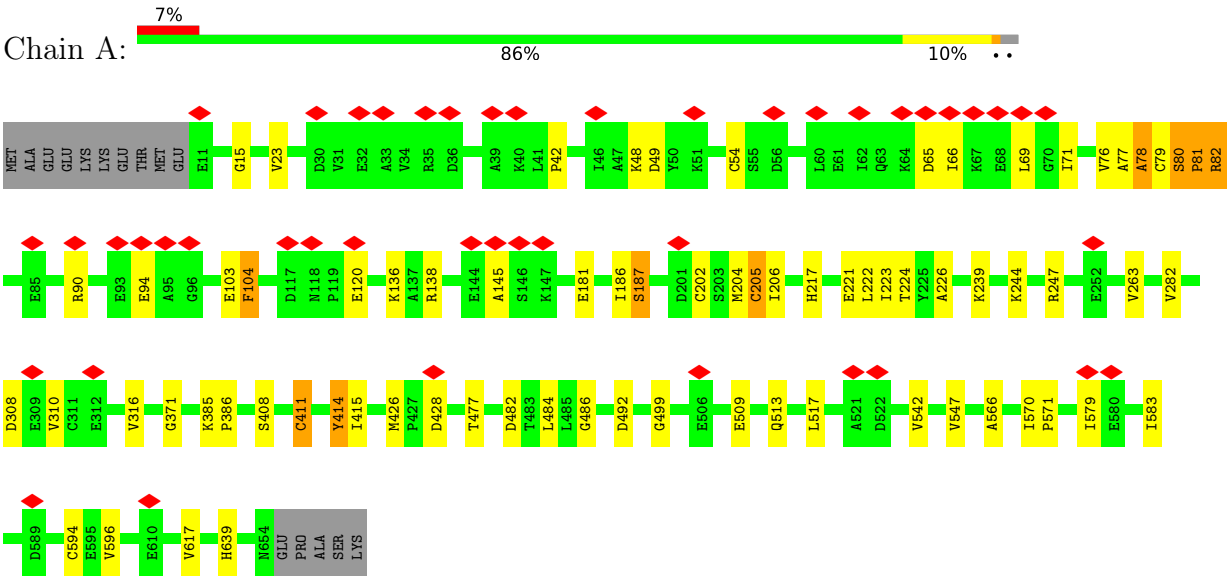
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	AltConf
11	A	5	Total O 5 5	0
11	E	3	Total O 3 3	0
11	D	1	Total O 1 1	0
11	C	1	Total O 1 1	0
11	a	4	Total O 4 4	0

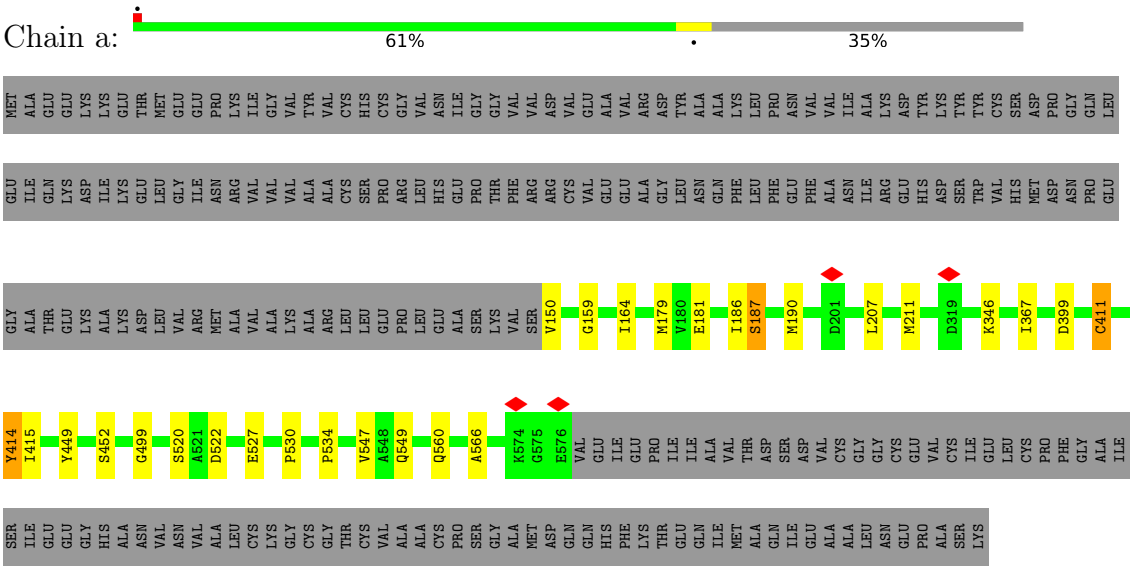
3 Residue-property plots (i)

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

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

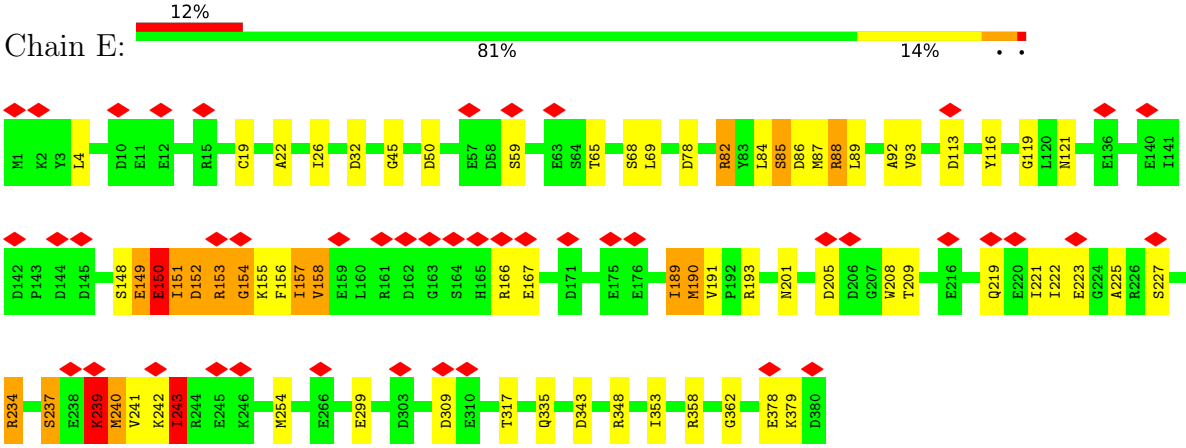


• Molecule 1: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit A



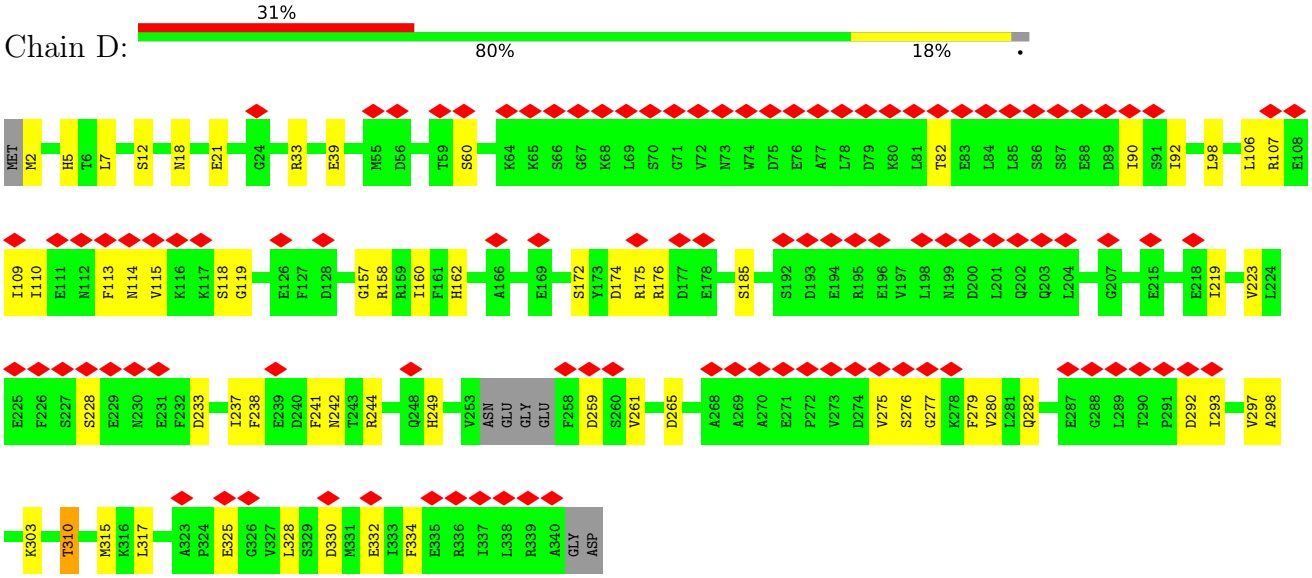
• Molecule 2: Formate dehydrogenase, beta subunit

Chain E:



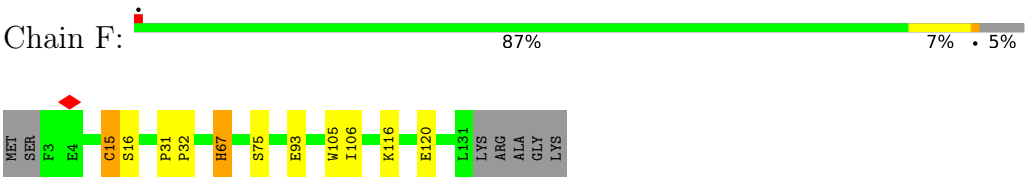
• Molecule 3: Formate dehydrogenase, alpha subunit

Chain D:



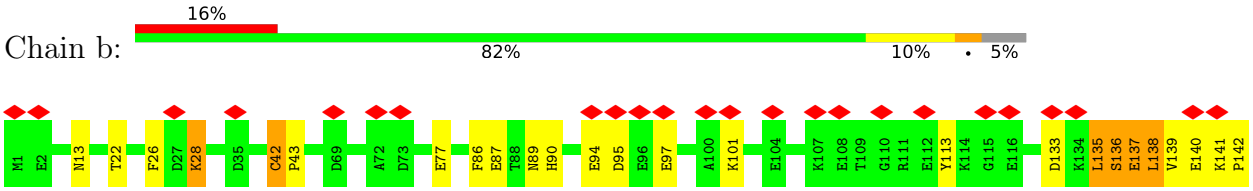
• Molecule 4: Methyl viologen-reducing hydrogenase, subunit D-related protein

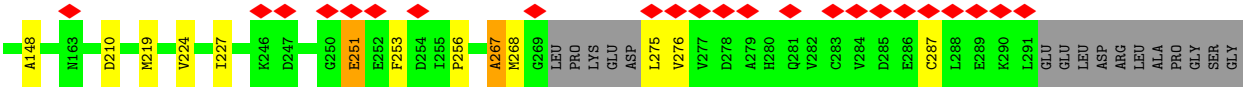
Chain F:



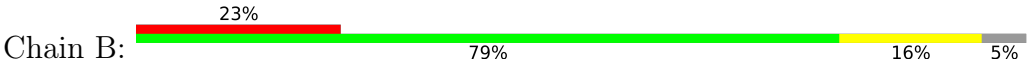
• Molecule 5: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit B

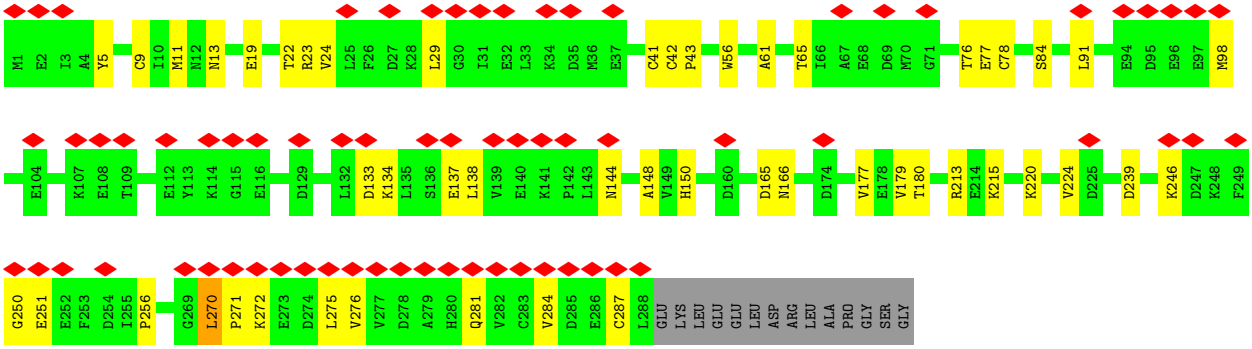
Chain b:



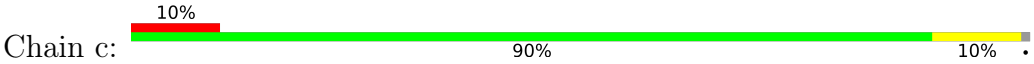


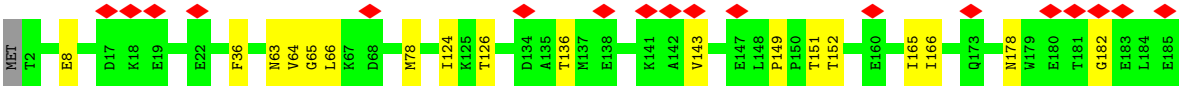
• Molecule 5: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit B



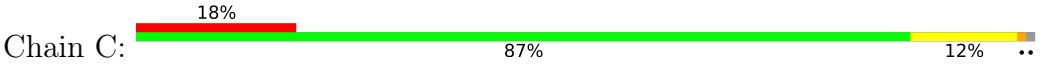


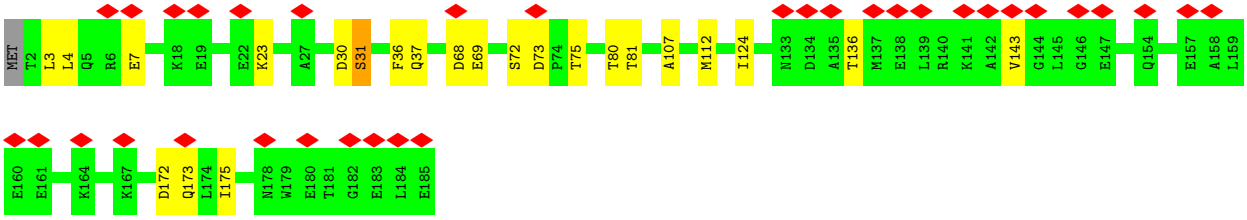
• Molecule 6: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit C





• Molecule 6: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit C





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76528	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	41.608	Depositor
Minimum map value	-25.218	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.047	Depositor
Recommended contour level	7.34	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, FES, 9S8, SF4

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	0.52	16/5008 (0.3%)	0.51	10/6777 (0.1%)
1	a	0.17	0/3336	0.31	0/4509
2	E	1.00	30/3076 (1.0%)	0.88	25/4144 (0.6%)
3	D	0.37	1/2587 (0.0%)	0.50	3/3523 (0.1%)
4	F	0.78	4/1066 (0.4%)	0.51	2/1434 (0.1%)
5	B	0.15	0/2260	0.39	1/3049 (0.0%)
5	b	0.51	7/2250 (0.3%)	0.66	12/3032 (0.4%)
6	C	0.17	0/1451	0.40	3/1956 (0.2%)
6	c	0.54	4/1451 (0.3%)	0.54	5/1956 (0.3%)
All	All	0.54	62/22485 (0.3%)	0.55	61/30380 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	E	0	3
All	All	0	4

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	89	LEU	C-O	-18.55	1.00	1.23
4	F	67	HIS	C-O	-15.91	1.04	1.23
2	E	189	ILE	C-O	-15.63	1.07	1.24
6	c	65	GLY	C-O	-13.64	1.06	1.24
1	A	81	PRO	C-O	-12.84	1.08	1.24
2	E	155	LYS	C-O	-12.38	1.09	1.24
2	E	190	MET	C-O	-11.36	1.09	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	88	ARG	C-O	-10.98	1.10	1.24
1	A	76	VAL	C-O	-10.63	1.12	1.24
1	A	103	GLU	C-O	-10.57	1.10	1.23
2	E	82	ARG	C-O	-10.57	1.11	1.24
2	E	158	VAL	C-O	-10.50	1.12	1.24
2	E	157	ILE	C-O	-10.22	1.14	1.24
4	F	16	SER	CA-CB	-9.66	1.38	1.53
2	E	156	PHE	C-O	-9.50	1.12	1.23
2	E	232	GLU	C-O	-9.02	1.12	1.24
6	c	66	LEU	C-O	-8.90	1.13	1.23
1	A	205	CYS	C-N	-8.67	1.23	1.33
3	D	119	GLY	C-O	-8.54	1.14	1.24
4	F	15	CYS	C-N	-8.33	1.22	1.33
2	E	234	ARG	C-O	-8.29	1.14	1.23
2	E	231	ILE	C-O	-8.17	1.16	1.24
1	A	104	PHE	C-O	-8.08	1.14	1.24
2	E	84	LEU	C-O	-8.02	1.12	1.24
1	A	77	ALA	C-O	-8.01	1.14	1.24
2	E	150	GLU	C-O	-7.96	1.14	1.23
2	E	243	ILE	C-O	-7.81	1.15	1.24
1	A	80	SER	CA-CB	-7.72	1.39	1.53
2	E	233	ALA	C-O	-7.66	1.14	1.23
6	c	64	VAL	C-O	-7.51	1.14	1.24
2	E	149	GLU	C-O	-7.51	1.14	1.23
1	A	205	CYS	C-O	-7.50	1.14	1.24
5	b	251	GLU	C-O	-7.50	1.14	1.24
2	E	237	SER	C-O	-7.39	1.14	1.23
1	A	104	PHE	C-N	-7.09	1.24	1.33
1	A	79	CYS	C-O	-6.87	1.15	1.24
5	b	267	ALA	CA-CB	-6.83	1.42	1.53
5	b	142	PRO	C-O	-6.77	1.15	1.23
4	F	16	SER	C-O	-6.70	1.16	1.24
1	A	80	SER	C-O	-6.69	1.15	1.24
2	E	152	ASP	C-N	-6.65	1.25	1.33
2	E	88	ARG	C-N	-6.62	1.25	1.33
2	E	240	MET	C-O	-6.55	1.16	1.24
5	b	135	LEU	C-O	-6.15	1.16	1.24
1	A	386	PRO	N-CD	-5.81	1.39	1.47
1	A	82	ARG	C-O	-5.76	1.16	1.24
2	E	151	ILE	C-O	-5.69	1.17	1.24
2	E	87	MET	C-O	-5.63	1.17	1.24
2	E	152	ASP	C-O	-5.55	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	b	141	LYS	C-O	-5.49	1.19	1.24
2	E	156	PHE	C-N	-5.38	1.25	1.33
2	E	82	ARG	C-N	-5.35	1.26	1.33
2	E	85	SER	C-N	-5.22	1.26	1.33
1	A	204	MET	C-N	-5.21	1.26	1.33
2	E	154	GLY	C-O	-5.18	1.16	1.24
2	E	84	LEU	C-N	-5.17	1.27	1.34
5	b	136	SER	CA-CB	-5.13	1.44	1.53
1	A	78	ALA	CA-CB	-5.11	1.44	1.53
5	b	137	GLU	C-O	-5.10	1.18	1.24
6	c	65	GLY	C-N	-5.09	1.27	1.33
1	A	81	PRO	N-CA	-5.05	1.40	1.47
2	E	237	SER	CA-CB	-5.05	1.45	1.53

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	86	ASP	CB-CA-C	-10.23	93.84	111.23
2	E	153	ARG	CB-CA-C	9.53	123.79	111.50
1	A	205	CYS	CA-CB-SG	-9.10	93.47	114.40
2	E	153	ARG	N-CA-C	-8.89	99.01	111.81
2	E	234	ARG	CA-C-O	-8.61	112.23	121.36
4	F	67	HIS	CB-CG-CD2	8.13	141.78	131.20
4	F	67	HIS	CB-CG-ND1	-8.02	110.67	122.70
5	b	267	ALA	N-CA-C	-7.83	99.98	110.55
3	D	113	PHE	N-CA-C	-7.74	103.40	112.92
5	b	267	ALA	CA-C-O	-7.68	112.75	121.81
2	E	85	SER	CA-C-N	-7.48	112.03	123.17
2	E	85	SER	C-N-CA	-7.48	112.03	123.17
5	b	137	GLU	N-CA-C	-7.43	103.18	111.28
2	E	87	MET	CA-C-O	-7.40	112.87	120.71
3	D	114	ASN	CB-CA-C	-7.36	99.39	112.27
5	b	141	LYS	N-CA-CB	-7.26	98.25	111.03
2	E	234	ARG	N-CA-C	-7.23	98.76	108.74
1	A	81	PRO	N-CA-CB	-7.14	95.68	103.39
5	b	140	GLU	N-CA-CB	-7.13	100.05	110.53
2	E	151	ILE	CA-C-O	-7.11	112.61	120.72
2	E	150	GLU	CA-C-O	-7.06	113.71	121.33
6	c	63	ASN	CA-C-N	7.02	132.30	120.64
6	c	63	ASN	C-N-CA	7.02	132.30	120.64
6	c	63	ASN	O-C-N	-6.80	114.39	122.15
1	A	206	ILE	N-CA-C	-6.46	106.50	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	b	26	PHE	N-CA-C	6.31	120.24	112.54
5	b	137	GLU	O-C-N	-6.30	115.44	122.12
2	E	148	SER	O-C-N	-6.14	116.81	123.26
6	C	31	SER	N-CA-C	6.11	118.74	111.71
1	A	104	PHE	CA-CB-CG	6.04	119.84	113.80
6	c	66	LEU	CA-C-O	-6.03	115.11	122.41
2	E	149	GLU	CB-CG-CD	6.02	122.83	112.60
5	b	251	GLU	N-CA-CB	-5.96	100.73	110.21
5	b	142	PRO	CB-CA-C	5.95	119.13	111.46
2	E	242	LYS	CA-C-O	-5.94	114.12	120.42
6	C	7	GLU	N-CA-C	5.93	121.17	113.88
1	A	78	ALA	N-CA-CB	-5.90	100.52	110.49
2	E	378	GLU	N-CA-C	-5.82	102.15	110.59
6	c	165	ILE	N-CA-C	-5.76	104.89	110.42
2	E	239	LYS	CA-C-N	5.75	128.46	120.29
2	E	239	LYS	C-N-CA	5.75	128.46	120.29
5	b	142	PRO	N-CA-C	-5.63	102.36	111.14
2	E	85	SER	N-CA-C	5.60	118.14	111.71
6	C	7	GLU	N-CA-CB	-5.49	103.29	110.59
2	E	86	ASP	CA-C-O	-5.43	114.43	121.17
1	A	145	ALA	N-CA-C	-5.32	103.00	110.50
2	E	237	SER	CB-CA-C	-5.26	99.86	109.54
2	E	84	LEU	CA-C-N	5.20	127.76	120.28
2	E	84	LEU	C-N-CA	5.20	127.76	120.28
1	A	104	PHE	CB-CA-C	-5.20	100.30	109.70
1	A	217	HIS	N-CA-C	-5.19	102.60	110.28
2	E	237	SER	N-CA-C	-5.15	103.24	110.50
2	E	379	LYS	CB-CA-C	-5.14	103.99	111.14
1	A	66	ILE	N-CA-C	-5.11	105.51	110.42
5	b	28	LYS	N-CA-C	-5.11	106.31	112.54
5	b	28	LYS	N-CA-CB	5.11	118.87	110.39
2	E	241	VAL	N-CA-C	-5.08	104.75	111.09
1	A	371	GLY	N-CA-C	-5.07	106.09	112.23
2	E	157	ILE	CA-C-O	-5.07	114.99	120.67
5	B	220	LYS	N-CA-C	5.05	116.78	111.28
3	D	114	ASN	N-CA-C	5.02	116.78	110.91

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	82	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	E	153	ARG	Sidechain
2	E	234	ARG	Mainchain
2	E	88	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	4919	4875	4877	41	0
1	a	3276	3263	3263	17	0
2	E	3020	2863	2908	48	0
3	D	2534	2459	2458	33	0
4	F	1037	989	989	6	0
5	B	2223	2188	2188	34	0
5	b	2215	2183	2182	28	0
6	C	1426	1435	1435	15	0
6	c	1426	1436	1435	8	0
7	A	48	0	0	0	0
7	C	16	0	0	0	0
7	D	8	0	0	0	0
7	E	32	0	0	0	0
7	a	24	0	0	0	0
7	c	16	0	0	0	0
8	A	53	31	31	1	0
8	E	53	31	31	14	0
8	a	53	30	31	0	0
9	F	4	0	0	0	0
10	B	16	0	0	2	0
10	b	16	0	0	0	0
11	A	5	0	0	0	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
11	E	3	0	0	0	0
11	a	4	0	0	2	0
All	All	22429	21783	21828	219	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 5.

All (219) 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)
2:E:19:CYS:SG	8:E:405:FAD:O3'	2.25	0.94
6:C:73:ASP:OD2	6:C:75:THR:OG1	1.91	0.87
3:D:92:ILE:HD12	3:D:115:VAL:HG21	1.58	0.83
5:B:5:TYR:OH	5:B:22:THR:HG21	1.77	0.82
2:E:69:LEU:H	8:E:405:FAD:H2A	1.50	0.74
1:a:449:TYR:OH	11:a:801:HOH:O	2.04	0.74
3:D:107:ARG:HD2	3:D:249:HIS:O	1.87	0.74
3:D:109:ILE:HD11	3:D:334:PHE:HB3	1.69	0.72
3:D:282:GLN:NE2	3:D:330:ASP:OD1	2.22	0.72
3:D:174:ASP:OD1	3:D:175:ARG:N	2.24	0.71
1:a:150:VAL:N	11:a:802:HOH:O	2.23	0.71
5:B:19:GLU:O	5:B:22:THR:HG22	1.92	0.70
1:A:385:LYS:HD3	1:A:426:MET:SD	2.33	0.69
2:E:69:LEU:N	8:E:405:FAD:H2A	2.08	0.69
3:D:92:ILE:CD1	3:D:115:VAL:HG21	2.21	0.69
1:a:190:MET:HG2	1:a:207:LEU:HD22	1.75	0.69
1:A:23:VAL:HG12	1:A:23:VAL:O	1.93	0.69
6:c:124:ILE:HG12	6:c:166:ILE:HD13	1.75	0.68
5:B:22:THR:CB	5:B:77:GLU:OE2	2.41	0.68
3:D:12:SER:HB2	3:D:310:THR:HG23	1.74	0.68
2:E:19:CYS:HG	8:E:405:FAD:HO3'	1.27	0.67
2:E:353:ILE:HD11	4:F:93:GLU:HG3	1.76	0.66
3:D:244:ARG:NH1	3:D:310:THR:O	2.29	0.65
1:A:120:GLU:N	1:A:120:GLU:OE1	2.29	0.65
2:E:335:GLN:OE1	3:D:33:ARG:NH2	2.29	0.65
10:B:401:9S8:FE4	10:B:401:9S8:S1	1.89	0.64
2:E:19:CYS:O	2:E:209:THR:OG1	2.14	0.64
5:B:256:PRO:HG2	5:B:287:CYS:HB2	1.80	0.64
5:b:268:MET:O	5:b:268:MET:HG2	1.99	0.63
1:a:520:SER:OG	1:a:522:ASP:OD1	2.16	0.62
1:A:136:LYS:NZ	1:A:639:HIS:O	2.33	0.61
2:E:69:LEU:H	8:E:405:FAD:C2A	2.13	0.61
6:C:68:ASP:O	6:C:72:SER:OG	2.19	0.60
2:E:151:ILE:O	2:E:152:ASP:OD1	2.20	0.60
5:b:87:GLU:HA	5:b:90:HIS:NE2	2.17	0.60
5:B:11:MET:SD	5:B:77:GLU:OE1	2.59	0.60
2:E:239:LYS:O	2:E:243:ILE:HD12	2.03	0.59
2:E:19:CYS:HB2	8:E:405:FAD:O1P	2.02	0.59
2:E:150:GLU:OE2	2:E:152:ASP:CG	2.46	0.59
5:b:139:VAL:HG23	5:b:267:ALA:HB1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:133:ASP:O	5:B:137:GLU:HG3	2.03	0.59
5:B:133:ASP:OD1	5:B:134:LYS:N	2.35	0.59
2:E:150:GLU:OE2	2:E:152:ASP:OD1	2.20	0.59
5:B:22:THR:OG1	5:B:77:GLU:OE2	2.18	0.58
3:D:109:ILE:HD11	3:D:334:PHE:CB	2.33	0.58
5:b:138:LEU:HB3	5:b:268:MET:HE2	1.85	0.58
2:E:150:GLU:CD	2:E:152:ASP:OD2	2.47	0.58
2:E:209:THR:HG23	8:E:405:FAD:H5'2	1.84	0.58
2:E:45:GLY:N	2:E:50:ASP:O	2.34	0.58
1:a:549:GLN:OE1	1:a:560:GLN:NE2	2.34	0.58
5:b:86:PHE:O	5:b:90:HIS:CD2	2.57	0.58
5:b:136:SER:O	5:b:139:VAL:HG12	2.03	0.57
5:B:13:ASN:C	6:C:136:THR:HG21	2.30	0.57
3:D:5:HIS:ND1	3:D:18:ASN:OD1	2.37	0.57
2:E:157:ILE:HG12	2:E:167:GLU:HG2	1.85	0.57
2:E:237:SER:H	2:E:240:MET:HE3	1.70	0.57
2:E:205:ASP:OD1	2:E:208:TRP:CD1	2.57	0.56
1:a:346:LYS:NZ	1:a:399:ASP:OD2	2.38	0.56
3:D:174:ASP:OD2	3:D:176:ARG:NH2	2.39	0.56
2:E:152:ASP:C	2:E:154:GLY:H	2.14	0.55
3:D:259:ASP:O	3:D:277:GLY:N	2.39	0.55
5:B:29:LEU:HD23	5:B:138:LEU:CD1	2.36	0.55
1:A:223:ILE:HG22	1:A:226:ALA:HB3	1.87	0.55
1:A:517:LEU:HD21	1:A:542:VAL:HG11	1.89	0.55
5:b:256:PRO:HG3	5:b:287:CYS:HB2	1.87	0.55
6:C:107:ALA:O	6:C:112:MET:HE2	2.07	0.54
5:B:239:ASP:OD2	5:B:281:GLN:N	2.40	0.54
5:b:13:ASN:C	6:c:136:THR:HG21	2.33	0.54
2:E:209:THR:HG23	8:E:405:FAD:C5'	2.38	0.54
3:D:280:VAL:HG22	3:D:293:ILE:HD11	1.90	0.53
5:b:28:LYS:HD3	5:b:268:MET:SD	2.48	0.53
5:B:24:VAL:HG11	5:B:270:LEU:HD11	1.91	0.53
2:E:92:ALA:HB3	8:E:405:FAD:H8A	1.91	0.53
5:B:13:ASN:O	6:C:136:THR:HG21	2.07	0.53
3:D:98:LEU:O	3:D:242:ASN:ND2	2.35	0.53
3:D:279:PHE:N	3:D:292:ASP:OD2	2.42	0.52
5:B:276:VAL:HG22	6:C:143:VAL:HG11	1.90	0.52
2:E:92:ALA:CB	8:E:405:FAD:H8A	2.40	0.52
2:E:152:ASP:C	2:E:154:GLY:N	2.68	0.52
3:D:237:ILE:HA	3:D:310:THR:HG21	1.92	0.52
5:B:76:THR:HG22	5:B:78:CYS:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:PRO:O	1:A:138:ARG:NH1	2.43	0.51
1:A:181:GLU:OE1	8:A:706:FAD:O3B	2.28	0.51
1:A:385:LYS:HD3	1:A:426:MET:CE	2.40	0.51
2:E:19:CYS:SG	2:E:201:ASN:HB3	2.50	0.51
1:A:23:VAL:O	1:A:23:VAL:CG1	2.58	0.51
5:B:22:THR:HB	5:B:77:GLU:OE2	2.10	0.51
1:a:415:ILE:HD11	1:a:499:GLY:HA3	1.93	0.50
1:A:202:CYS:SG	1:A:205:CYS:SG	3.10	0.50
1:A:428:ASP:OD1	1:A:428:ASP:N	2.39	0.50
1:A:223:ILE:HG22	1:A:226:ALA:CB	2.42	0.50
5:b:210:ASP:OD1	6:C:4:LEU:HD11	2.12	0.50
1:A:594:CYS:SG	1:A:596:VAL:HG22	2.52	0.50
6:C:173:GLN:OE1	6:C:173:GLN:HA	2.12	0.49
1:A:54:CYS:SG	1:A:54:CYS:O	2.70	0.49
2:E:22:ALA:O	2:E:26:ILE:HD12	2.12	0.49
2:E:191:VAL:HB	2:E:193:ARG:NH1	2.28	0.49
5:b:148:ALA:HB2	5:b:224:VAL:HG11	1.94	0.49
2:E:32:ASP:OD1	2:E:59:SER:OG	2.23	0.49
2:E:254:MET:HA	2:E:254:MET:HE2	1.95	0.49
2:E:358:ARG:O	2:E:362:GLY:N	2.41	0.48
3:D:315:MET:HE2	3:D:317:LEU:HD21	1.95	0.48
5:B:9:CYS:N	10:B:402:9S8:S7	2.86	0.48
2:E:150:GLU:OE2	2:E:152:ASP:OD2	2.32	0.48
5:b:275:LEU:O	5:b:276:VAL:C	2.56	0.48
1:A:566:ALA:HB2	1:a:566:ALA:HB2	1.95	0.48
1:a:547:VAL:HG12	1:a:547:VAL:O	2.14	0.48
2:E:343:ASP:OD2	3:D:162:HIS:NE2	2.37	0.48
5:b:267:ALA:O	5:b:268:MET:HB3	2.14	0.48
5:B:42:CYS:N	5:B:43:PRO:HA	2.29	0.48
1:a:527:GLU:HG3	1:a:534:PRO:HA	1.96	0.48
2:E:225:ALA:HB1	2:E:231:ILE:HG12	1.94	0.48
1:A:48:LYS:HD2	1:A:65:ASP:OD2	2.14	0.48
3:D:265:ASP:N	3:D:265:ASP:OD1	2.46	0.48
4:F:116:LYS:NZ	4:F:120:GLU:OE2	2.42	0.48
2:E:65:THR:O	8:E:405:FAD:H3B	2.13	0.47
5:b:268:MET:O	5:b:268:MET:CG	2.61	0.47
1:A:224:THR:OG1	1:A:247:ARG:NH2	2.47	0.47
5:B:5:TYR:HH	5:B:22:THR:HG21	1.78	0.47
5:B:150:HIS:CE1	5:B:215:LYS:HE2	2.49	0.47
1:A:477:THR:OG1	1:A:492:ASP:OD2	2.29	0.46
1:a:159:GLY:N	1:a:181:GLU:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:405:FAD:N3A	8:E:405:FAD:H2B	2.31	0.46
1:A:186:ILE:O	1:A:187:SER:CB	2.63	0.46
1:a:186:ILE:O	1:a:187:SER:CB	2.63	0.46
2:E:158:VAL:HG22	2:E:166:ARG:HB2	1.97	0.46
2:E:223:GLU:OE2	2:E:223:GLU:HA	2.16	0.46
3:D:12:SER:HA	3:D:241:PHE:HA	1.98	0.46
4:F:120:GLU:OE1	4:F:120:GLU:HA	2.16	0.46
5:b:89:ASN:OD1	5:b:113:TYR:OH	2.32	0.45
5:b:101:LYS:O	5:b:101:LYS:HD3	2.16	0.45
6:C:80:THR:O	6:C:81:THR:OG1	2.28	0.45
1:a:414:TYR:CD1	1:a:414:TYR:C	2.94	0.45
1:A:408:SER:HB2	1:A:411:CYS:SG	2.56	0.45
5:B:61:ALA:O	5:B:65:THR:HG23	2.16	0.45
2:E:4:LEU:CD1	2:E:222:ILE:HG21	2.46	0.45
2:E:205:ASP:OD1	2:E:208:TRP:HD1	1.97	0.45
1:A:90:ARG:O	1:A:94:GLU:OE2	2.35	0.45
1:A:414:TYR:CD1	1:A:414:TYR:C	2.94	0.45
2:E:93:VAL:O	2:E:119:GLY:HA2	2.17	0.45
5:b:42:CYS:N	5:b:43:PRO:HA	2.32	0.45
6:C:124:ILE:HD12	6:C:175:ILE:HD11	1.99	0.44
5:b:95:ASP:OD2	5:b:95:ASP:C	2.59	0.44
2:E:189:ILE:O	2:E:190:MET:HE2	2.16	0.44
3:D:2:MET:O	3:D:21:GLU:N	2.41	0.44
4:F:67:HIS:HA	4:F:105:TRP:HB3	1.99	0.44
5:b:22:THR:OG1	5:b:77:GLU:OE1	2.35	0.44
1:a:164:ILE:HA	1:a:179:MET:HE1	1.99	0.44
5:B:56:TRP:NE1	5:B:84:SER:OG	2.48	0.44
3:D:39:GLU:OE1	3:D:158:ARG:NH1	2.51	0.44
1:A:415:ILE:HD11	1:A:499:GLY:HA3	2.00	0.44
3:D:106:LEU:HD12	3:D:106:LEU:O	2.18	0.44
1:A:482:ASP:O	1:A:486:GLY:N	2.51	0.44
3:D:261:VAL:HG22	3:D:275:VAL:HG13	1.98	0.44
1:a:186:ILE:O	1:a:211:MET:HE3	2.18	0.44
1:A:484:LEU:HD13	6:C:37:GLN:CB	2.48	0.44
1:A:49:ASP:OD1	1:A:49:ASP:N	2.51	0.43
2:E:68:SER:HG	8:E:405:FAD:HO2'	1.62	0.43
5:B:177:VAL:O	5:B:180:THR:OG1	2.34	0.43
3:D:238:PHE:H	3:D:310:THR:CG2	2.31	0.43
3:D:298:ALA:O	3:D:303:LYS:NZ	2.47	0.43
1:A:263:VAL:HG11	1:A:310:VAL:HG21	2.00	0.43
5:B:22:THR:HG23	5:B:23:ARG:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:148:ALA:HB2	5:B:224:VAL:HG11	2.00	0.43
1:A:224:THR:O	1:A:244:LYS:NZ	2.44	0.43
5:b:90:HIS:O	5:b:94:GLU:HG3	2.19	0.43
5:B:91:LEU:HD21	5:B:98:MET:SD	2.58	0.43
1:A:570:ILE:HB	1:A:571:PRO:HD3	1.98	0.43
2:E:223:GLU:O	2:E:227:SER:OG	2.31	0.43
5:B:213:ARG:NH2	5:B:251:GLU:OE1	2.44	0.43
5:B:284:VAL:O	5:B:284:VAL:CG1	2.67	0.43
3:D:297:VAL:HA	3:D:328:LEU:O	2.19	0.43
1:A:308:ASP:OD1	1:A:316:VAL:CG1	2.67	0.43
3:D:261:VAL:HG22	3:D:275:VAL:CG1	2.49	0.43
1:A:65:ASP:HA	1:A:69:LEU:HD23	2.01	0.42
1:A:222:LEU:HG	1:A:224:THR:HG23	2.00	0.42
1:A:282:VAL:O	1:A:282:VAL:HG13	2.18	0.42
2:E:78:ASP:OD1	2:E:82:ARG:NE	2.52	0.42
3:D:90:ILE:O	3:D:115:VAL:HG13	2.19	0.42
5:b:133:ASP:O	5:b:137:GLU:HG3	2.19	0.42
5:B:271:PRO:O	5:B:272:LYS:HB2	2.19	0.42
6:C:124:ILE:CD1	6:C:175:ILE:HD11	2.50	0.42
5:b:101:LYS:HE2	5:b:101:LYS:HA	2.02	0.42
5:b:251:GLU:HG3	5:b:253:PHE:CE1	2.54	0.42
6:C:30:ASP:OD1	6:C:31:SER:N	2.53	0.42
6:C:172:ASP:OD1	6:C:173:GLN:N	2.53	0.42
1:a:527:GLU:OE2	1:a:530:PRO:HA	2.20	0.42
2:E:225:ALA:CB	2:E:231:ILE:HG12	2.49	0.42
1:A:547:VAL:O	1:A:547:VAL:HG12	2.19	0.42
5:b:219:MET:SD	5:b:227:ILE:HG12	2.60	0.41
1:A:509:GLU:O	1:A:513:GLN:HG2	2.20	0.41
5:B:144:ASN:OD1	5:B:144:ASN:C	2.63	0.41
6:c:78:MET:HE3	6:C:3:LEU:HD12	2.02	0.41
1:A:80:SER:HA	1:A:81:PRO:HD2	1.85	0.41
2:E:113:ASP:OD1	2:E:113:ASP:C	2.63	0.41
3:D:110:ILE:HG23	3:D:115:VAL:HB	2.02	0.41
5:b:13:ASN:O	6:c:136:THR:HG21	2.20	0.41
2:E:116:TYR:HD2	2:E:221:ILE:HD11	1.85	0.41
4:F:15:CYS:HB3	4:F:106:ILE:O	2.20	0.41
5:B:246:LYS:O	5:B:250:GLY:HA2	2.20	0.41
3:D:157:GLY:HA2	3:D:160:ILE:HD12	2.02	0.41
5:B:275:LEU:HD12	5:B:275:LEU:H	1.84	0.41
6:c:126:THR:O	6:c:152:THR:OG1	2.38	0.41
1:A:411:CYS:HA	1:A:414:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:165:ASP:OD1	5:B:166:ASN:N	2.50	0.41
1:A:583:ILE:HD13	1:A:617:VAL:HG22	2.03	0.41
3:D:219:ILE:HG12	3:D:223:VAL:HG23	2.02	0.41
4:F:31:PRO:HA	4:F:32:PRO:HD3	1.93	0.41
6:c:149:PRO:O	6:c:151:THR:N	2.53	0.41
6:c:178:ASN:O	6:c:182:GLY:N	2.54	0.41
1:A:15:GLY:HA3	1:A:71:ILE:HD13	2.02	0.41
1:A:221:GLU:HG3	1:A:223:ILE:HD11	2.02	0.41
2:E:219:GLN:HA	2:E:219:GLN:OE1	2.21	0.41
5:b:276:VAL:CG2	6:c:143:VAL:HG21	2.51	0.40
5:b:97:GLU:OE1	5:b:97:GLU:HA	2.21	0.40
5:b:135:LEU:HA	5:b:138:LEU:HD12	2.03	0.40
5:B:284:VAL:O	5:B:284:VAL:HG12	2.21	0.40
1:a:411:CYS:HA	1:a:414:TYR:CD2	2.56	0.40
2:E:121:ASN:O	8:E:405:FAD:C9A	2.70	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	642/659 (97%)	626 (98%)	14 (2%)	2 (0%)	36	43
1	a	425/659 (64%)	415 (98%)	9 (2%)	1 (0%)	43	52
2	E	378/380 (100%)	368 (97%)	10 (3%)	0	100	100
3	D	331/342 (97%)	317 (96%)	14 (4%)	0	100	100
4	F	127/136 (93%)	125 (98%)	2 (2%)	0	100	100
5	B	286/302 (95%)	280 (98%)	6 (2%)	0	100	100
5	b	282/302 (93%)	273 (97%)	9 (3%)	0	100	100
6	C	182/185 (98%)	178 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	c	182/185 (98%)	179 (98%)	3 (2%)	0	100 100
All	All	2835/3150 (90%)	2761 (97%)	71 (2%)	3 (0%)	49 59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	SER
1	a	187	SER
1	A	78	ALA

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	534/547 (98%)	529 (99%)	5 (1%)	70 82
1	a	356/547 (65%)	352 (99%)	4 (1%)	65 79
2	E	328/329 (100%)	318 (97%)	10 (3%)	36 48
3	D	270/292 (92%)	258 (96%)	12 (4%)	25 33
4	F	107/112 (96%)	106 (99%)	1 (1%)	70 82
5	B	242/255 (95%)	239 (99%)	3 (1%)	63 77
5	b	242/255 (95%)	240 (99%)	2 (1%)	73 84
6	C	154/155 (99%)	151 (98%)	3 (2%)	50 65
6	c	154/155 (99%)	152 (99%)	2 (1%)	61 76
All	All	2387/2647 (90%)	2345 (98%)	42 (2%)	51 66

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	PHE
1	A	239	LYS
1	A	411	CYS
1	A	414	TYR

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Mol	Chain	Res	Type
1	A	579	ILE
2	E	85	SER
2	E	149	GLU
2	E	150	GLU
2	E	232	GLU
2	E	239	LYS
2	E	243	ILE
2	E	299	GLU
2	E	309	ASP
2	E	317	THR
2	E	348	ARG
3	D	7	LEU
3	D	60	SER
3	D	82	THR
3	D	118	SER
3	D	172	SER
3	D	185	SER
3	D	228	SER
3	D	233	ASP
3	D	276	SER
3	D	310	THR
3	D	325	GLU
3	D	332	GLU
4	F	75	SER
5	b	42	CYS
5	b	138	LEU
5	B	41	CYS
5	B	179	VAL
5	B	270	LEU
6	c	8	GLU
6	c	36	PHE
6	C	23	LYS
6	C	36	PHE
6	C	69	GLU
1	a	367	ILE
1	a	411	CYS
1	a	414	TYR
1	a	452	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	612	HIS
1	A	648	GLN
2	E	121	ASN
2	E	201	ASN
3	D	142	ASN
3	D	188	HIS
4	F	67	HIS
5	b	235	HIS
5	b	281	GLN
5	B	150	HIS
6	c	5	GLN
6	c	63	ASN
6	c	178	ASN
1	a	471	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)

26 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	$\#\|Z\| > 2$
10	9S8	B	401	5	2,10,10	5.48	2 (100%)	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	SF4	A	702	1	0,12,12	-	-	-		
10	9S8	b	401	5	2,10,10	5.70	1 (50%)	-		
7	SF4	E	401	2	0,12,12	-	-	-		
7	SF4	E	403	2	0,12,12	-	-	-		
7	SF4	A	705	1	0,12,12	-	-	-		
8	FAD	A	706	-	56,58,58	0.54	0	81,89,89	0.67	1 (1%)
7	SF4	D	401	3	0,12,12	-	-	-		
7	SF4	A	701	1	0,12,12	-	-	-		
9	FES	F	201	4	0,4,4	-	-	-		
7	SF4	A	704	1	0,12,12	-	-	-		
10	9S8	b	402	5	2,10,10	5.64	2 (100%)	-		
7	SF4	c	201	6	0,12,12	-	-	-		
7	SF4	A	707	1	0,12,12	-	-	-		
8	FAD	E	405	-	56,58,58	0.51	0	81,89,89	0.72	1 (1%)
7	SF4	a	704	1	0,12,12	-	-	-		
7	SF4	C	202	6	0,12,12	-	-	-		
7	SF4	a	702	1	0,12,12	-	-	-		
8	FAD	a	701	-	56,58,58	0.54	0	81,89,89	0.67	1 (1%)
7	SF4	A	703	1	0,12,12	-	-	-		
7	SF4	c	202	6	0,12,12	-	-	-		
10	9S8	B	402	5	2,10,10	1.20	0	-		
7	SF4	E	404	2	0,12,12	-	-	-		
7	SF4	a	703	1	0,12,12	-	-	-		
7	SF4	E	402	2	0,12,12	-	-	-		
7	SF4	C	201	6	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
10	9S8	B	401	5	-	-	0/3/3/3
7	SF4	A	702	1	-	-	0/6/5/5
10	9S8	b	401	5	-	-	0/3/3/3
7	SF4	E	401	2	-	-	0/6/5/5
7	SF4	E	403	2	-	-	0/6/5/5
7	SF4	A	705	1	-	-	0/6/5/5
7	SF4	D	401	3	-	-	0/6/5/5
8	FAD	A	706	-	-	1/34/50/50	0/6/6/6
7	SF4	A	701	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FES	F	201	4	-	-	0/1/1/1
7	SF4	A	704	1	-	-	0/6/5/5
10	9S8	b	402	5	-	-	0/3/3/3
7	SF4	c	201	6	-	-	0/6/5/5
7	SF4	A	707	1	-	-	0/6/5/5
8	FAD	E	405	-	-	8/34/50/50	0/6/6/6
7	SF4	a	704	1	-	-	0/6/5/5
7	SF4	C	202	6	-	-	0/6/5/5
7	SF4	a	702	1	-	-	0/6/5/5
8	FAD	a	701	-	-	2/34/50/50	0/6/6/6
7	SF4	A	703	1	-	-	0/6/5/5
7	SF4	c	202	6	-	-	0/6/5/5
10	9S8	B	402	5	-	-	0/3/3/3
7	SF4	E	404	2	-	-	0/6/5/5
7	SF4	a	703	1	-	-	0/6/5/5
7	SF4	E	402	2	-	-	0/6/5/5
7	SF4	C	201	6	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	b	401	9S8	S3-FE4	-8.05	2.05	2.24
10	b	402	9S8	S3-FE4	-7.22	2.07	2.24
10	B	401	9S8	S3-FE4	-7.17	2.08	2.24
10	b	402	9S8	S5-FE4	-3.40	2.16	2.24
10	B	401	9S8	S5-FE4	-2.92	2.18	2.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	405	FAD	O4B-C1B-C2B	-2.10	102.07	106.64
8	a	701	FAD	C4-N3-C2	-2.08	121.80	125.64
8	A	706	FAD	C4-N3-C2	-2.07	121.82	125.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	405	FAD	C5'-O5'-P-O1P
8	E	405	FAD	C5'-O5'-P-O2P
8	E	405	FAD	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
8	E	405	FAD	C2B-C1B-N9A-C4A
8	E	405	FAD	C2B-C1B-N9A-C8A
8	E	405	FAD	O4B-C1B-N9A-C8A
8	E	405	FAD	C5'-O5'-P-O3P
8	A	706	FAD	O4B-C4B-C5B-O5B
8	E	405	FAD	O4B-C4B-C5B-O5B
8	a	701	FAD	O4B-C4B-C5B-O5B
8	a	701	FAD	C2B-C1B-N9A-C8A

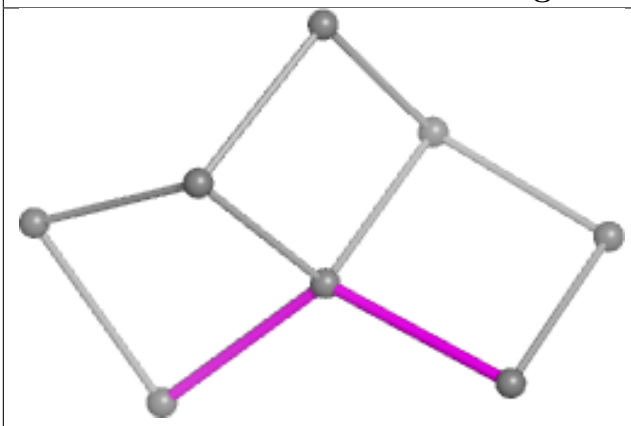
There are no ring outliers.

4 monomers are involved in 17 short contacts:

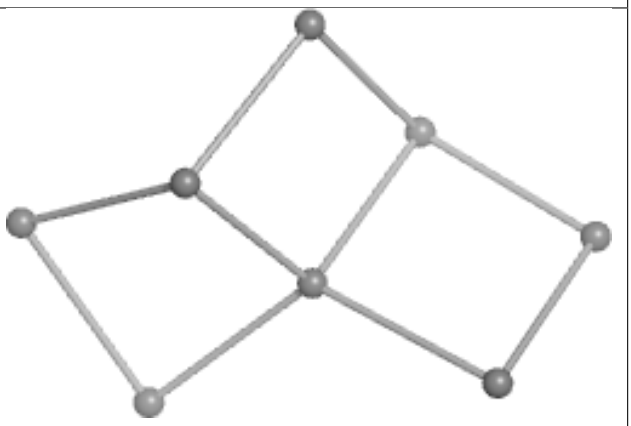
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	401	9S8	1	0
8	A	706	FAD	1	0
8	E	405	FAD	14	0
10	B	402	9S8	1	0

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.

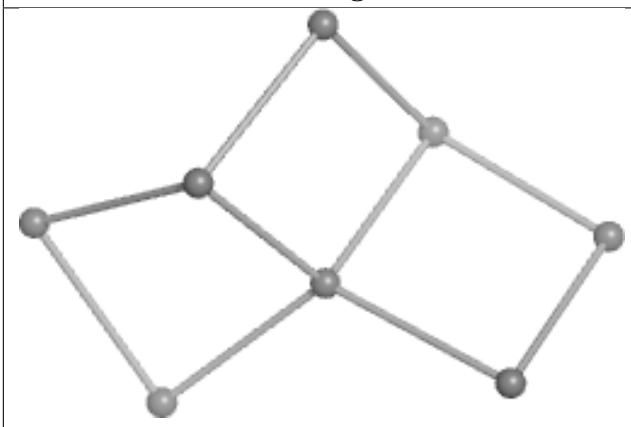
Ligand 9S8 B 401



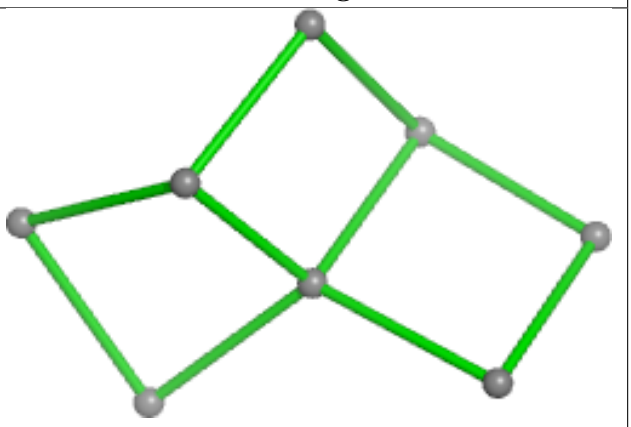
Bond lengths



Bond angles

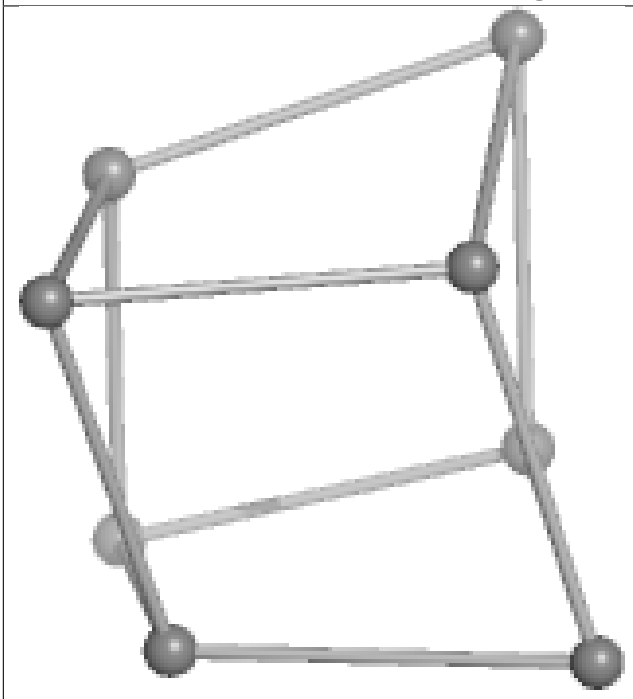


Torsions

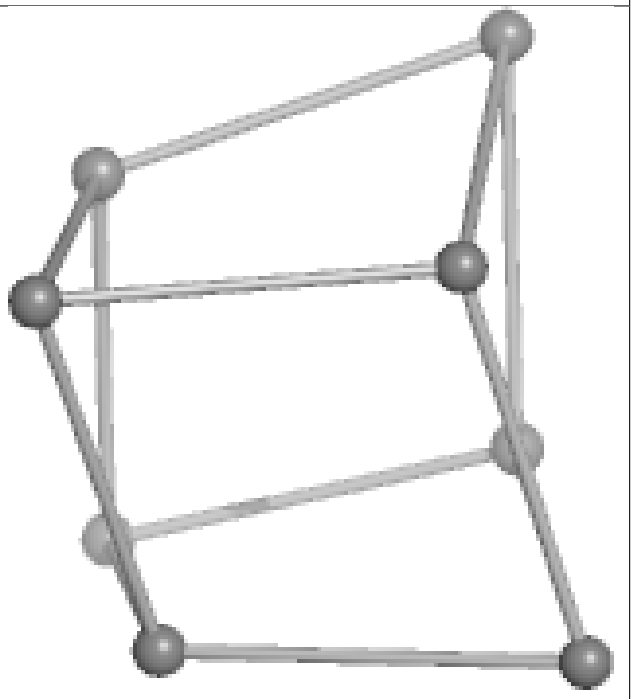


Rings

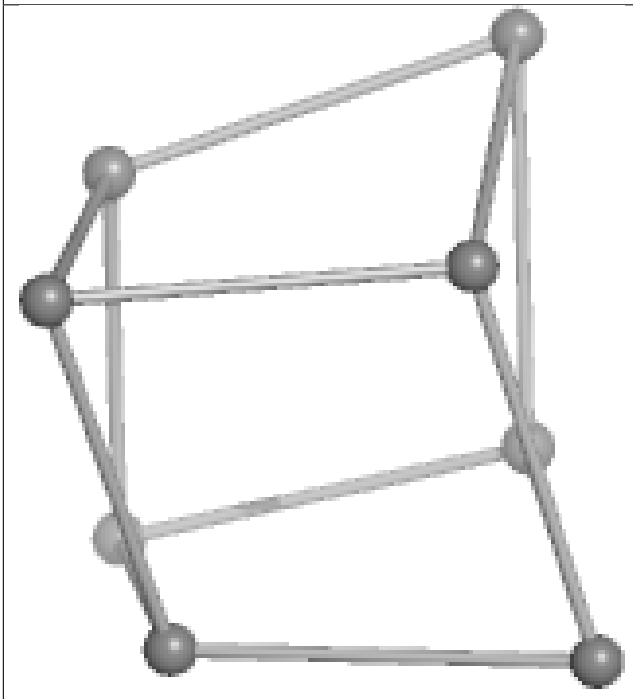
Ligand SF4 A 702



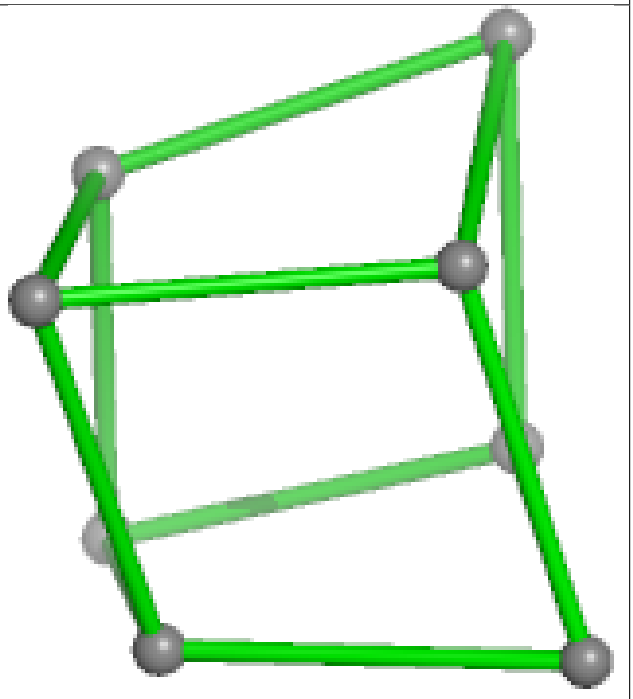
Bond lengths



Bond angles

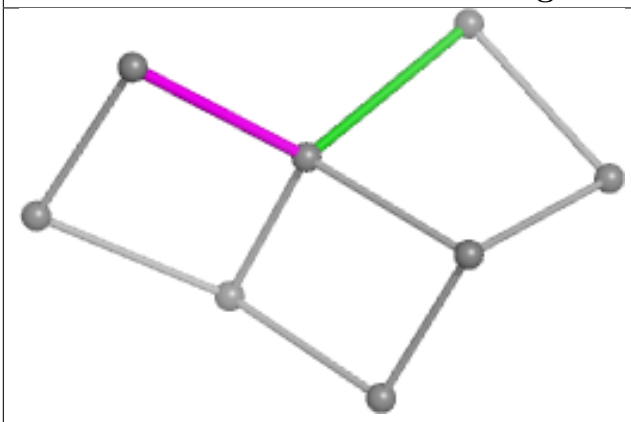


Torsions

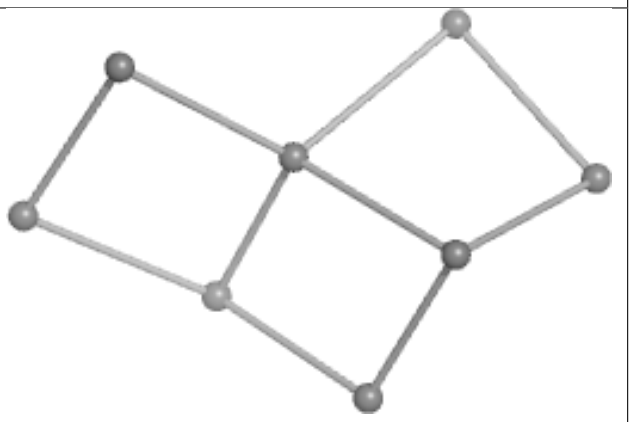


Rings

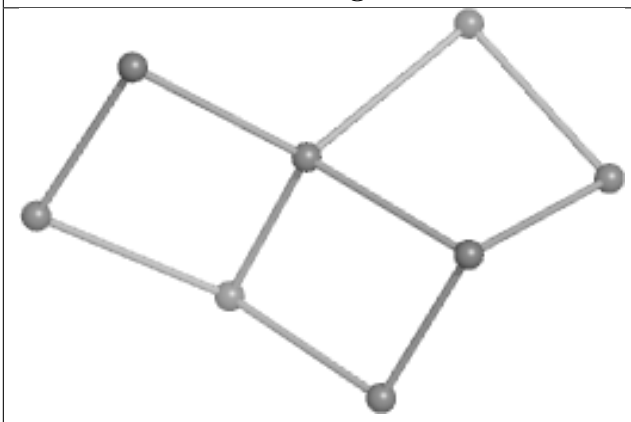
Ligand 9S8 b 401



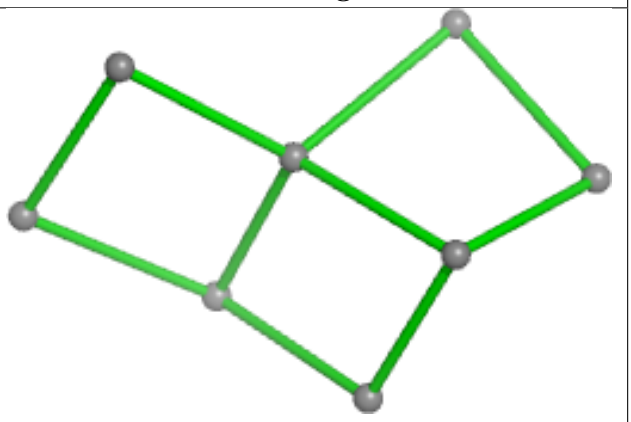
Bond lengths



Bond angles

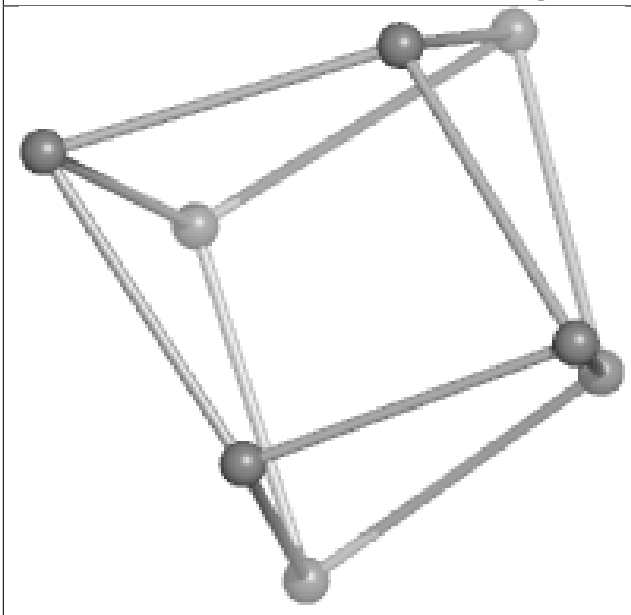


Torsions

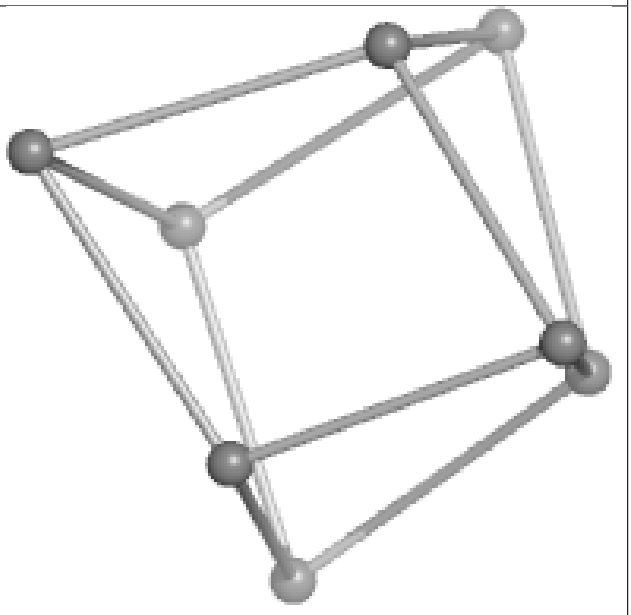


Rings

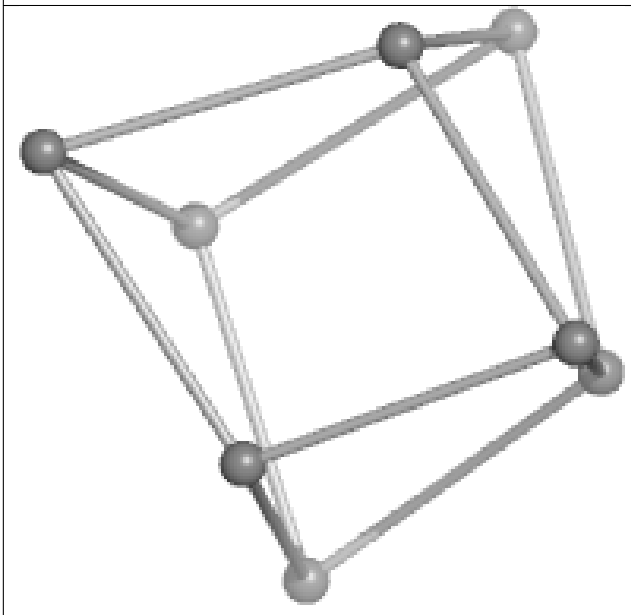
Ligand SF4 E 401



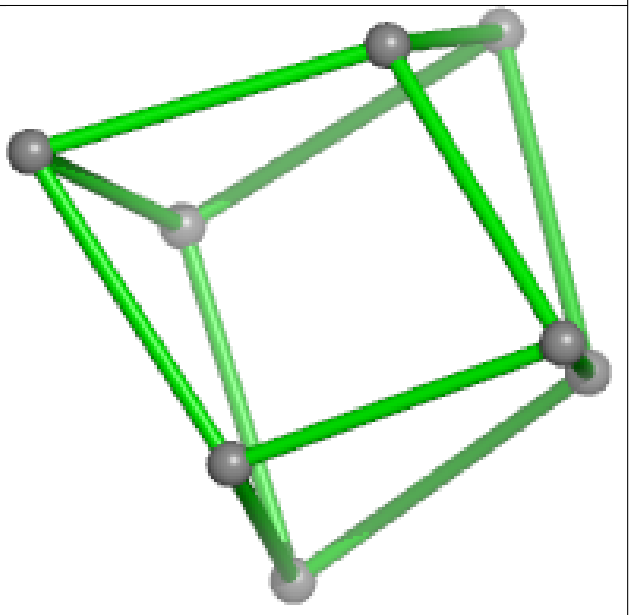
Bond lengths



Bond angles

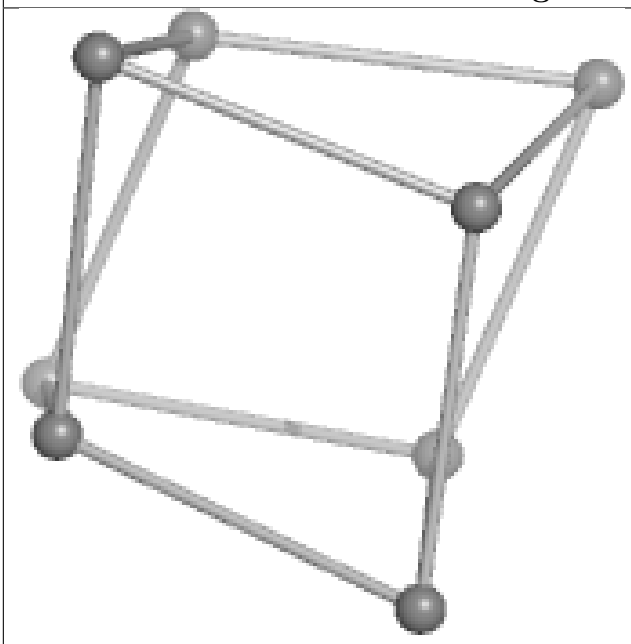


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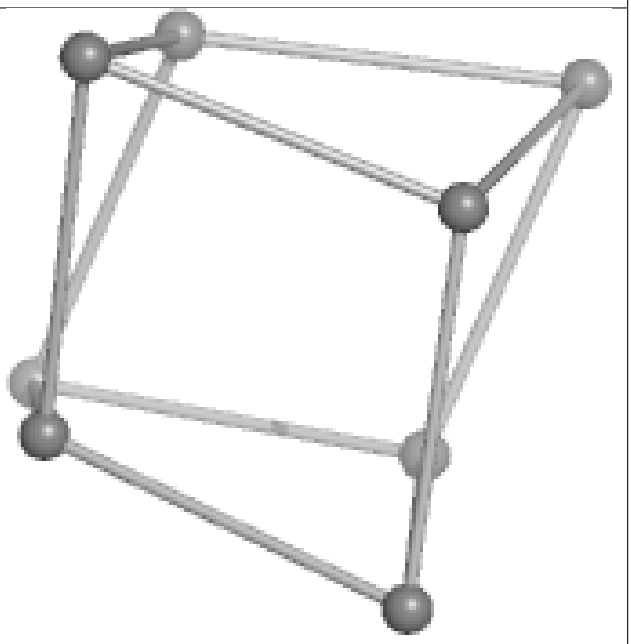


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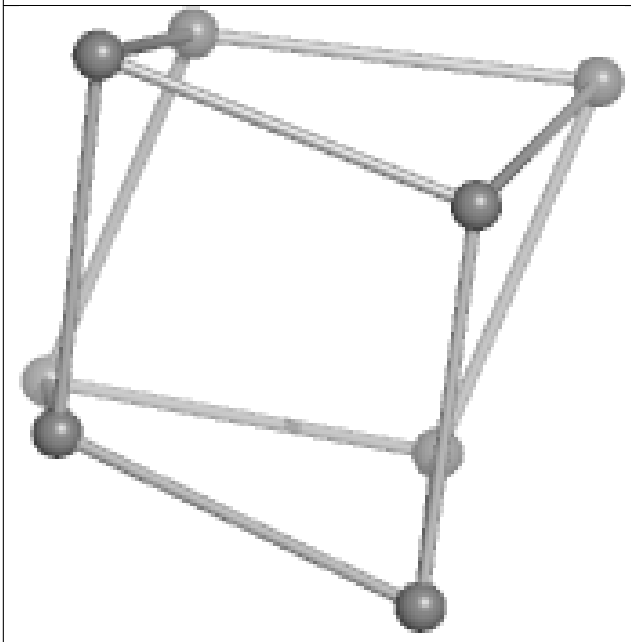
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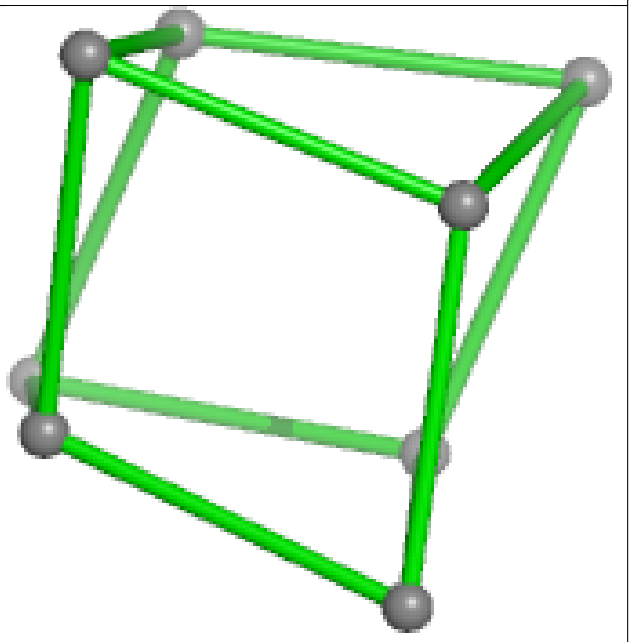
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Bond angles

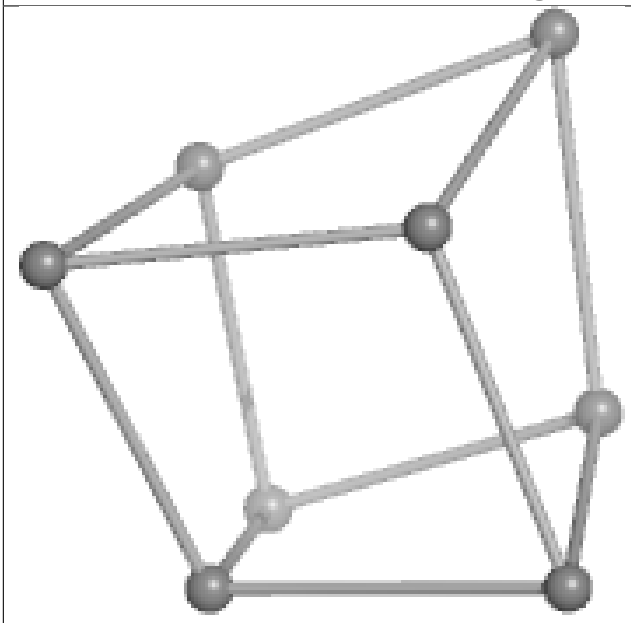


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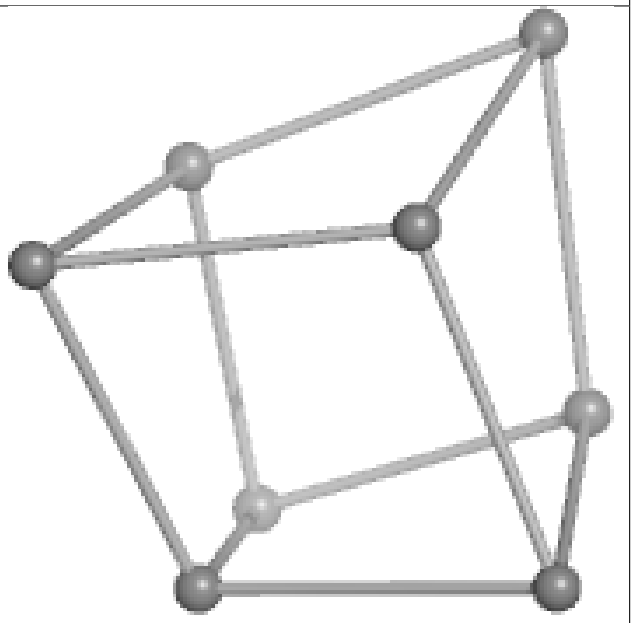


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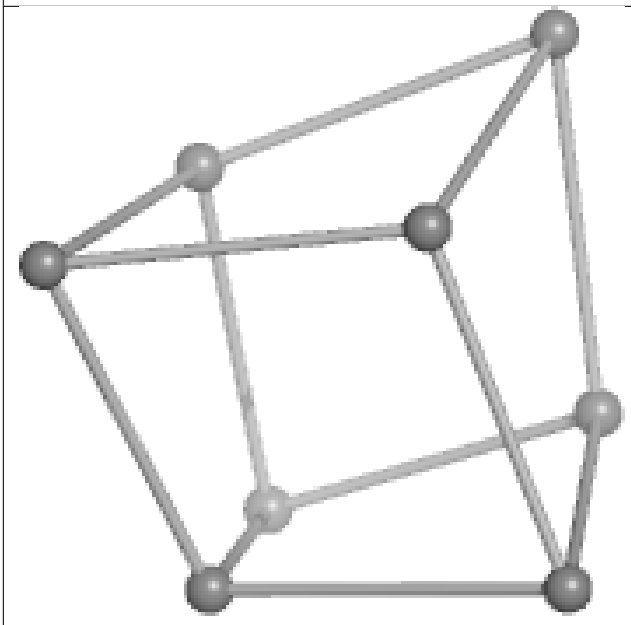
Ligand SF4 A 705



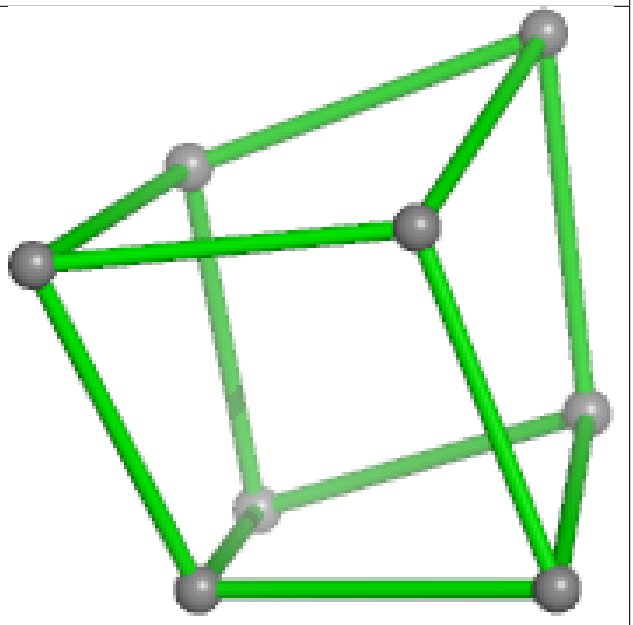
Bond lengths



Bond angles

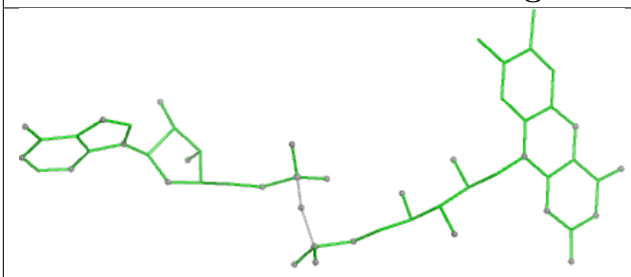


Torsions



Rings

Ligand FAD A 706



Bond lengths



Bond angles

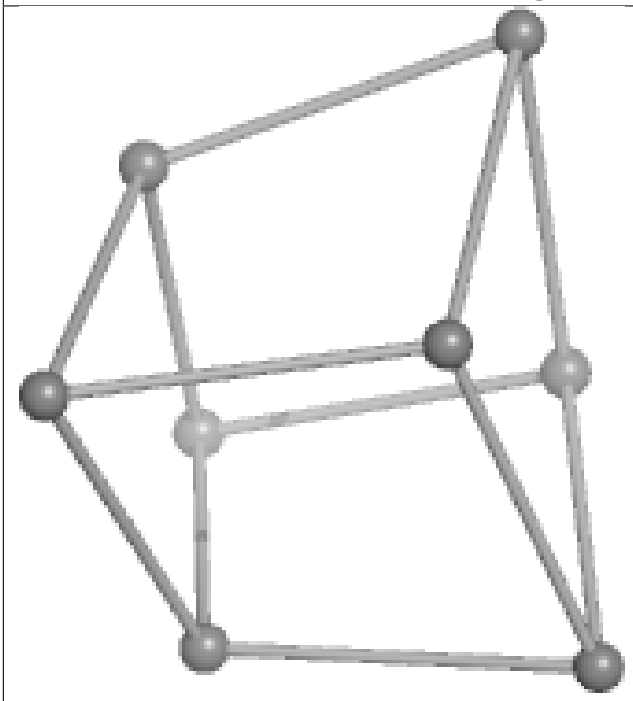


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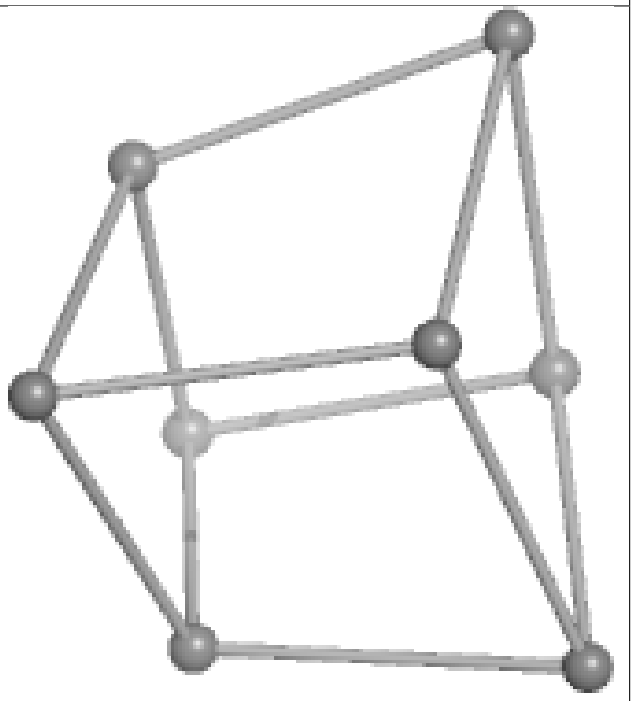


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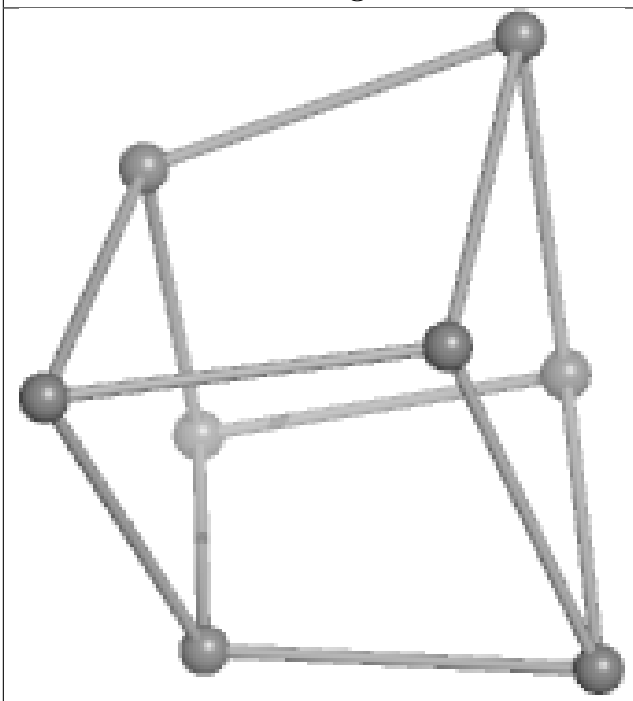
Ligand SF4 D 401



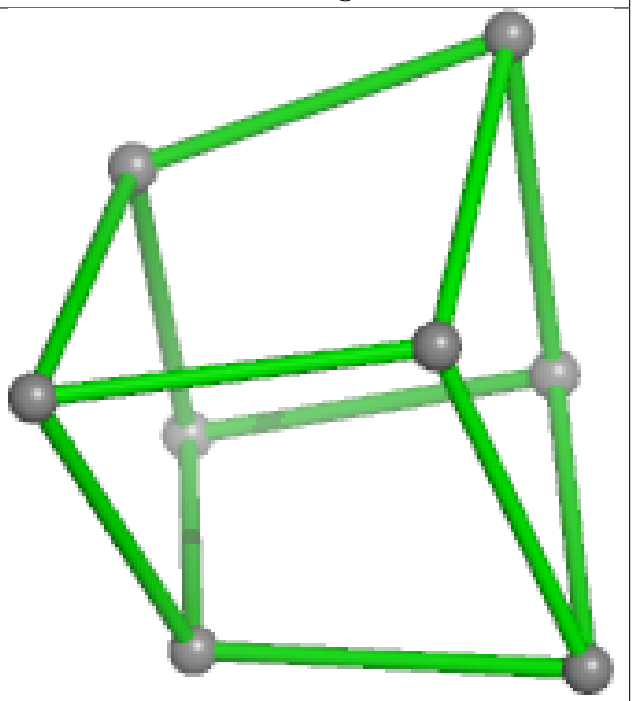
Bond lengths



Bond angles

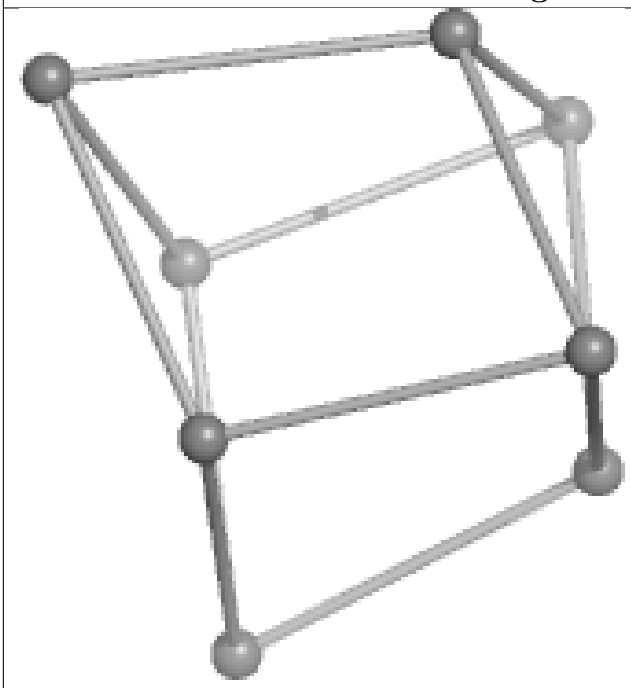


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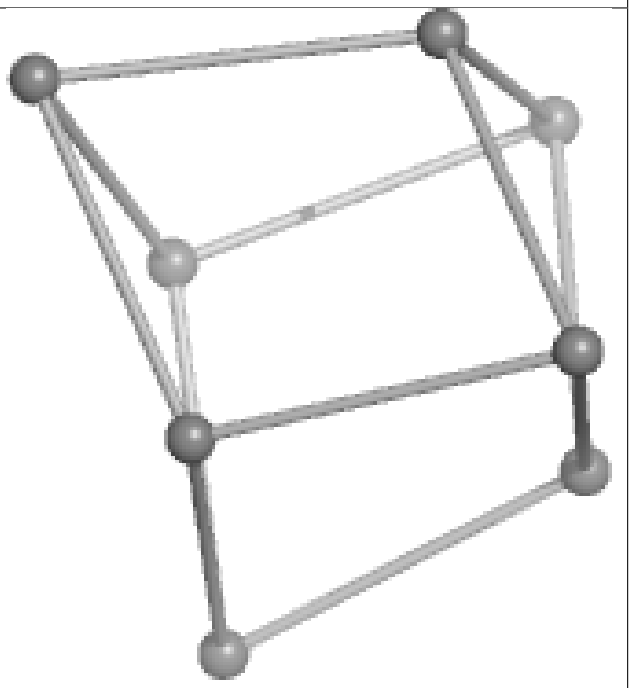


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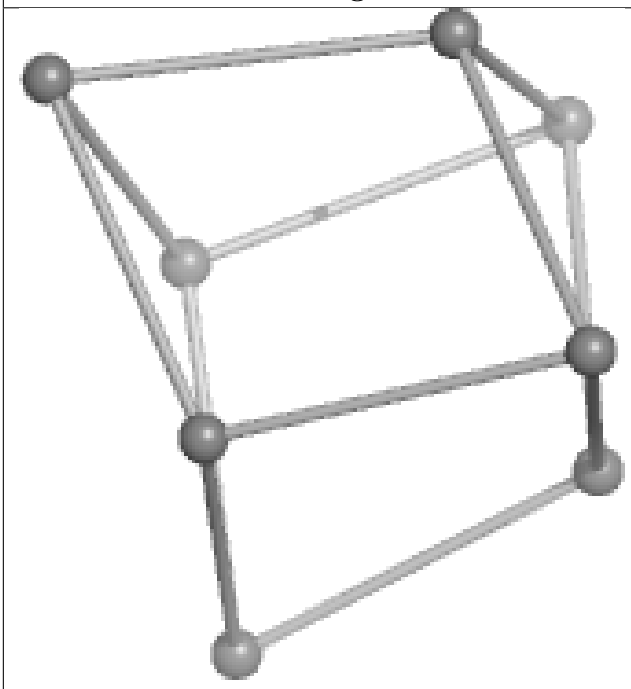
Ligand SF4 A 701



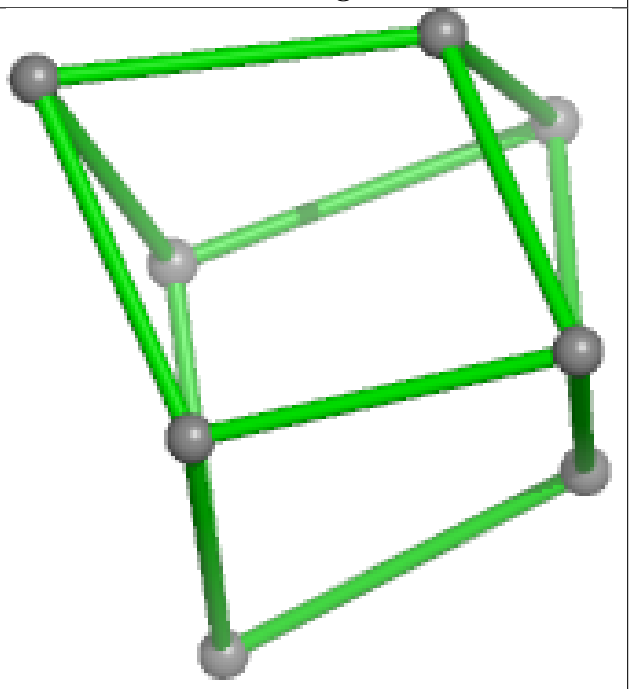
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Bond angles

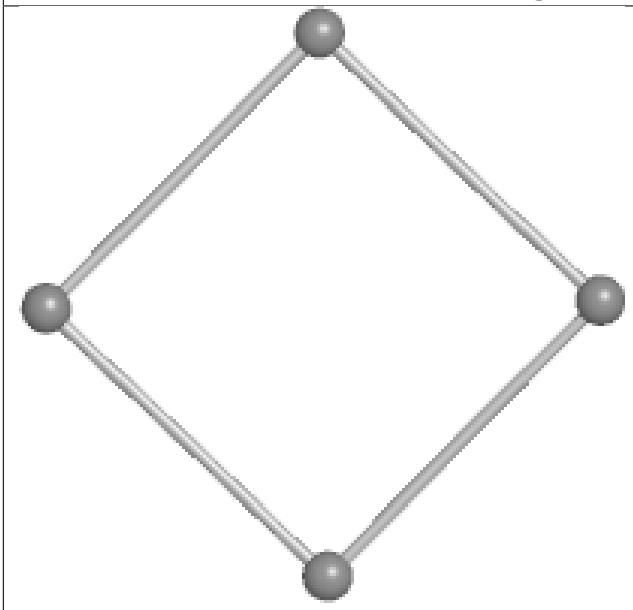


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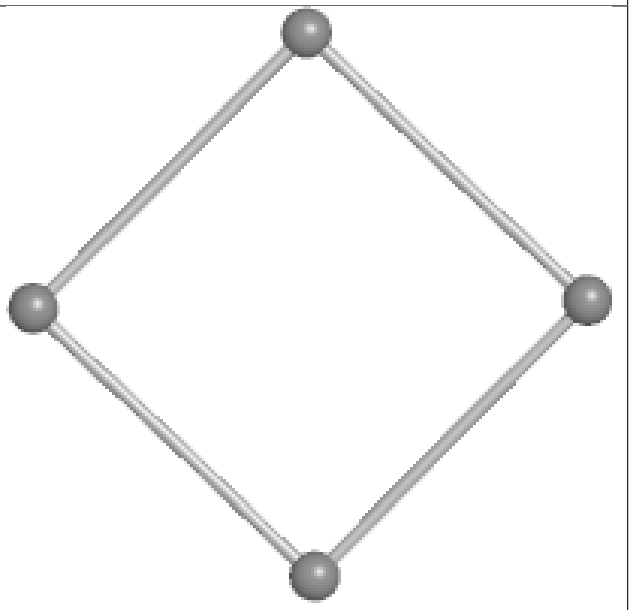


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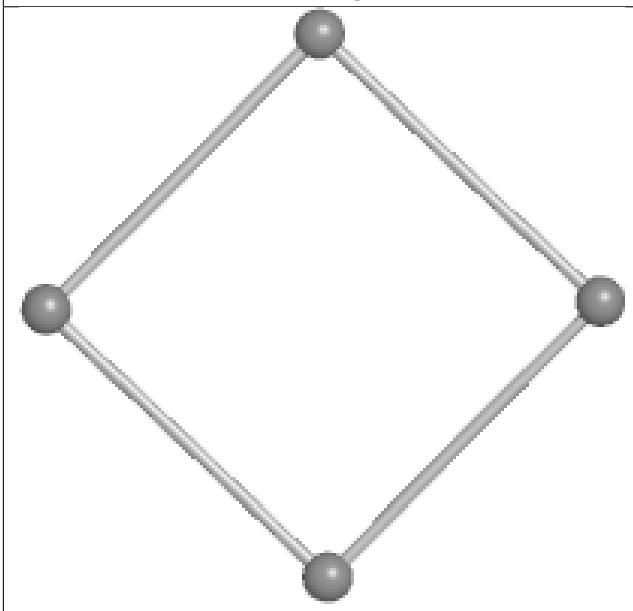
Ligand FES F 201



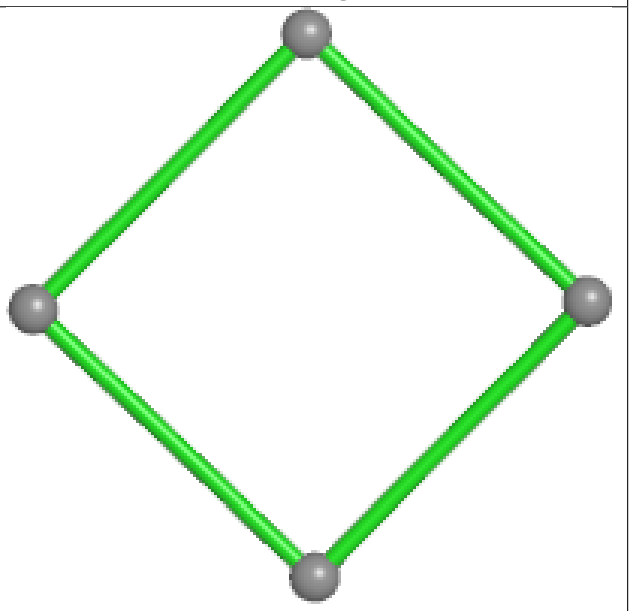
Bond lengths



Bond angles

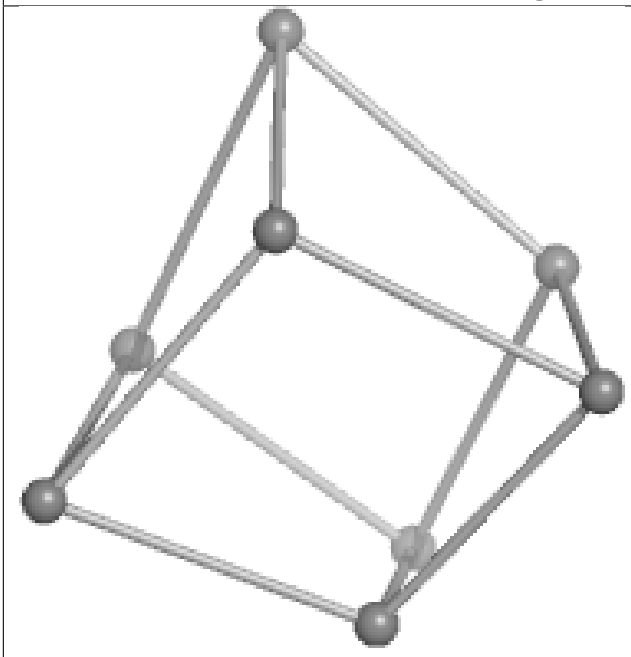


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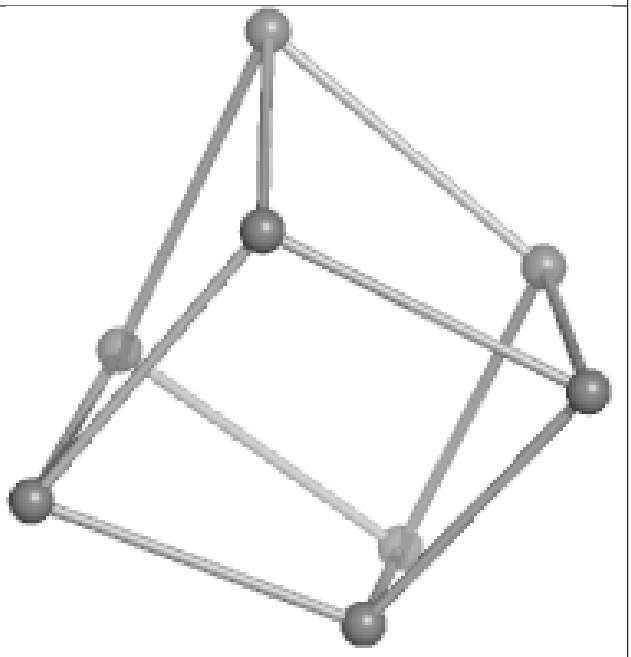


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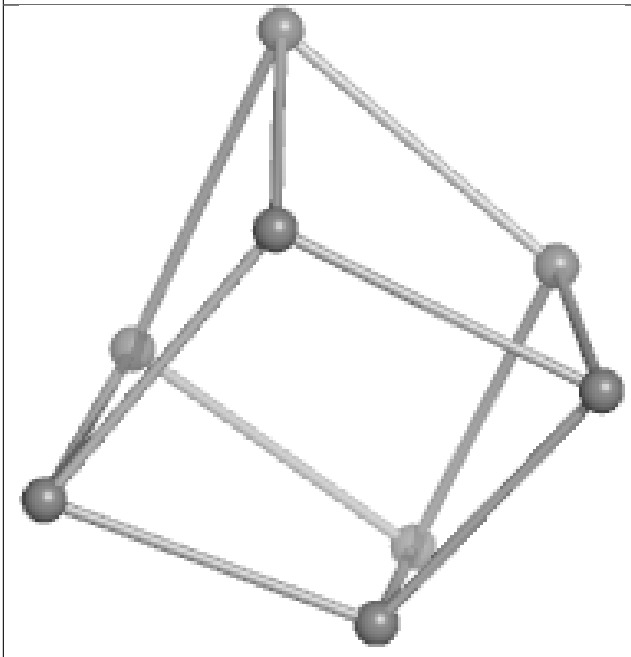
Ligand SF4 A 704



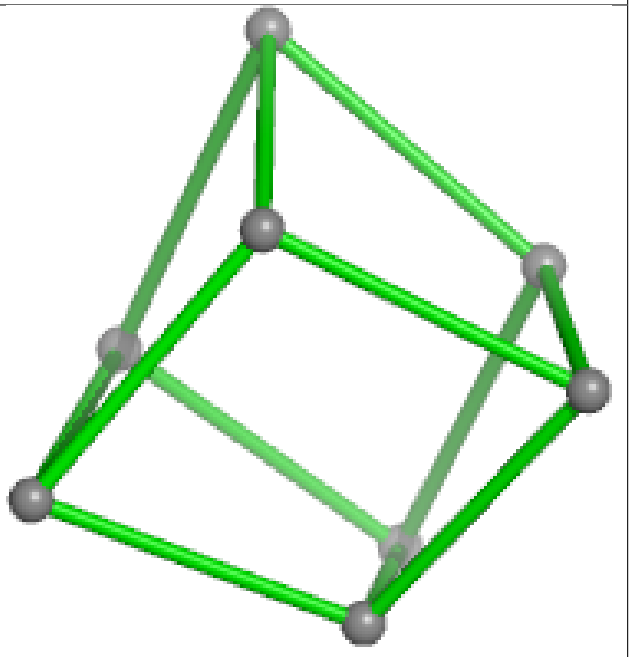
Bond lengths



Bond angles

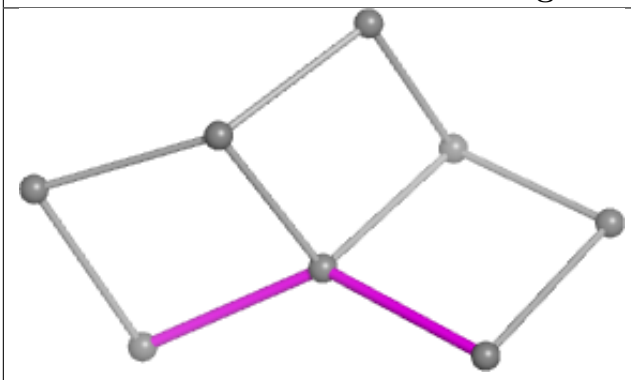


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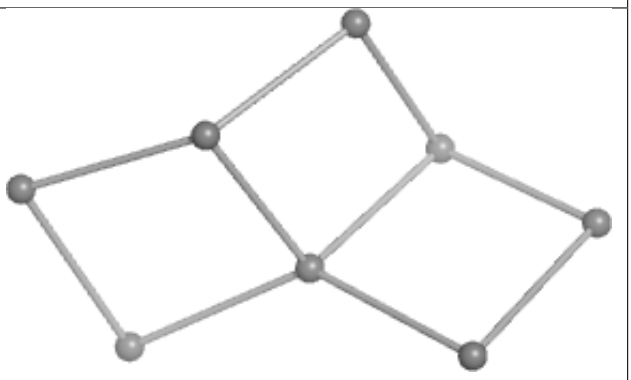


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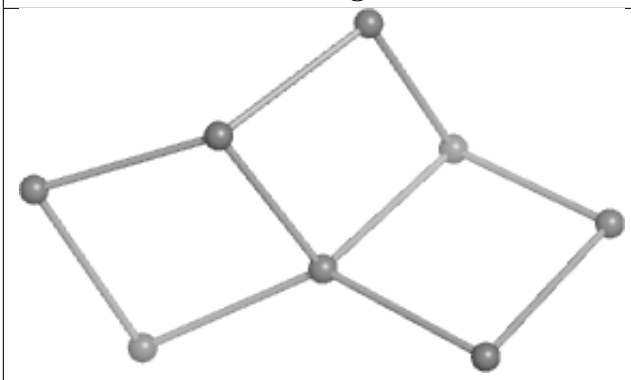
Ligand 9S8 b 402



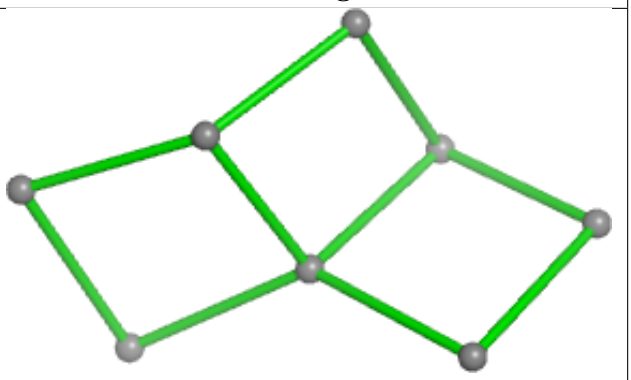
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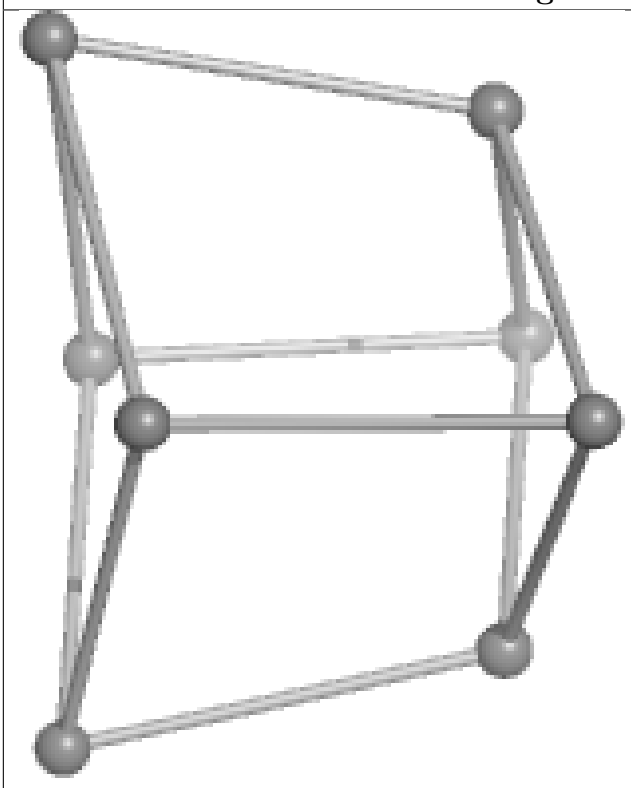


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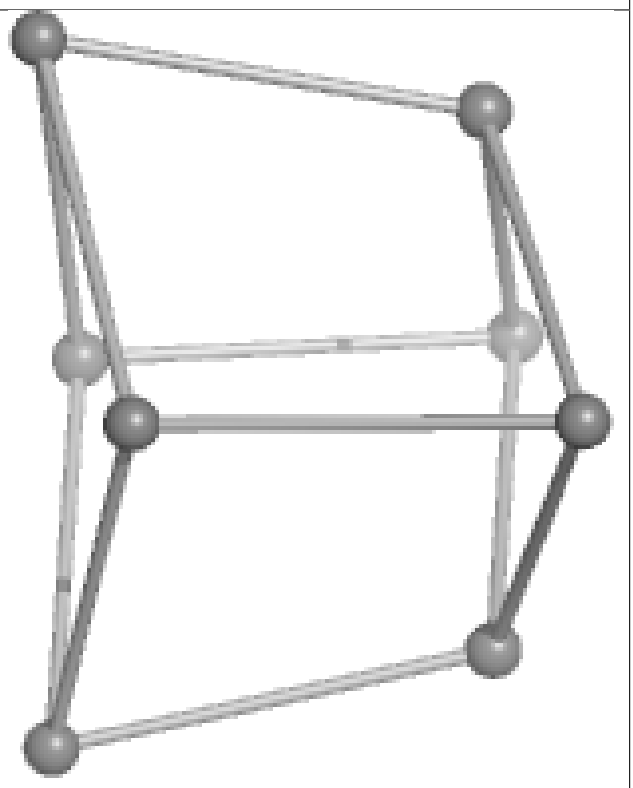


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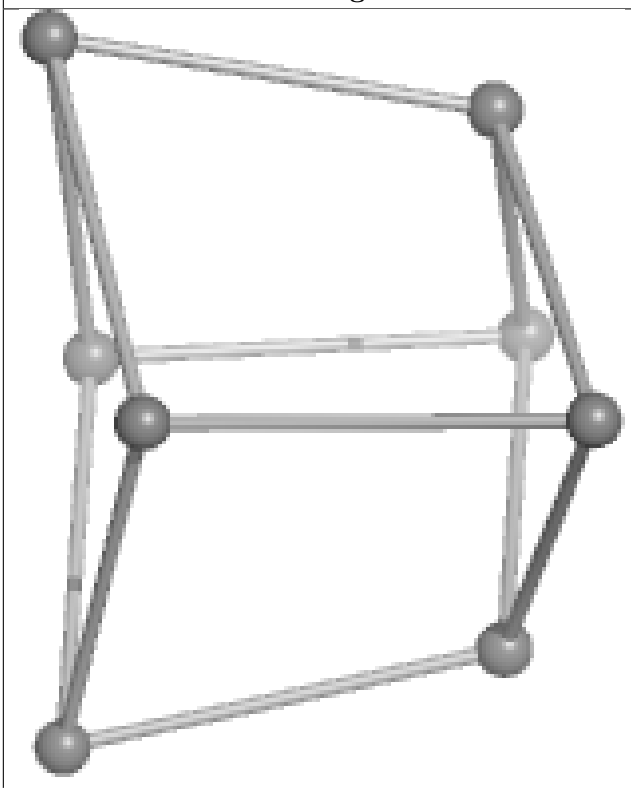
Ligand SF4 c 201



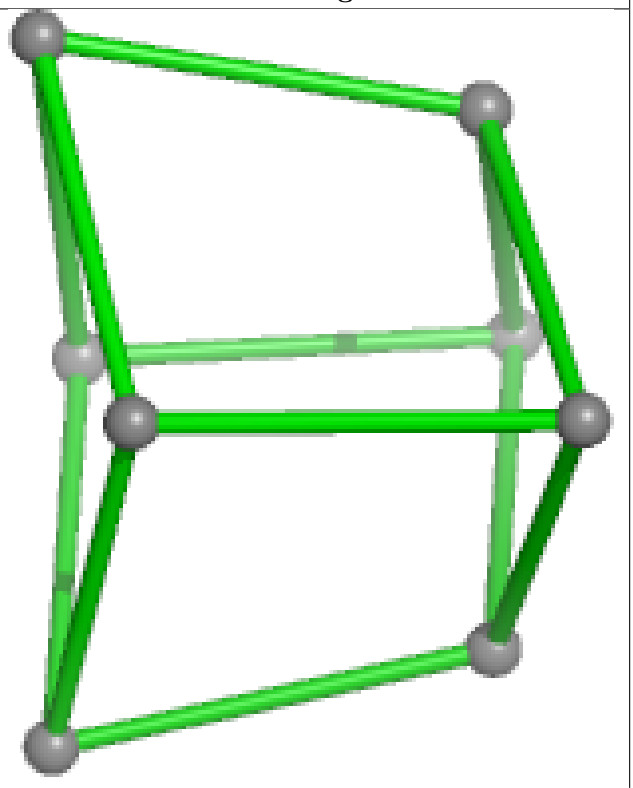
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Bond angles

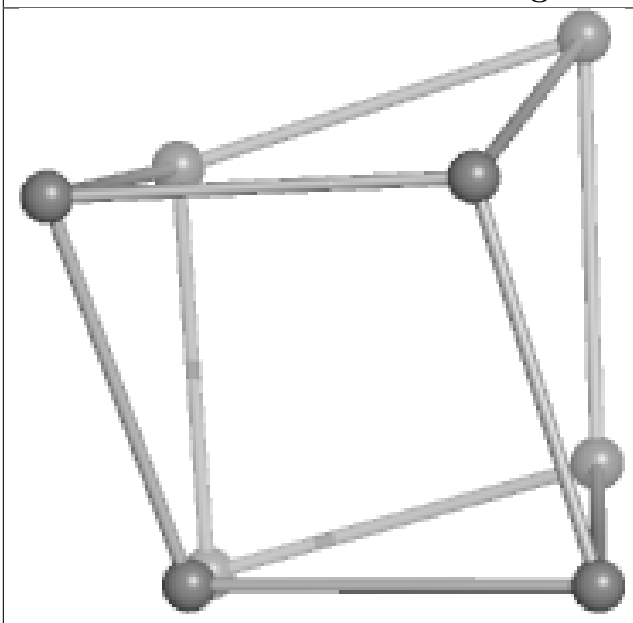


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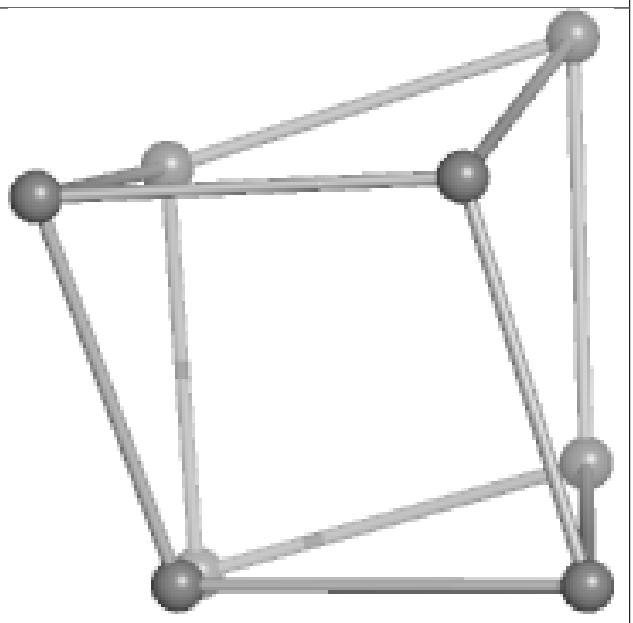


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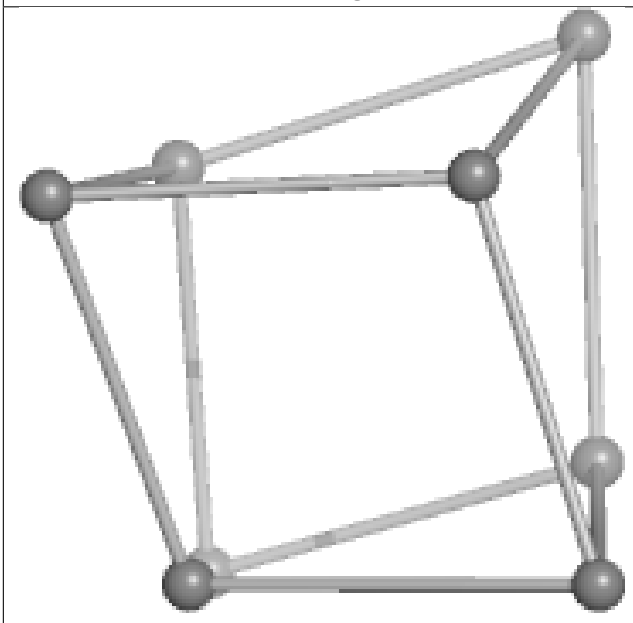
Ligand SF4 A 707



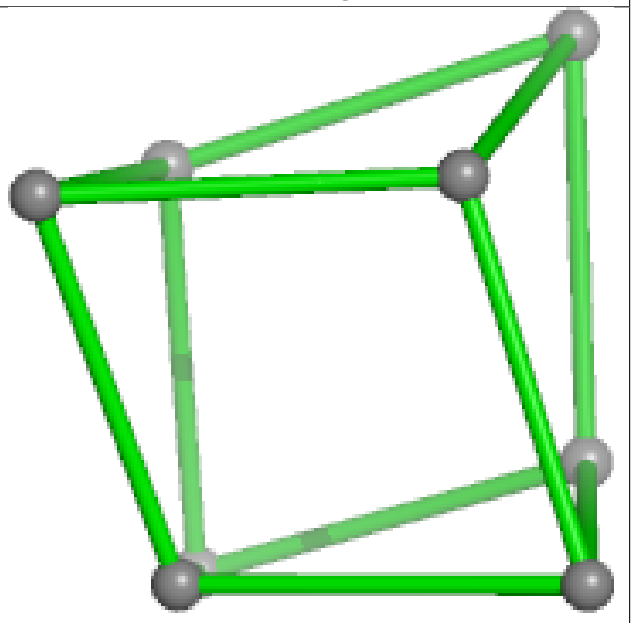
Bond lengths



Bond angles

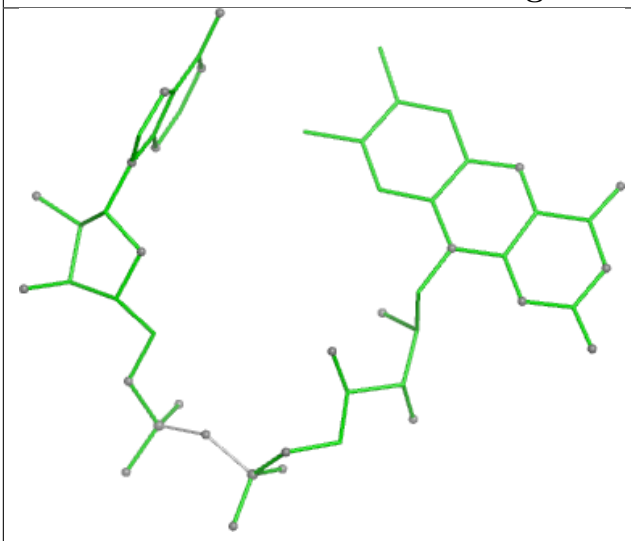


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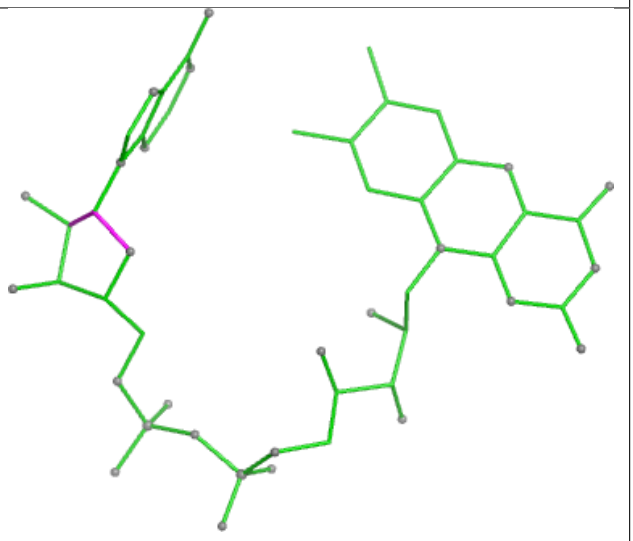


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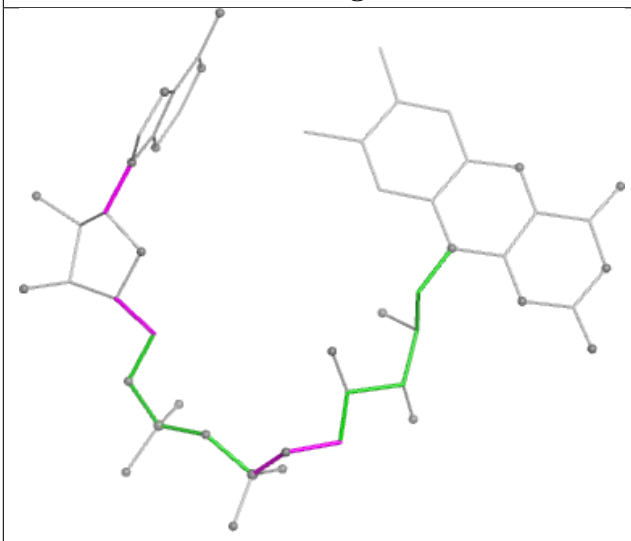
Ligand FAD E 405



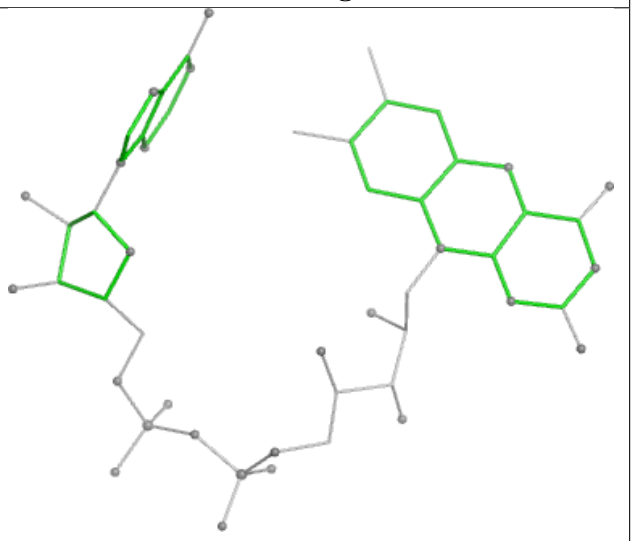
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Bond angles

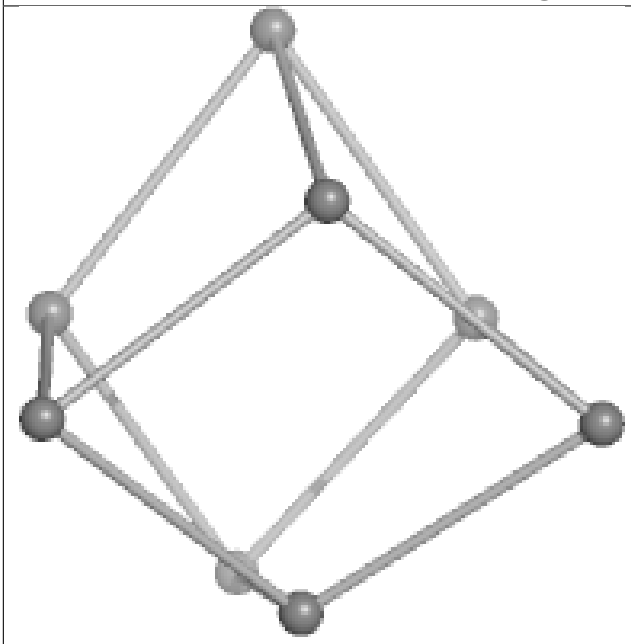


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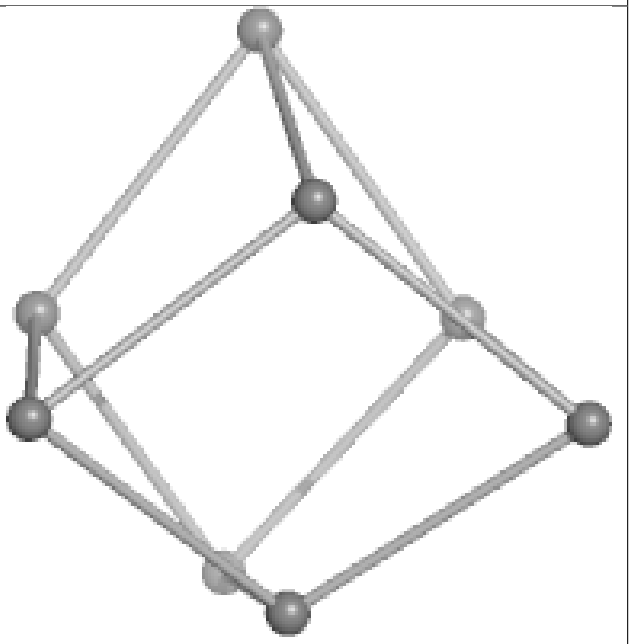


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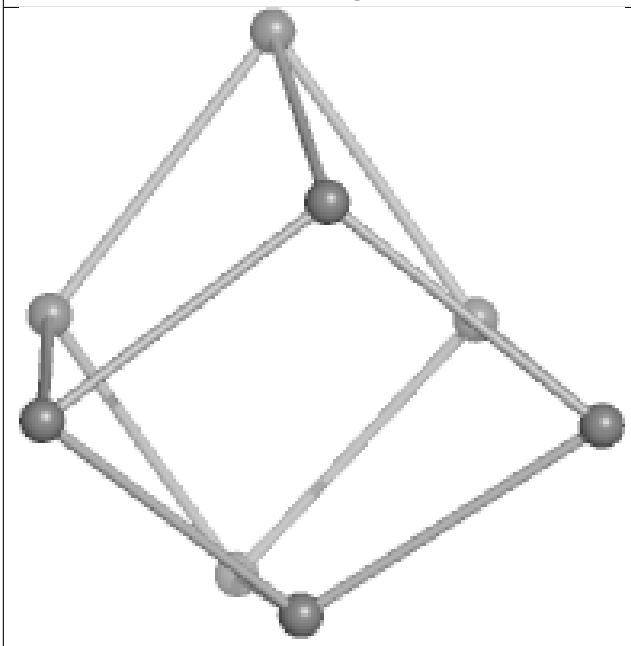
Ligand SF4 a 704



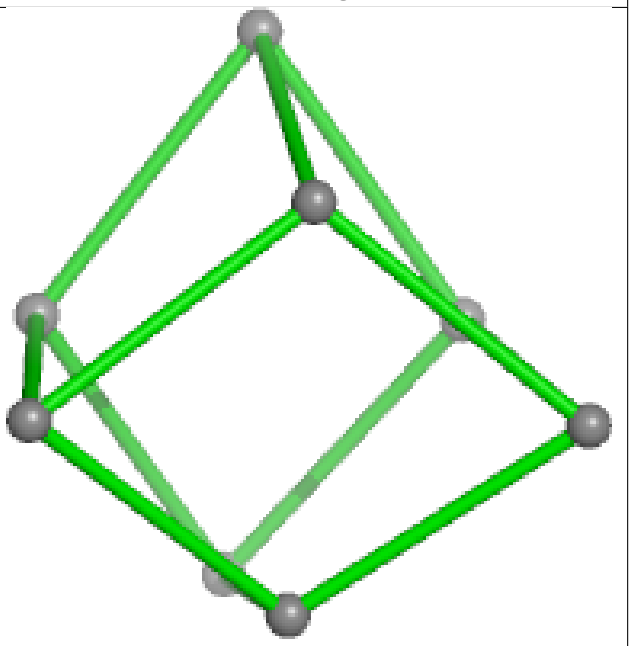
Bond lengths



Bond angles

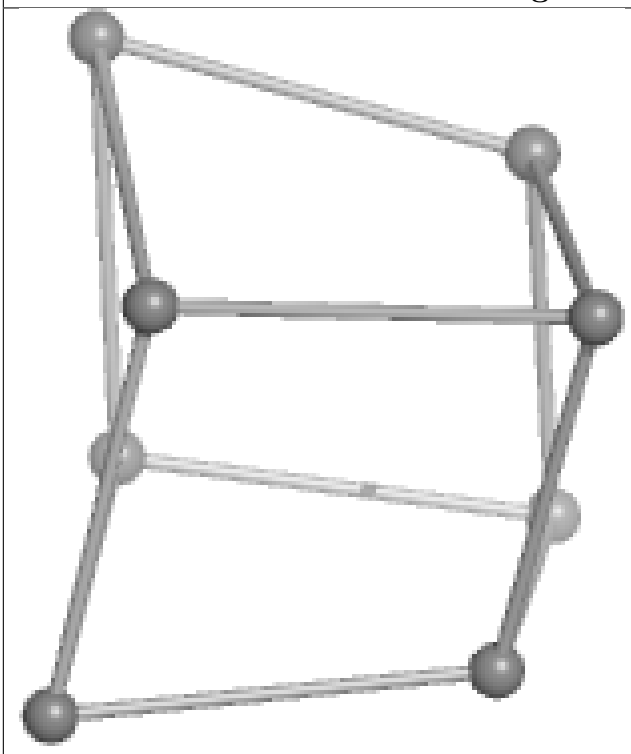


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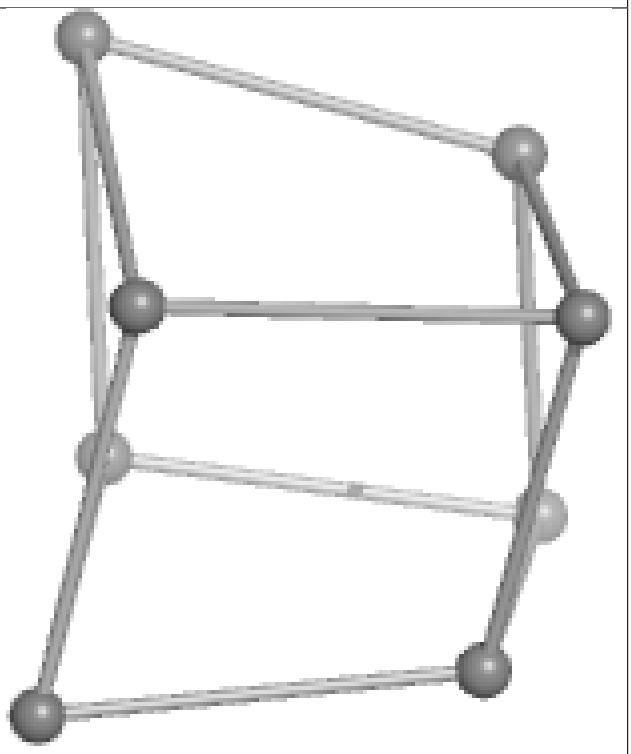


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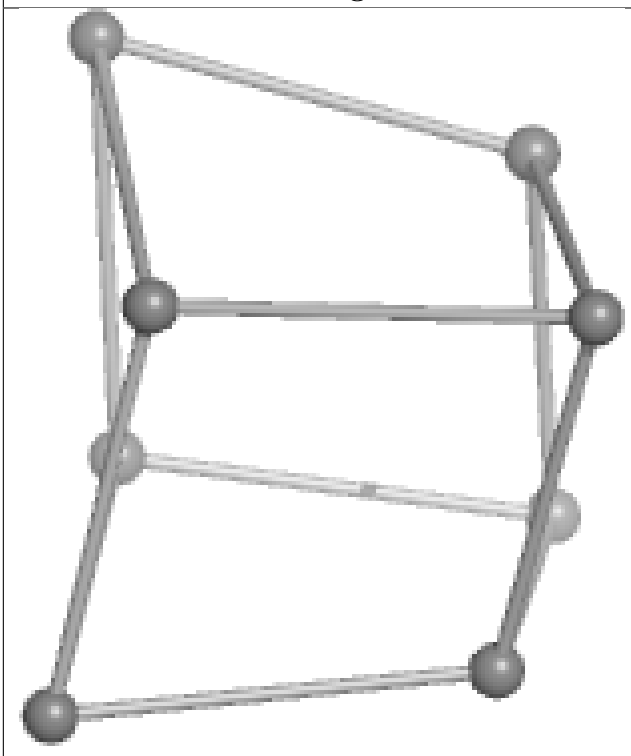
Ligand SF4 C 202



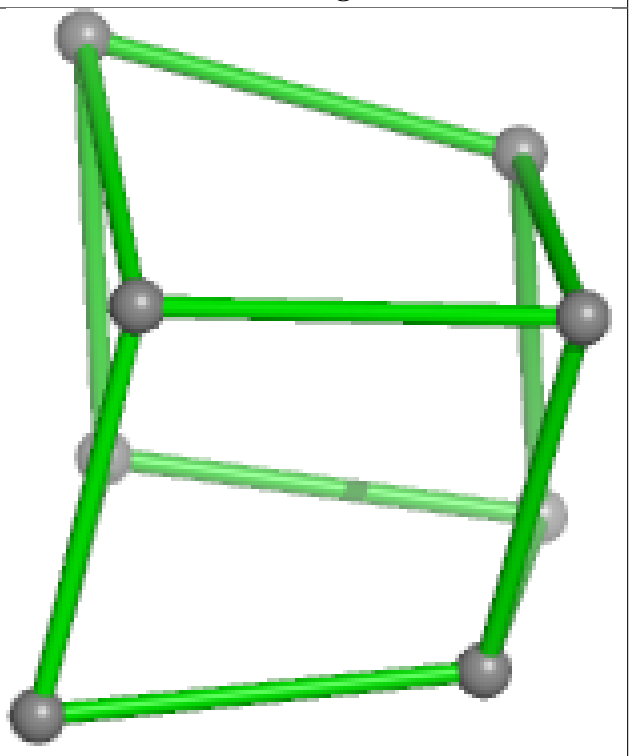
Bond lengths



Bond angles

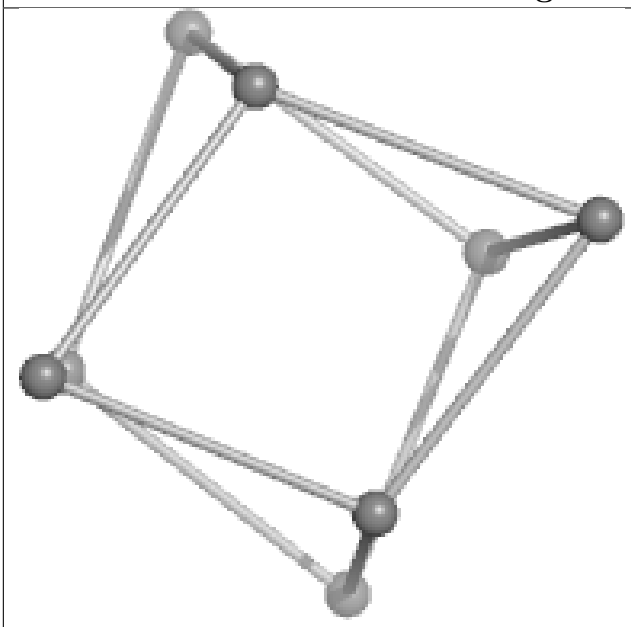


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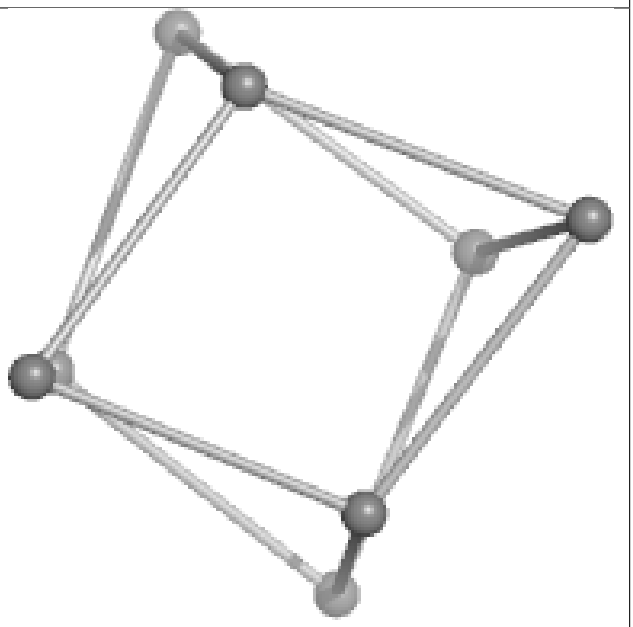


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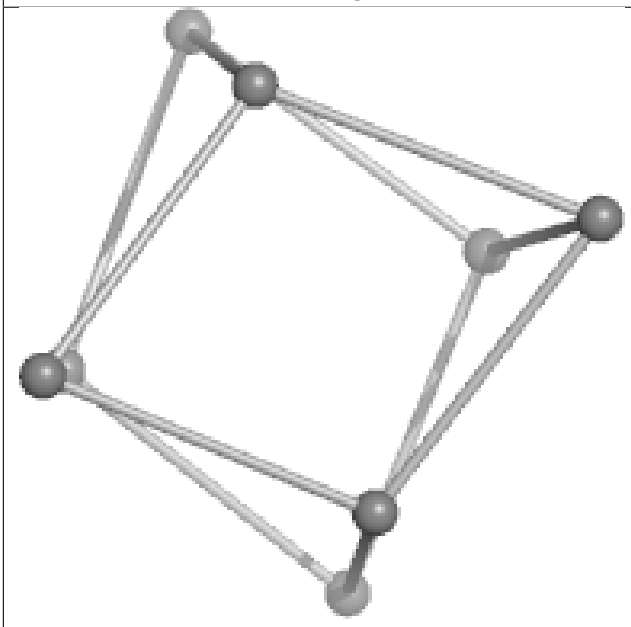
Ligand SF4 a 702



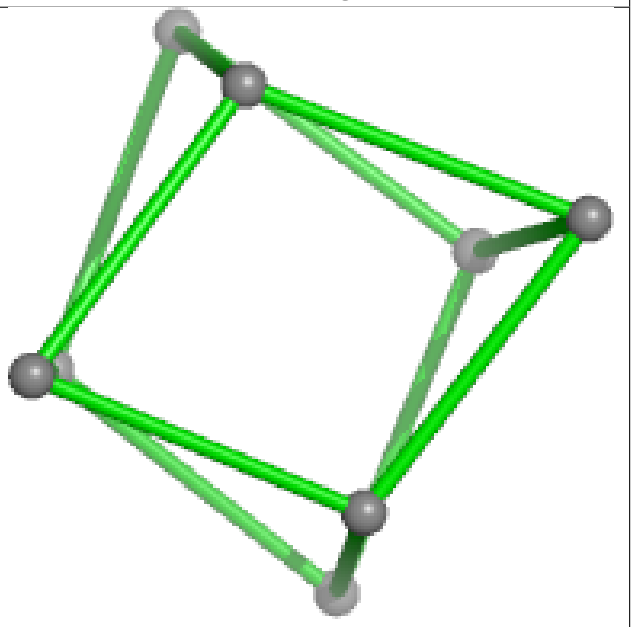
Bond lengths



Bond angles

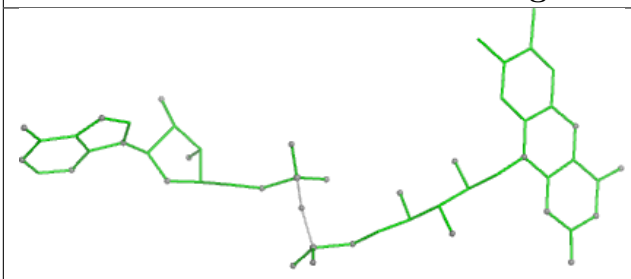


Torsions



Rings

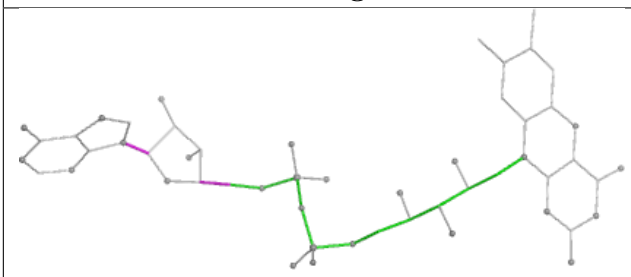
Ligand FAD a 701



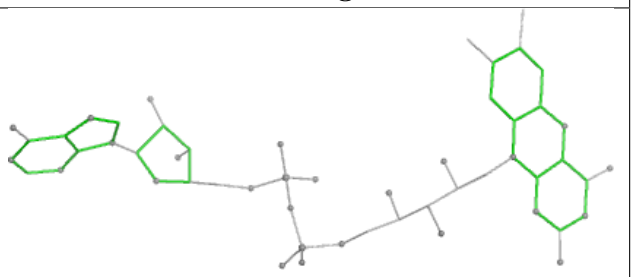
Bond lengths



Bond angles

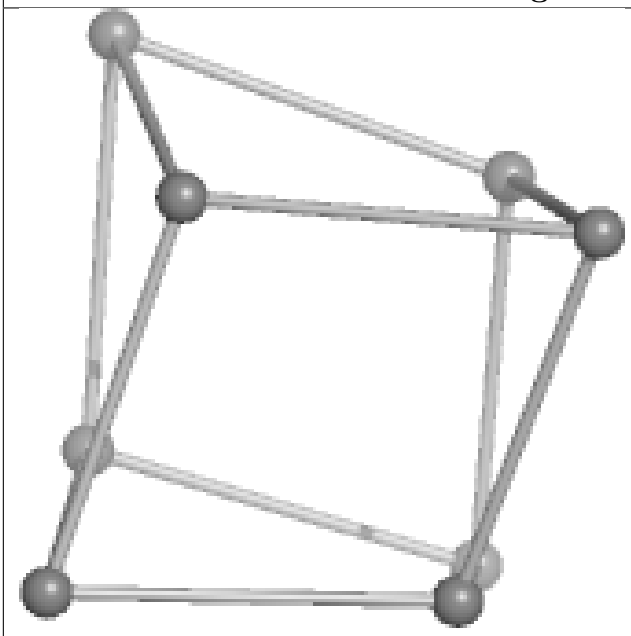


Torsions

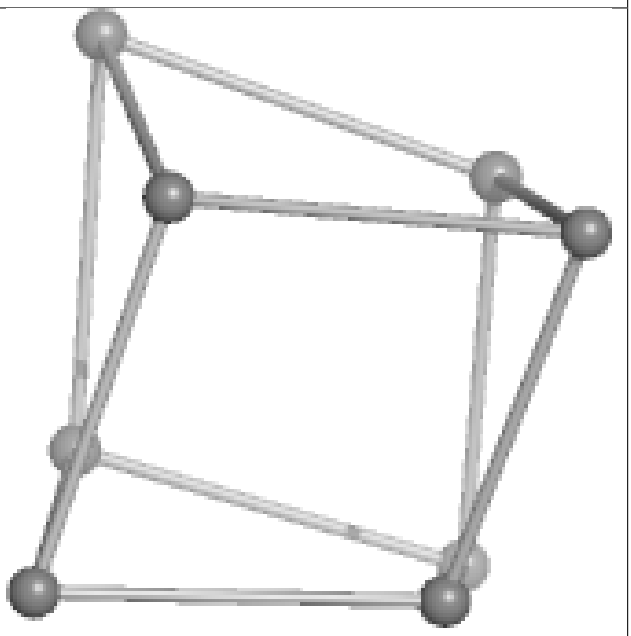


Rings

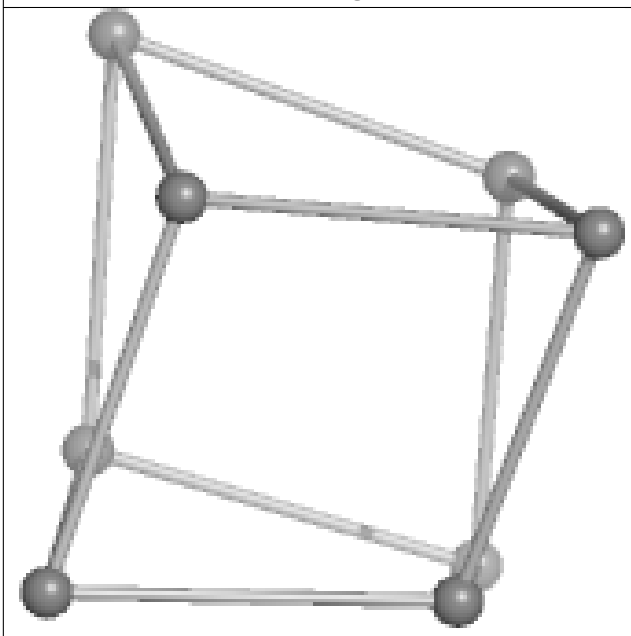
Ligand SF4 A 703



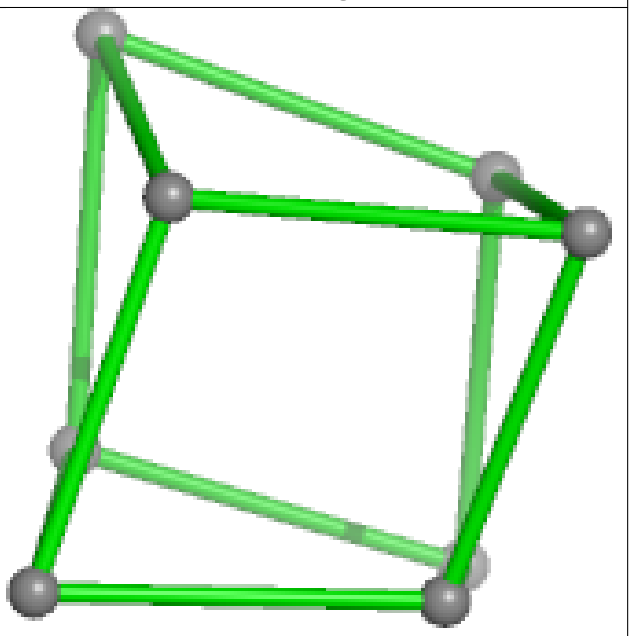
Bond lengths



Bond angles

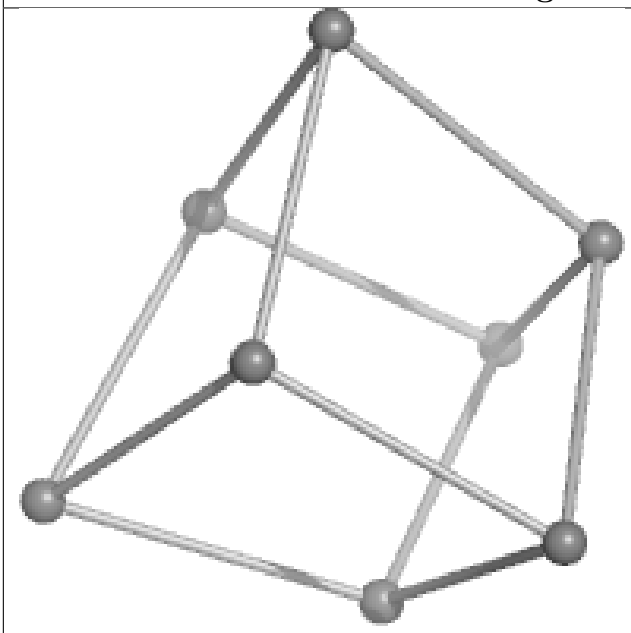


Torsions

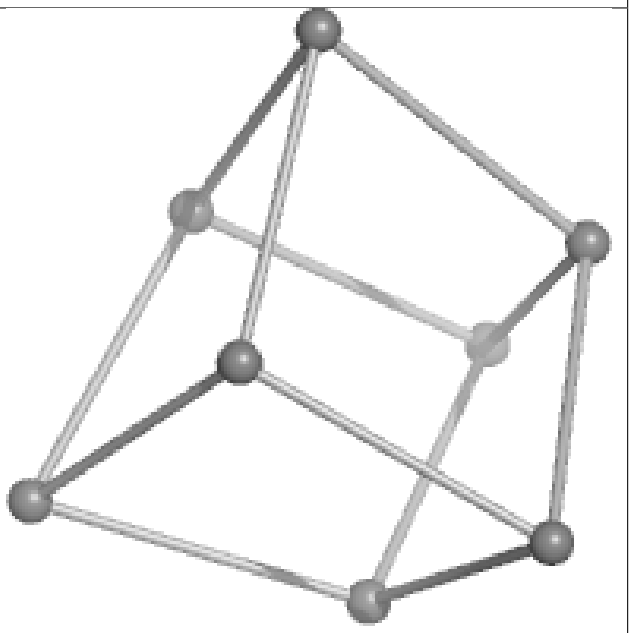


Rings

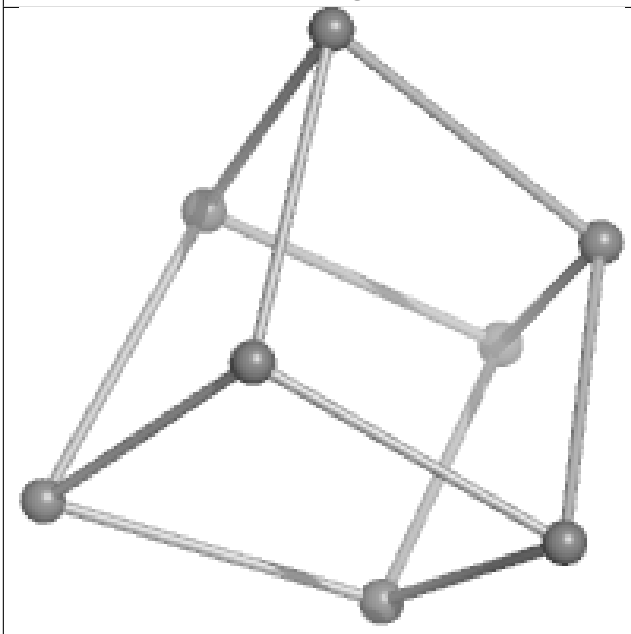
Ligand SF4 c 202



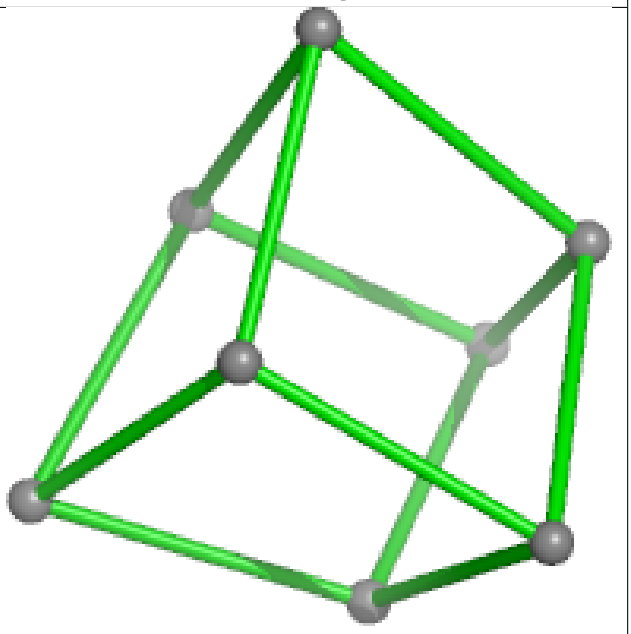
Bond lengths



Bond angles

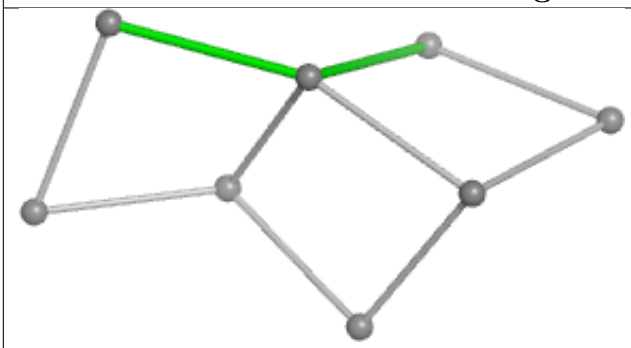


Torsions

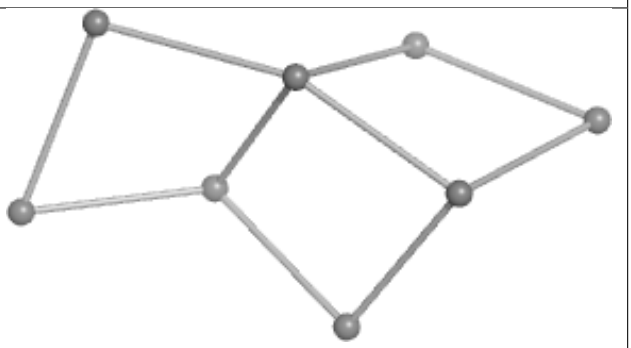


Rings

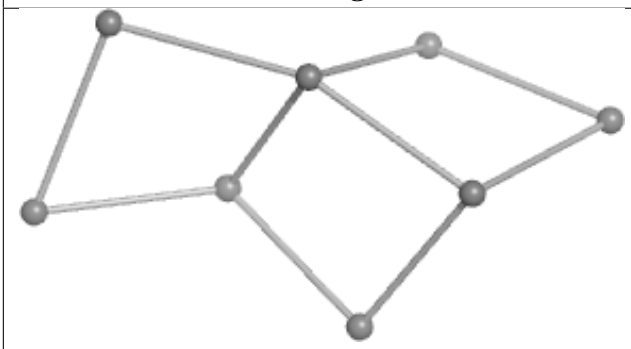
Ligand 9S8 B 402



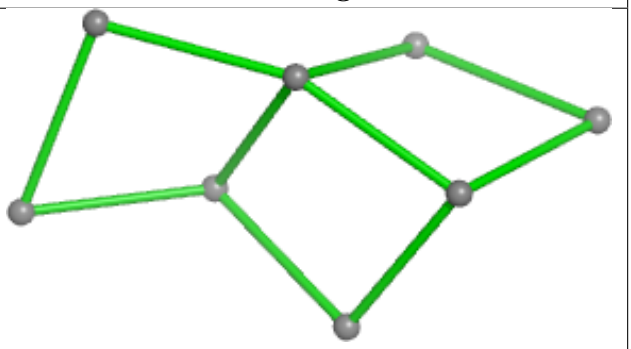
Bond lengths



Bond angles

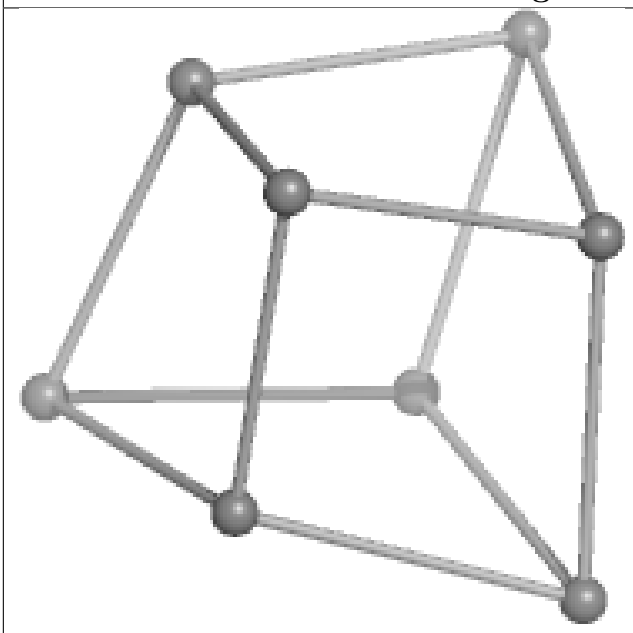


Torsions

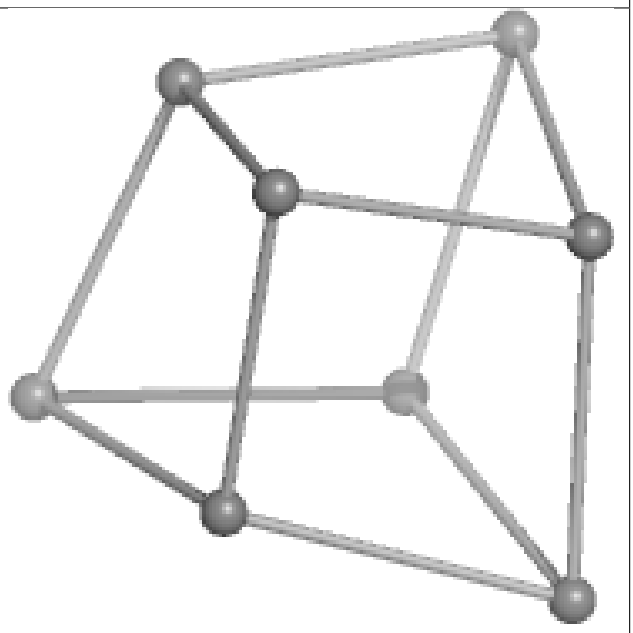


Rings

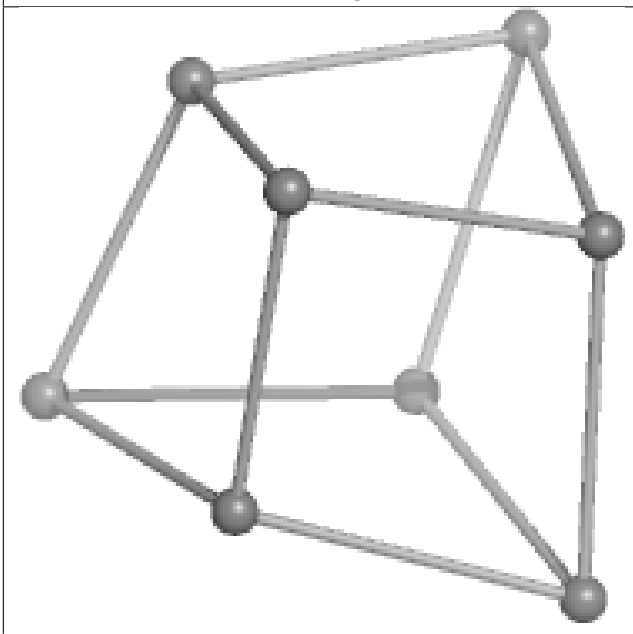
Ligand SF4 E 404



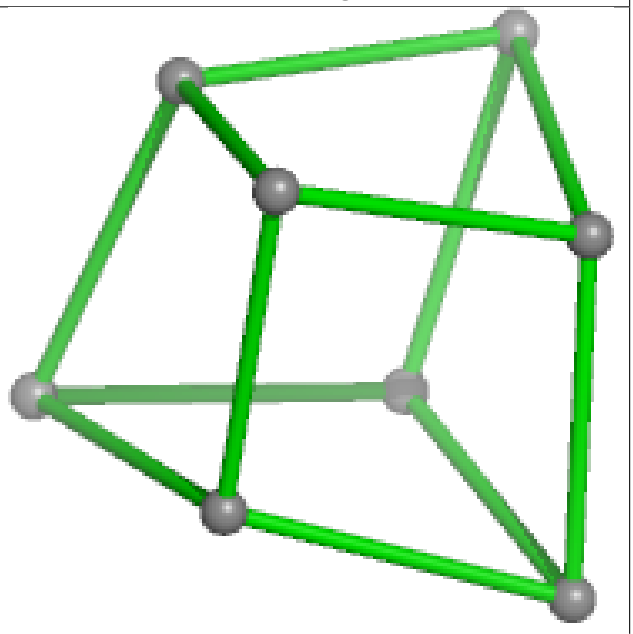
Bond lengths



Bond angles

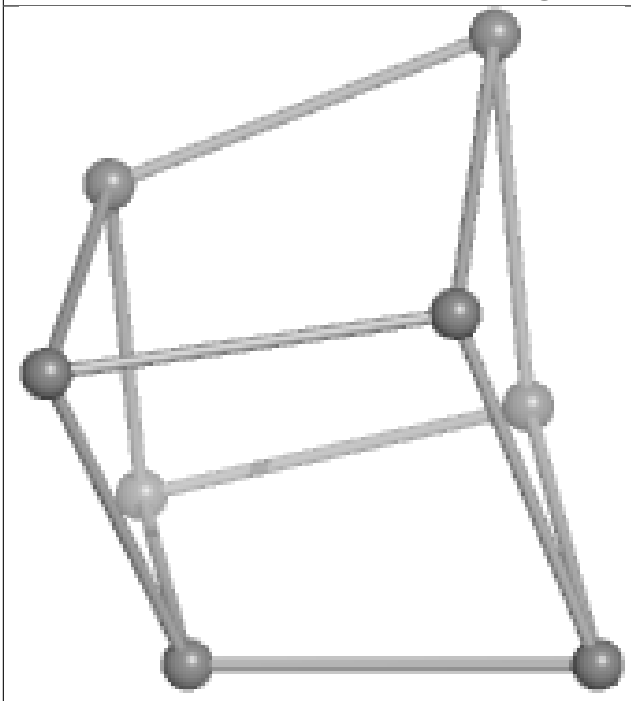


Torsions

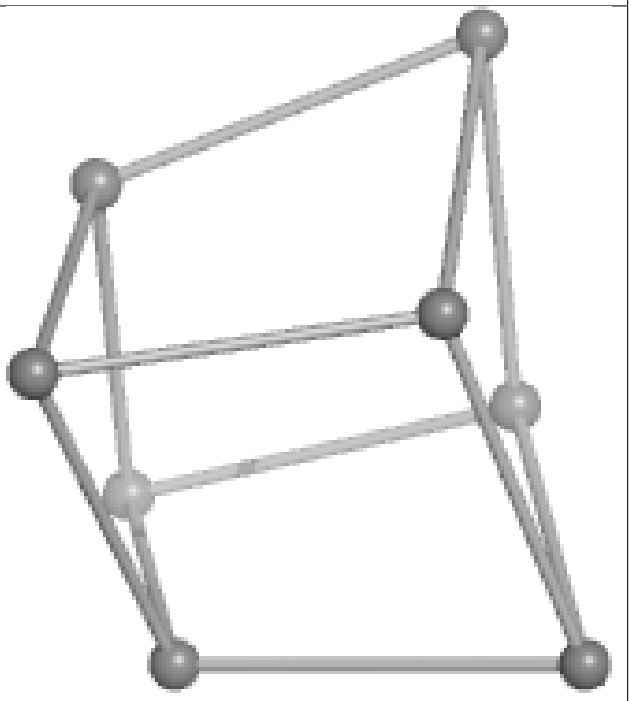


Rings

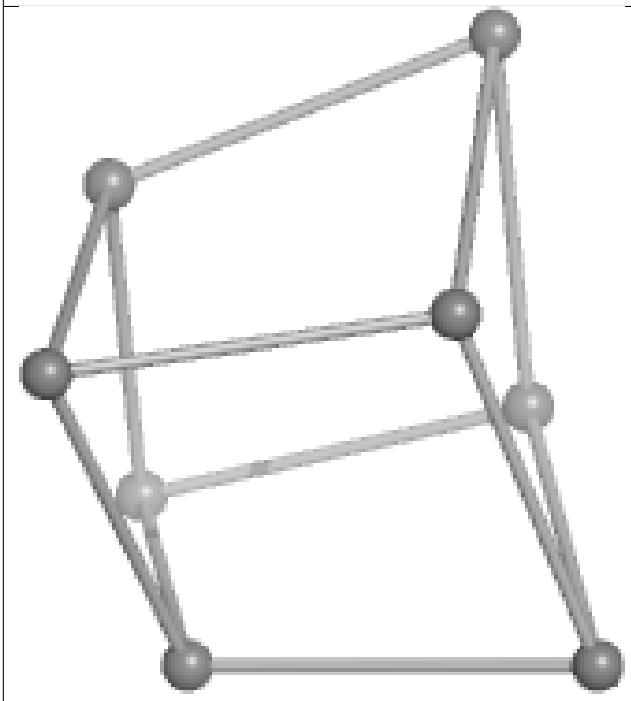
Ligand SF4 a 703



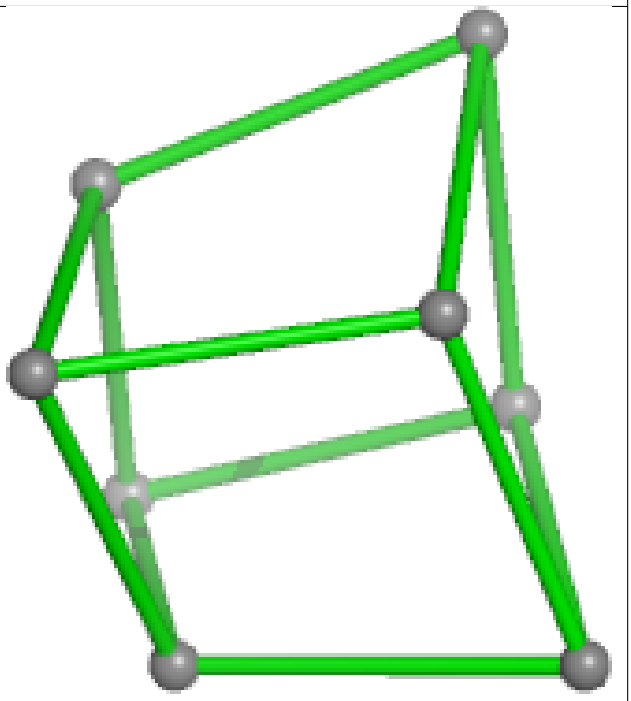
Bond lengths



Bond angles

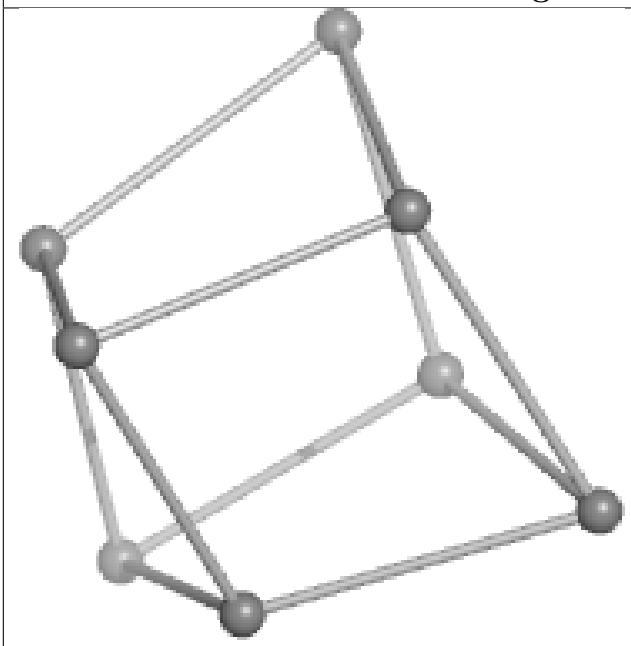


Torsions

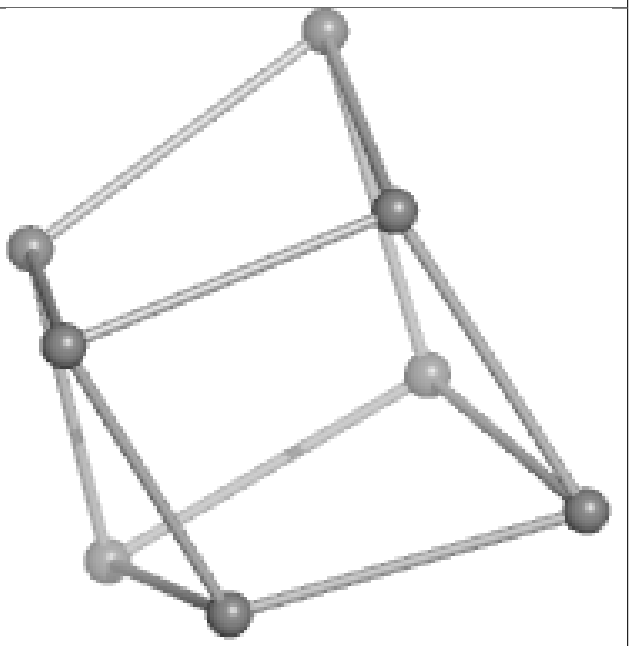


Rings

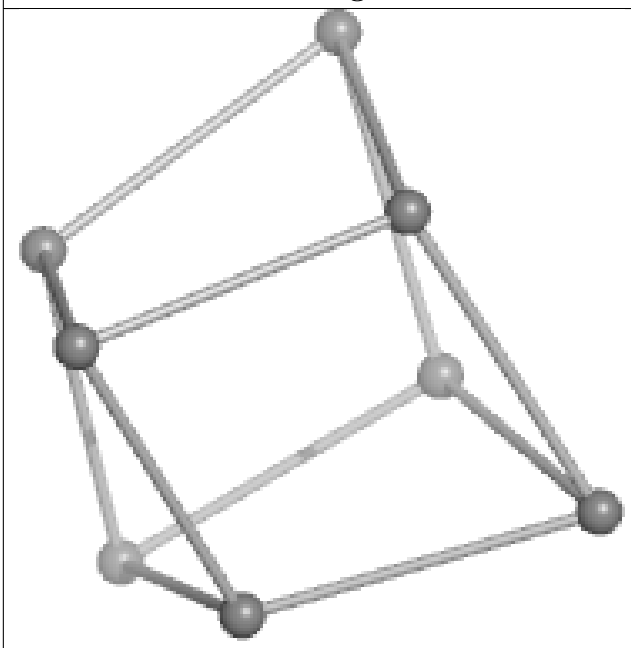
Ligand SF4 E 402



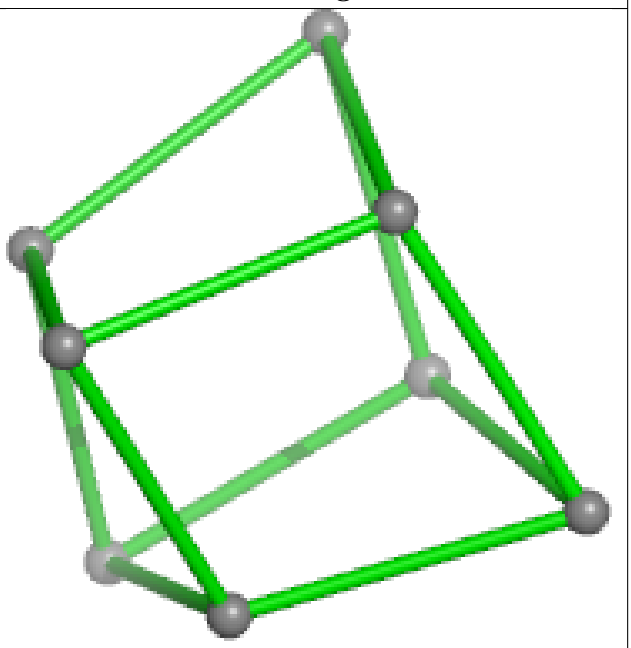
Bond lengths



Bond angles

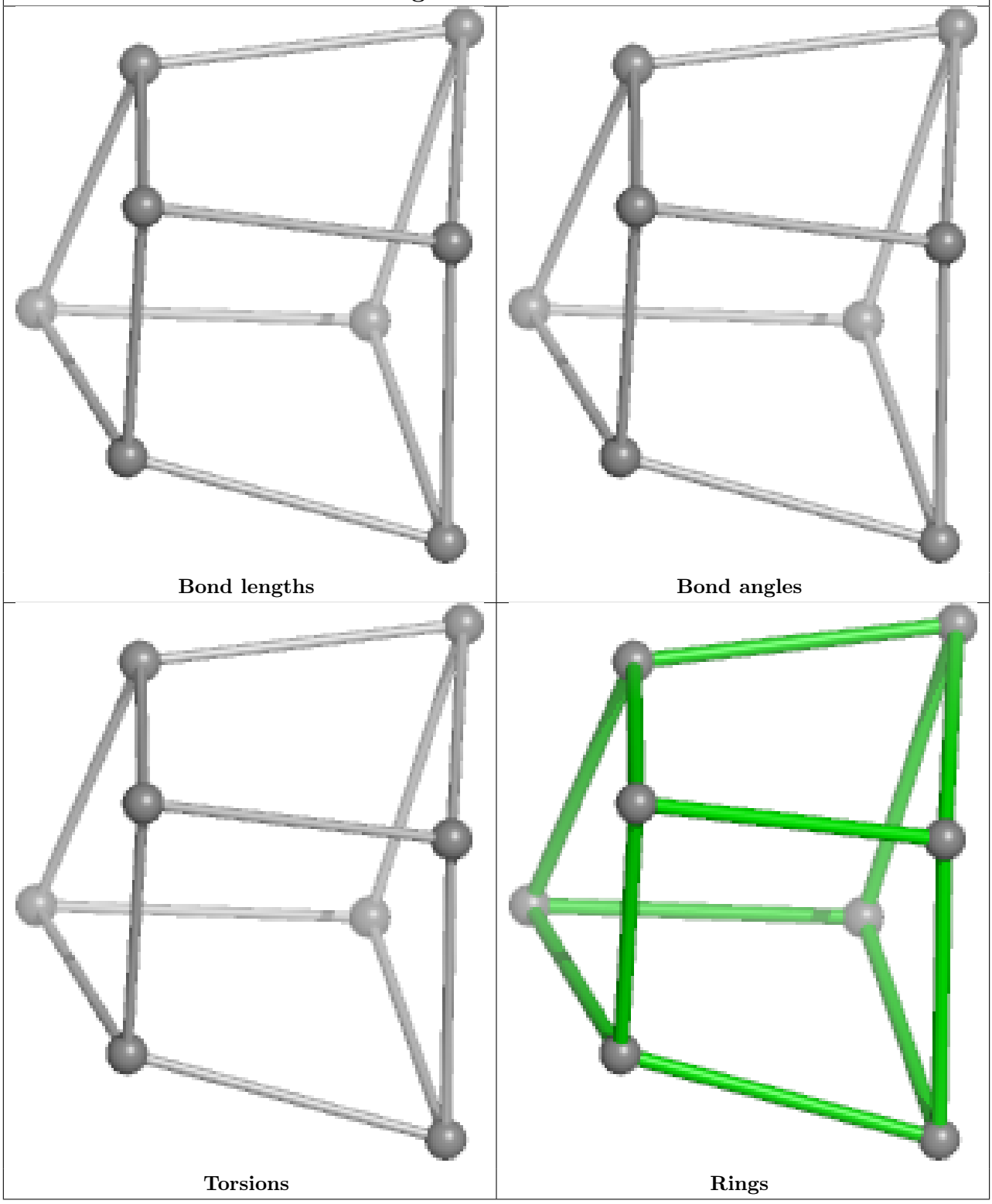


Torsions



Rings

Ligand SF4 C 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

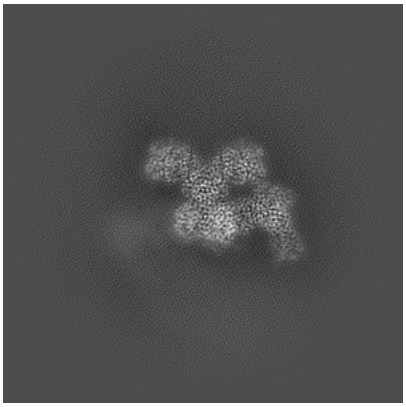
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19538. These allow visual inspection of the internal detail of the map and identification of artifacts.

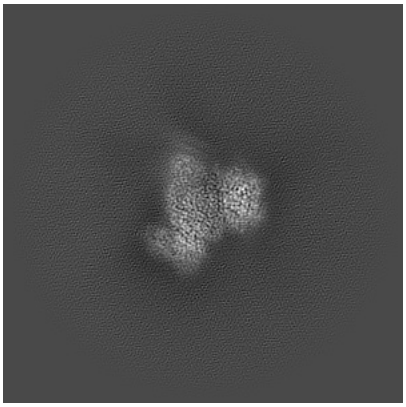
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

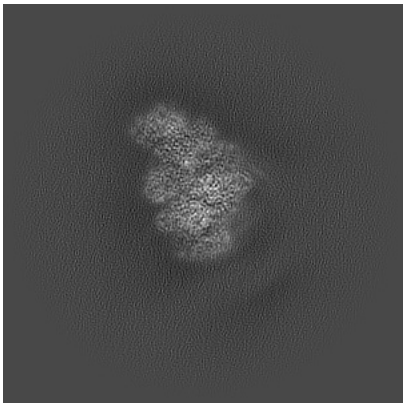
6.1.1 Primary map



X



Y

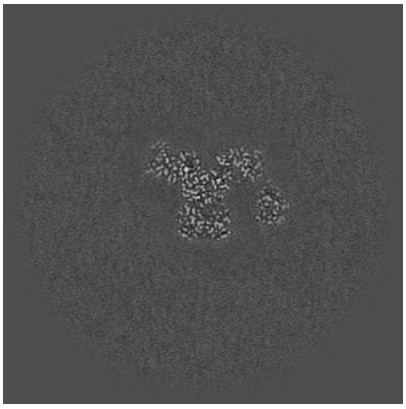


Z

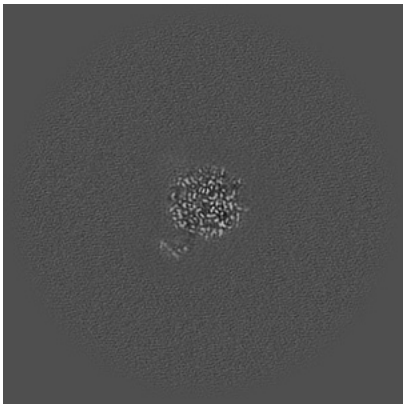
The images above show the map projected in three orthogonal directions.

6.2 Central slices

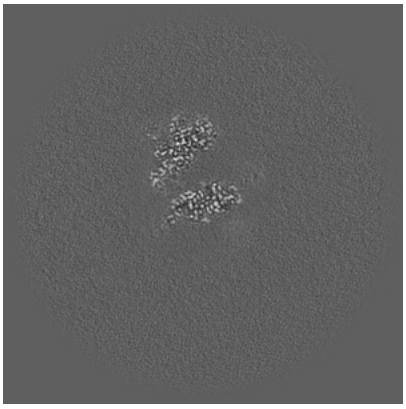
6.2.1 Primary map



X Index: 224



Y Index: 224

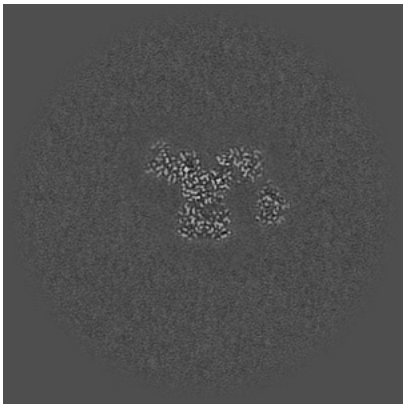


Z Index: 224

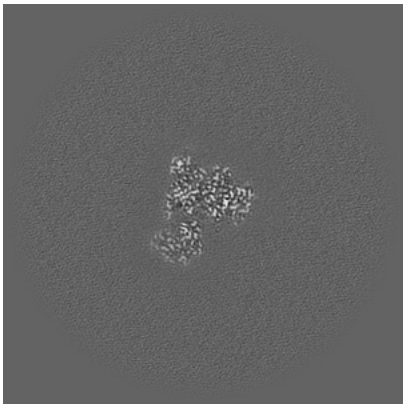
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

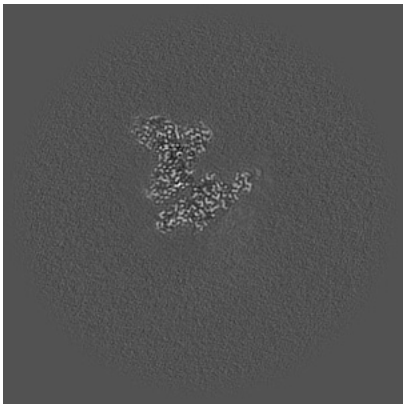
6.3.1 Primary map



X Index: 224



Y Index: 240

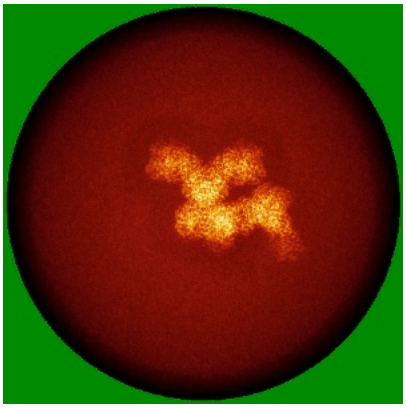


Z Index: 208

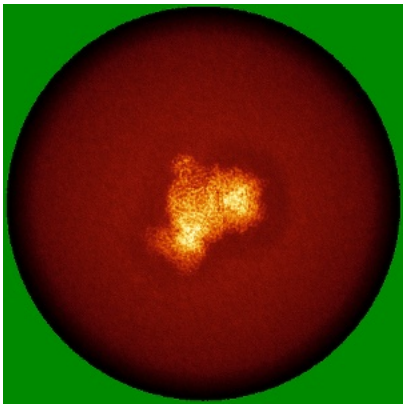
The images above show the largest variance slices of the map in three orthogonal directions.

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

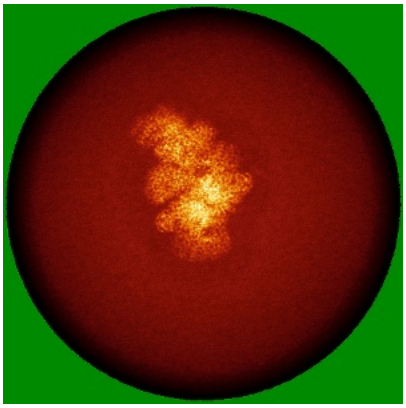
6.4.1 Primary map



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

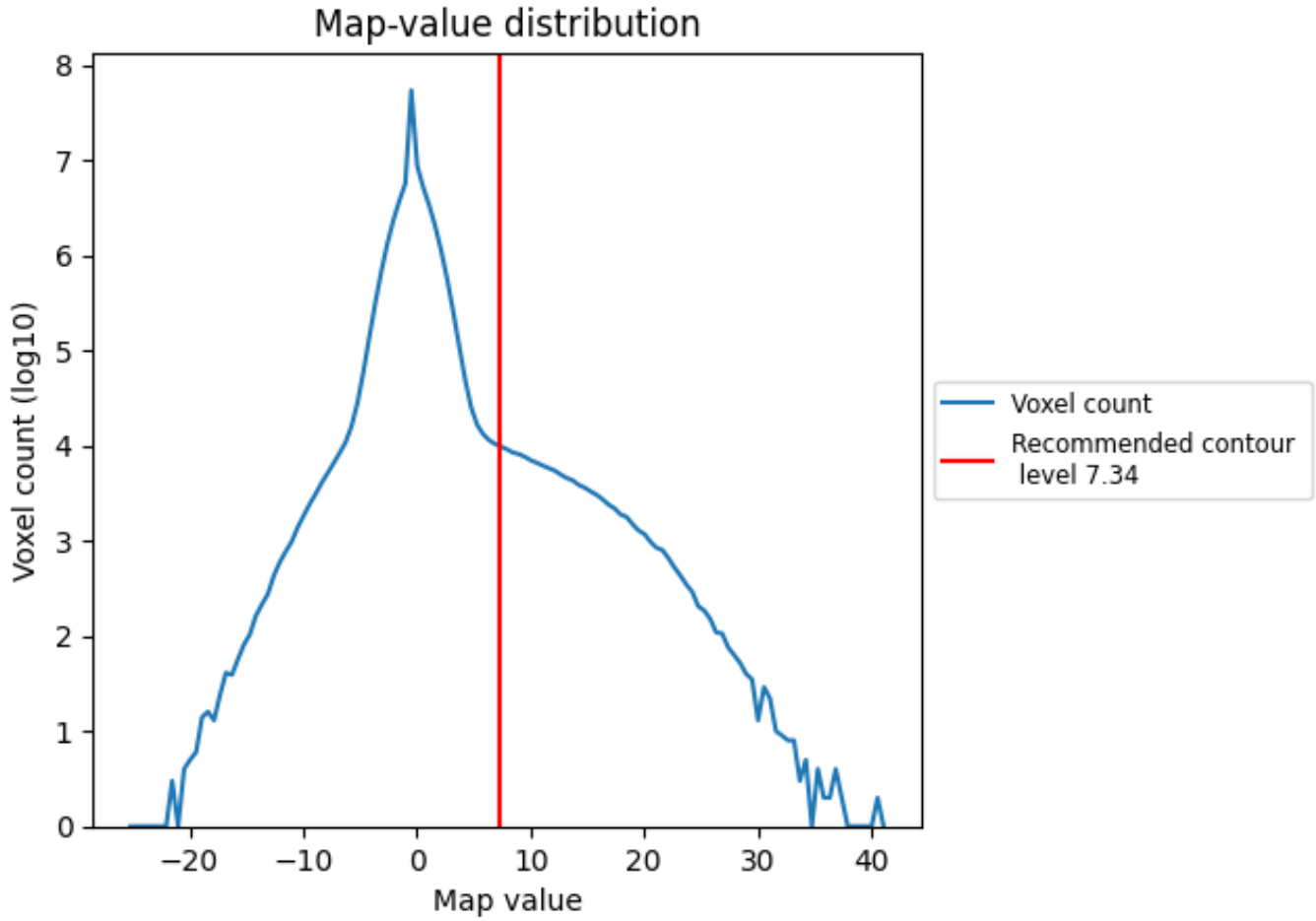
6.6 Mask visualisation (i)

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

7 Map analysis

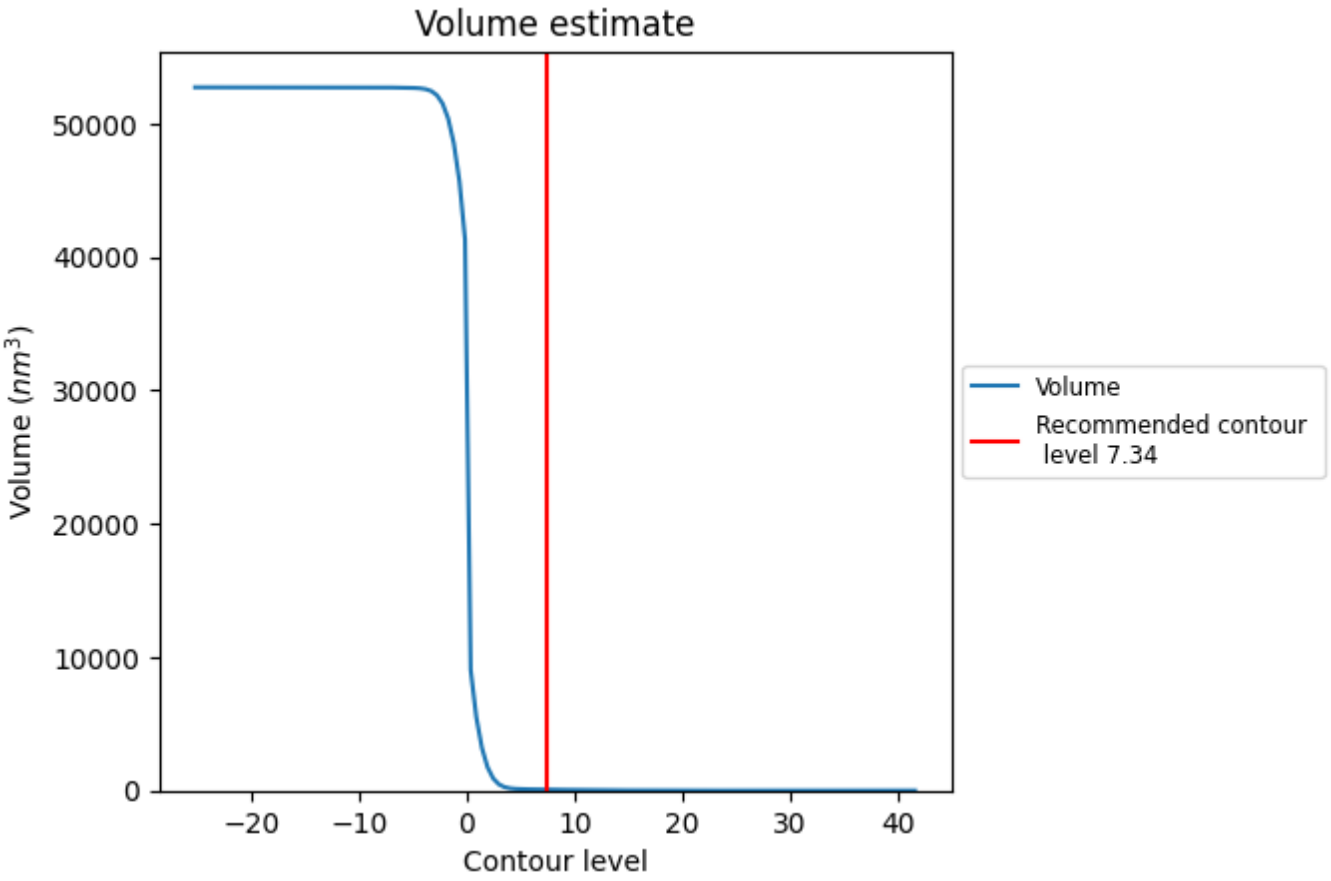
This section contains the results of statistical analysis of the map.

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.

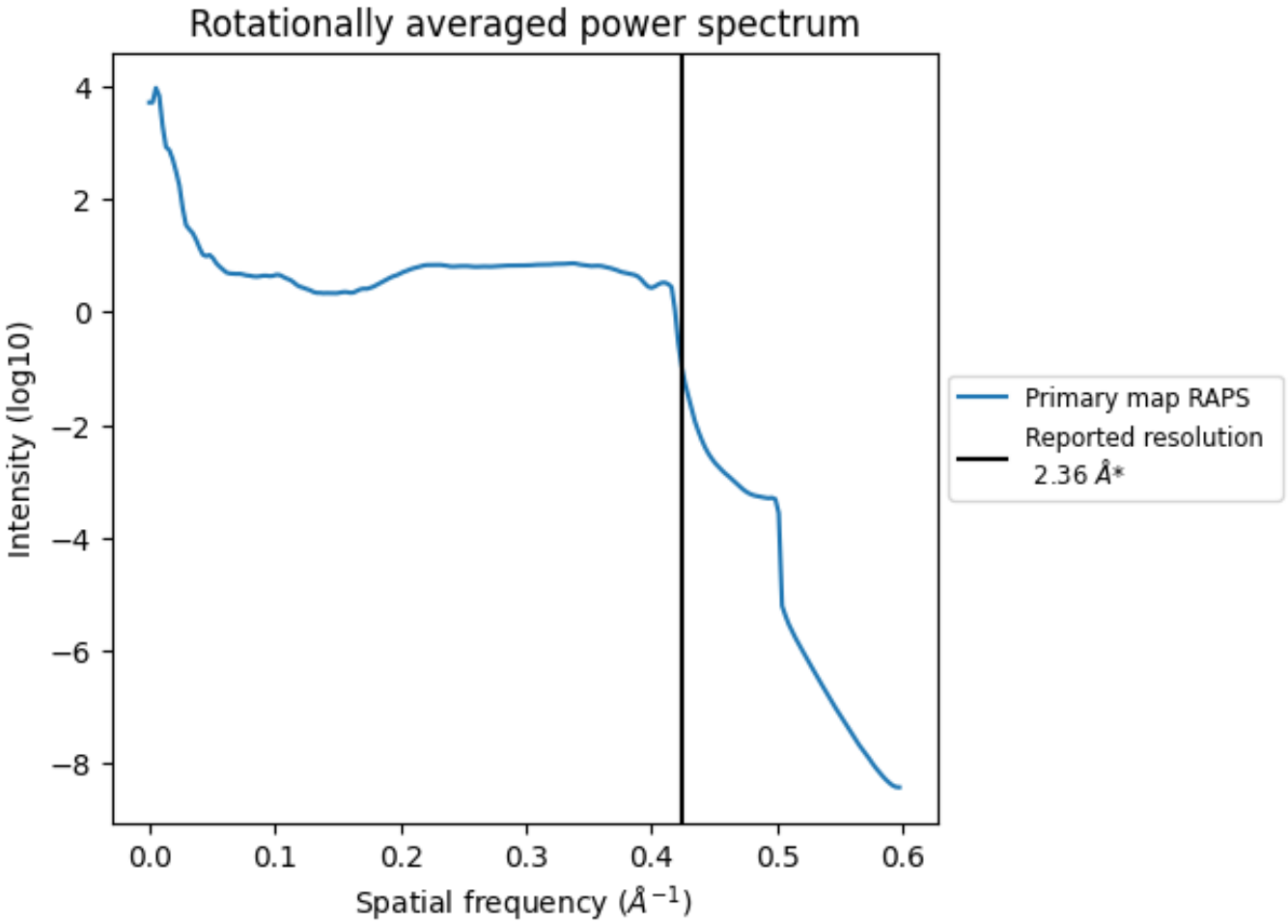
7.2 Volume estimate



The volume at the recommended contour level is 73 nm^3; this corresponds to an approximate mass of 66 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 0.424 Å^{-1}

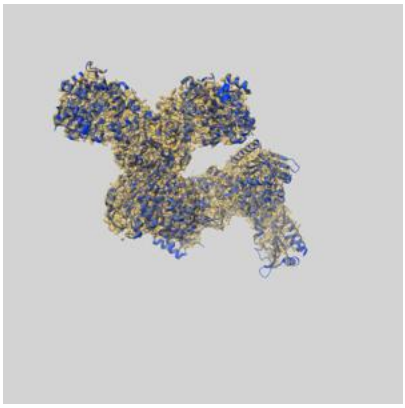
8 Fourier-Shell correlation (i)

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

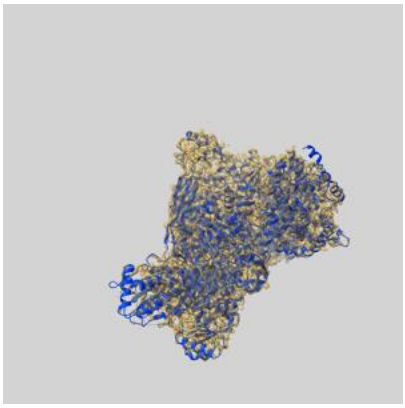
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19538 and PDB model 8RVY. Per-residue inclusion information can be found in section 3 on page 9.

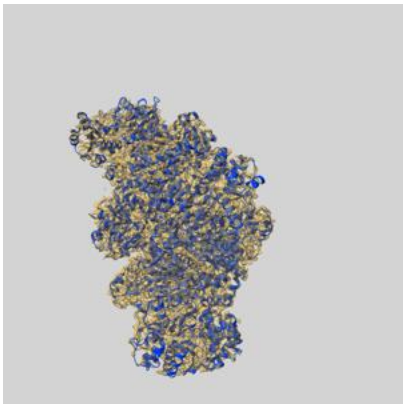
9.1 Map-model overlay



X



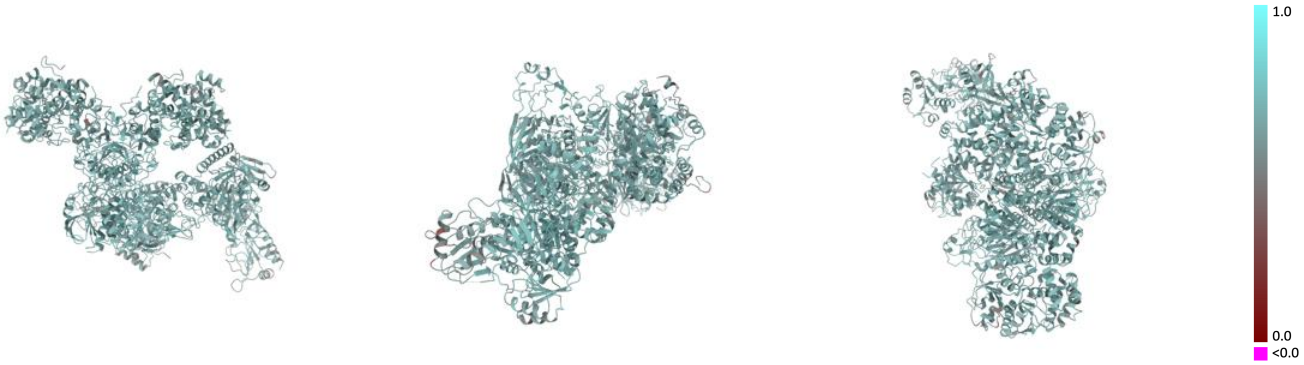
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.34 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.

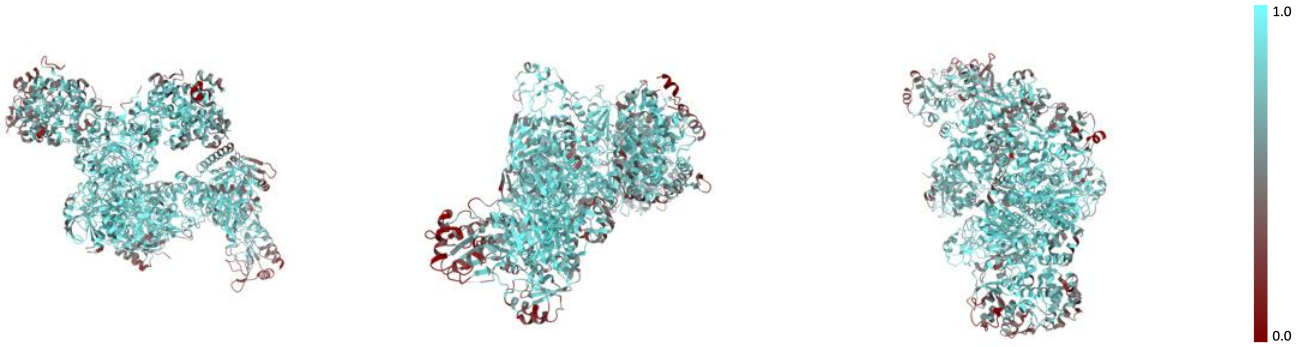
9.2 Q-score mapped to coordinate model (i)



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.

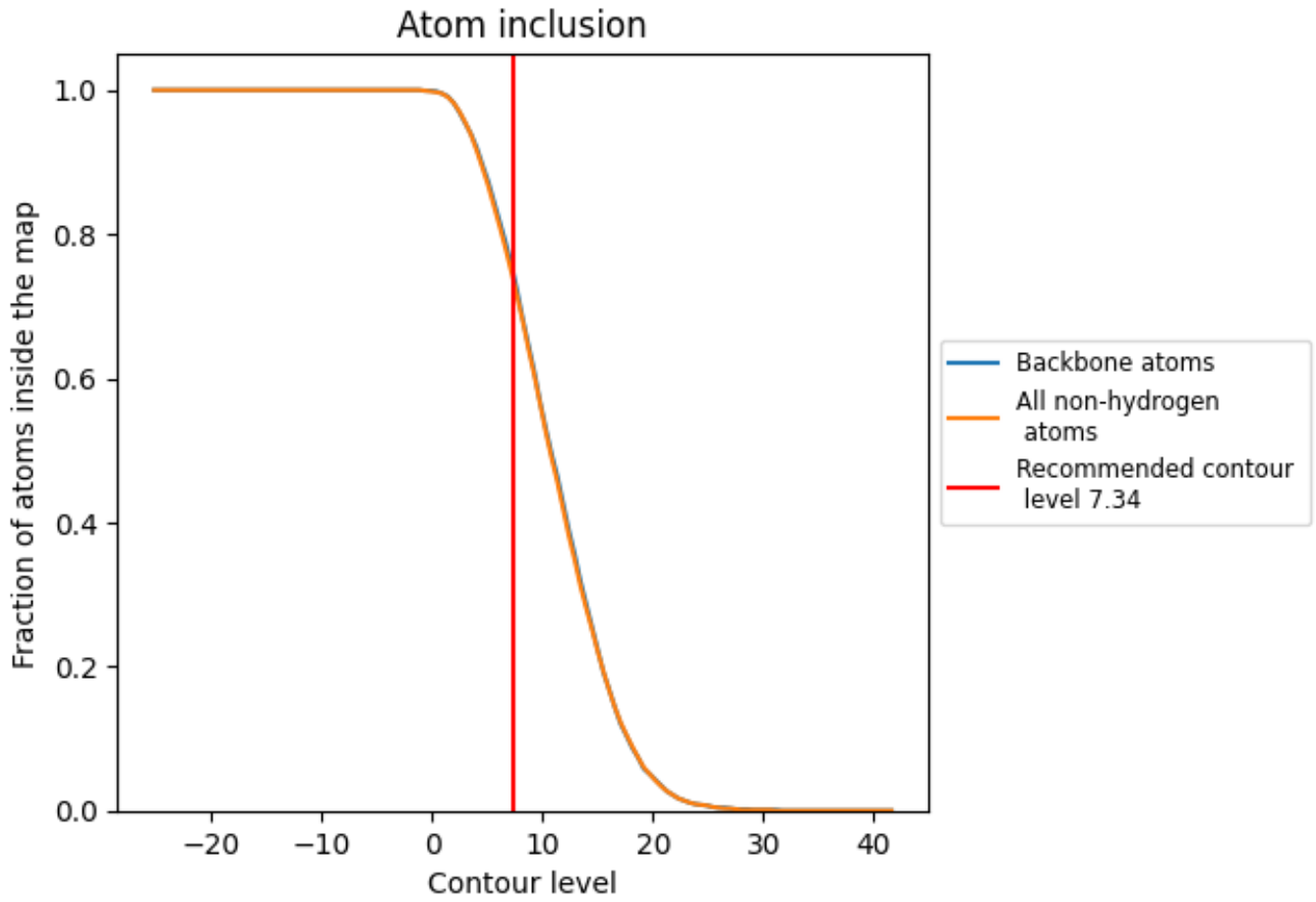
9.3 Atom inclusion mapped to coordinate model (i)



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 (7.34).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 74% 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 (7.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7360	0.6480
A	0.7920	0.6540
B	0.6230	0.6300
C	0.7020	0.6400
D	0.5940	0.6220
E	0.7680	0.6520
F	0.8700	0.6790
a	0.8460	0.6670
b	0.6940	0.6400
c	0.7480	0.6450

