wwPDB EM Validation Summary Report (i)

Aug 23, 2026 – 10:34 am BST

PDB ID	:	6TGA / pdb_00006tga
EMDB ID	:	EMD-10496
Title	:	Cryo-EM Structure of as isolated form of NAD+-dependent Formate Dehydrogenase from Rhodobacter capsulatus
Authors	:	Wendler, P.; Radon, C.; Mittelstaedt, G.
Deposited on	:	2019-11-15
Resolution	:	3.26 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:

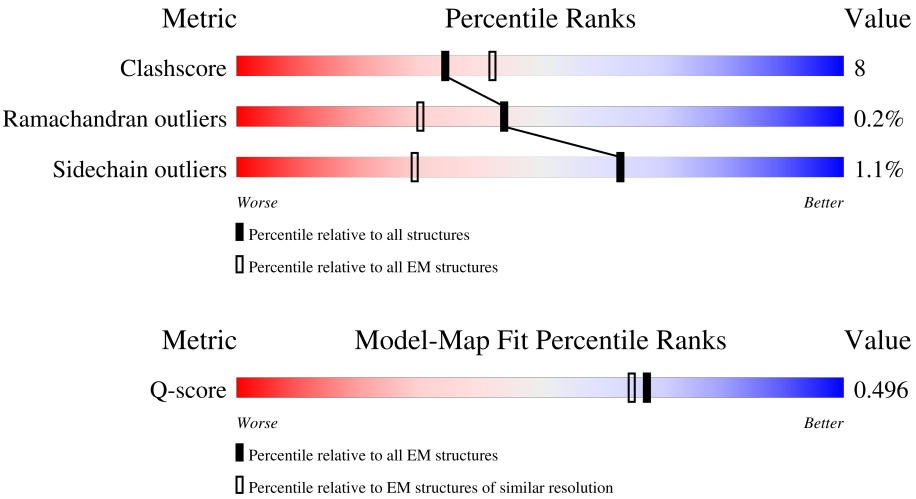
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.26 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	14557 (2.76 - 3.76)

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	958	81% 17%
1	E	958	81% 18%
2	B	500	6% 83% 16%
2	F	500	6% 82% 17%

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Mol	Chain	Length	Quality of chain
3	C	150	6% 83% 15%
3	G	150	6% 81% 17%
4	D	71	8% 80% 15%
4	H	71	8% 77% 18%

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
8	SF4	A	1007	-	-	X	-
8	SF4	E	1007	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 25324 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 Formate dehydrogenase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	949	Total	C	N	O	S	0	0
			7261	4518	1316	1378	49		
1	E	949	Total	C	N	O	S	0	0
			7261	4518	1316	1378	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	493	Total	C	N	O	S	0	0
			3645	2318	636	663	28		
2	F	493	Total	C	N	O	S	0	0
			3645	2318	636	663	28		

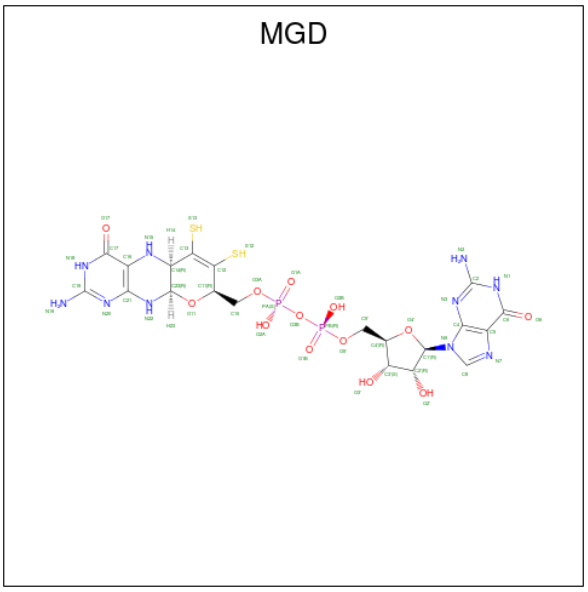
- Molecule 3 is a protein called Formate dehydrogenase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	148	Total	C	N	O	S	0	0
			1076	674	197	197	8		
3	C	148	Total	C	N	O	S	0	0
			1076	674	197	197	8		

- Molecule 4 is a protein called NAD-dependent formate dehydrogenase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	69	Total	C	N	O	S	0	0
			505	321	93	89	2		
4	H	69	Total	C	N	O	S	0	0
			505	321	93	89	2		

- Molecule 5 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).

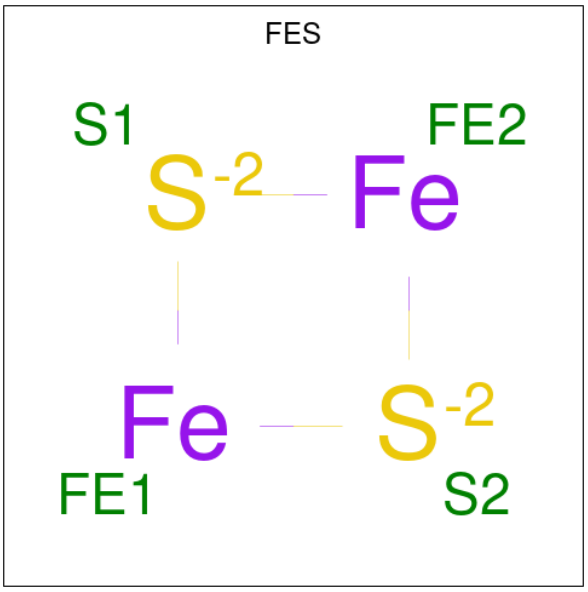


Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
5	A	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
5	E	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
5	E	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	

- Molecule 6 is MOLYBDENUM(VI) ION (CCD ID: 6MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

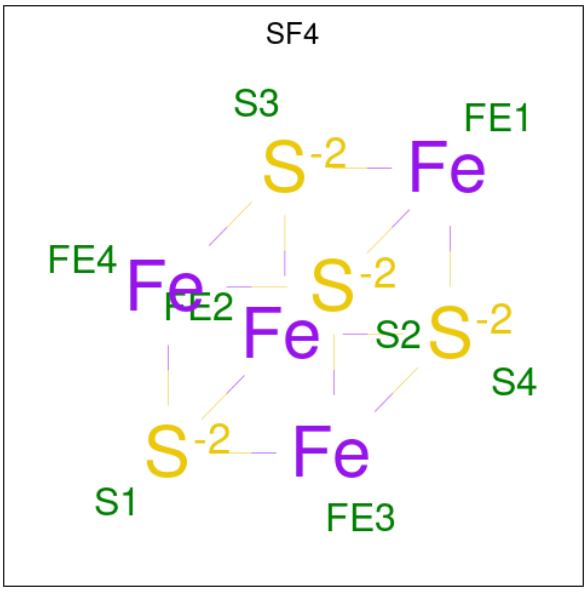
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mo	0
			1	1	
6	E	1	Total	Mo	0
			1	1	

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



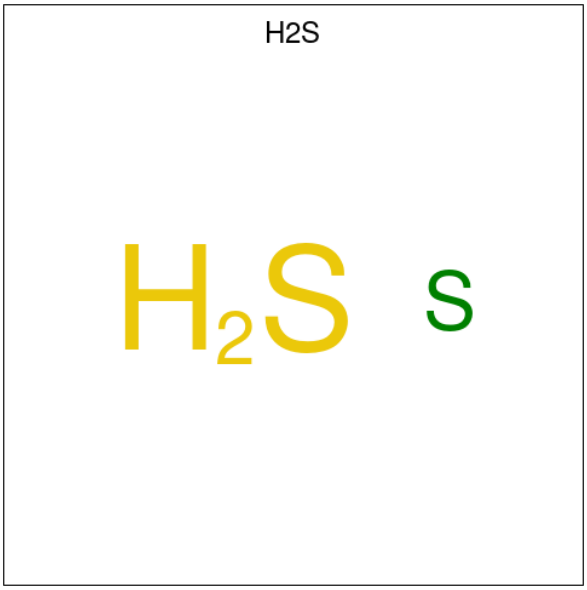
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total Fe S 4 2 2	0
7	G	1	Total Fe S 4 2 2	0
7	E	1	Total Fe S 4 2 2	0
7	C	1	Total Fe S 4 2 2	0

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H_2S) (labeled as "Ligand of Interest" by depositor).



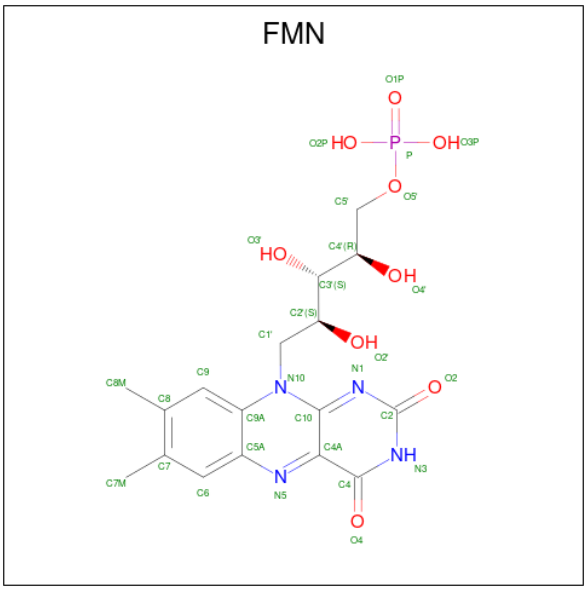
Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total S 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
9	E	1	Total S 1 1	0

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



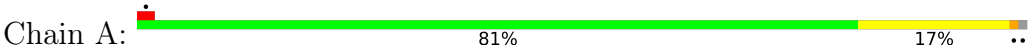
Mol	Chain	Residues	Atoms	AltConf
10	B	1	Total C N O P 31 17 4 9 1	0
10	F	1	Total C N O P 31 17 4 9 1	0

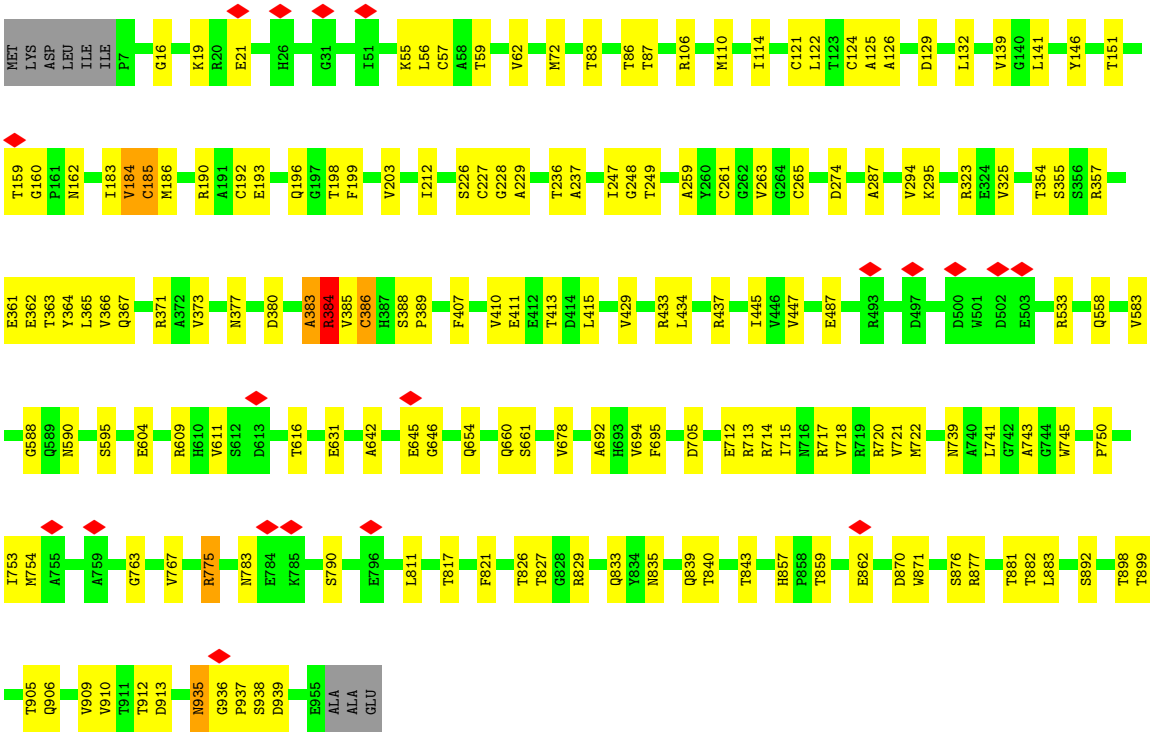
3 Residue-property plots (i)

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: Formate dehydrogenase subunit alpha

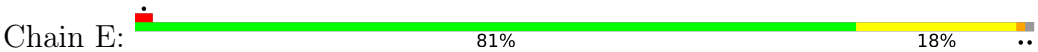
Chain A:

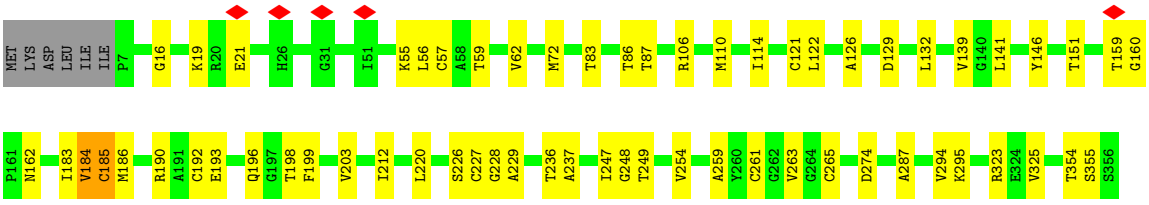


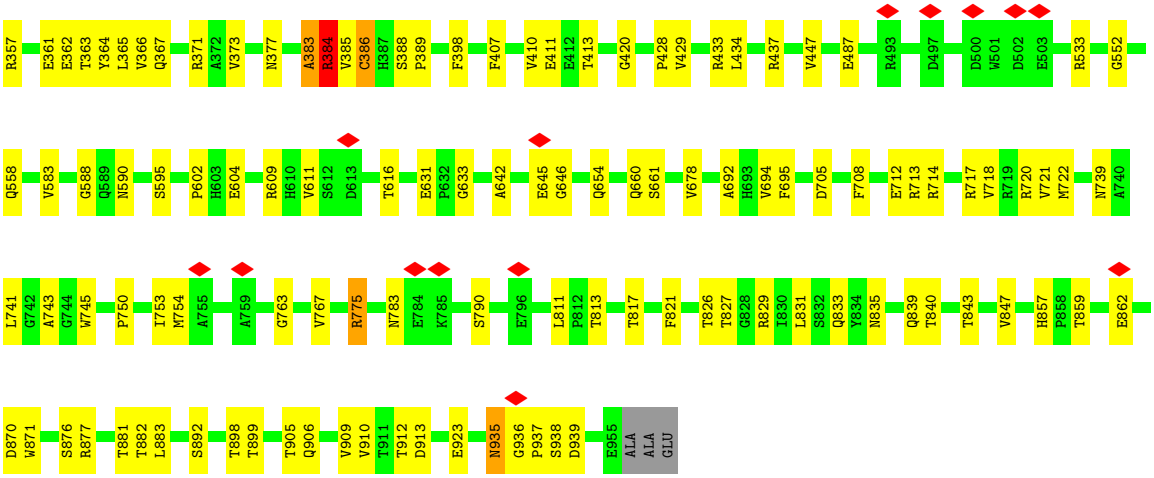


• Molecule 1: Formate dehydrogenase subunit alpha

Chain E:



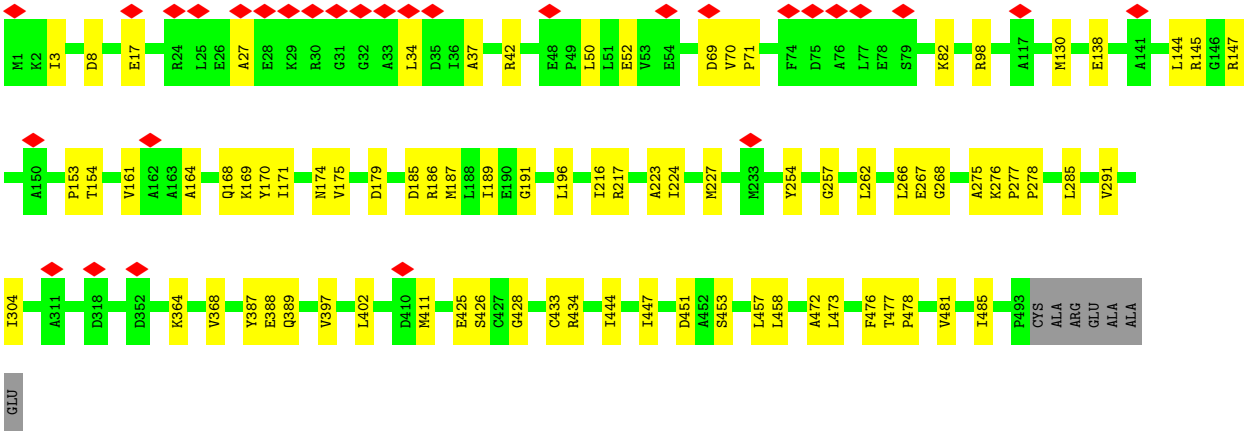




• Molecule 2: Formate dehydrogenase subunit beta

Chain B:

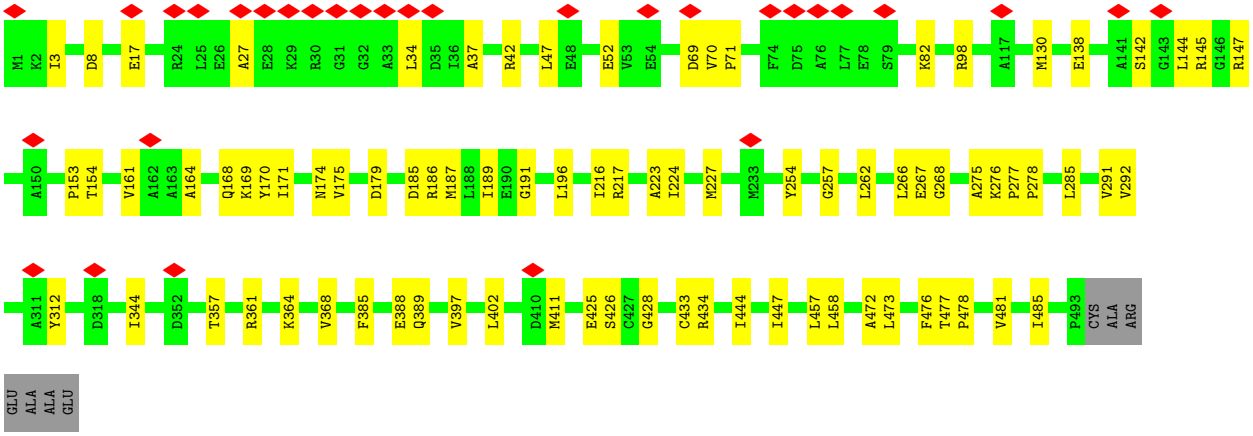




• Molecule 2: Formate dehydrogenase subunit beta

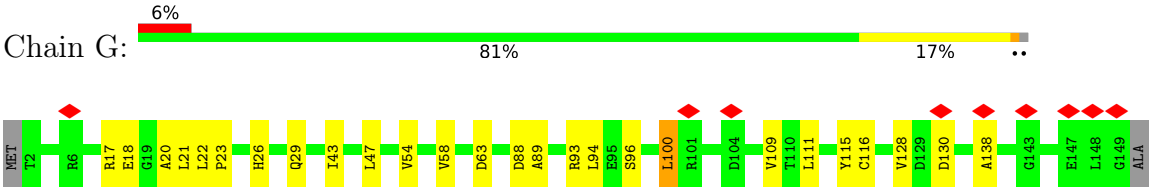
Chain F:





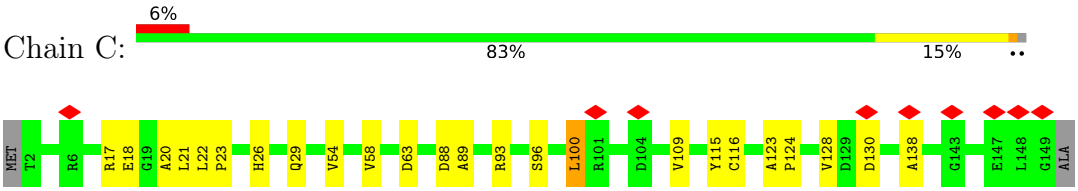
• Molecule 3: Formate dehydrogenase subunit gamma

Chain G:



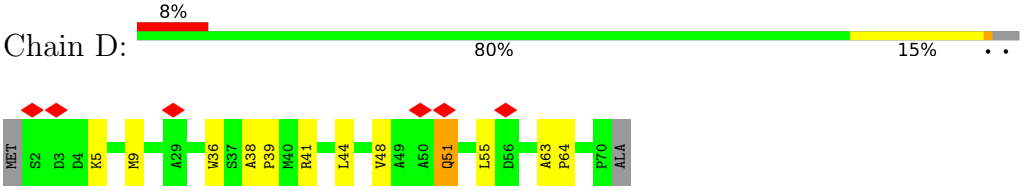
• Molecule 3: Formate dehydrogenase subunit gamma

Chain C:



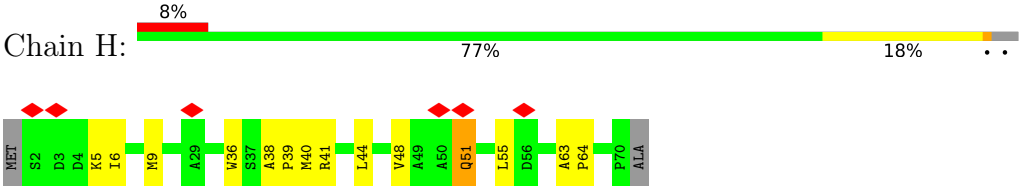
• Molecule 4: NAD-dependent formate dehydrogenase subunit delta

Chain D:



• Molecule 4: NAD-dependent formate dehydrogenase subunit delta

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	366558	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND4 was used to estimate contrast transfer function parameters. CTF correction was done in Relion 3.0.	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.163	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0112	Depositor
Map size (Å)	241.15201, 241.15201, 241.15201	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.628, 0.628, 0.628	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, SF4, FES, H2S, 6MO, MGD

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	0.39	0/7426	0.69	5/10113 (0.0%)
1	E	0.39	0/7426	0.69	5/10113 (0.0%)
2	B	0.38	0/3724	0.68	2/5045 (0.0%)
2	F	0.37	0/3724	0.67	2/5045 (0.0%)
3	C	0.39	0/1091	0.69	0/1479
3	G	0.39	0/1091	0.69	0/1479
4	D	0.39	0/518	0.66	0/710
4	H	0.39	0/518	0.65	0/710
All	All	0.39	0/25518	0.69	14/34694 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	276	LYS	CA-C-N	-6.39	113.80	120.38
2	B	276	LYS	C-N-CA	-6.39	113.80	120.38
2	F	276	LYS	CA-C-N	-6.36	113.83	120.38
2	F	276	LYS	C-N-CA	-6.36	113.83	120.38
1	E	383	ALA	CA-C-N	5.85	132.71	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7261	0	7057	125	0
1	E	7261	0	7057	131	0
2	B	3645	0	3659	54	0
2	F	3645	0	3659	56	0
3	C	1076	0	1084	14	0
3	G	1076	0	1084	15	0
4	D	505	0	510	10	0
4	H	505	0	510	11	0
5	A	94	0	42	11	0
5	E	94	0	42	11	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	A	4	0	0	0	0
7	C	4	0	0	0	0
7	E	4	0	0	0	0
7	G	4	0	0	0	0
8	A	32	0	0	3	0
8	B	8	0	0	1	0
8	E	32	0	0	3	0
8	F	8	0	0	1	0
9	A	1	0	0	0	0
9	E	1	0	0	0	0
10	B	31	0	19	0	0
10	F	31	0	19	1	0
All	All	25324	0	24742	404	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 8.

The worst 5 of 404 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:THR:HG21	1:A:363:THR:HG23	1.35	1.08
1:E:354:THR:HG21	1:E:363:THR:HG23	1.35	1.06
2:F:145:ARG:HA	2:F:153:PRO:HA	1.49	0.91
1:A:882:THR:OG1	1:A:937:PRO:O	1.91	0.89
1:E:882:THR:OG1	1:E:937:PRO:O	1.91	0.88

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	947/958 (99%)	891 (94%)	53 (6%)	3 (0%)	36	66
1	E	947/958 (99%)	891 (94%)	53 (6%)	3 (0%)	36	66
2	B	491/500 (98%)	465 (95%)	26 (5%)	0	100	100
2	F	491/500 (98%)	465 (95%)	26 (5%)	0	100	100
3	C	146/150 (97%)	136 (93%)	10 (7%)	0	100	100
3	G	146/150 (97%)	136 (93%)	10 (7%)	0	100	100
4	D	67/71 (94%)	66 (98%)	1 (2%)	0	100	100
4	H	67/71 (94%)	66 (98%)	1 (2%)	0	100	100
All	All	3302/3358 (98%)	3116 (94%)	180 (6%)	6 (0%)	44	70

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	CYS
1	A	384	ARG
1	E	185	CYS
1	E	384	ARG
1	A	184	VAL

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	765/772 (99%)	756 (99%)	9 (1%)	63	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	765/772 (99%)	756 (99%)	9 (1%)	63 74
2	B	363/367 (99%)	362 (100%)	1 (0%)	86 86
2	F	363/367 (99%)	361 (99%)	2 (1%)	78 81
3	C	102/103 (99%)	99 (97%)	3 (3%)	37 60
3	G	102/103 (99%)	99 (97%)	3 (3%)	37 60
4	D	50/51 (98%)	49 (98%)	1 (2%)	48 66
4	H	50/51 (98%)	49 (98%)	1 (2%)	48 66
All	All	2560/2586 (99%)	2531 (99%)	29 (1%)	63 75

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	19	LYS
3	C	130	ASP
1	E	274	ASP
2	F	142	SER
1	E	226	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	270	HIS
3	C	91	GLN
1	E	473	ASN
2	F	382	HIS
1	E	387	HIS

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 24 ligands modelled in this entry, 2 are monoatomic and 2 are modelled with single atom - leaving 20 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	$\#\|Z\| > 2$
8	SF4	E	1005	1	0,12,12	-	-	-		
5	MGD	A	1001	6	45,52,52	4.42	24 (53%)	54,81,81	2.29	15 (27%)
5	MGD	A	1002	6	45,52,52	4.43	26 (57%)	54,81,81	2.13	13 (24%)
8	SF4	E	1007	1	0,12,12	-	-	-		
8	SF4	F	602	2	0,12,12	-	-	-		
7	FES	A	1004	1	0,4,4	-	-	-		
8	SF4	E	1006	1	0,12,12	-	-	-		
10	FMN	B	601	-	33,33,33	2.08	5 (15%)	48,50,50	1.25	6 (12%)
7	FES	E	1004	1	0,4,4	-	-	-		
8	SF4	A	1005	1	0,12,12	-	-	-		
8	SF4	A	1007	1	0,12,12	-	-	-		
8	SF4	E	1008	1	0,12,12	-	-	-		
8	SF4	A	1006	1	0,12,12	-	-	-		
7	FES	G	201	3	0,4,4	-	-	-		
5	MGD	E	1002	6	45,52,52	4.43	26 (57%)	54,81,81	2.13	13 (24%)
8	SF4	B	602	2	0,12,12	-	-	-		
5	MGD	E	1001	6	45,52,52	4.42	24 (53%)	54,81,81	2.29	15 (27%)
10	FMN	F	601	-	33,33,33	2.08	5 (15%)	48,50,50	1.26	6 (12%)
7	FES	C	201	3	0,4,4	-	-	-		
8	SF4	A	1008	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
8	SF4	E	1005	1	-	-	0/6/5/5
5	MGD	A	1001	6	-	4/22/66/66	0/6/6/6
5	MGD	A	1002	6	-	12/22/66/66	0/6/6/6
8	SF4	E	1007	1	-	-	0/6/5/5
8	SF4	F	602	2	-	-	0/6/5/5
7	FES	A	1004	1	-	-	0/1/1/1
8	SF4	E	1006	1	-	-	0/6/5/5
10	FMN	B	601	-	-	7/18/18/18	0/3/3/3
7	FES	E	1004	1	-	-	0/1/1/1
8	SF4	A	1005	1	-	-	0/6/5/5
8	SF4	A	1007	1	-	-	0/6/5/5
8	SF4	E	1008	1	-	-	0/6/5/5
8	SF4	A	1006	1	-	-	0/6/5/5
7	FES	G	201	3	-	-	0/1/1/1
5	MGD	E	1002	6	-	12/22/66/66	0/6/6/6
8	SF4	B	602	2	-	-	0/6/5/5
5	MGD	E	1001	6	-	4/22/66/66	0/6/6/6
10	FMN	F	601	-	-	7/18/18/18	0/3/3/3
7	FES	C	201	3	-	-	0/1/1/1
8	SF4	A	1008	1	-	-	0/6/5/5

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1002	MGD	C21-N20	11.11	1.52	1.36
5	E	1002	MGD	C21-N20	11.11	1.52	1.36
5	A	1001	MGD	C21-N20	10.91	1.52	1.36
5	E	1001	MGD	C21-N20	10.82	1.52	1.36
5	A	1001	MGD	C23-C14	10.12	1.61	1.53

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1001	MGD	O11-C23-N22	6.18	114.92	108.57
5	E	1001	MGD	O11-C23-N22	6.10	114.84	108.57
5	E	1001	MGD	O4'-C1'-N9	5.81	121.64	108.36
5	A	1001	MGD	O4'-C1'-N9	5.80	121.63	108.36
5	E	1001	MGD	C2-N3-C4	5.51	122.13	112.30

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	MGD	C5'-O5'-PB-O2B
5	A	1001	MGD	C5'-O5'-PB-O3B
5	A	1002	MGD	C5'-O5'-PB-O3B
5	A	1002	MGD	C10-O3A-PA-O1A
5	A	1002	MGD	O4'-C4'-C5'-O5'

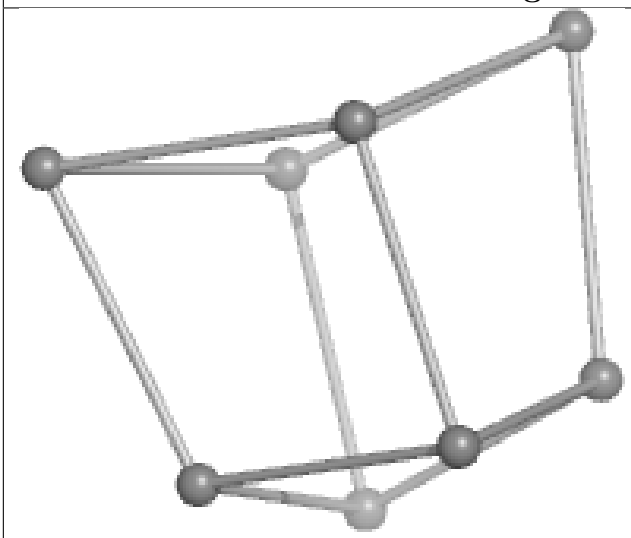
There are no ring outliers.

11 monomers are involved in 31 short contacts:

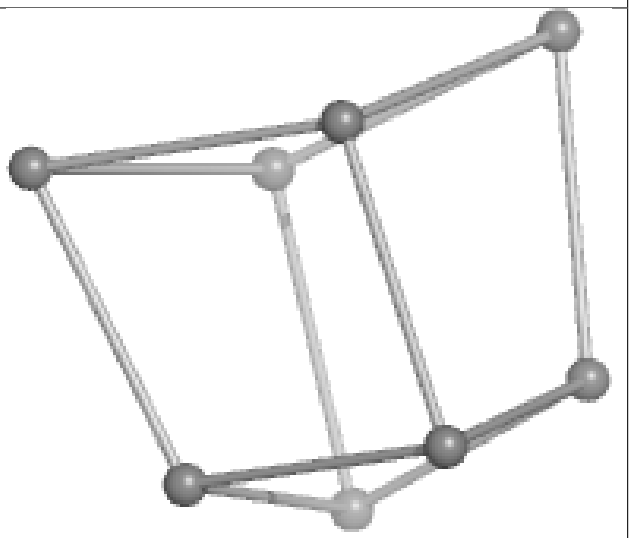
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	1005	SF4	1	0
5	A	1001	MGD	7	0
5	A	1002	MGD	4	0
8	E	1007	SF4	2	0
8	F	602	SF4	1	0
8	A	1005	SF4	1	0
8	A	1007	SF4	2	0
5	E	1002	MGD	4	0
8	B	602	SF4	1	0
5	E	1001	MGD	7	0
10	F	601	FMN	1	0

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.

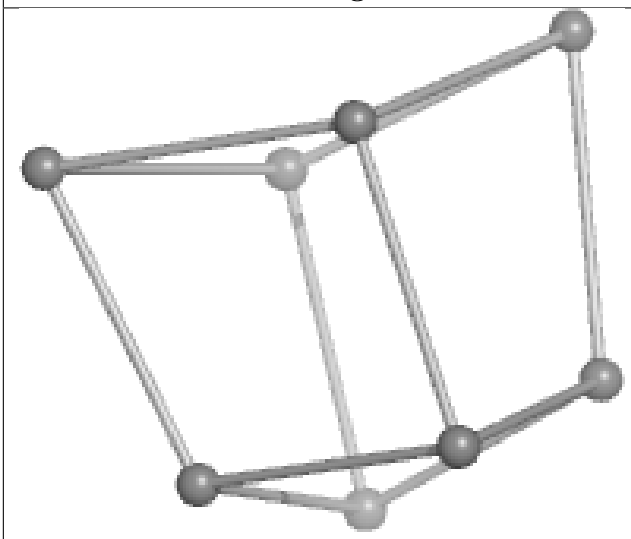
Ligand SF4 E 1005



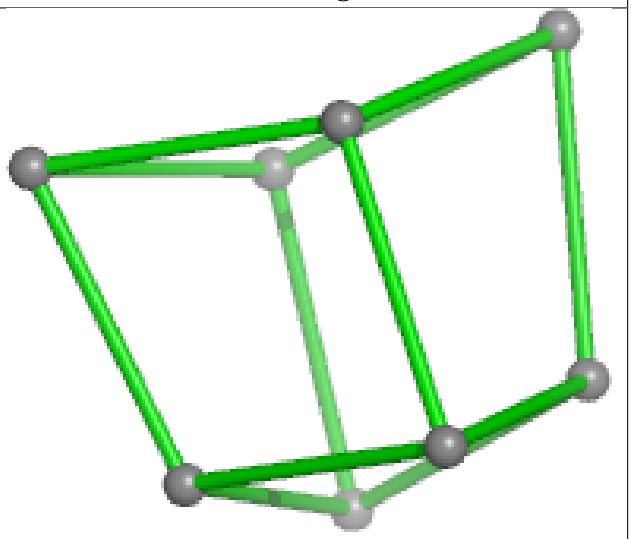
Bond lengths



Bond angles

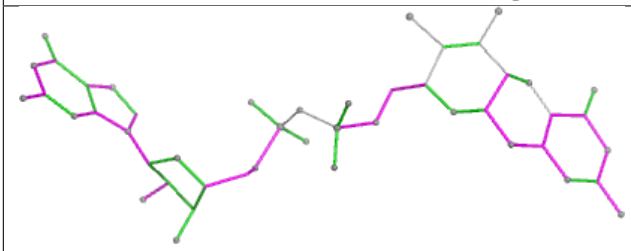


Torsions

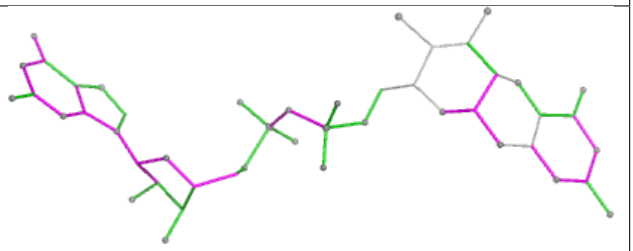


Rings

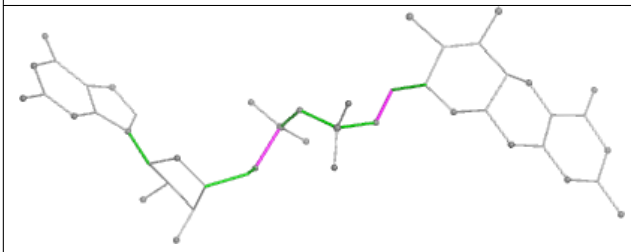
Ligand MGD A 1001



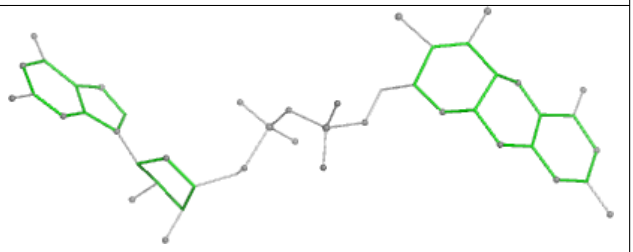
Bond lengths



Bond angles

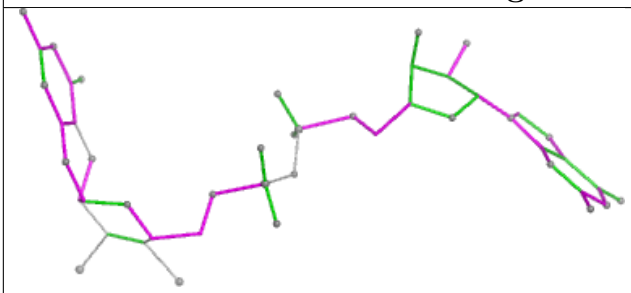


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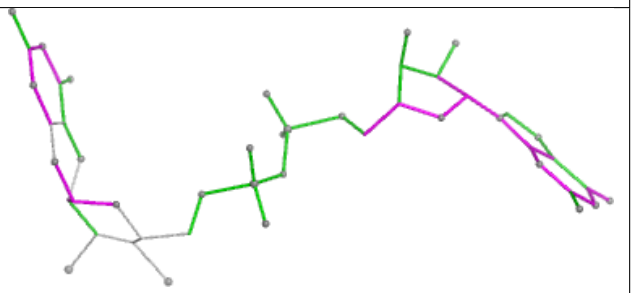


Rings

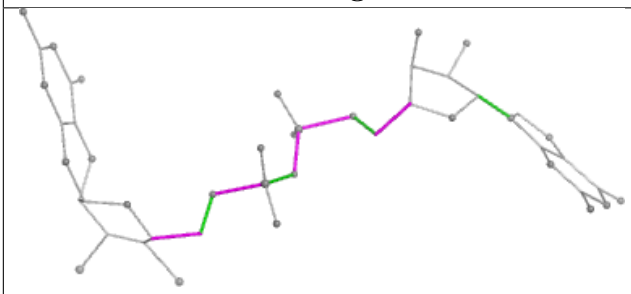
Ligand MGD A 1002



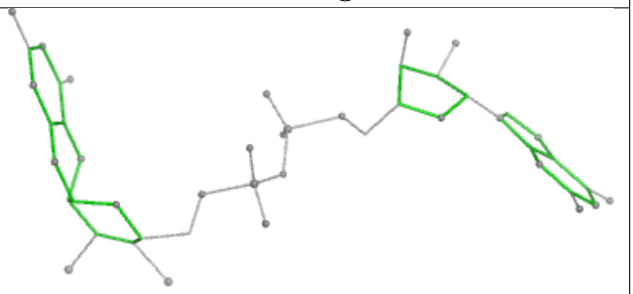
Bond lengths



Bond angles

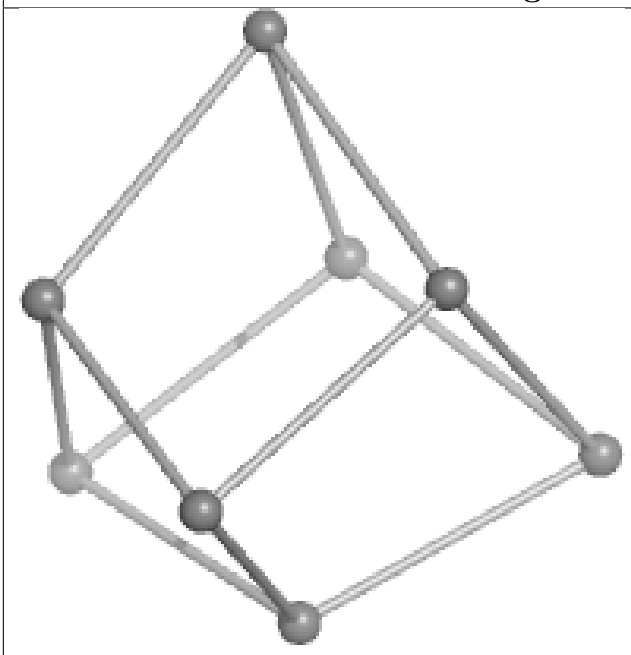


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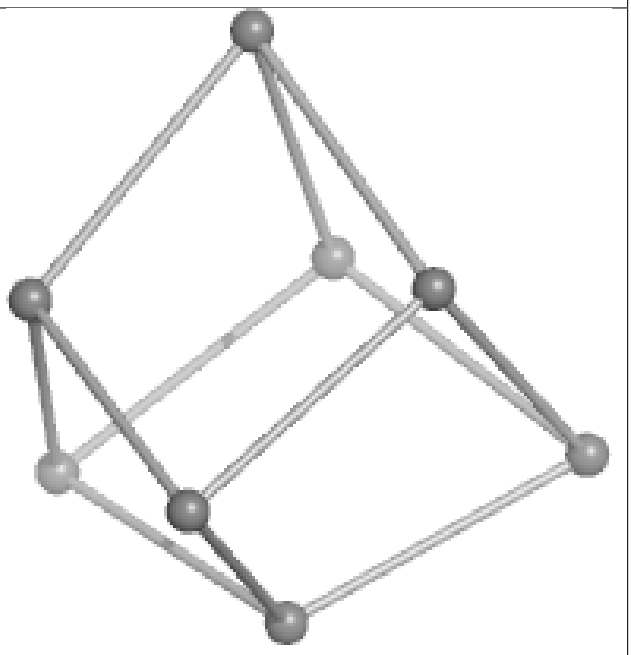


Rings

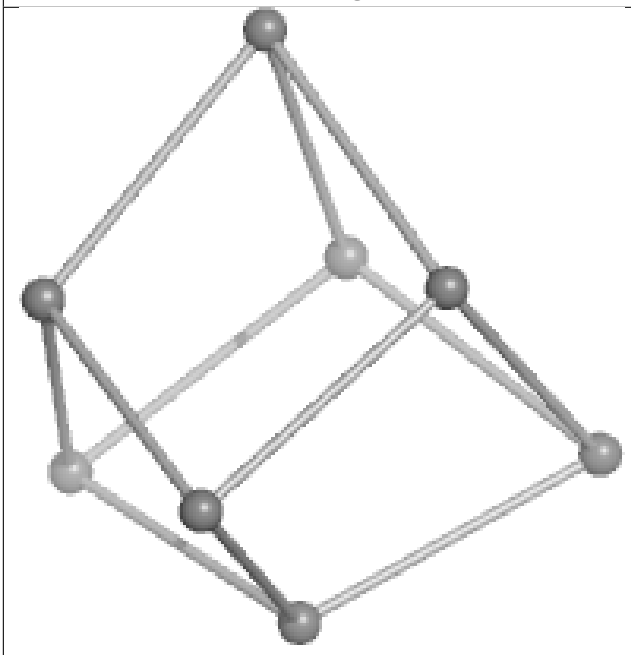
Ligand SF4 E 1007



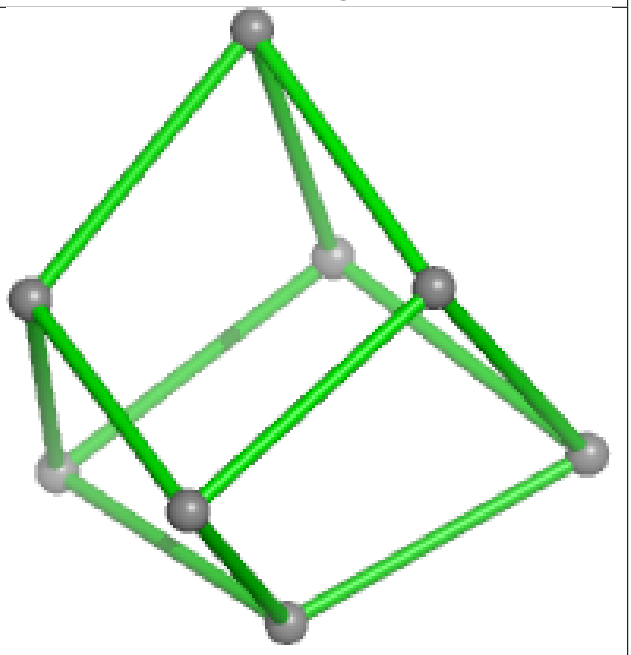
Bond lengths



Bond angles

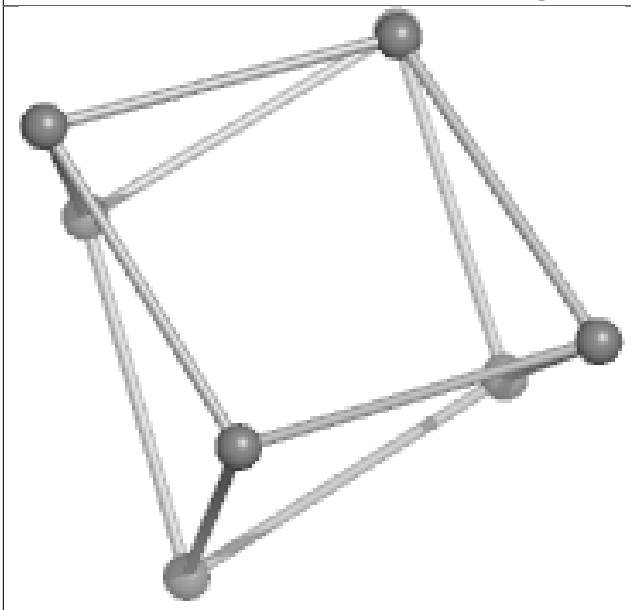


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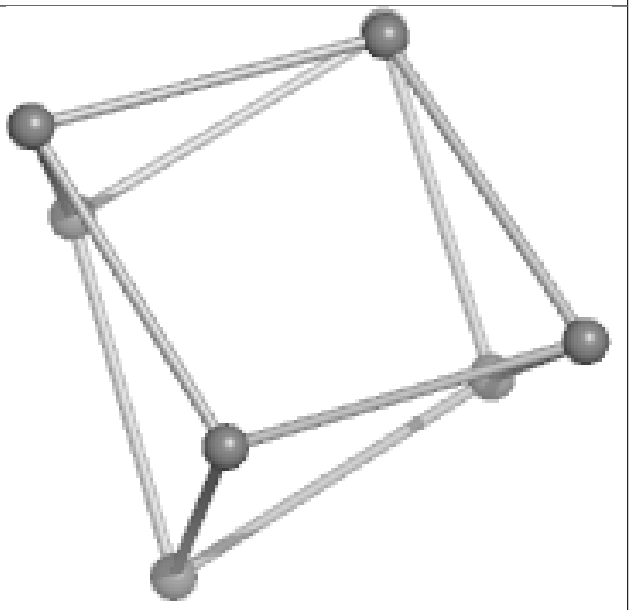


Rings

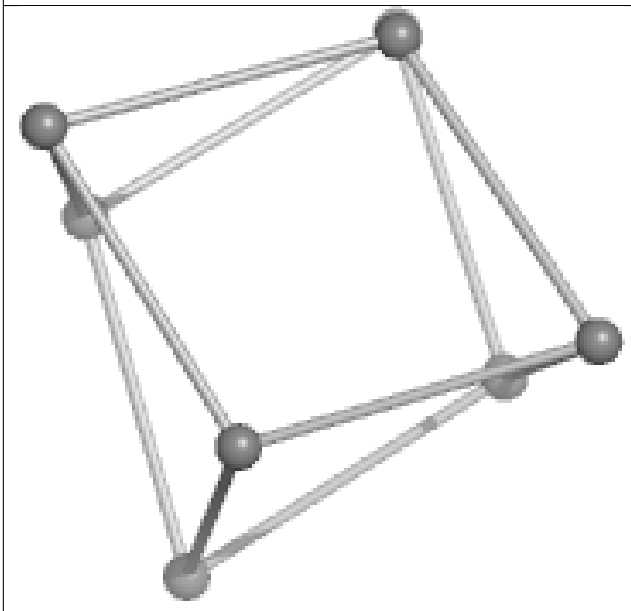
Ligand SF4 F 602



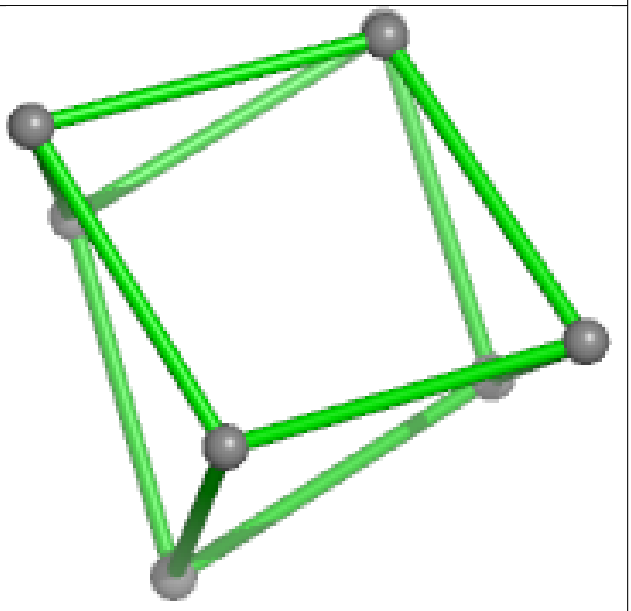
Bond lengths



Bond angles

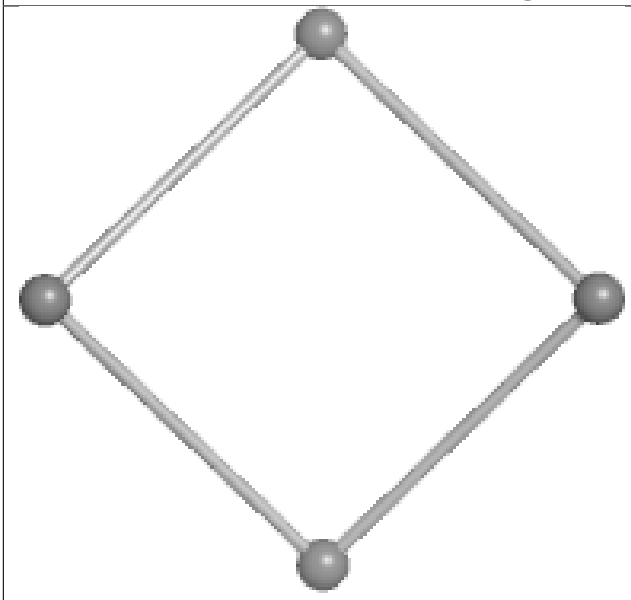


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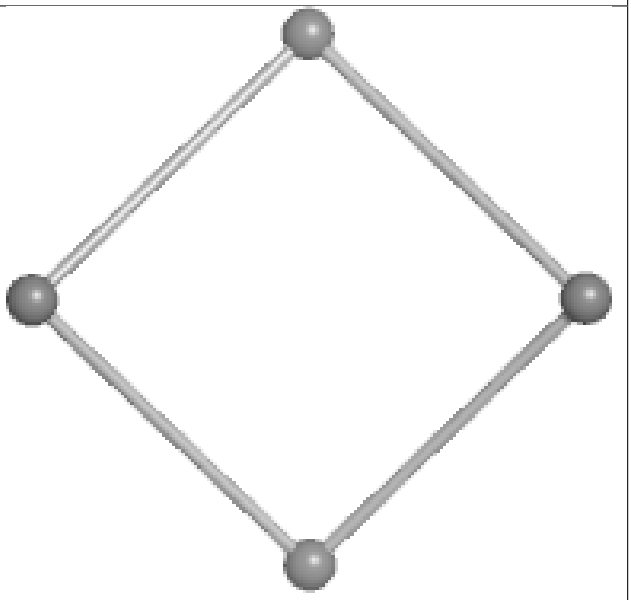


Rings

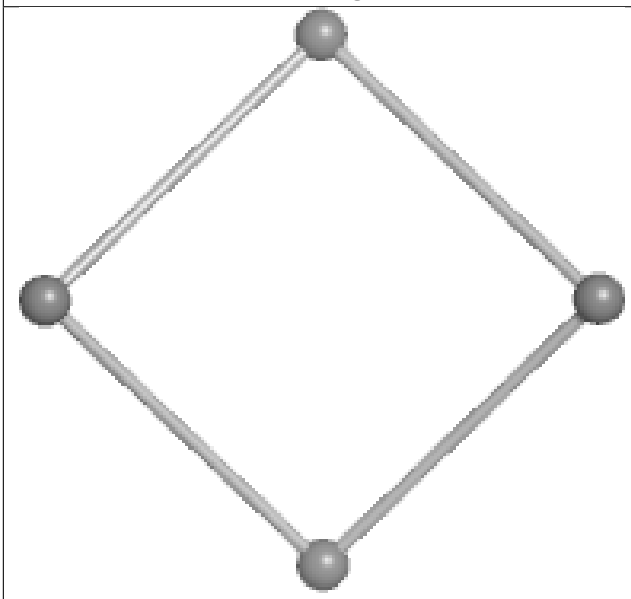
Ligand FES A 1004



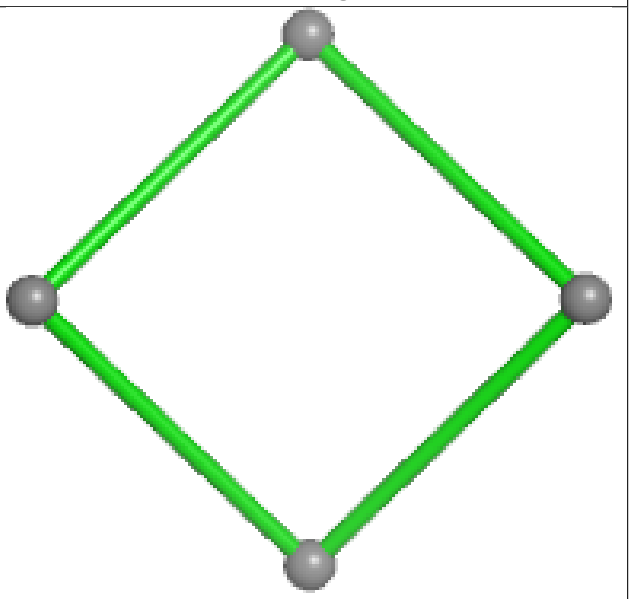
Bond lengths



Bond angles

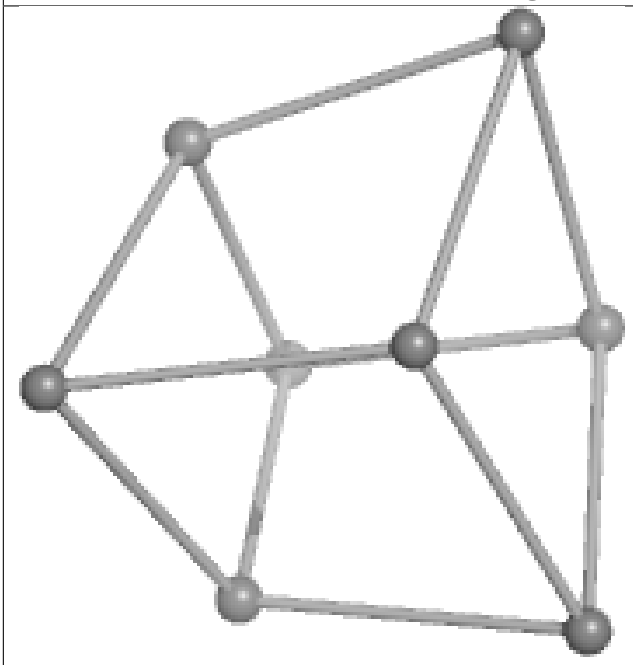


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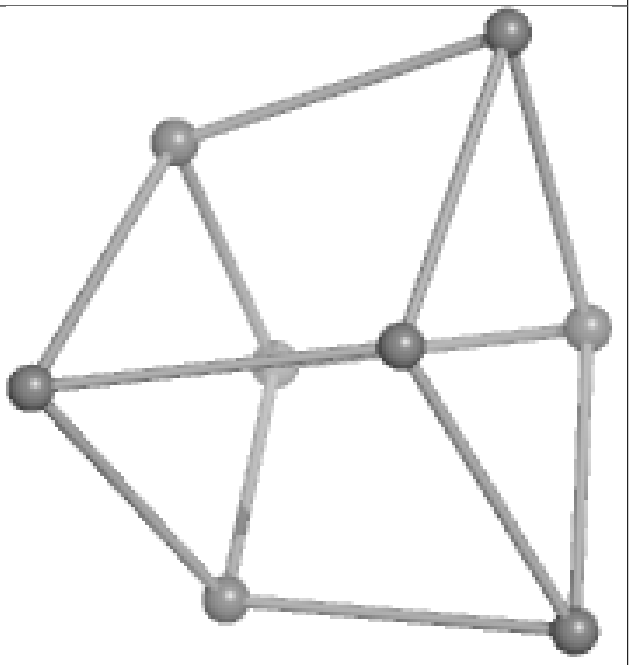


Rings

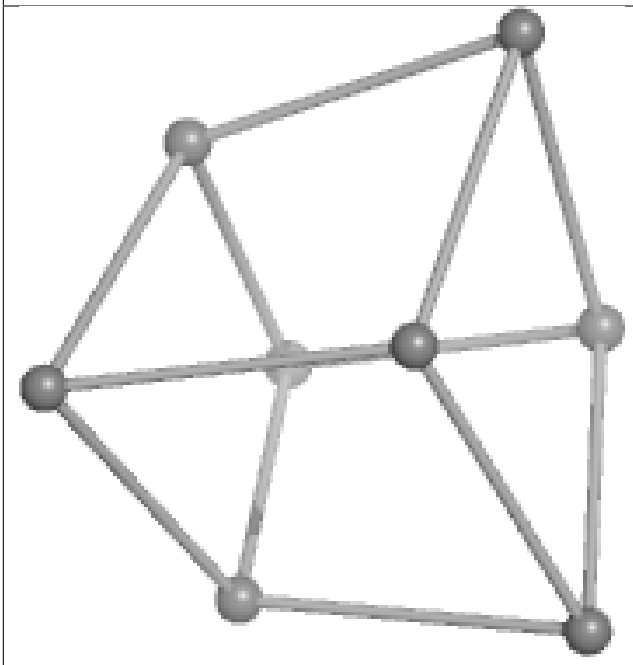
Ligand SF4 E 1006



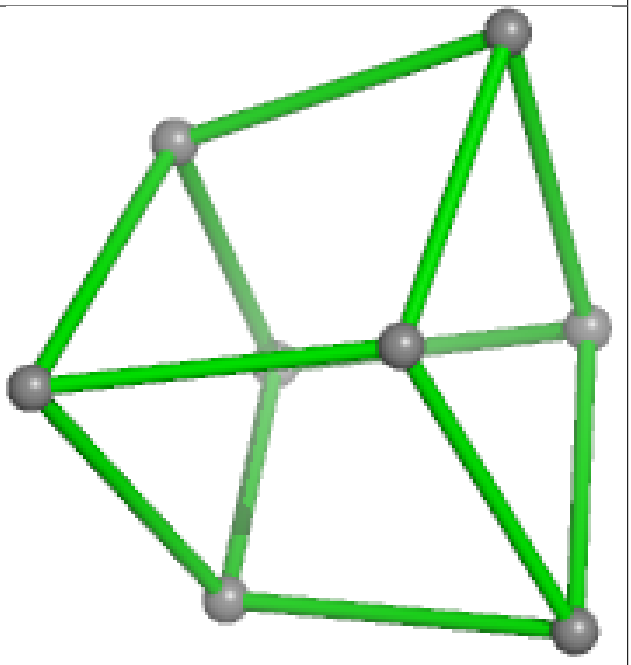
Bond lengths



Bond angles

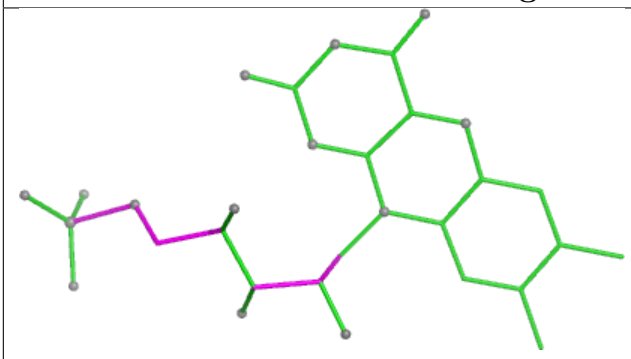


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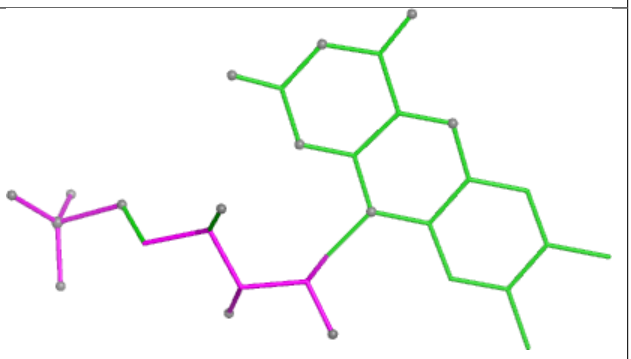


Rings

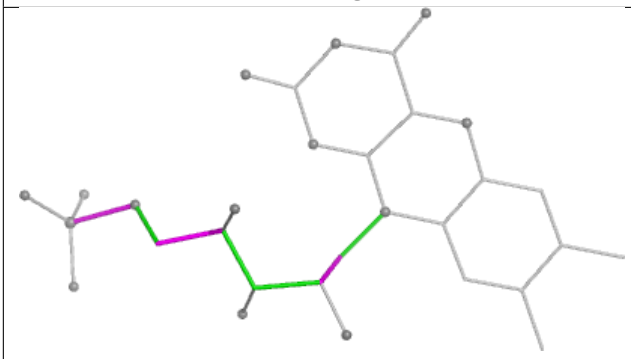
Ligand FMN B 601



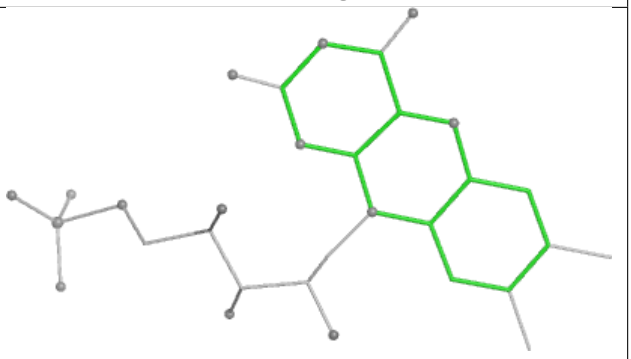
Bond lengths



Bond angles

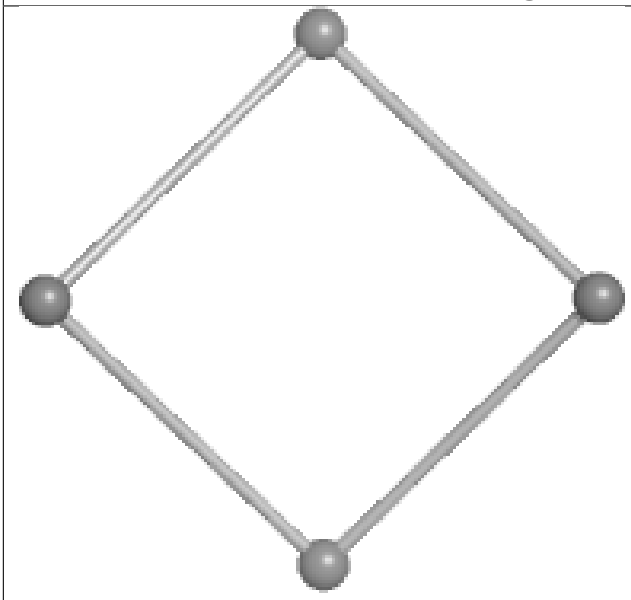


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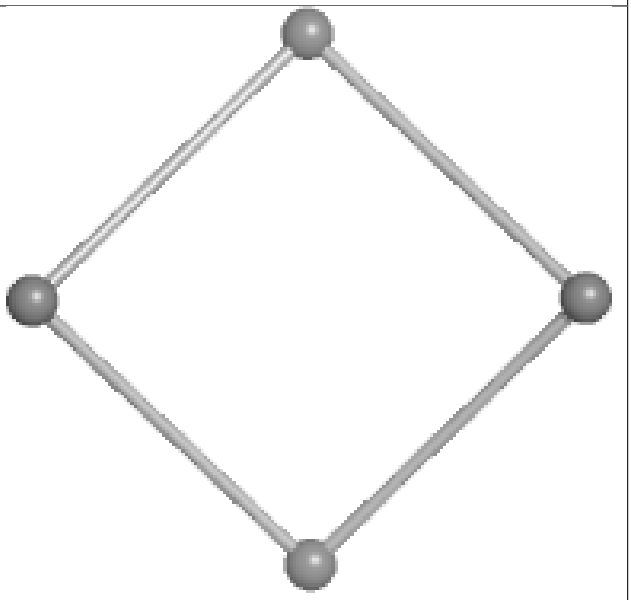


Rings

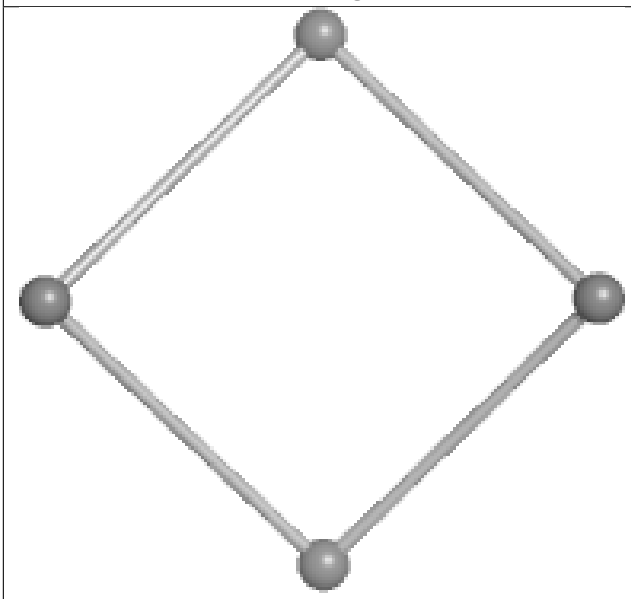
Ligand FES E 1004



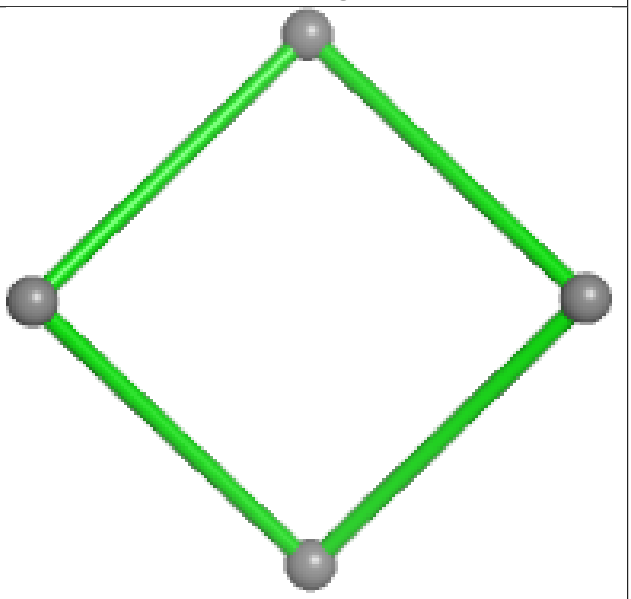
Bond lengths



Bond angles

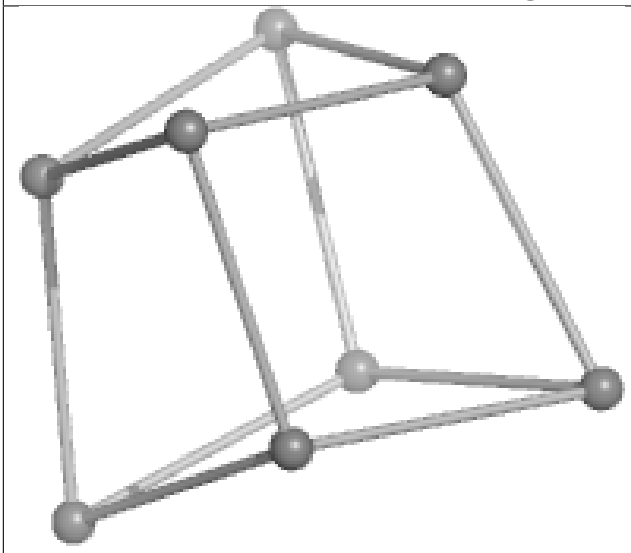


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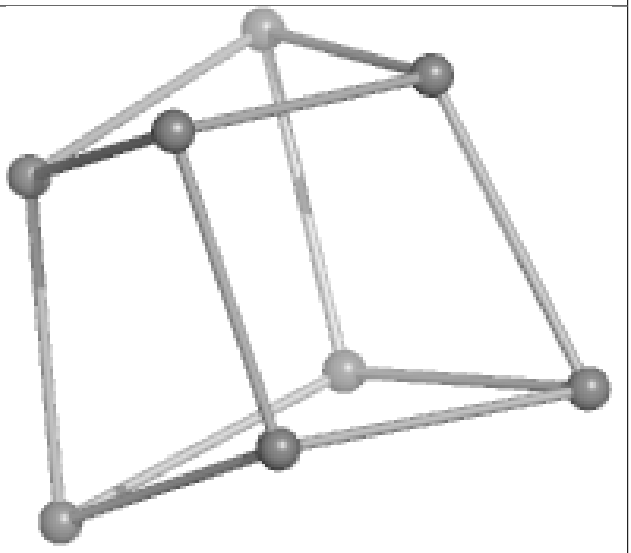


Rings

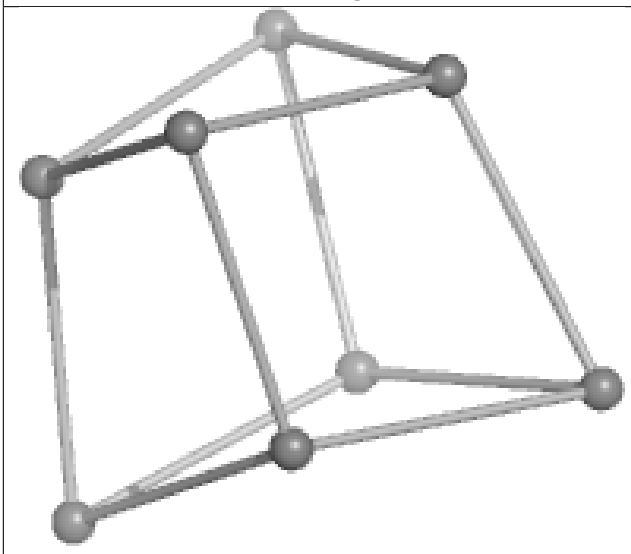
Ligand SF4 A 1005



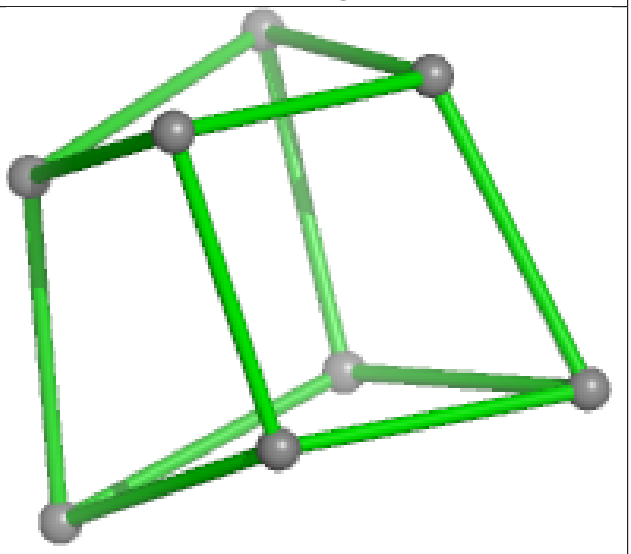
Bond lengths



Bond angles

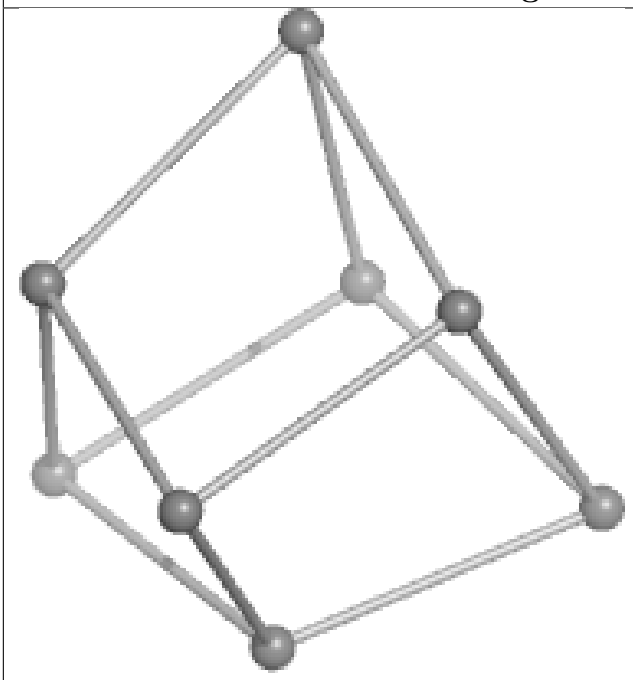


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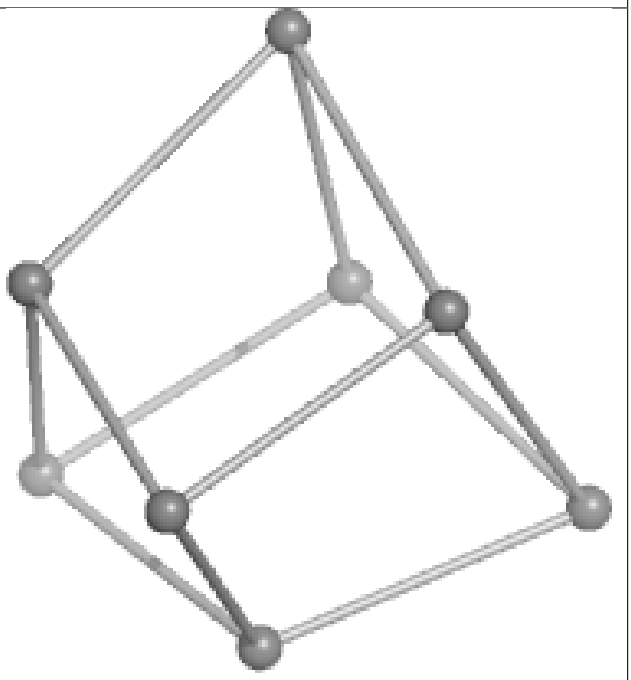


Rings

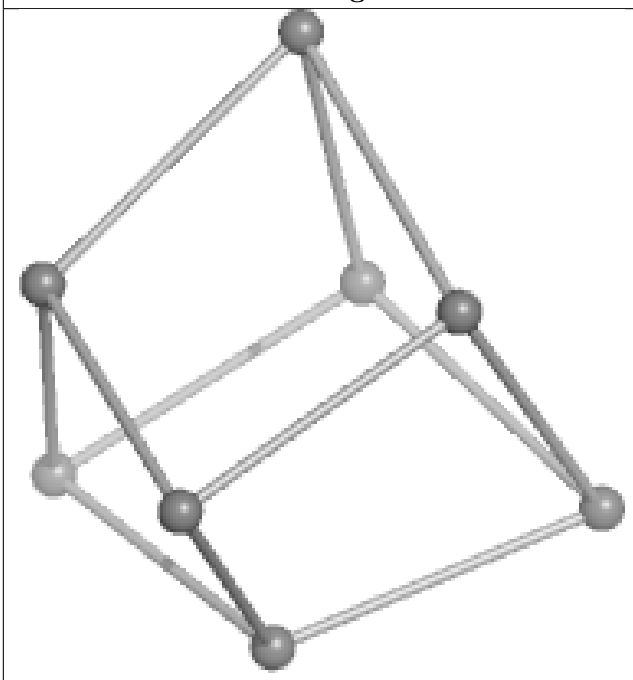
Ligand SF4 A 1007



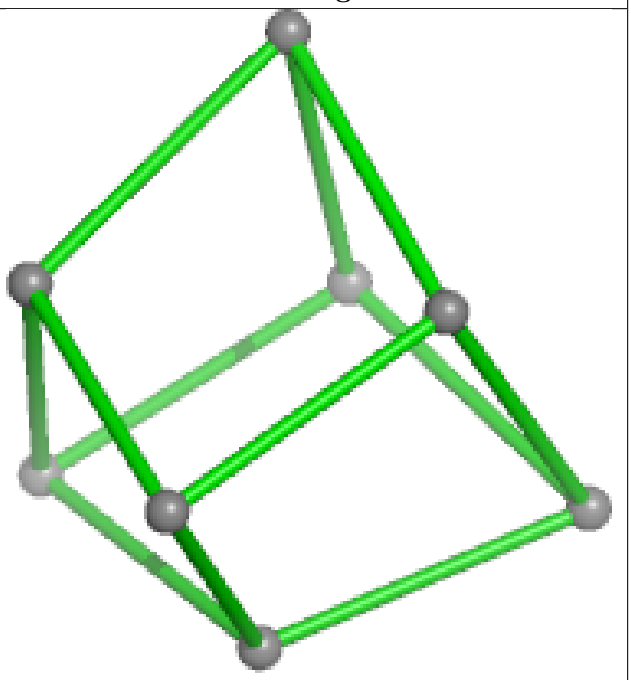
Bond lengths



Bond angles

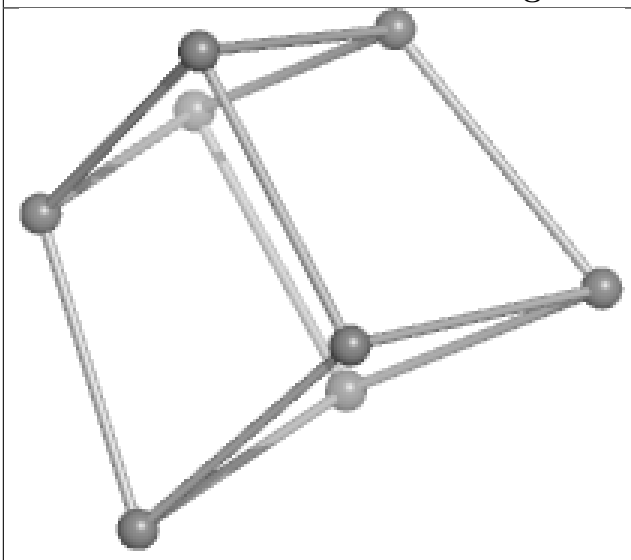


Torsions

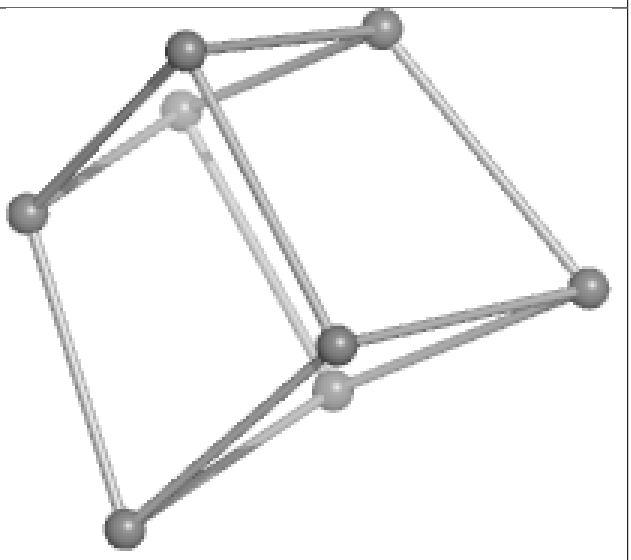


Rings

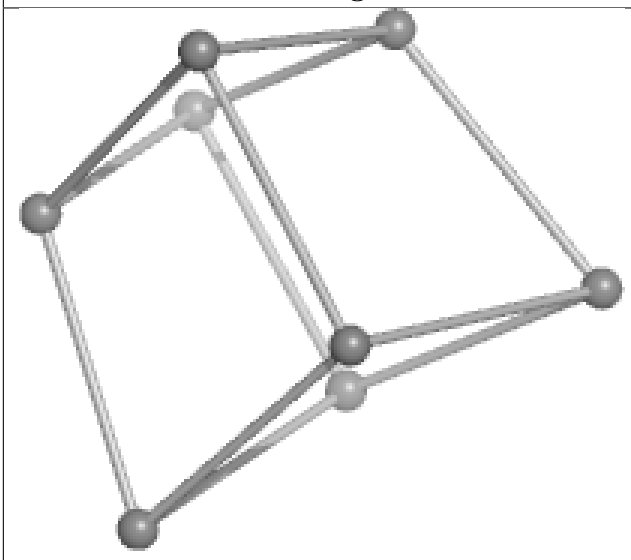
Ligand SF4 E 1008



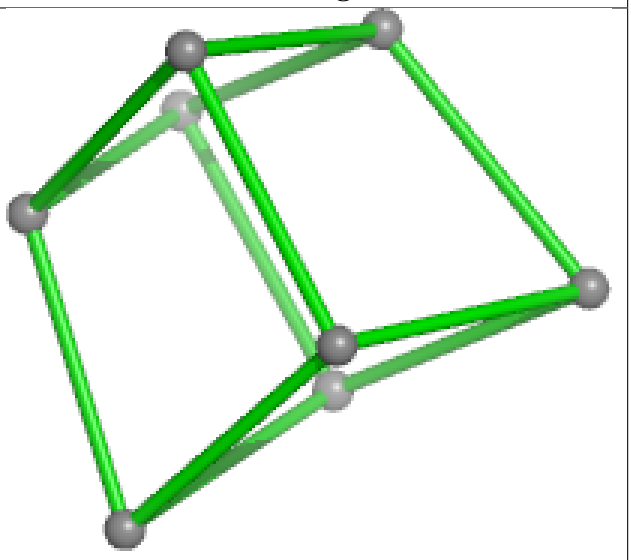
Bond lengths



Bond angles

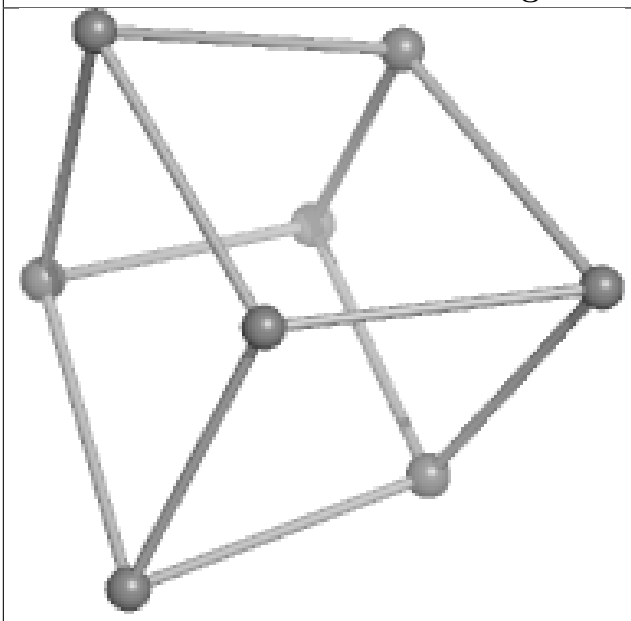


Torsions

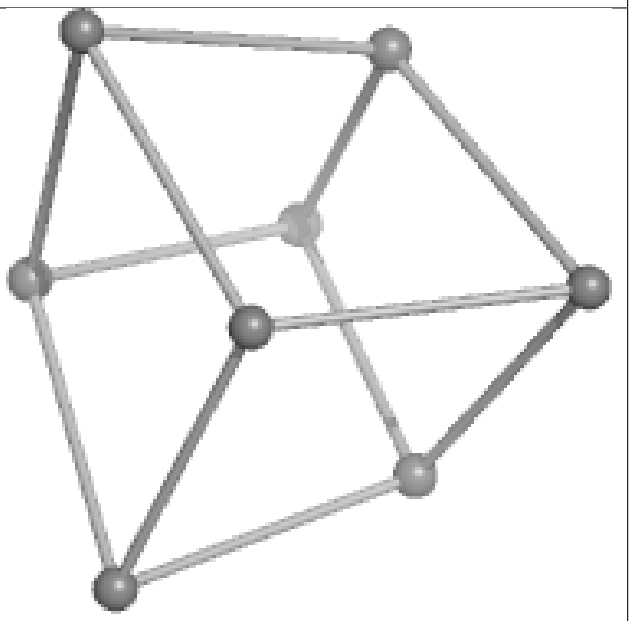


Rings

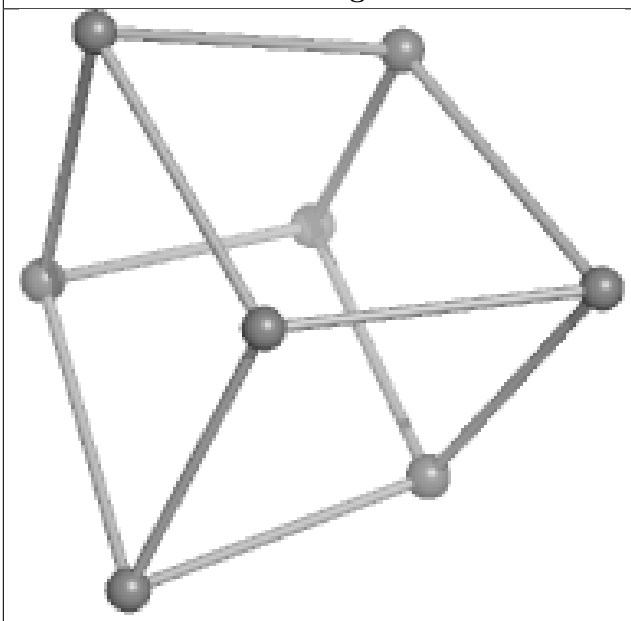
Ligand SF4 A 1006



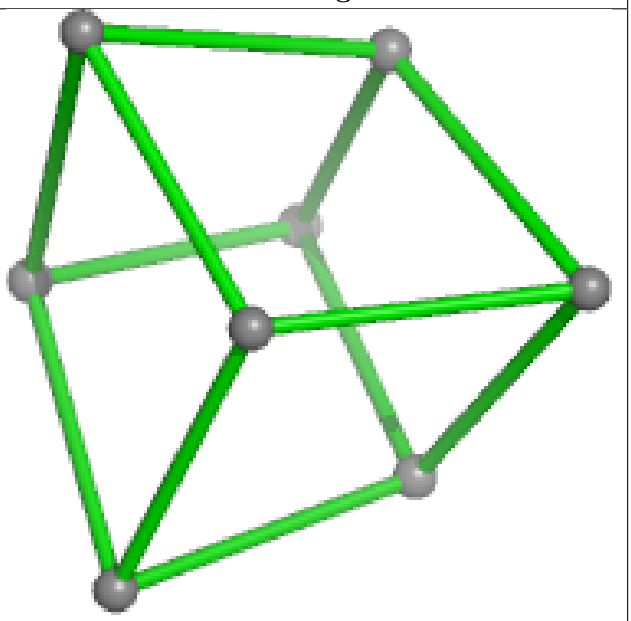
Bond lengths



Bond angles

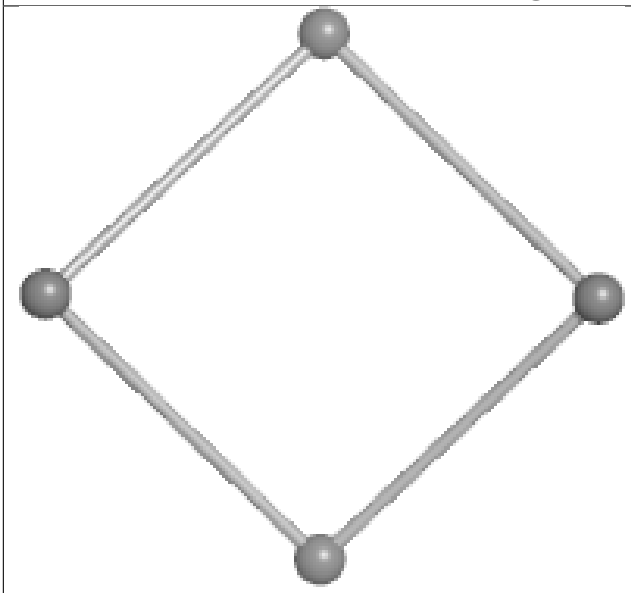


Torsions

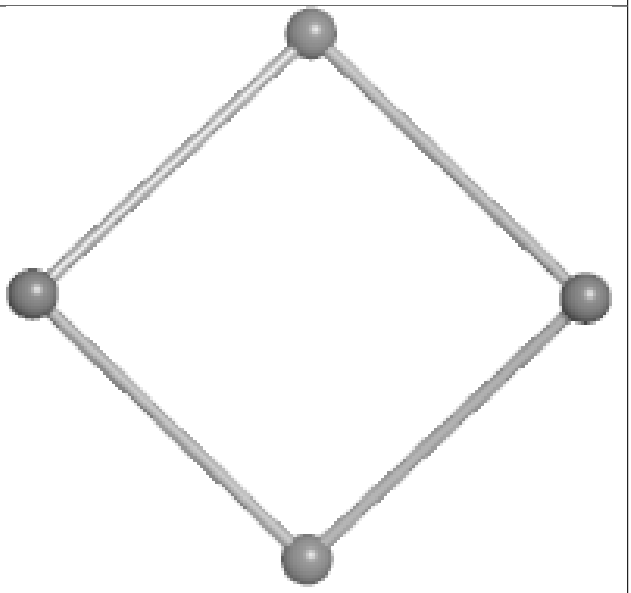


Rings

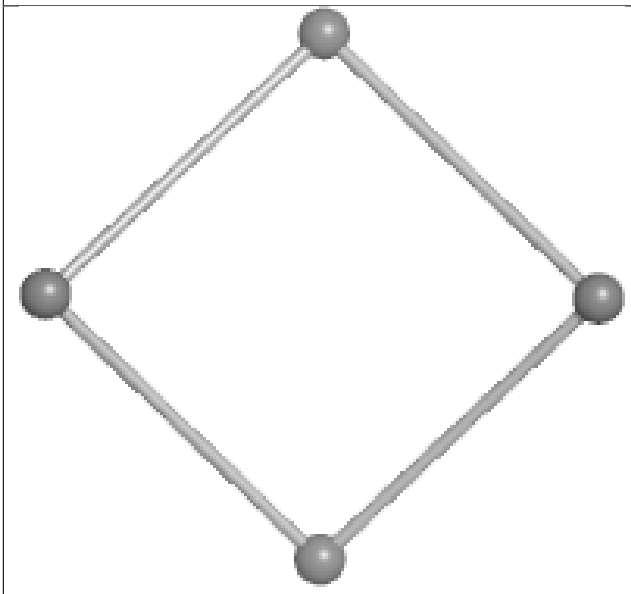
Ligand FES G 201



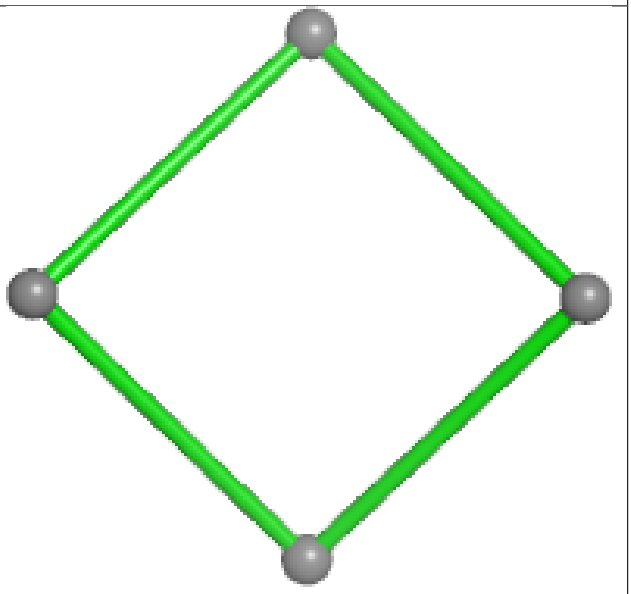
Bond lengths



Bond angles

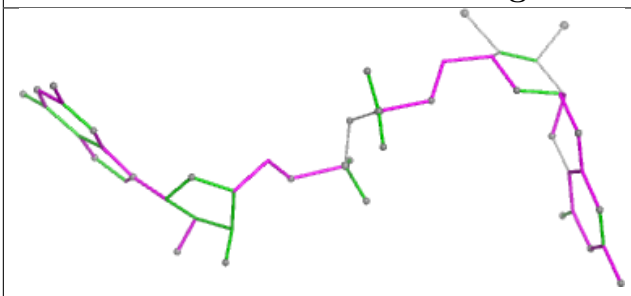


Torsions

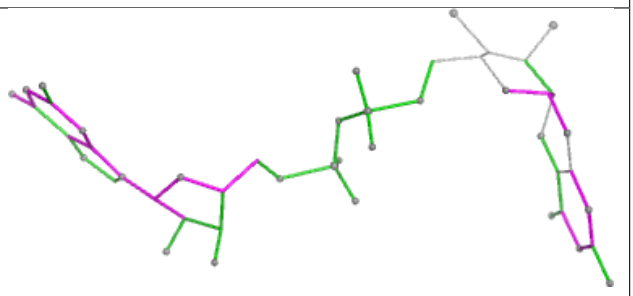


Rings

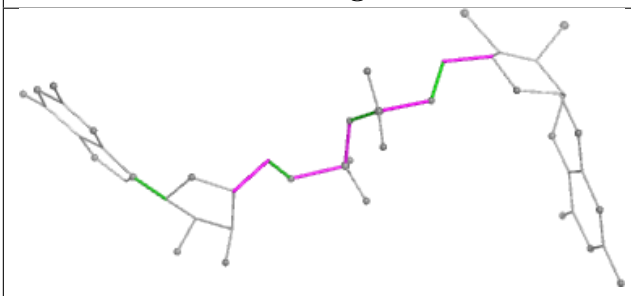
Ligand MGD E 1002



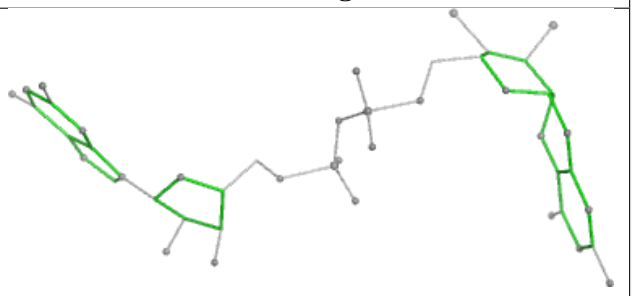
Bond lengths



Bond angles

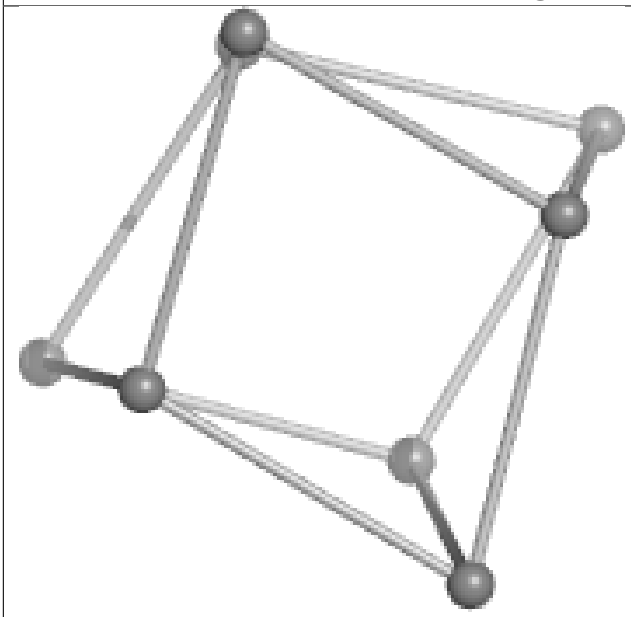


Torsions

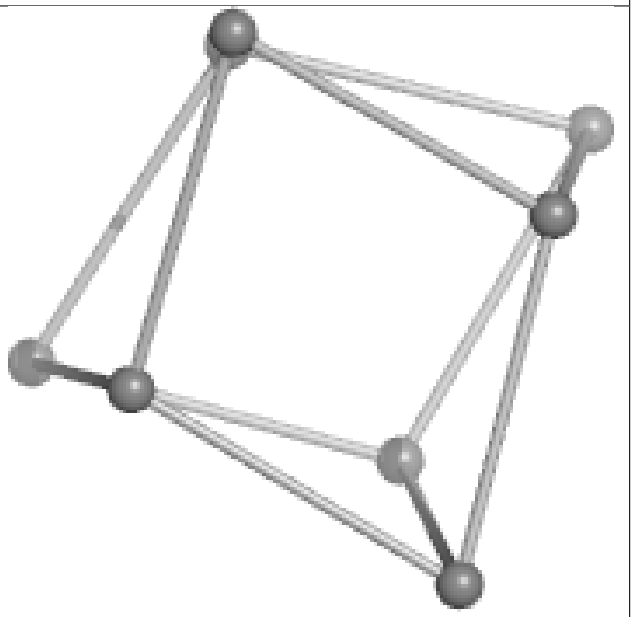


Rings

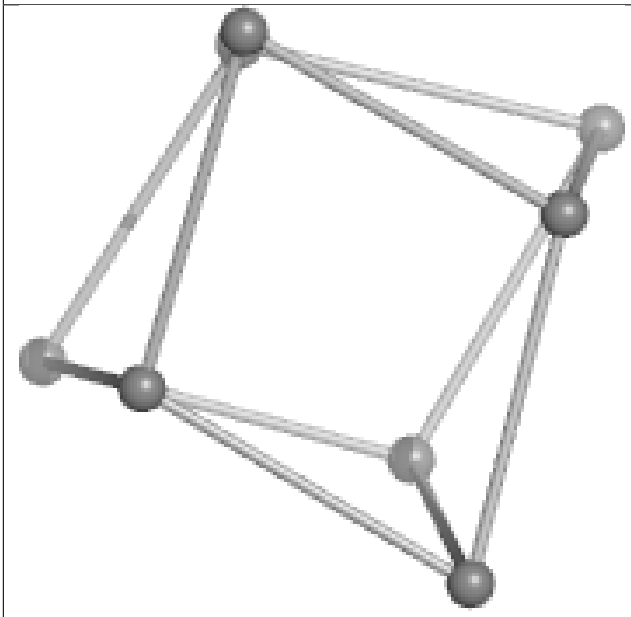
Ligand SF4 B 602



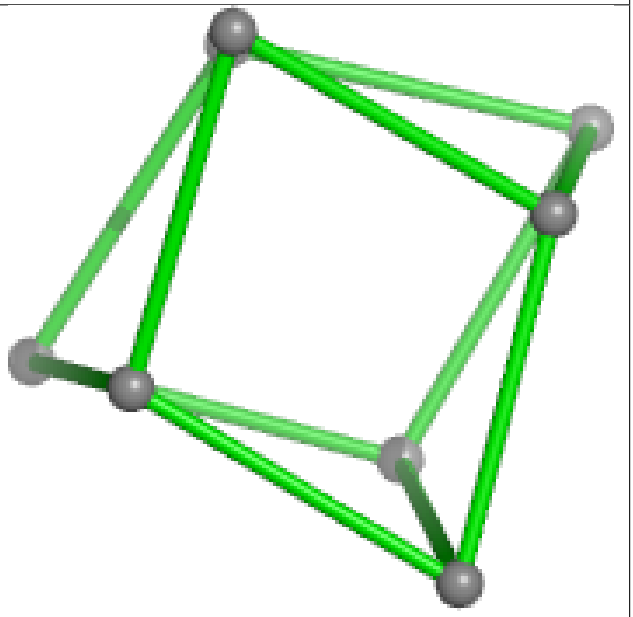
Bond lengths



Bond angles

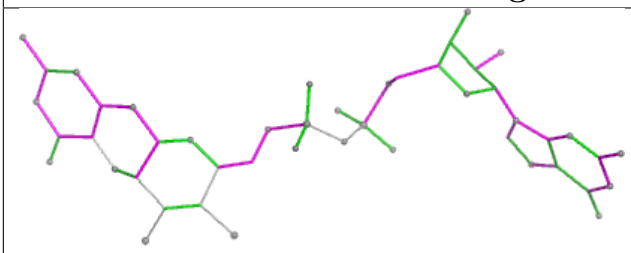


Torsions

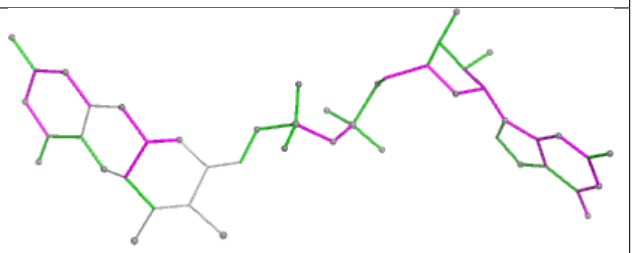


Rings

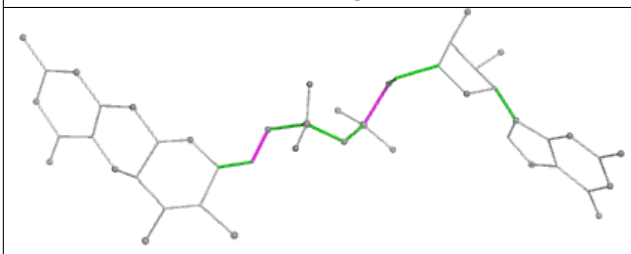
Ligand MGD E 1001



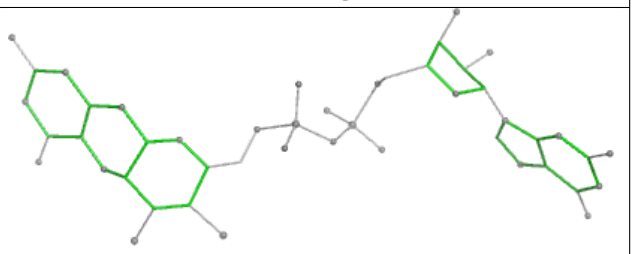
Bond lengths



Bond angles

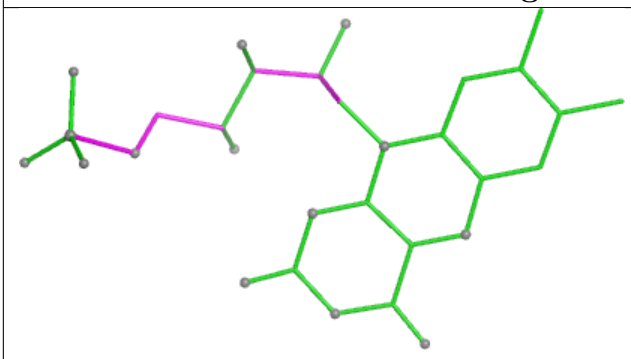


Torsions

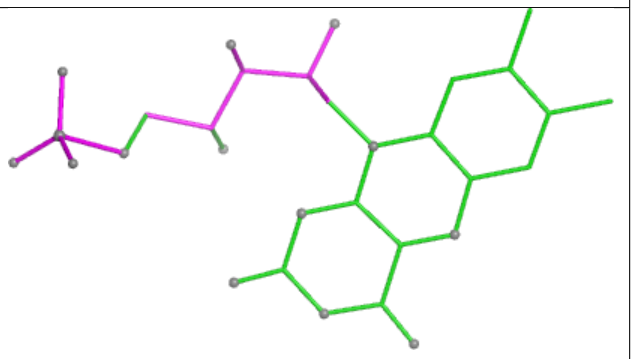


Rings

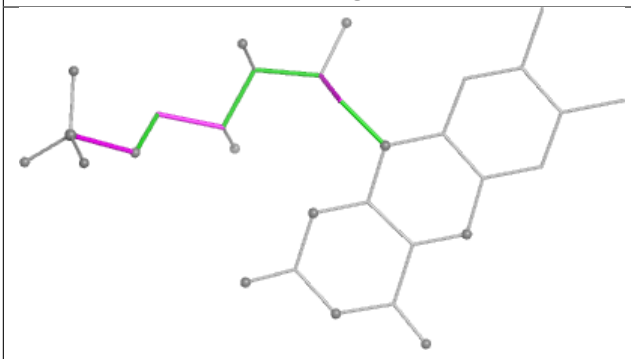
Ligand FMN F 601



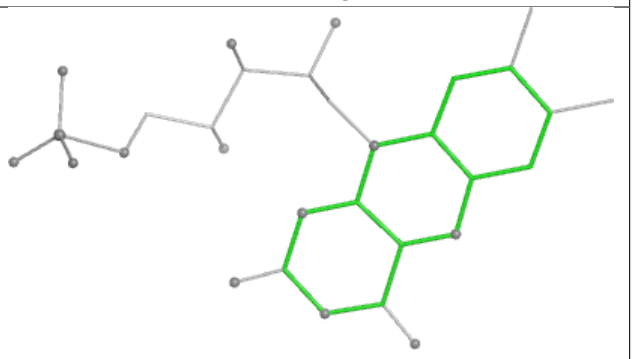
Bond lengths



Bond angles

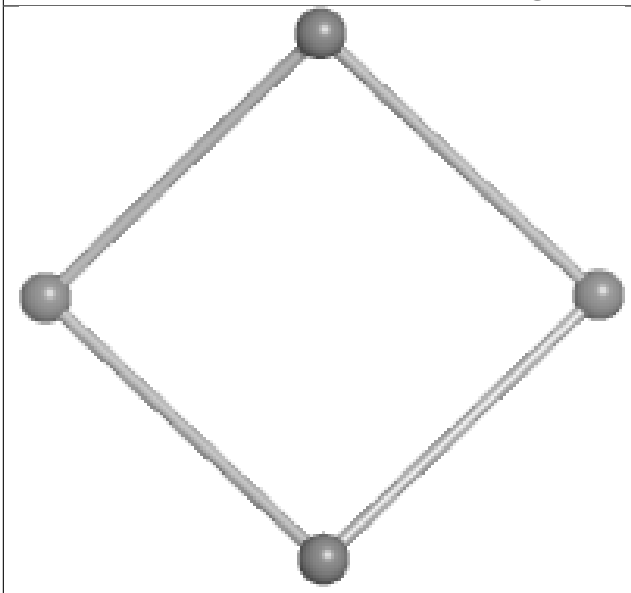


Torsions

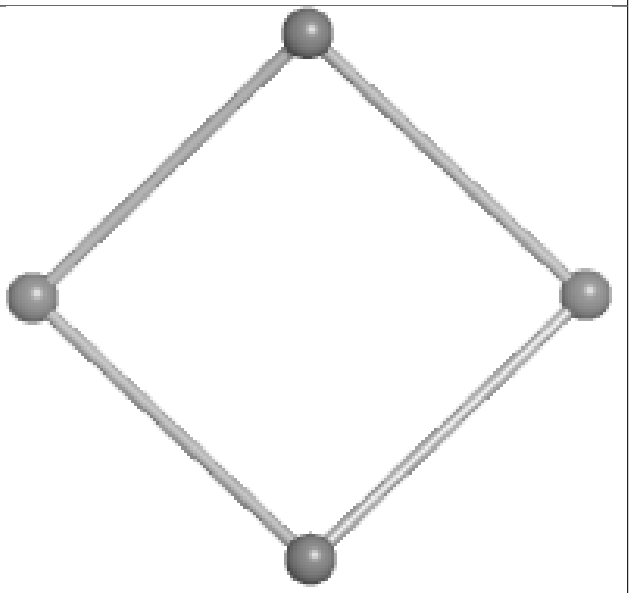


Rings

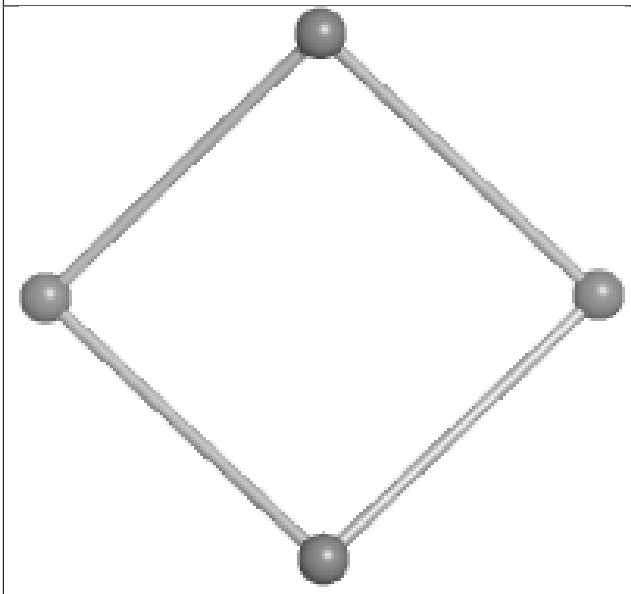
Ligand FES C 201



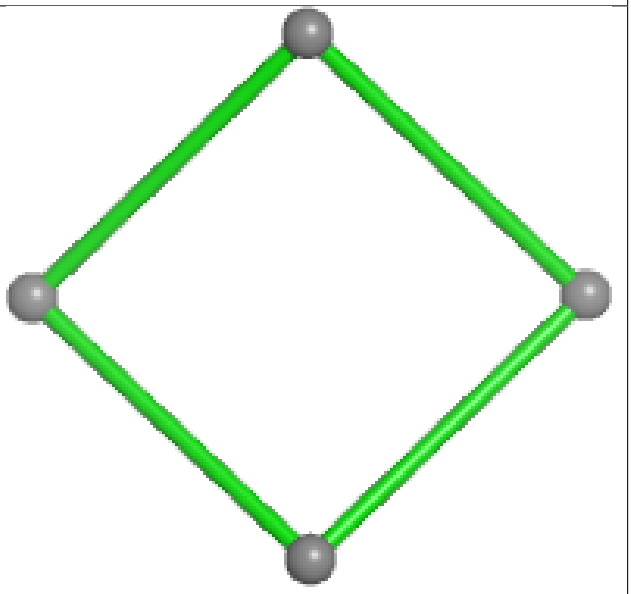
Bond lengths



Bond angles

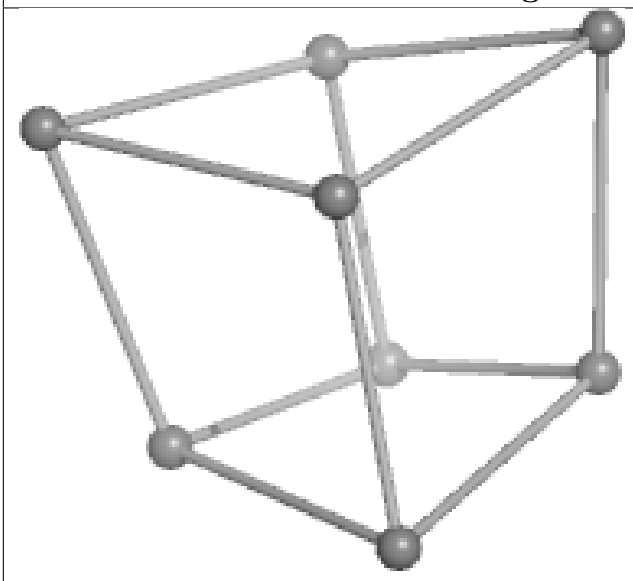


Torsions

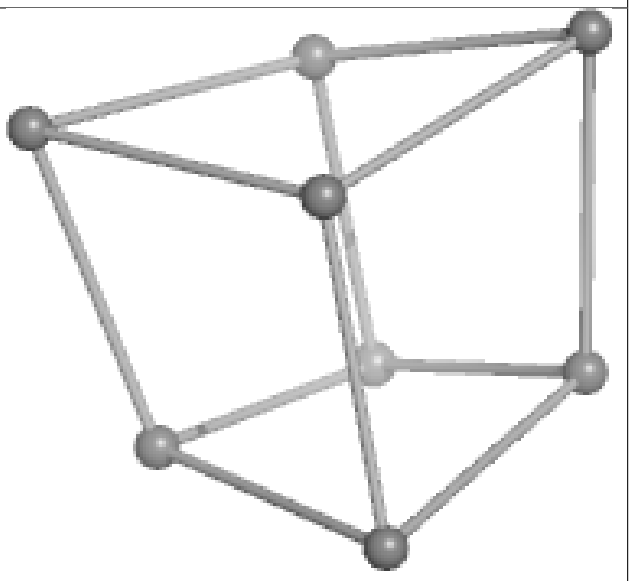


Rings

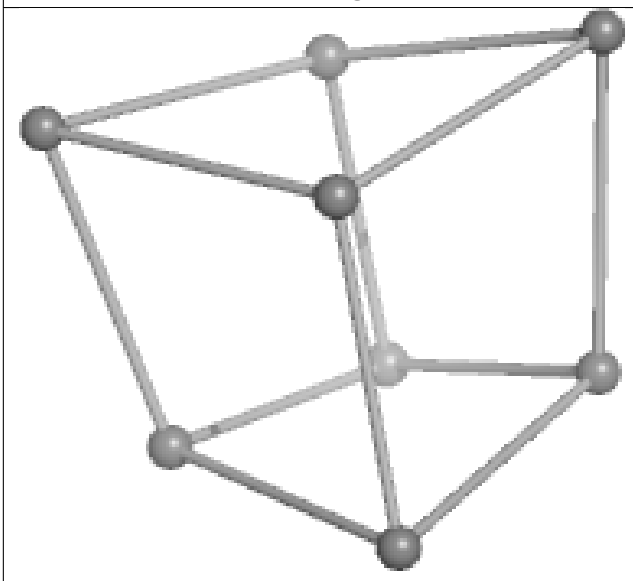
Ligand SF4 A 1008



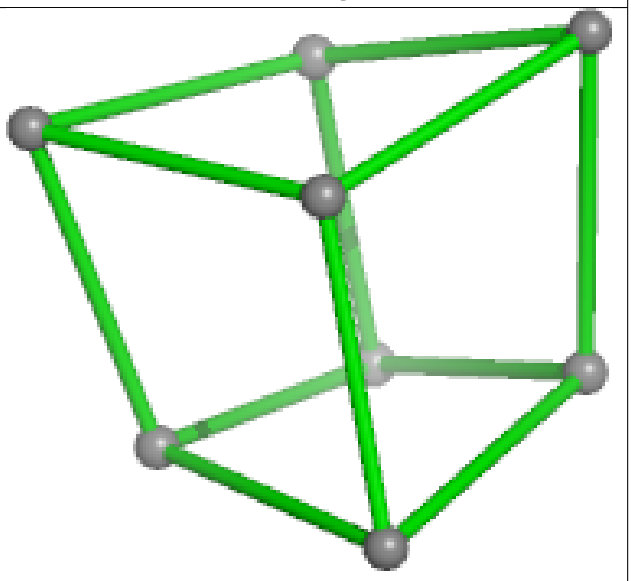
Bond lengths



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.

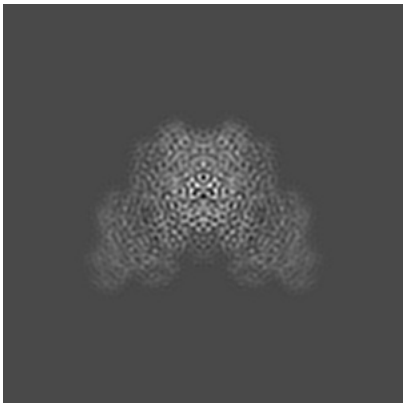
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10496. These allow visual inspection of the internal detail of the map and identification of artifacts.

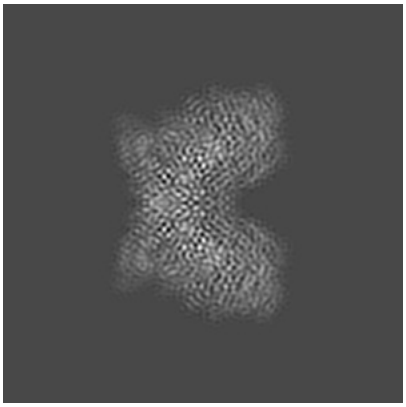
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

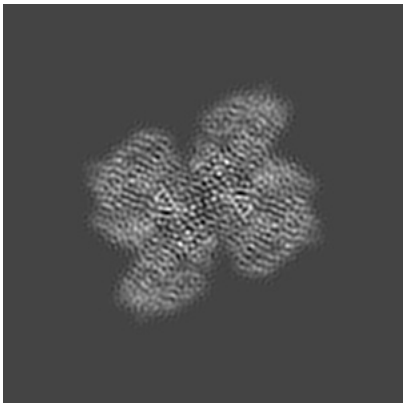
6.1.1 Primary map



X



Y

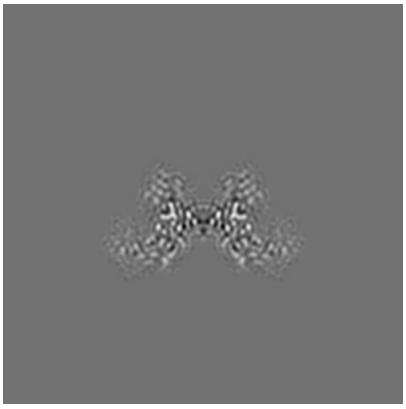


Z

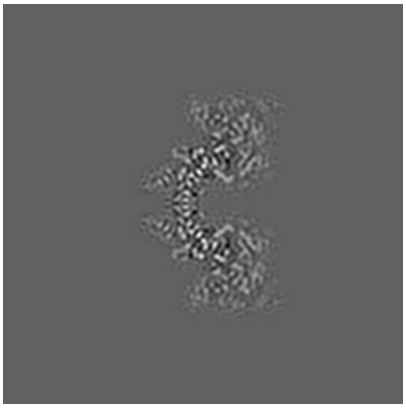
The images above show the map projected in three orthogonal directions.

6.2 Central slices

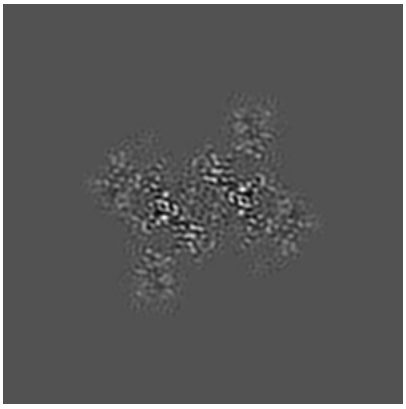
6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

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

6.3 Largest variance slices (i)

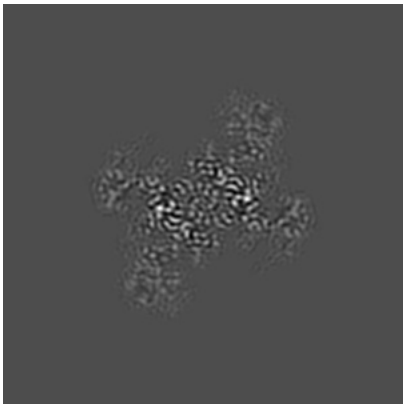
6.3.1 Primary map



X Index: 152



Y Index: 180

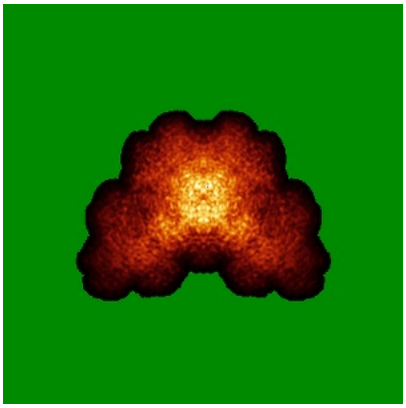


Z Index: 188

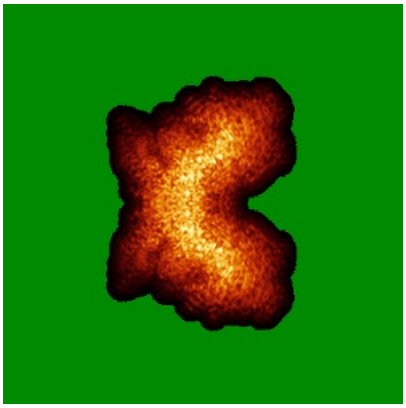
The images above show the largest variance slices of the map in three orthogonal directions.

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

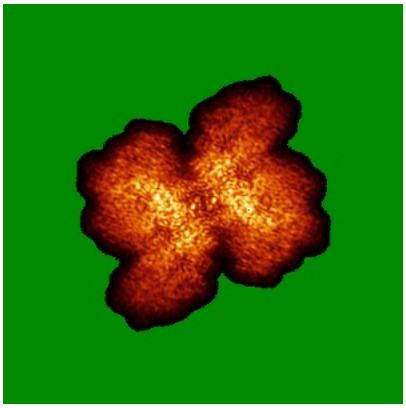
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0112. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

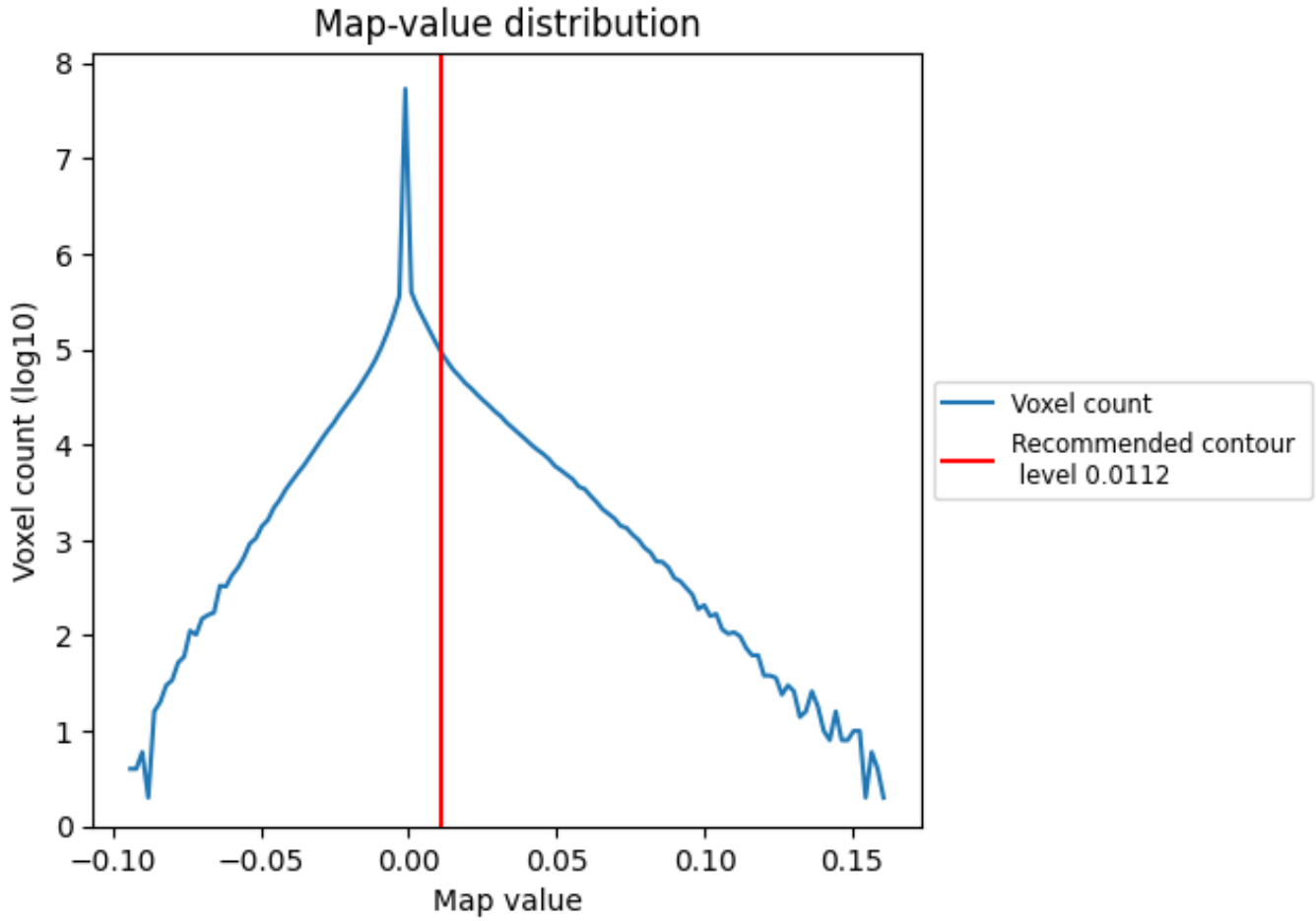
6.6 Mask visualisation (i)

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

7 Map analysis

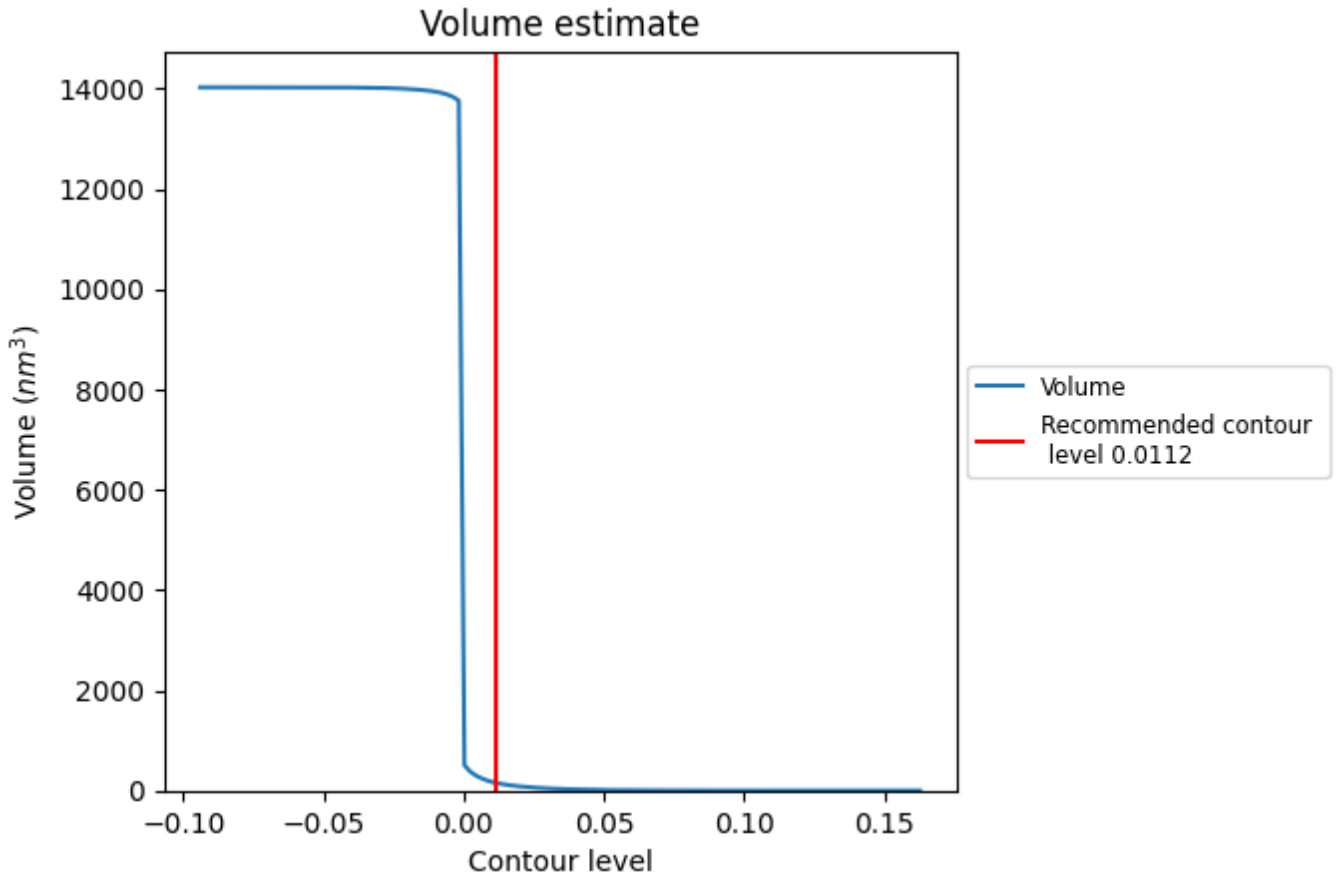
This section contains the results of statistical analysis of the map.

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.

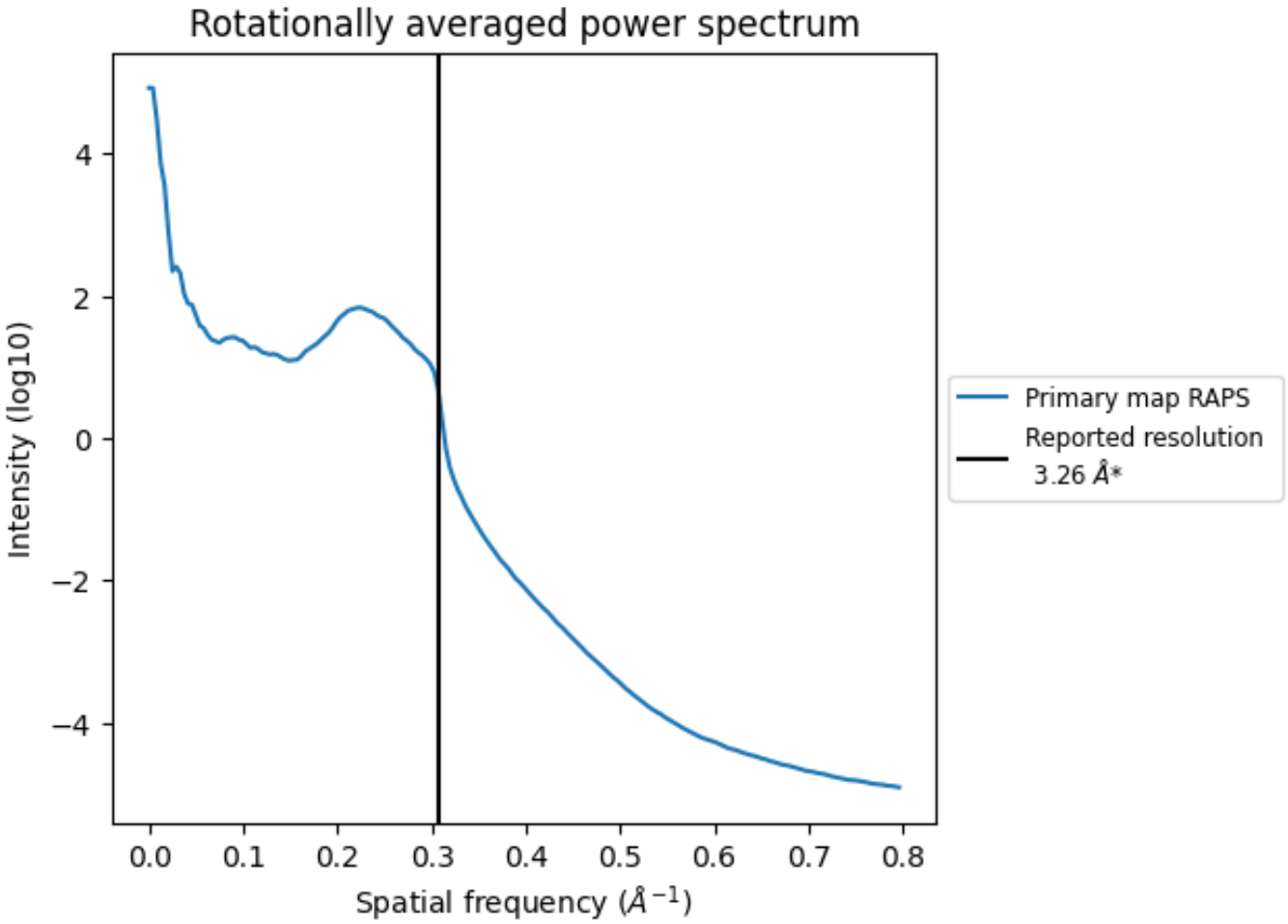
7.2 Volume estimate (i)



The volume at the recommended contour level is 157 nm^3; this corresponds to an approximate mass of 142 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)

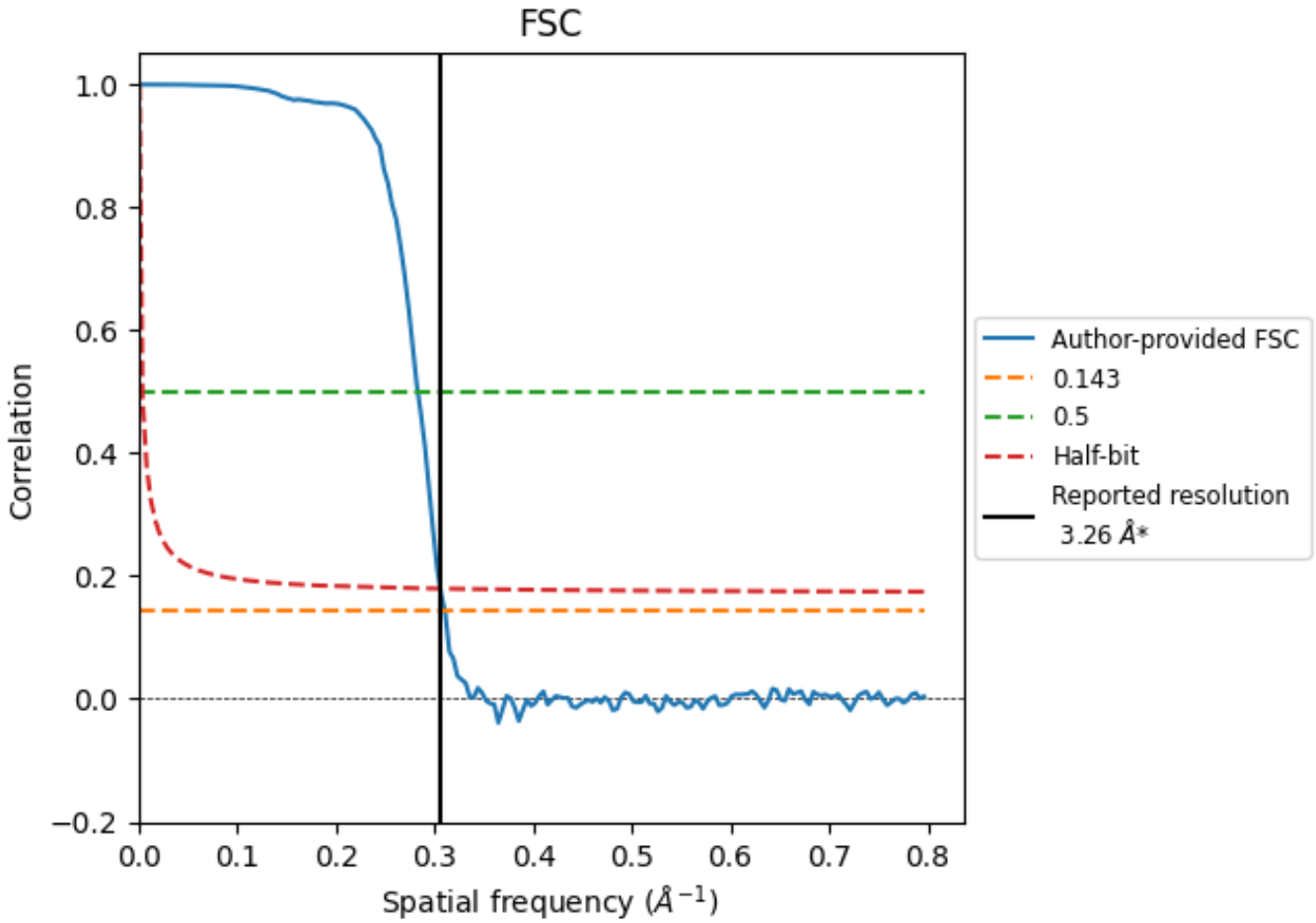


*Reported resolution corresponds to spatial frequency of 0.307 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.307 Å^{-1}

8.2 Resolution estimates (i)

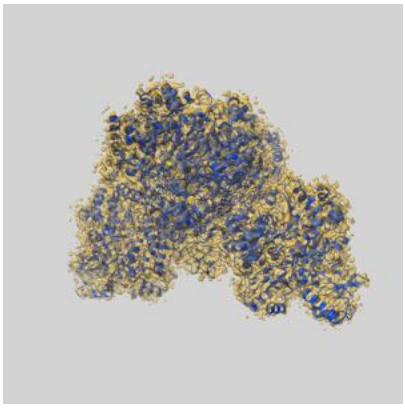
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	3.22	3.53	3.27
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

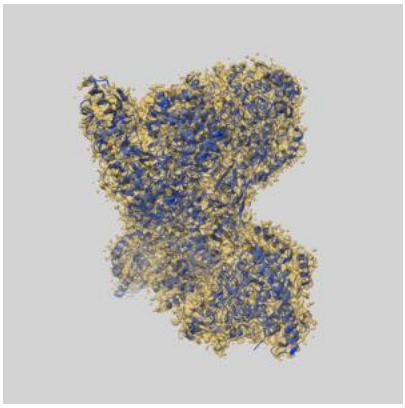
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10496 and PDB model 6TGA. Per-residue inclusion information can be found in section 3 on page 9.

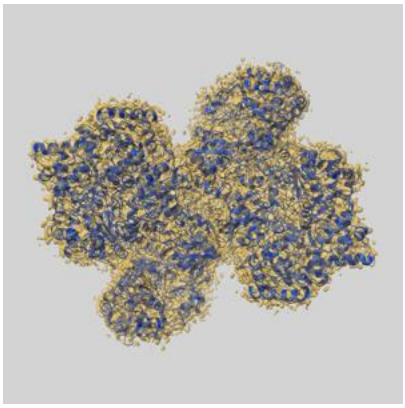
9.1 Map-model overlay



X



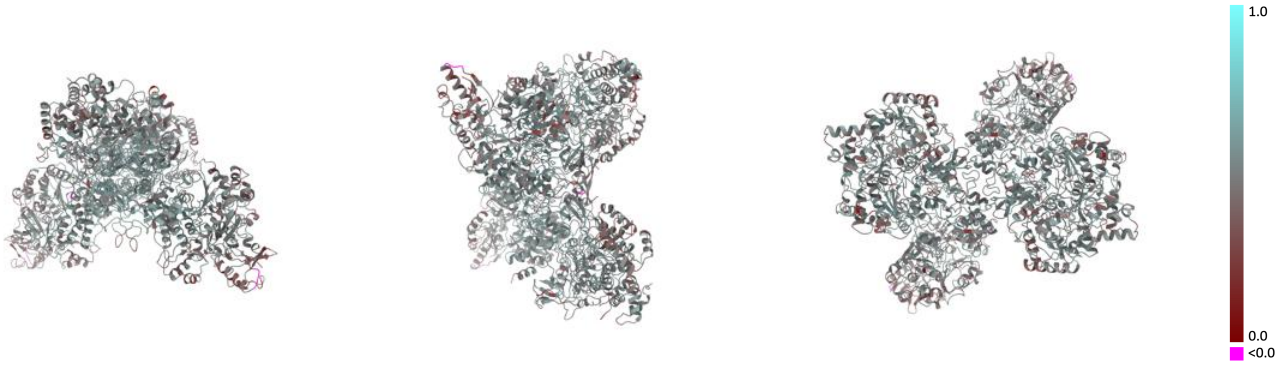
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0112 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.

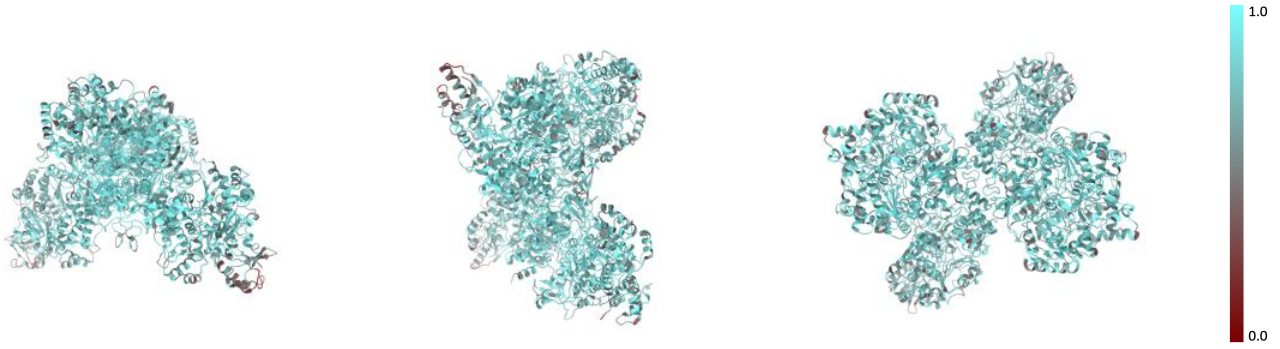
9.2 Q-score mapped to coordinate model (i)



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.

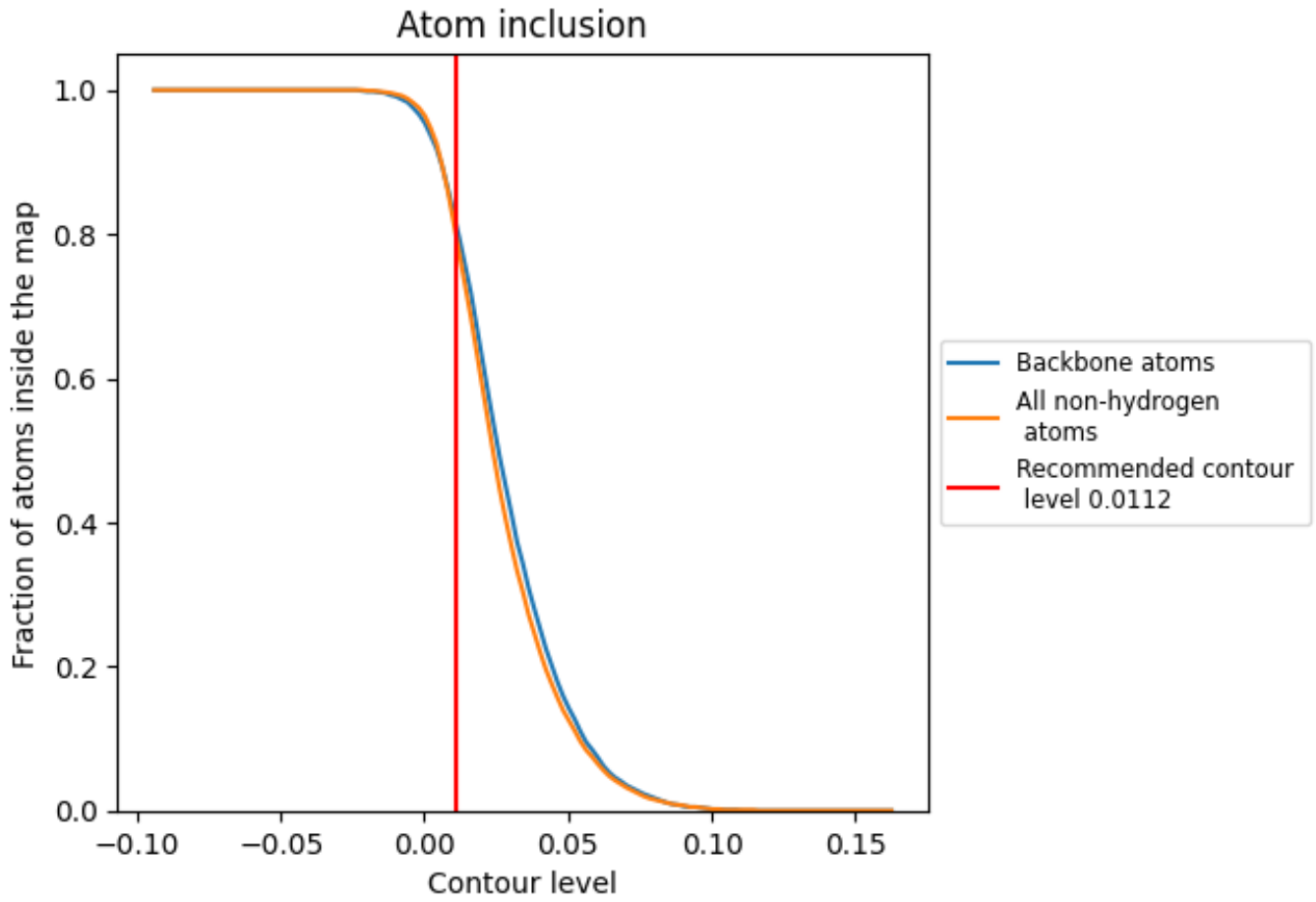
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0112).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7960	0.4960
A	0.8230	0.5080
B	0.7640	0.4830
C	0.7670	0.4830
D	0.7080	0.4650
E	0.8230	0.5070
F	0.7640	0.4820
G	0.7670	0.4820
H	0.7120	0.4730

