Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2025 – 02:18 am GMT

PDB ID	:	8RU7
Title	:	Desulfovibrio desulfuricans [FeFe]-hydrogenase variant with both subunits linked by a 13 amino acid linker peptide derived from CpI of Clostridium pasteurianum
Authors	:	Bikbaev, K.; Jaenecke, J.; Winkler, M.; Span, I.
Deposited on	:	2024-01-30
Resolution	:	1.32 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

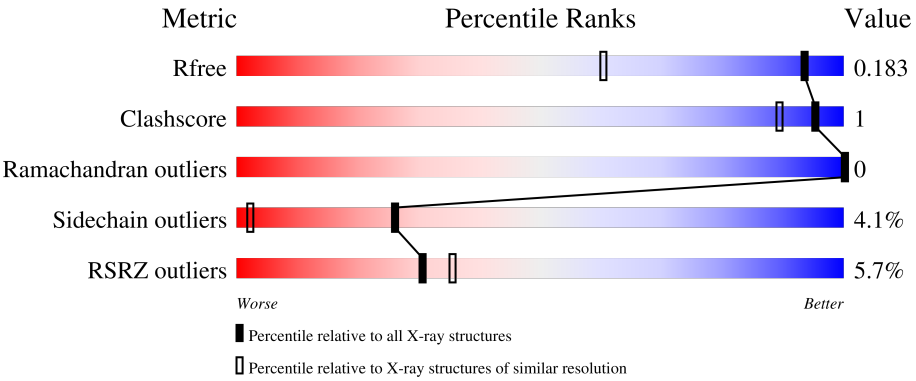
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 1.32 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}	164625	2202 (1.34-1.30)
Clashscore	180529	2378 (1.34-1.30)
Ramachandran outliers	177936	2325 (1.34-1.30)
Sidechain outliers	177891	2325 (1.34-1.30)
RSRZ outliers	164620	2199 (1.34-1.30)

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	492	5% 86% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7639 atoms, of which 3692 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.

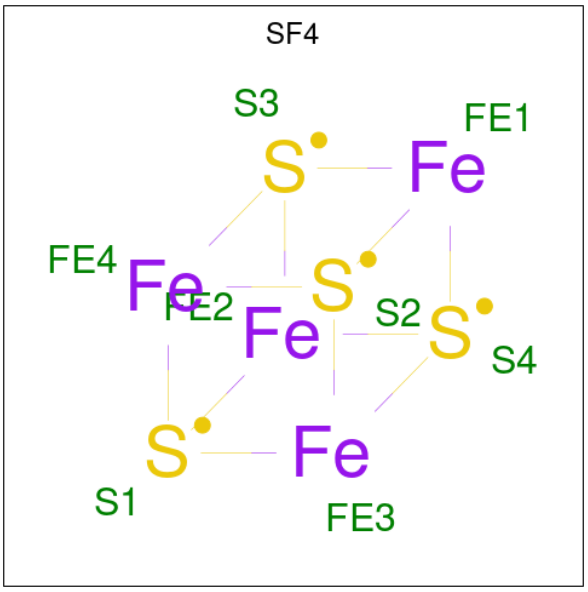
- Molecule 1 is a protein called Periplasmic [Fe] hydrogenase large subunit,CpI,Periplasmic [Fe] hydrogenase small subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	471	7371	2345	3685	617	687	37	302	14	0

There are 10 discrepancies between the modelled and reference sequences:

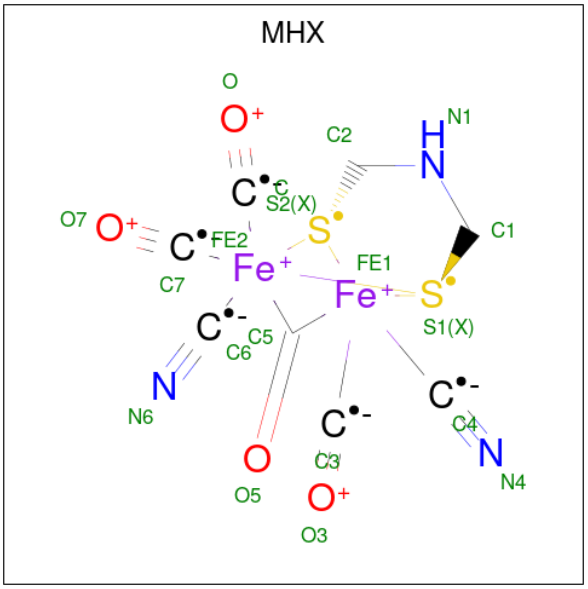
Chain	Residue	Modelled	Actual	Comment	Reference
A	483	SER	-	expression tag	UNP P07603
A	484	ALA	-	expression tag	UNP P07603
A	485	TRP	-	expression tag	UNP P07603
A	486	SER	-	expression tag	UNP P07603
A	487	HIS	-	expression tag	UNP P07603
A	488	PRO	-	expression tag	UNP P07603
A	489	GLN	-	expression tag	UNP P07603
A	490	PHE	-	expression tag	UNP P07603
A	491	GLU	-	expression tag	UNP P07603
A	492	LYS	-	expression tag	UNP P07603

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0

- Molecule 3 is Binuclear [FeFe], di(thiomethyl)amine, carbon monoxide, cyanide cluster (-CO form) (three-letter code: MHX) (formula: $C_8H_5Fe_2N_3O_4S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Fe	H	N	O	S	1	0
			26	8	2	7	3	4	2		

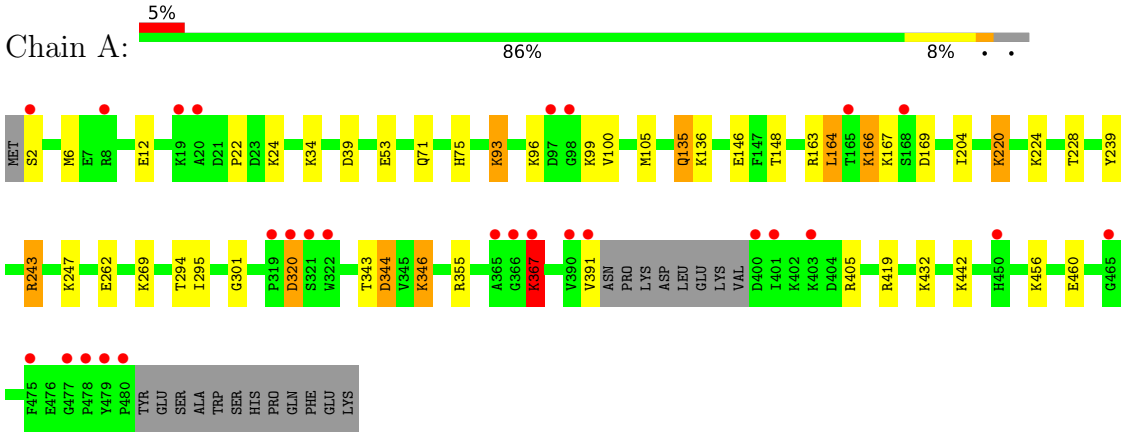
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	218	Total	O	0	0
			218	218		

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: Periplasmic [Fe] hydrogenase large subunit,CpI,Periplasmic [Fe] hydrogenase small subunit



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.18Å 88.77Å 53.04Å 90.00° 110.27° 90.00°	Depositor
Resolution (Å)	47.11 – 1.32 47.11 – 1.32	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.11-1.32) 97.5 (47.11-1.32)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 1.32Å)	Xtriage
Refinement program	REFMAC 5.8.0425, REFMAC 5.8.0425	Depositor
R, R_{free}	0.161 , 0.181 0.162 , 0.183	Depositor DCC
R_{free} test set	4959 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	14.9	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7639	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MHX

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	1.65	22/3835 (0.6%)	2.04	35/5186 (0.7%)

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	6

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320[A]	ASP	CB-CG	49.47	2.55	1.51
1	A	320[B]	ASP	CB-CG	49.47	2.55	1.51
1	A	135	GLN	CD-OE1	26.42	1.82	1.24
1	A	460	GLU	CD-OE1	24.92	1.53	1.25
1	A	136	LYS	CE-NZ	18.31	1.94	1.49
1	A	460	GLU	CD-OE2	-18.00	1.05	1.25
1	A	93	LYS	CG-CD	17.03	2.10	1.52
1	A	346	LYS	CE-NZ	-16.99	1.06	1.49
1	A	34	LYS	CE-NZ	-16.47	1.07	1.49
1	A	456	LYS	CE-NZ	14.06	1.84	1.49
1	A	96	LYS	CD-CE	14.02	1.86	1.51
1	A	247	LYS	CE-NZ	-13.19	1.16	1.49
1	A	367	LYS	C-O	-11.93	1.00	1.23
1	A	53	GLU	CG-CD	-10.07	1.36	1.51
1	A	24	LYS	CE-NZ	8.81	1.71	1.49
1	A	169	ASP	CB-CG	-7.85	1.35	1.51
1	A	367	LYS	CA-C	7.56	1.72	1.52
1	A	269	LYS	CD-CE	6.91	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346	LYS	CD-CE	6.52	1.67	1.51
1	A	220	LYS	CE-NZ	5.84	1.63	1.49
1	A	344	ASP	CG-OD2	5.81	1.38	1.25
1	A	367	LYS	CA-CB	5.30	1.65	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	320[A]	ASP	CB-CG-OD2	-70.95	54.45	118.30
1	A	320[B]	ASP	CB-CG-OD2	-70.95	54.45	118.30
1	A	320[A]	ASP	CB-CG-OD1	-48.54	74.62	118.30
1	A	320[B]	ASP	CB-CG-OD1	-48.54	74.62	118.30
1	A	456	LYS	CD-CE-NZ	-14.57	78.19	111.70
1	A	136	LYS	CD-CE-NZ	-11.69	84.81	111.70
1	A	367	LYS	CA-C-N	-10.49	94.11	117.20
1	A	220	LYS	CD-CE-NZ	-10.37	87.86	111.70
1	A	320[A]	ASP	CA-CB-CG	9.83	135.03	113.40
1	A	320[B]	ASP	CA-CB-CG	9.83	135.03	113.40
1	A	344	ASP	OD1-CG-OD2	-9.75	104.77	123.30
1	A	34	LYS	CD-CE-NZ	-9.39	90.11	111.70
1	A	166	LYS	CA-CB-CG	8.80	132.76	113.40
1	A	460	GLU	CG-CD-OE2	8.59	135.48	118.30
1	A	355	ARG	NE-CZ-NH1	-8.47	116.06	120.30
1	A	405	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	A	24	LYS	CD-CE-NZ	-8.31	92.58	111.70
1	A	367	LYS	N-CA-C	8.10	132.87	111.00
1	A	135	GLN	OE1-CD-NE2	-6.71	106.46	121.90
1	A	367	LYS	O-C-N	-6.66	112.05	122.70
1	A	344	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	243	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	96	LYS	CD-CE-NZ	6.12	125.76	111.70
1	A	460	GLU	OE1-CD-OE2	-6.07	116.02	123.30
1	A	164	LEU	CB-CG-CD2	6.05	121.28	111.00
1	A	53	GLU	CB-CG-CD	6.03	130.48	114.20
1	A	367	LYS	CB-CA-C	-5.68	99.05	110.40
1	A	346	LYS	CD-CE-NZ	5.55	124.47	111.70
1	A	460	GLU	CG-CD-OE1	-5.55	107.20	118.30
1	A	355	ARG	CG-CD-NE	-5.50	100.24	111.80
1	A	419	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	343	THR	CA-CB-CG2	5.17	119.64	112.40
1	A	163	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	355	ARG	NE-CZ-NH2	5.11	122.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	146	GLU	CG-CD-OE2	-5.10	108.10	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	GLN	Sidechain
1	A	243	ARG	Sidechain
1	A	320[A]	ASP	Sidechain
1	A	320[B]	ASP	Sidechain
1	A	344	ASP	Sidechain
1	A	367	LYS	Mainchain

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	3686	3685	3635	7	0
2	A	24	0	0	0	0
3	A	19	7	0	1	0
4	A	218	0	0	0	0
All	All	3947	3692	3635	8	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.

All (8) 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:71:GLN:O	1:A:75:HIS:HD2	1.88	0.57
3:A:504:MHX:N1	3:A:504:MHX:C	2.73	0.52
1:A:105[B]:MET:HE3	1:A:204:ILE:HD11	1.95	0.49
1:A:105[B]:MET:HE1	1:A:228:THR:HB	1.96	0.47
1:A:99:LYS:HG2	1:A:100:VAL:HG23	1.97	0.47
1:A:22:PRO:HB2	1:A:239:TYR:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6[B]:MET:SD	1:A:262:GLU:HG2	2.60	0.42
1:A:295:ILE:O	1:A:301:GLY:HA3	2.19	0.42

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	482/492 (98%)	471 (98%)	11 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	401/406 (99%)	383 (96%)	18 (4%)	23 2

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	12	GLU
1	A	39	ASP
1	A	93	LYS

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Mol	Chain	Res	Type
1	A	148[A]	THR
1	A	148[B]	THR
1	A	148[C]	THR
1	A	164	LEU
1	A	166	LYS
1	A	167	LYS
1	A	220	LYS
1	A	224	LYS
1	A	294	THR
1	A	346	LYS
1	A	367	LYS
1	A	391	VAL
1	A	432	LYS
1	A	442	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	75	HIS
1	A	174	GLN
1	A	441	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)

4 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	$\#\|Z\| > 2$
2	SF4	A	501	1	0,12,12	-	-	-		
2	SF4	A	502	1	0,12,12	-	-	-		
3	MHX	A	504	1	12,21,21	4.17	6 (50%)	2,42,42	0.58	0
2	SF4	A	503	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
2	SF4	A	501	1	-	-	0/6/5/5
2	SF4	A	502	1	-	-	0/6/5/5
3	MHX	A	504	1	-	-	0/5/3/3
2	SF4	A	503	1	-	-	0/6/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	504	MHX	C2-S2	-8.48	1.69	1.85
3	A	504	MHX	C1-S1	-7.47	1.71	1.85
3	A	504	MHX	O5-C5	6.03	1.27	1.17
3	A	504	MHX	C6-N6	4.71	1.25	1.15
3	A	504	MHX	O-C	3.29	1.22	1.14
3	A	504	MHX	C6-FE2	-2.50	1.87	1.95

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

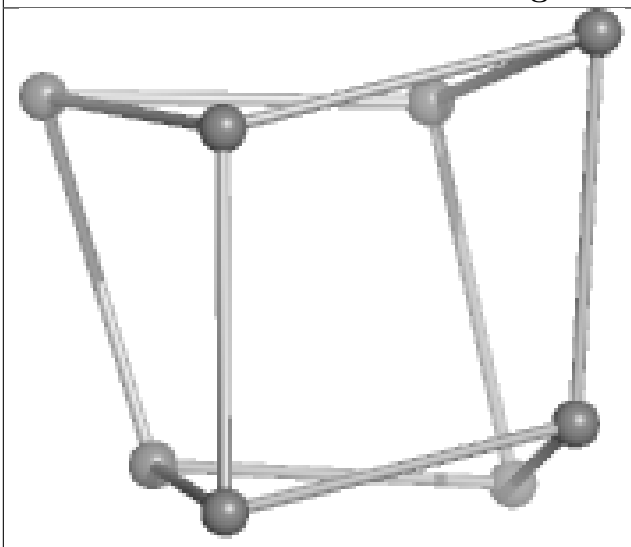
There are no ring outliers.

1 monomer is involved in 1 short contact:

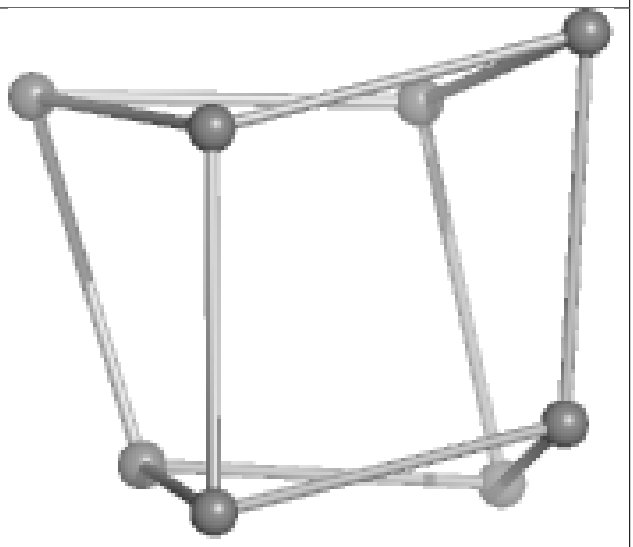
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	MHX	1	0

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.

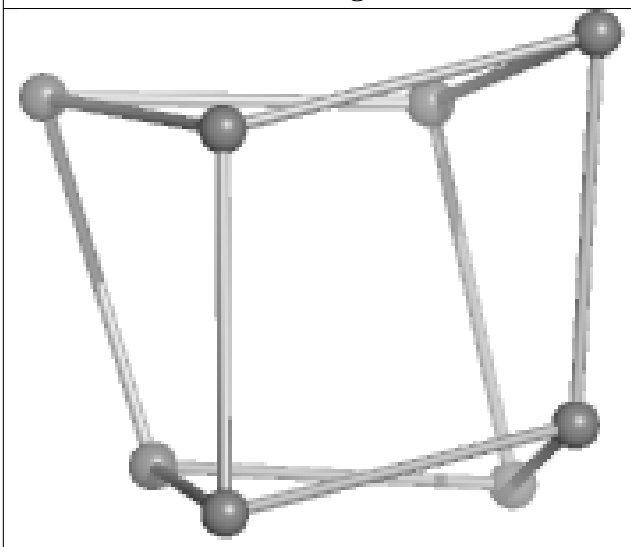
Ligand SF4 A 501



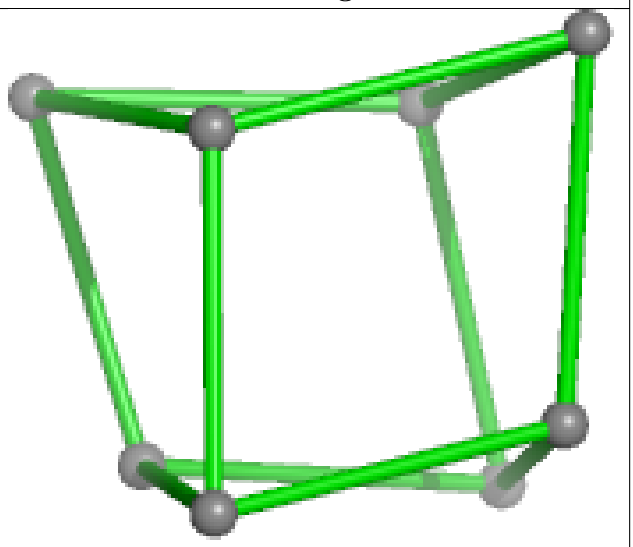
Bond lengths



Bond angles

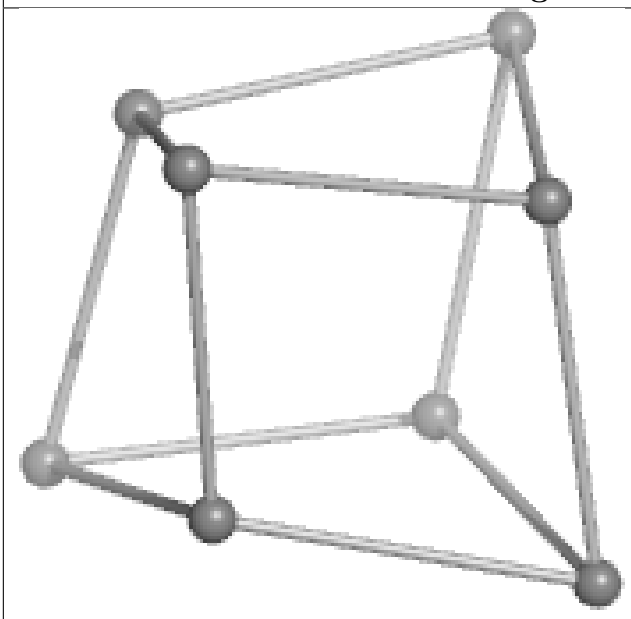


Torsions

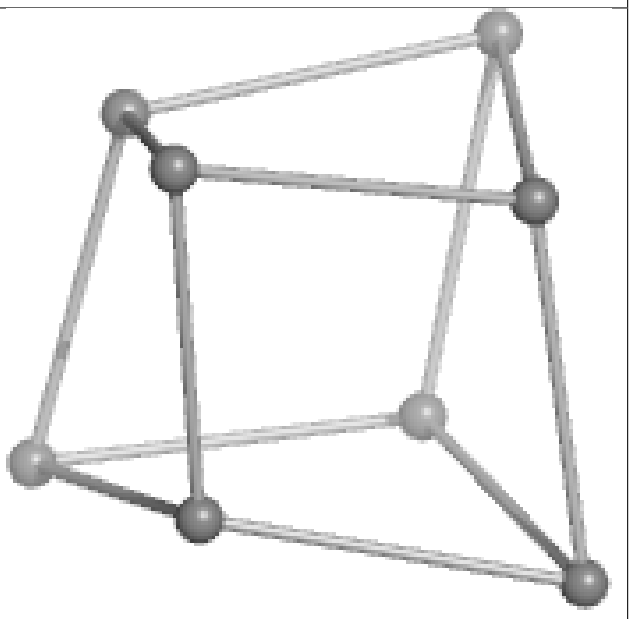


Rings

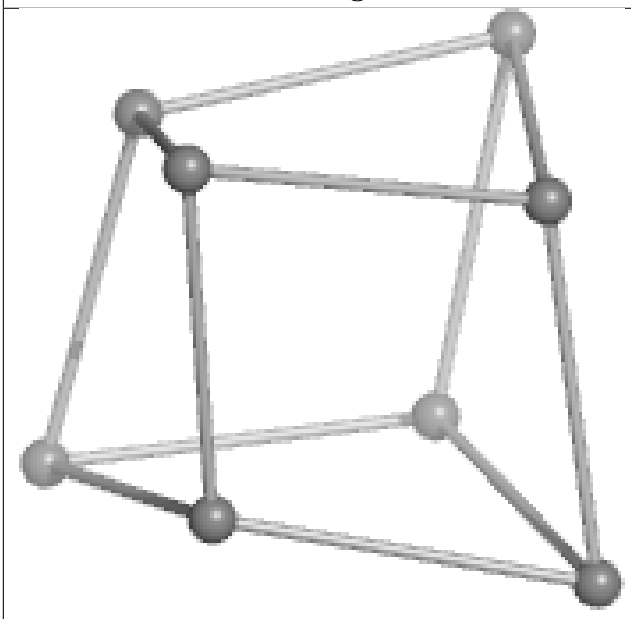
Ligand SF4 A 502



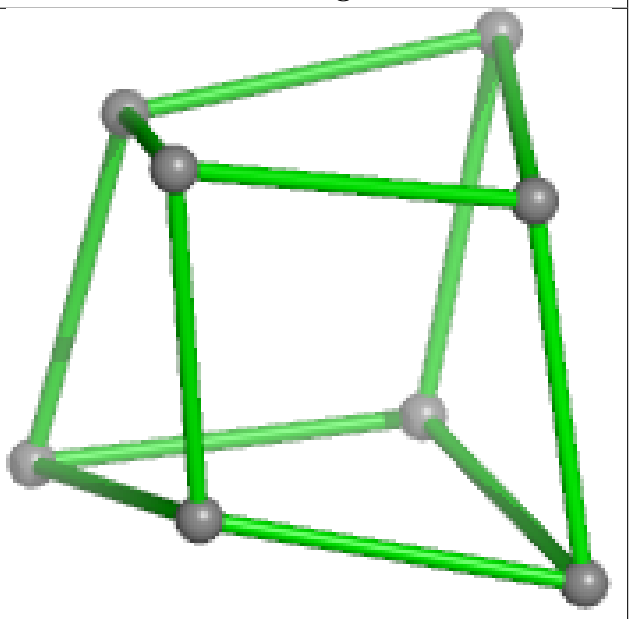
Bond lengths



Bond angles

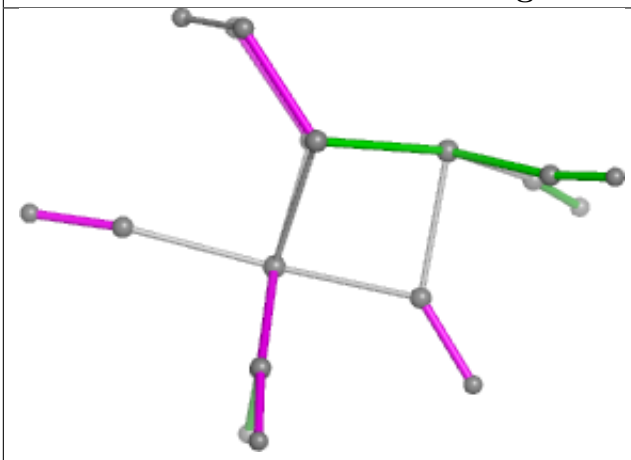


Torsions

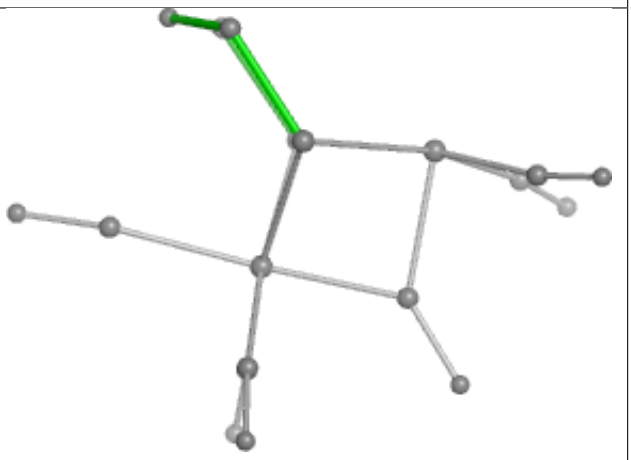


Rings

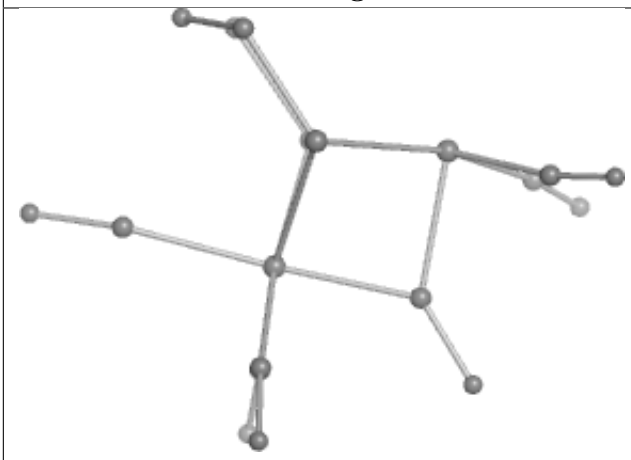
Ligand MHX A 504



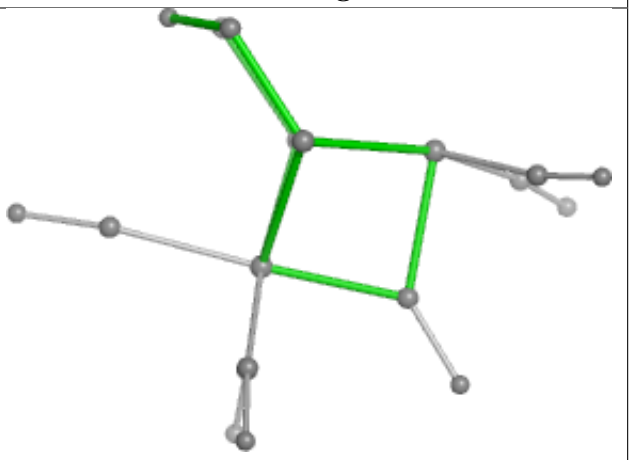
Bond lengths



Bond angles

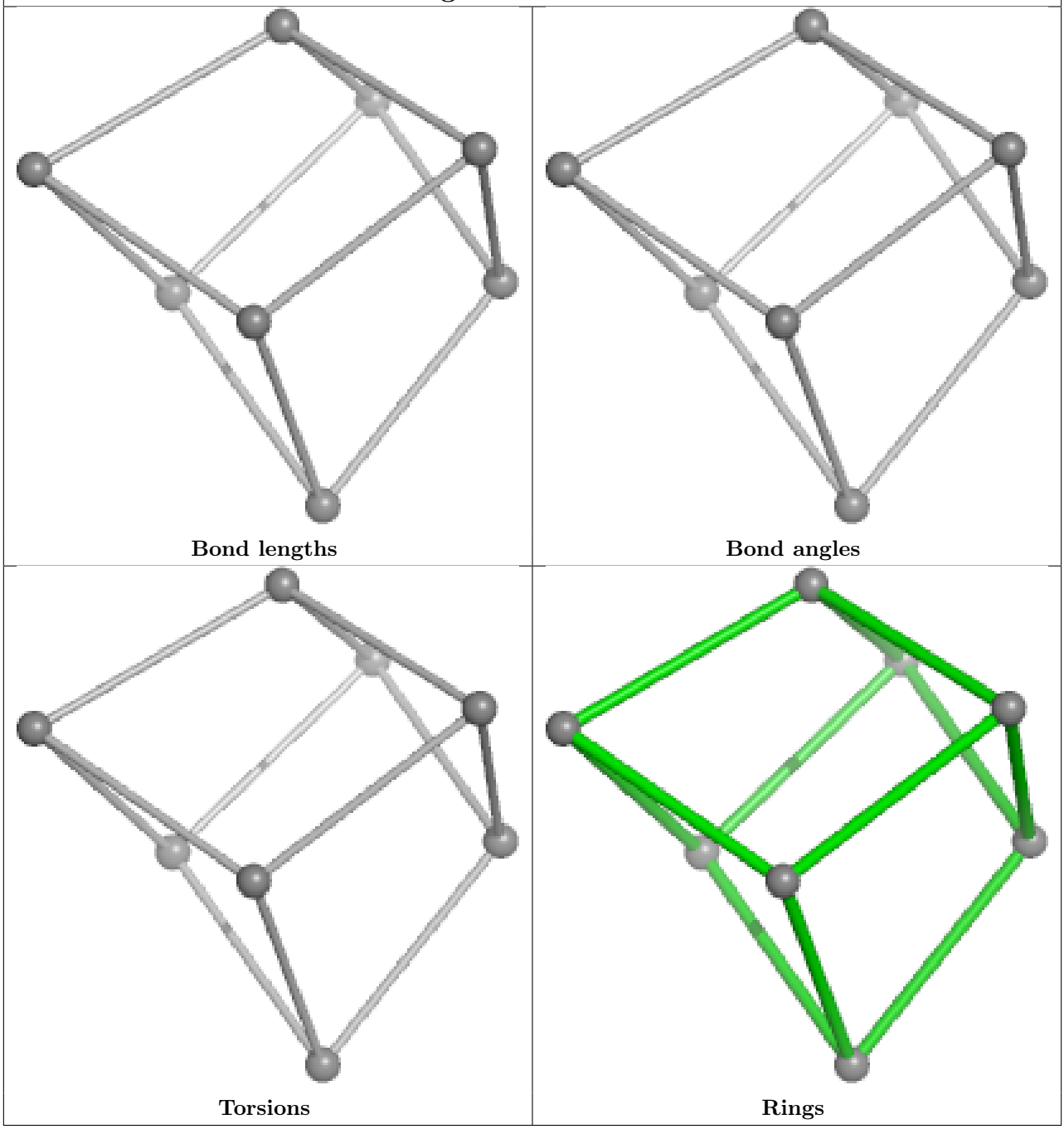


Torsions



Rings

Ligand SF4 A 503



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	471/492 (95%)	0.17	27 (5%) 30 35	6, 17, 35, 71	41 (8%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	475	PHE	11.3
1	A	367	LYS	5.4
1	A	477	GLY	5.3
1	A	391	VAL	5.2
1	A	390	VAL	4.1
1	A	480	PRO	3.8
1	A	97	ASP	3.6
1	A	478[A]	PRO	3.6
1	A	320[A]	ASP	3.5
1	A	2	SER	3.0
1	A	168	SER	3.0
1	A	400	ASP	2.9
1	A	19	LYS	2.9
1	A	365	ALA	2.7
1	A	401	ILE	2.7
1	A	319[A]	PRO	2.7
1	A	20	ALA	2.5
1	A	8	ARG	2.5
1	A	165	THR	2.4
1	A	321	SER	2.2
1	A	98	GLY	2.2
1	A	465	GLY	2.1
1	A	450	HIS	2.1
1	A	366	GLY	2.1
1	A	479[A]	TYR	2.1
1	A	322	TRP	2.0
1	A	403	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

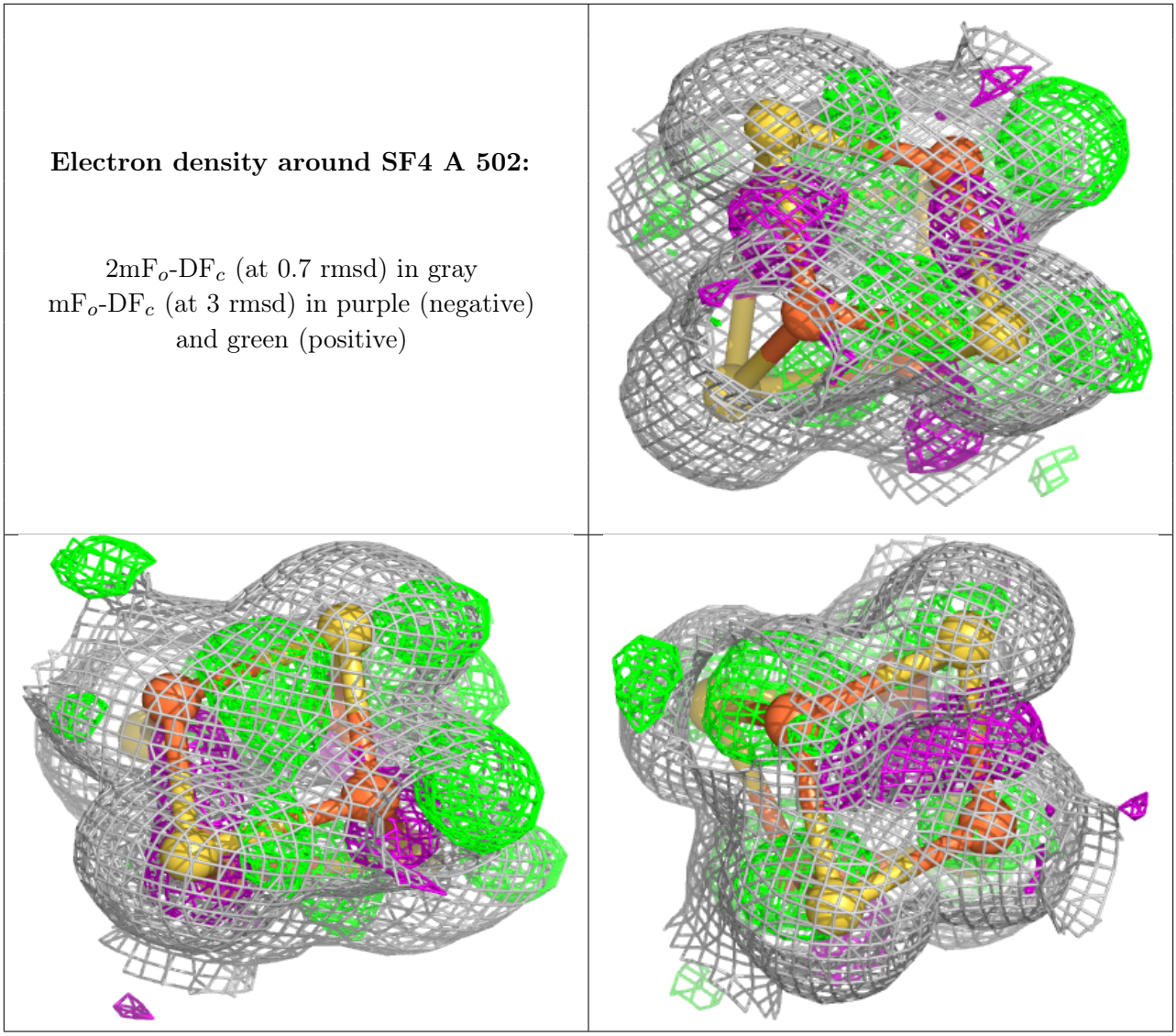
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	SF4	A	502	8/8	0.97	0.06	19,20,23,23	0
2	SF4	A	501	8/8	0.99	0.03	13,14,14,15	0
3	MHX	A	504	19/19	0.99	0.06	9,13,17,18	26
2	SF4	A	503	8/8	1.00	0.02	11,11,11,12	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.

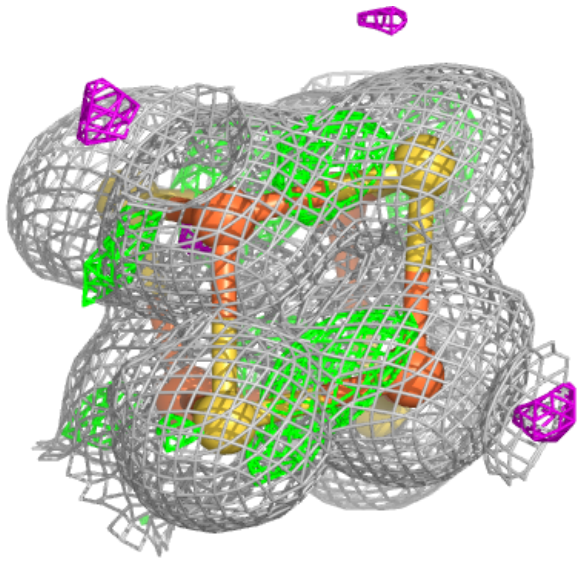
Electron density around SF4 A 502:

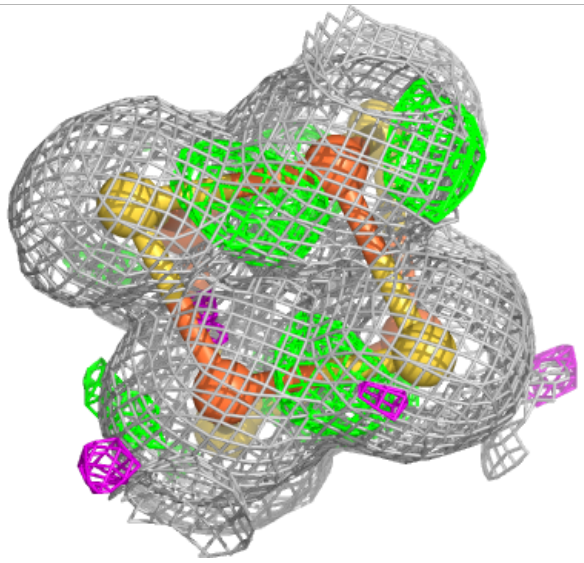
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

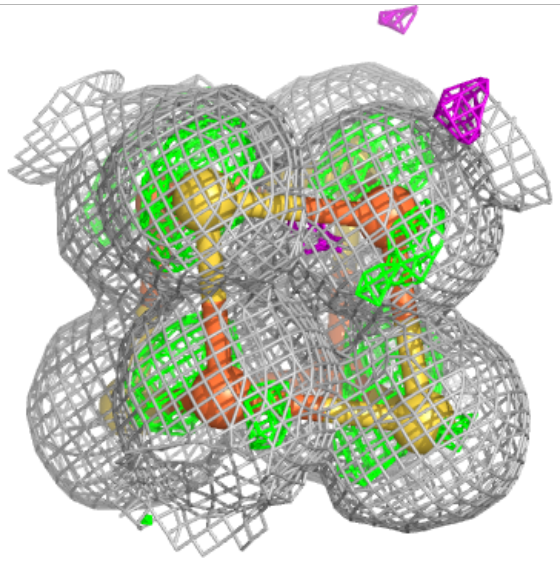


Electron density around SF4 A 501:

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

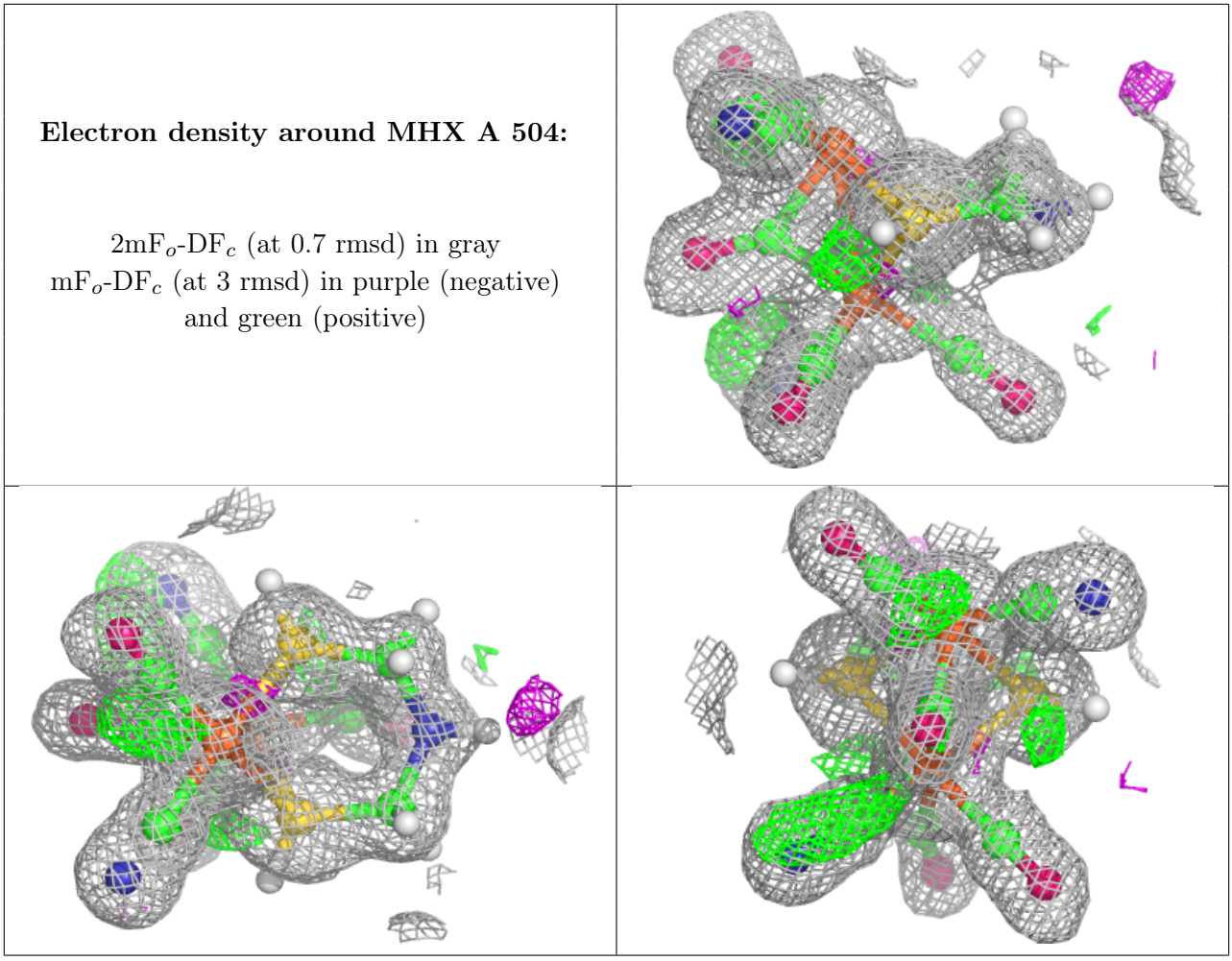






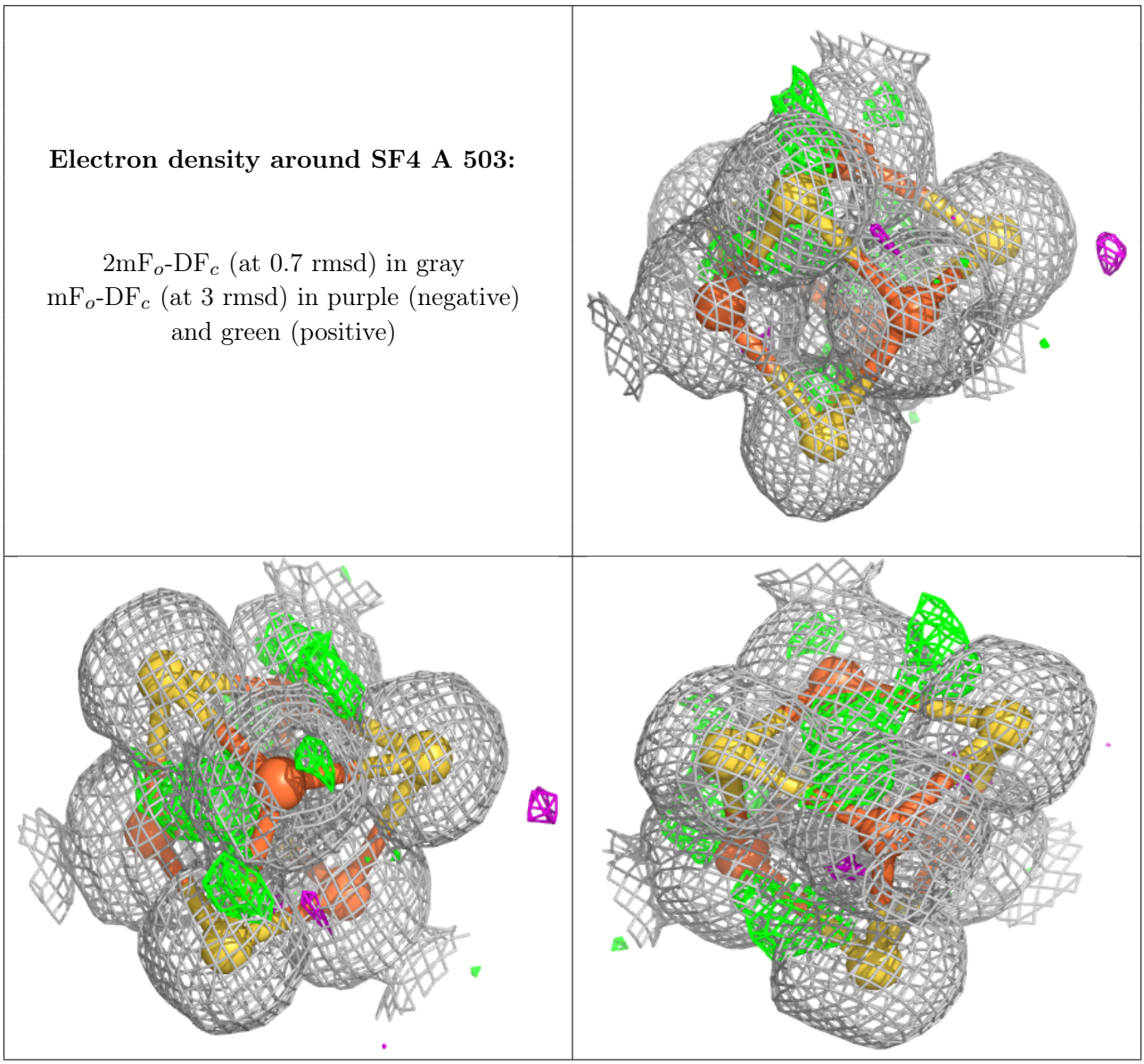
Electron density around MHX A 504:

$2mF_o$-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 A 503:

$2mF_o$-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.