Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2023 – 04:07 PM EDT

PDB ID	:	8G5W
Title	:	Structure of the Class II Fructose-1,6-Bisphophatase from Francisella tularensis complexed with native metal cofactor Mn++
Authors	:	Abad-Zapatero, C.; Selezneva, A.I.
Deposited on	:	2023-02-14
Resolution	:	2.00 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:

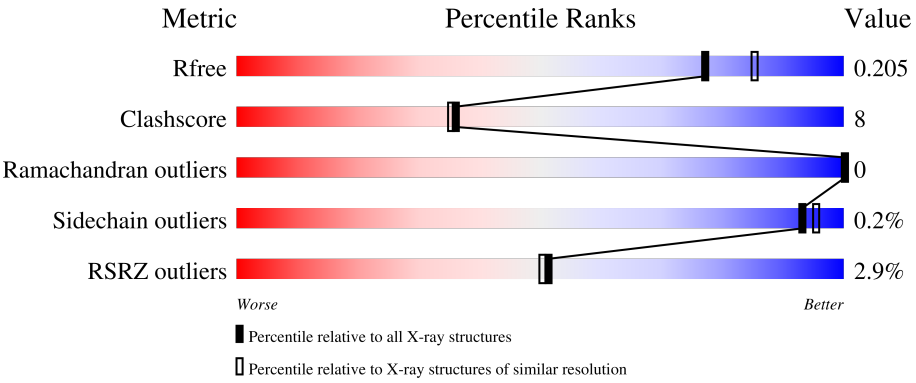
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	348	6% 76% 18% 6%
1	B	348	3% 80% 13% • 6%
1	C	348	2% 83% 11% 6%
1	D	348	% 77% 15% 8%

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
2	GOL	A	403	-	X	-	-
2	GOL	D	404	-	X	-	-
2	GOL	D	405	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20268 atoms, of which 9916 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 Fructose-1,6-bisphosphatase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	H	N	O	S	0	0	0
			4887	1507	2454	432	478	16			
1	B	328	Total	C	H	N	O	S	0	0	0
			4887	1507	2454	432	478	16			
1	C	328	Total	C	H	N	O	S	0	0	0
			4887	1507	2454	432	478	16			
1	D	321	Total	C	H	N	O	S	0	0	0
			4794	1477	2411	425	465	16			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A0E2ZJY0
A	-18	GLY	-	expression tag	UNP A0A0E2ZJY0
A	-17	SER	-	expression tag	UNP A0A0E2ZJY0
A	-16	SER	-	expression tag	UNP A0A0E2ZJY0
A	-15	HIS	-	expression tag	UNP A0A0E2ZJY0
A	-14	HIS	-	expression tag	UNP A0A0E2ZJY0
A	-13	HIS	-	expression tag	UNP A0A0E2ZJY0
A	-12	HIS	-	expression tag	UNP A0A0E2ZJY0
A	-11	HIS	-	expression tag	UNP A0A0E2ZJY0
A	-10	HIS	-	expression tag	UNP A0A0E2ZJY0
A	-9	SER	-	expression tag	UNP A0A0E2ZJY0
A	-8	SER	-	expression tag	UNP A0A0E2ZJY0
A	-7	GLY	-	expression tag	UNP A0A0E2ZJY0
A	-6	LEU	-	expression tag	UNP A0A0E2ZJY0
A	-5	VAL	-	expression tag	UNP A0A0E2ZJY0
A	-4	PRO	-	expression tag	UNP A0A0E2ZJY0
A	-3	ARG	-	expression tag	UNP A0A0E2ZJY0
A	-2	GLY	-	expression tag	UNP A0A0E2ZJY0
A	-1	SER	-	expression tag	UNP A0A0E2ZJY0
A	0	HIS	-	expression tag	UNP A0A0E2ZJY0
B	-19	MET	-	initiating methionine	UNP A0A0E2ZJY0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A0A0E2ZJY0
B	-17	SER	-	expression tag	UNP A0A0E2ZJY0
B	-16	SER	-	expression tag	UNP A0A0E2ZJY0
B	-15	HIS	-	expression tag	UNP A0A0E2ZJY0
B	-14	HIS	-	expression tag	UNP A0A0E2ZJY0
B	-13	HIS	-	expression tag	UNP A0A0E2ZJY0
B	-12	HIS	-	expression tag	UNP A0A0E2ZJY0
B	-11	HIS	-	expression tag	UNP A0A0E2ZJY0
B	-10	HIS	-	expression tag	UNP A0A0E2ZJY0
B	-9	SER	-	expression tag	UNP A0A0E2ZJY0
B	-8	SER	-	expression tag	UNP A0A0E2ZJY0
B	-7	GLY	-	expression tag	UNP A0A0E2ZJY0
B	-6	LEU	-	expression tag	UNP A0A0E2ZJY0
B	-5	VAL	-	expression tag	UNP A0A0E2ZJY0
B	-4	PRO	-	expression tag	UNP A0A0E2ZJY0
B	-3	ARG	-	expression tag	UNP A0A0E2ZJY0
B	-2	GLY	-	expression tag	UNP A0A0E2ZJY0
B	-1	SER	-	expression tag	UNP A0A0E2ZJY0
B	0	HIS	-	expression tag	UNP A0A0E2ZJY0
C	-19	MET	-	initiating methionine	UNP A0A0E2ZJY0
C	-18	GLY	-	expression tag	UNP A0A0E2ZJY0
C	-17	SER	-	expression tag	UNP A0A0E2ZJY0
C	-16	SER	-	expression tag	UNP A0A0E2ZJY0
C	-15	HIS	-	expression tag	UNP A0A0E2ZJY0
C	-14	HIS	-	expression tag	UNP A0A0E2ZJY0
C	-13	HIS	-	expression tag	UNP A0A0E2ZJY0
C	-12	HIS	-	expression tag	UNP A0A0E2ZJY0
C	-11	HIS	-	expression tag	UNP A0A0E2ZJY0
C	-10	HIS	-	expression tag	UNP A0A0E2ZJY0
C	-9	SER	-	expression tag	UNP A0A0E2ZJY0
C	-8	SER	-	expression tag	UNP A0A0E2ZJY0
C	-7	GLY	-	expression tag	UNP A0A0E2ZJY0
C	-6	LEU	-	expression tag	UNP A0A0E2ZJY0
C	-5	VAL	-	expression tag	UNP A0A0E2ZJY0
C	-4	PRO	-	expression tag	UNP A0A0E2ZJY0
C	-3	ARG	-	expression tag	UNP A0A0E2ZJY0
C	-2	GLY	-	expression tag	UNP A0A0E2ZJY0
C	-1	SER	-	expression tag	UNP A0A0E2ZJY0
C	0	HIS	-	expression tag	UNP A0A0E2ZJY0
D	-19	MET	-	initiating methionine	UNP A0A0E2ZJY0
D	-18	GLY	-	expression tag	UNP A0A0E2ZJY0
D	-17	SER	-	expression tag	UNP A0A0E2ZJY0

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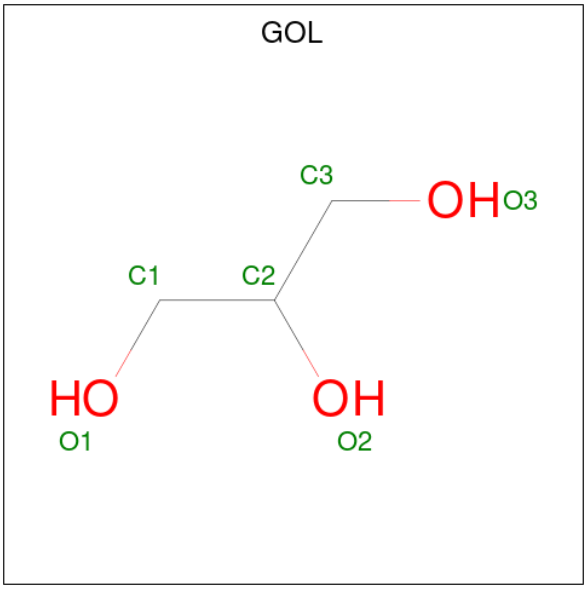
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A0A0E2ZJY0
D	-15	HIS	-	expression tag	UNP A0A0E2ZJY0
D	-14	HIS	-	expression tag	UNP A0A0E2ZJY0
D	-13	HIS	-	expression tag	UNP A0A0E2ZJY0
D	-12	HIS	-	expression tag	UNP A0A0E2ZJY0
D	-11	HIS	-	expression tag	UNP A0A0E2ZJY0
D	-10	HIS	-	expression tag	UNP A0A0E2ZJY0
D	-9	SER	-	expression tag	UNP A0A0E2ZJY0
D	-8	SER	-	expression tag	UNP A0A0E2ZJY0
D	-7	GLY	-	expression tag	UNP A0A0E2ZJY0
D	-6	LEU	-	expression tag	UNP A0A0E2ZJY0
D	-5	VAL	-	expression tag	UNP A0A0E2ZJY0
D	-4	PRO	-	expression tag	UNP A0A0E2ZJY0
D	-3	ARG	-	expression tag	UNP A0A0E2ZJY0
D	-2	GLY	-	expression tag	UNP A0A0E2ZJY0
D	-1	SER	-	expression tag	UNP A0A0E2ZJY0
D	0	HIS	-	expression tag	UNP A0A0E2ZJY0

- 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	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			13	3	7	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mn 1 1	0	0

- Molecule 4 is water.

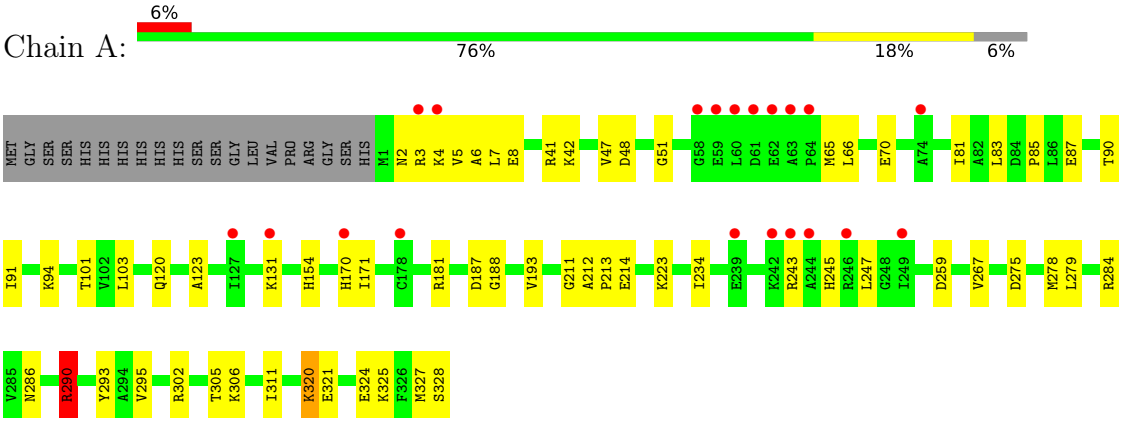
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	88	Total O 88 88	0	0
4	B	105	Total O 105 105	0	0
4	C	194	Total O 194 194	0	0
4	D	171	Total O 171 171	0	0

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.

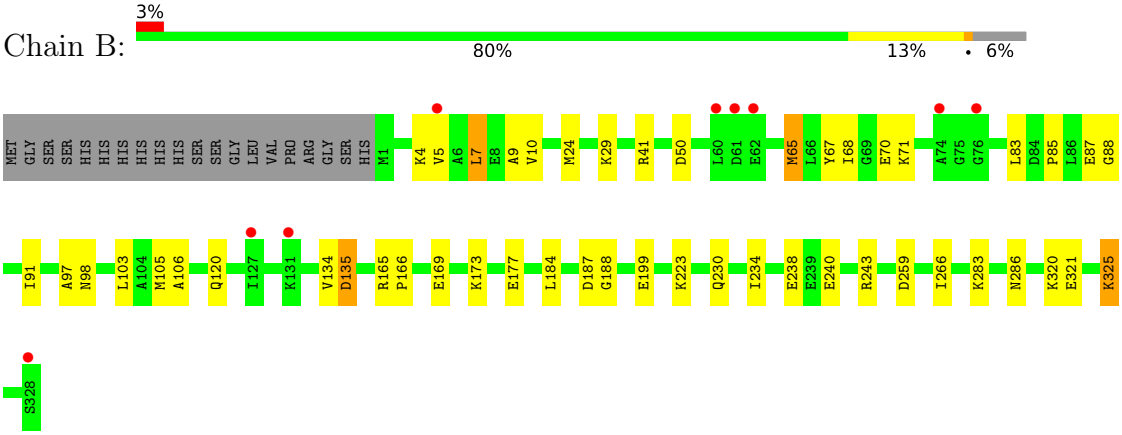
• Molecule 1: Fructose-1,6-bisphosphatase

Chain A:



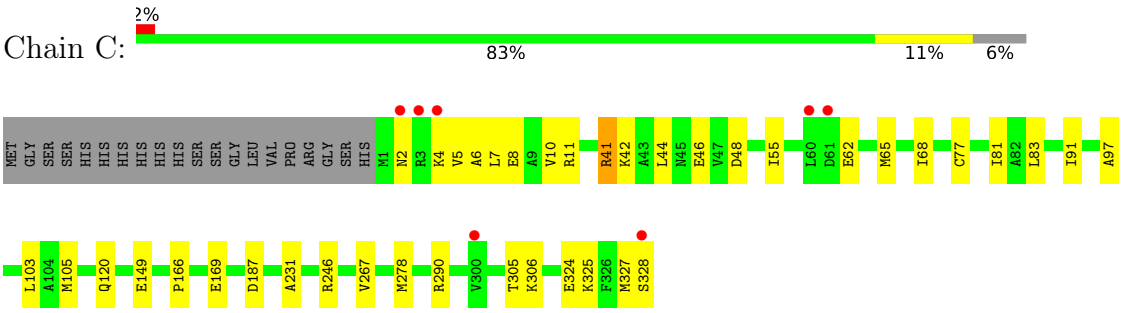
• Molecule 1: Fructose-1,6-bisphosphatase

Chain B:



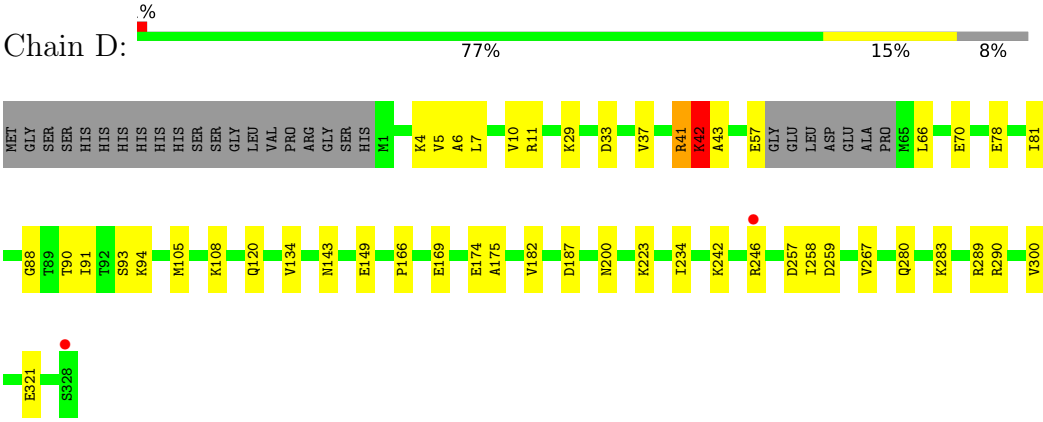
• Molecule 1: Fructose-1,6-bisphosphatase

Chain C:



• Molecule 1: Fructose-1,6-bisphosphatase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	63.84Å 75.88Å 77.62Å 67.83° 68.14° 76.37°	Depositor
Resolution (Å)	37.37 – 2.00 37.37 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.0 (37.37-2.00) 97.7 (37.37-1.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, REFMAC 5.8.0158	Depositor
R, R_{free}	0.161 , 0.204 0.161 , 0.205	Depositor DCC
R_{free} test set	4120 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 52.2	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	20268	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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: MN, 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	0.51	0/2459	0.71	3/3317 (0.1%)
1	B	0.69	5/2459 (0.2%)	0.87	10/3317 (0.3%)
1	C	0.60	0/2459	0.79	4/3317 (0.1%)
1	D	0.80	3/2407 (0.1%)	0.88	7/3244 (0.2%)
All	All	0.66	8/9784 (0.1%)	0.81	24/13195 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	42	LYS	CE-NZ	-21.90	0.94	1.49
1	B	325	LYS	CE-NZ	15.84	1.88	1.49
1	D	78	GLU	CB-CG	-8.65	1.35	1.52
1	B	325	LYS	CD-CE	8.43	1.72	1.51
1	B	29	LYS	CE-NZ	7.15	1.67	1.49
1	D	42	LYS	CD-CE	6.39	1.67	1.51
1	B	238	GLU	CB-CG	-5.89	1.41	1.52
1	B	325	LYS	CG-CD	-5.30	1.34	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	135	ASP	CB-CG-OD1	13.67	130.60	118.30
1	D	42	LYS	CD-CE-NZ	13.33	142.37	111.70
1	B	238	GLU	OE1-CD-OE2	-8.62	112.96	123.30
1	B	238	GLU	CG-CD-OE1	8.59	135.48	118.30
1	A	290	ARG	CG-CD-NE	-7.98	95.04	111.80
1	C	41	ARG	NE-CZ-NH1	-7.31	116.65	120.30
1	C	62	GLU	OE1-CD-OE2	-7.29	114.55	123.30
1	D	42	LYS	CG-CD-CE	6.65	131.84	111.90
1	B	65	MET	CG-SD-CE	6.49	110.59	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	41	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	7	LEU	CB-CG-CD2	-5.94	100.89	111.00
1	D	200	ASN	CB-CA-C	5.90	122.21	110.40
1	B	135	ASP	OD1-CG-OD2	-5.88	112.13	123.30
1	D	41	ARG	CG-CD-NE	-5.87	99.47	111.80
1	D	78	GLU	CA-CB-CG	5.75	126.06	113.40
1	A	320	LYS	CB-CG-CD	-5.64	96.94	111.60
1	A	320	LYS	CD-CE-NZ	-5.64	98.73	111.70
1	B	134	VAL	C-N-CA	-5.43	108.12	121.70
1	B	238	GLU	CG-CD-OE2	-5.23	107.84	118.30
1	C	41	ARG	NE-CZ-NH2	5.13	122.86	120.30
1	D	78	GLU	OE1-CD-OE2	-5.10	117.18	123.30
1	C	278	MET	CG-SD-CE	-5.10	92.05	100.20
1	B	199	GLU	CA-CB-CG	5.04	124.50	113.40
1	B	325	LYS	CA-CB-CG	5.01	124.43	113.40

There are no chirality outliers.

There are no planarity outliers.

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	2433	2454	2456	51	0
1	B	2433	2454	2456	40	0
1	C	2433	2454	2456	40	0
1	D	2383	2411	2413	41	0
2	A	30	40	39	4	0
2	B	24	32	32	3	0
2	C	24	32	32	5	0
2	D	30	39	38	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	88	0	0	2	0
4	B	105	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	194	0	0	4	0
4	D	171	0	0	7	0
All	All	10352	9916	9922	158	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (158) 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:B:325:LYS:CE	1:B:325:LYS:NZ	1.88	1.36
1:D:11:ARG:NH2	4:D:501:HOH:O	1.86	1.08
1:A:131:LYS:NZ	1:A:259:ASP:OD2	1.90	1.04
1:B:50:ASP:OD1	1:B:71:LYS:NZ	2.02	0.93
1:B:173:LYS:O	1:B:177:GLU:HG2	1.71	0.90
1:A:3:ARG:HD2	1:A:3:ARG:H	1.37	0.88
1:B:173:LYS:NZ	4:B:502:HOH:O	2.12	0.82
1:A:284:ARG:HH12	2:A:405:GOL:H12	1.41	0.82
1:B:165:ARG:NH2	4:B:501:HOH:O	2.12	0.81
1:B:41:ARG:HE	1:B:65:MET:HE2	1.44	0.80
1:D:174:GLU:OE2	4:D:502:HOH:O	2.02	0.77
1:C:11:ARG:NH2	1:C:46:GLU:OE2	2.19	0.75
1:C:2:ASN:O	1:C:5:VAL:HG22	1.88	0.74
1:C:68:ILE:HD11	2:C:602:GOL:H11	1.68	0.74
1:C:81:ILE:HD13	1:C:105:MET:HG2	1.69	0.74
1:B:4:LYS:HE3	1:C:4:LYS:HD2	1.72	0.71
1:D:81:ILE:HD13	1:D:105:MET:HG2	1.71	0.71
1:D:166:PRO:O	1:D:169:GLU:HG3	1.92	0.70
1:B:173:LYS:HA	1:B:173:LYS:HE2	1.75	0.68
1:C:77:CYS:SG	4:C:735:HOH:O	2.51	0.68
1:A:290:ARG:HD2	1:A:293:TYR:CD1	2.28	0.68
1:D:90:THR:O	1:D:94:LYS:HG2	1.95	0.66
1:A:3:ARG:HA	1:A:302:ARG:HH12	1.61	0.66
1:C:83:LEU:CD2	1:C:103:LEU:HD13	2.26	0.66
1:C:44:LEU:HD11	1:C:83:LEU:HD11	1.79	0.63
1:D:10:VAL:HG12	1:D:300:VAL:HB	1.80	0.63
1:C:2:ASN:HB3	1:C:4:LYS:HG2	1.81	0.63
1:B:240:GLU:HG2	1:B:243:ARG:HH12	1.64	0.63
1:B:41:ARG:HE	1:B:65:MET:CE	2.12	0.62
1:D:120:GLN:HG3	1:D:234:ILE:HD11	1.82	0.62
1:D:283:LYS:HE2	2:D:404:GOL:O2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LYS:HD2	1:B:184:LEU:HD12	1.83	0.61
1:D:43:ALA:HA	4:D:501:HOH:O	2.00	0.60
1:C:83:LEU:HD21	1:C:103:LEU:HD13	1.84	0.60
1:A:41:ARG:HD3	1:A:65:MET:HE3	1.82	0.60
1:B:4:LYS:CE	1:C:4:LYS:HD2	2.32	0.60
1:A:286:ASN:OD1	2:A:405:GOL:H11	2.01	0.60
1:A:243:ARG:O	1:A:247:LEU:HD23	2.03	0.59
1:B:91:ILE:HD11	1:B:187:ASP:HB3	1.85	0.59
1:D:41:ARG:HG2	1:D:41:ARG:HH11	1.67	0.59
1:A:275:ASP:HB3	2:A:401:GOL:H11	1.85	0.59
1:B:7:LEU:O	1:B:10:VAL:HG12	2.03	0.58
1:B:87:GLU:OE2	1:B:188:GLY:HA2	2.03	0.58
1:D:41:ARG:HG2	1:D:41:ARG:NH1	2.19	0.58
1:A:245:HIS:NE2	4:A:501:HOH:O	2.25	0.57
1:D:5:VAL:HG12	1:D:105:MET:CE	2.34	0.57
1:A:223:LYS:HE2	1:A:259:ASP:OD1	2.04	0.57
1:D:318:ASP:HB3	1:D:321:GLU:OE1	2.07	0.55
1:C:68:ILE:HD11	2:C:602:GOL:C1	2.36	0.54
1:A:81:ILE:CG2	1:A:83:LEU:HD21	2.39	0.53
1:A:120:GLN:HG3	1:A:234:ILE:HD11	1.90	0.53
1:A:4:LYS:HD2	1:D:4:LYS:NZ	2.24	0.53
1:B:41:ARG:NE	1:B:65:MET:HE2	2.18	0.53
1:D:88:GLY:HA3	1:D:91:ILE:HD12	1.91	0.52
1:A:41:ARG:HD3	1:A:65:MET:CE	2.39	0.52
1:C:97:ALA:HB1	2:C:604:GOL:H31	1.92	0.52
1:A:83:LEU:CD2	1:A:103:LEU:HD13	2.40	0.52
1:D:29:LYS:HA	1:D:93:SER:OG	2.09	0.51
1:B:7:LEU:HB3	1:C:7:LEU:HB3	1.92	0.51
1:A:311:ILE:HG12	1:D:311:ILE:HG12	1.93	0.51
1:D:6:ALA:HA	1:D:267:VAL:HG11	1.91	0.51
1:A:90:THR:H	2:A:402:GOL:H2	1.74	0.51
1:D:91:ILE:HA	1:D:94:LYS:HE2	1.93	0.51
1:C:7:LEU:O	1:C:10:VAL:HG12	2.12	0.50
1:C:91:ILE:HD11	1:C:187:ASP:HB3	1.93	0.50
1:A:290:ARG:HD2	1:A:293:TYR:CE1	2.46	0.50
1:B:7:LEU:HD22	1:C:7:LEU:HD22	1.92	0.50
1:C:290:ARG:HD3	4:C:790:HOH:O	2.12	0.50
1:D:91:ILE:HD11	1:D:187:ASP:HB3	1.92	0.50
1:D:66:LEU:HA	1:D:70:GLU:OE2	2.13	0.49
1:D:81:ILE:CG2	1:D:83:LEU:HD23	2.42	0.49
1:A:293:TYR:CE2	1:A:295:VAL:HG22	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:PRO:O	1:B:169:GLU:HG2	2.12	0.49
1:D:108:LYS:C	1:D:108:LYS:HD2	2.32	0.49
1:D:289:ARG:HG2	1:D:290:ARG:HD2	1.93	0.49
1:A:2:ASN:O	1:A:5:VAL:HG22	2.12	0.48
1:B:68:ILE:HG13	2:B:401:GOL:H12	1.95	0.48
1:A:87:GLU:OE2	1:A:188:GLY:HA2	2.13	0.48
1:A:320:LYS:HE3	1:A:320:LYS:HB2	1.49	0.48
1:A:321:GLU:OE1	1:A:325:LYS:HE2	2.13	0.48
1:A:278:MET:HG2	1:A:279:LEU:HG	1.96	0.48
1:B:4:LYS:HD2	1:C:48:ASP:OD2	2.14	0.48
1:A:6:ALA:HA	1:A:267:VAL:HG11	1.96	0.48
1:C:41:ARG:HE	1:C:65:MET:HE3	1.79	0.48
1:A:212:ALA:N	1:A:213:PRO:CD	2.77	0.47
1:C:149:GLU:OE1	4:C:701:HOH:O	2.20	0.47
1:D:5:VAL:HG12	1:D:105:MET:HE1	1.95	0.47
1:A:91:ILE:HD11	1:A:187:ASP:HB3	1.94	0.47
1:C:246:ARG:HD3	4:C:805:HOH:O	2.13	0.47
1:C:81:ILE:CD1	1:C:105:MET:HG2	2.43	0.47
1:B:41:ARG:NE	1:B:65:MET:CE	2.75	0.47
1:B:135:ASP:HB2	1:B:230:GLN:OE1	2.15	0.47
1:C:41:ARG:NE	1:C:65:MET:HE3	2.30	0.47
1:D:37:VAL:HG22	1:D:85:PRO:HG2	1.97	0.46
1:A:8:GLU:HG2	1:A:47:VAL:HG22	1.97	0.46
1:B:5:VAL:HG12	1:B:105:MET:HE1	1.97	0.46
1:D:81:ILE:HG21	1:D:83:LEU:HD23	1.97	0.46
1:C:42:LYS:HD2	1:C:328:SER:HB3	1.98	0.46
1:A:4:LYS:HD2	1:D:4:LYS:HZ2	1.81	0.46
1:A:170:HIS:CE1	1:A:171:ILE:HG13	2.51	0.46
1:C:324:GLU:HB2	1:C:327:MET:CE	2.46	0.46
1:C:166:PRO:O	1:C:169:GLU:HG2	2.15	0.45
1:C:290:ARG:HG3	1:C:290:ARG:NH1	2.31	0.45
1:C:324:GLU:HB2	1:C:327:MET:HE2	1.98	0.45
1:B:286:ASN:ND2	4:B:508:HOH:O	2.43	0.45
1:A:290:ARG:HD3	4:A:524:HOH:O	2.16	0.45
1:D:42:LYS:HE3	4:D:521:HOH:O	2.16	0.45
1:B:5:VAL:HG12	1:B:105:MET:CE	2.47	0.45
1:B:83:LEU:HD12	1:B:85:PRO:HD3	1.98	0.45
1:C:41:ARG:HD3	1:C:65:MET:HE2	1.99	0.45
1:B:120:GLN:NE2	1:B:234:ILE:HD11	2.32	0.45
1:C:120:GLN:O	1:C:231:ALA:HA	2.18	0.44
1:D:223:LYS:HE3	1:D:259:ASP:OD1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:LYS:HD3	1:C:325:LYS:HA	1.75	0.44
1:D:175:ALA:HB3	1:D:182:VAL:HG21	1.99	0.44
1:A:7:LEU:HD12	1:D:7:LEU:HD22	2.00	0.44
1:C:41:ARG:HD3	1:C:65:MET:CE	2.47	0.44
1:A:3:ARG:H	1:A:3:ARG:CD	2.15	0.43
1:B:4:LYS:HB2	1:C:8:GLU:OE2	2.17	0.43
1:C:55:ILE:HA	2:C:602:GOL:H11	2.00	0.43
1:A:51:GLY:HA3	1:A:81:ILE:HD11	1.99	0.43
1:B:321:GLU:OE1	1:B:325:LYS:HE2	2.18	0.43
1:C:6:ALA:HA	1:C:267:VAL:HG11	2.01	0.43
1:D:149:GLU:OE1	4:D:503:HOH:O	2.20	0.43
1:D:94:LYS:HE3	4:D:630:HOH:O	2.18	0.43
1:D:280:GLN:NE2	4:D:514:HOH:O	2.52	0.43
1:A:42:LYS:HD2	1:A:328:SER:HB2	2.01	0.42
1:A:81:ILE:HG21	1:A:83:LEU:HD21	2.01	0.42
1:A:154:HIS:HB2	1:B:320:LYS:O	2.19	0.42
1:A:290:ARG:CD	1:A:293:TYR:CD1	3.01	0.42
1:B:9:ALA:HB1	1:B:103:LEU:HD23	2.02	0.42
1:B:106:ALA:HB2	1:B:266:ILE:HD13	2.01	0.42
1:A:293:TYR:HE2	1:A:295:VAL:HG22	1.84	0.42
1:A:321:GLU:HB3	1:A:325:LYS:HD3	2.01	0.42
1:B:67:TYR:CE2	1:B:70:GLU:HB2	2.55	0.42
1:A:324:GLU:HB3	1:A:327:MET:CE	2.50	0.42
1:D:33:ASP:OD2	1:D:57:GLU:OE2	2.38	0.42
1:D:257:ASP:CG	1:D:258:ILE:N	2.73	0.42
1:C:97:ALA:CB	2:C:604:GOL:H31	2.50	0.42
1:A:305:THR:O	1:A:306:LYS:HB2	2.20	0.42
1:B:68:ILE:CD1	2:B:401:GOL:H12	2.50	0.42
1:B:223:LYS:HE3	1:B:259:ASP:OD1	2.19	0.42
1:B:283:LYS:HE2	2:B:402:GOL:O2	2.19	0.41
1:A:293:TYR:CE2	1:A:295:VAL:CG2	3.03	0.41
1:A:211:GLY:HA3	1:A:214:GLU:OE2	2.21	0.41
1:B:97:ALA:O	1:B:98:ASN:HB2	2.20	0.41
1:D:29:LYS:HB3	1:D:29:LYS:HE2	1.72	0.41
1:A:48:ASP:OD2	1:D:4:LYS:HD2	2.21	0.41
1:A:66:LEU:N	1:A:70:GLU:OE1	2.53	0.41
1:A:181:ARG:HB3	1:B:24:MET:O	2.20	0.41
1:B:88:GLY:HA3	1:B:91:ILE:HD12	2.03	0.41
1:C:305:THR:O	1:C:306:LYS:HB2	2.21	0.41
1:D:242:LYS:O	1:D:246:ARG:HG3	2.21	0.41
1:A:123:ALA:CB	1:A:193:VAL:HG13	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ARG:HG3	1:C:290:ARG:HH11	1.87	0.40
1:A:85:PRO:O	1:A:101:THR:HG22	2.21	0.40
1:C:81:ILE:CG2	1:C:83:LEU:HD21	2.51	0.40
1:D:134:VAL:HA	1:D:143:ASN:OD1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	326/348 (94%)	319 (98%)	7 (2%)	0	100	100
1	B	326/348 (94%)	321 (98%)	5 (2%)	0	100	100
1	C	326/348 (94%)	321 (98%)	5 (2%)	0	100	100
1	D	317/348 (91%)	314 (99%)	3 (1%)	0	100	100
All	All	1295/1392 (93%)	1275 (98%)	20 (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	254/271 (94%)	253 (100%)	1 (0%)	91	93
1	B	254/271 (94%)	254 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	254/271 (94%)	254 (100%)	0	100 100
1	D	249/271 (92%)	248 (100%)	1 (0%)	91 93
All	All	1011/1084 (93%)	1009 (100%)	2 (0%)	93 95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	ARG
1	D	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	B	170	HIS
1	D	253	ASN
1	D	280	GLN
1	D	286	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
2	GOL	A	403	-	5,5,5	2.73	2 (40%)	5,5,5	3.32	4 (80%)
2	GOL	A	404	-	5,5,5	0.67	0	5,5,5	1.07	0
2	GOL	B	403	-	5,5,5	1.06	0	5,5,5	0.94	0
2	GOL	D	403	-	5,5,5	0.84	0	5,5,5	0.76	0
2	GOL	D	405	-	5,5,5	3.03	3 (60%)	5,5,5	1.85	2 (40%)
2	GOL	D	401	-	5,5,5	0.78	0	5,5,5	0.72	0
2	GOL	A	405	-	5,5,5	0.75	0	5,5,5	1.05	0
2	GOL	D	404	-	5,5,5	1.15	1 (20%)	5,5,5	1.44	1 (20%)
2	GOL	D	402	-	5,5,5	0.94	0	5,5,5	0.81	0
2	GOL	A	401	-	5,5,5	0.89	0	5,5,5	0.97	0
2	GOL	B	402	-	5,5,5	0.84	0	5,5,5	0.83	0
2	GOL	C	602	-	5,5,5	1.37	1 (20%)	5,5,5	1.16	0
2	GOL	C	603	-	5,5,5	0.92	0	5,5,5	1.21	1 (20%)
2	GOL	C	601	-	5,5,5	0.85	0	5,5,5	1.04	0
2	GOL	A	402	-	5,5,5	1.08	0	5,5,5	1.43	1 (20%)
2	GOL	B	404	-	5,5,5	0.94	0	5,5,5	1.32	1 (20%)
2	GOL	B	401	-	5,5,5	0.97	0	5,5,5	1.02	0
2	GOL	C	604	-	5,5,5	0.64	0	5,5,5	1.05	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	A	403	-	-	2/4/4/4	-
2	GOL	A	404	-	-	3/4/4/4	-
2	GOL	B	403	-	-	1/4/4/4	-
2	GOL	D	403	-	-	4/4/4/4	-
2	GOL	D	405	-	-	4/4/4/4	-
2	GOL	D	401	-	-	3/4/4/4	-
2	GOL	A	405	-	-	0/4/4/4	-
2	GOL	D	404	-	-	4/4/4/4	-
2	GOL	D	402	-	-	0/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	402	-	-	4/4/4/4	-
2	GOL	C	602	-	-	0/4/4/4	-
2	GOL	C	603	-	-	1/4/4/4	-
2	GOL	C	601	-	-	4/4/4/4	-
2	GOL	A	402	-	-	2/4/4/4	-
2	GOL	B	404	-	-	2/4/4/4	-
2	GOL	B	401	-	-	2/4/4/4	-
2	GOL	C	604	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	403	GOL	C3-C2	-4.86	1.31	1.51
2	D	405	GOL	O3-C3	4.45	1.61	1.42
2	D	405	GOL	C3-C2	-4.13	1.34	1.51
2	A	403	GOL	O2-C2	-3.02	1.34	1.43
2	D	405	GOL	O2-C2	2.63	1.51	1.43
2	C	602	GOL	O1-C1	2.43	1.52	1.42
2	D	404	GOL	O2-C2	-2.09	1.37	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	403	GOL	C3-C2-C1	-5.01	92.22	111.70
2	D	405	GOL	O1-C1-C2	-3.37	94.03	110.20
2	A	403	GOL	O1-C1-C2	-3.21	94.81	110.20
2	A	403	GOL	O2-C2-C1	-3.15	95.24	109.12
2	A	402	GOL	C3-C2-C1	-2.88	100.52	111.70
2	A	403	GOL	O2-C2-C3	2.74	121.20	109.12
2	B	404	GOL	C3-C2-C1	-2.39	102.42	111.70
2	C	603	GOL	C3-C2-C1	-2.31	102.74	111.70
2	D	405	GOL	O2-C2-C1	-2.08	99.96	109.12
2	D	404	GOL	O3-C3-C2	-2.04	100.42	110.20

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	GOL	C1-C2-C3-O3
2	A	402	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	403	GOL	O2-C2-C3-O3
2	B	401	GOL	C1-C2-C3-O3
2	B	402	GOL	O1-C1-C2-C3
2	B	404	GOL	O1-C1-C2-C3
2	C	601	GOL	O1-C1-C2-C3
2	C	601	GOL	C1-C2-C3-O3
2	D	403	GOL	O1-C1-C2-O2
2	D	403	GOL	O1-C1-C2-C3
2	D	403	GOL	C1-C2-C3-O3
2	D	404	GOL	O1-C1-C2-C3
2	D	404	GOL	C1-C2-C3-O3
2	D	405	GOL	C1-C2-C3-O3
2	B	401	GOL	O2-C2-C3-O3
2	C	601	GOL	O2-C2-C3-O3
2	D	404	GOL	O2-C2-C3-O3
2	A	404	GOL	O1-C1-C2-C3
2	B	402	GOL	C1-C2-C3-O3
2	D	401	GOL	O1-C1-C2-C3
2	D	405	GOL	O1-C1-C2-C3
2	A	404	GOL	O1-C1-C2-O2
2	B	402	GOL	O1-C1-C2-O2
2	C	601	GOL	O1-C1-C2-O2
2	D	403	GOL	O2-C2-C3-O3
2	D	405	GOL	O1-C1-C2-O2
2	D	405	GOL	O2-C2-C3-O3
2	B	402	GOL	O2-C2-C3-O3
2	B	404	GOL	O1-C1-C2-O2
2	D	404	GOL	O1-C1-C2-O2
2	B	403	GOL	O2-C2-C3-O3
2	A	404	GOL	O2-C2-C3-O3
2	C	603	GOL	O1-C1-C2-O2
2	D	401	GOL	C1-C2-C3-O3
2	D	401	GOL	O1-C1-C2-O2
2	A	403	GOL	C1-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	405	GOL	2	0
2	D	404	GOL	1	0
2	A	401	GOL	1	0

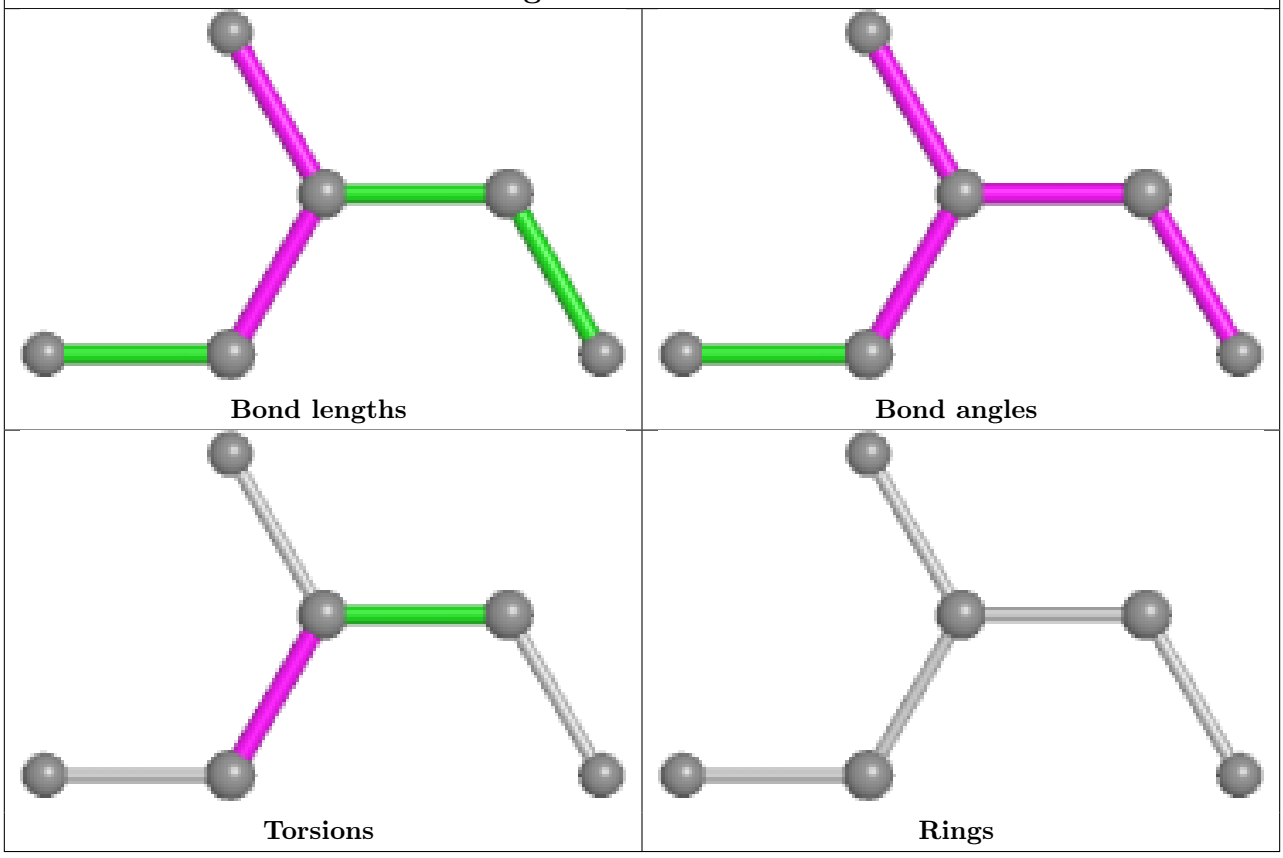
Continued on next page...

Continued from previous page...

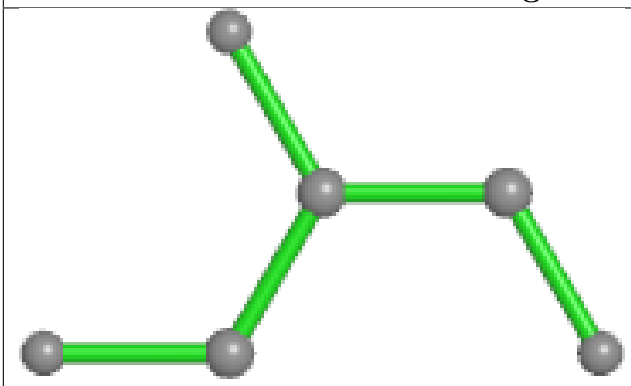
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	GOL	1	0
2	C	602	GOL	3	0
2	A	402	GOL	1	0
2	B	401	GOL	2	0
2	C	604	GOL	2	0

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.

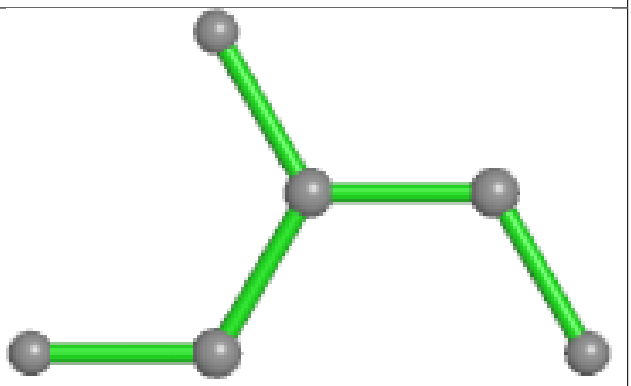
Ligand GOL A 403



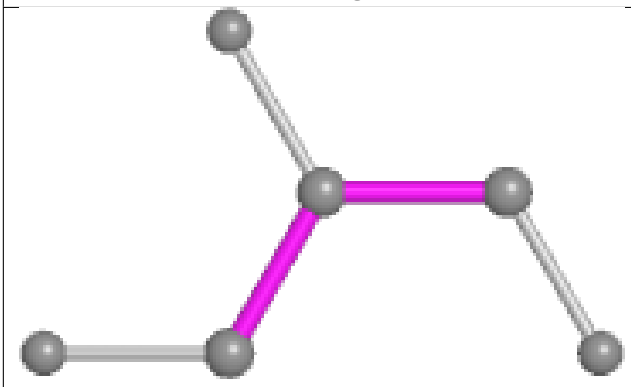
Ligand GOL A 404



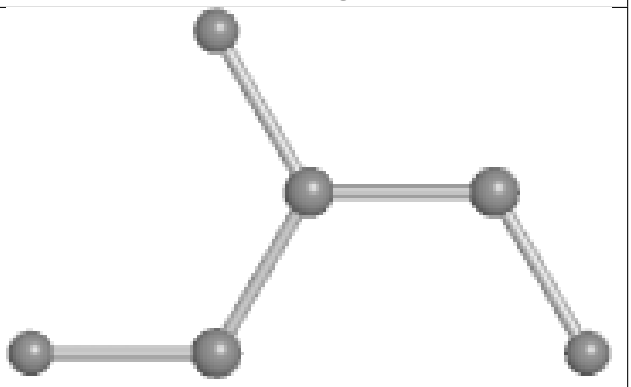
Bond lengths



Bond angles

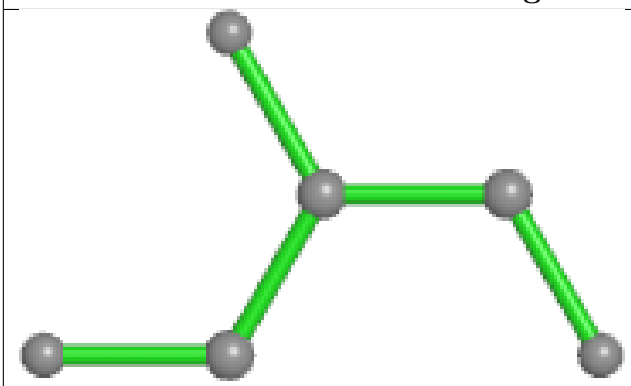


Torsions

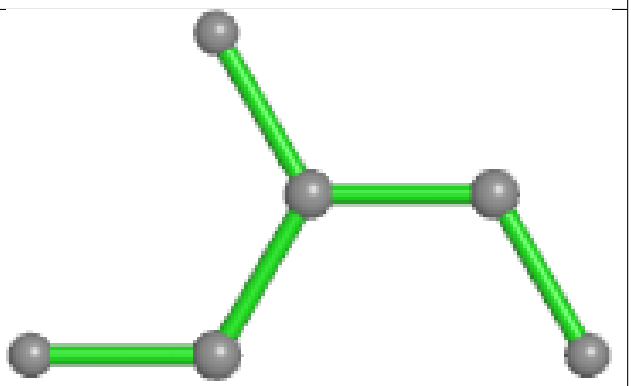


Rings

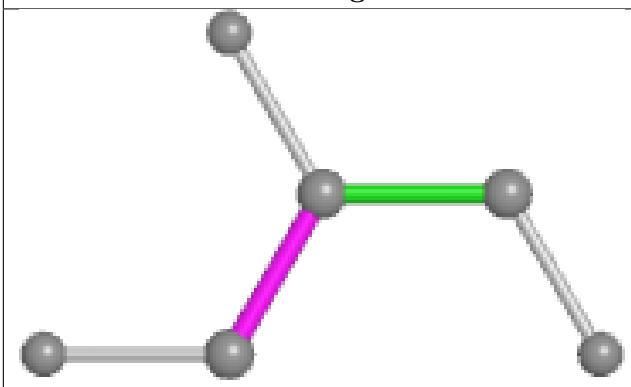
Ligand GOL B 403



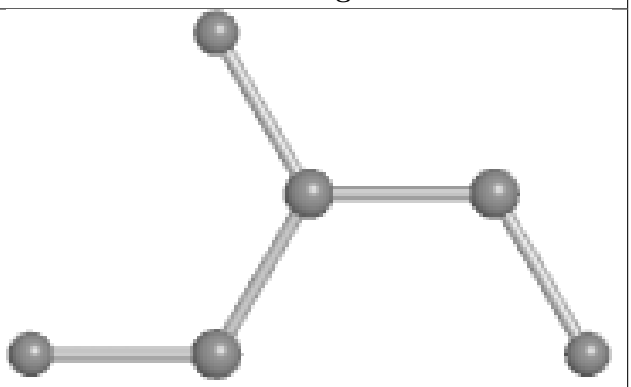
Bond lengths



Bond angles

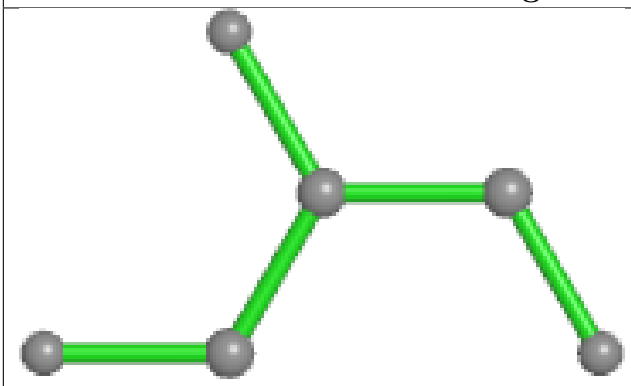


Torsions

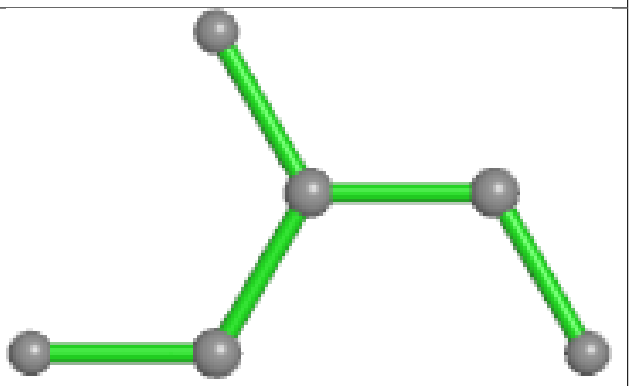


Rings

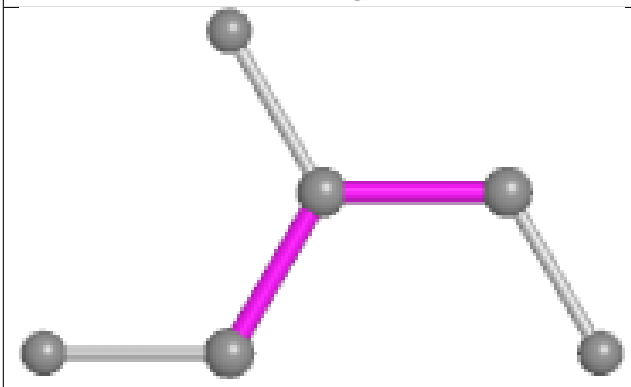
Ligand GOL D 403



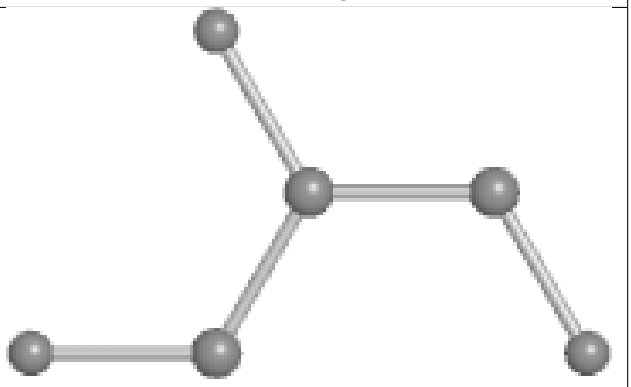
Bond lengths



Bond angles

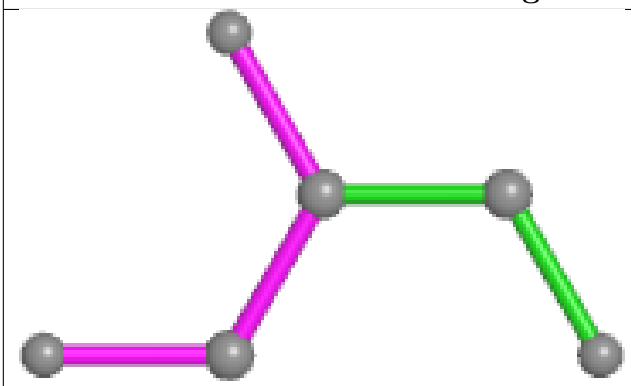


Torsions

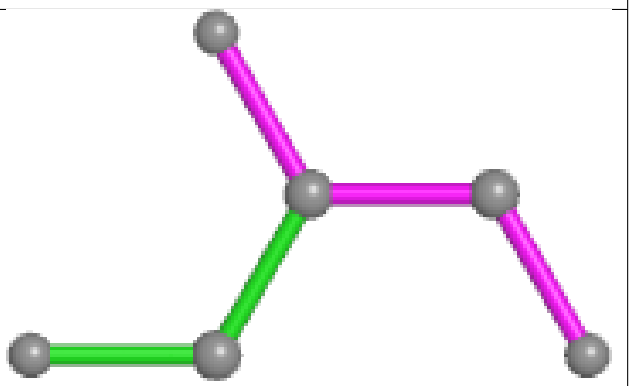


Rings

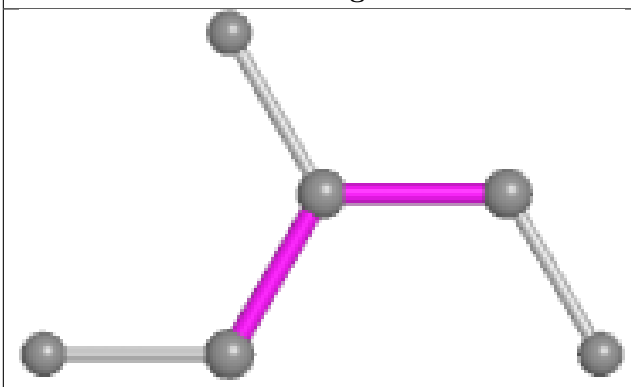
Ligand GOL D 405



Bond lengths



Bond angles



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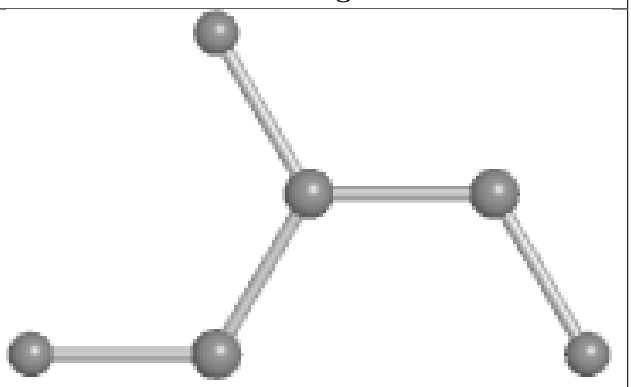
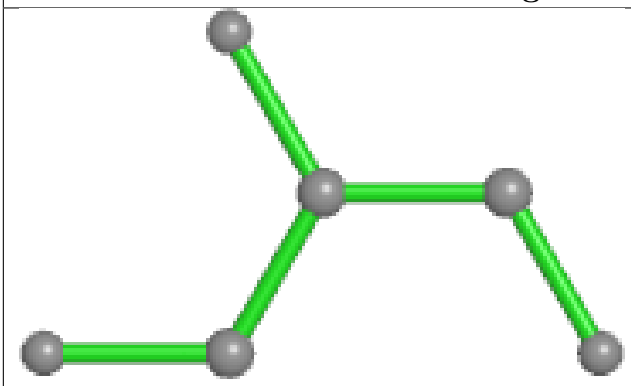
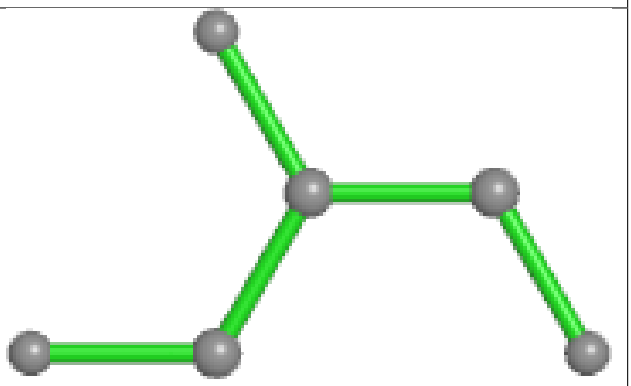


Rings

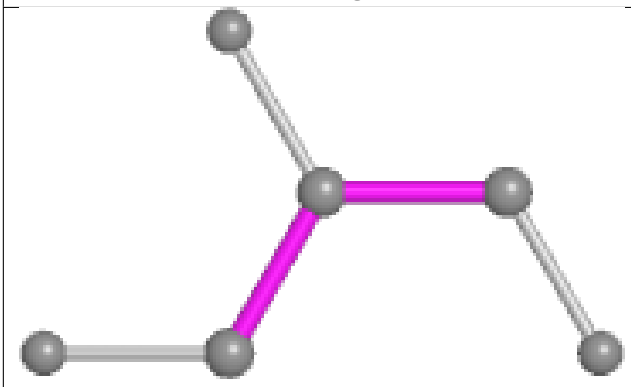
Ligand GOL D 401



Bond lengths



Bond angles



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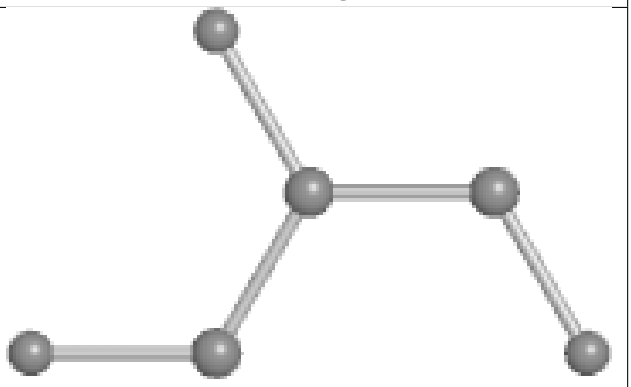
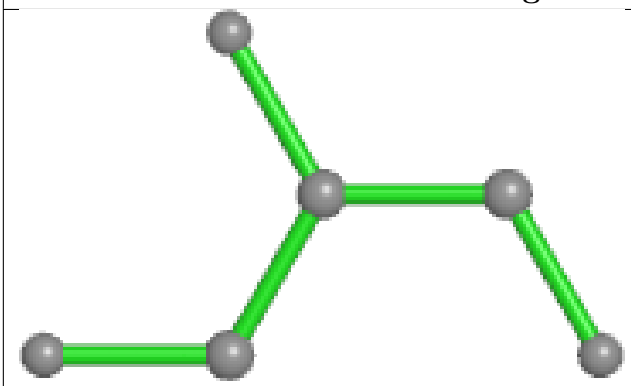


Rings

Ligand GOL A 405



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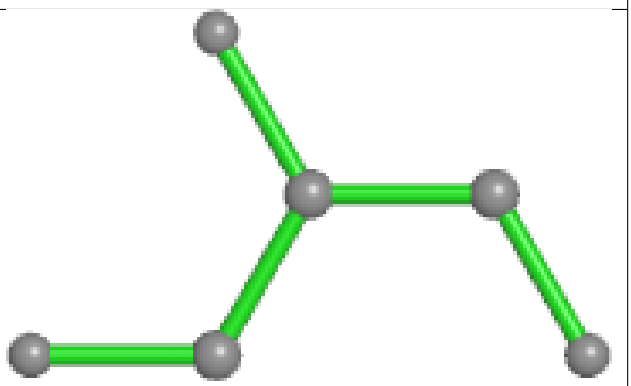

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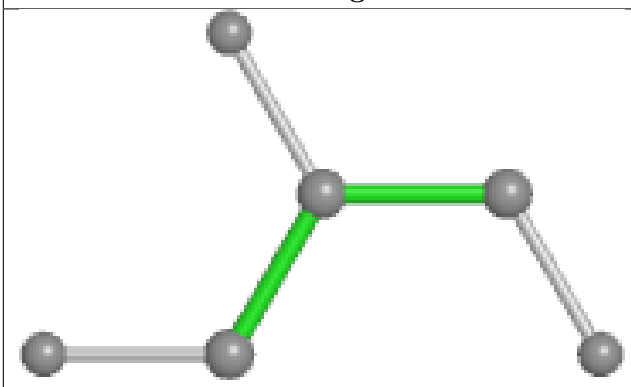

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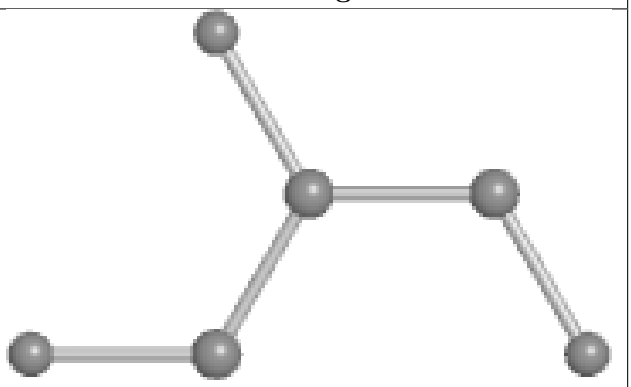

Rings

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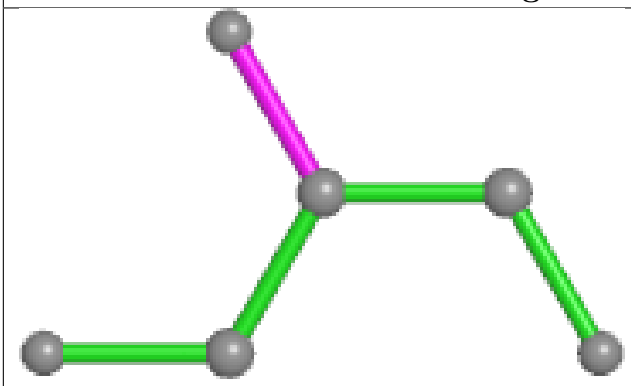

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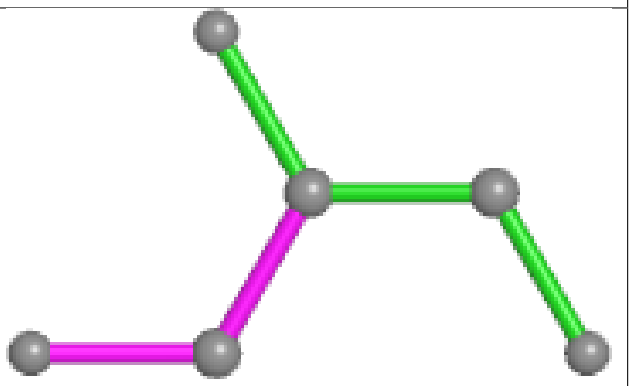
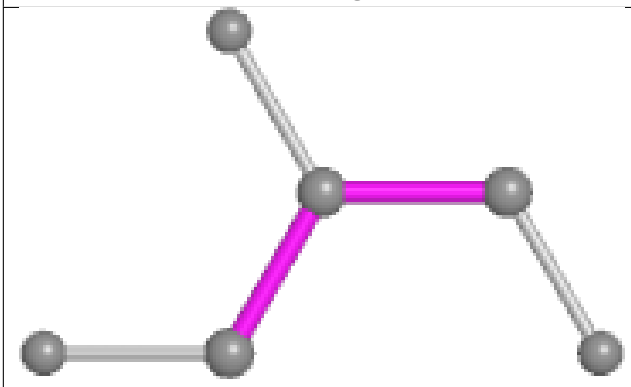


Bond angles



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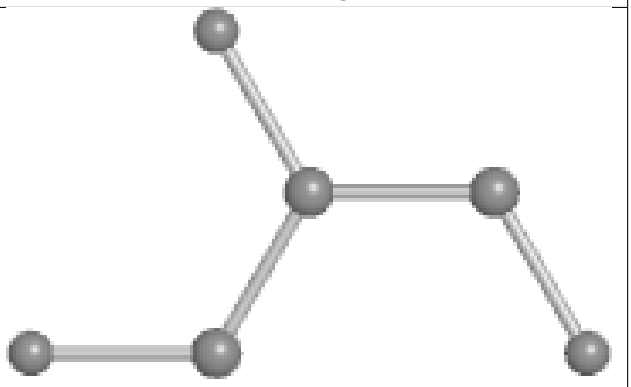
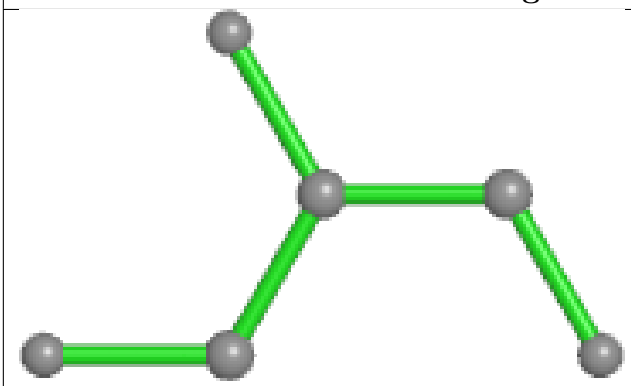


Rings

Ligand GOL D 402



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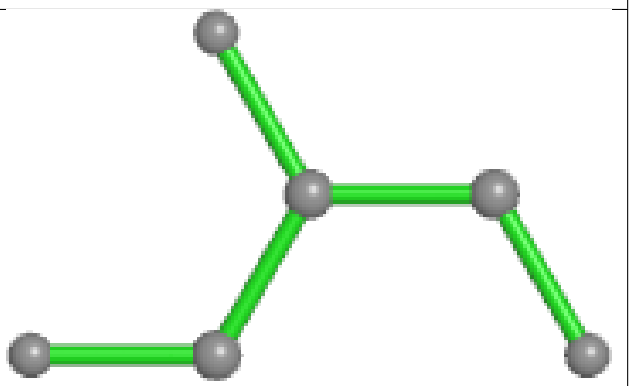
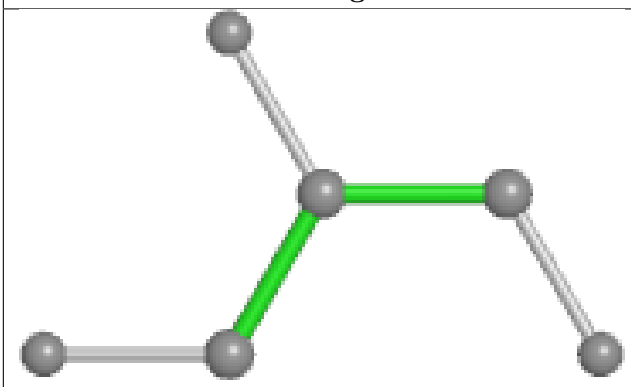


Bond angles



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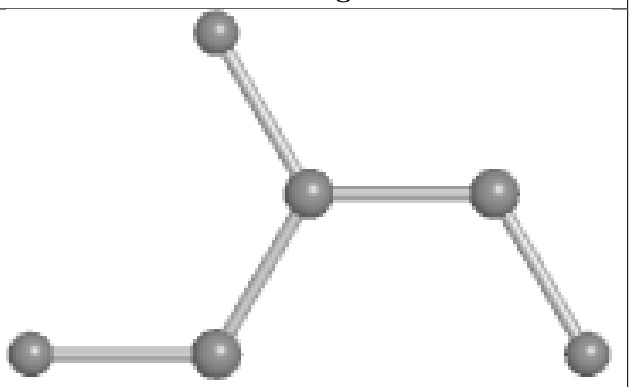
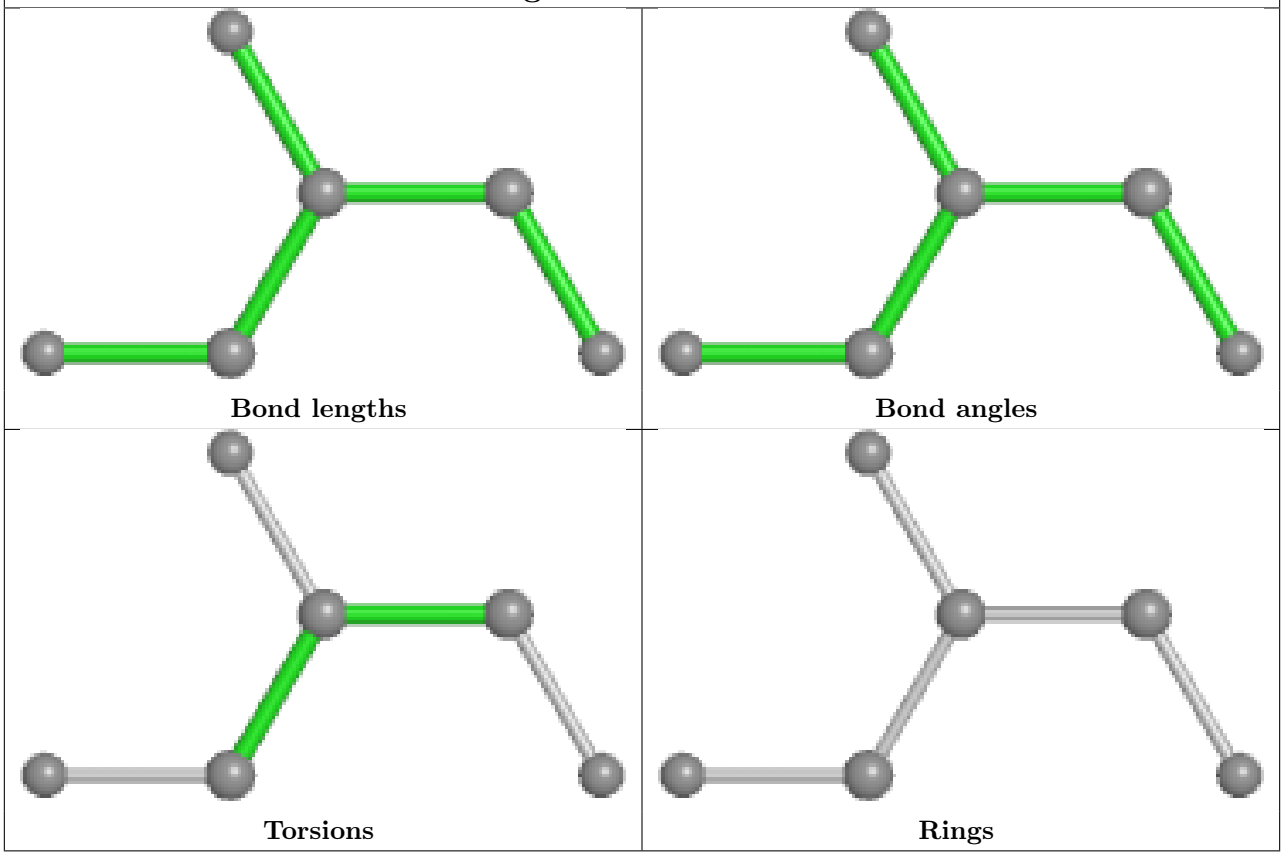
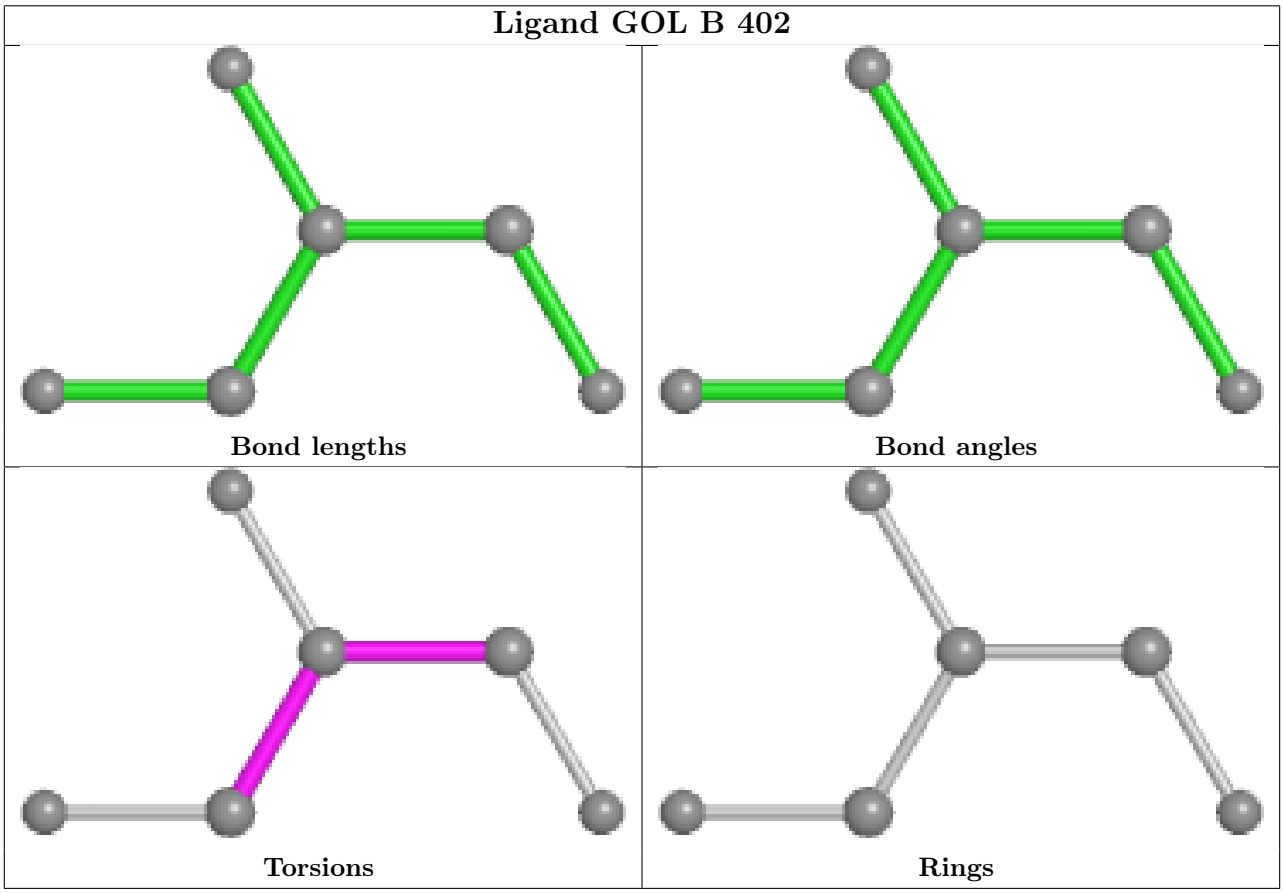


Rings

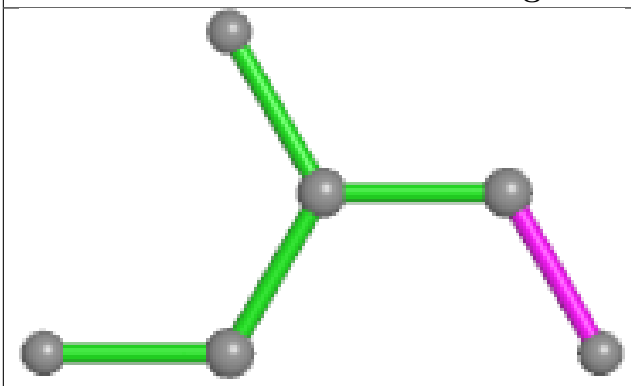
Ligand GOL A 401



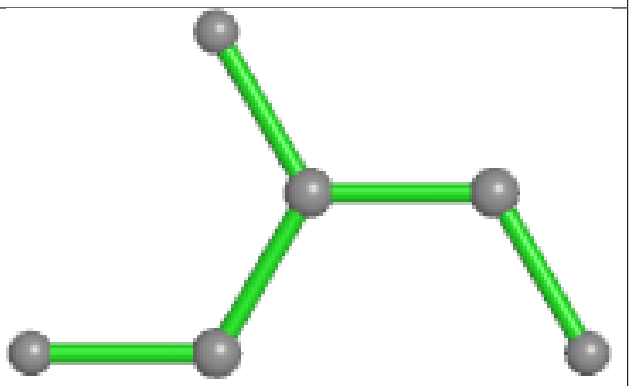
Ligand GOL B 402



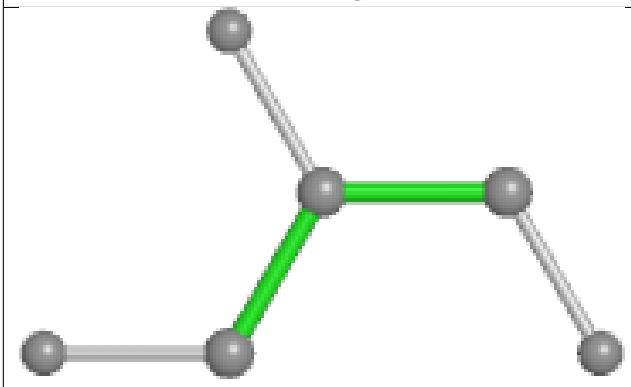
Ligand GOL C 602



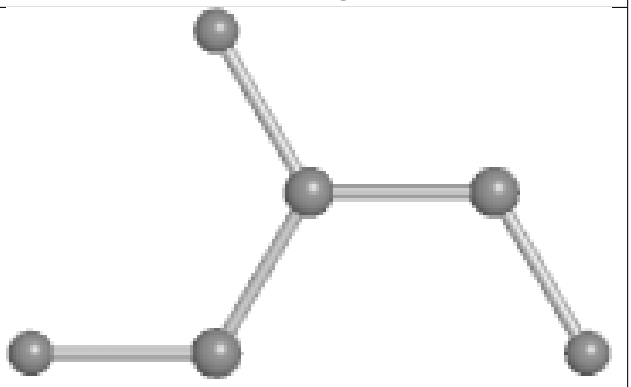
Bond lengths



Bond angles

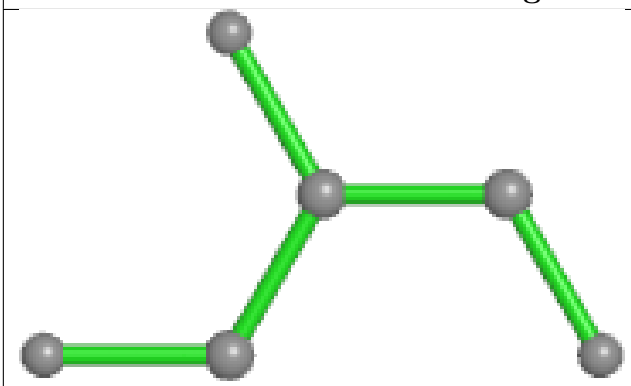


Torsions

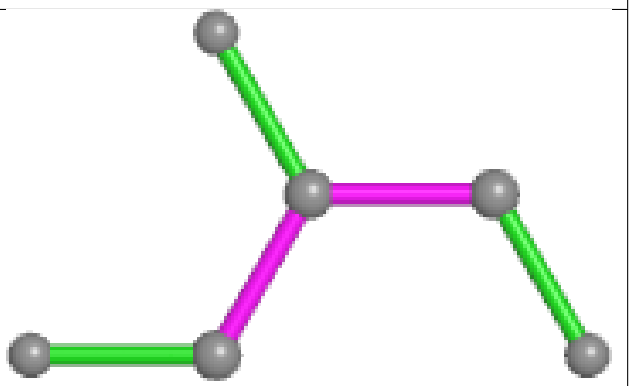


Rings

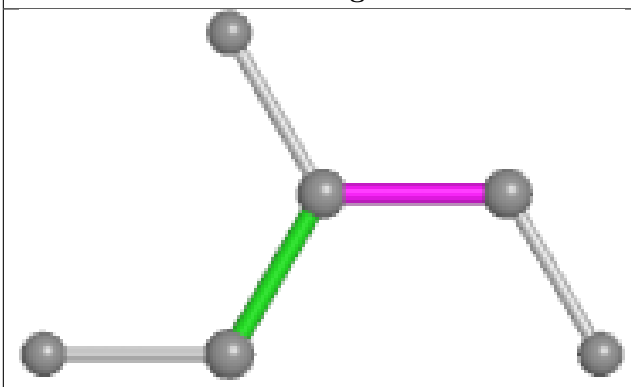
Ligand GOL C 603



Bond lengths



Bond angles



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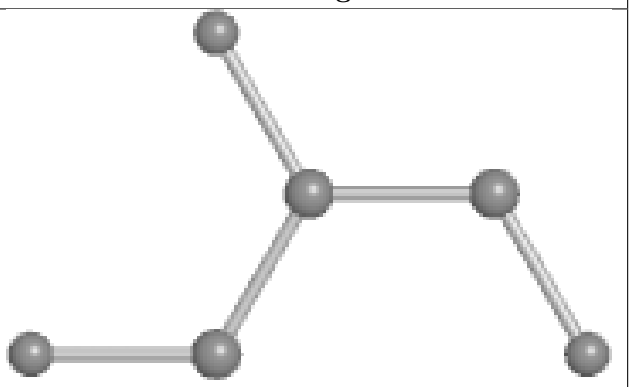
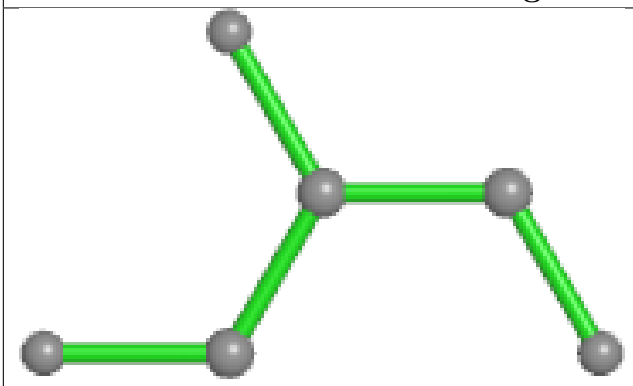
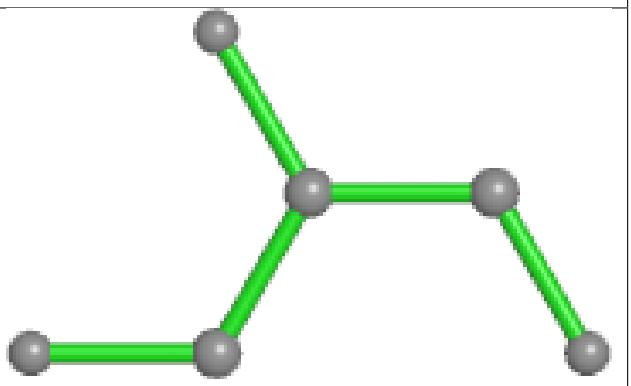


Rings

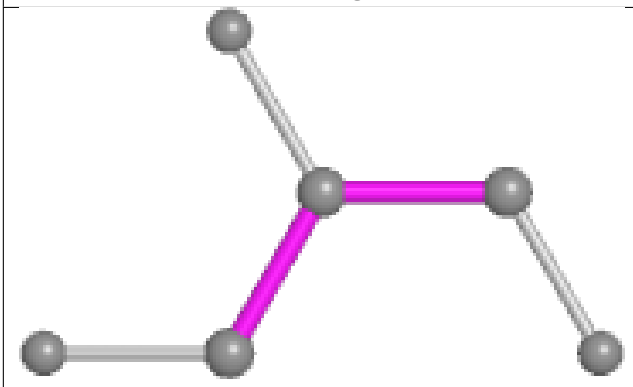
Ligand GOL C 601



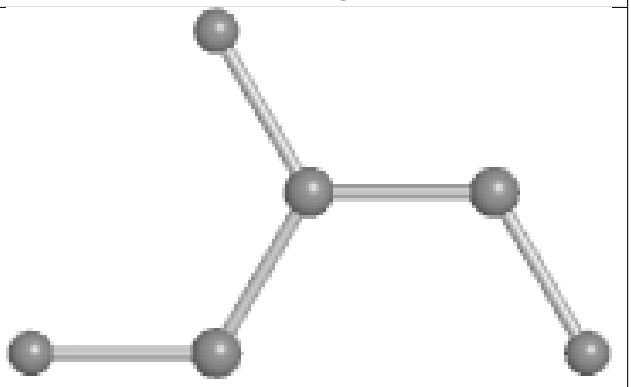
Bond lengths



Bond angles

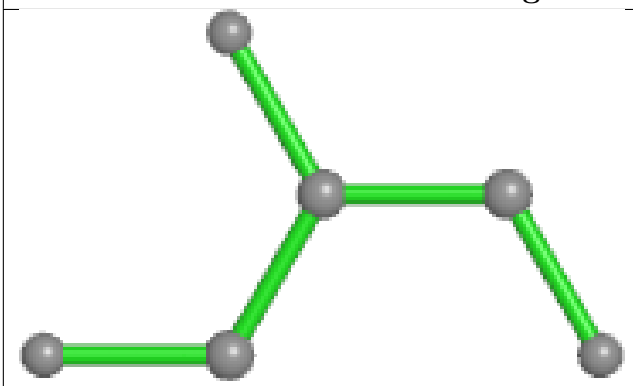


Torsions



Rings

Ligand GOL A 402



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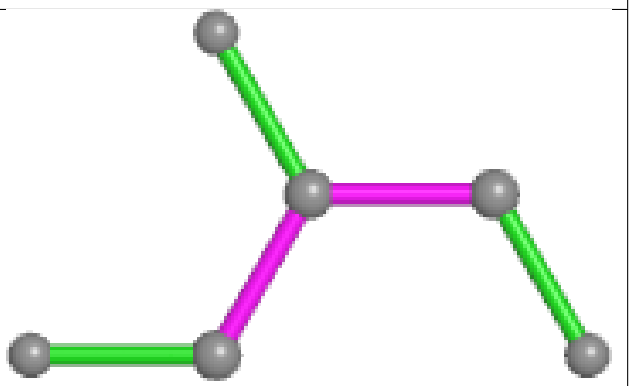
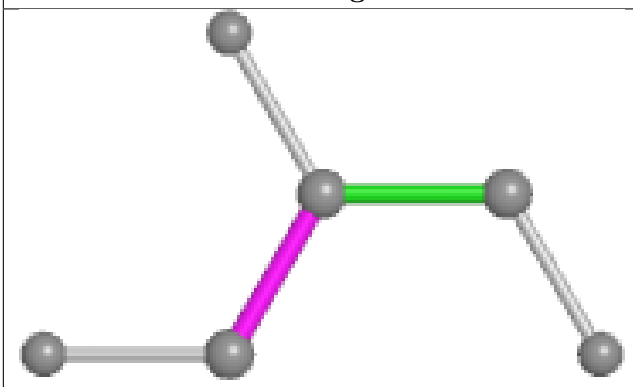
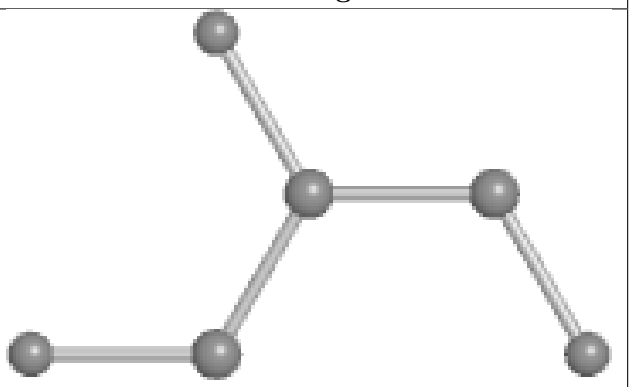


Bond angles

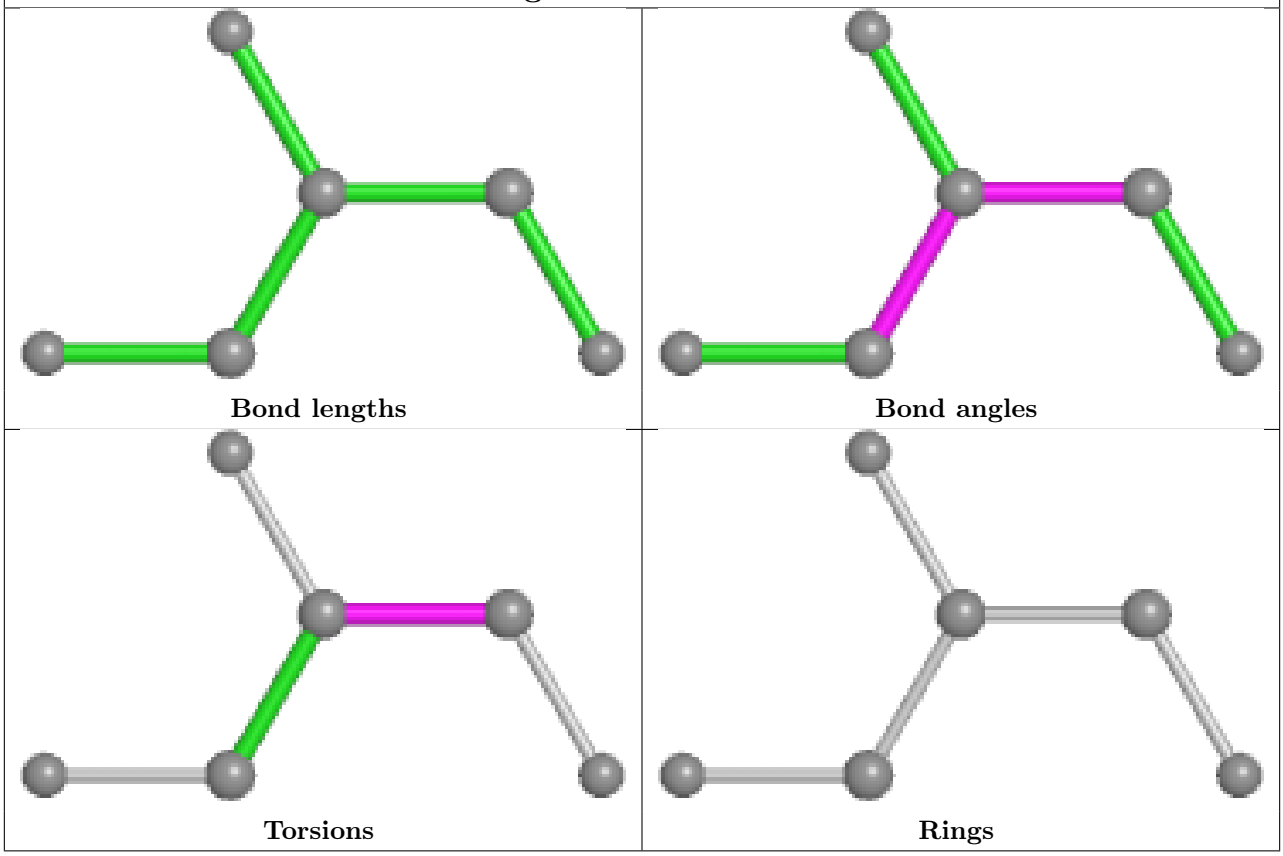


Torsions

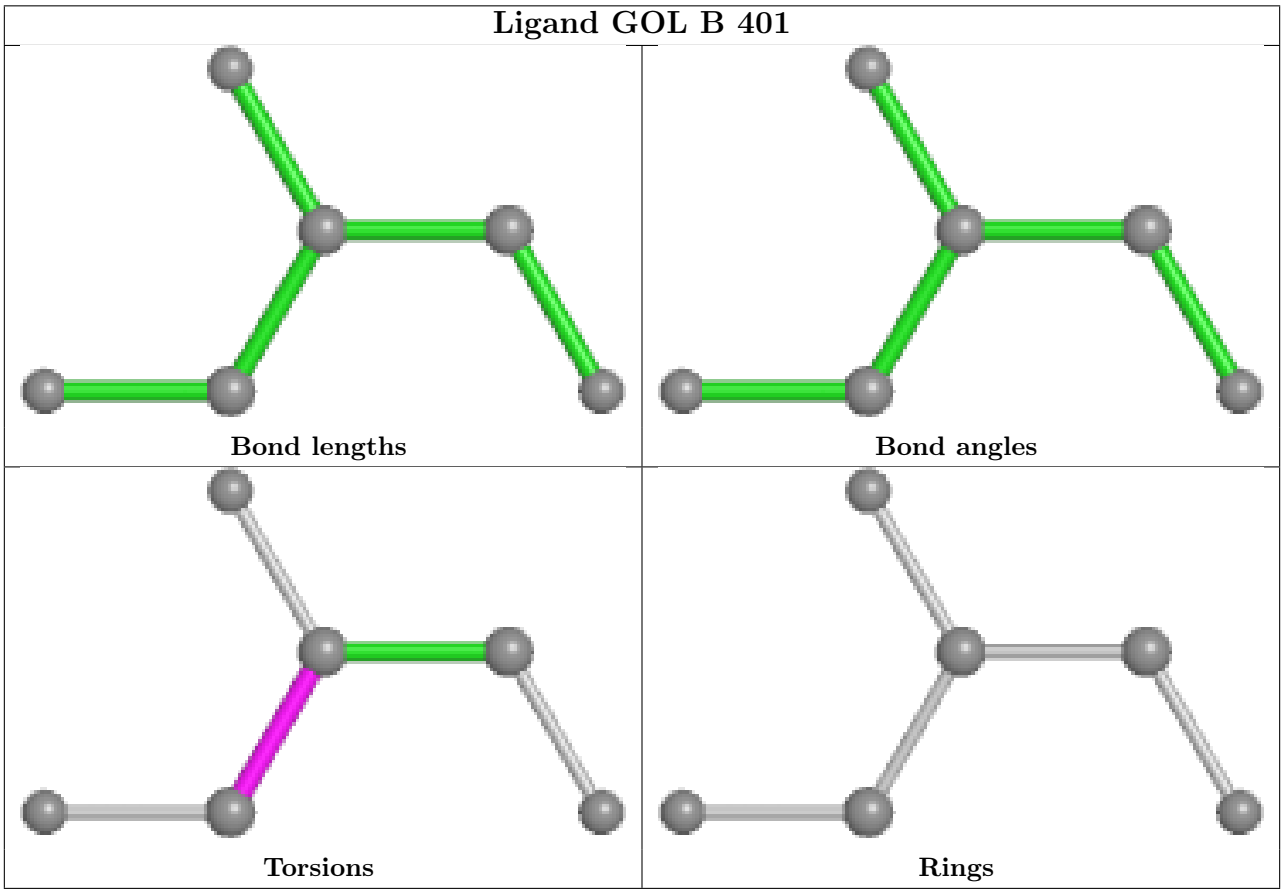


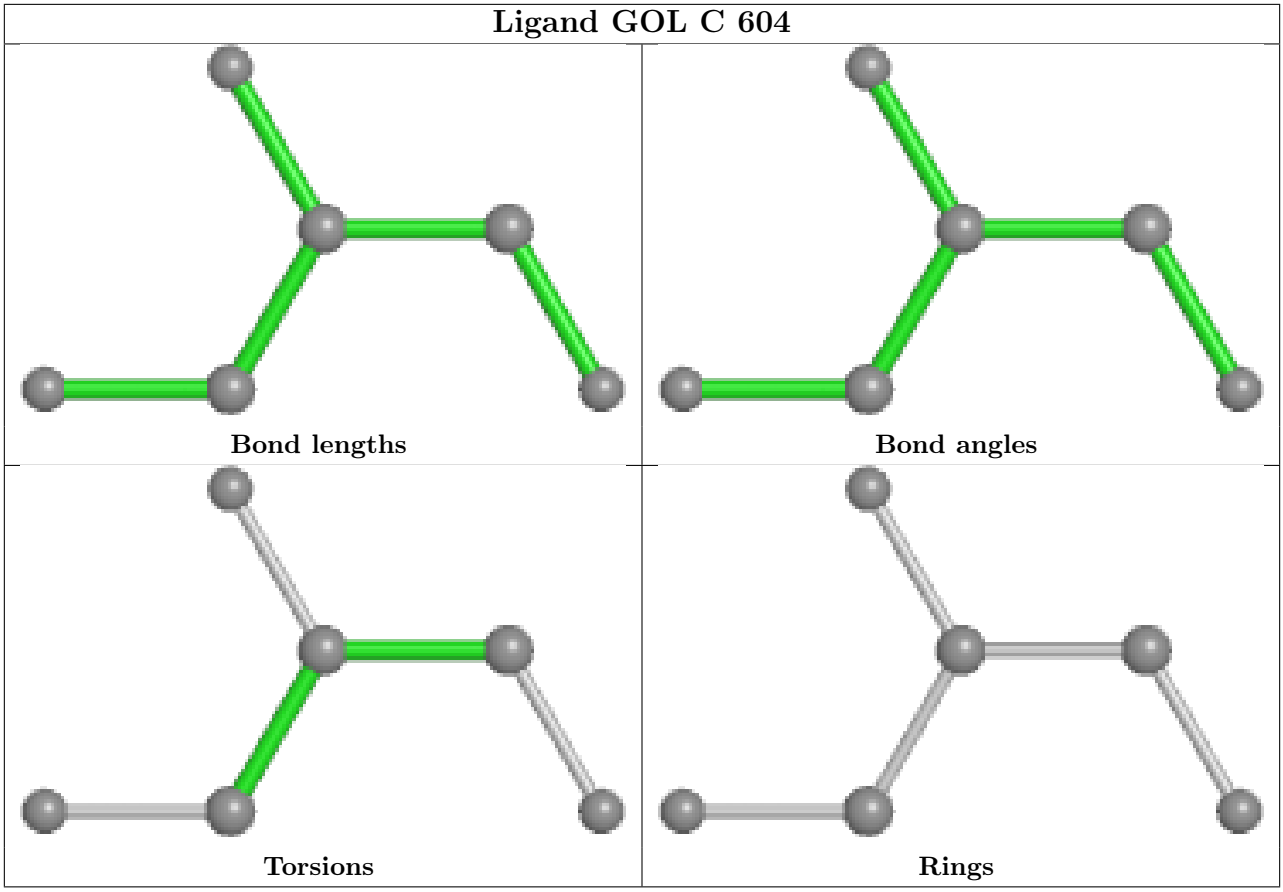
Rings

Ligand GOL B 404



Ligand GOL B 401





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	328/348 (94%)	0.32	20 (6%)	21	20	24, 43, 95, 130	0
1	B	328/348 (94%)	0.08	9 (2%)	54	53	26, 41, 69, 116	0
1	C	328/348 (94%)	-0.16	7 (2%)	63	62	17, 29, 61, 111	0
1	D	321/348 (92%)	-0.16	2 (0%)	89	88	17, 29, 57, 84	0
All	All	1305/1392 (93%)	0.02	38 (2%)	51	50	17, 36, 71, 130	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	LYS	7.2
1	A	246	ARG	5.6
1	A	4	LYS	5.3
1	B	127	ILE	4.2
1	A	60	LEU	4.1
1	B	328	SER	3.9
1	B	60	LEU	3.8
1	D	328	SER	3.8
1	A	62	GLU	3.7
1	A	249	ILE	3.4
1	B	61	ASP	3.4
1	A	58	GLY	3.2
1	A	61	ASP	3.1
1	A	3	ARG	3.0
1	C	2	ASN	3.0
1	A	131	LYS	2.9
1	C	61	ASP	2.7
1	B	5	VAL	2.6
1	A	244	ALA	2.6
1	A	64	PRO	2.6
1	B	74	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	60	LEU	2.5
1	B	62	GLU	2.4
1	A	178	CYS	2.4
1	A	170	HIS	2.3
1	A	243	ARG	2.3
1	A	127	ILE	2.3
1	A	74	ALA	2.2
1	D	246	ARG	2.2
1	B	76	GLY	2.2
1	A	63	ALA	2.2
1	C	328	SER	2.2
1	C	300	VAL	2.2
1	C	4	LYS	2.2
1	C	3	ARG	2.1
1	A	59	GLU	2.1
1	A	239	GLU	2.1
1	B	131	LYS	2.1

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
3	MN	A	406	1/1	0.38	0.24	103,103,103,103	0
2	GOL	D	402	6/6	0.47	0.34	60,85,102,102	0
3	MN	B	405	1/1	0.49	0.14	98,98,98,98	0
2	GOL	D	405	6/6	0.67	0.38	53,67,87,101	0
2	GOL	D	403	6/6	0.69	0.29	46,71,85,90	0
2	GOL	C	602	6/6	0.71	0.20	39,60,75,79	0

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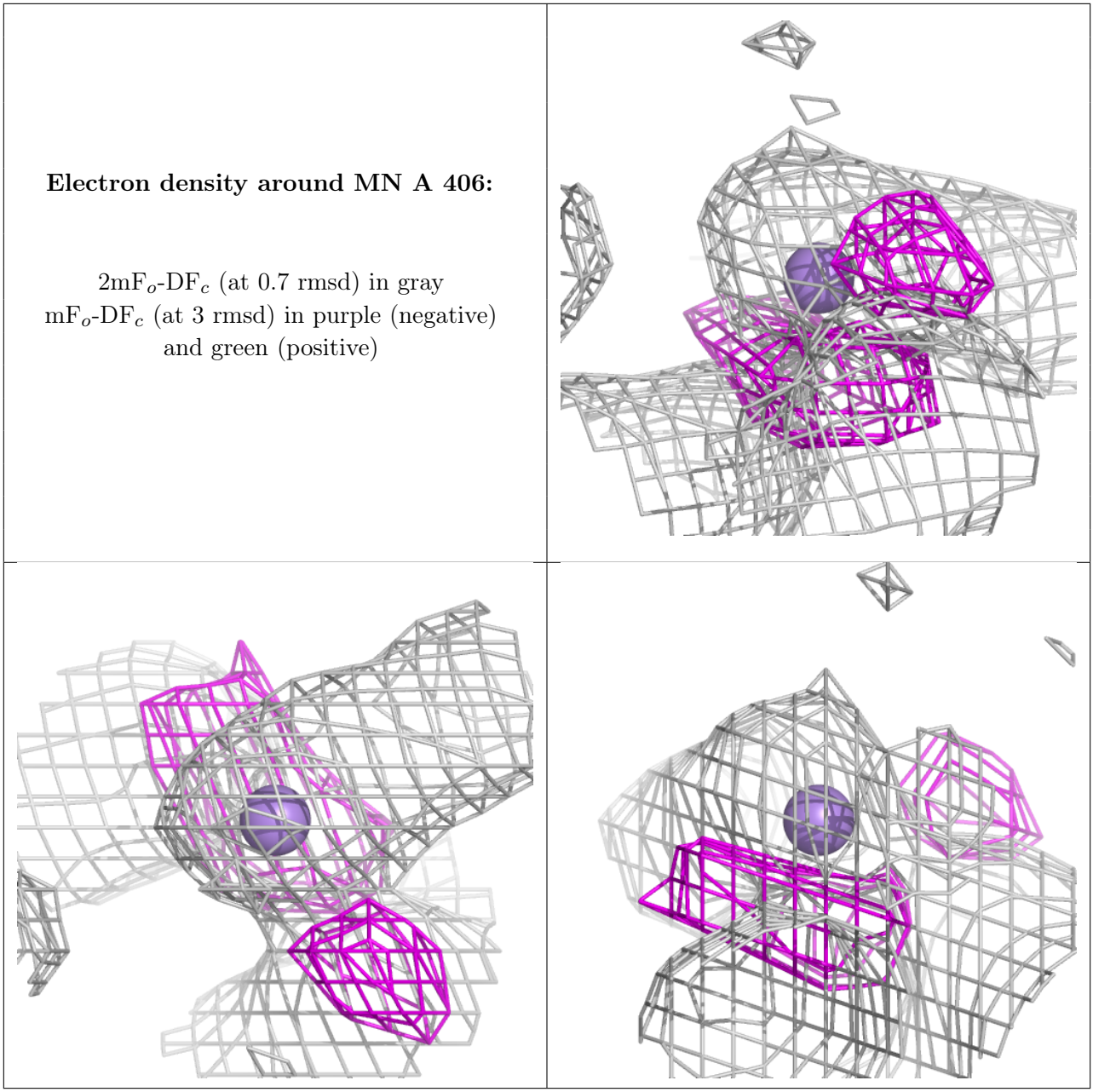
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	B	403	6/6	0.77	0.21	48,72,91,91	0
2	GOL	C	601	6/6	0.81	0.47	58,76,96,96	0
2	GOL	A	401	6/6	0.82	0.16	57,69,76,77	0
2	GOL	B	401	6/6	0.84	0.21	48,68,81,82	0
2	GOL	D	404	6/6	0.85	0.19	37,47,58,61	0
2	GOL	C	604	6/6	0.85	0.16	49,59,70,74	0
2	GOL	A	405	6/6	0.87	0.19	53,66,79,79	0
2	GOL	A	403	6/6	0.89	0.29	53,64,77,78	0
2	GOL	B	402	6/6	0.89	0.19	39,50,60,67	0
2	GOL	B	404	6/6	0.90	0.28	52,65,77,78	0
2	GOL	A	402	6/6	0.90	0.11	51,63,73,80	0
2	GOL	D	401	6/6	0.90	0.19	43,66,83,100	0
3	MN	D	406	1/1	0.91	0.14	117,117,117,117	0
2	GOL	C	603	6/6	0.93	0.15	41,55,66,70	0
3	MN	C	605	1/1	0.94	0.19	64,64,64,64	0
2	GOL	A	404	6/6	0.94	0.13	36,46,54,61	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.

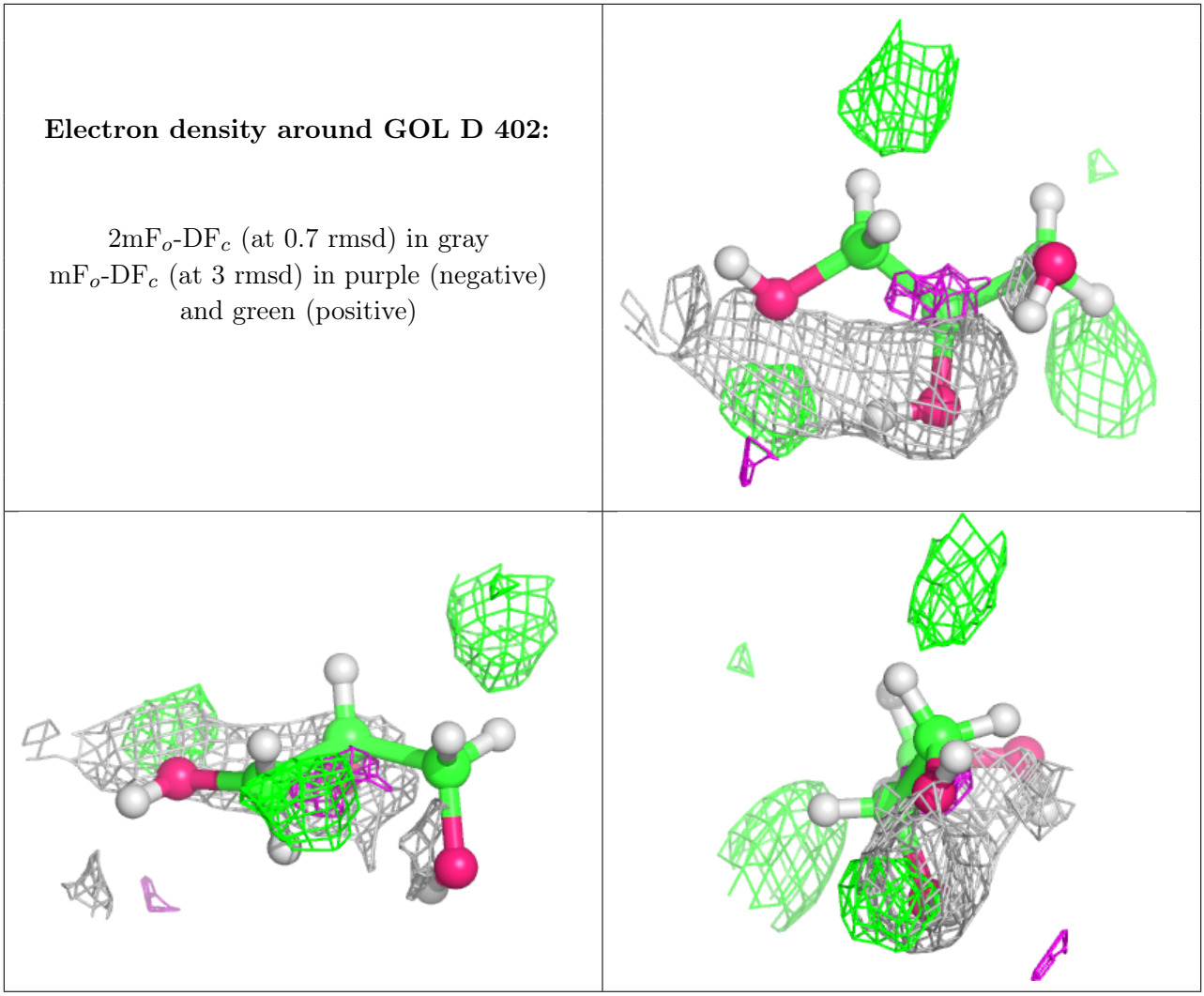
Electron density around MN A 406:

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



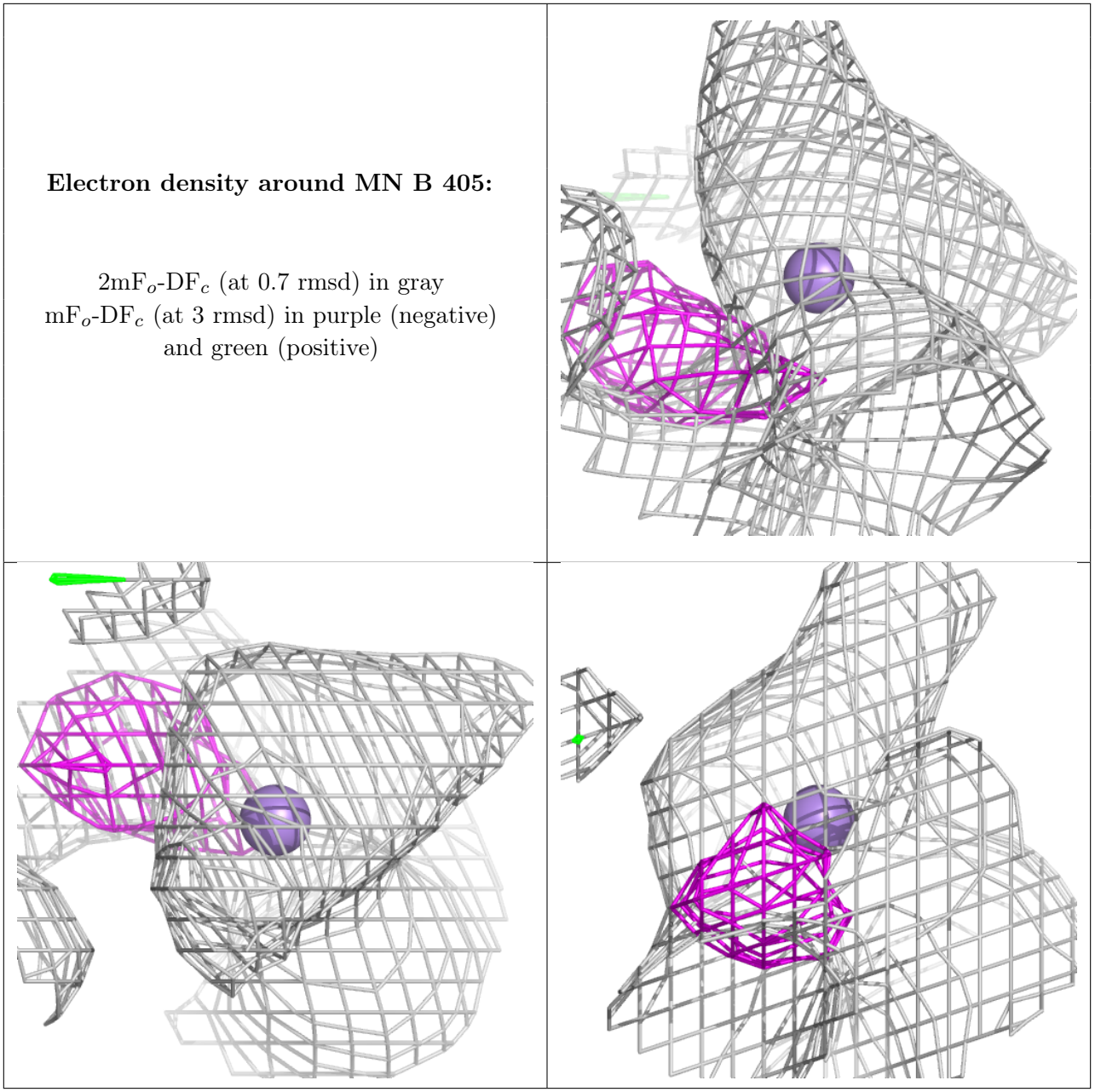
Electron density around GOL D 402:

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



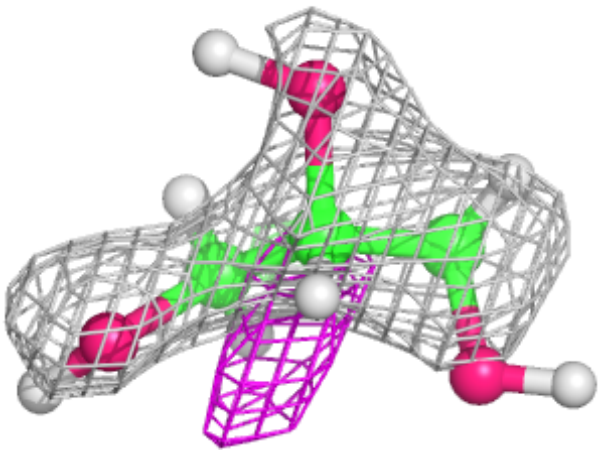
Electron density around MN B 405:

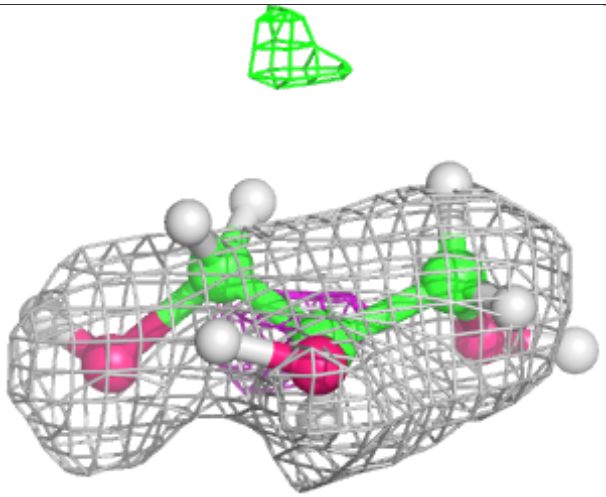
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

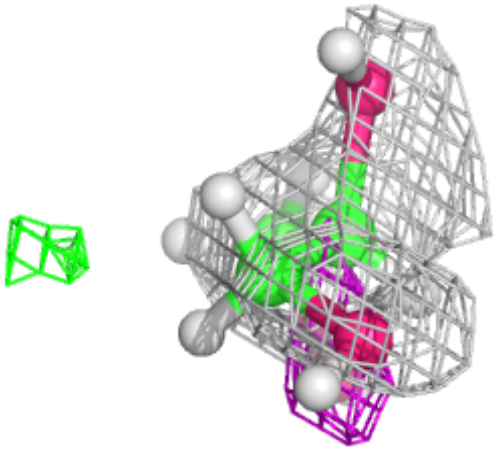


Electron density around GOL D 405:

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

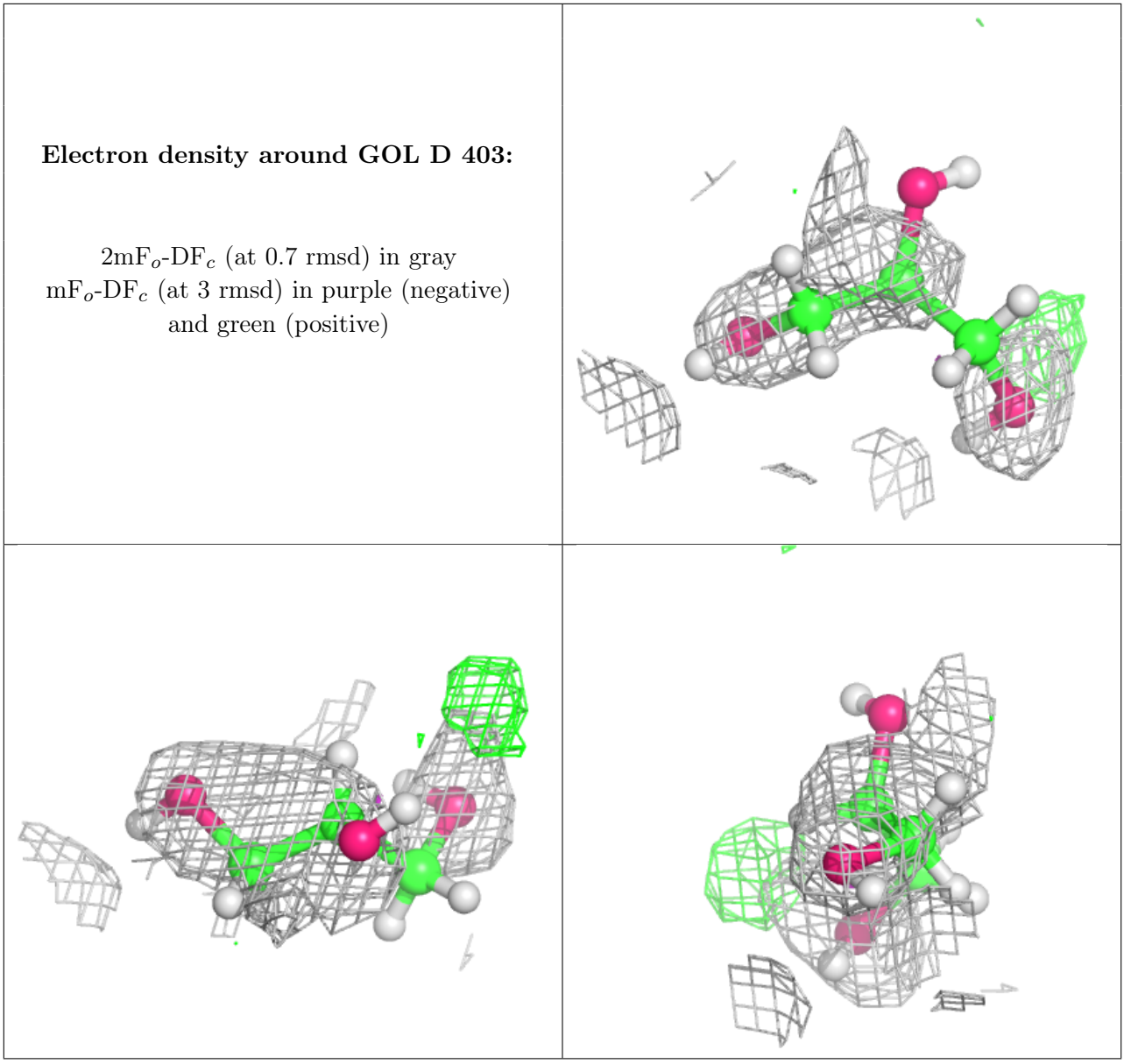






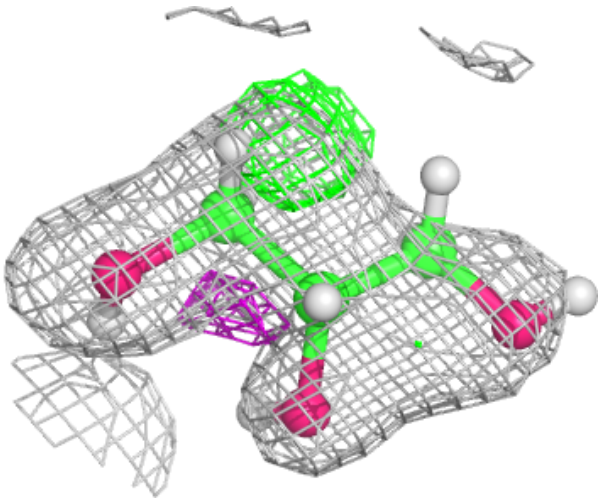
Electron density around GOL D 403:

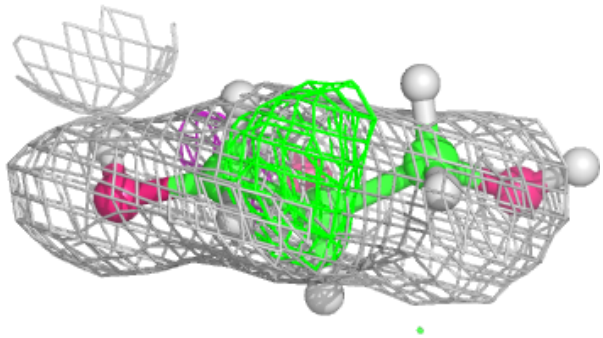
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

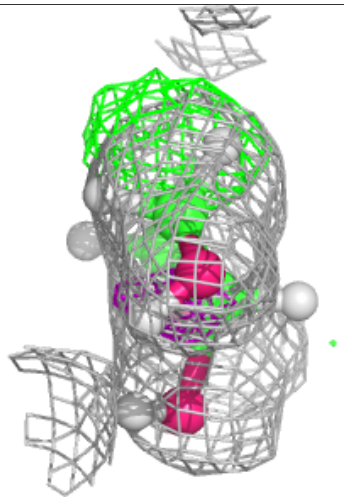


Electron density around GOL C 602:

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

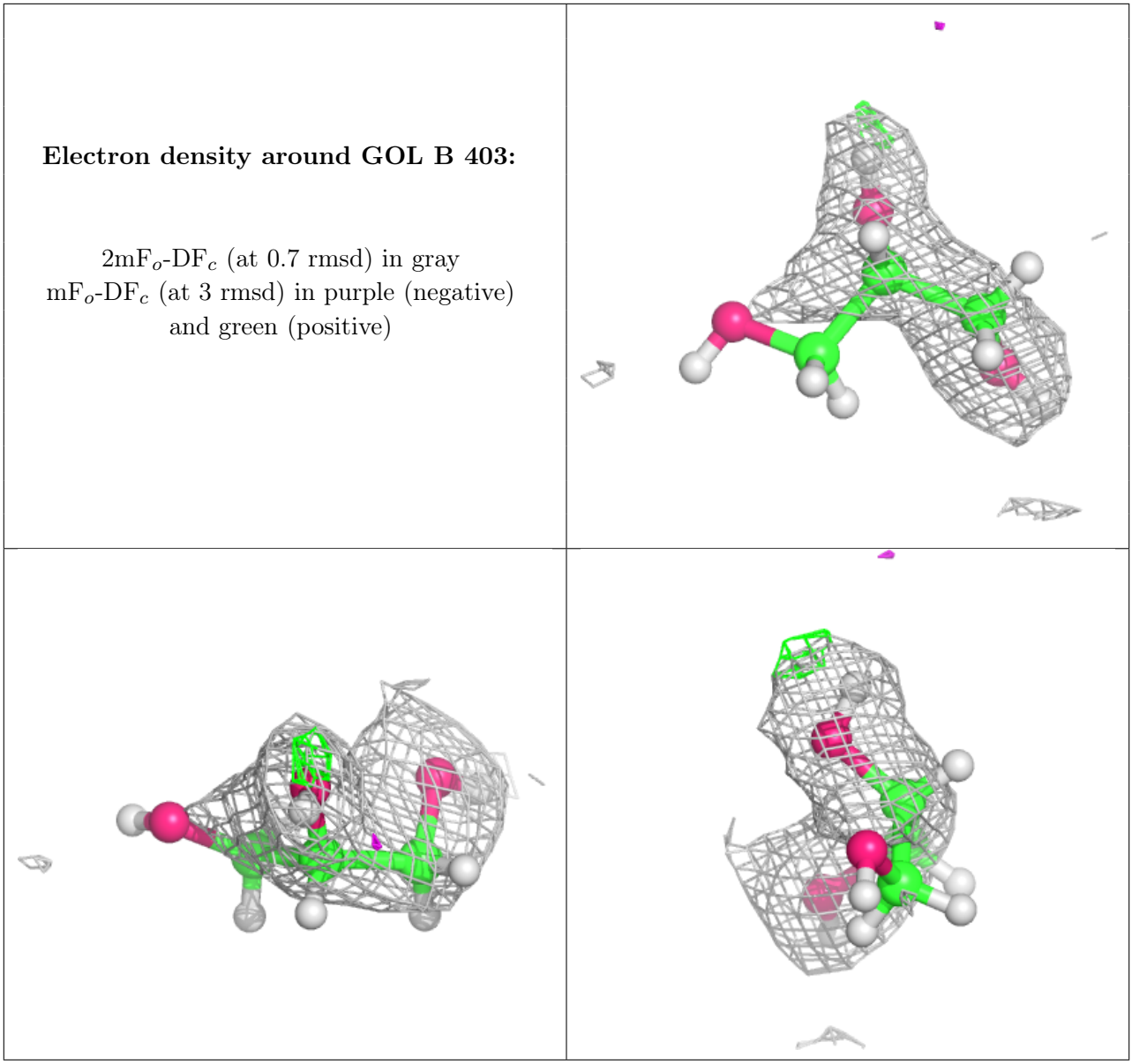






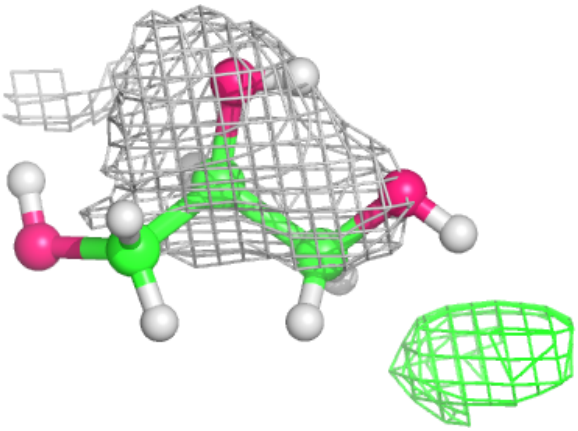
Electron density around GOL B 403:

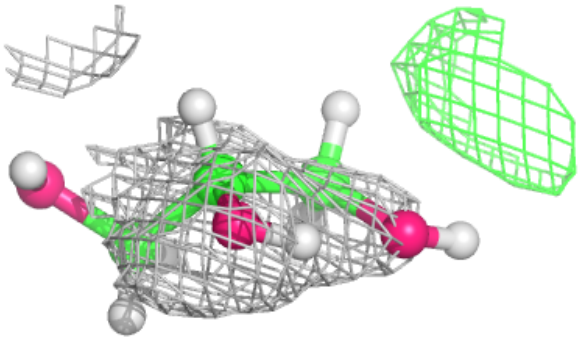
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

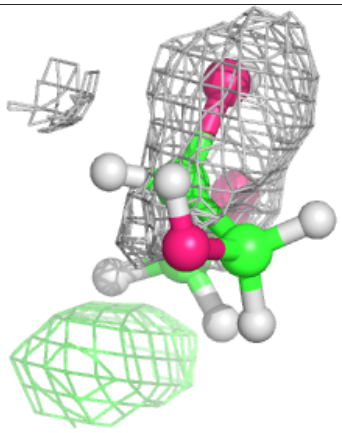


Electron density around GOL C 601:

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

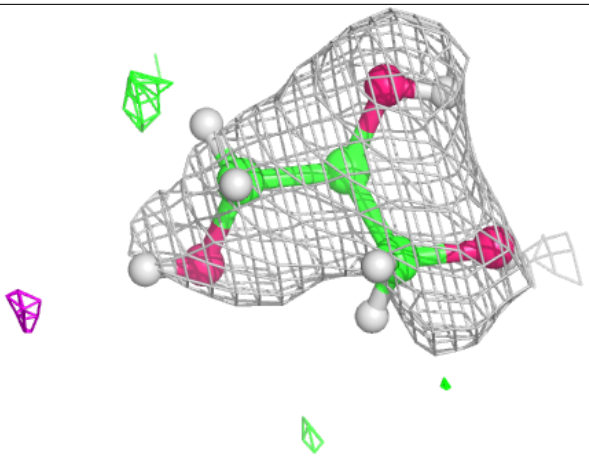


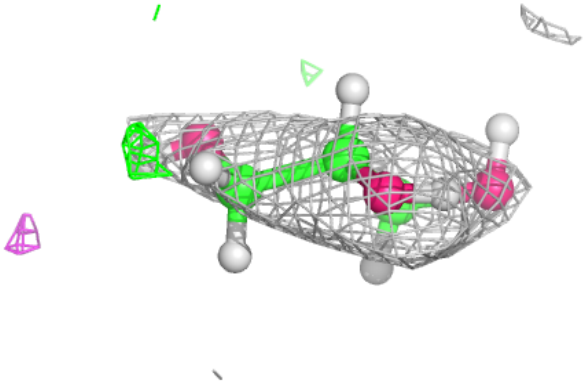


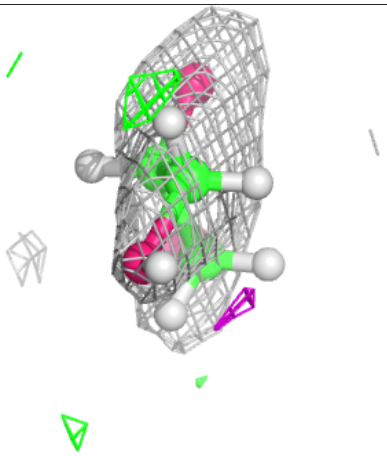


Electron density around GOL A 401:

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







Electron density around GOL B 401:

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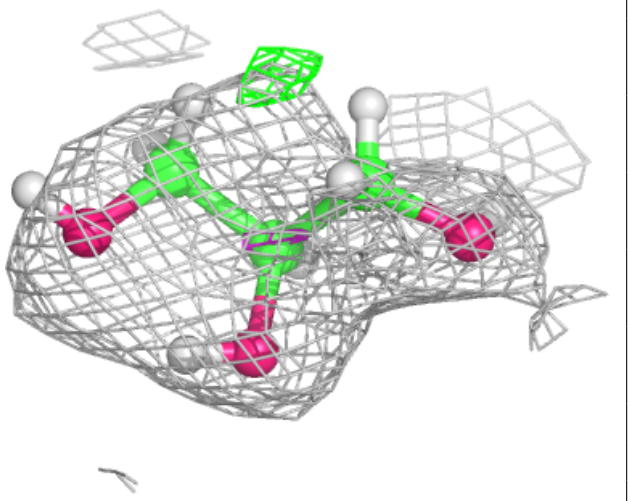
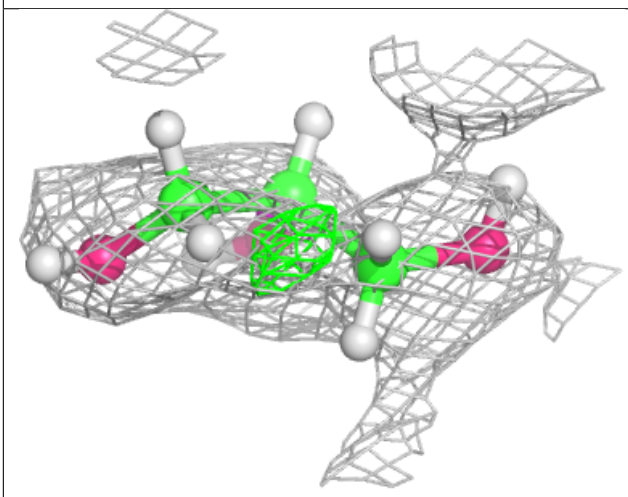
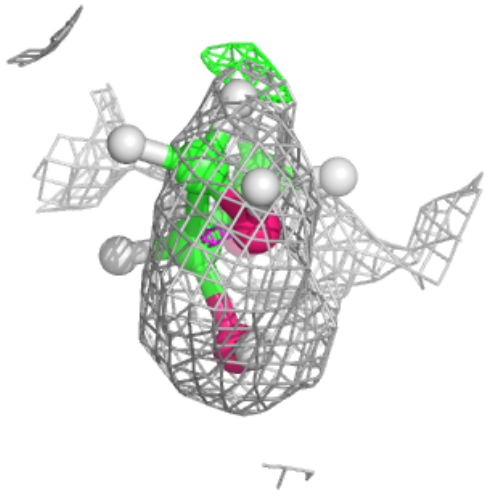
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

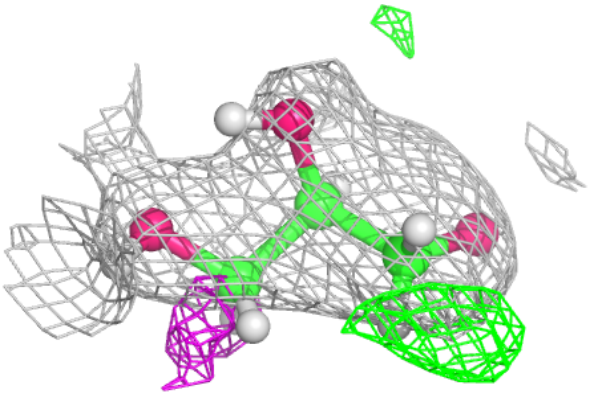


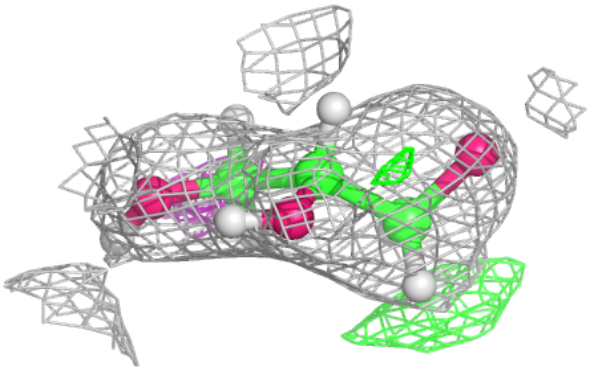


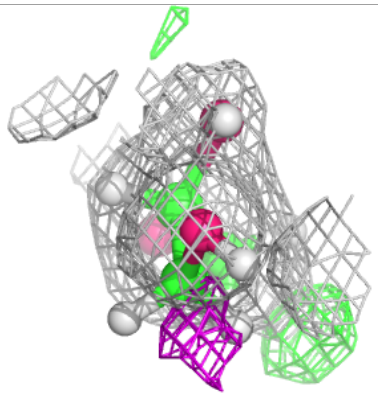


Electron density around GOL D 404:

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

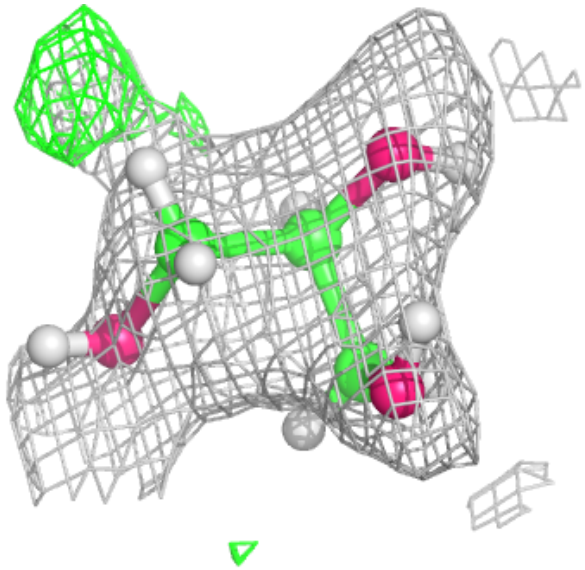


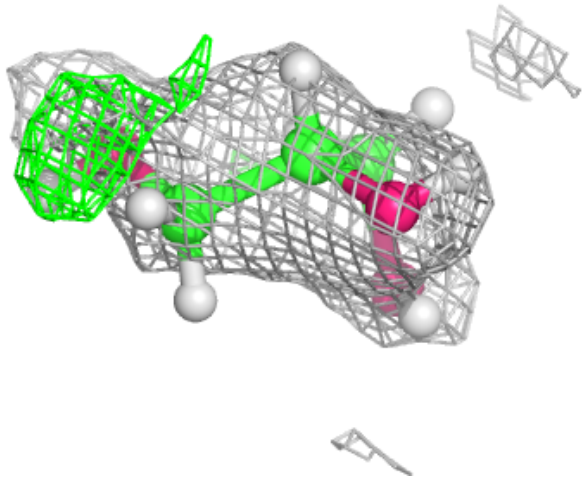


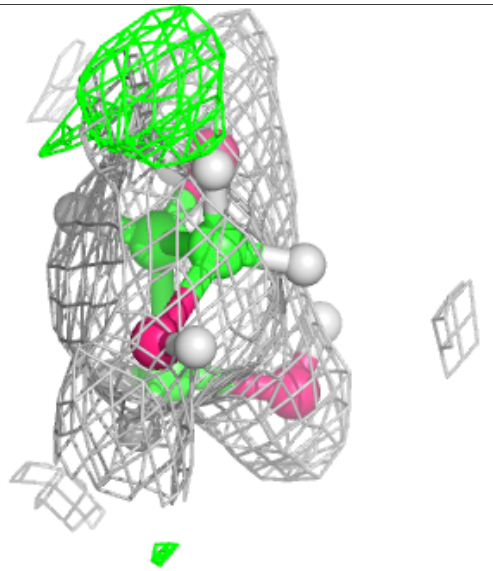


Electron density around GOL C 604:

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

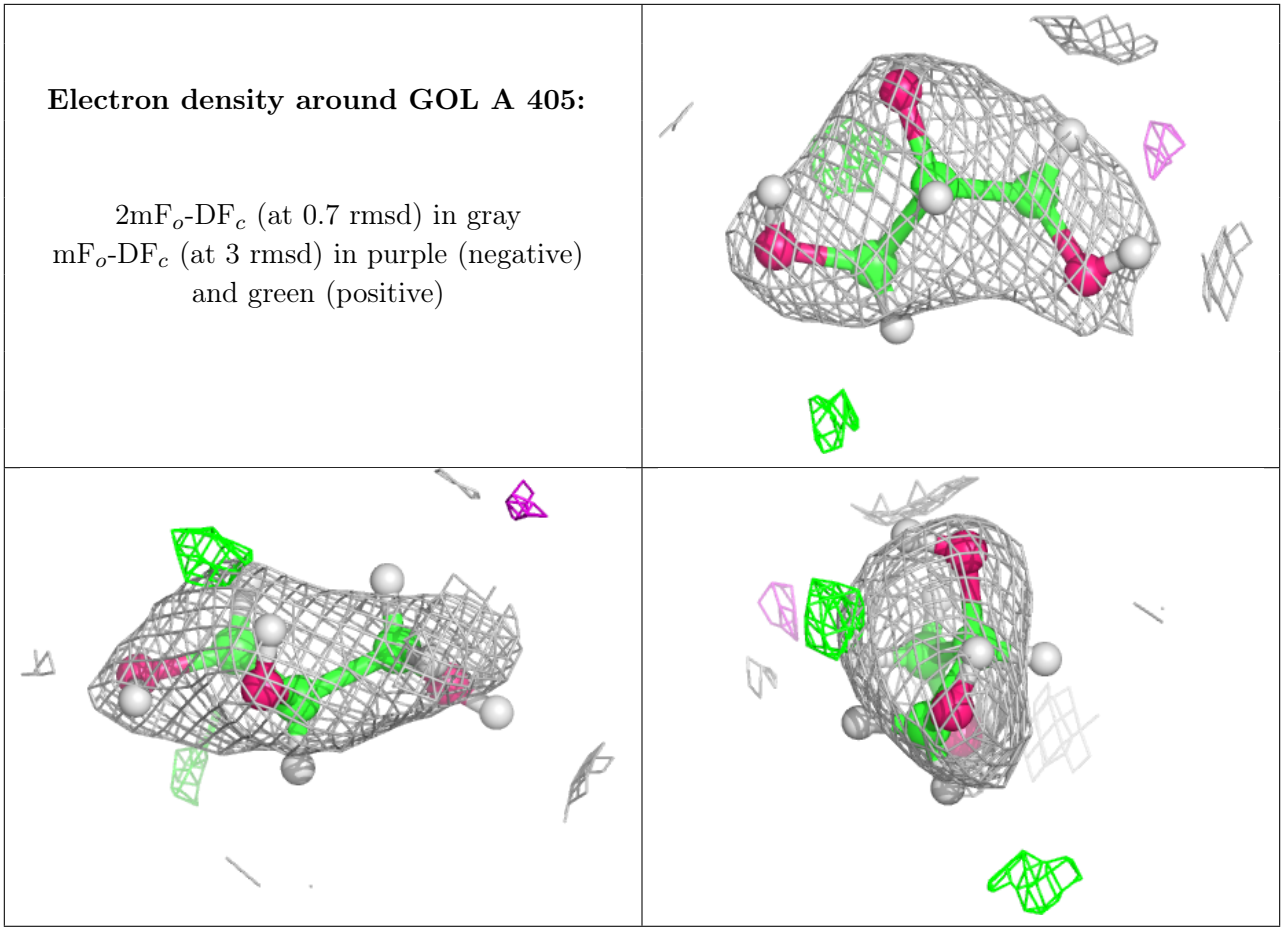






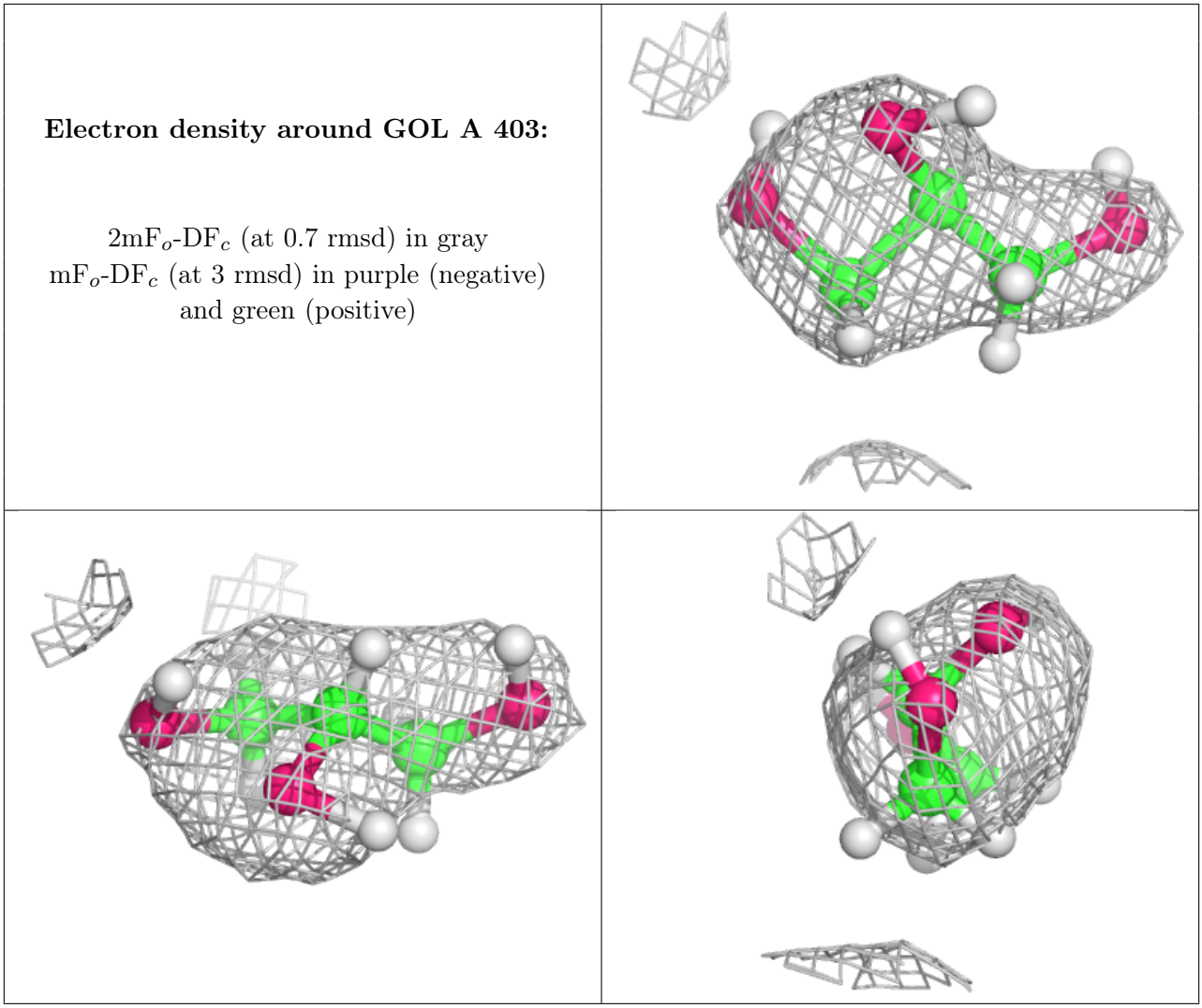
Electron density around GOL A 405:

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



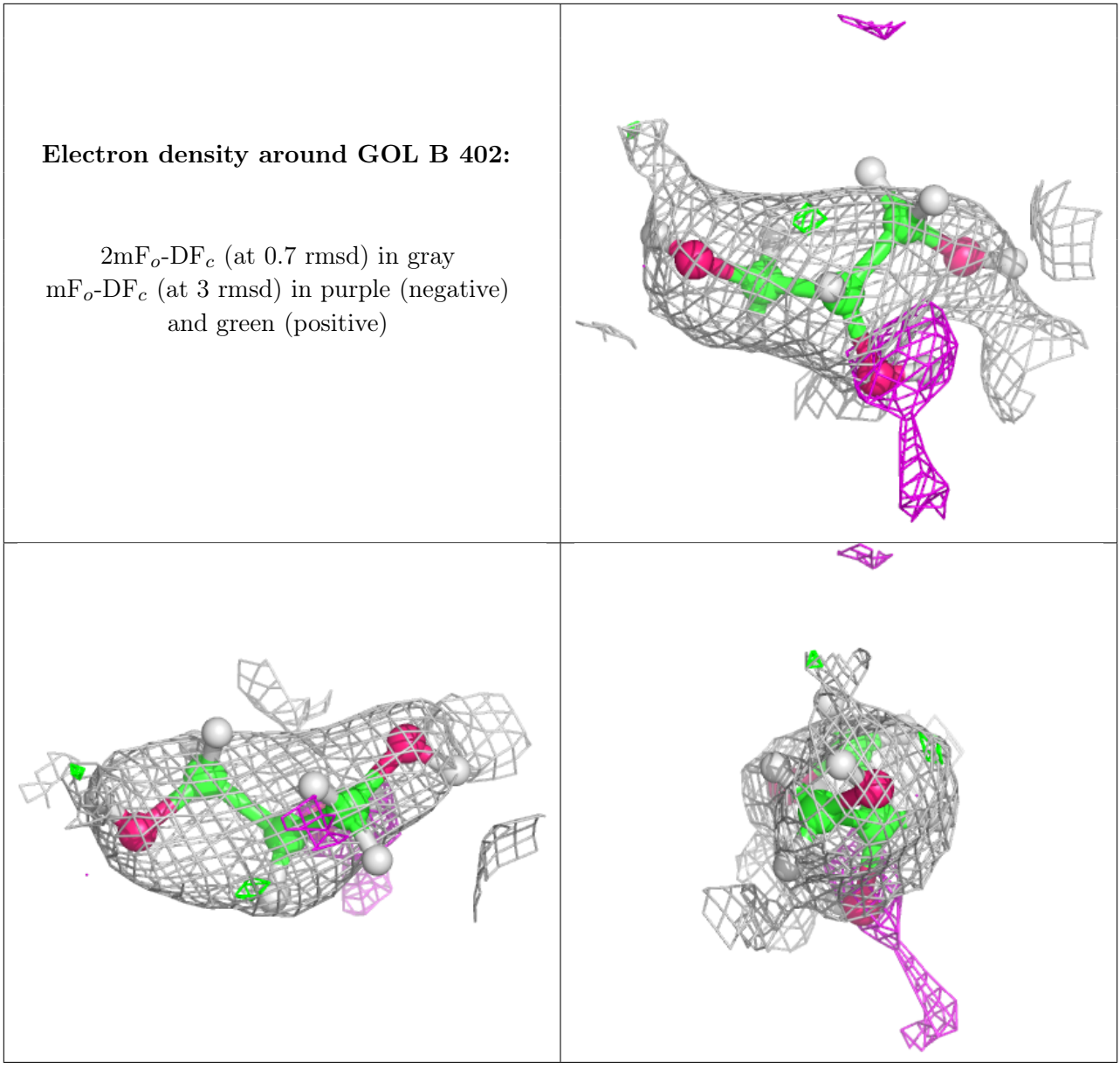
Electron density around GOL A 403:

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



Electron density around GOL B 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 B 404:

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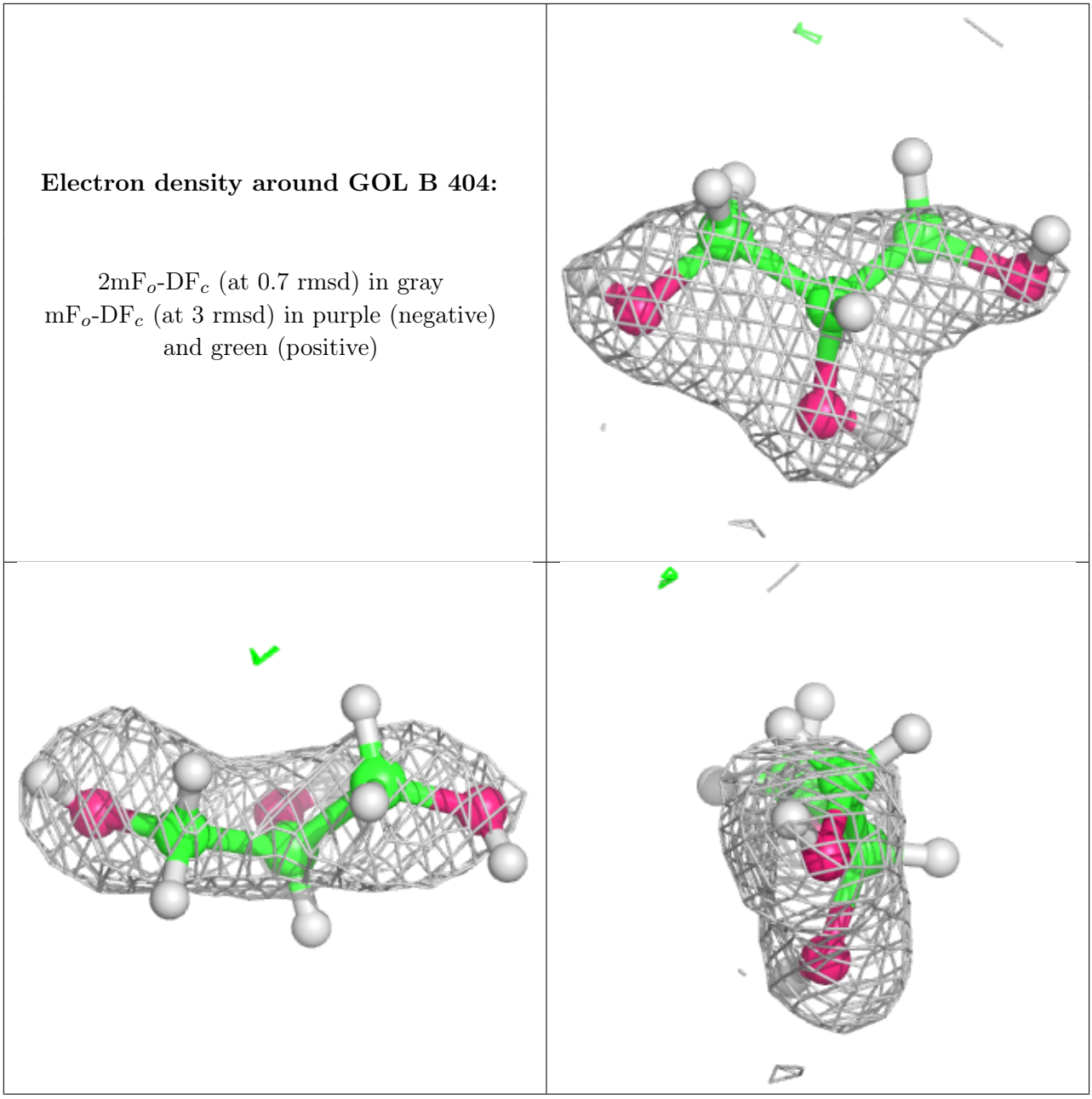
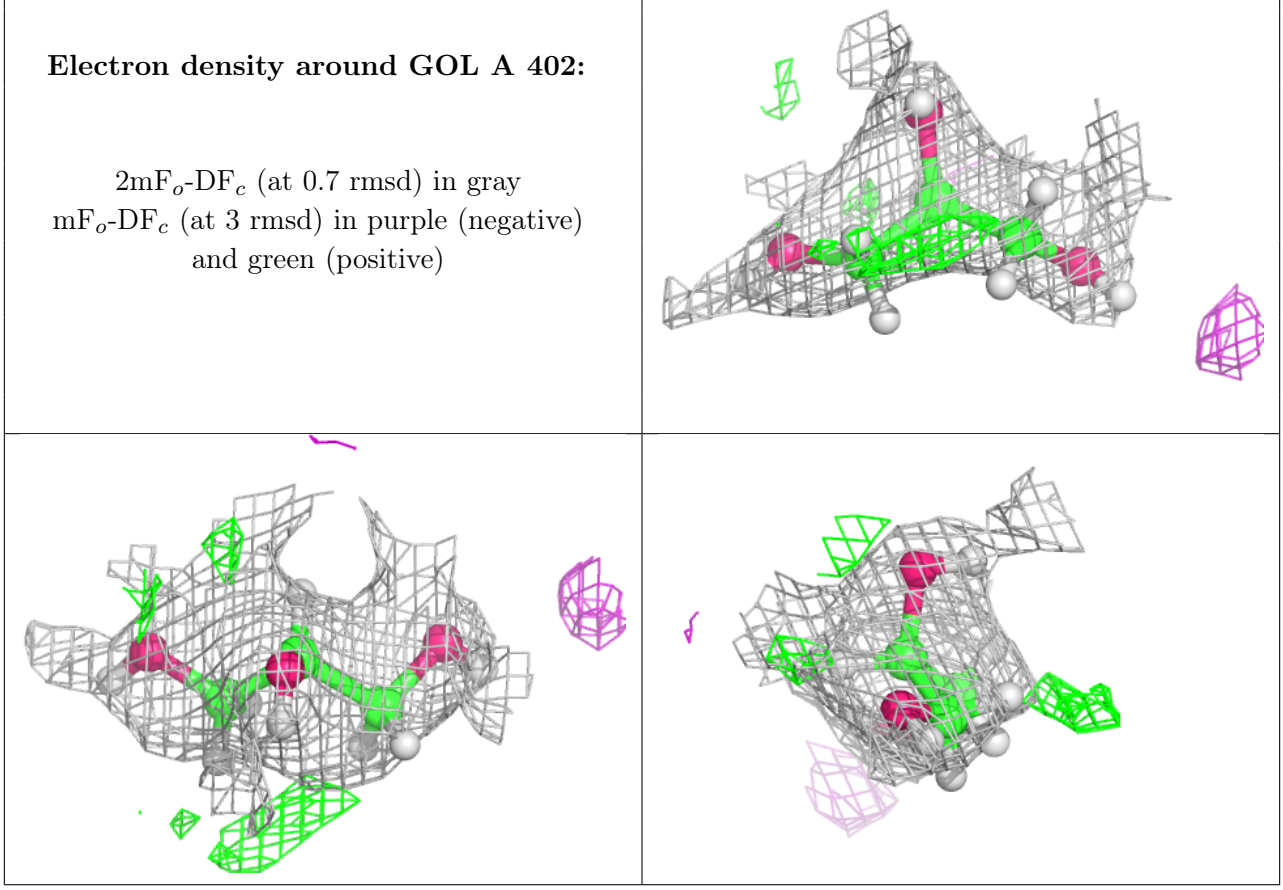
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around GOL 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 D 401:

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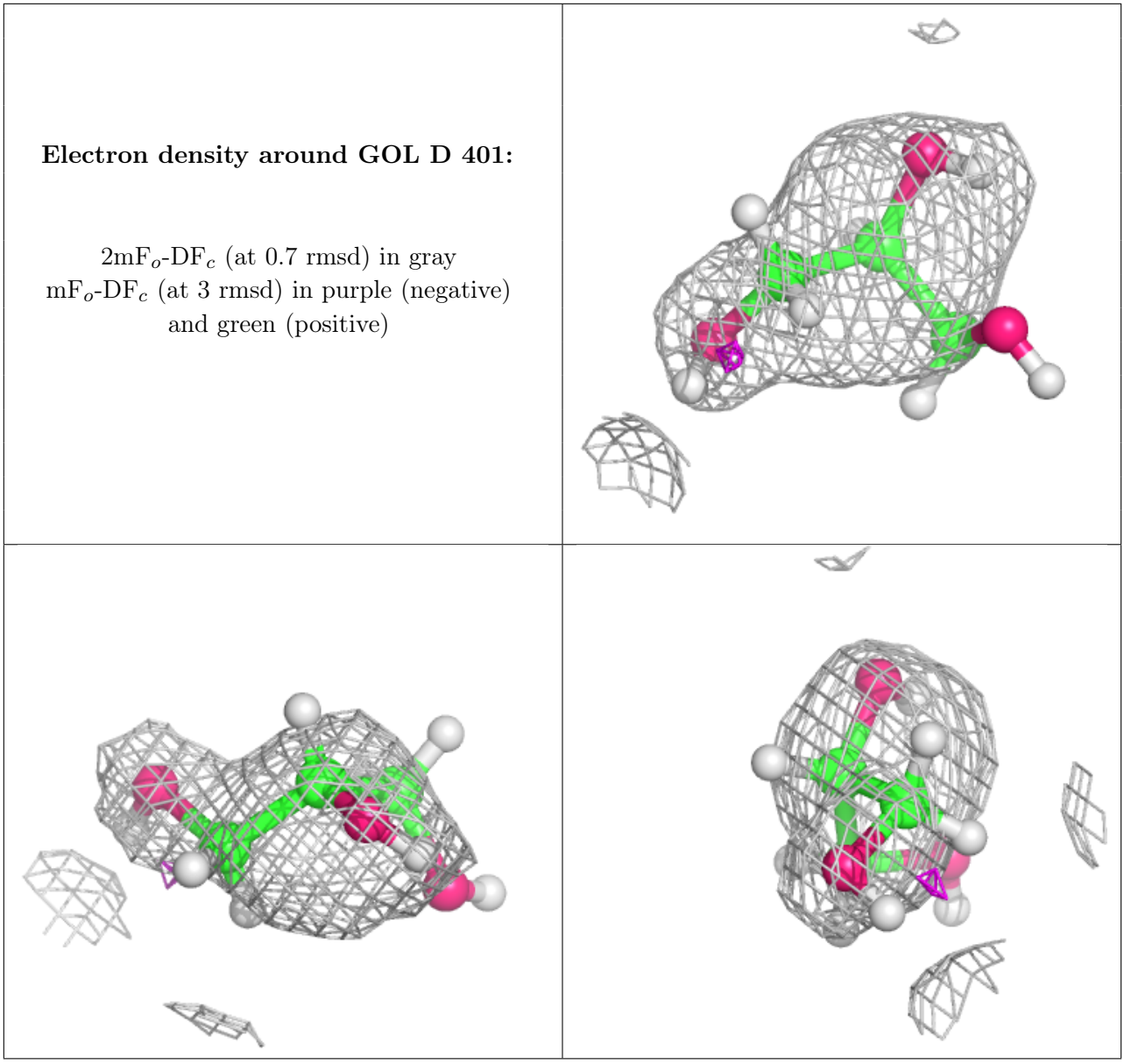
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MN D 406:

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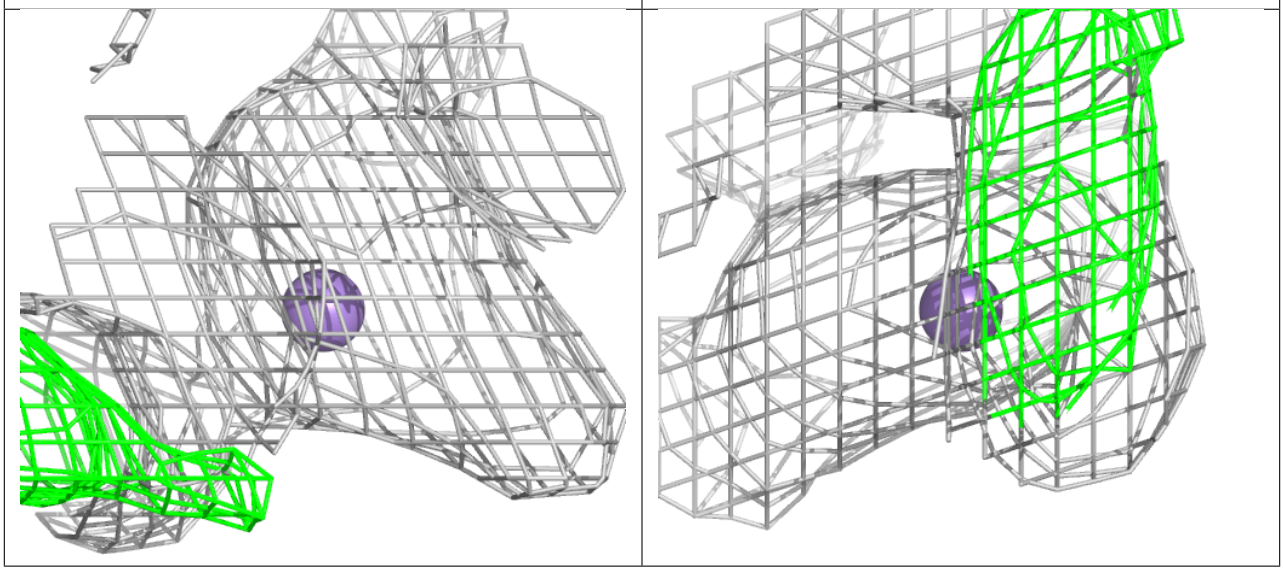
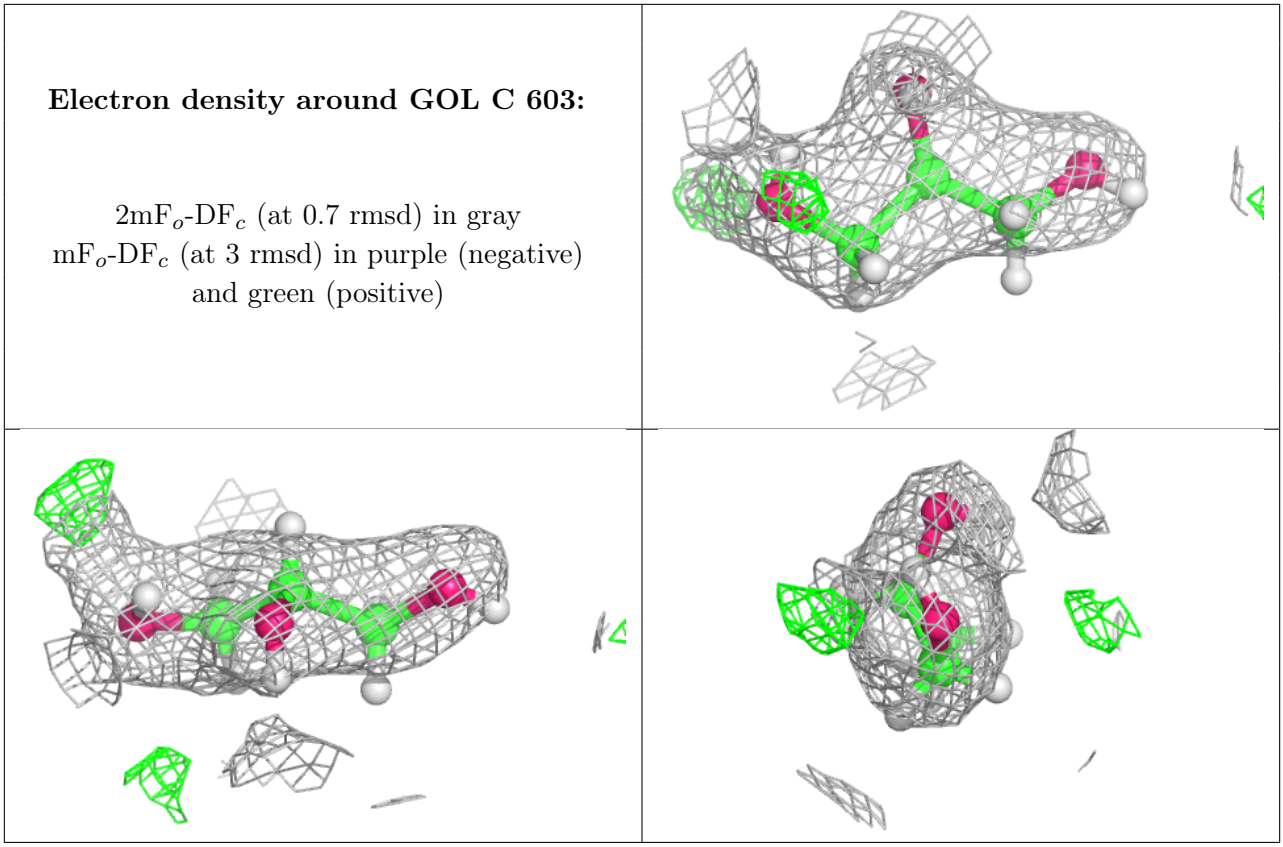
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



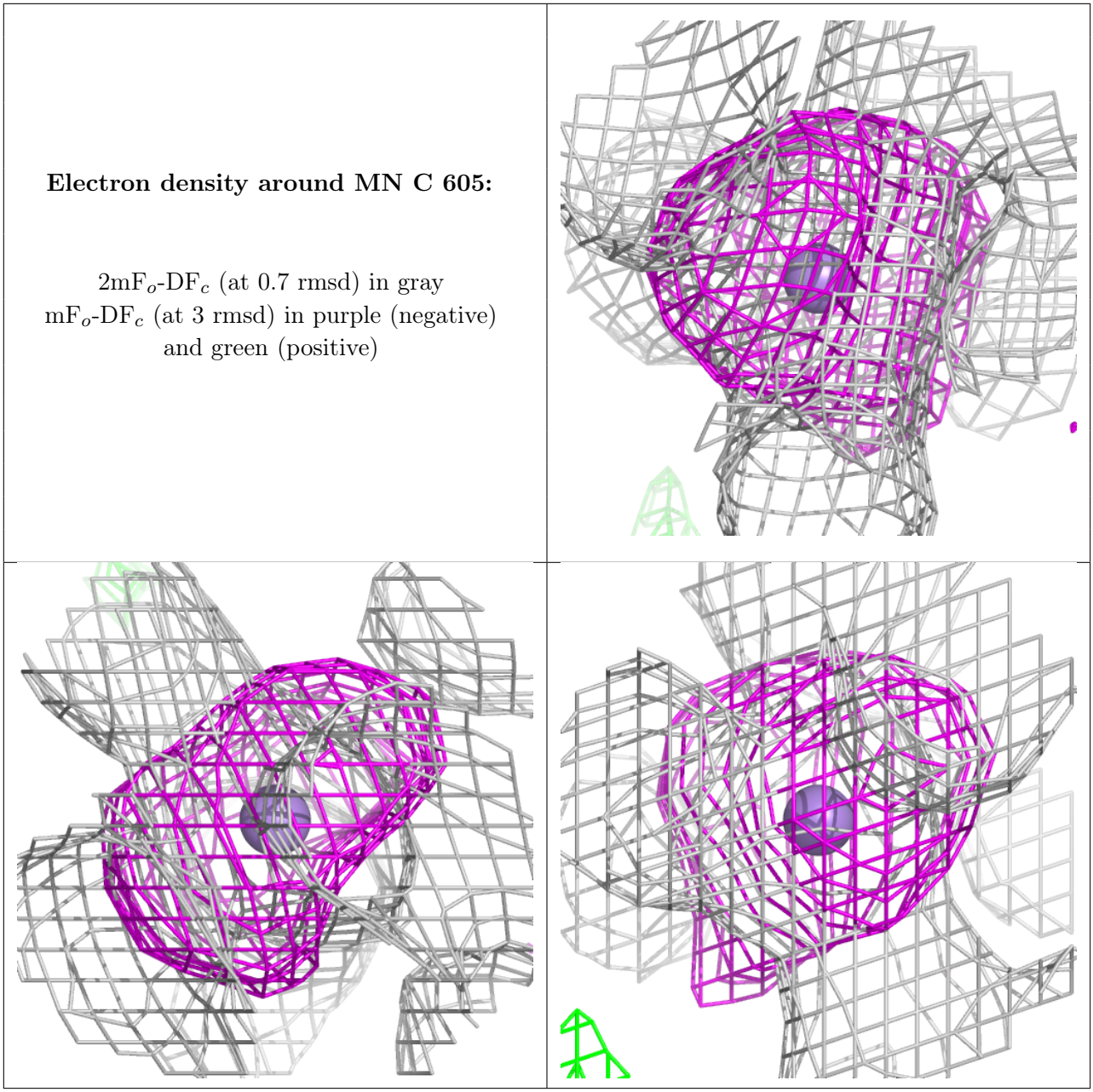
Electron density around GOL C 603:

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



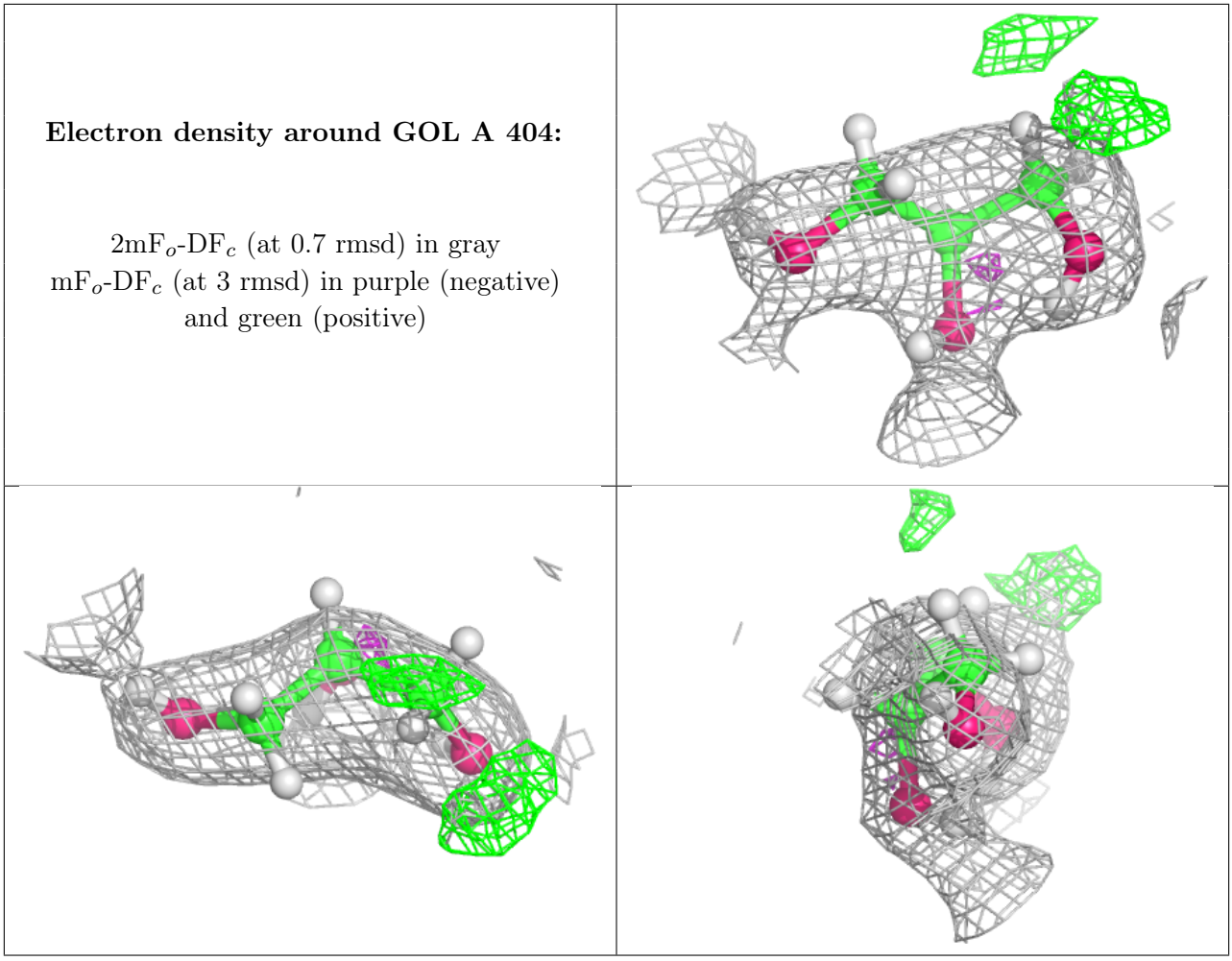
Electron density around MN C 605:

$2mF_o$-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.