wwPDB X-ray Structure Validation Summary Report (i)

Aug 25, 2026 – 07:19 am BST

PDB ID	:	9R52 / pdb_00009r52
Title	:	Dimeric state of the F420-reducing hydrogenase from Methanothermococcus thermolithotrophicus in crystalline form 2
Authors	:	Jespersen, M.; Lemaire, O.N.; Wagner, T.
Deposited on	:	2025-05-08
Resolution	:	1.65 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

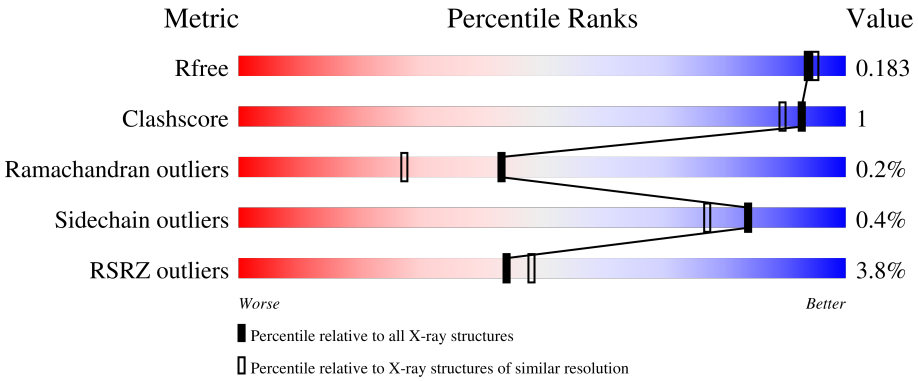
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	410	92%
2	B	282	11% 96%
3	C	241	2% 94% 5%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 15123 atoms, of which 7193 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 F420-reducing [NiFe]-hydrogenase from Methanothermococcus thermolithotrophicus alpha subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	392	6174	1970	3077	529	583	15	0	6	0

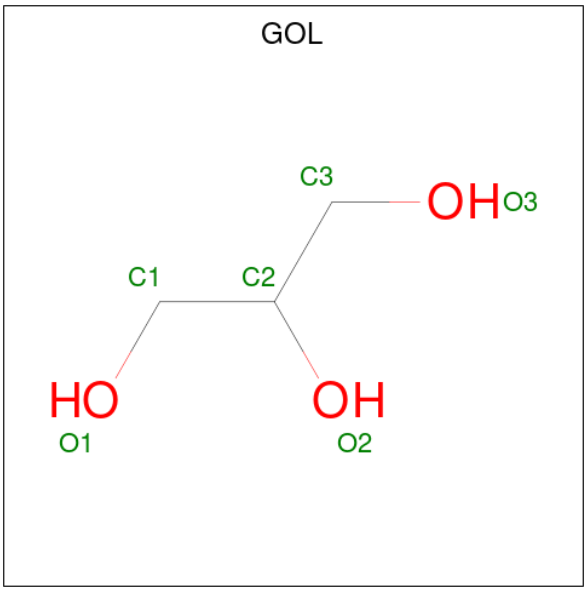
- Molecule 2 is a protein called F420-reducing [NiFe]-hydrogenase from Methanothermococcus thermolithotrophicus beta subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	278	4336	1373	2191	351	406	15	0	0	0

- Molecule 3 is a protein called F420-reducing [NiFe]-hydrogenase from Methanothermococcus thermolithotrophicus gamma subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	240	3653	1135	1845	301	351	21	0	2	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	B	1	Total C H O 14 3 8 3	0	0
4	B	1	Total C H O 14 3 8 3	0	0
4	C	1	Total C H O 14 3 8 3	0	0
4	C	1	Total C H O 14 3 8 3	0	0
4	C	1	Total C H O 14 3 8 3	0	0

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

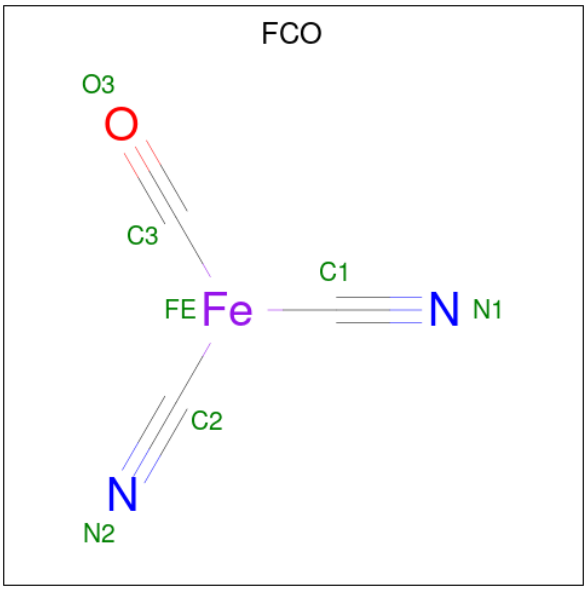
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Fe 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Fe 1 1	0	0

- Molecule 6 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: C_3FeN_2O) (labeled as "Ligand of Interest" by depositor).

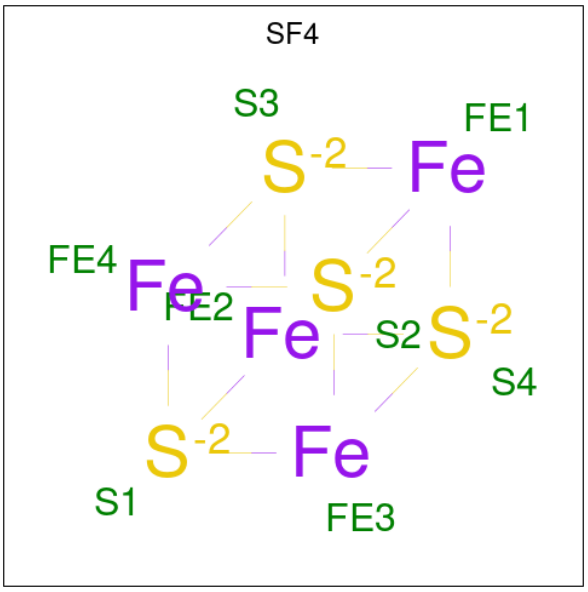


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C Fe N O 7 3 1 2 1	0	0

- Molecule 7 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

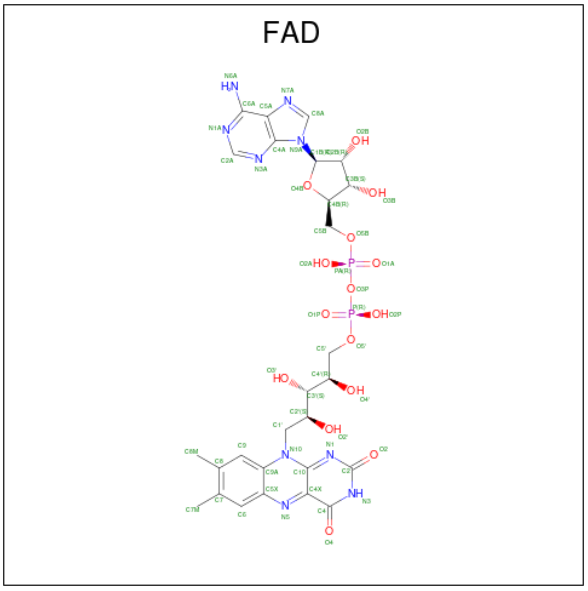
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ni 1 1	0	0

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



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

- Molecule 9 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					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	1
			53	27	9	15	2		

- Molecule 10 is water.

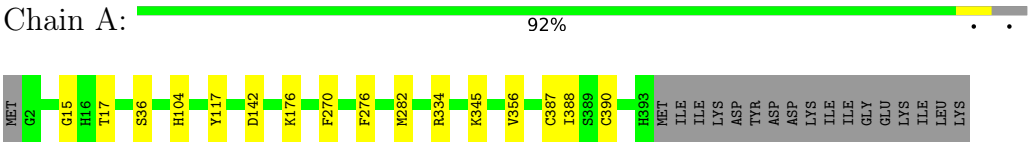
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	340	Total	O	0	4
			340	340		
10	B	180	Total	O	0	11
			180	180		
10	C	205	Total	O	0	3
			205	205		

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

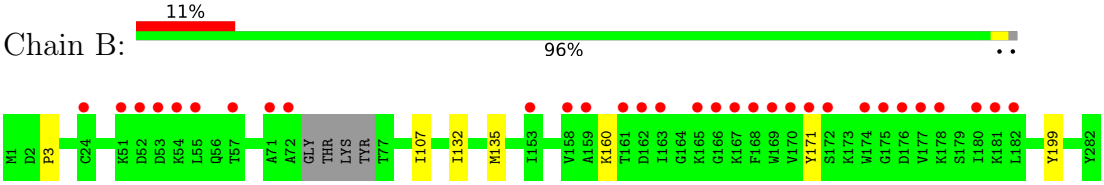
• Molecule 1: F420-reducing [NiFe]-hydrogenase from Methanothermococcus thermolithotrophicus alpha subunit

Chain A:



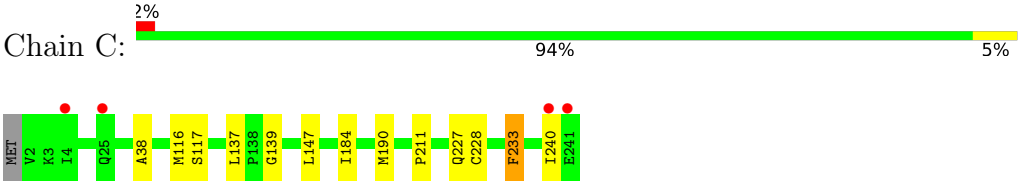
• Molecule 2: F420-reducing [NiFe]-hydrogenase from Methanothermococcus thermolithotrophicus beta subunit

Chain B:



• Molecule 3: F420-reducing [NiFe]-hydrogenase from Methanothermococcus thermolithotrophicus gamma subunit

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	95.03Å 163.48Å 128.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.41 – 1.65 64.41 – 1.65	Depositor EDS
% Data completeness (in resolution range)	77.3 (64.41-1.65) 77.3 (64.41-1.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 1.65Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.141 , 0.183 0.143 , 0.183	Depositor DCC
R_{free} test set	4605 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.008 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.016 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	15123	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.36	0/3197	0.62	1/4327 (0.0%)
2	B	0.37	0/2185	0.59	0/2947
3	C	0.43	0/1838	0.66	2/2488 (0.1%)
All	All	0.38	0/7220	0.62	3/9762 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	139	GLY	CA-C-O	-6.81	117.53	122.23
1	A	142	ASP	CA-CB-CG	5.29	117.89	112.60
3	C	233	PHE	N-CA-CB	5.14	116.52	110.71

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	3097	3077	3051	12	0
2	B	2145	2191	2191	4	0
3	C	1808	1845	1833	6	0
4	A	30	40	40	0	0
4	B	12	16	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	18	24	24	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	7	0	0	1	0
7	A	1	0	0	0	0
8	B	8	0	0	0	0
8	C	24	0	0	0	0
9	B	53	0	31	1	0
10	A	340	0	0	2	0
10	B	180	0	0	0	0
10	C	205	0	0	0	0
All	All	7930	7193	7186	21	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 1.

The worst 5 of 21 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:17:THR:HG23	1:A:388:ILE:HG13	1.58	0.84
3:C:137:LEU:CD1	3:C:147:LEU:HD23	2.34	0.57
1:A:345:LYS:NZ	10:A:601:HOH:O	2.38	0.57
3:C:137:LEU:HD13	3:C:147:LEU:HD23	1.87	0.55
3:C:116:MET:HE3	3:C:117:SER:HA	1.90	0.53

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 X-ray entries followed by that with respect to entries of similar resolution.

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	396/410 (97%)	386 (98%)	10 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	274/282 (97%)	267 (97%)	6 (2%)	1 (0%)	30 15
3	C	240/241 (100%)	227 (95%)	12 (5%)	1 (0%)	30 15
All	All	910/933 (98%)	880 (97%)	28 (3%)	2 (0%)	43 27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	38	ALA
2	B	3	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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	335/347 (96%)	334 (100%)	1 (0%)	86 80
2	B	235/238 (99%)	235 (100%)	0	100 100
3	C	206/205 (100%)	204 (99%)	2 (1%)	68 52
All	All	776/790 (98%)	773 (100%)	3 (0%)	84 77

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	HIS
3	C	190	MET
3	C	240	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	185	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	A	505	-	5,5,5	0.63	0	5,5,5	0.93	0
4	GOL	B	404	-	5,5,5	0.09	0	5,5,5	0.33	0
4	GOL	A	504	-	5,5,5	0.66	0	5,5,5	0.90	0
8	SF4	B	401	2	0,12,12	-	-	-		
4	GOL	A	503	-	5,5,5	0.66	0	5,5,5	1.03	0
4	GOL	C	305	-	5,5,5	0.56	0	5,5,5	0.87	0
4	GOL	A	502	-	5,5,5	0.08	0	5,5,5	0.39	0
4	GOL	C	306	-	5,5,5	0.09	0	5,5,5	0.34	0
4	GOL	B	403	-	5,5,5	0.62	0	5,5,5	0.95	0
8	SF4	C	304	3	0,12,12	-	-	-		
4	GOL	C	301	-	5,5,5	0.10	0	5,5,5	0.32	0
8	SF4	C	302	3	0,12,12	-	-	-		
8	SF4	C	303	3	0,12,12	-	-	-		
9	FAD	B	402[A]	-	56,58,58	0.49	0	81,89,89	0.45	0
4	GOL	A	506	-	5,5,5	0.46	0	5,5,5	0.87	0
6	FCO	A	508	1,7	1,6,6	3.26	1 (100%)	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	505	-	-	0/4/4/4	-
4	GOL	B	404	-	-	3/4/4/4	-
4	GOL	A	504	-	-	0/4/4/4	-
8	SF4	B	401	2	-	-	0/6/5/5
4	GOL	A	503	-	-	0/4/4/4	-
4	GOL	C	305	-	-	0/4/4/4	-
4	GOL	A	502	-	-	2/4/4/4	-
4	GOL	C	306	-	-	1/4/4/4	-
4	GOL	B	403	-	-	4/4/4/4	-
8	SF4	C	304	3	-	-	0/6/5/5
4	GOL	C	301	-	-	2/4/4/4	-
8	SF4	C	302	3	-	-	0/6/5/5
8	SF4	C	303	3	-	-	0/6/5/5
9	FAD	B	402[A]	-	-	4/34/50/50	0/6/6/6
4	GOL	A	506	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	508	FCO	O3-C3	3.26	1.20	1.16

There are no bond angle outliers.

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	GOL	C1-C2-C3-O3
4	A	502	GOL	O2-C2-C3-O3
4	B	403	GOL	C1-C2-C3-O3
4	B	404	GOL	O1-C1-C2-O2
4	B	404	GOL	O1-C1-C2-C3

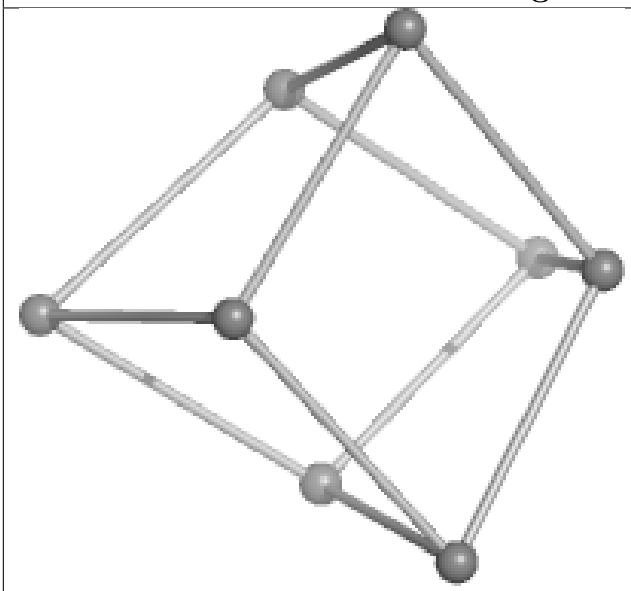
There are no ring outliers.

2 monomers are involved in 2 short contacts:

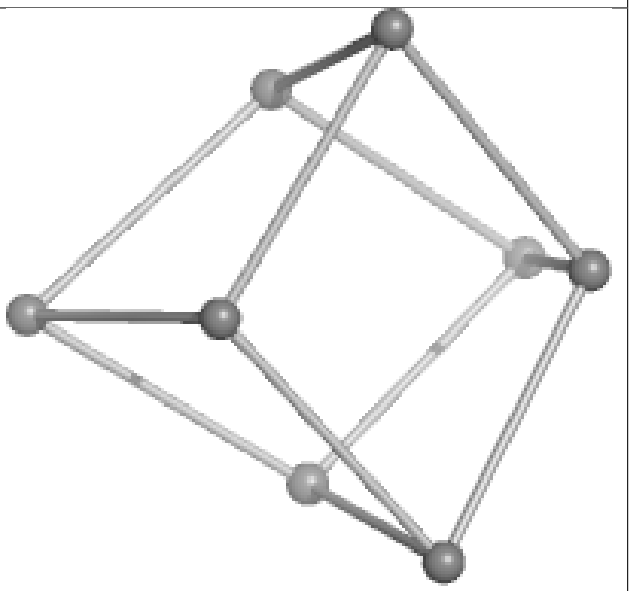
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	402[A]	FAD	1	0
6	A	508	FCO	1	0

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.

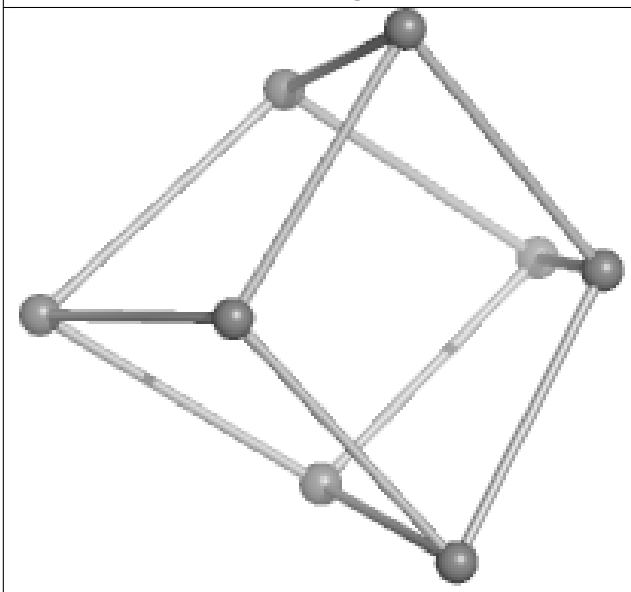
Ligand SF4 B 401



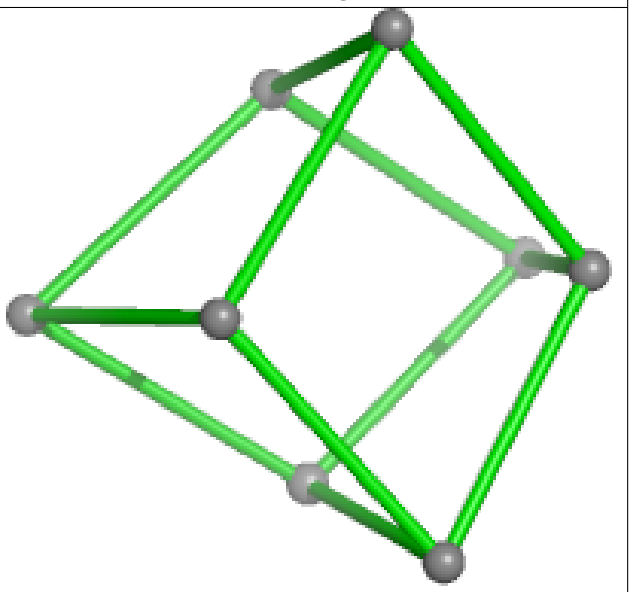
Bond lengths



Bond angles

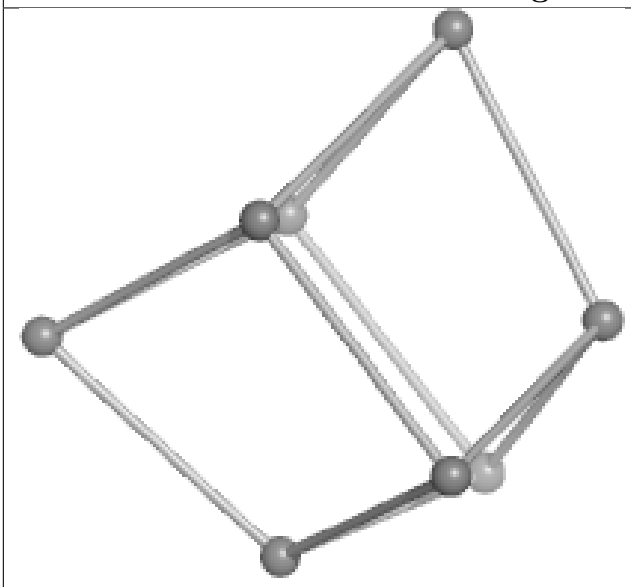


Torsions

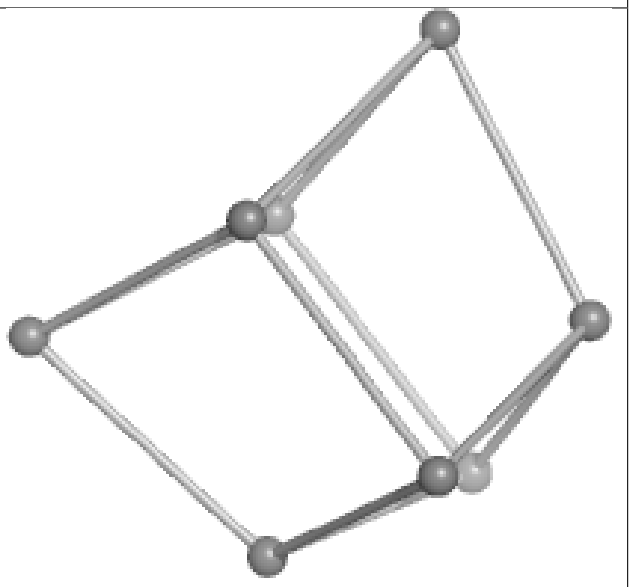


Rings

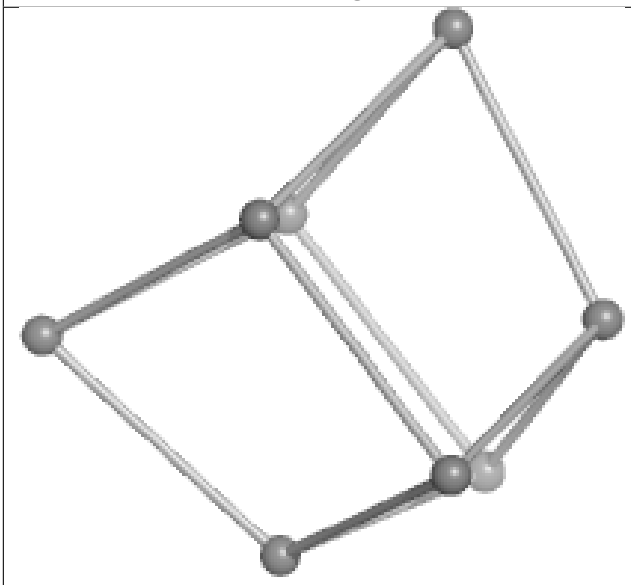
Ligand SF4 C 304



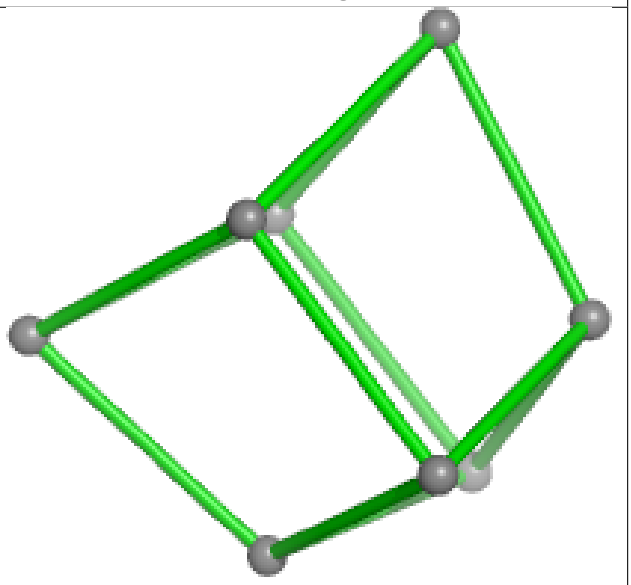
Bond lengths



Bond angles

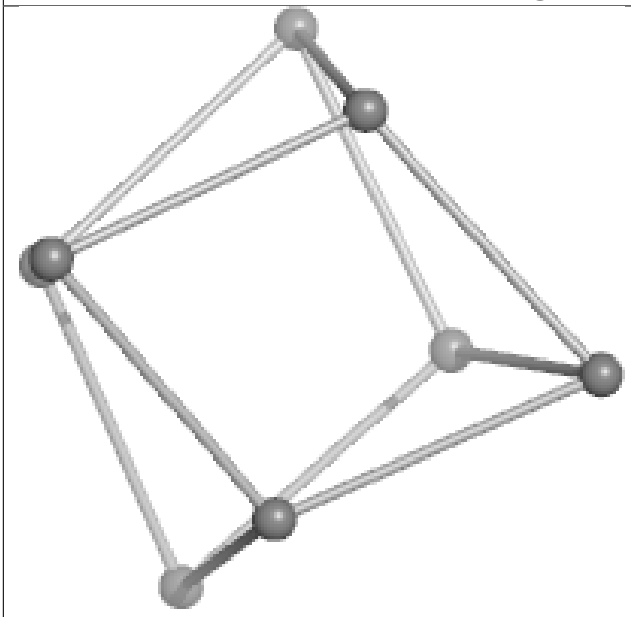


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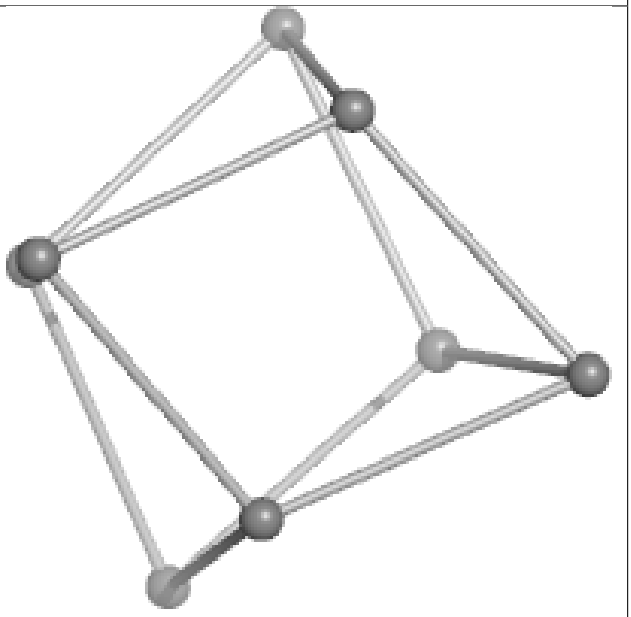


Rings

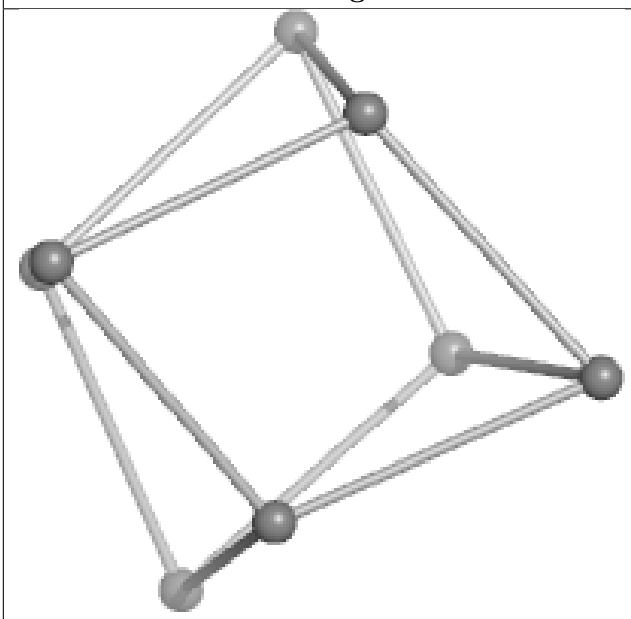
Ligand SF4 C 302



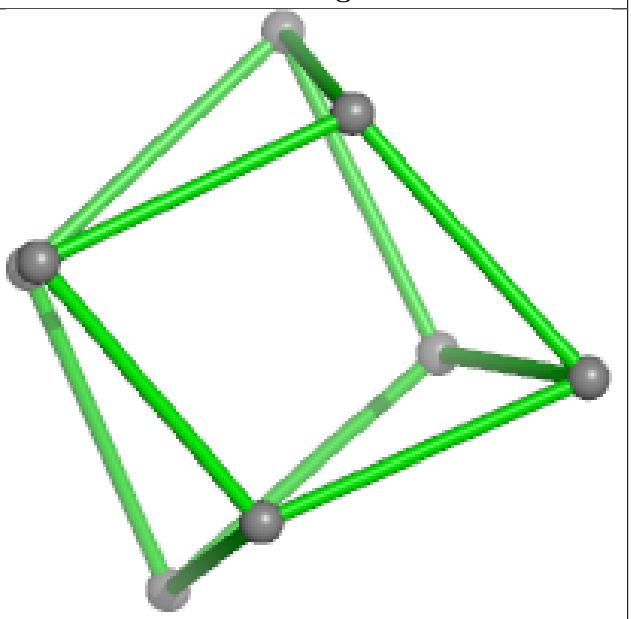
Bond lengths



Bond angles

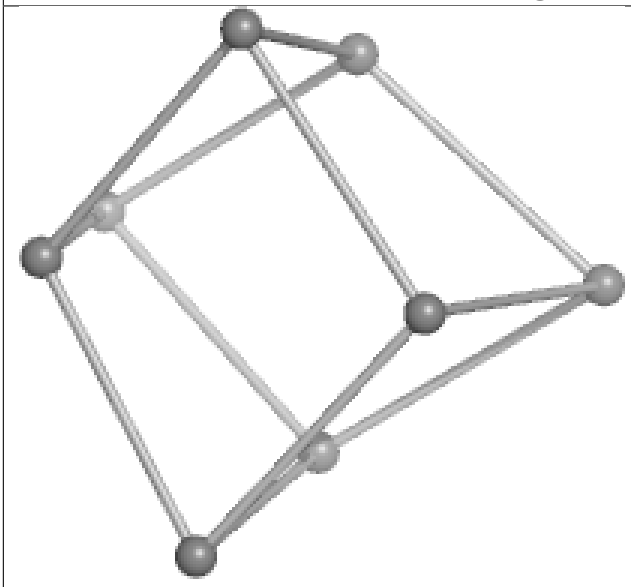


Torsions

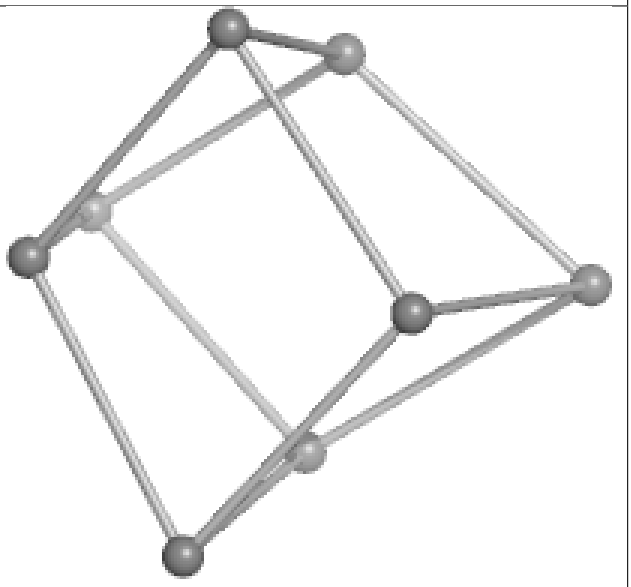


Rings

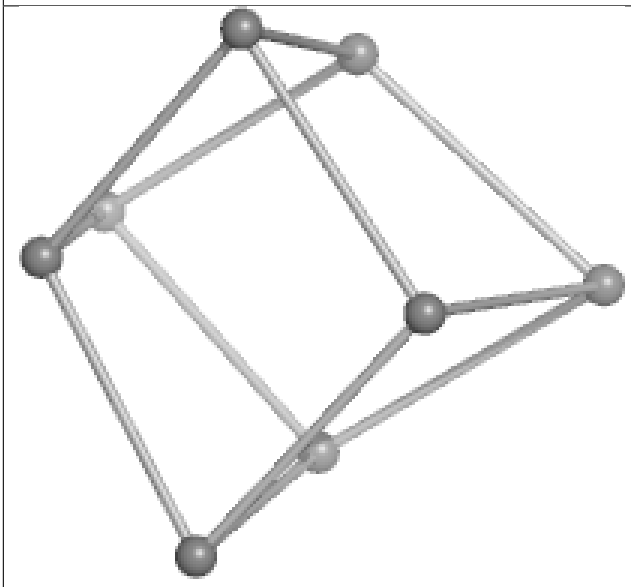
Ligand SF4 C 303



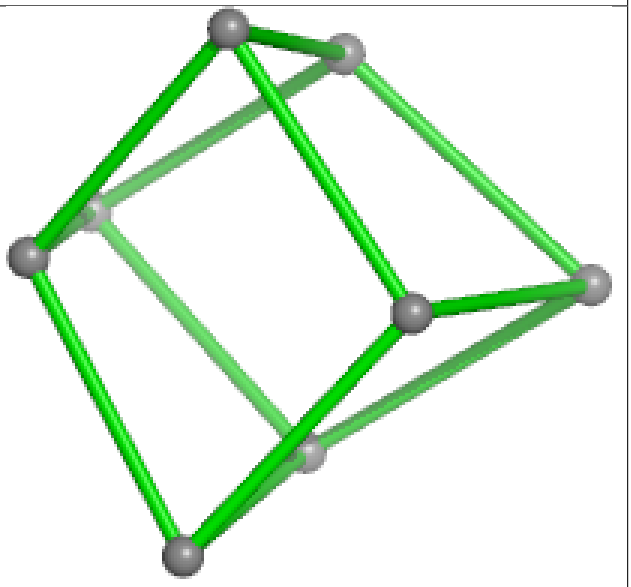
Bond lengths



Bond angles

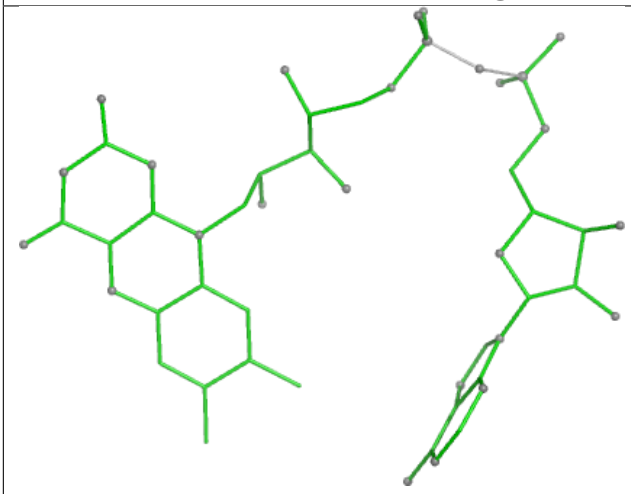


Torsions

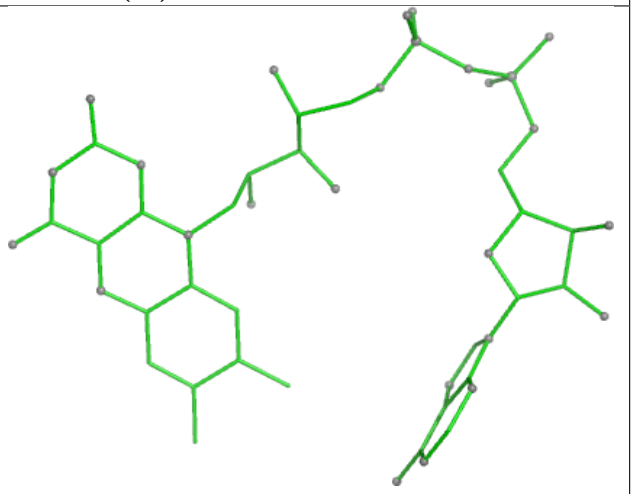


Rings

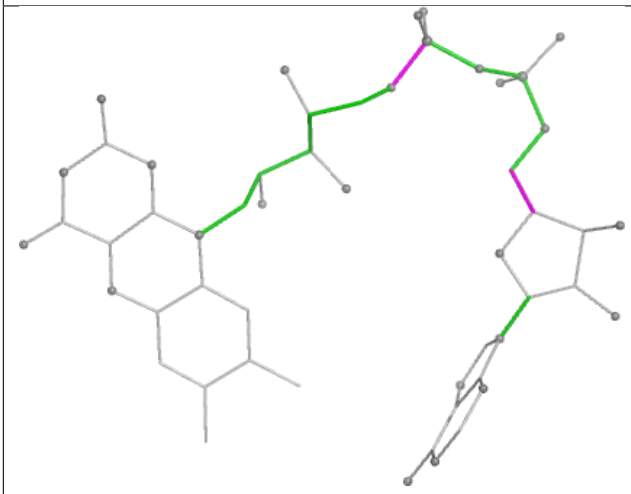
Ligand FAD B 402 (A)



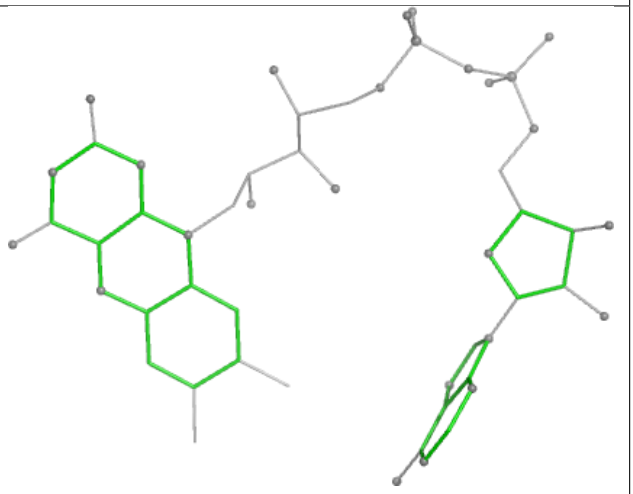
Bond lengths



Bond angles

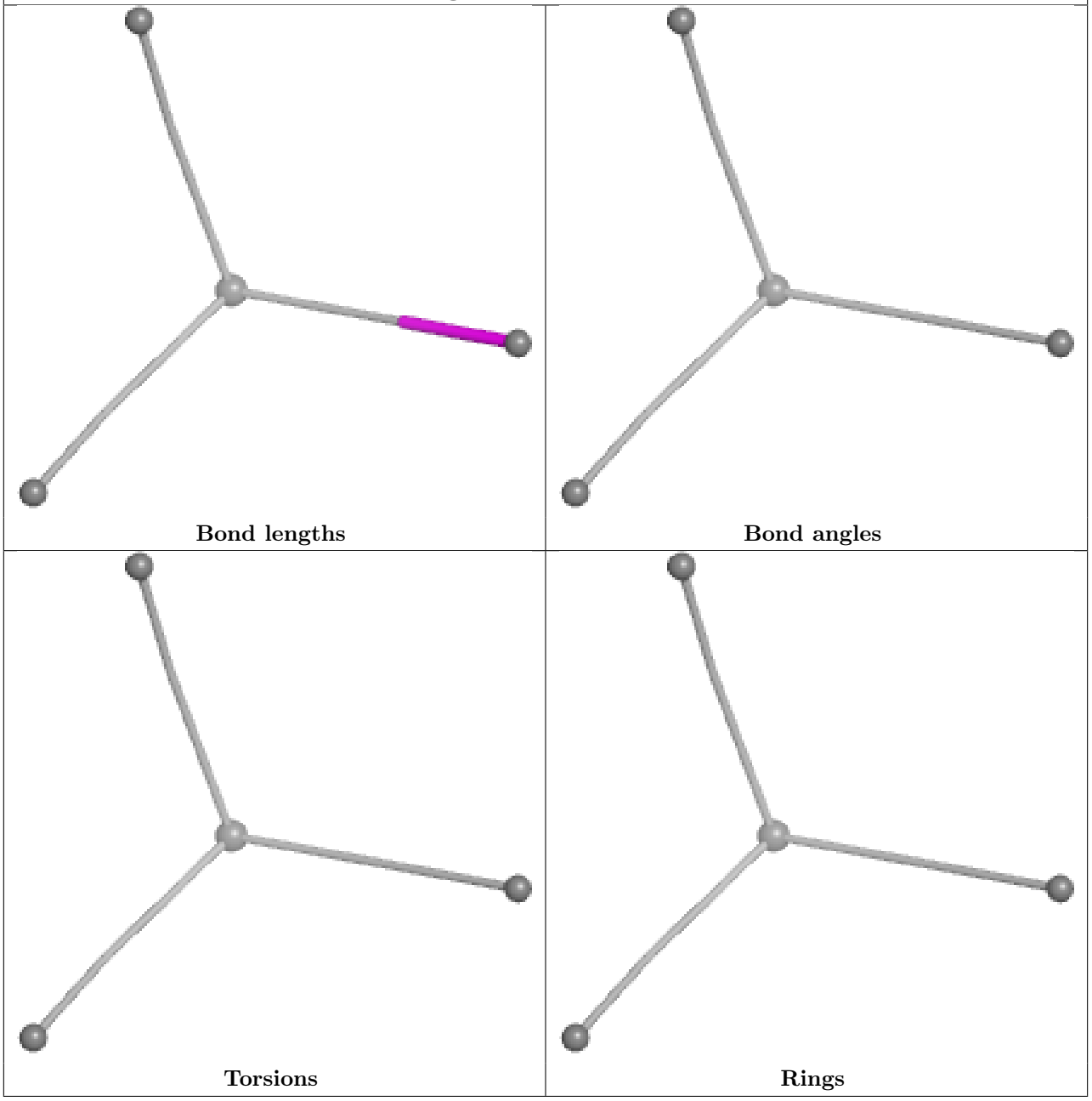


Torsions



Rings

Ligand FCO A 508



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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	392/410 (95%)	-0.55	0 100 100	15, 31, 52, 75	3 (0%)
2	B	278/282 (98%)	0.28	31 (11%) 10 11	23, 40, 95, 119	0
3	C	240/241 (99%)	-0.43	4 (1%) 69 74	21, 30, 51, 94	1 (0%)
All	All	910/933 (97%)	-0.27	35 (3%) 44 48	15, 33, 79, 119	4 (0%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	163	ILE	5.6
2	B	182	LEU	5.4
2	B	174	TRP	5.3
2	B	55	LEU	5.2
2	B	169	TRP	5.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

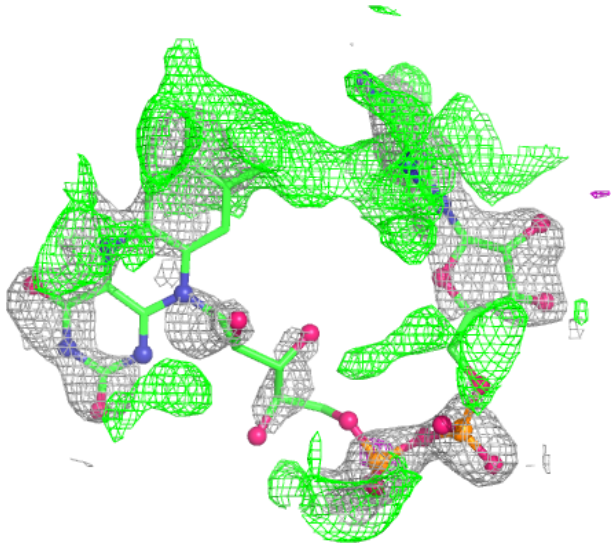
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

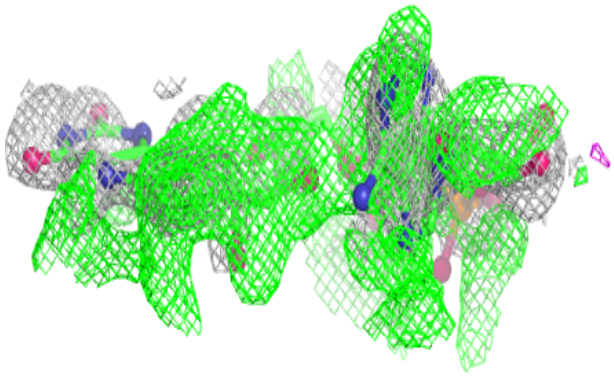
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	B	404	6/6	0.56	0.14	54,65,66,66	0
4	GOL	C	306	6/6	0.65	0.14	53,63,65,65	0
4	GOL	B	403	6/6	0.66	0.14	74,89,91,91	0
4	GOL	C	301	6/6	0.74	0.16	49,58,62,64	0
4	GOL	A	503	6/6	0.74	0.15	70,84,86,86	0
4	GOL	A	502	6/6	0.75	0.16	41,57,67,69	0
9	FAD	B	402[A]	53/53	0.75	0.28	41,45,48,48	53
4	GOL	A	505	6/6	0.77	0.18	65,78,80,81	0
4	GOL	A	504	6/6	0.79	0.16	64,77,78,78	0
4	GOL	C	305	6/6	0.79	0.12	74,89,91,91	0
4	GOL	A	506	6/6	0.89	0.11	57,69,73,73	0
5	FE	B	405	1/1	0.98	0.07	58,58,58,58	0
6	FCO	A	508	7/7	0.99	0.06	21,22,24,24	0
7	NI	A	509	1/1	1.00	0.06	25,25,25,25	0
8	SF4	B	401	8/8	1.00	0.02	28,29,30,30	0
8	SF4	C	302	8/8	1.00	0.03	21,22,22,22	0
8	SF4	C	303	8/8	1.00	0.02	22,22,23,24	0
8	SF4	C	304	8/8	1.00	0.02	22,22,23,24	0
5	FE	A	507	1/1	1.00	0.03	24,24,24,24	0

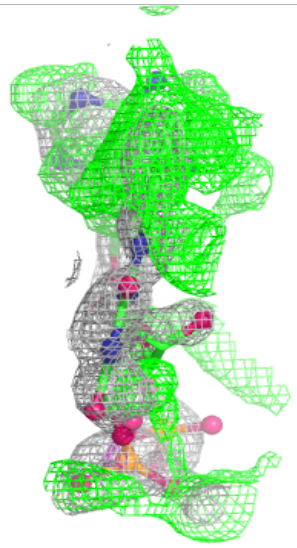
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD B 402 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

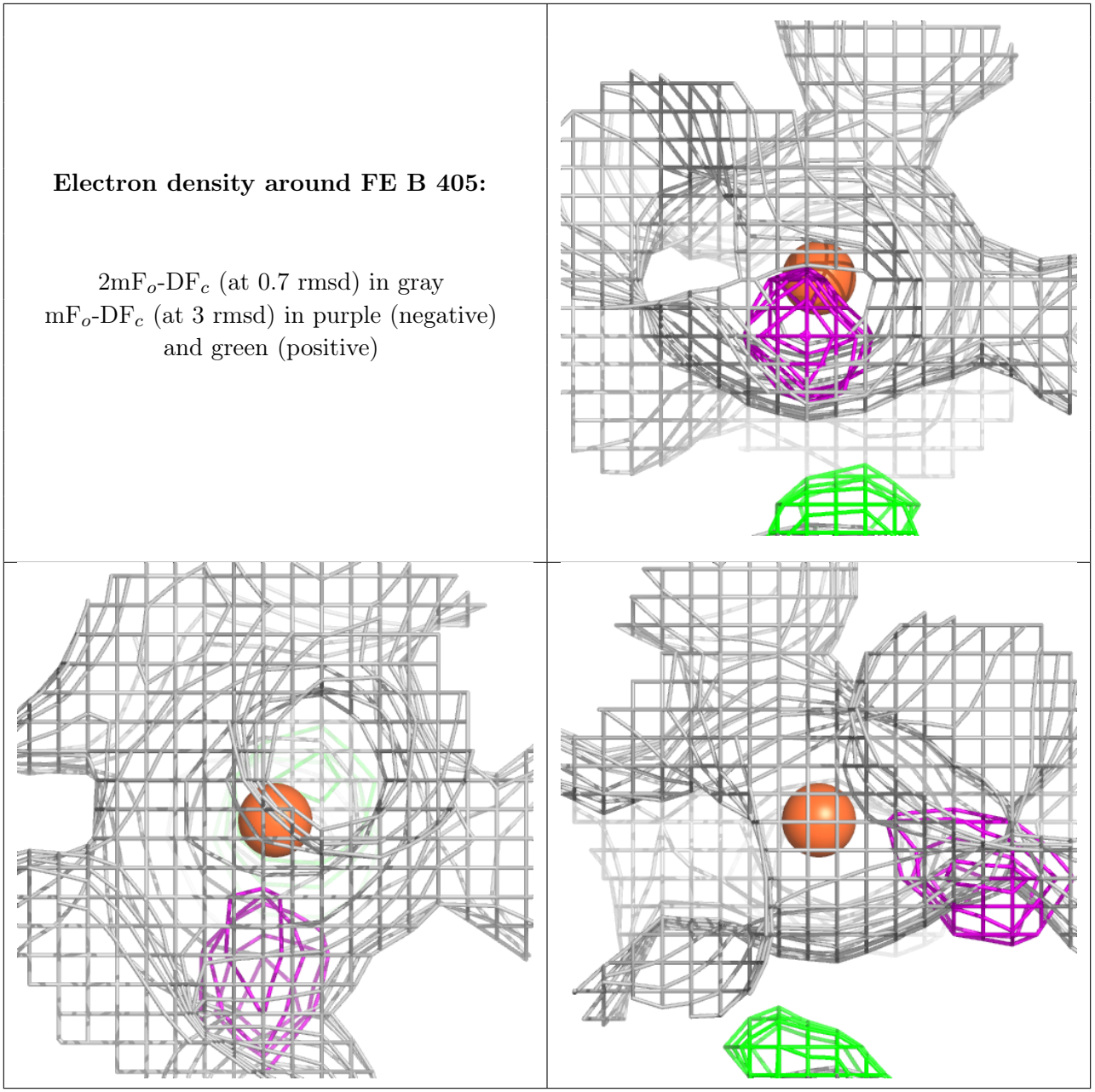






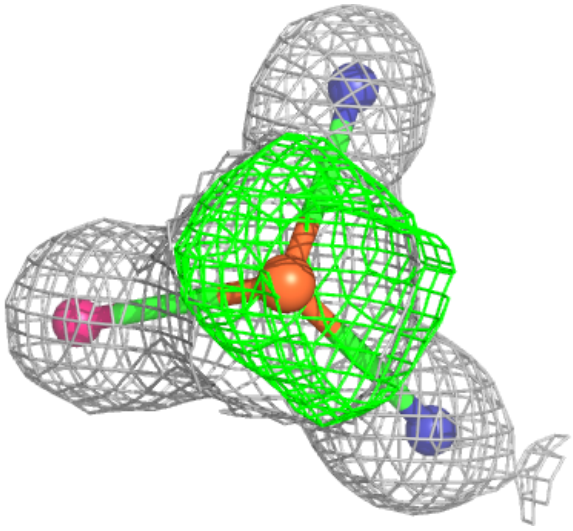
Electron density around FE B 405:

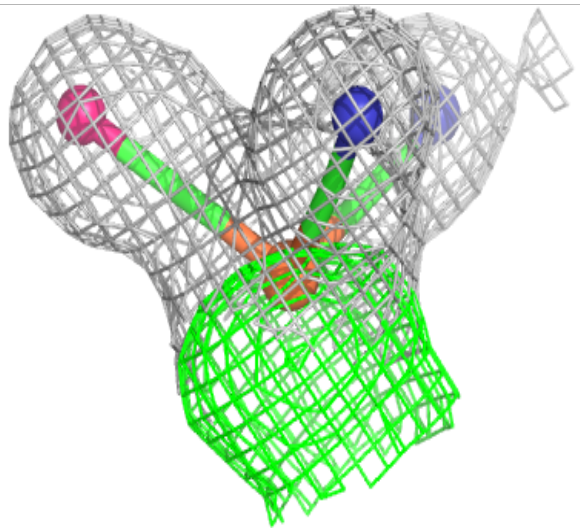
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

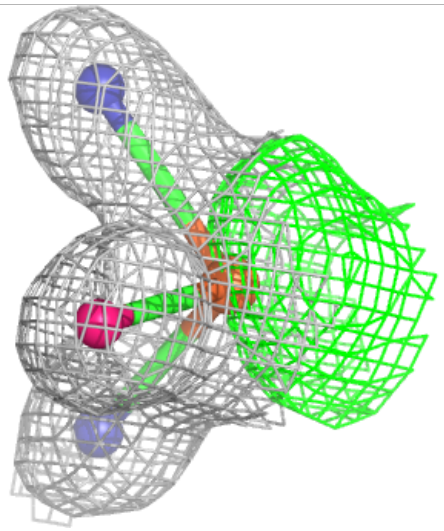


Electron density around FCO A 508:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

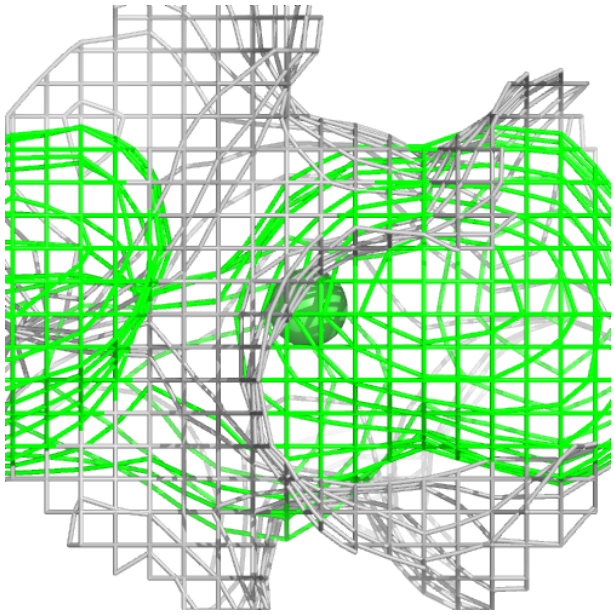


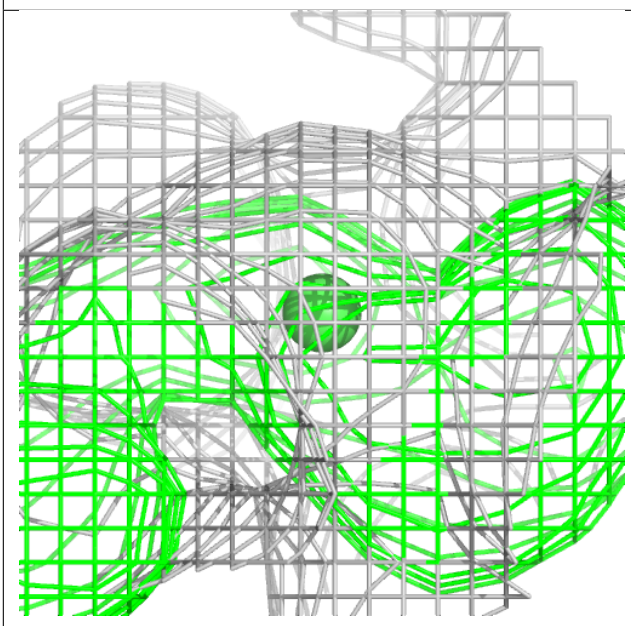


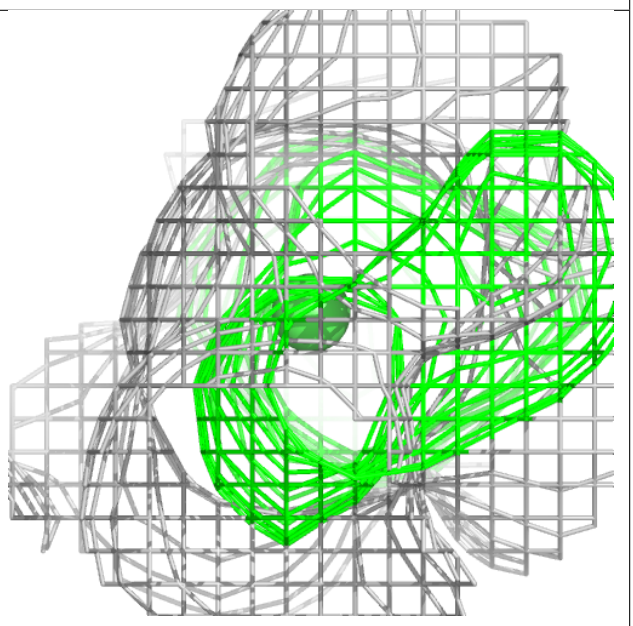


Electron density around NI A 509:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

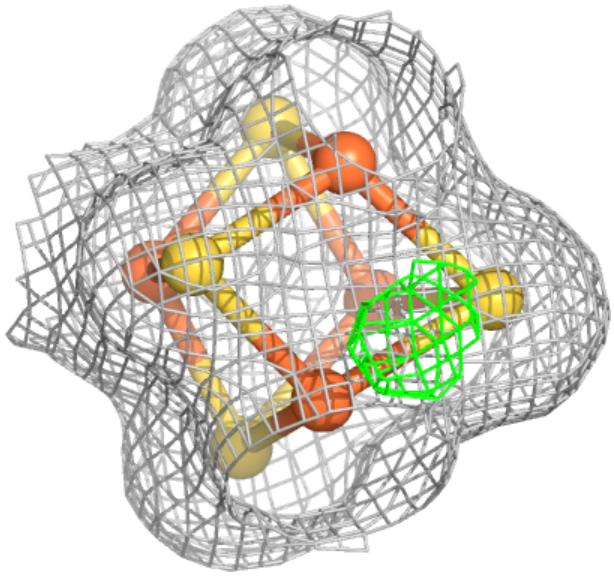


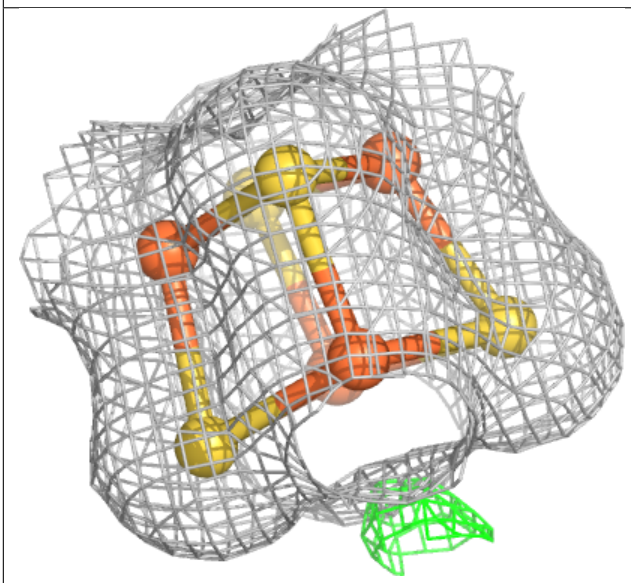


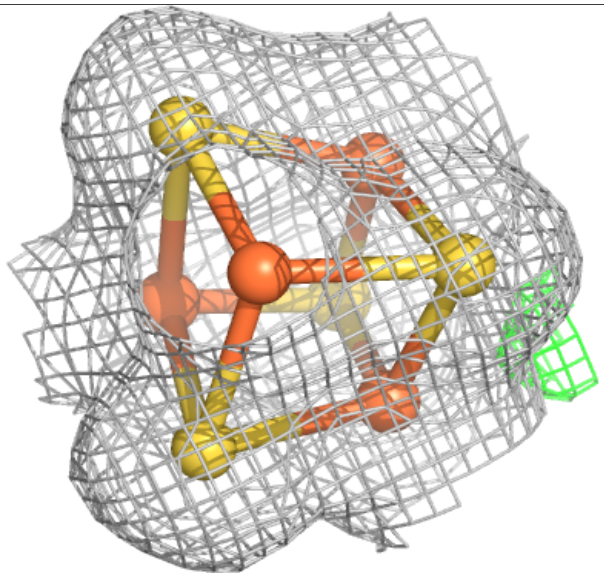


Electron density around SF4 B 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

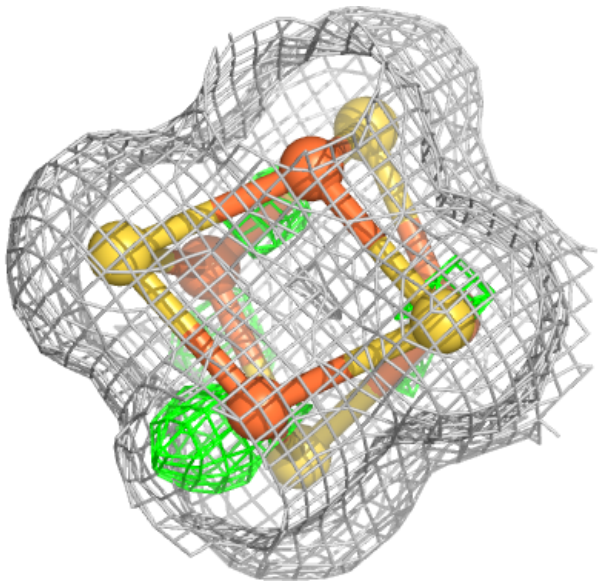


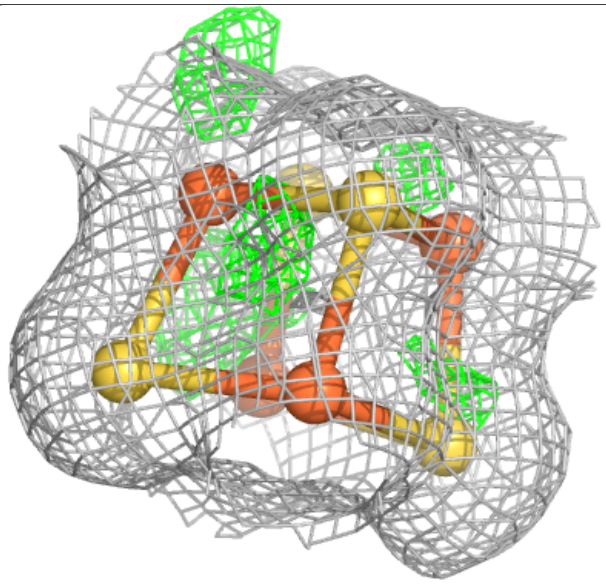


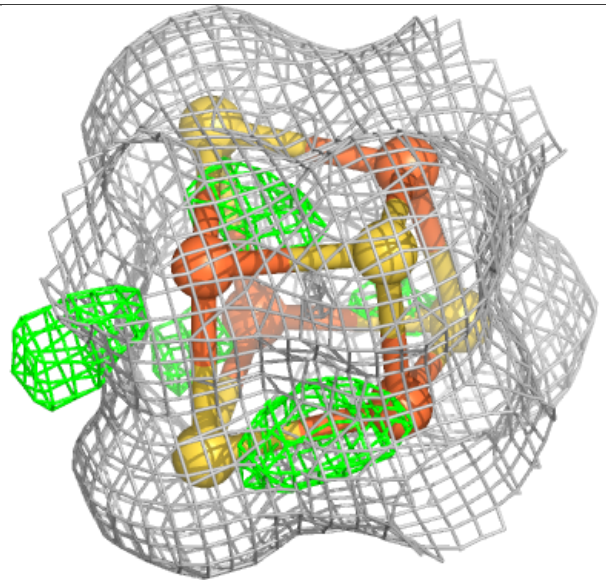


Electron density around SF4 C 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

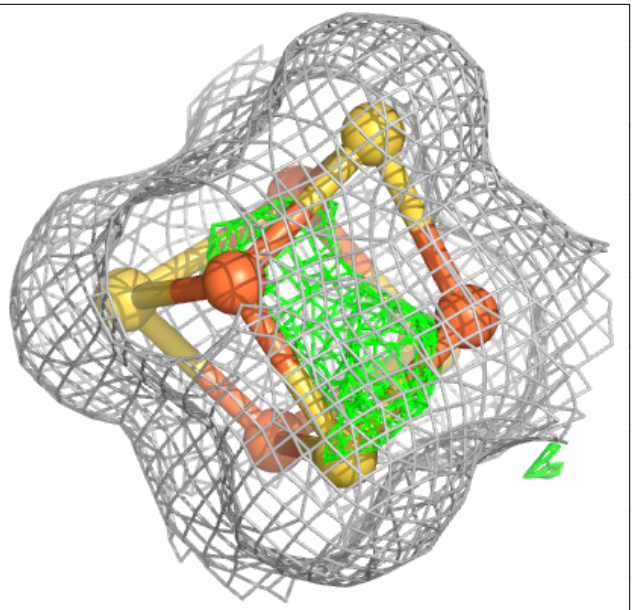


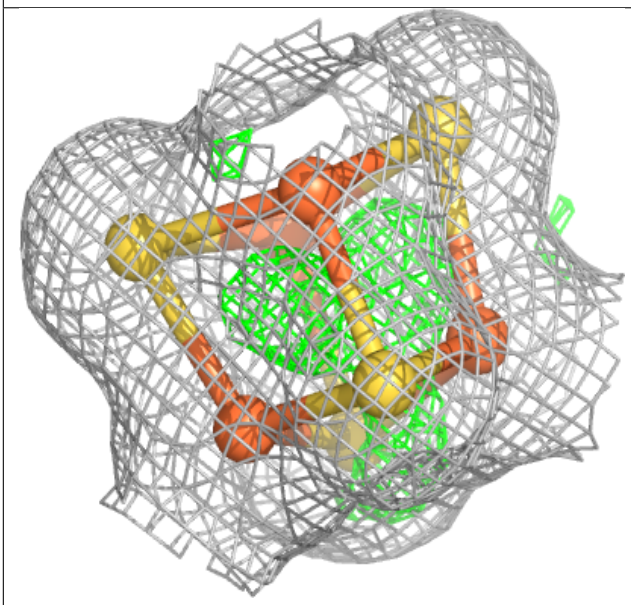


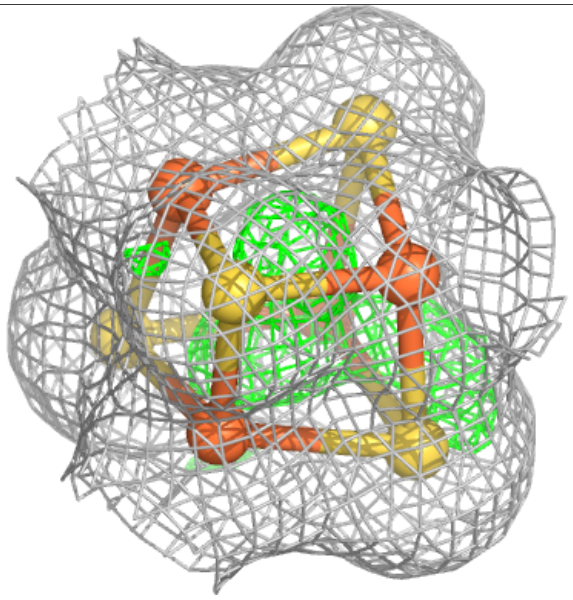


Electron density around SF4 C 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

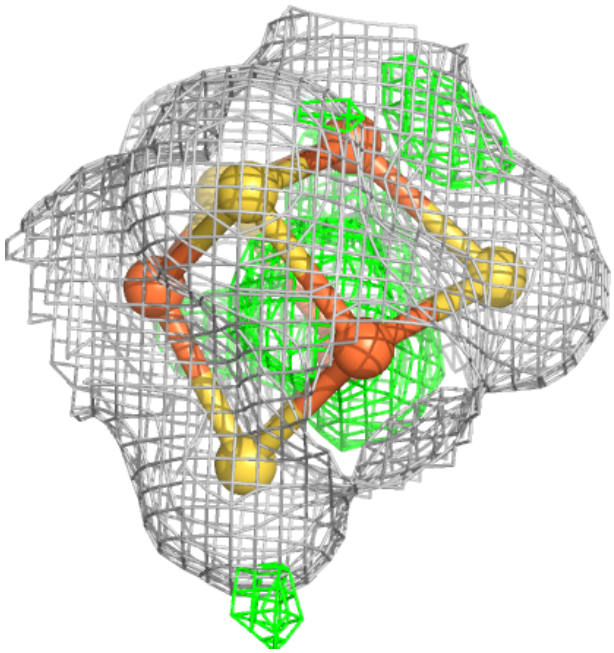


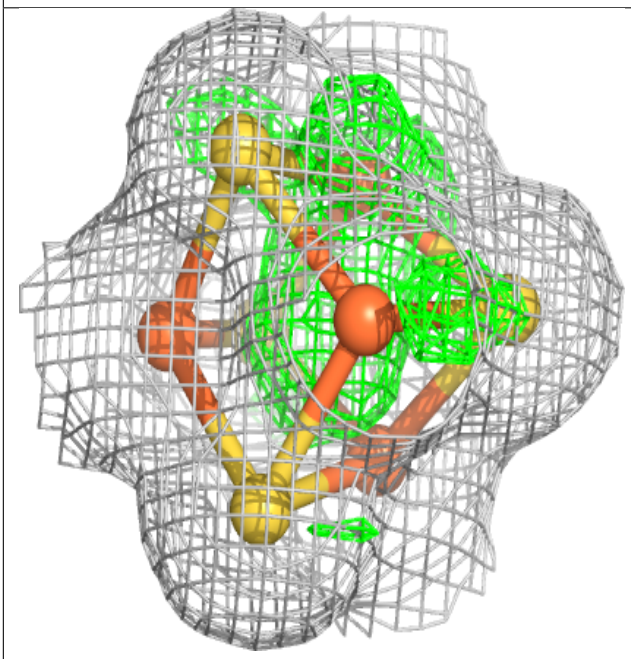


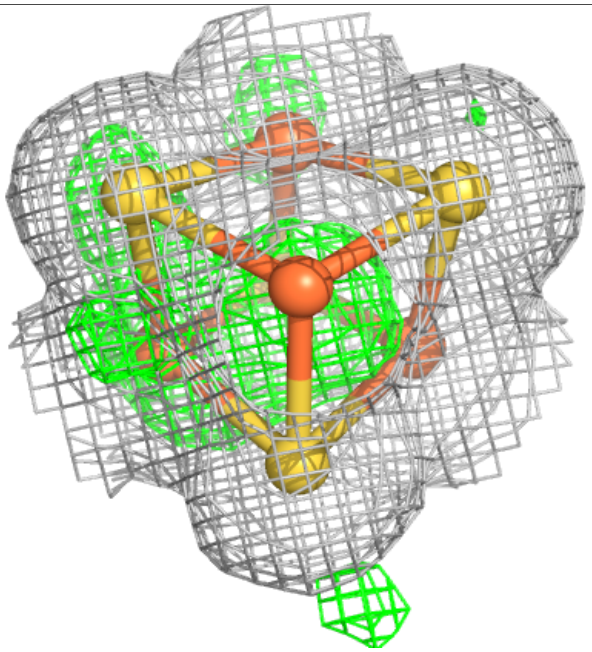


Electron density around SF4 C 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

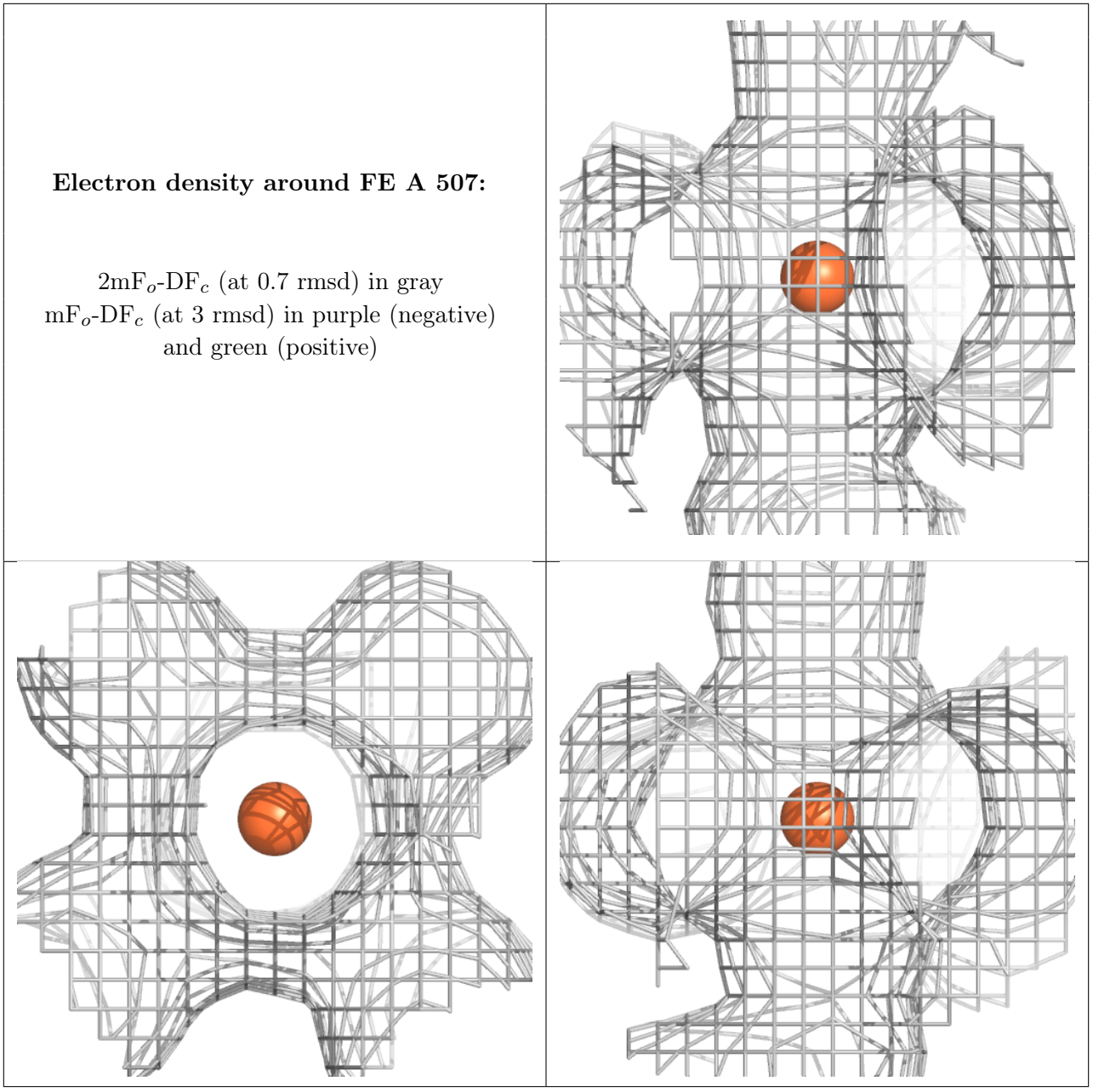






Electron density around FE A 507:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.