wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2023 – 10:27 am BST

PDB ID	:	8B5O
Title	:	Structure of haloalkane dehalogenase DmmarA from Mycobacterium marinum at pH 5.5
Authors	:	Snajdarova, K.; Marek, M.
Deposited on	:	2022-09-23
Resolution	:	1.60 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:

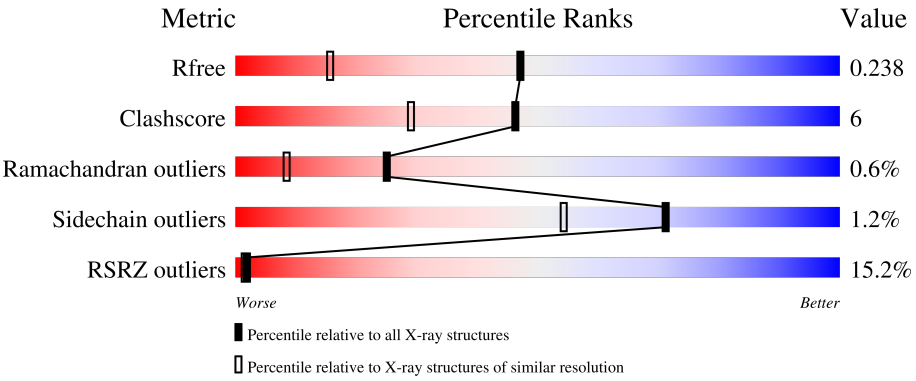
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.60 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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	296	89% 7% ·
1	B	296	90% 5% 5%
1	C	296	86% 9% ·
1	D	296	56% 66% 25% · · 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FMT	A	402	-	X	-	-
3	FMT	A	403	-	X	-	-
3	FMT	A	405	-	X	-	-
3	FMT	A	406	-	X	-	-
3	FMT	B	304	-	X	-	-
3	FMT	B	305	-	X	-	-
3	FMT	B	306	-	X	-	-
3	FMT	C	302	-	X	-	-
3	FMT	C	304	-	X	-	-
3	FMT	C	305	-	X	-	-
3	FMT	C	307	-	X	-	-
3	FMT	C	308	-	X	-	-
3	FMT	D	301	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9744 atoms, of which 0 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 Haloalkane dehalogenase DhaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	3	0
			2257	1438	393	417	9			
1	B	282	Total	C	N	O	S	0	1	0
			2230	1422	386	413	9			
1	C	284	Total	C	N	O	S	0	3	0
			2268	1444	397	418	9			
1	D	277	Total	C	N	O	S	0	1	0
			2194	1401	377	407	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	HIS	-	expression tag	UNP B2HR89
A	292	HIS	-	expression tag	UNP B2HR89
A	293	HIS	-	expression tag	UNP B2HR89
A	294	HIS	-	expression tag	UNP B2HR89
A	295	HIS	-	expression tag	UNP B2HR89
A	296	HIS	-	expression tag	UNP B2HR89
B	291	HIS	-	expression tag	UNP B2HR89
B	292	HIS	-	expression tag	UNP B2HR89
B	293	HIS	-	expression tag	UNP B2HR89
B	294	HIS	-	expression tag	UNP B2HR89
B	295	HIS	-	expression tag	UNP B2HR89
B	296	HIS	-	expression tag	UNP B2HR89
C	291	HIS	-	expression tag	UNP B2HR89
C	292	HIS	-	expression tag	UNP B2HR89
C	293	HIS	-	expression tag	UNP B2HR89
C	294	HIS	-	expression tag	UNP B2HR89
C	295	HIS	-	expression tag	UNP B2HR89
C	296	HIS	-	expression tag	UNP B2HR89
D	291	HIS	-	expression tag	UNP B2HR89
D	292	HIS	-	expression tag	UNP B2HR89
D	293	HIS	-	expression tag	UNP B2HR89

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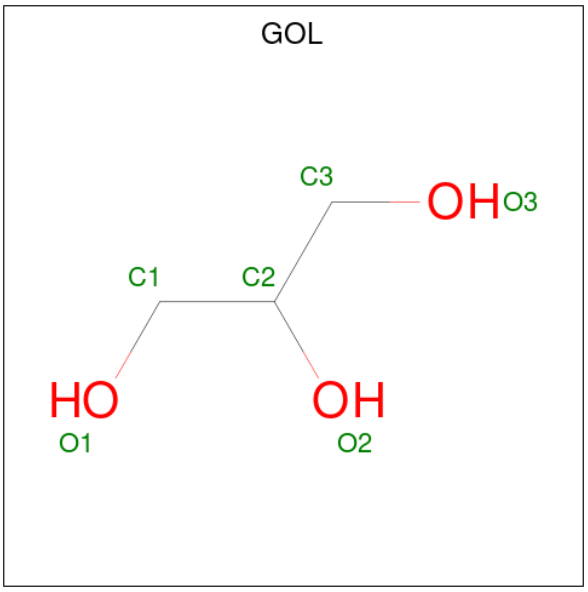
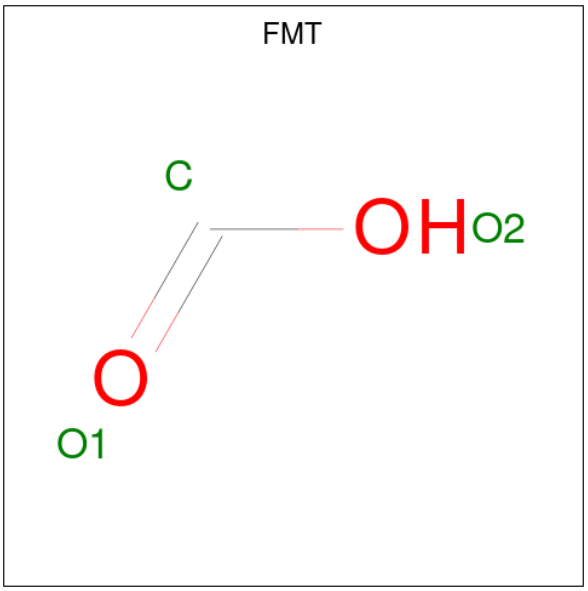
Chain	Residue	Modelled	Actual	Comment	Reference
D	294	HIS	-	expression tag	UNP B2HR89
D	295	HIS	-	expression tag	UNP B2HR89
D	296	HIS	-	expression tag	UNP B2HR89

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

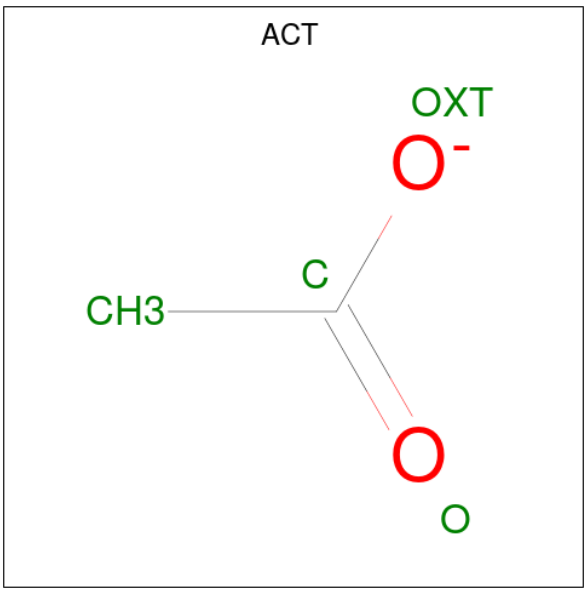
- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$) (labeled as

"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0

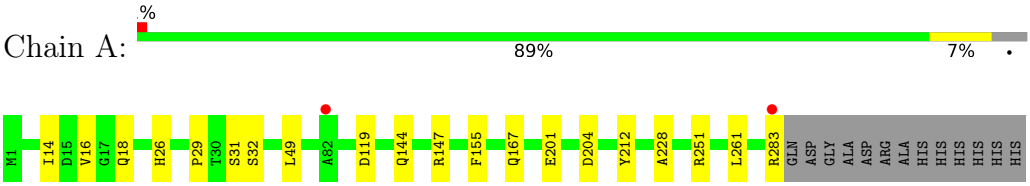
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	229	Total O 229 229	0	0
5	B	187	Total O 187 187	0	0
5	C	246	Total O 248 248	0	2
5	D	46	Total O 46 46	0	0

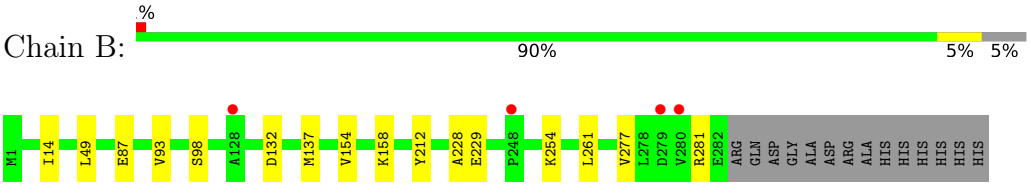
3 Residue-property plots (i)

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 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.

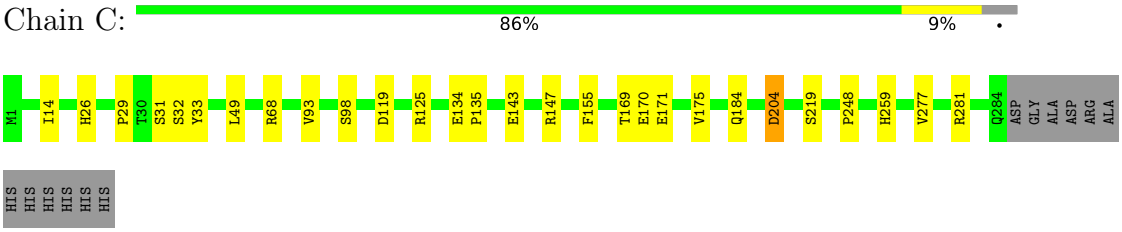
• Molecule 1: Haloalkane dehalogenase DhaA



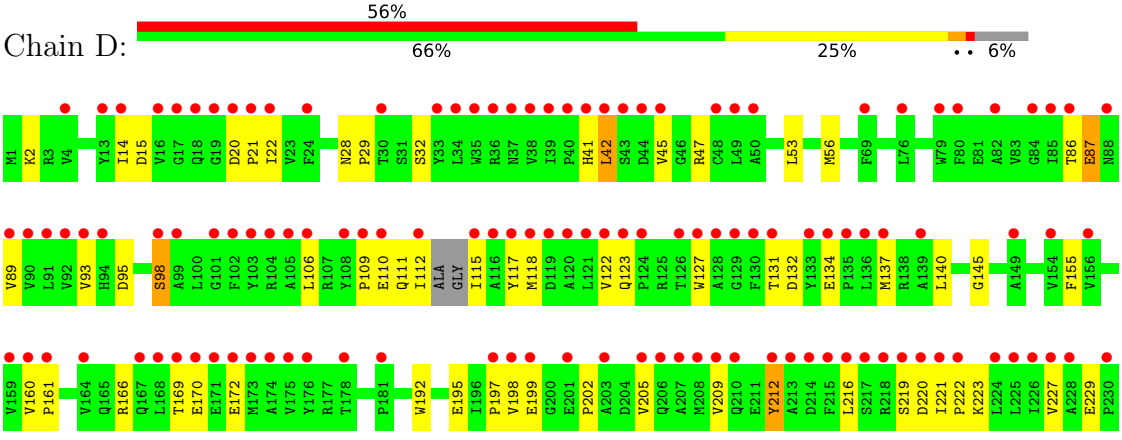
• Molecule 1: Haloalkane dehalogenase DhaA

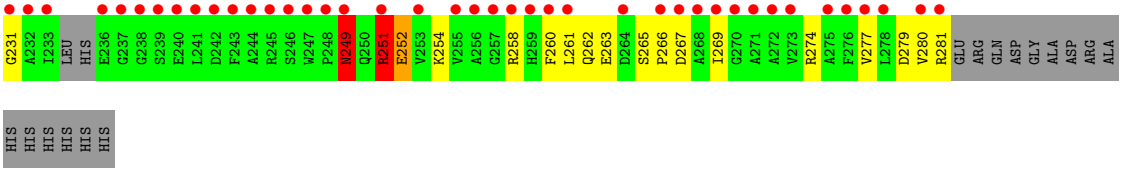


• Molecule 1: Haloalkane dehalogenase DhaA



• Molecule 1: Haloalkane dehalogenase DhaA




G231
A232
I233
LEU
HIS
E236
G237
G238
S239
E240
L241
D242
P243
A244
R245
S246
W247
P248
N249
Q250
R251
E252
V253
K254
V255
A256
G257
R258
H259
F260
L261
Q262
E263
D264
S265
P266
D267
A268
I269
G270
A271
A272
V273
R274
A275
F276
V277
L278
D279
V280
R281
GLU
ARG
GLN
ASP
GLY
ALA
ASP
ARG
ALA
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.70Å 60.77Å 104.78Å 90.00° 105.49° 90.00°	Depositor
Resolution (Å)	43.70 – 1.60 43.70 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (43.70-1.60) 98.8 (43.70-1.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.14-3260	Depositor
R, R_{free}	0.198 , 0.238 0.198 , 0.238	Depositor DCC
R_{free} test set	7081 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	17.8	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9744	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: ACT, FMT, GOL

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	0.67	0/2318	0.77	1/3158 (0.0%)
1	B	0.64	0/2291	0.75	1/3122 (0.0%)
1	C	0.73	0/2329	0.79	2/3172 (0.1%)
1	D	0.46	0/2249	0.61	0/3064
All	All	0.63	0/9187	0.73	4/12516 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	204	ASP	CB-CG-OD1	6.53	124.17	118.30
1	C	204	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	137	MET	CG-SD-CE	-5.21	91.87	100.20
1	C	125	ARG	NE-CZ-NH1	-5.02	117.79	120.30

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	2257	0	2208	11	0
1	B	2230	0	2180	10	0
1	C	2268	0	2221	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2194	0	2144	74	0
2	A	12	0	16	1	0
2	B	12	0	16	0	0
2	C	18	0	24	0	0
3	A	12	0	8	1	0
3	B	9	0	6	0	0
3	C	15	0	10	0	0
3	D	3	0	2	0	0
4	B	4	0	3	0	0
5	A	229	0	0	4	0
5	B	187	0	0	2	0
5	C	248	0	0	3	0
5	D	46	0	0	0	0
All	All	9744	0	8838	112	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 6.

The worst 5 of 112 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:D:53:LEU:HB2	1:D:56:MET:HE3	1.23	1.16
1:D:95:ASP:O	1:D:98:SER:HB3	1.63	0.98
1:D:42:LEU:HD22	1:D:45:VAL:CG2	1.99	0.91
1:D:42:LEU:HD22	1:D:45:VAL:HG21	1.59	0.82
1:A:144[A]:GLN:NE2	5:A:503:HOH:O	2.23	0.71

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	284/296 (96%)	274 (96%)	9 (3%)	1 (0%)	34 15
1	B	281/296 (95%)	271 (96%)	10 (4%)	0	100 100
1	C	285/296 (96%)	274 (96%)	11 (4%)	0	100 100
1	D	272/296 (92%)	248 (91%)	18 (7%)	6 (2%)	6 1
All	All	1122/1184 (95%)	1067 (95%)	48 (4%)	7 (1%)	25 8

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	251	ARG
1	D	252	GLU
1	D	87	GLU
1	D	249	ASN
1	D	42	LEU

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	237/244 (97%)	232 (98%)	5 (2%)	53 29
1	B	234/244 (96%)	233 (100%)	1 (0%)	91 84
1	C	238/244 (98%)	238 (100%)	0	100 100
1	D	231/244 (95%)	225 (97%)	6 (3%)	46 21
All	All	940/976 (96%)	928 (99%)	12 (1%)	71 50

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	134	GLU
1	D	170	GLU
1	D	251	ARG
1	D	212	TYR
1	A	251[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	167	GLN
1	C	18	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

21 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	GOL	C	301	-	5,5,5	0.57	0	5,5,5	0.70	0
2	GOL	B	301	-	5,5,5	0.47	0	5,5,5	0.29	0
3	FMT	A	402	-	2,2,2	3.04	2 (100%)	1,1,1	1.51	0
3	FMT	B	306	-	2,2,2	3.04	2 (100%)	1,1,1	1.52	0
3	FMT	B	305	-	2,2,2	3.00	2 (100%)	1,1,1	1.62	0
3	FMT	A	406	-	2,2,2	2.95	2 (100%)	1,1,1	1.36	0
3	FMT	A	405	-	2,2,2	3.09	2 (100%)	1,1,1	1.75	0
4	ACT	B	303	-	3,3,3	1.04	0	3,3,3	0.65	0
2	GOL	C	303	-	5,5,5	0.50	0	5,5,5	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FMT	C	305	-	2,2,2	3.00	2 (100%)	1,1,1	1.63	0
3	FMT	A	403	-	2,2,2	3.04	2 (100%)	1,1,1	1.36	0
3	FMT	D	301	-	2,2,2	3.35	2 (100%)	1,1,1	1.35	0
3	FMT	C	302	-	2,2,2	3.16	2 (100%)	1,1,1	1.25	0
2	GOL	C	306	-	5,5,5	0.45	0	5,5,5	0.27	0
2	GOL	A	401	-	5,5,5	0.29	0	5,5,5	0.57	0
3	FMT	B	304	-	2,2,2	2.96	2 (100%)	1,1,1	1.51	0
2	GOL	B	302	-	5,5,5	0.65	0	5,5,5	0.74	0
3	FMT	C	307	-	2,2,2	3.17	2 (100%)	1,1,1	0.76	0
2	GOL	A	404	-	5,5,5	0.49	0	5,5,5	0.27	0
3	FMT	C	304	-	2,2,2	2.98	2 (100%)	1,1,1	1.68	0
3	FMT	C	308	-	2,2,2	2.97	2 (100%)	1,1,1	1.71	0

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	GOL	C	301	-	-	0/4/4/4	-
2	GOL	B	301	-	-	2/4/4/4	-
2	GOL	B	302	-	-	4/4/4/4	-
2	GOL	C	303	-	-	2/4/4/4	-
2	GOL	A	404	-	-	2/4/4/4	-
2	GOL	C	306	-	-	2/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	FMT	O1-C	3.98	1.43	1.22
3	C	307	FMT	O1-C	3.70	1.41	1.22
3	C	302	FMT	O1-C	3.68	1.41	1.22
3	A	402	FMT	O1-C	3.67	1.41	1.22
3	B	306	FMT	O1-C	3.57	1.41	1.22

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	GOL	C1-C2-C3-O3
2	B	302	GOL	C1-C2-C3-O3
2	B	302	GOL	O2-C2-C3-O3
2	A	401	GOL	C1-C2-C3-O3
2	A	404	GOL	C1-C2-C3-O3

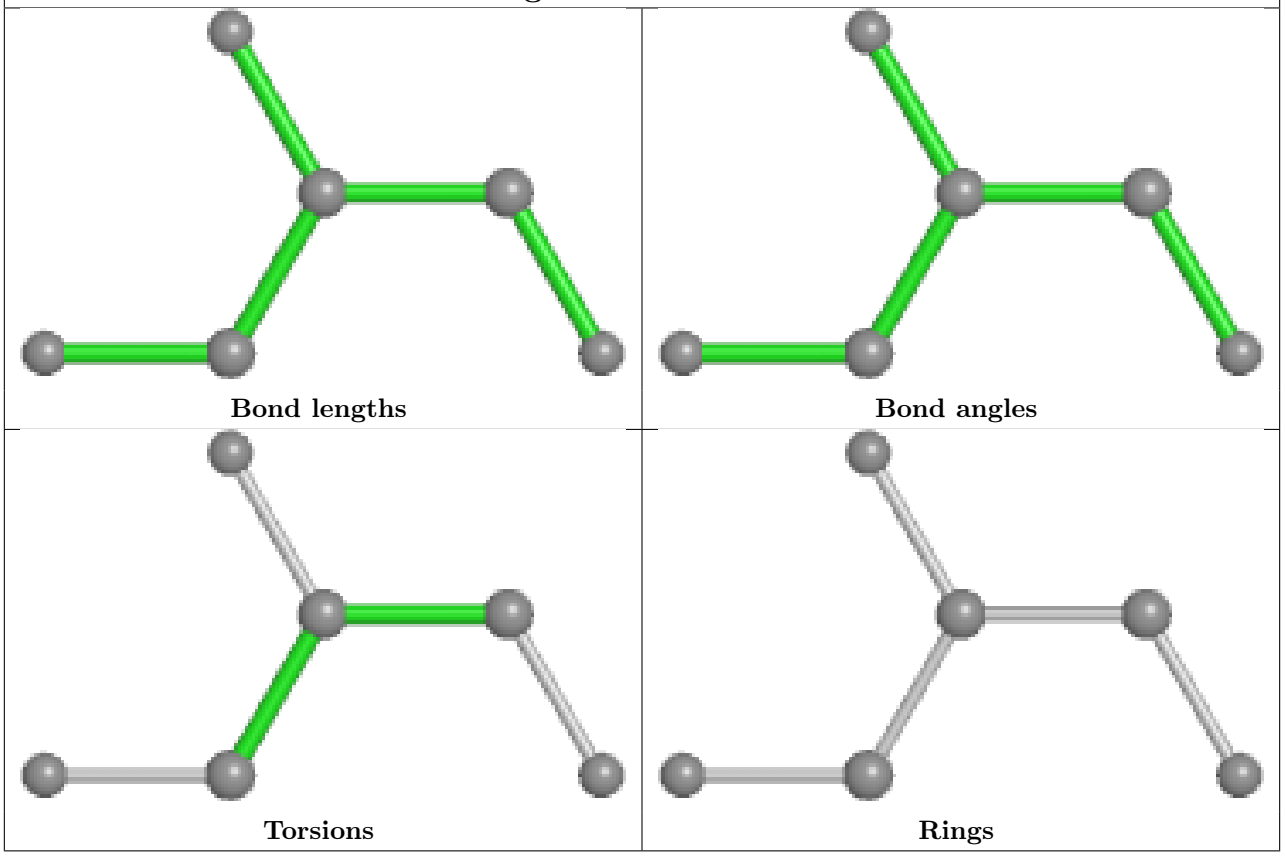
There are no ring outliers.

2 monomers are involved in 2 short contacts:

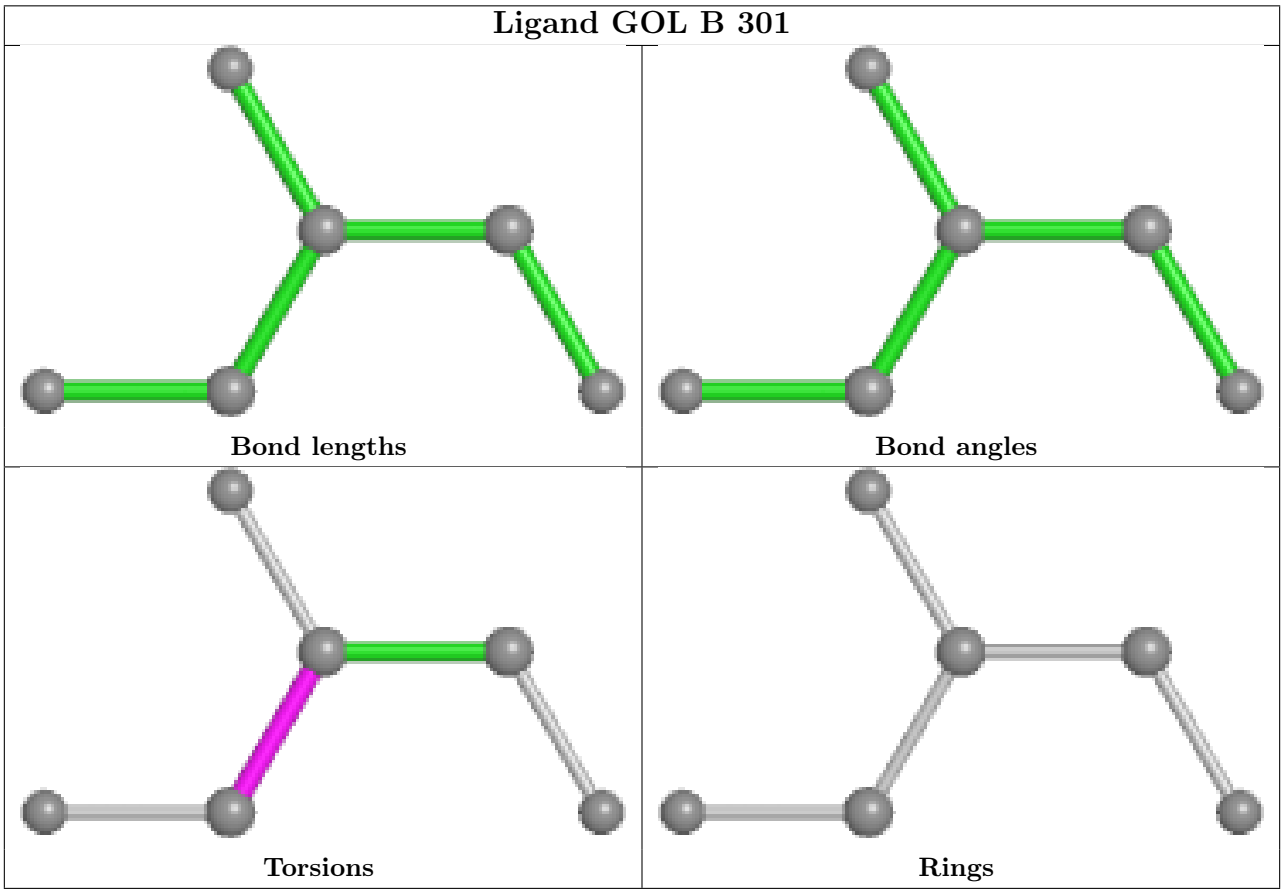
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	406	FMT	1	0
2	A	401	GOL	1	0

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.

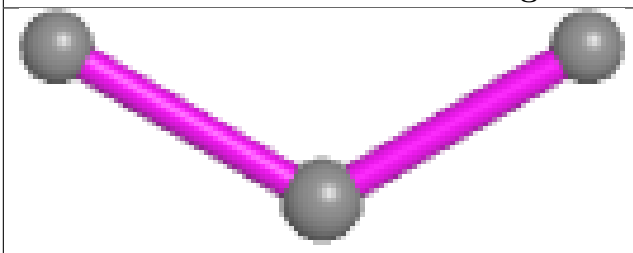
Ligand GOL C 301



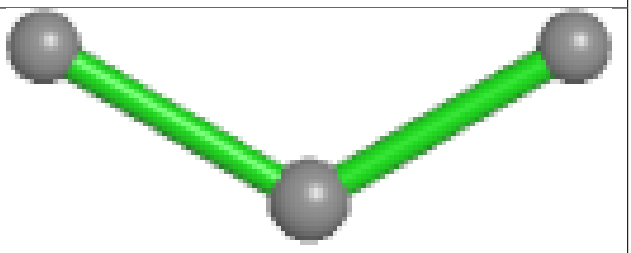
Ligand GOL B 301



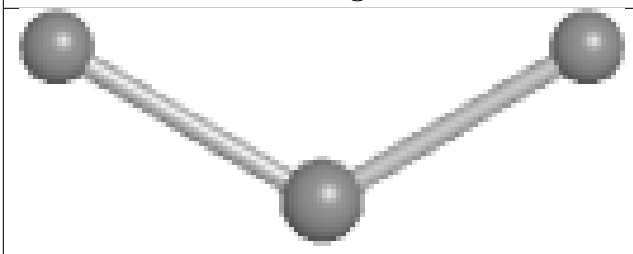
Ligand FMT A 402



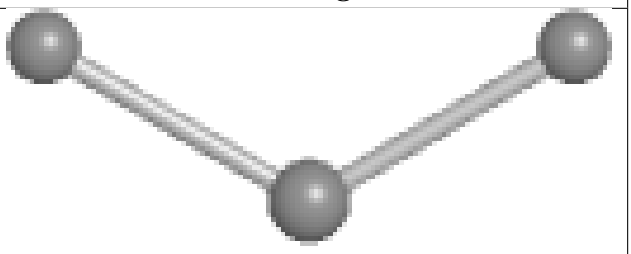
Bond lengths



Bond angles

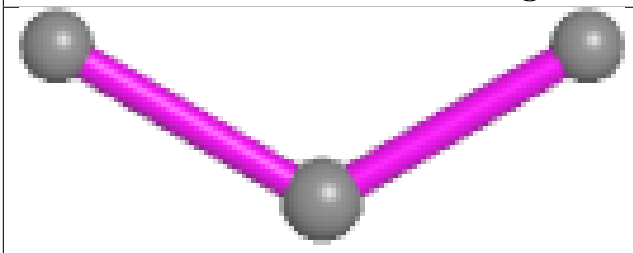


Torsions

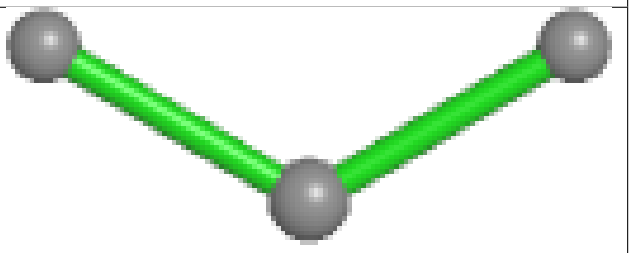


Rings

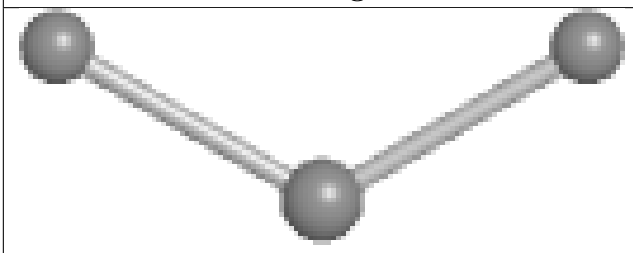
Ligand FMT B 306



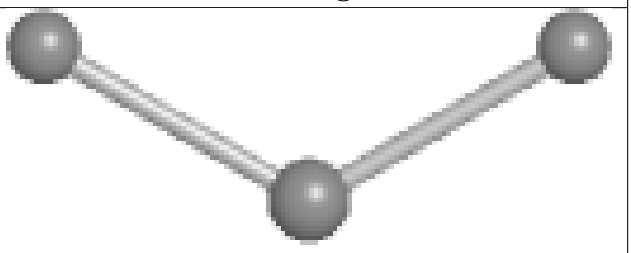
Bond lengths



Bond angles

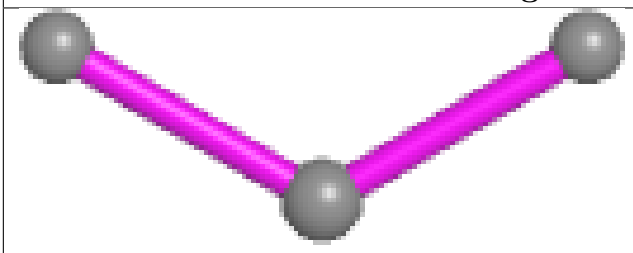


Torsions

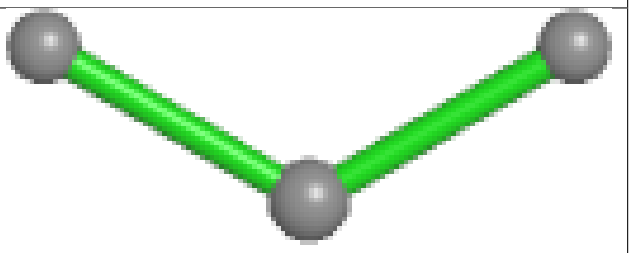


Rings

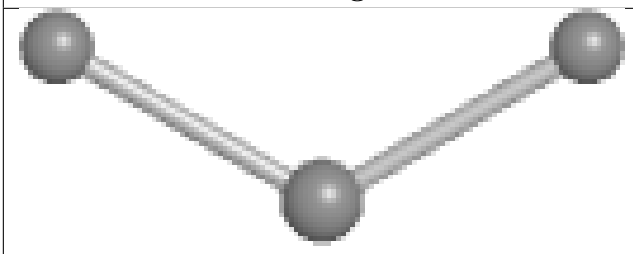
Ligand FMT B 305



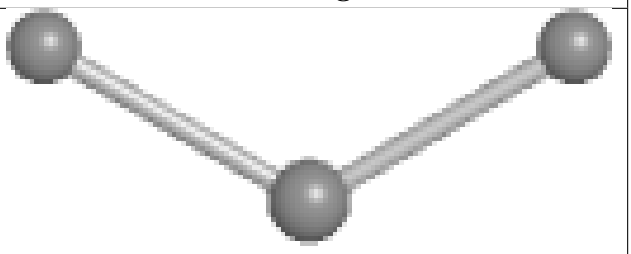
Bond lengths



Bond angles

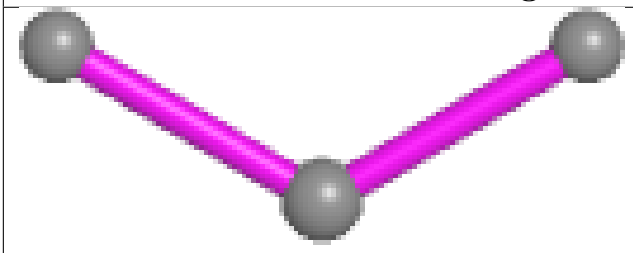


Torsions

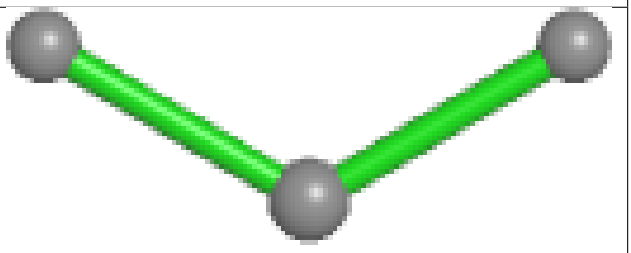


Rings

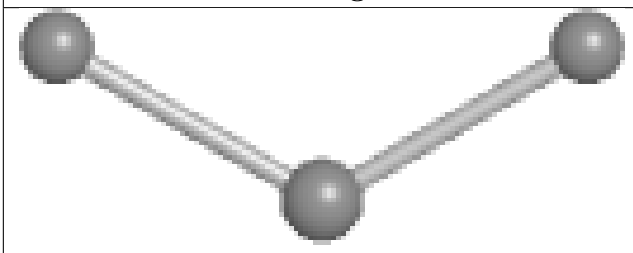
Ligand FMT A 406



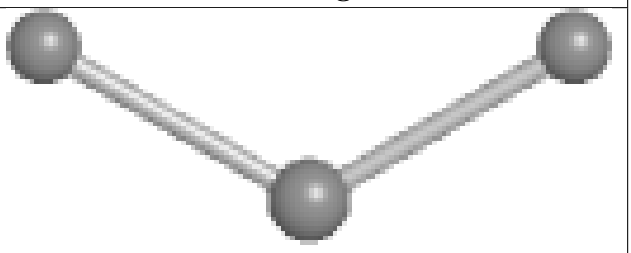
Bond lengths



Bond angles

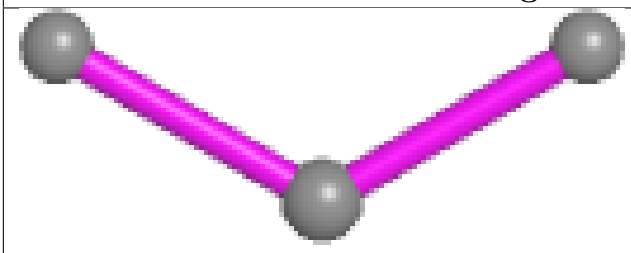


Torsions



Rings

Ligand FMT A 405



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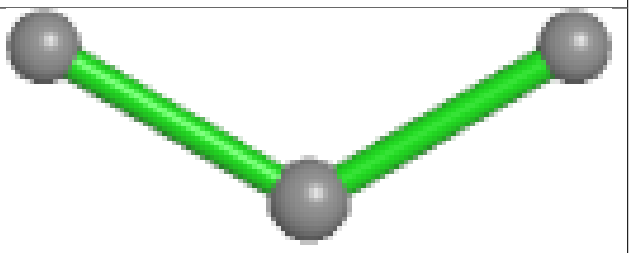
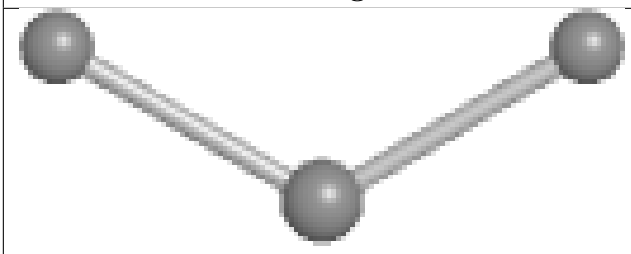


Bond angles



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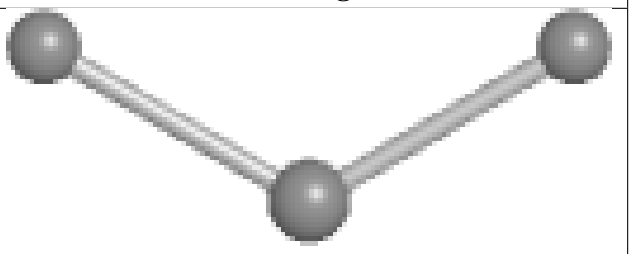
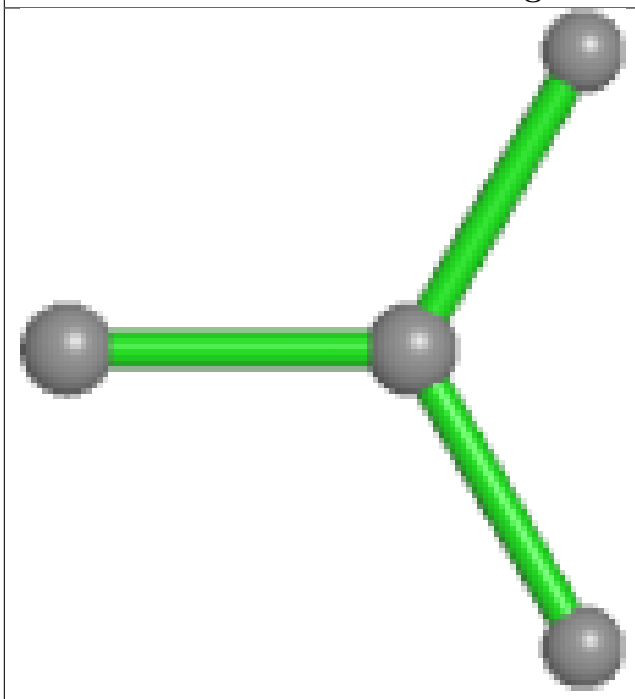
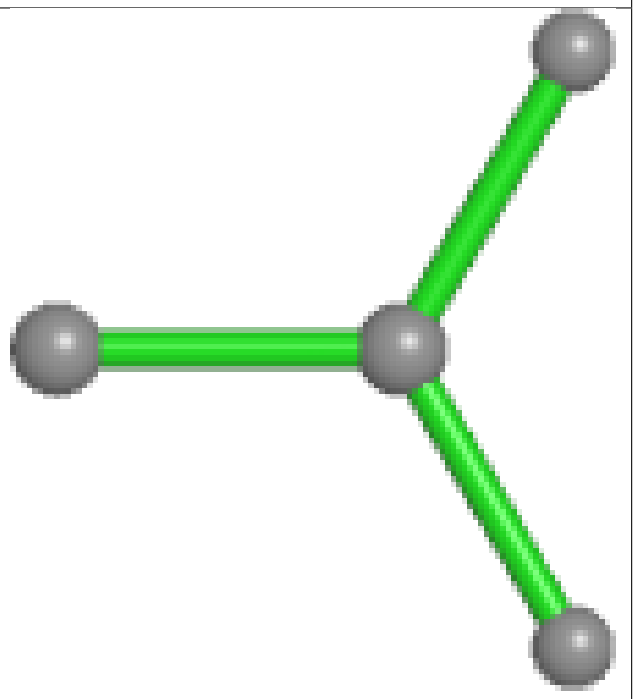


Rings

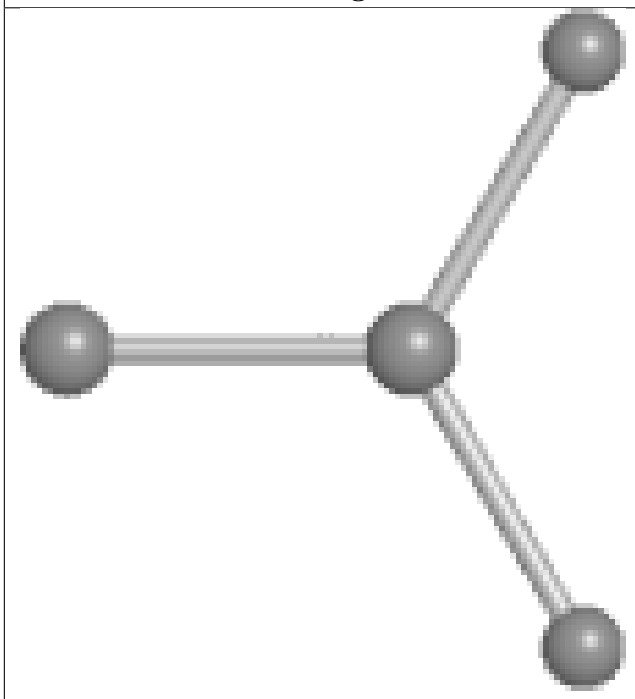
Ligand ACT B 303



Bond lengths



Bond angles



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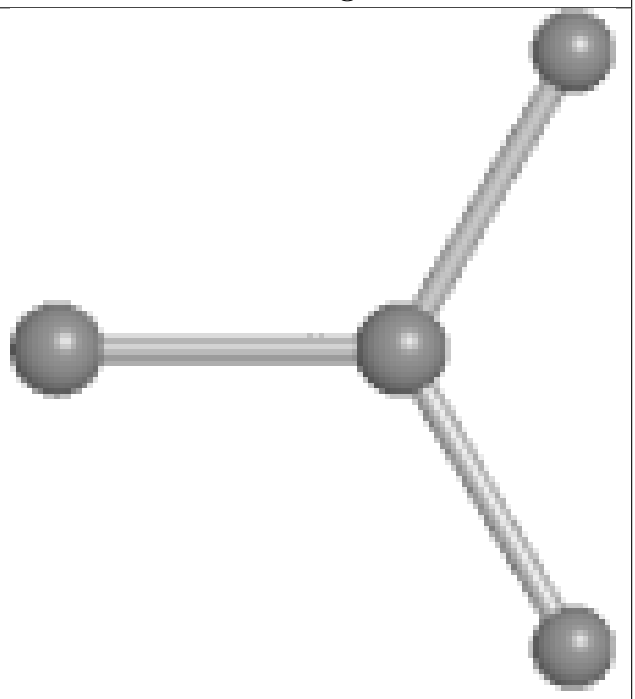
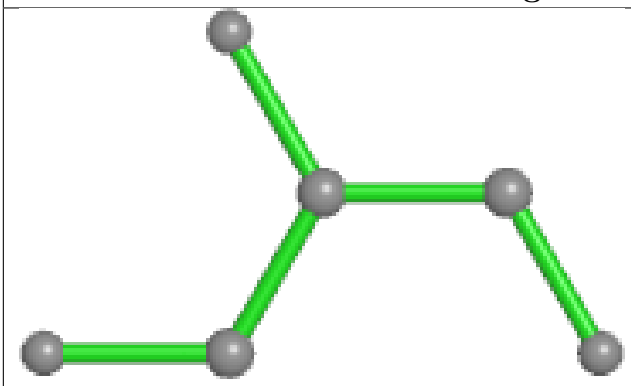


Rings

Ligand GOL C 303



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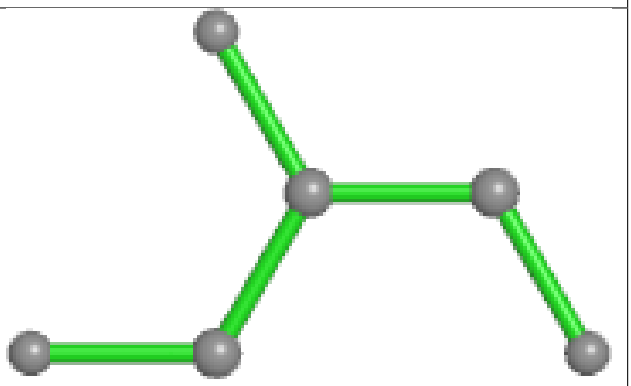
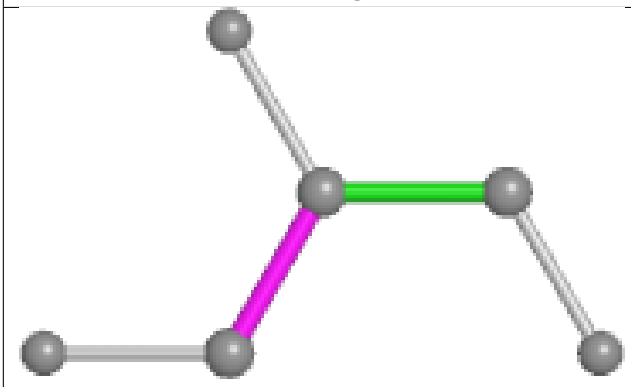


Bond angles



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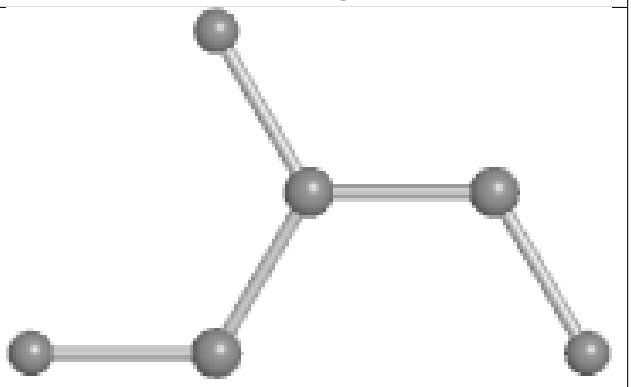
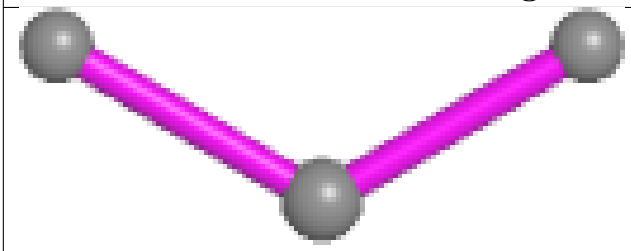
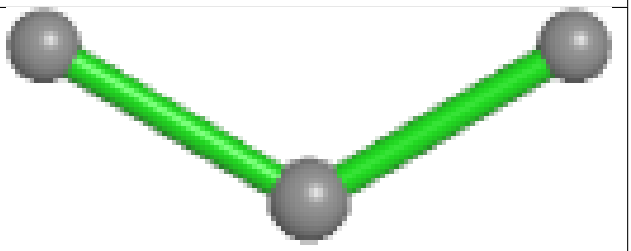


Rings

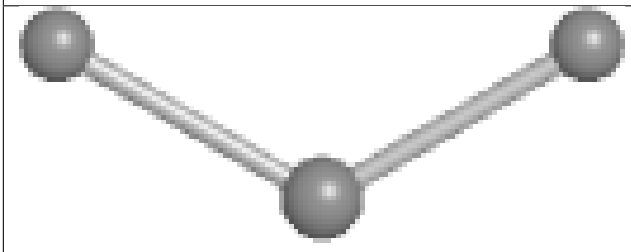
Ligand FMT C 305



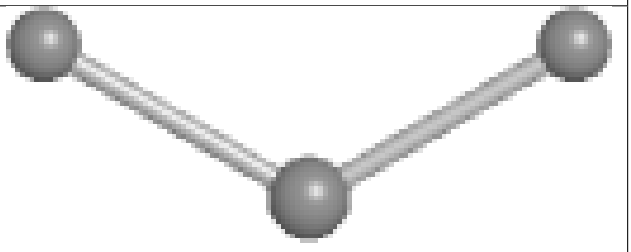
Bond lengths



Bond angles

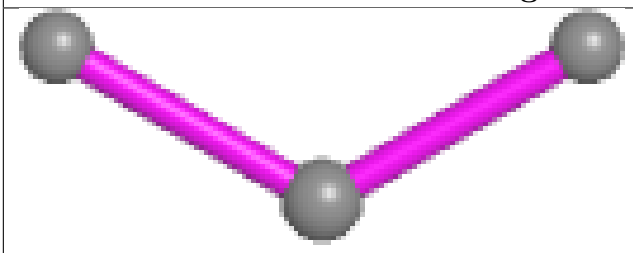


Torsions

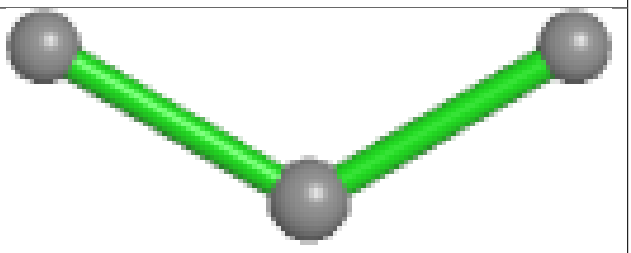


Rings

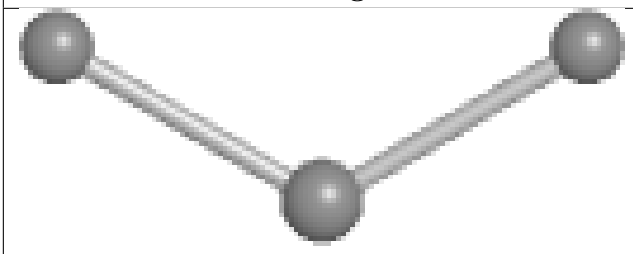
Ligand FMT A 403



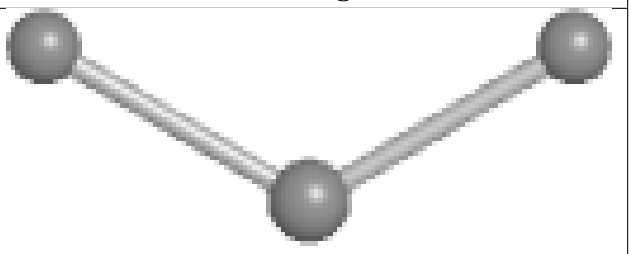
Bond lengths



Bond angles

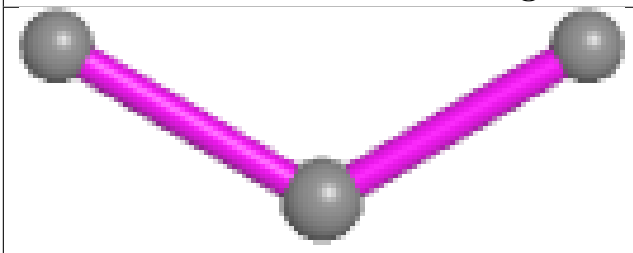


Torsions

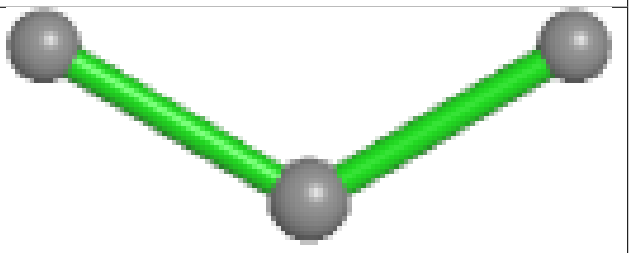


Rings

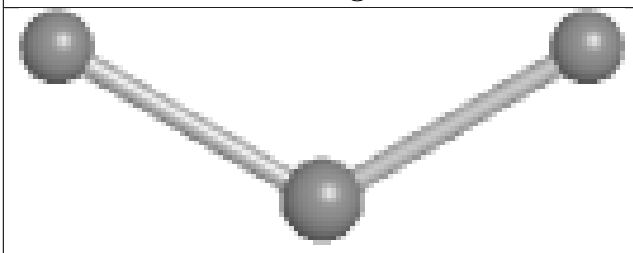
Ligand FMT D 301



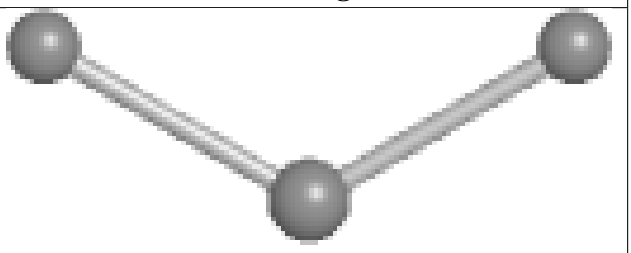
Bond lengths



Bond angles

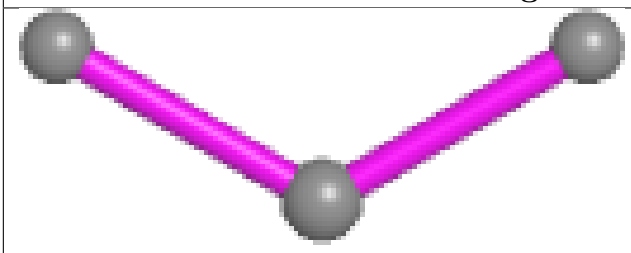


Torsions



Rings

Ligand FMT C 302



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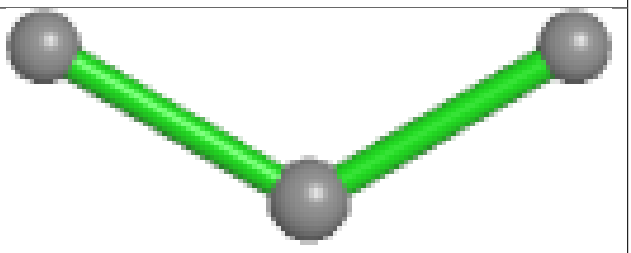
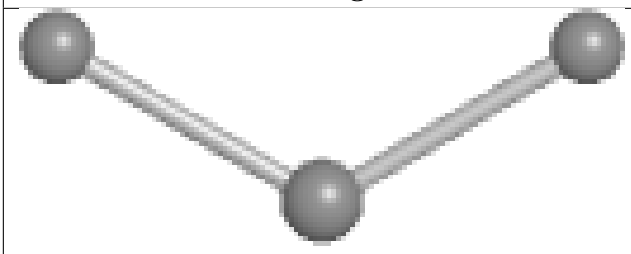
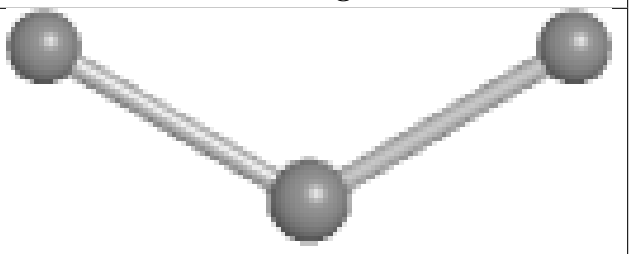


Bond angles

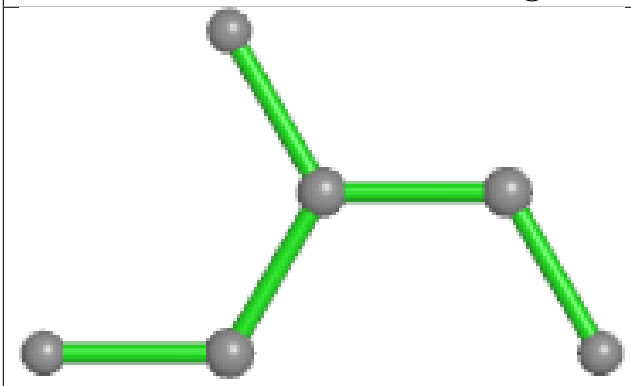


Torsions

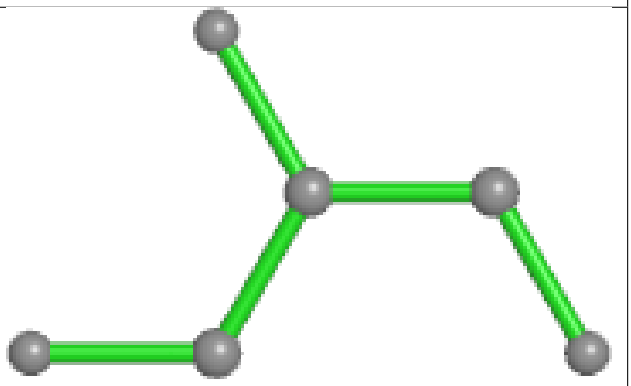


Rings

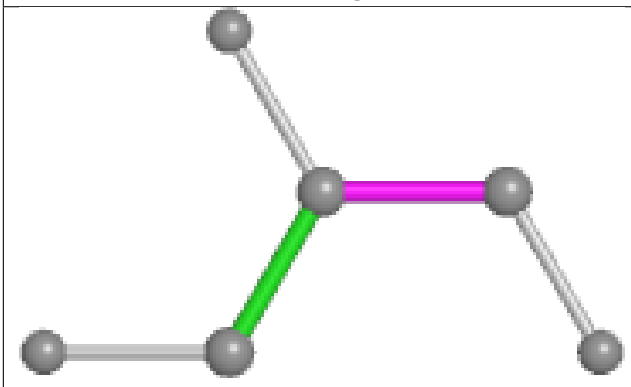
Ligand GOL C 306



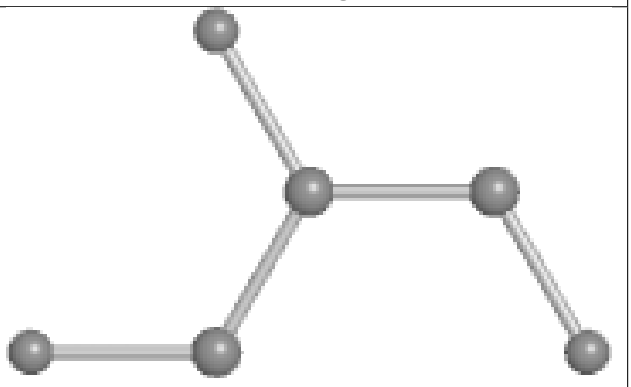
Bond lengths



Bond angles

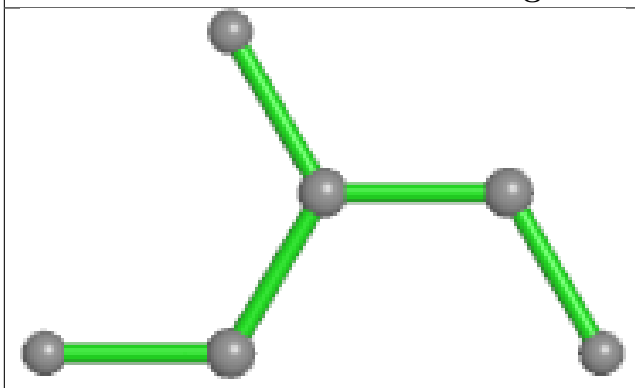


Torsions

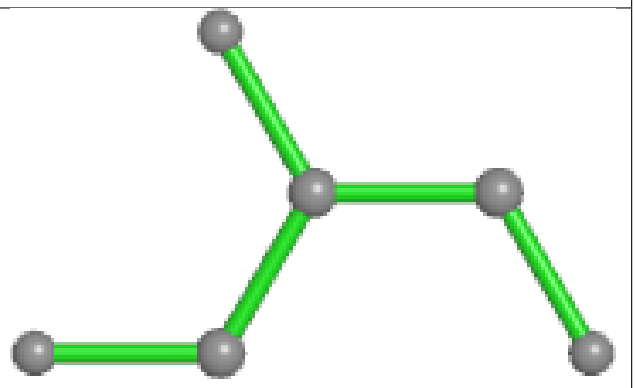


Rings

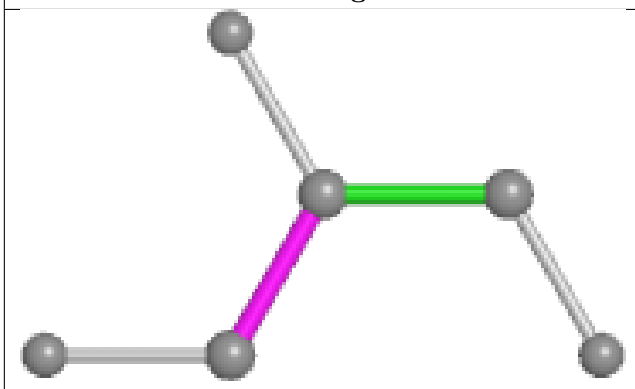
Ligand GOL A 401



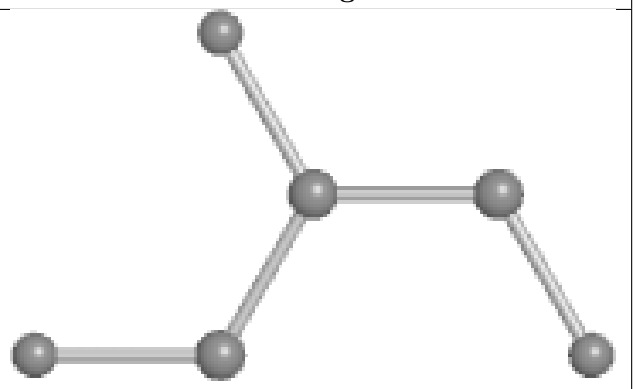
Bond lengths



Bond angles

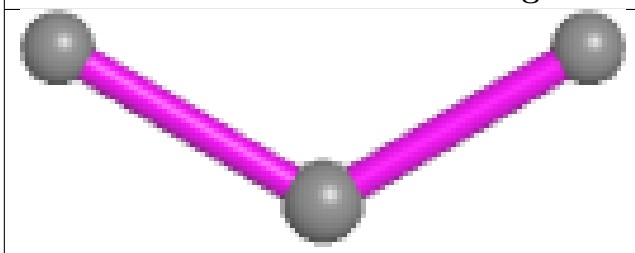


Torsions

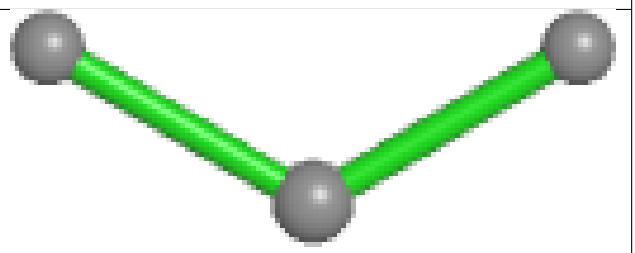


Rings

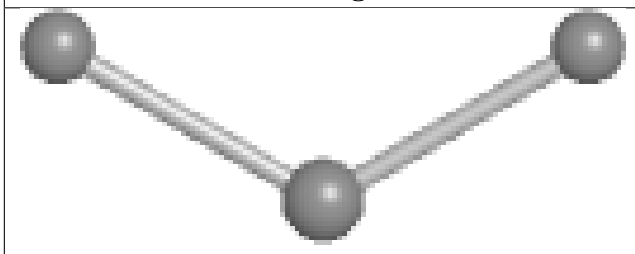
Ligand FMT B 304



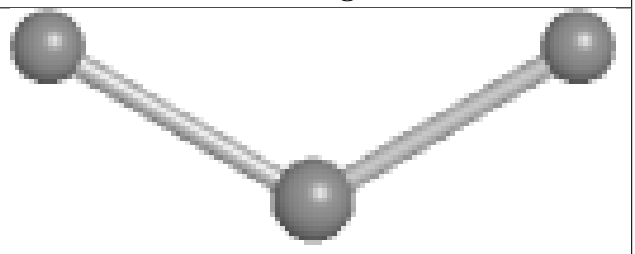
Bond lengths



Bond angles

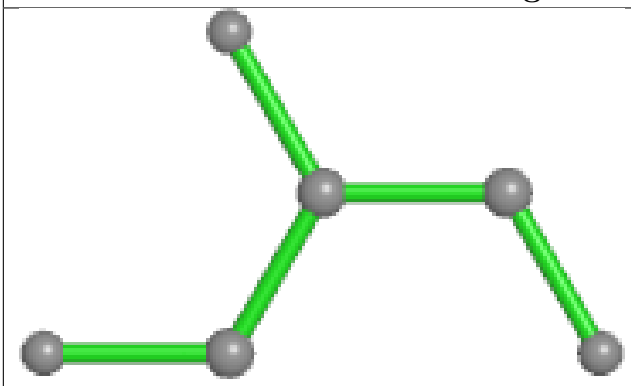


Torsions

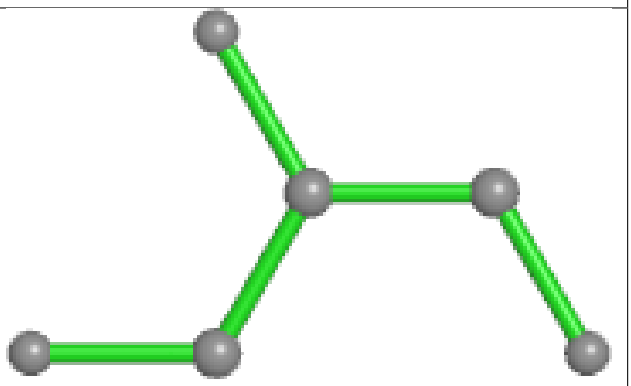


Rings

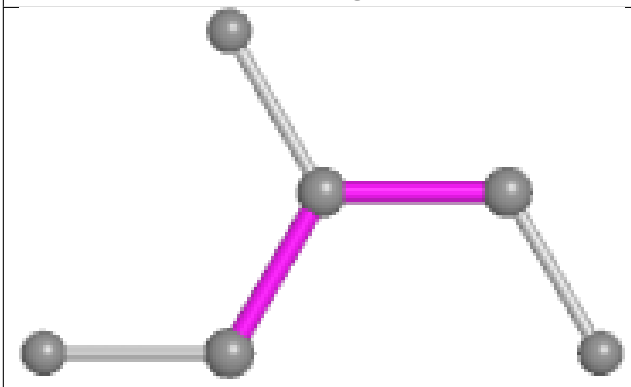
Ligand GOL B 302



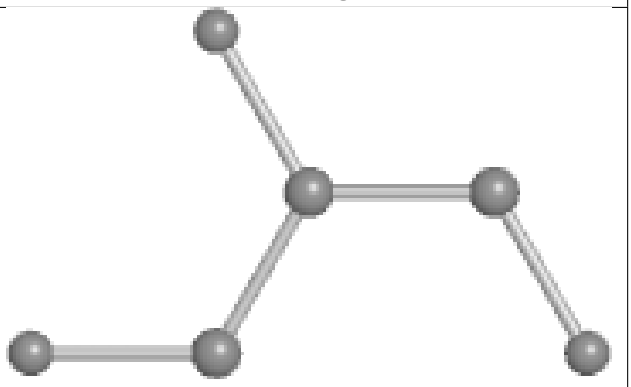
Bond lengths



Bond angles

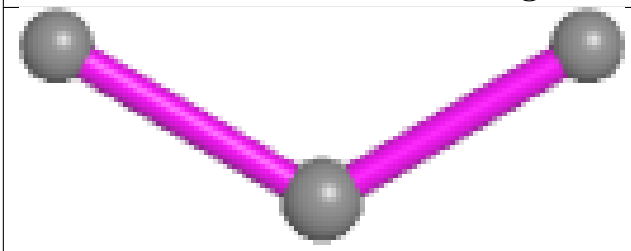


Torsions

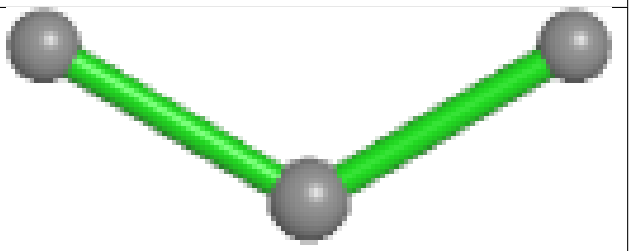


Rings

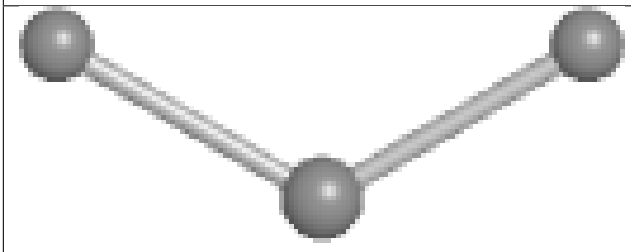
Ligand FMT C 307



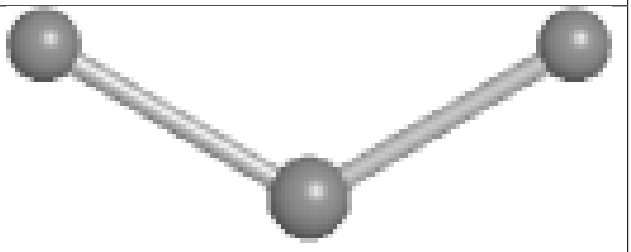
Bond lengths



Bond angles

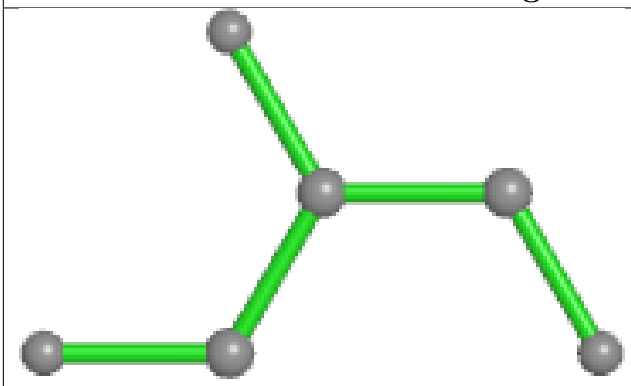


Torsions

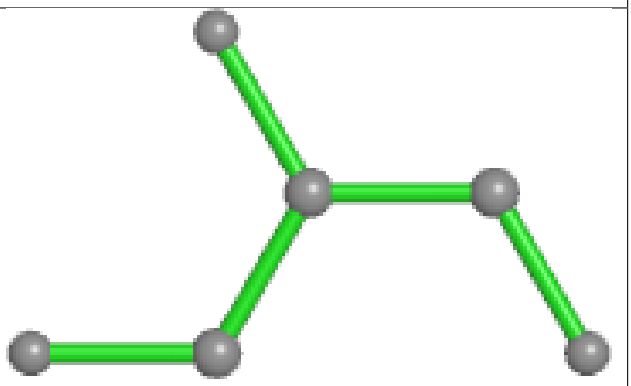


Rings

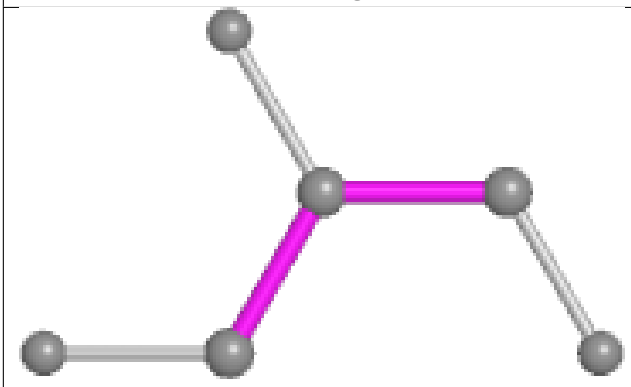
Ligand GOL A 404



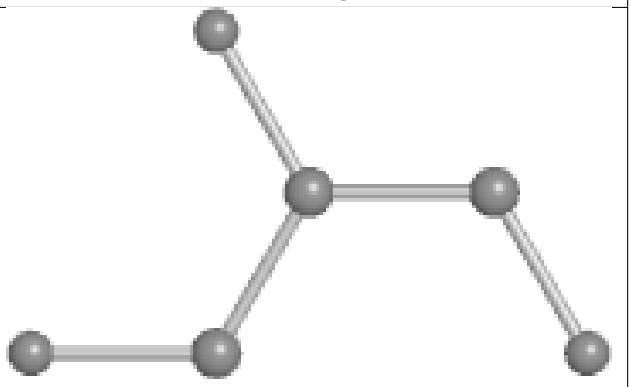
Bond lengths



Bond angles

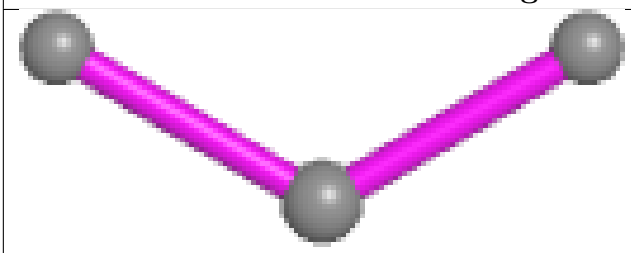


Torsions

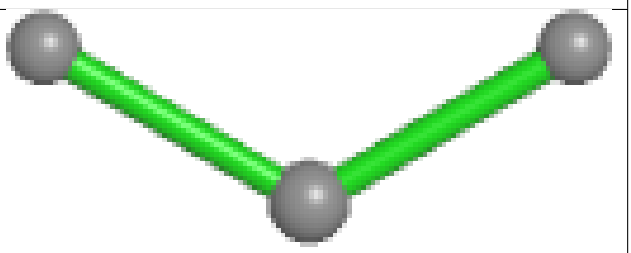


Rings

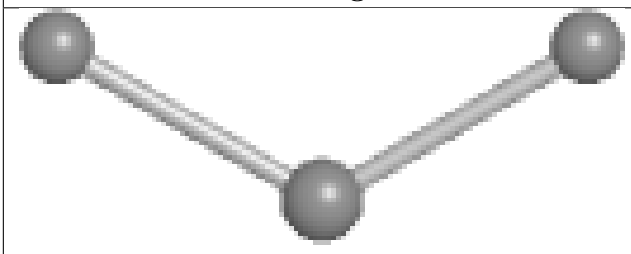
Ligand FMT C 304



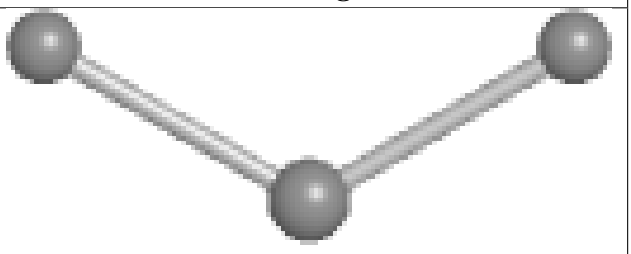
Bond lengths



Bond angles

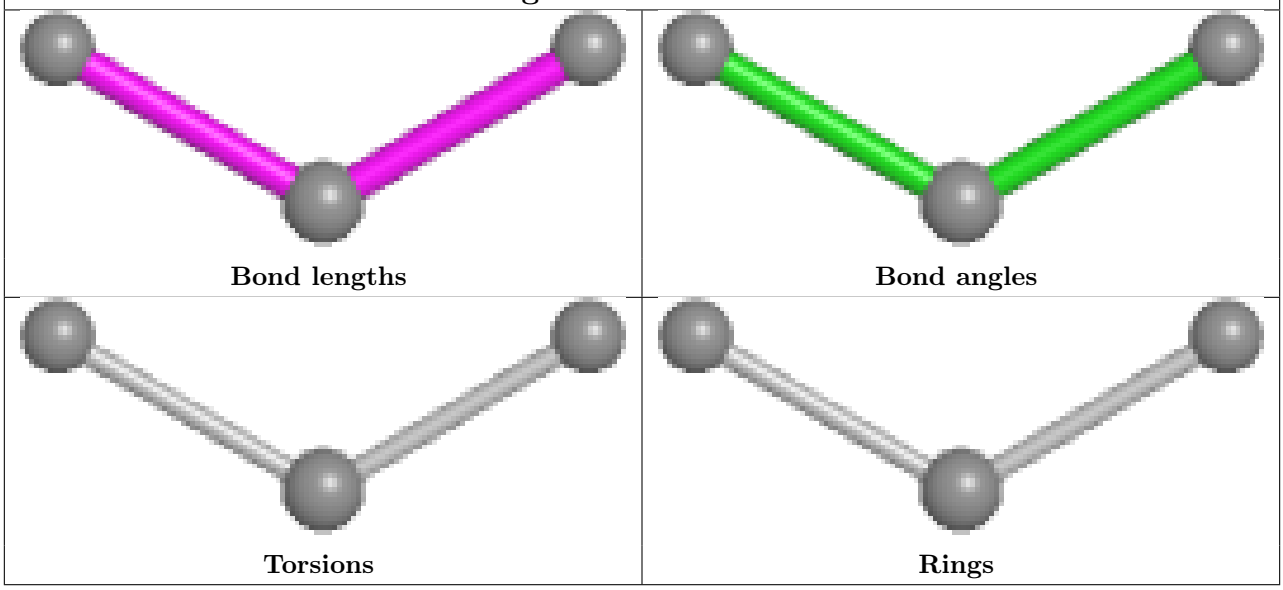


Torsions



Rings

Ligand FMT C 308



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	283/296 (95%)	0.11	2 (0%) 87 87	12, 20, 32, 71	0
1	B	282/296 (95%)	0.09	4 (1%) 75 75	12, 22, 35, 55	0
1	C	284/296 (95%)	0.01	0 100 100	12, 18, 29, 47	0
1	D	277/296 (93%)	2.89	165 (59%) 0 0	20, 50, 85, 145	0
All	All	1126/1184 (95%)	0.76	171 (15%) 2 1	12, 23, 64, 145	0

The worst 5 of 171 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	244	ALA	19.9
1	D	247	TRP	11.6
1	D	277	VAL	11.0
1	D	253	VAL	9.4
1	D	216	LEU	9.3

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 monosaccharides in this entry.

6.4 Ligands

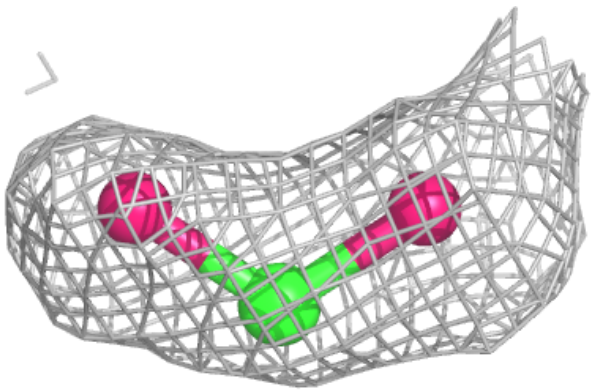
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

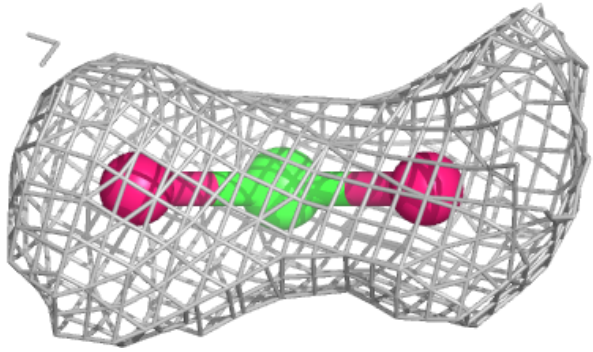
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FMT	C	302	3/3	0.71	0.13	49,49,52,52	0
3	FMT	C	304	3/3	0.76	0.14	56,56,59,61	0
2	GOL	B	301	6/6	0.78	0.14	59,61,63,68	0
2	GOL	C	303	6/6	0.81	0.15	47,51,54,56	0
2	GOL	B	302	6/6	0.82	0.17	25,46,54,55	0
3	FMT	A	405	3/3	0.83	0.13	37,37,41,42	0
3	FMT	B	306	3/3	0.84	0.15	50,50,52,54	0
3	FMT	A	406	3/3	0.85	0.21	43,43,45,47	0
2	GOL	A	401	6/6	0.86	0.10	28,30,34,35	0
3	FMT	C	305	3/3	0.87	0.10	56,56,60,63	0
2	GOL	C	301	6/6	0.88	0.14	24,33,36,37	0
3	FMT	B	304	3/3	0.88	0.12	46,46,48,53	0
3	FMT	C	308	3/3	0.88	0.18	33,33,38,40	0
3	FMT	A	403	3/3	0.89	0.10	37,37,42,43	0
3	FMT	D	301	3/3	0.89	0.08	26,26,29,33	0
4	ACT	B	303	4/4	0.89	0.10	24,31,35,39	0
2	GOL	C	306	6/6	0.91	0.10	26,43,48,50	0
3	FMT	C	307	3/3	0.92	0.12	20,20,21,22	0
3	FMT	B	305	3/3	0.94	0.08	34,34,39,43	0
3	FMT	A	402	3/3	0.95	0.08	24,24,26,27	0
2	GOL	A	404	6/6	0.96	0.08	22,32,44,53	0

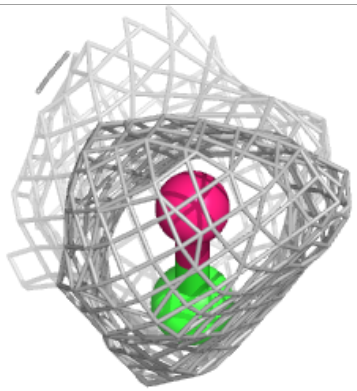
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMT 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)

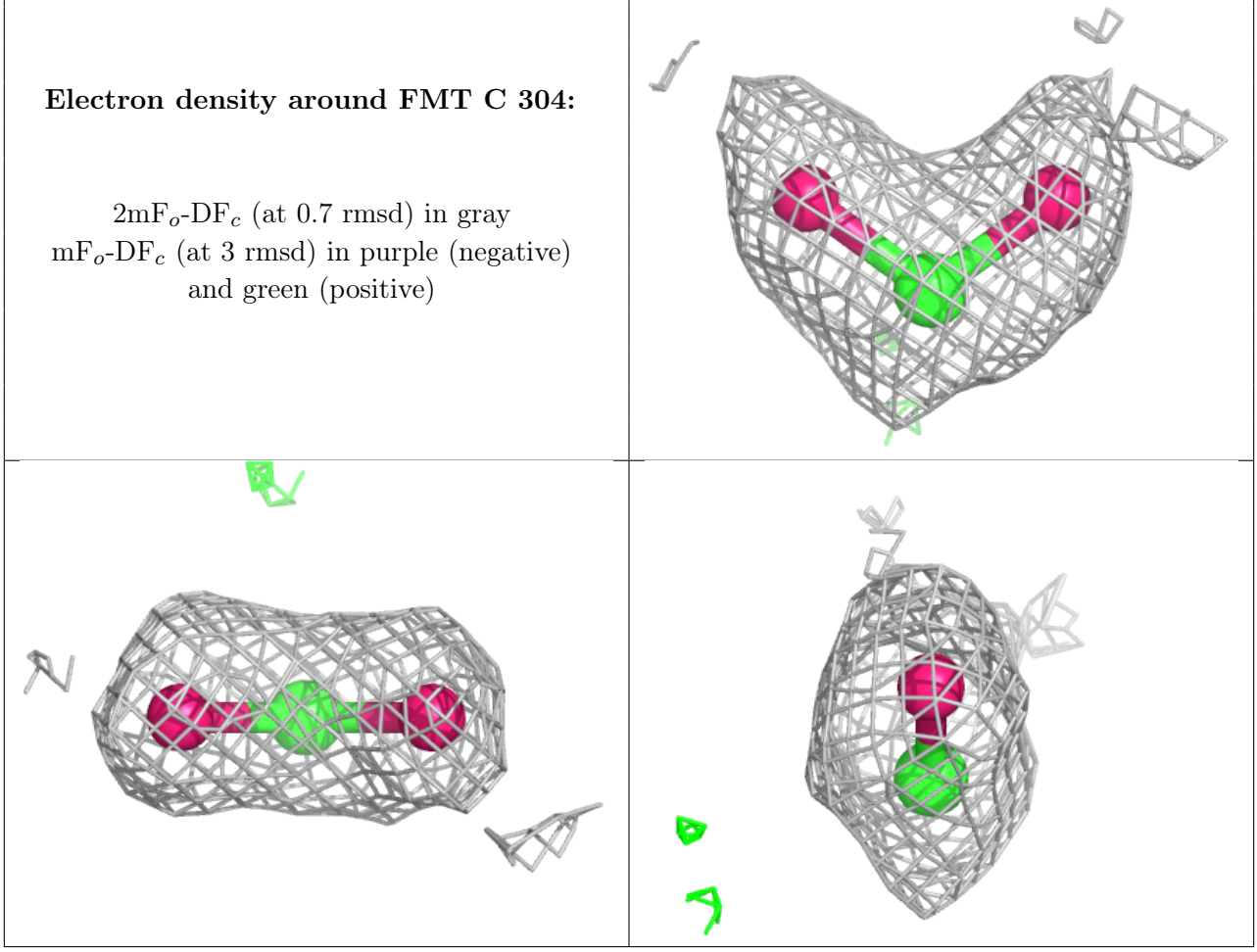






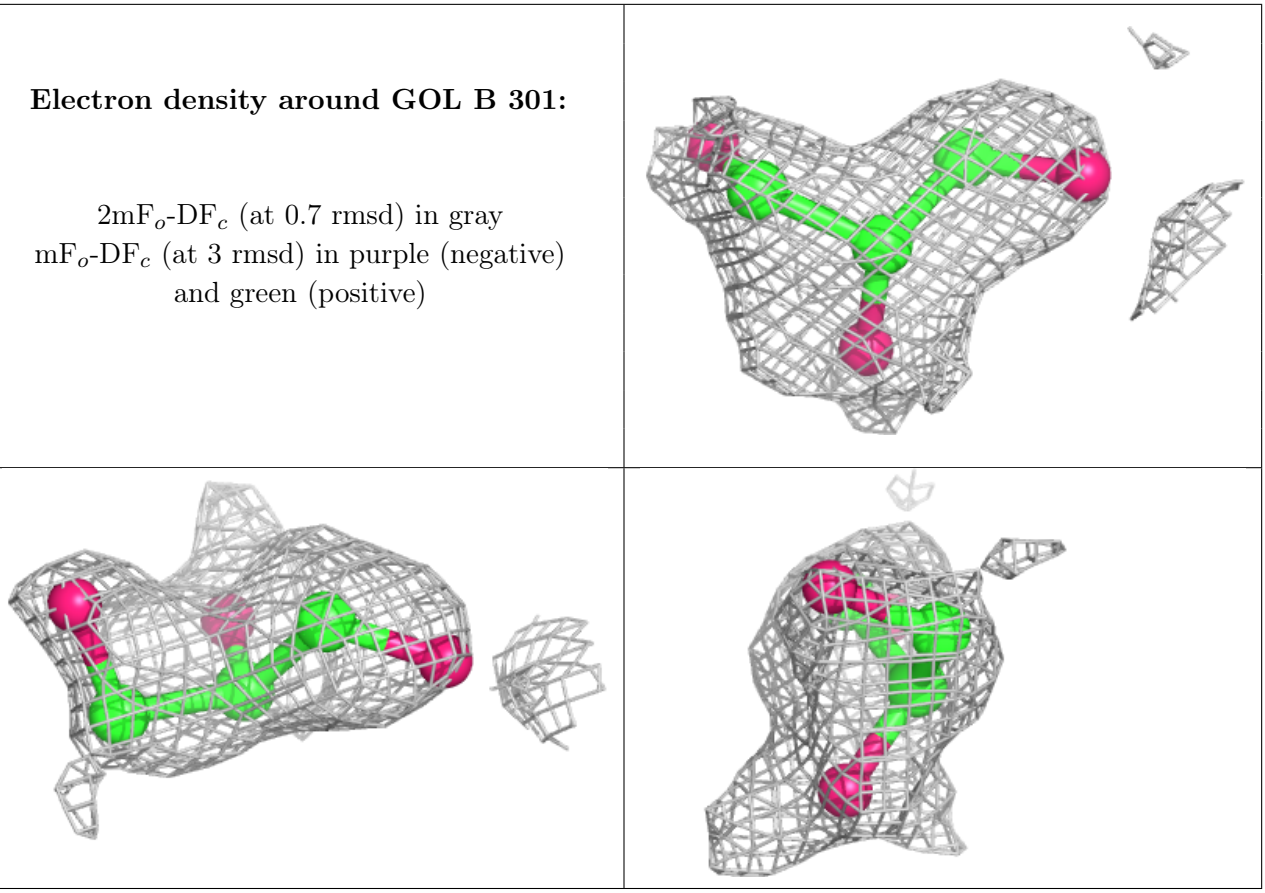
Electron density around FMT C 304:

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



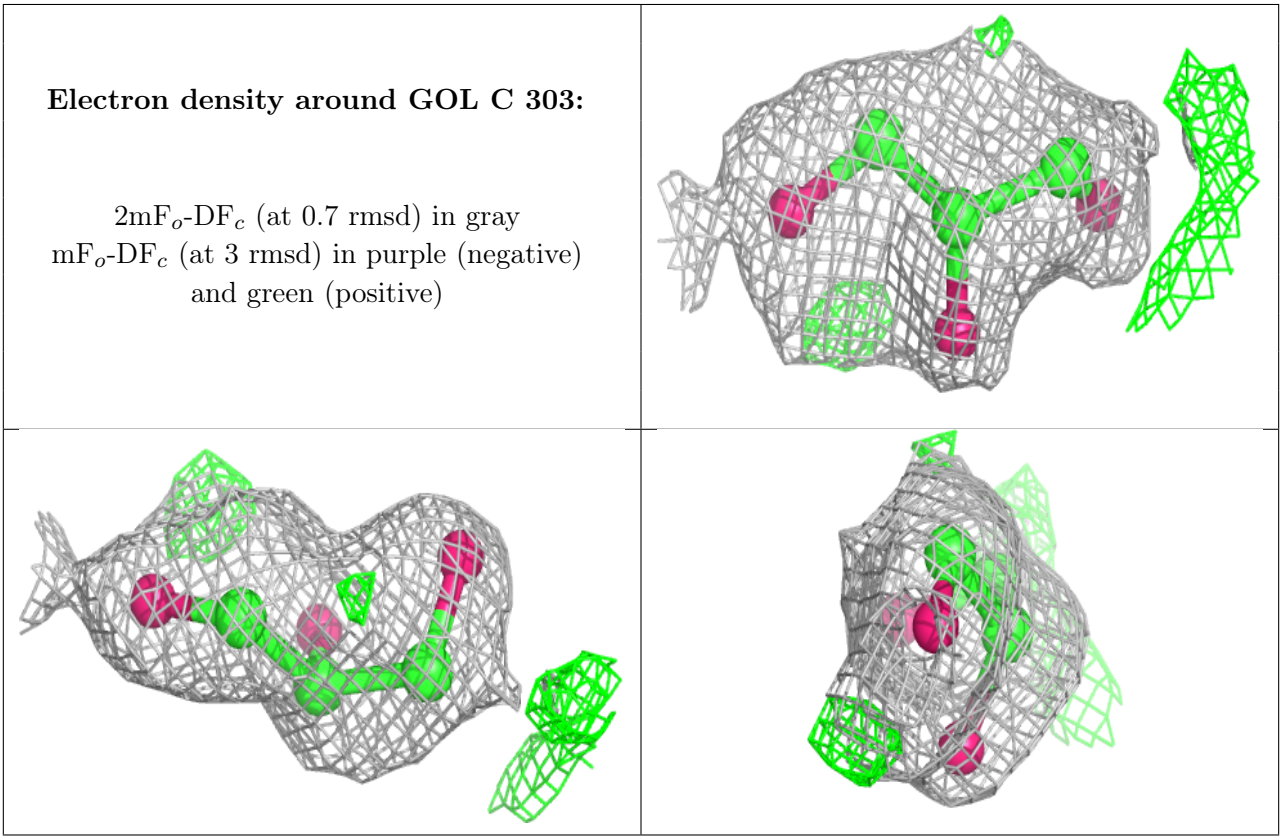
Electron density around GOL B 301:

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



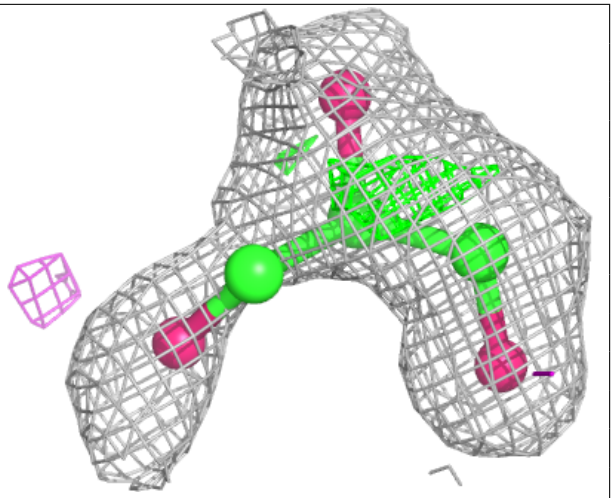
Electron density around GOL C 303:

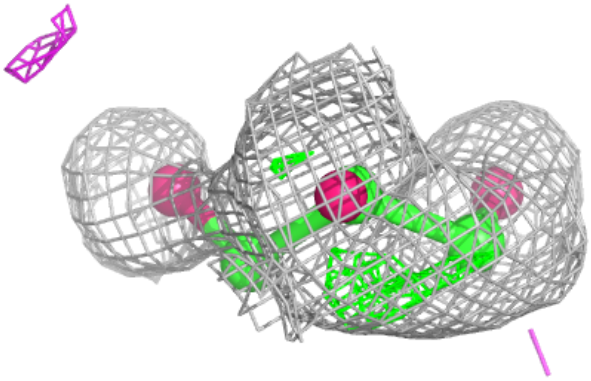
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

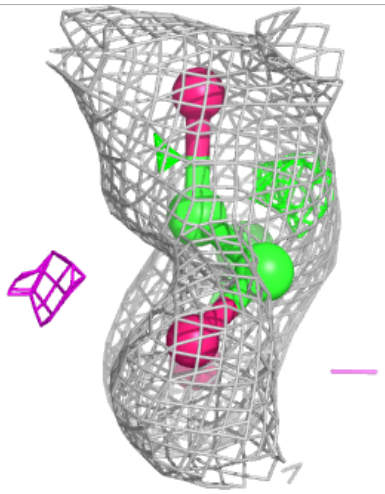


Electron density around GOL B 302:

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

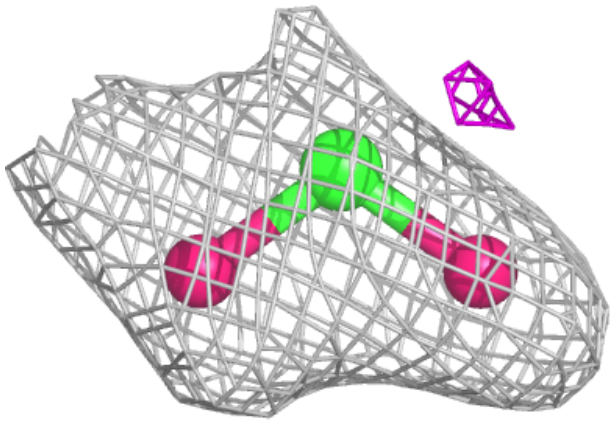


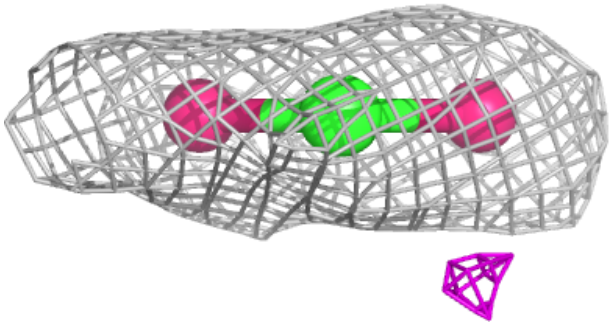


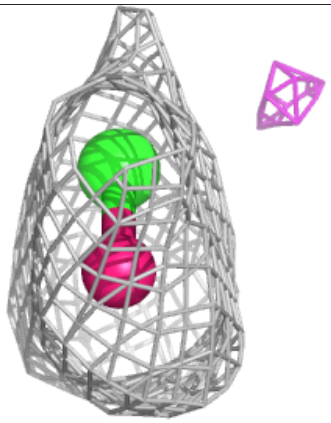


Electron density around FMT A 405:

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

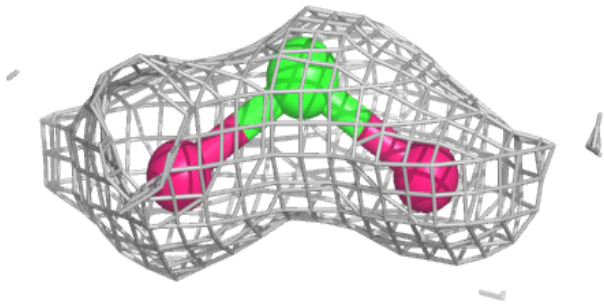


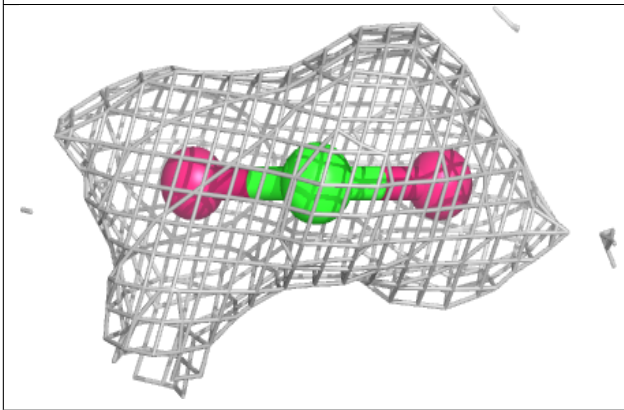


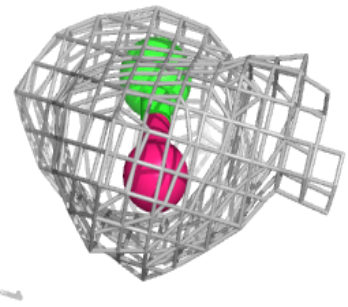


Electron density around FMT B 306:

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

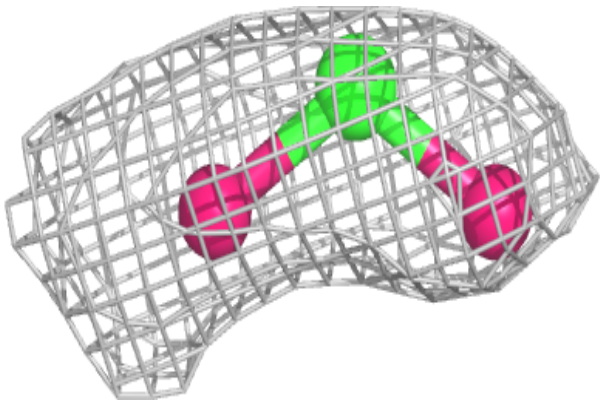


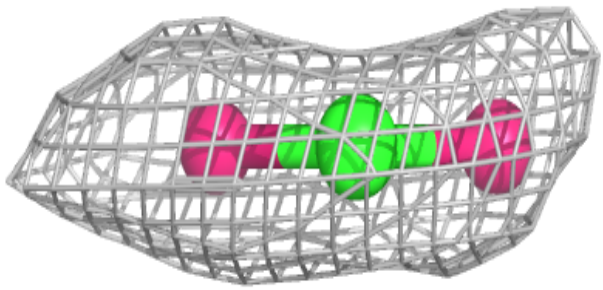


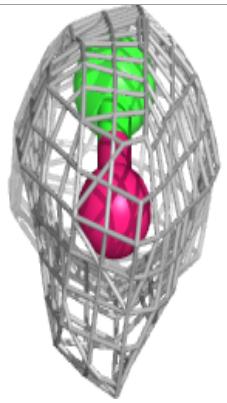


Electron density around FMT A 406:

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

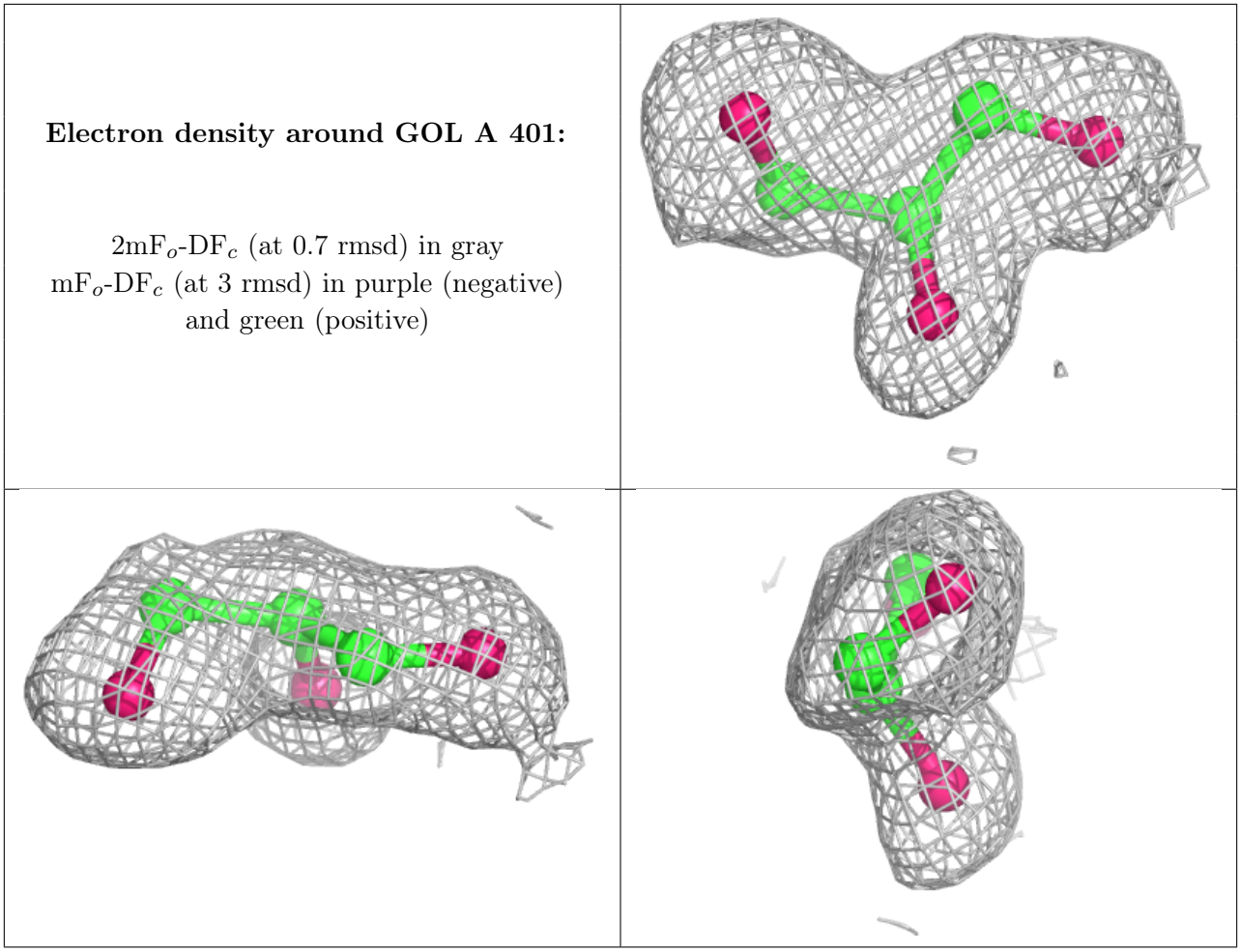






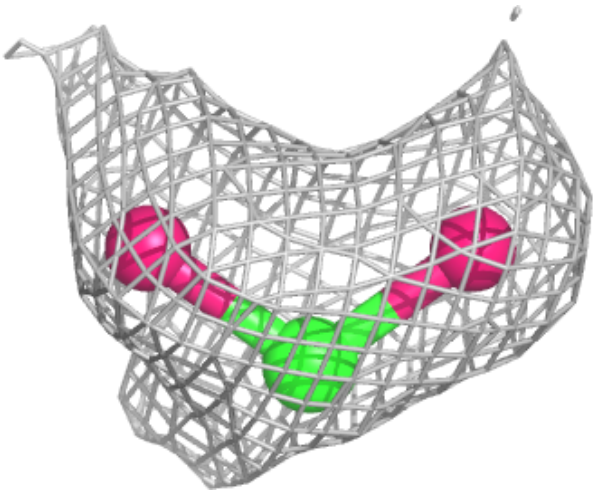
Electron density around GOL A 401:

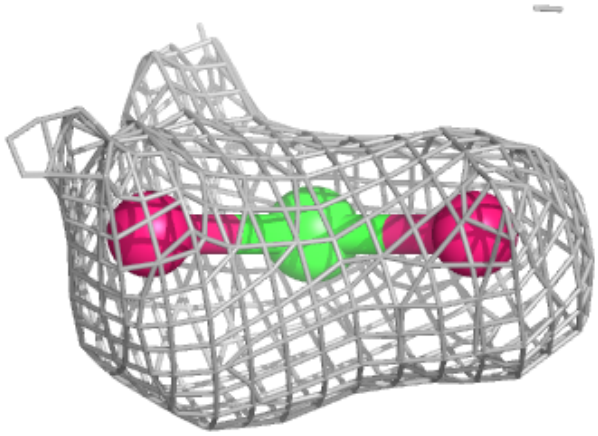
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

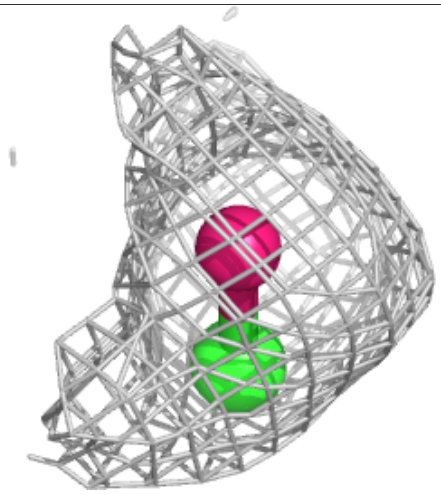


Electron density around FMT C 305:

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

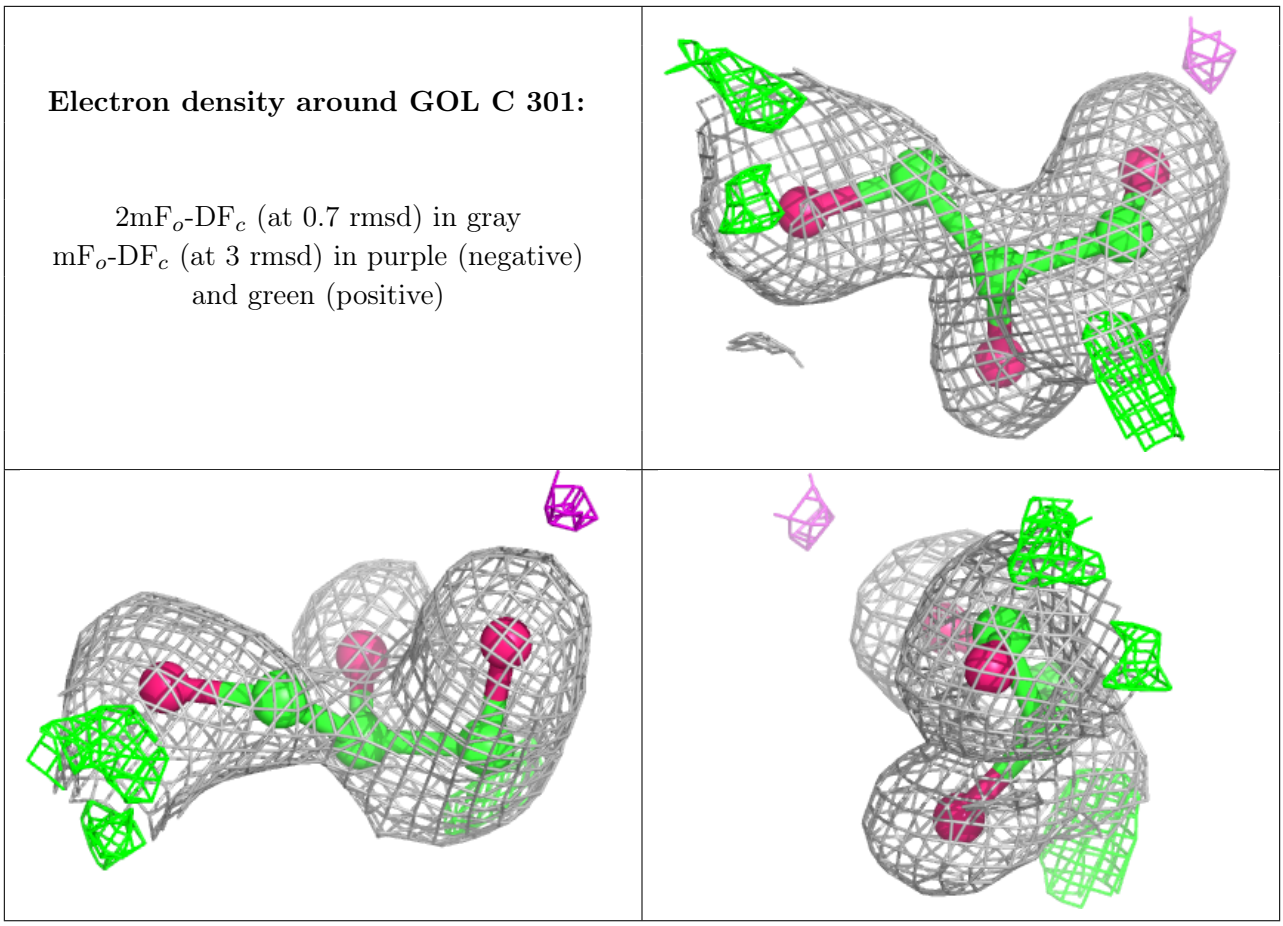






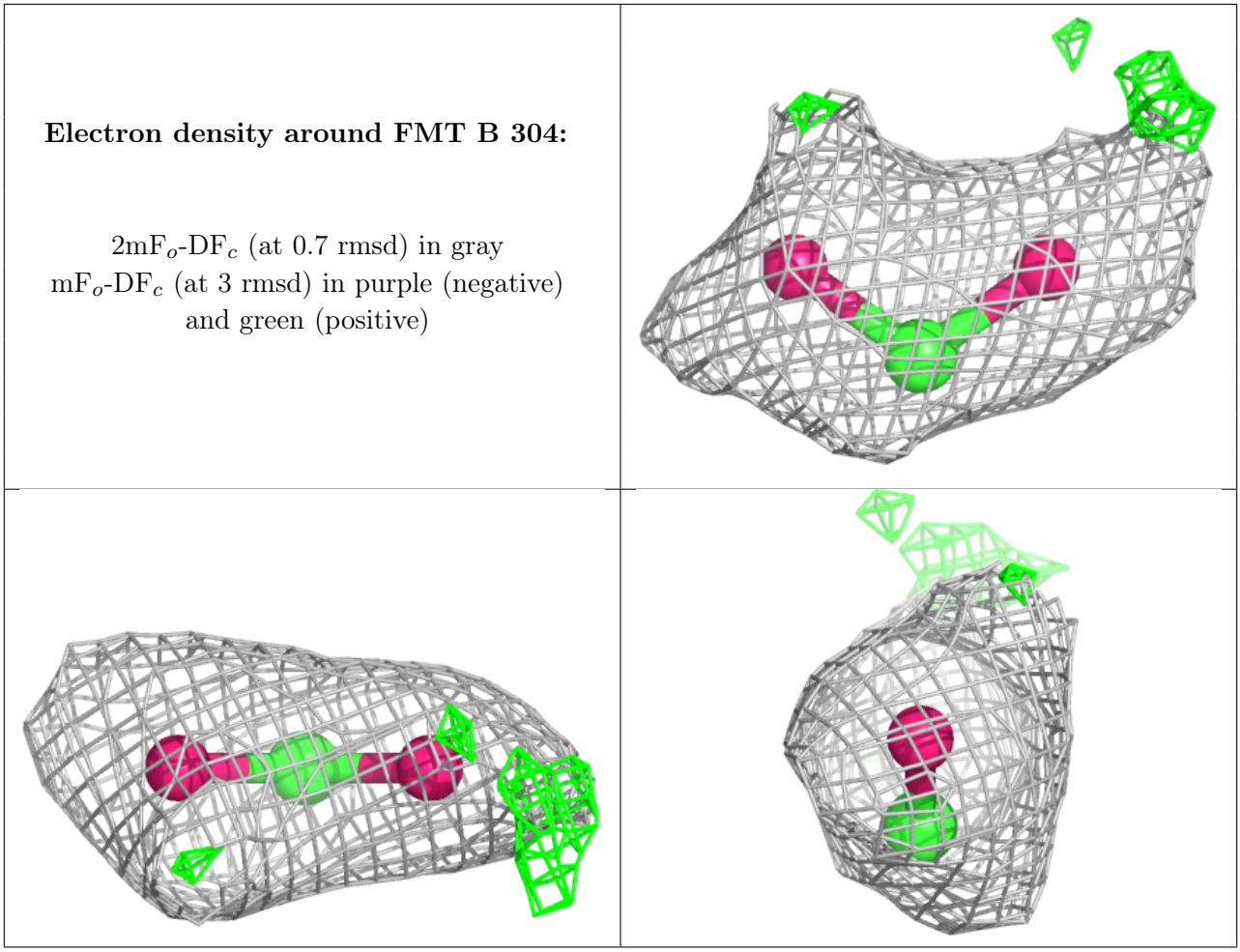
Electron density around GOL C 301:

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



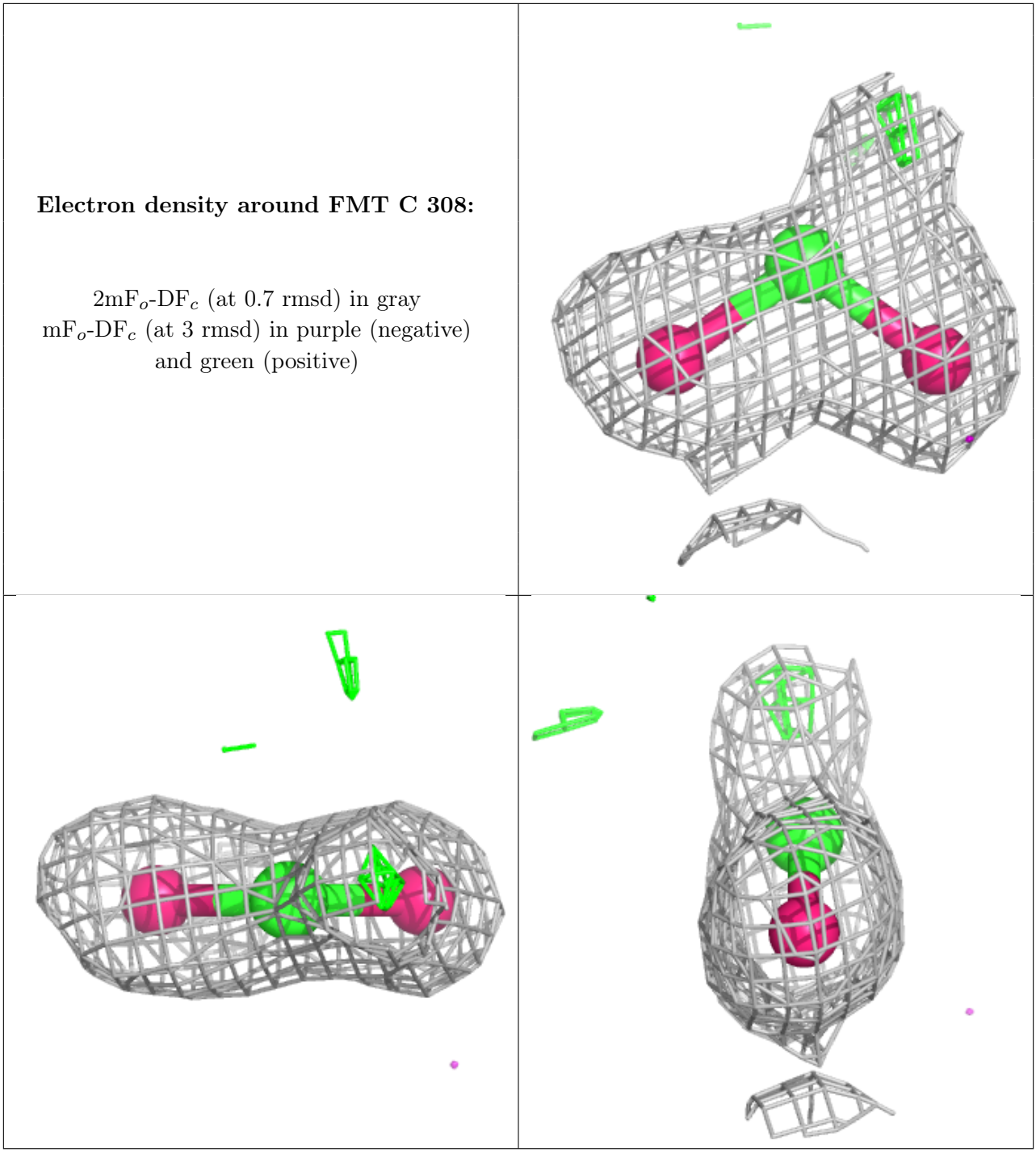
Electron density around FMT B 304:

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



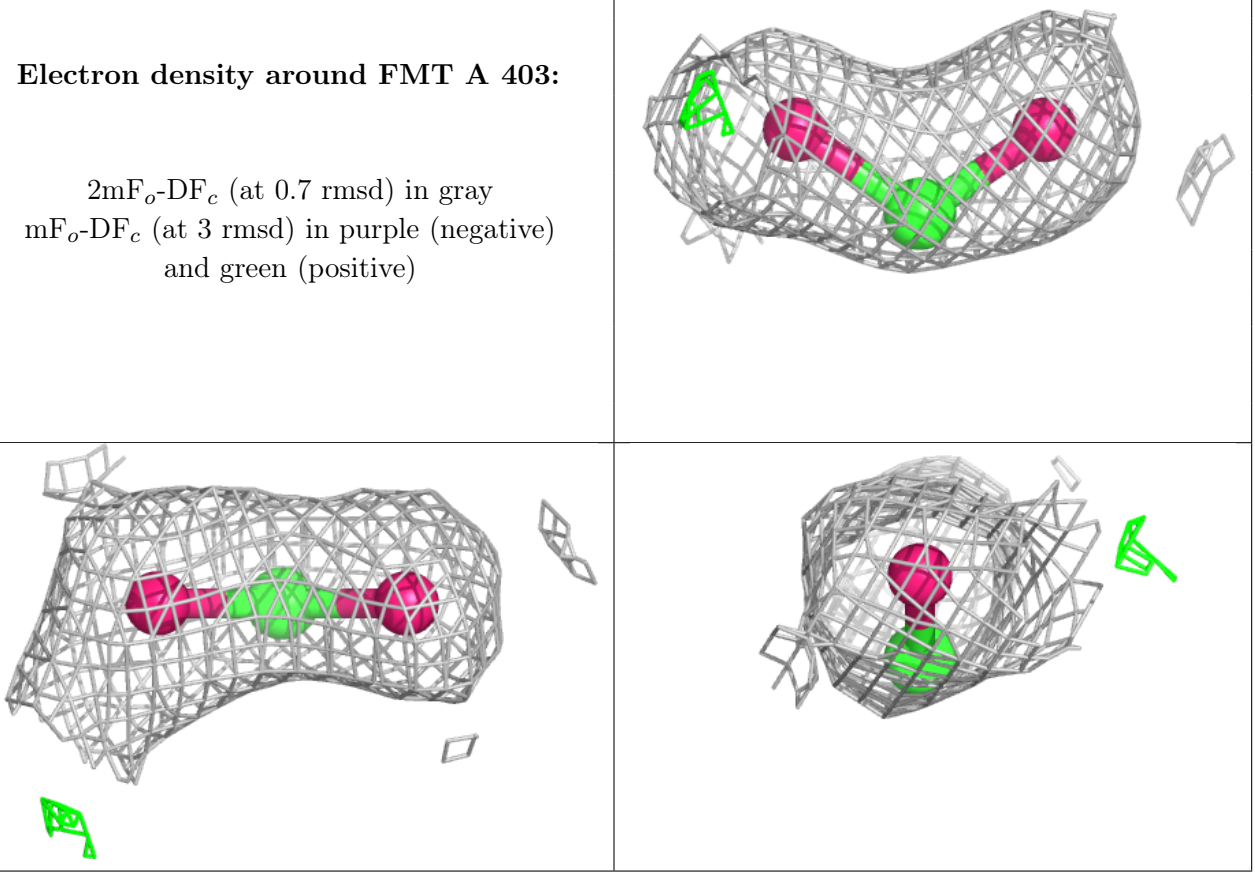
Electron density around FMT C 308:

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



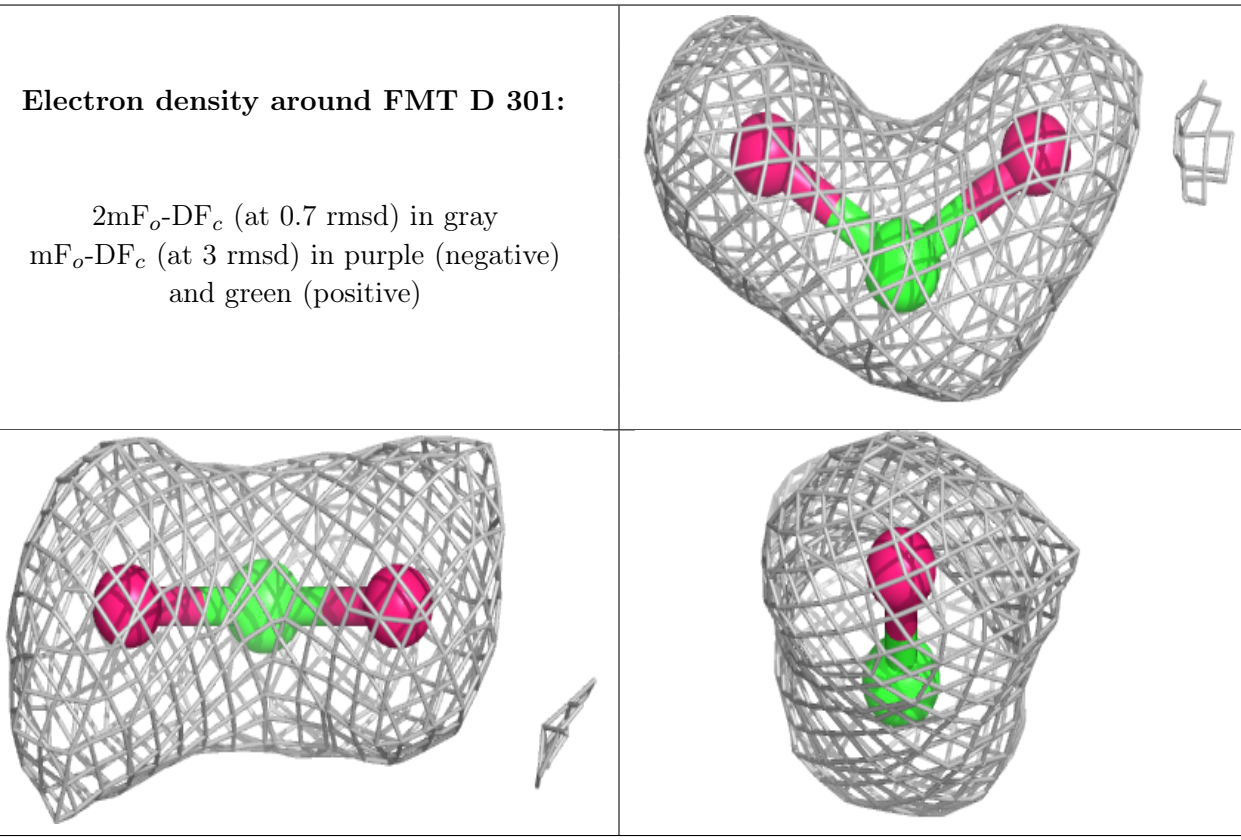
Electron density around FMT A 403:

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



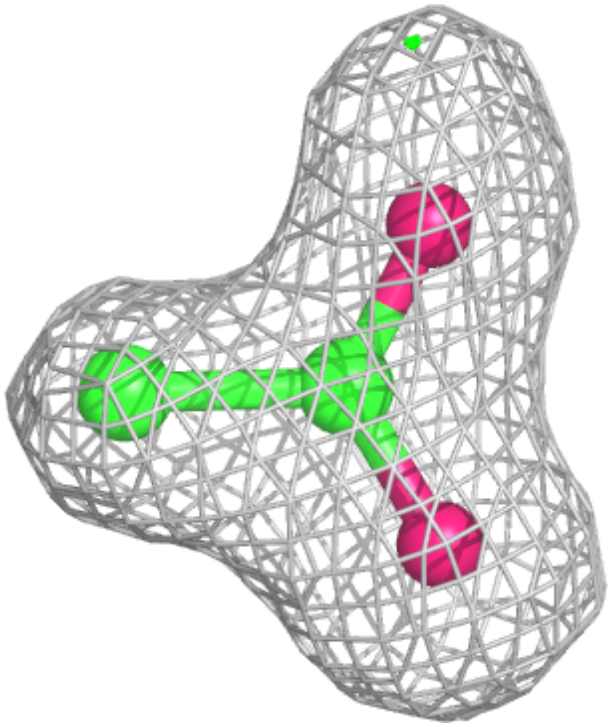
Electron density around FMT D 301:

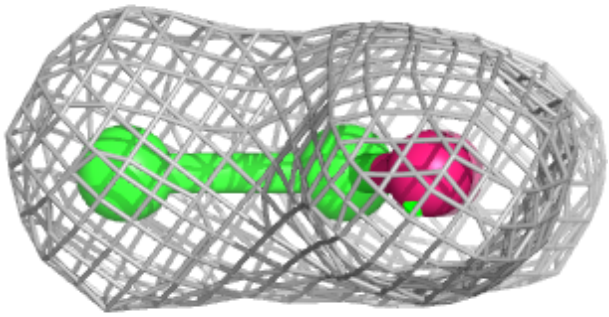
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

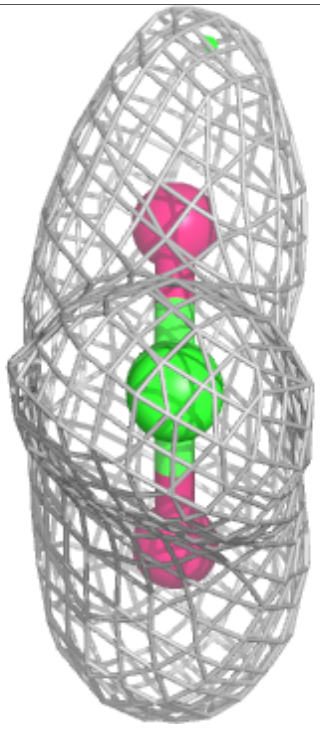


Electron density around ACT B 303:

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

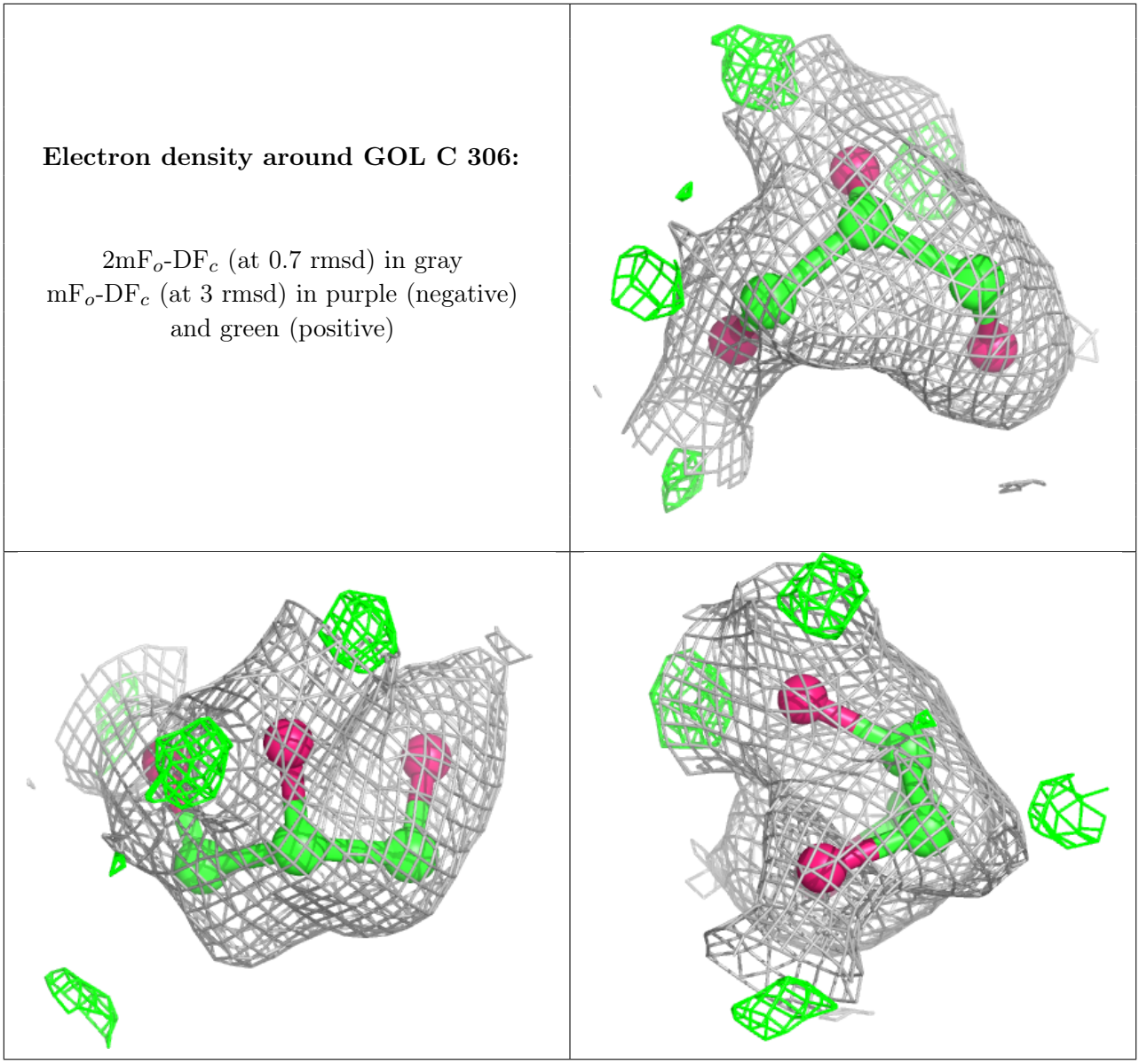






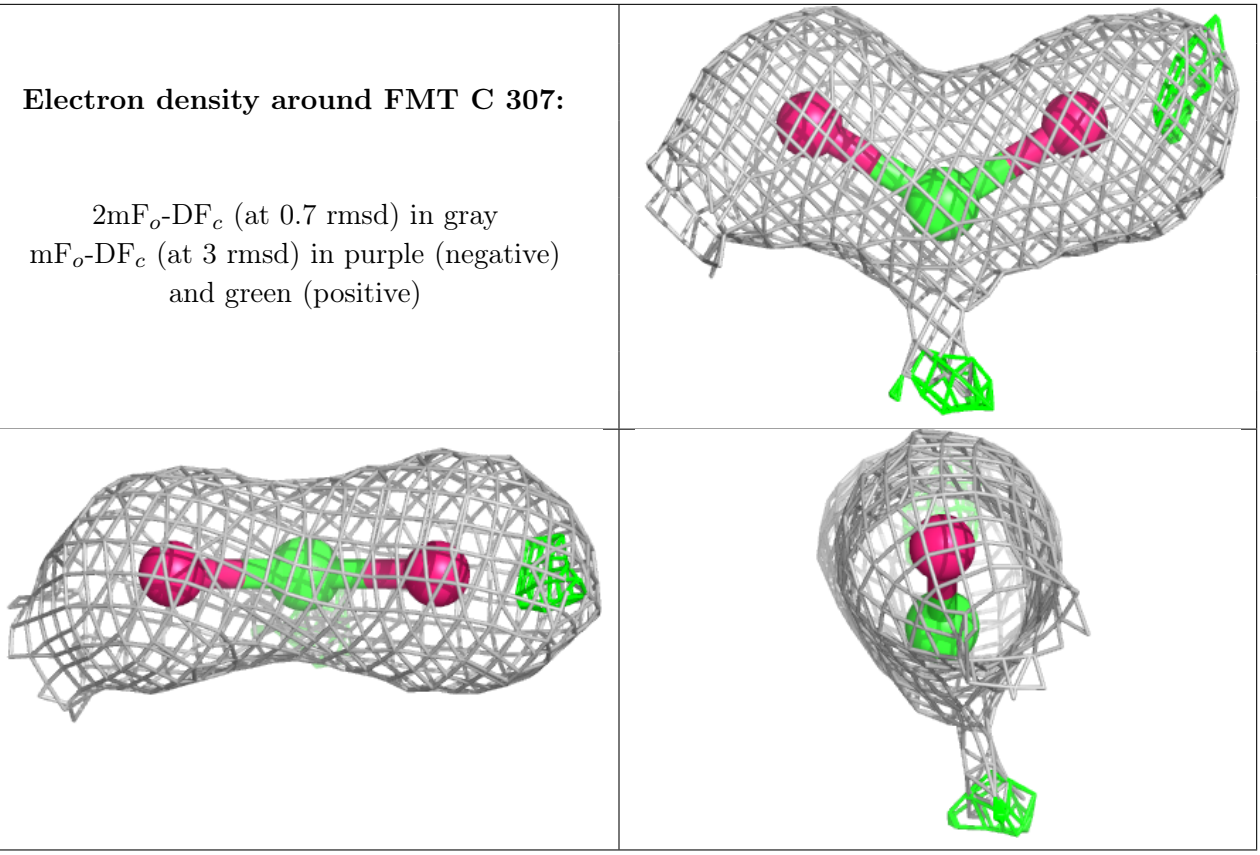
Electron density around GOL C 306:

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



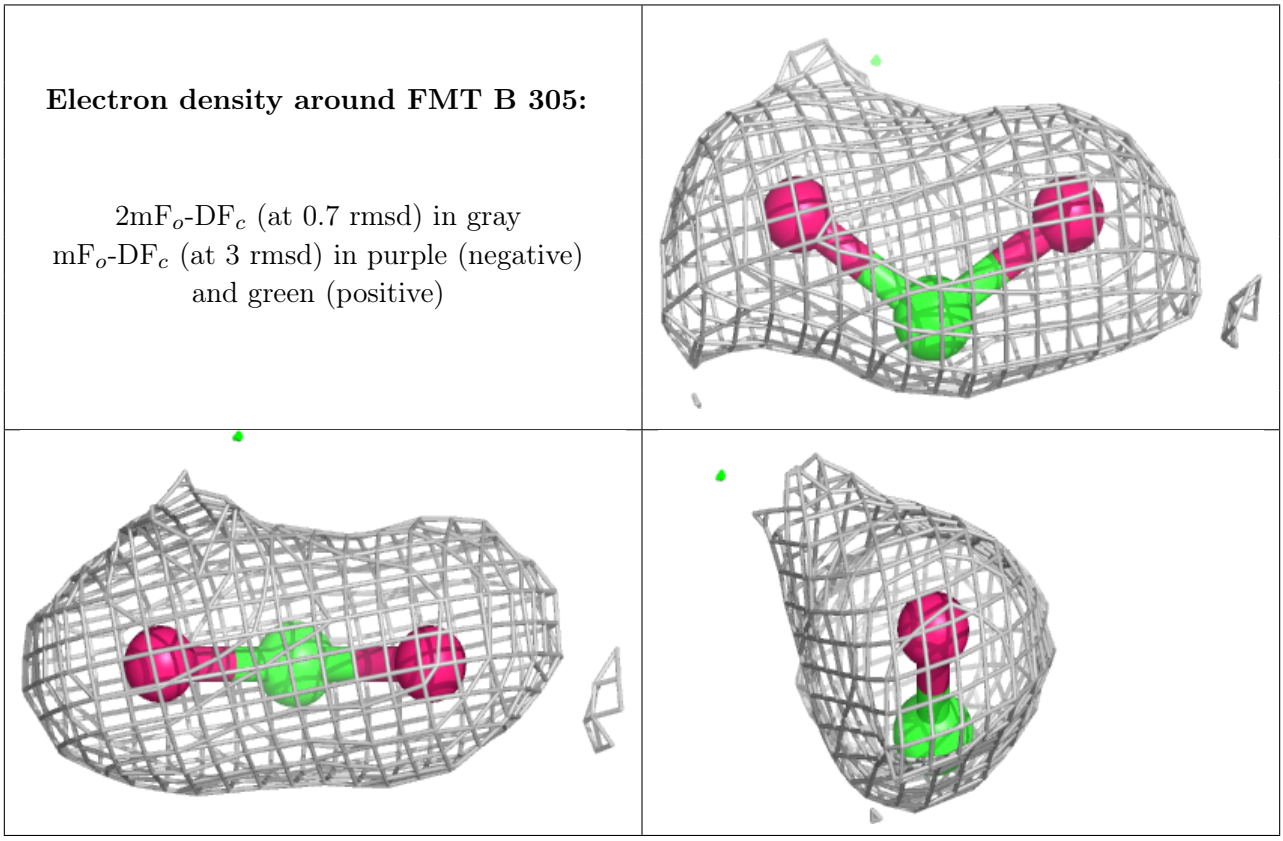
Electron density around FMT C 307:

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



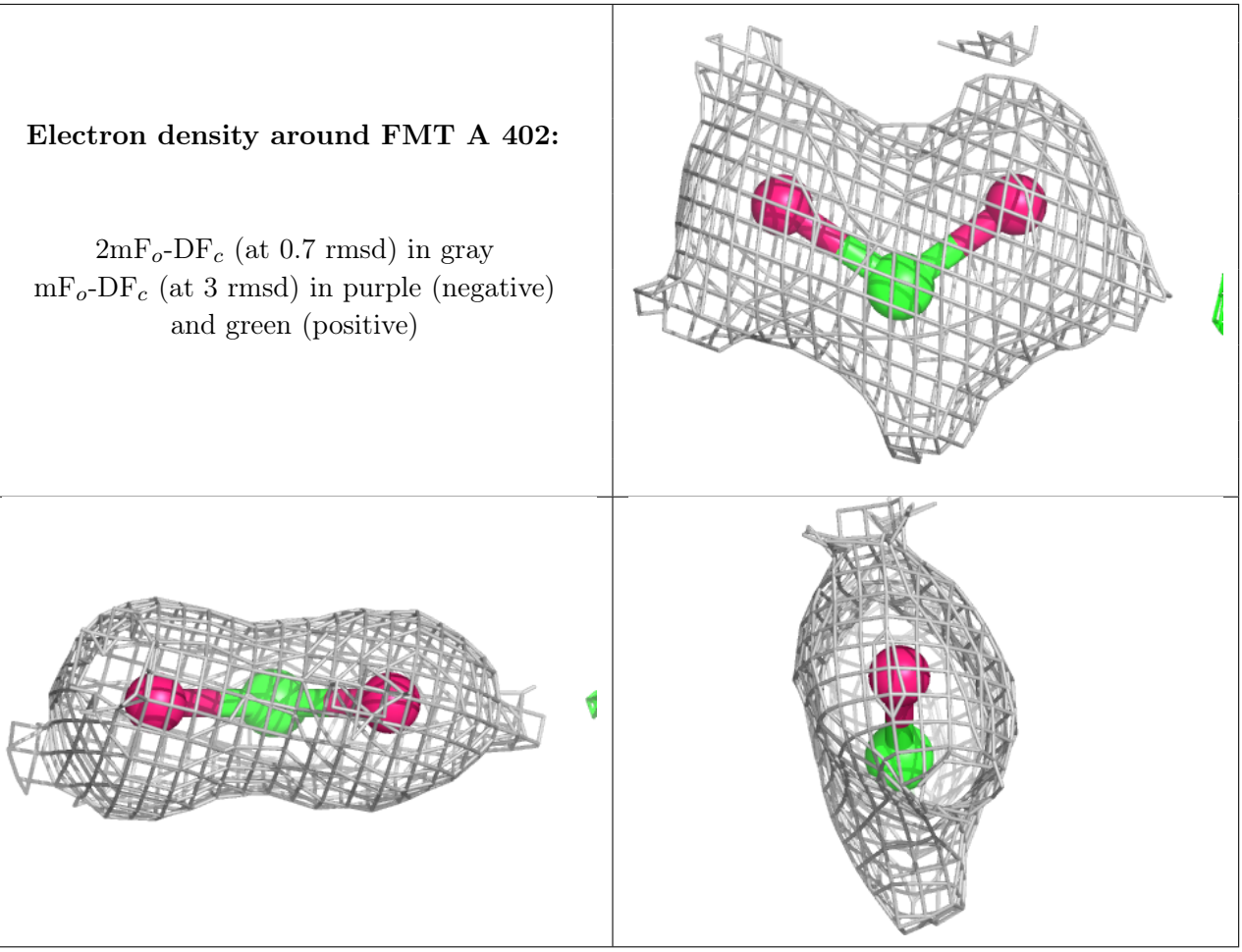
Electron density around FMT B 305:

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



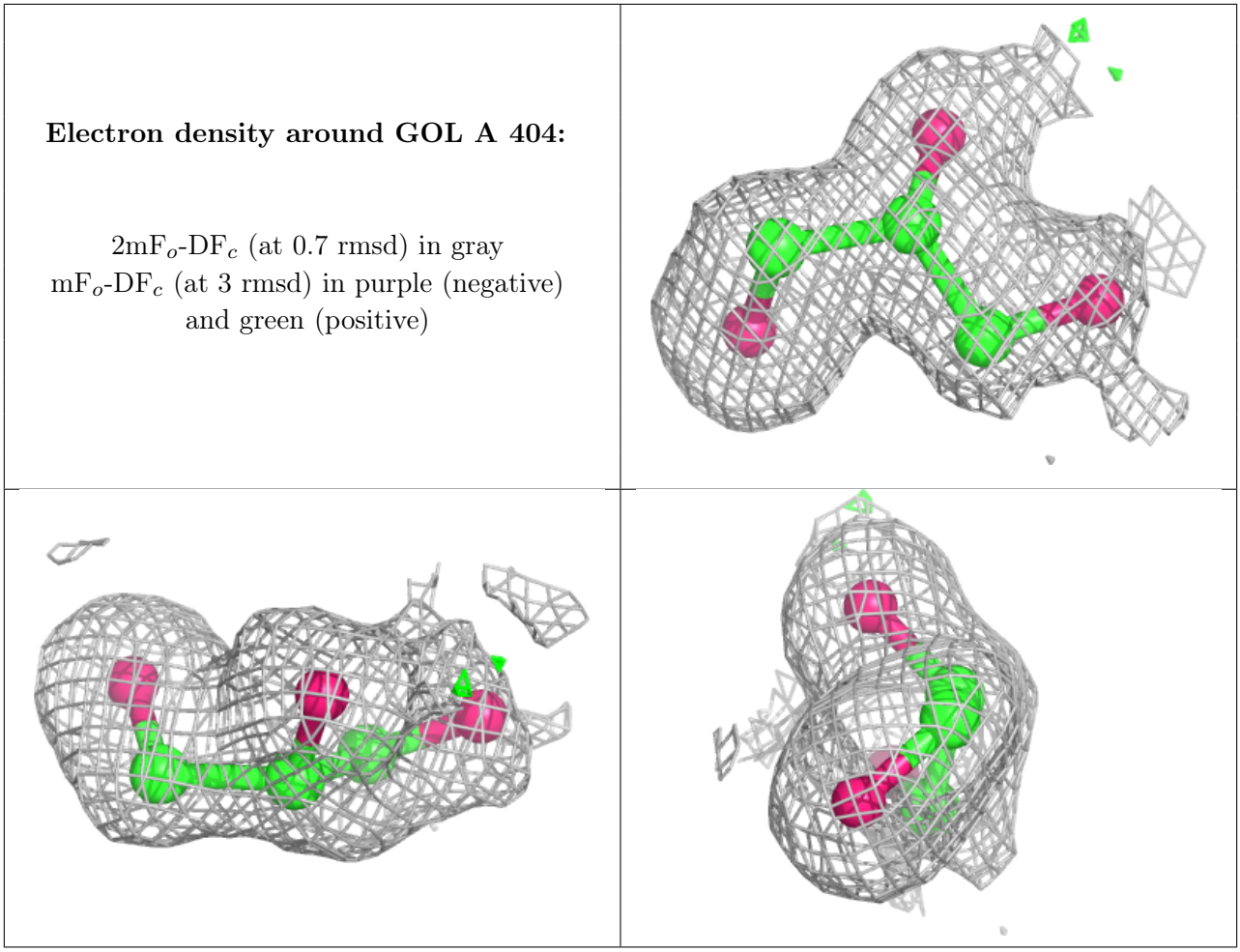
Electron density around FMT A 402:

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



Electron density around GOL A 404:

$2mF_o$-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.