Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2024 – 02:16 PM EST

PDB ID	:	8TE4
Title	:	Crystal structure of the methyltransferase domain of R882H/N879A DNMT3A homotetramer
Authors	:	Lu, J.W.; Song, J.K.
Deposited on	:	2023-07-05
Resolution	:	2.65 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:

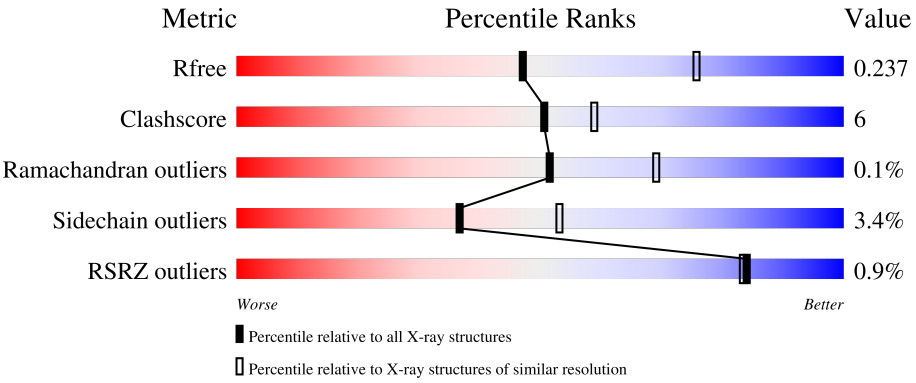
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	287	81% 14% 5%
1	B	287	83% 12% .
1	C	287	84% 11% . .
1	D	287	80% 14% . .
1	E	287	% 46% 9% 45%

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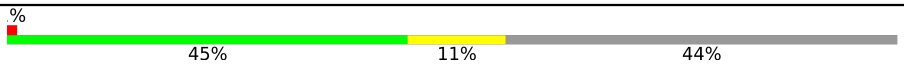
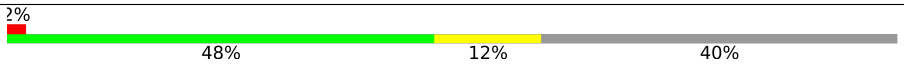
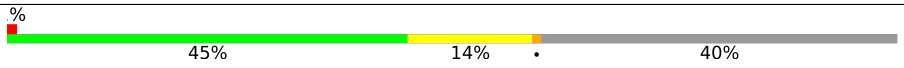
Mol	Chain	Length	Quality of chain
1	F	287	
1	G	287	
1	H	287	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14869 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 DNA (cytosine-5)-methyltransferase 3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	3	0
			2199	1409	391	385	14			
1	B	275	Total	C	N	O	S	0	3	0
			2206	1414	391	387	14			
1	C	275	Total	C	N	O	S	0	3	0
			2205	1414	391	386	14			
1	E	158	Total	C	N	O	S	0	0	0
			1254	821	217	211	5			
1	H	171	Total	C	N	O	S	0	0	0
			1361	885	238	232	6			
1	F	161	Total	C	N	O	S	0	0	0
			1265	829	215	215	6			
1	D	275	Total	C	N	O	S	0	4	0
			2217	1421	394	388	14			
1	G	173	Total	C	N	O	S	0	0	0
			1354	882	235	231	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	626	GLY	-	expression tag	UNP Q9Y6K1
A	627	SER	-	expression tag	UNP Q9Y6K1
A	879	ALA	ASN	engineered mutation	UNP Q9Y6K1
A	882	HIS	ARG	engineered mutation	UNP Q9Y6K1
B	626	GLY	-	expression tag	UNP Q9Y6K1
B	627	SER	-	expression tag	UNP Q9Y6K1
B	879	ALA	ASN	engineered mutation	UNP Q9Y6K1
B	882	HIS	ARG	engineered mutation	UNP Q9Y6K1
C	626	GLY	-	expression tag	UNP Q9Y6K1
C	627	SER	-	expression tag	UNP Q9Y6K1
C	879	ALA	ASN	engineered mutation	UNP Q9Y6K1
C	882	HIS	ARG	engineered mutation	UNP Q9Y6K1
E	626	GLY	-	expression tag	UNP Q9Y6K1

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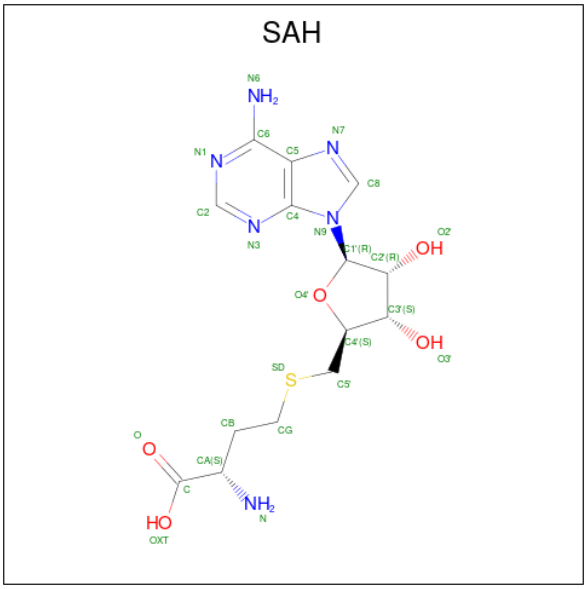
Chain	Residue	Modelled	Actual	Comment	Reference
E	627	SER	-	expression tag	UNP Q9Y6K1
E	879	ALA	ASN	engineered mutation	UNP Q9Y6K1
E	882	HIS	ARG	engineered mutation	UNP Q9Y6K1
H	626	GLY	-	expression tag	UNP Q9Y6K1
H	627	SER	-	expression tag	UNP Q9Y6K1
H	879	ALA	ASN	engineered mutation	UNP Q9Y6K1
H	882	HIS	ARG	engineered mutation	UNP Q9Y6K1
F	626	GLY	-	expression tag	UNP Q9Y6K1
F	627	SER	-	expression tag	UNP Q9Y6K1
F	879	ALA	ASN	engineered mutation	UNP Q9Y6K1
F	882	HIS	ARG	engineered mutation	UNP Q9Y6K1
D	626	GLY	-	expression tag	UNP Q9Y6K1
D	627	SER	-	expression tag	UNP Q9Y6K1
D	879	ALA	ASN	engineered mutation	UNP Q9Y6K1
D	882	HIS	ARG	engineered mutation	UNP Q9Y6K1
G	626	GLY	-	expression tag	UNP Q9Y6K1
G	627	SER	-	expression tag	UNP Q9Y6K1
G	879	ALA	ASN	engineered mutation	UNP Q9Y6K1
G	882	HIS	ARG	engineered mutation	UNP Q9Y6K1

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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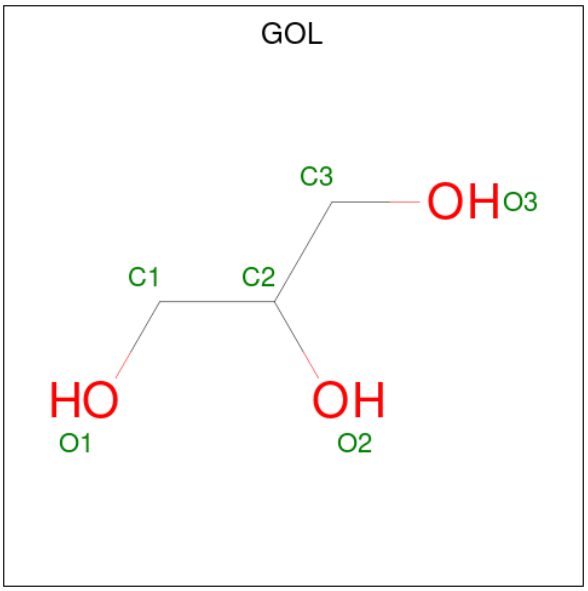
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O S 26 14 6 5 1	0	0
2	C	1	Total C N O S 26 14 6 5 1	0	0
2	D	1	Total C N O S 26 14 6 5 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 4 is water.

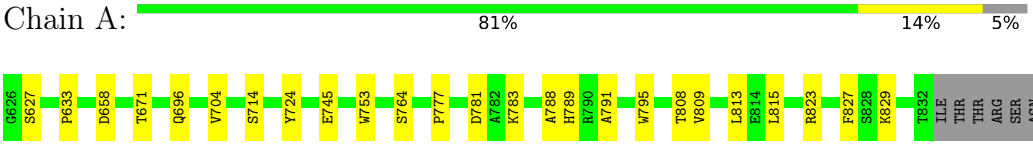
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	107	Total O 107 107	0	0
4	B	124	Total O 124 124	0	0
4	C	122	Total O 122 122	0	0
4	E	36	Total O 36 36	0	0
4	H	29	Total O 29 29	0	0
4	F	34	Total O 34 34	0	0
4	D	119	Total O 119 119	0	0
4	G	37	Total O 37 37	0	0

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.

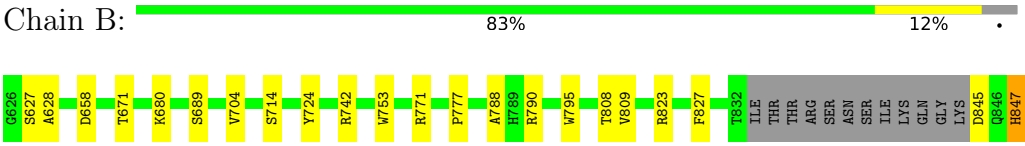
• Molecule 1: DNA (cytosine-5)-methyltransferase 3A

Chain A:



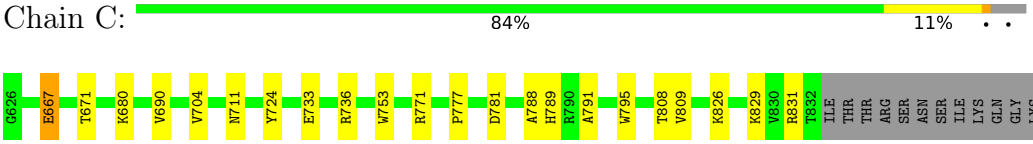
• Molecule 1: DNA (cytosine-5)-methyltransferase 3A

Chain B:



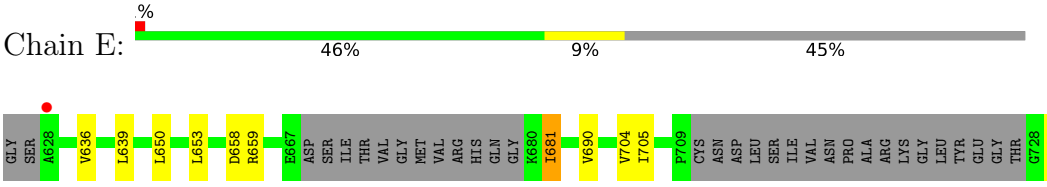
• Molecule 1: DNA (cytosine-5)-methyltransferase 3A

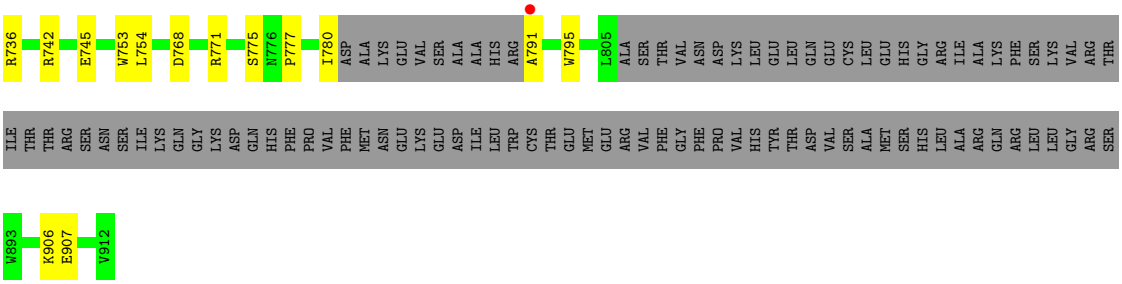
Chain C:



• Molecule 1: DNA (cytosine-5)-methyltransferase 3A

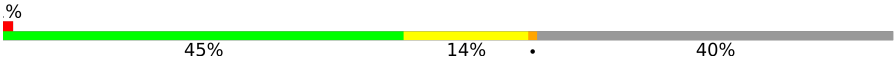
Chain E:

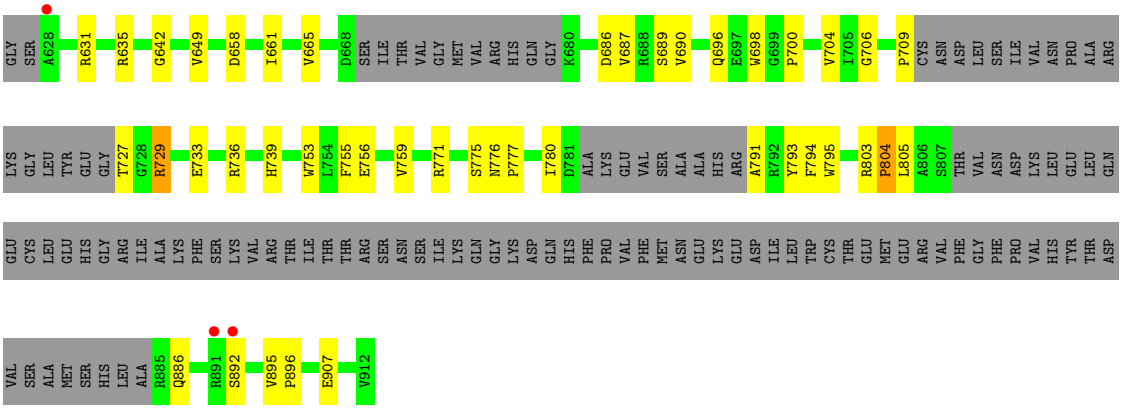




• Molecule 1: DNA (cytosine-5)-methyltransferase 3A

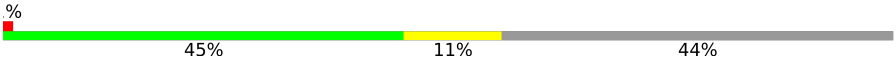
Chain H:

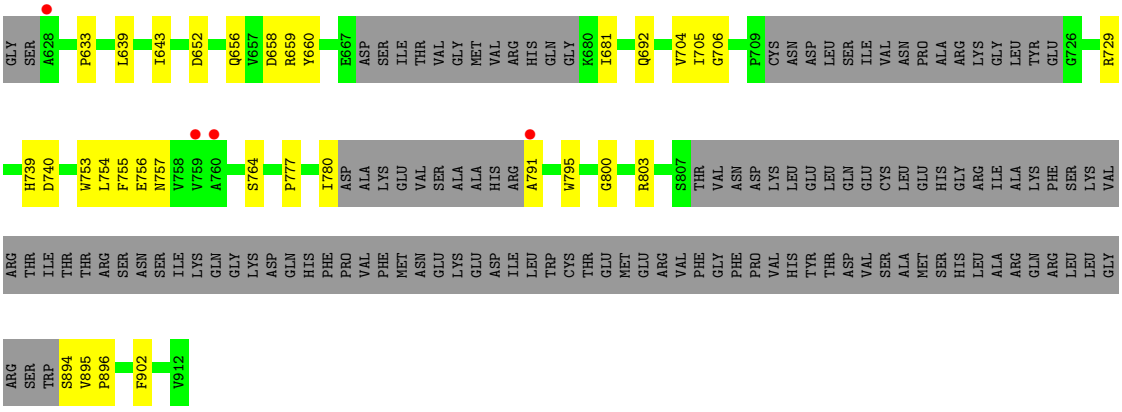




• Molecule 1: DNA (cytosine-5)-methyltransferase 3A

Chain F:

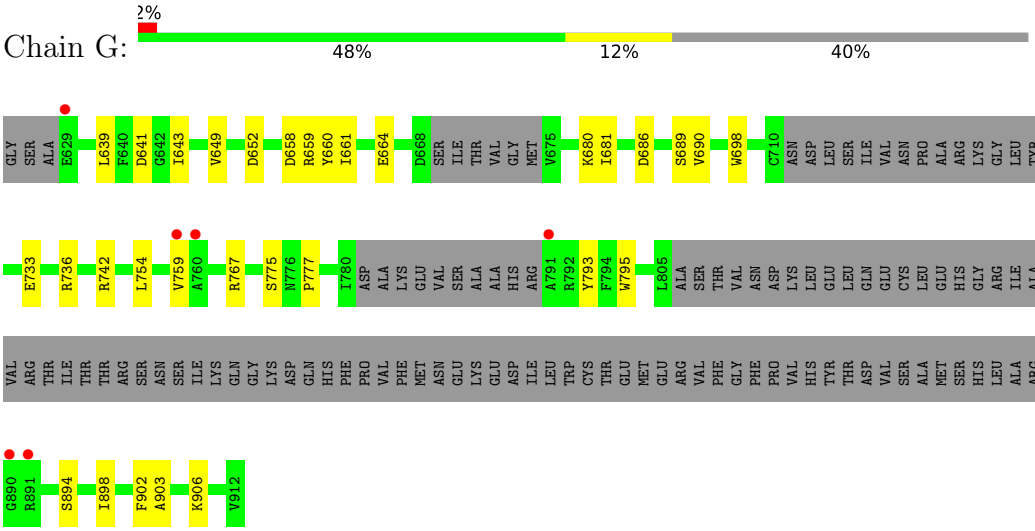




• Molecule 1: DNA (cytosine-5)-methyltransferase 3A

Chain D:

• Molecule 1: DNA (cytosine-5)-methyltransferase 3A



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	178.07Å 178.07Å 109.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.76 – 2.65 46.76 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.76-2.65) 99.3 (46.76-2.65)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.203 , 0.236 0.203 , 0.237	Depositor DCC
R_{free} test set	1995 reflections (1.77%)	wwPDB-VP
Wilson B-factor (Å^2)	53.1	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.478 for -h,-k,l 0.479 for h,-h-k,-l 0.478 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14869	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: SAH, 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	0.33	0/2262	0.53	0/3054
1	B	0.26	0/2269	0.52	0/3064
1	C	0.26	0/2268	0.52	0/3064
1	D	0.26	0/2283	0.53	0/3083
1	E	0.26	0/1287	0.50	0/1739
1	F	0.26	0/1296	0.53	0/1749
1	G	0.26	0/1386	0.54	0/1872
1	H	0.26	0/1394	0.53	0/1880
All	All	0.27	0/14445	0.52	0/19505

There are no bond length outliers.

There are no bond angle outliers.

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	2199	0	2170	23	0
1	B	2206	0	2172	26	0
1	C	2205	0	2168	24	0
1	D	2217	0	2185	29	0
1	E	1254	0	1215	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1265	0	1235	18	0
1	G	1354	0	1311	15	0
1	H	1361	0	1335	25	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	0	0
3	A	30	0	40	2	0
3	B	30	0	40	1	0
3	C	12	0	16	0	0
3	D	24	0	32	2	0
4	A	107	0	0	0	0
4	B	124	0	0	2	0
4	C	122	0	0	1	0
4	D	119	0	0	2	0
4	E	36	0	0	1	0
4	F	34	0	0	0	0
4	G	37	0	0	0	0
4	H	29	0	0	1	0
All	All	14869	0	13995	160	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.

All (160) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:PRO:HD2	1:A:858:ILE:HA	1.61	0.82
1:D:643:ILE:HD11	1:D:888:LEU:HD13	1.69	0.73
1:B:849:PRO:HG2	1:B:859:LEU:HD23	1.71	0.72
1:H:709:PRO:HG3	1:H:892:SER:HB3	1.72	0.72
1:H:780:ILE:O	1:H:791:ALA:HA	1.90	0.71
1:B:847:HIS:O	1:B:847:HIS:ND1	2.24	0.70
1:B:851:PHE:HE1	1:B:856:GLU:HG3	1.58	0.68
1:E:690:VAL:O	1:E:736:ARG:NH2	2.27	0.67
1:C:849:PRO:HD2	1:C:858:ILE:HA	1.77	0.67
1:C:887:ARG:HH21	1:C:891:ARG:HH22	1.43	0.66
1:G:690:VAL:O	1:G:736:ARG:NH2	2.30	0.65
1:B:628:ALA:HB3	3:B:1006:GOL:H32	1.79	0.64
1:H:895:VAL:H	1:H:896:PRO:HD2	1.62	0.63
1:C:690:VAL:O	1:C:736:ARG:NH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:SER:HB2	1:H:804:PRO:HD2	1.81	0.63
1:H:727:THR:N	4:H:1001:HOH:O	2.32	0.63
1:C:680:LYS:NZ	1:E:907:GLU:OE1	2.32	0.62
1:A:885:ARG:NH2	1:B:876:ASP:OD1	2.32	0.62
1:B:790:ARG:NH2	1:B:890:GLY:O	2.32	0.62
1:D:783:LYS:O	1:D:829:LYS:NZ	2.32	0.62
1:C:882:HIS:ND1	4:C:1101:HOH:O	2.31	0.61
1:D:790:ARG:NH2	1:D:890:GLY:O	2.33	0.61
1:G:643:ILE:HD12	1:G:889:LEU:HD11	1.83	0.60
1:D:712:ASP:HB2	1:D:727:THR:HG22	1.82	0.60
1:H:690:VAL:O	1:H:736:ARG:NH2	2.35	0.60
1:C:878:SER:O	1:C:878:SER:OG	2.20	0.60
1:C:733:GLU:OE1	1:C:736:ARG:NH1	2.35	0.59
1:D:643:ILE:HG23	1:D:874:TYR:HE2	1.68	0.59
1:A:808:THR:OG1	1:A:809:VAL:N	2.36	0.58
1:E:733:GLU:OE1	1:E:736:ARG:NH1	2.38	0.57
1:A:671:THR:HG21	1:A:878:SER:HB2	1.86	0.57
1:D:690:VAL:O	1:D:736:ARG:NH2	2.36	0.57
1:B:808:THR:OG1	1:B:809:VAL:N	2.38	0.57
1:C:808:THR:OG1	1:C:809:VAL:N	2.39	0.56
1:F:780:ILE:O	1:F:791:ALA:HA	2.05	0.56
1:A:878:SER:O	1:A:878:SER:OG	2.23	0.56
1:D:808:THR:OG1	1:D:809:VAL:N	2.39	0.56
1:B:680:LYS:NZ	1:H:907:GLU:OE1	2.36	0.55
1:D:831[A]:ARG:NH2	3:D:1005:GOL:O3	2.39	0.55
1:E:777:PRO:HB3	1:E:795:TRP:CE2	2.41	0.55
1:E:742:ARG:NH2	4:E:1001:HOH:O	2.39	0.54
1:B:851:PHE:CE1	1:B:856:GLU:HG3	2.41	0.54
1:B:658:ASP:O	1:H:631:ARG:NH2	2.41	0.54
1:D:831[A]:ARG:NH1	3:D:1005:GOL:O2	2.35	0.53
1:H:661:ILE:HD12	1:H:698:TRP:HB3	1.91	0.53
1:F:639:LEU:HD13	1:F:639:LEU:O	2.09	0.52
1:F:895:VAL:N	1:F:896:PRO:HD2	2.24	0.52
1:A:633:PRO:HB2	1:A:658:ASP:HB2	1.91	0.52
1:H:649:VAL:HG22	1:H:895:VAL:HG13	1.91	0.52
1:H:777:PRO:HB3	1:H:795:TRP:CE2	2.45	0.52
1:D:826:LYS:HE2	1:D:851:PHE:CZ	2.46	0.51
1:F:633:PRO:HB3	1:F:656:GLN:HB3	1.92	0.51
1:C:878:SER:HA	1:D:860:TRP:CE2	2.46	0.50
1:F:729:ARG:HG3	1:F:729:ARG:HH11	1.77	0.50
1:D:849:PRO:HG2	1:D:859:LEU:CD2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:TYR:CD1	1:F:729:ARG:HA	2.47	0.49
1:D:692:GLN:NE2	4:D:1105:HOH:O	2.44	0.49
1:D:849:PRO:HG2	1:D:859:LEU:HD23	1.94	0.49
1:B:878:SER:O	1:B:878:SER:OG	2.27	0.49
1:C:789:HIS:HB2	1:C:831:ARG:HB3	1.94	0.49
1:B:671:THR:HG21	1:B:878:SER:HB2	1.94	0.49
1:B:771:ARG:HH22	1:E:733:GLU:CD	2.16	0.48
1:H:803:ARG:O	1:H:805:LEU:N	2.45	0.48
1:B:845:ASP:N	4:B:1107:HOH:O	2.46	0.48
1:H:895:VAL:N	1:H:896:PRO:HD2	2.28	0.48
1:A:875:THR:O	1:A:885:ARG:HD3	2.14	0.48
1:A:878:SER:HA	1:B:860:TRP:CE2	2.49	0.48
1:C:860:TRP:CE2	1:D:878:SER:HA	2.49	0.48
1:H:665:VAL:HG12	1:H:687:VAL:HG11	1.95	0.48
1:F:800:GLY:O	1:F:803:ARG:NH1	2.47	0.47
1:D:733:GLU:OE1	1:D:736:ARG:NH1	2.47	0.47
1:D:768:ASP:OD1	1:D:771:ARG:NH1	2.47	0.47
1:F:729:ARG:HG3	1:F:729:ARG:NH1	2.29	0.47
1:G:641:ASP:O	1:G:889:LEU:HD12	2.13	0.47
1:E:639:LEU:O	1:E:639:LEU:HD13	2.14	0.47
1:E:653:LEU:HD22	1:E:906:LYS:HD2	1.96	0.47
1:H:729:ARG:NH1	1:H:733:GLU:OE2	2.48	0.47
1:G:733:GLU:OE1	1:G:736:ARG:NH1	2.48	0.47
1:G:759:VAL:HG23	1:G:793:TYR:CZ	2.50	0.47
1:G:777:PRO:HB3	1:G:795:TRP:CE2	2.50	0.47
1:A:827:PHE:HB3	3:A:1004:GOL:H12	1.97	0.46
1:B:724:TYR:CG	1:E:729:ARG:HB2	2.50	0.46
1:C:771:ARG:NH2	1:H:733:GLU:OE1	2.48	0.46
1:A:860:TRP:CE2	1:B:878:SER:HA	2.51	0.46
1:H:776:ASN:OD1	1:H:804:PRO:HA	2.15	0.46
1:D:878:SER:O	1:D:878:SER:OG	2.25	0.46
1:C:887:ARG:O	1:C:891:ARG:HG3	2.14	0.46
1:H:686:ASP:O	1:H:689:SER:OG	2.30	0.46
1:F:754:LEU:HD13	1:F:902:PHE:HE1	1.80	0.46
1:F:643:ILE:HD12	1:F:643:ILE:H	1.79	0.46
1:B:823:ARG:NH1	1:B:857:ASP:OD2	2.42	0.46
1:E:780:ILE:O	1:E:791:ALA:HA	2.15	0.46
1:F:777:PRO:HB3	1:F:795:TRP:CE2	2.51	0.46
1:G:903:ALA:O	1:G:906:LYS:HG2	2.15	0.46
1:C:724:TYR:CD2	1:H:729:ARG:HA	2.50	0.46
1:G:661:ILE:CD1	1:G:698:TRP:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:886:GLN:OE1	1:H:886:GLN:N	2.49	0.46
1:A:783:LYS:HB2	1:A:829:LYS:HD3	1.98	0.45
1:H:706:GLY:O	1:H:755:PHE:HA	2.16	0.45
1:A:789:HIS:HE1	3:A:1004:GOL:H32	1.81	0.45
1:C:671:THR:HG21	1:C:878:SER:HB2	1.99	0.45
1:B:864:MET:HB2	1:B:864:MET:HE3	1.76	0.45
1:C:826:LYS:HE2	1:C:851:PHE:CE2	2.52	0.45
1:C:877:VAL:HG23	1:C:878:SER:HB3	1.99	0.45
1:C:781:ASP:HA	1:C:791:ALA:HA	1.99	0.45
1:E:768:ASP:OD1	1:E:771:ARG:NH1	2.48	0.44
1:D:724:TYR:CD2	1:G:729:ARG:HA	2.52	0.44
1:A:851:PHE:CE1	1:A:856:GLU:HB3	2.51	0.44
1:B:777:PRO:HB3	1:B:795:TRP:CE2	2.52	0.44
1:H:759:VAL:HA	1:H:793:TYR:CD2	2.52	0.44
1:E:636:VAL:HG21	1:E:650:LEU:HD11	1.99	0.44
1:E:704:VAL:O	1:E:753:TRP:HA	2.18	0.44
1:H:635:ARG:NH1	1:H:700:PRO:HG2	2.33	0.44
1:D:887:ARG:O	1:D:891:ARG:HG3	2.18	0.44
1:A:887:ARG:O	1:A:891:ARG:HG3	2.18	0.44
1:G:660:TYR:HB3	1:G:681:ILE:HG23	1.99	0.44
1:B:883:LEU:HD12	1:B:883:LEU:HA	1.77	0.43
1:E:681:ILE:O	1:E:681:ILE:HG13	2.17	0.43
1:G:643:ILE:CD1	1:G:889:LEU:HD11	2.48	0.43
1:E:705:ILE:HG22	1:E:754:LEU:HB3	1.99	0.43
1:G:754:LEU:HD13	1:G:902:PHE:CE1	2.54	0.43
1:G:649:VAL:HG21	1:G:898:ILE:HG23	2.01	0.43
1:C:864:MET:HB3	1:C:889:LEU:HD13	2.00	0.43
1:A:815:LEU:HD11	1:A:859:LEU:HD21	1.99	0.43
1:D:777:PRO:HB3	1:D:795:TRP:CE2	2.54	0.43
1:D:671:THR:HG21	1:D:878:SER:HB2	2.01	0.43
1:F:706:GLY:O	1:F:755:PHE:HA	2.20	0.42
1:D:642:GLY:O	1:D:669:SER:HB3	2.19	0.42
1:A:847:HIS:HB3	1:A:848:PHE:H	1.54	0.42
1:F:756:GLU:HG2	1:F:757:ASN:N	2.34	0.42
1:B:788:ALA:HB2	1:B:867:VAL:CG1	2.49	0.42
1:B:887:ARG:O	1:B:891:ARG:HG3	2.20	0.42
1:F:660:TYR:HB3	1:F:681:ILE:HG23	2.00	0.42
1:A:777:PRO:HB3	1:A:795:TRP:CE2	2.55	0.42
1:D:882:HIS:HD2	4:D:1177:HOH:O	2.03	0.42
1:D:704:VAL:O	1:D:753:TRP:HA	2.20	0.41
1:H:704:VAL:O	1:H:753:TRP:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:895:VAL:N	1:F:896:PRO:CD	2.83	0.41
1:A:781:ASP:HA	1:A:791:ALA:HA	2.02	0.41
1:D:787:ALA:HA	1:D:829:LYS:HG2	2.02	0.41
1:C:777:PRO:HB3	1:C:795:TRP:CE2	2.55	0.41
1:H:756:GLU:HB2	1:H:794:PHE:CE2	2.55	0.41
1:D:788:ALA:HB2	1:D:867:VAL:CG1	2.51	0.41
1:B:704:VAL:O	1:B:753:TRP:HA	2.20	0.41
1:C:704:VAL:O	1:C:753:TRP:HA	2.20	0.41
1:G:639:LEU:HD13	1:G:639:LEU:O	2.20	0.41
1:B:742[A]:ARG:HD3	4:B:1108:HOH:O	2.19	0.41
1:D:859:LEU:HD12	1:D:863:GLU:HB2	2.03	0.41
1:A:906:LYS:HE2	1:A:906:LYS:HB2	1.83	0.41
1:C:788:ALA:HB2	1:C:867:VAL:CG1	2.51	0.41
1:C:887:ARG:HH21	1:C:891:ARG:NH2	2.15	0.41
1:G:686:ASP:O	1:G:689:SER:OG	2.35	0.41
1:A:788:ALA:HB2	1:A:867:VAL:CG1	2.51	0.41
1:F:705:ILE:HG22	1:F:754:LEU:HB3	2.02	0.40
1:F:704:VAL:O	1:F:753:TRP:HA	2.21	0.40
1:D:823:ARG:NH2	1:D:850:VAL:HG21	2.36	0.40
1:A:704:VAL:O	1:A:753:TRP:HA	2.21	0.40
1:F:692:GLN:HG2	1:F:740:ASP:CG	2.42	0.40
1:A:823:ARG:CZ	1:A:850:VAL:HG21	2.51	0.40
1:C:667:GLU:OE2	1:C:667:GLU:N	2.35	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	272/287 (95%)	265 (97%)	7 (3%)	0	100	100
1	B	274/287 (96%)	267 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	274/287 (96%)	266 (97%)	8 (3%)	0	100	100
1	D	275/287 (96%)	268 (98%)	7 (2%)	0	100	100
1	E	148/287 (52%)	142 (96%)	6 (4%)	0	100	100
1	F	151/287 (53%)	147 (97%)	4 (3%)	0	100	100
1	G	163/287 (57%)	156 (96%)	7 (4%)	0	100	100
1	H	161/287 (56%)	152 (94%)	7 (4%)	2 (1%)	13	19
All	All	1718/2296 (75%)	1663 (97%)	53 (3%)	2 (0%)	51	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	804	PRO
1	H	642	GLY

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	232/250 (93%)	226 (97%)	6 (3%)	46	64
1	B	232/250 (93%)	228 (98%)	4 (2%)	60	77
1	C	231/250 (92%)	227 (98%)	4 (2%)	60	77
1	D	233/250 (93%)	227 (97%)	6 (3%)	46	64
1	E	126/250 (50%)	121 (96%)	5 (4%)	31	47
1	F	127/250 (51%)	121 (95%)	6 (5%)	26	40
1	G	136/250 (54%)	124 (91%)	12 (9%)	10	14
1	H	139/250 (56%)	133 (96%)	6 (4%)	29	44
All	All	1456/2000 (73%)	1407 (97%)	49 (3%)	37	53

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	627	SER
1	A	696	GLN
1	A	714	SER
1	A	745	GLU
1	A	764	SER
1	A	813	LEU
1	B	627	SER
1	B	714	SER
1	B	827	PHE
1	B	847	HIS
1	C	667	GLU
1	C	711	ASN
1	C	829	LYS
1	C	878	SER
1	E	658	ASP
1	E	659	ARG
1	E	681	ILE
1	E	745	GLU
1	E	775	SER
1	H	658	ASP
1	H	696	GLN
1	H	729	ARG
1	H	739	HIS
1	H	771	ARG
1	H	775	SER
1	F	652	ASP
1	F	658	ASP
1	F	659	ARG
1	F	739	HIS
1	F	764	SER
1	F	894	SER
1	D	696	GLN
1	D	714	SER
1	D	736	ARG
1	D	757	ASN
1	D	771	ARG
1	D	882	HIS
1	G	652	ASP
1	G	658	ASP
1	G	659	ARG
1	G	664	GLU
1	G	680	LYS
1	G	742	ARG

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Mol	Chain	Res	Type
1	G	767	ARG
1	G	775	SER
1	G	887	ARG
1	G	888	LEU
1	G	889	LEU
1	G	894	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	789	HIS
1	B	656	GLN
1	D	656	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)

20 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	$\#\|Z\|>2$
3	GOL	A	1005	-	5,5,5	0.91	0	5,5,5	0.95	0
3	GOL	D	1002	-	5,5,5	0.92	0	5,5,5	0.99	0
3	GOL	B	1006	-	5,5,5	0.93	0	5,5,5	0.91	0
2	SAH	A	1001	-	24,28,28	1.20	3 (12%)	25,40,40	1.60	4 (16%)
3	GOL	A	1004	-	5,5,5	0.93	0	5,5,5	0.95	0
3	GOL	C	1003	-	5,5,5	0.90	0	5,5,5	1.02	0
2	SAH	D	1001	-	24,28,28	1.20	3 (12%)	25,40,40	1.61	4 (16%)
3	GOL	D	1004	-	5,5,5	0.91	0	5,5,5	0.98	0
3	GOL	D	1003	-	5,5,5	0.88	0	5,5,5	0.96	0
3	GOL	B	1002	-	5,5,5	0.93	0	5,5,5	0.95	0
3	GOL	B	1003	-	5,5,5	0.90	0	5,5,5	1.00	0
3	GOL	D	1005	-	5,5,5	0.90	0	5,5,5	1.03	0
2	SAH	C	1001	-	24,28,28	1.19	3 (12%)	25,40,40	1.60	4 (16%)
3	GOL	A	1002	-	5,5,5	0.90	0	5,5,5	0.96	0
3	GOL	C	1002	-	5,5,5	0.92	0	5,5,5	1.00	0
2	SAH	B	1001	-	24,28,28	1.20	3 (12%)	25,40,40	1.61	4 (16%)
3	GOL	A	1003	-	5,5,5	0.95	0	5,5,5	0.88	0
3	GOL	A	1006	-	5,5,5	0.96	0	5,5,5	0.97	0
3	GOL	B	1005	-	5,5,5	0.92	0	5,5,5	0.97	0
3	GOL	B	1004	-	5,5,5	0.93	0	5,5,5	0.95	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
3	GOL	A	1005	-	-	0/4/4/4	-
3	GOL	D	1002	-	-	4/4/4/4	-
3	GOL	B	1006	-	-	0/4/4/4	-
2	SAH	A	1001	-	-	2/11/31/31	0/3/3/3
3	GOL	A	1004	-	-	2/4/4/4	-
3	GOL	C	1003	-	-	0/4/4/4	-
2	SAH	D	1001	-	-	3/11/31/31	0/3/3/3
3	GOL	D	1004	-	-	2/4/4/4	-
3	GOL	D	1003	-	-	2/4/4/4	-
3	GOL	B	1002	-	-	0/4/4/4	-
3	GOL	B	1003	-	-	3/4/4/4	-
3	GOL	D	1005	-	-	2/4/4/4	-
2	SAH	C	1001	-	-	2/11/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1002	-	-	2/4/4/4	-
3	GOL	C	1002	-	-	0/4/4/4	-
2	SAH	B	1001	-	-	2/11/31/31	0/3/3/3
3	GOL	A	1003	-	-	3/4/4/4	-
3	GOL	A	1006	-	-	2/4/4/4	-
3	GOL	B	1005	-	-	2/4/4/4	-
3	GOL	B	1004	-	-	0/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	SAH	C2-N3	4.00	1.38	1.32
2	B	1001	SAH	C2-N3	3.99	1.38	1.32
2	C	1001	SAH	C2-N3	3.97	1.38	1.32
2	D	1001	SAH	C2-N3	3.96	1.38	1.32
2	A	1001	SAH	C2-N1	2.41	1.38	1.33
2	C	1001	SAH	C2-N1	2.40	1.38	1.33
2	D	1001	SAH	C2-N1	2.39	1.38	1.33
2	B	1001	SAH	C2-N1	2.36	1.38	1.33
2	D	1001	SAH	OXT-C	-2.13	1.23	1.30
2	A	1001	SAH	OXT-C	-2.12	1.23	1.30
2	B	1001	SAH	OXT-C	-2.12	1.23	1.30
2	C	1001	SAH	OXT-C	-2.06	1.23	1.30

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1001	SAH	N3-C2-N1	-5.56	119.99	128.68
2	B	1001	SAH	N3-C2-N1	-5.55	120.00	128.68
2	A	1001	SAH	N3-C2-N1	-5.55	120.01	128.68
2	C	1001	SAH	N3-C2-N1	-5.48	120.11	128.68
2	B	1001	SAH	OXT-C-O	-2.88	117.54	124.09
2	C	1001	SAH	C5'-SD-CG	-2.86	93.68	102.27
2	D	1001	SAH	OXT-C-O	-2.83	117.67	124.09
2	C	1001	SAH	OXT-C-O	-2.80	117.73	124.09
2	A	1001	SAH	OXT-C-O	-2.80	117.73	124.09
2	A	1001	SAH	C5'-SD-CG	-2.80	93.87	102.27
2	D	1001	SAH	C5'-SD-CG	-2.77	93.96	102.27
2	B	1001	SAH	C5'-SD-CG	-2.69	94.19	102.27
2	D	1001	SAH	OXT-C-CA	2.33	121.34	113.38
2	B	1001	SAH	OXT-C-CA	2.33	121.33	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	SAH	OXT-C-CA	2.29	121.20	113.38
2	C	1001	SAH	OXT-C-CA	2.28	121.17	113.38

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	SAH	N-CA-CB-CG
2	B	1001	SAH	N-CA-CB-CG
2	C	1001	SAH	N-CA-CB-CG
2	D	1001	SAH	N-CA-CB-CG
3	A	1003	GOL	O1-C1-C2-O2
3	A	1003	GOL	O1-C1-C2-C3
3	A	1004	GOL	C1-C2-C3-O3
3	A	1006	GOL	C1-C2-C3-O3
3	B	1003	GOL	O1-C1-C2-O2
3	B	1003	GOL	O1-C1-C2-C3
3	B	1005	GOL	O1-C1-C2-O2
3	B	1005	GOL	O1-C1-C2-C3
3	D	1002	GOL	O1-C1-C2-C3
3	D	1004	GOL	O1-C1-C2-C3
3	D	1005	GOL	O1-C1-C2-C3
3	D	1004	GOL	O1-C1-C2-O2
3	A	1002	GOL	O1-C1-C2-C3
3	D	1003	GOL	C1-C2-C3-O3
3	A	1006	GOL	O2-C2-C3-O3
3	A	1004	GOL	O2-C2-C3-O3
3	D	1002	GOL	O1-C1-C2-O2
3	D	1002	GOL	O2-C2-C3-O3
3	D	1005	GOL	O1-C1-C2-O2
2	A	1001	SAH	CB-CG-SD-C5'
2	B	1001	SAH	CB-CG-SD-C5'
2	D	1001	SAH	CB-CG-SD-C5'
3	D	1003	GOL	O2-C2-C3-O3
2	C	1001	SAH	CB-CG-SD-C5'
2	D	1001	SAH	C-CA-CB-CG
3	A	1003	GOL	C1-C2-C3-O3
3	A	1002	GOL	O1-C1-C2-O2
3	B	1003	GOL	O2-C2-C3-O3
3	D	1002	GOL	C1-C2-C3-O3

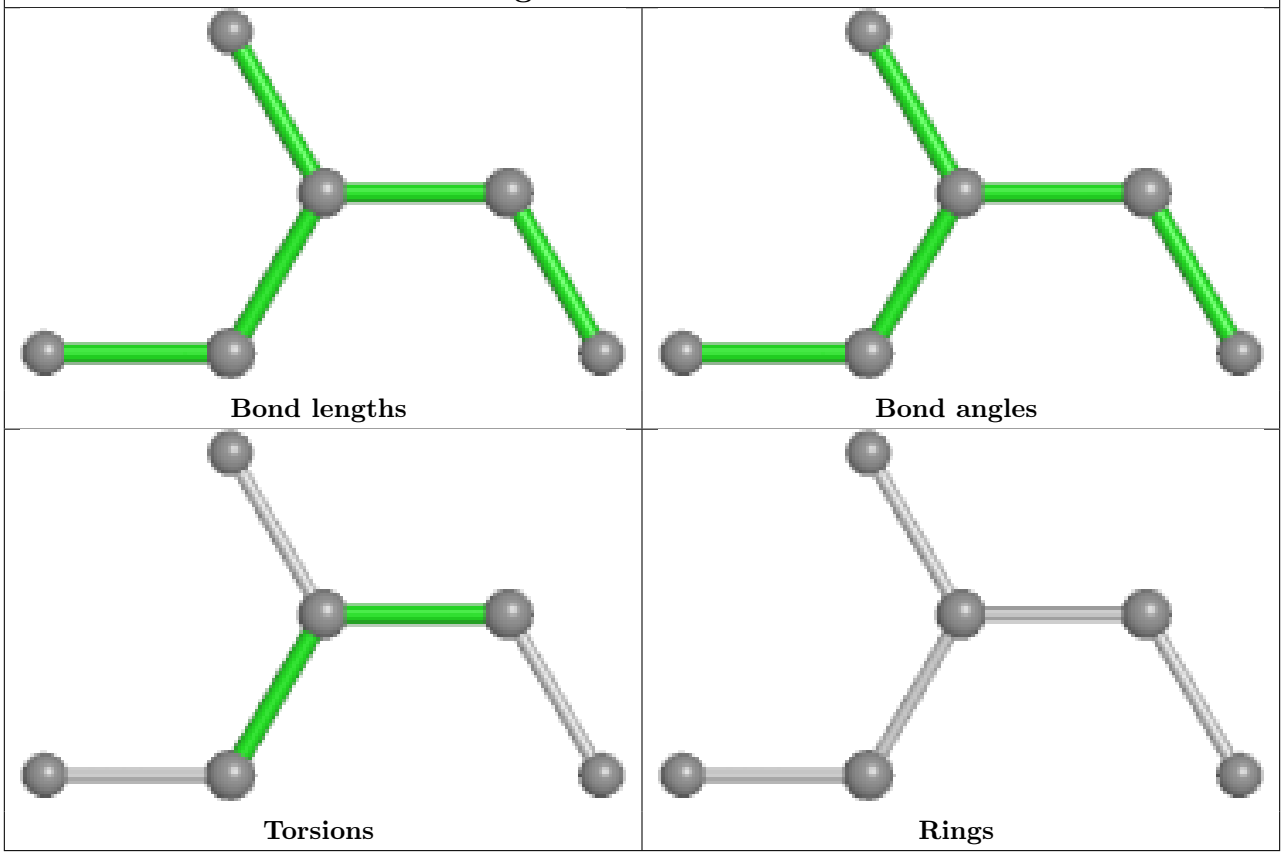
There are no ring outliers.

3 monomers are involved in 5 short contacts:

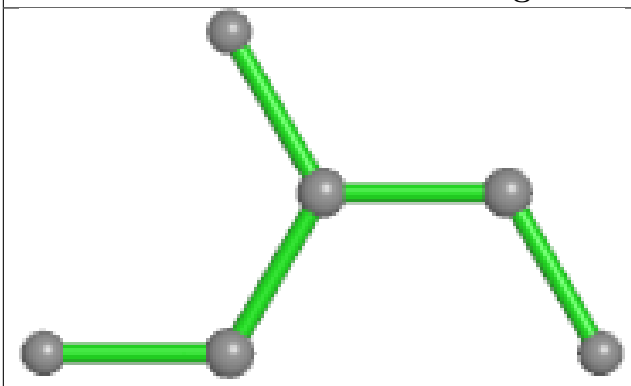
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1006	GOL	1	0
3	A	1004	GOL	2	0
3	D	1005	GOL	2	0

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.

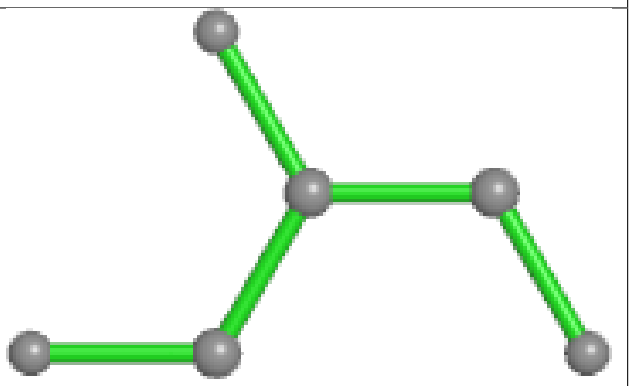
Ligand GOL A 1005



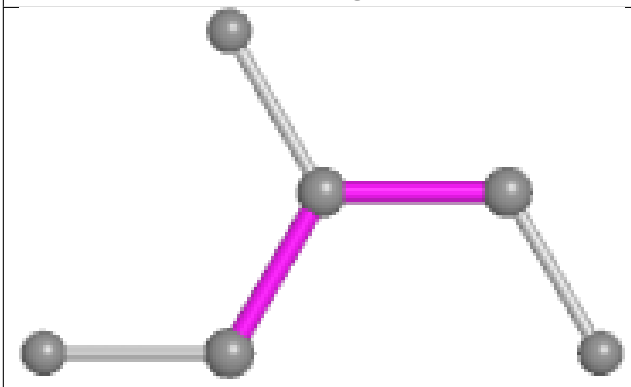
Ligand GOL D 1002



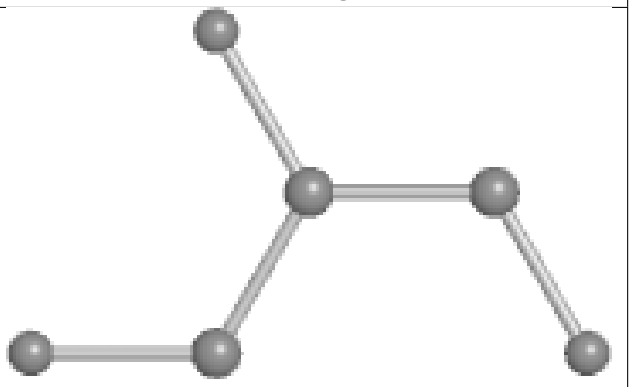
Bond lengths



Bond angles

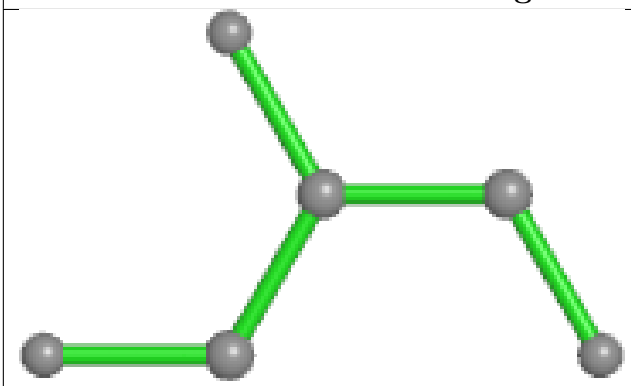


Torsions

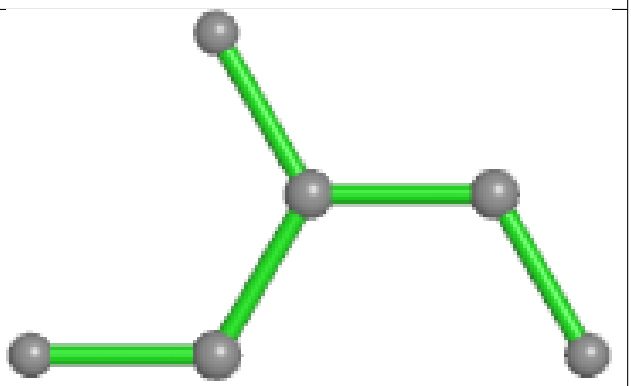


Rings

Ligand GOL B 1006



Bond lengths



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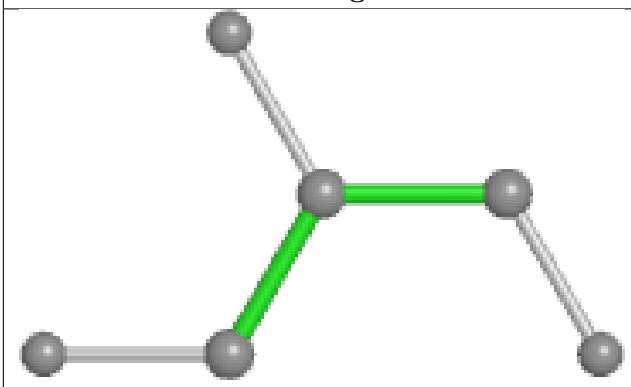
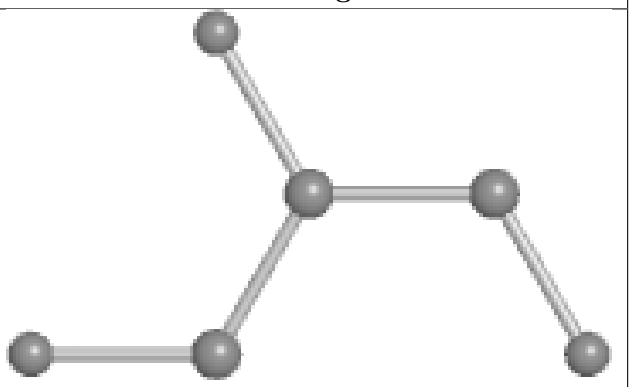
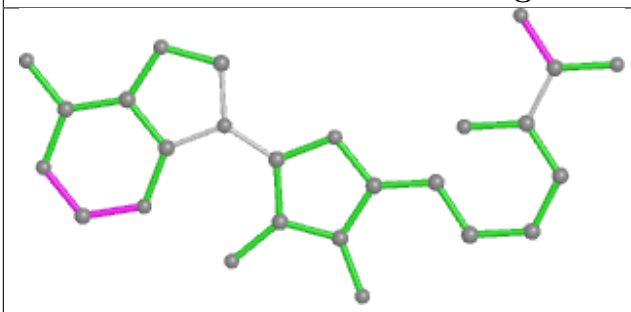


Torsions



Rings

Ligand SAH A 1001



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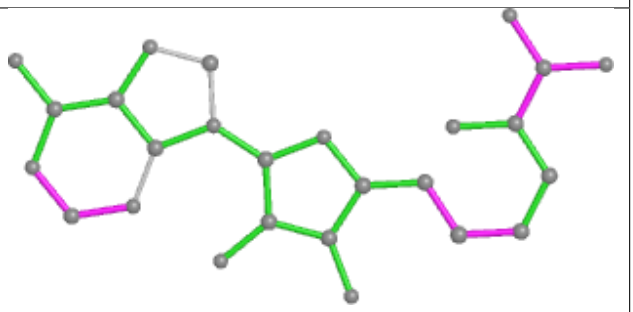
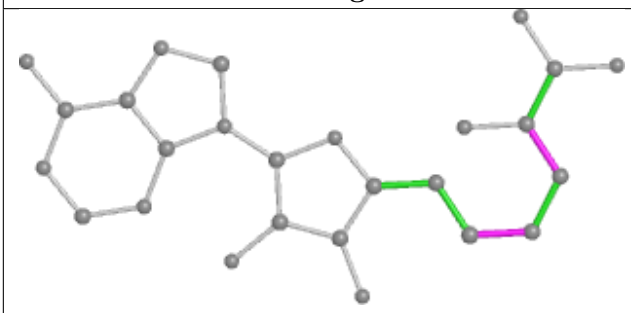
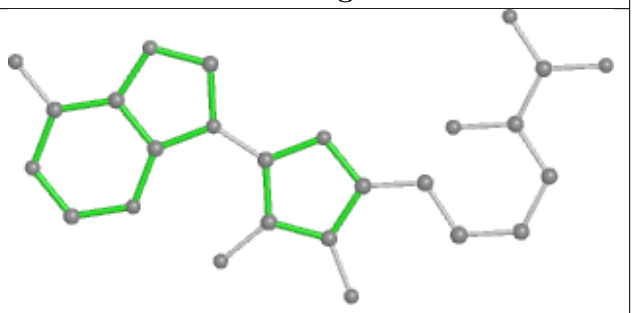


Bond angles

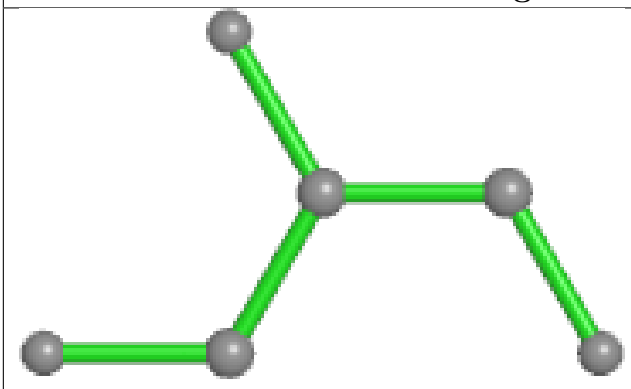


Torsions



Rings

Ligand GOL A 1004



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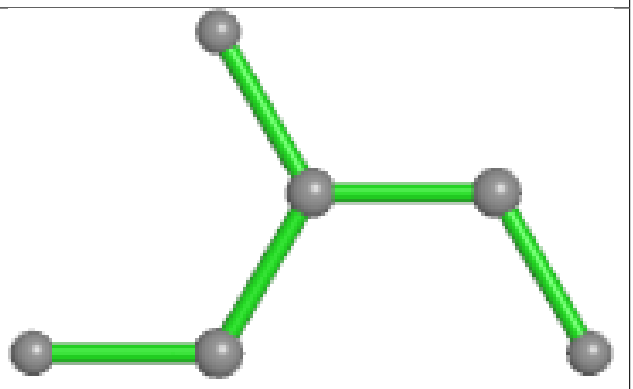

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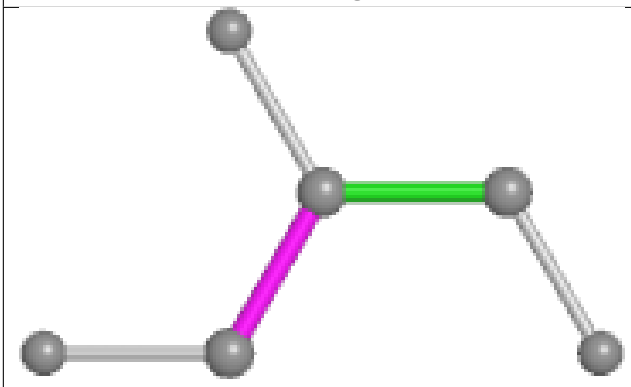

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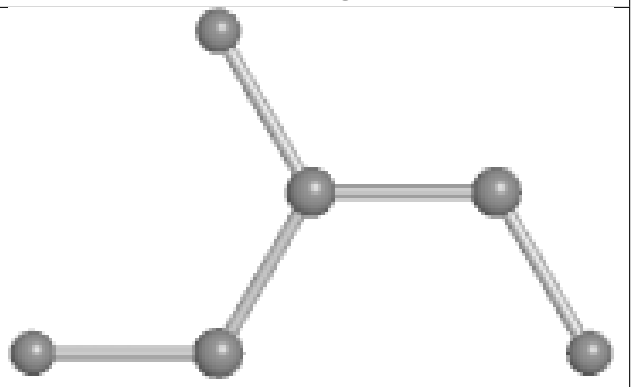
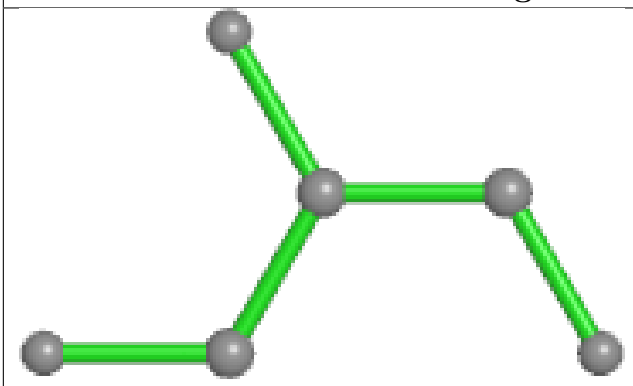


Rings

Ligand GOL C 1003



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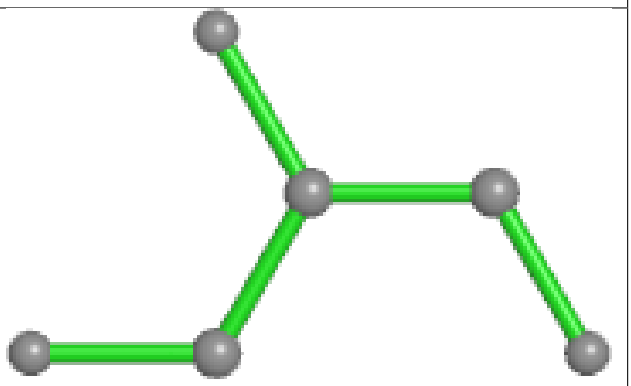

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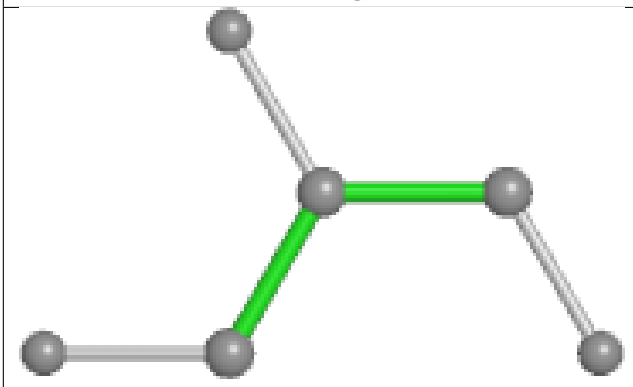

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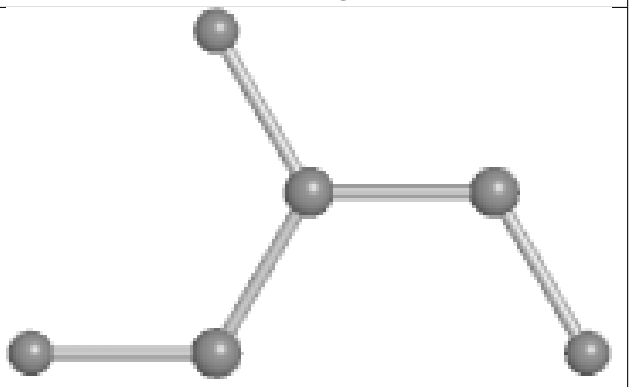
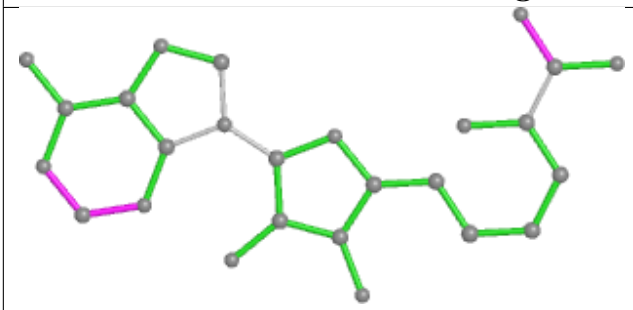


Rings

Ligand SAH D 1001



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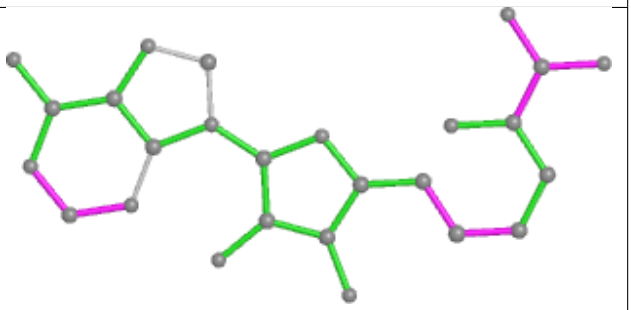

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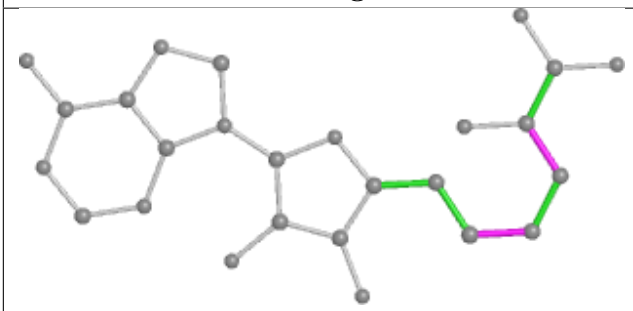

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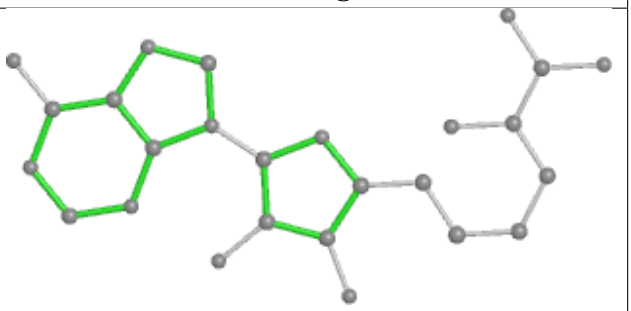
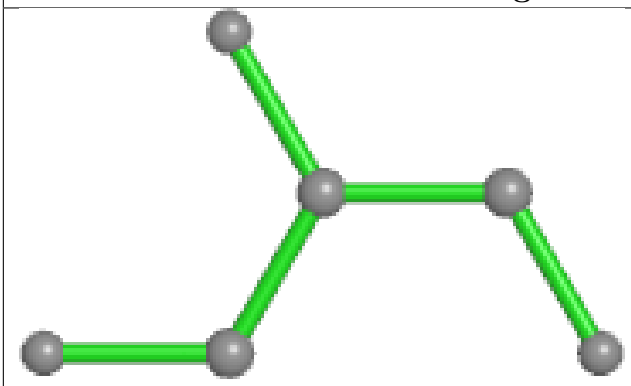


Rings

Ligand GOL D 1004



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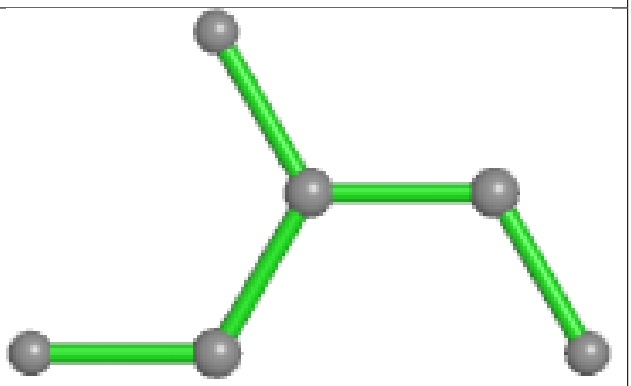

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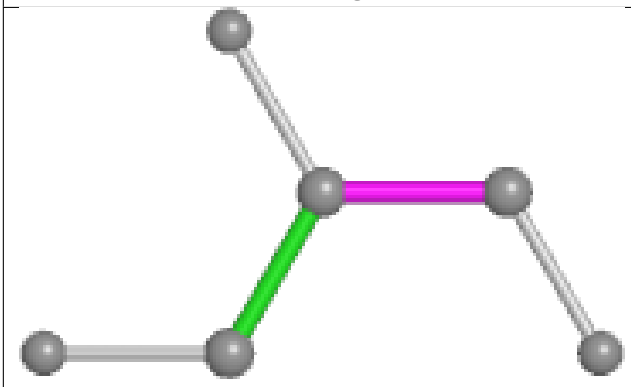

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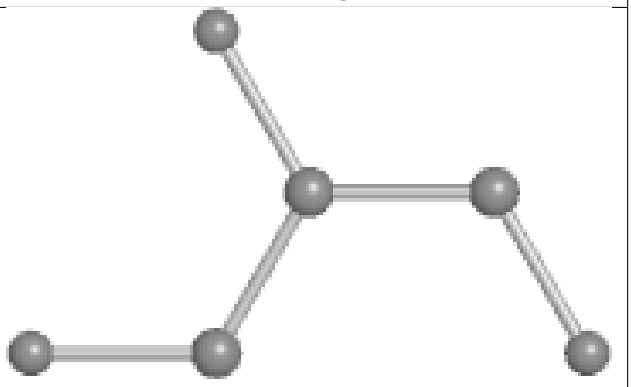
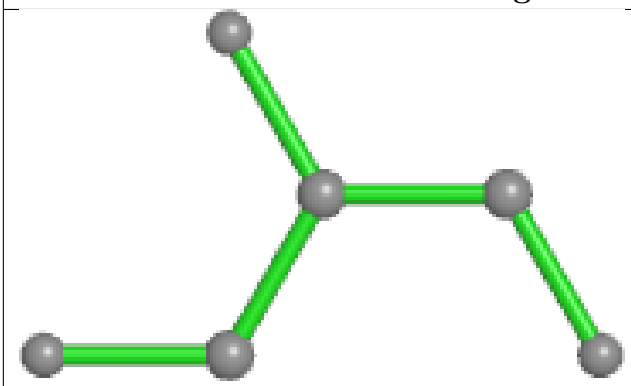


Rings

Ligand GOL D 1003



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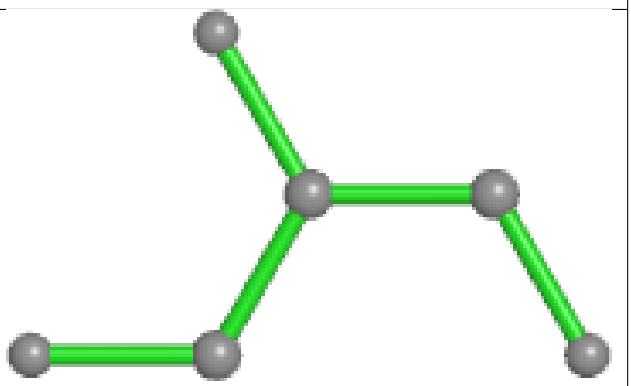
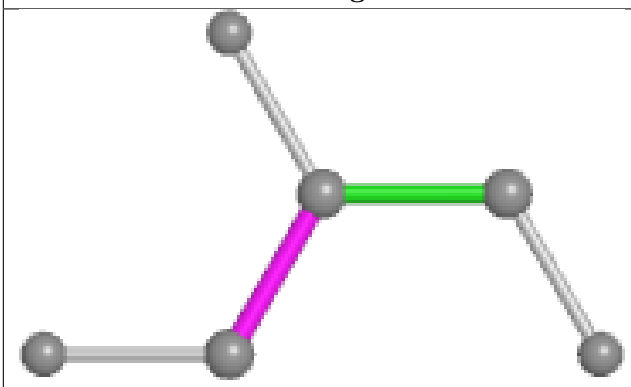


Bond angles



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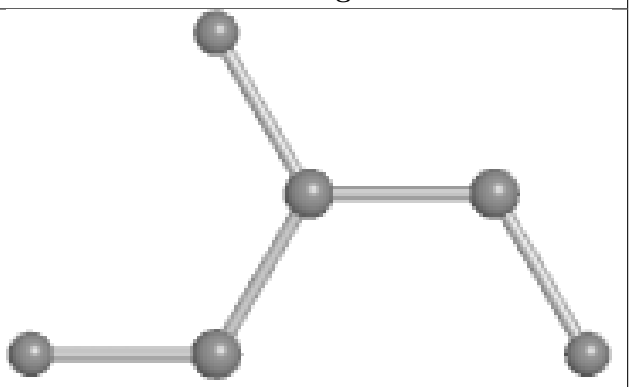
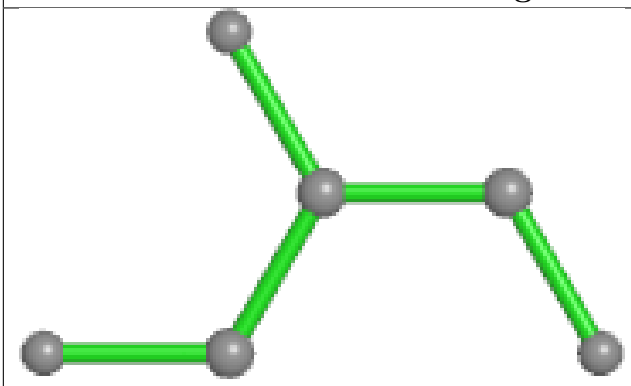
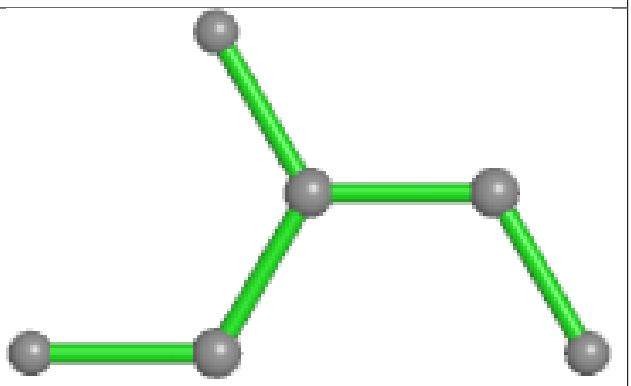


Rings

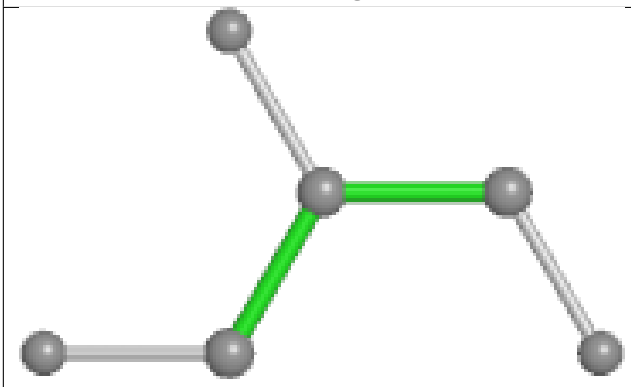
Ligand GOL B 1002



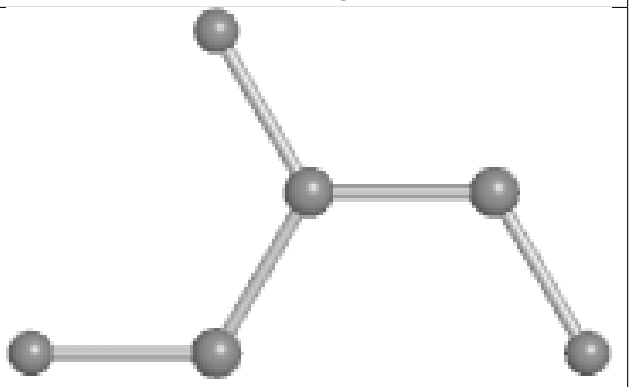
Bond lengths



Bond angles

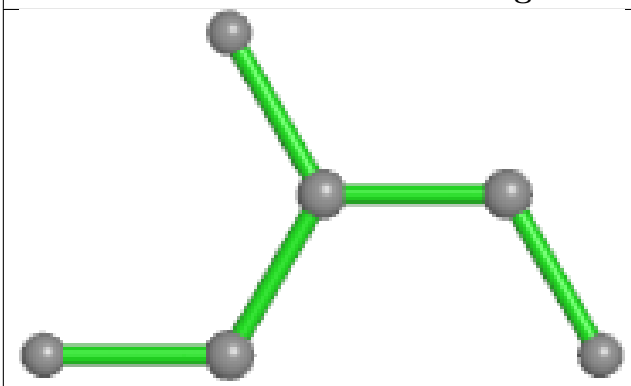


Torsions



Rings

Ligand GOL B 1003



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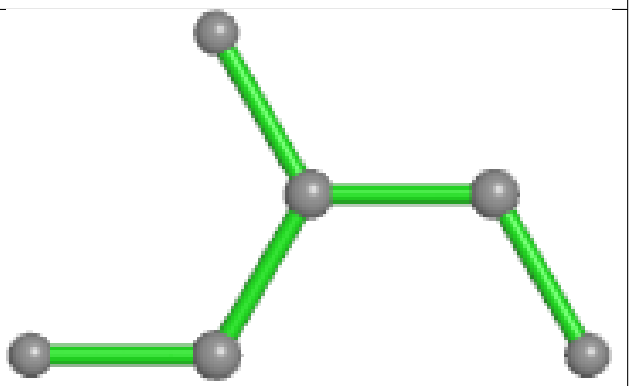

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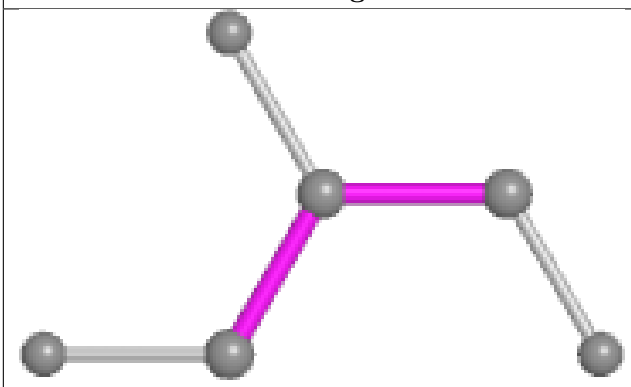

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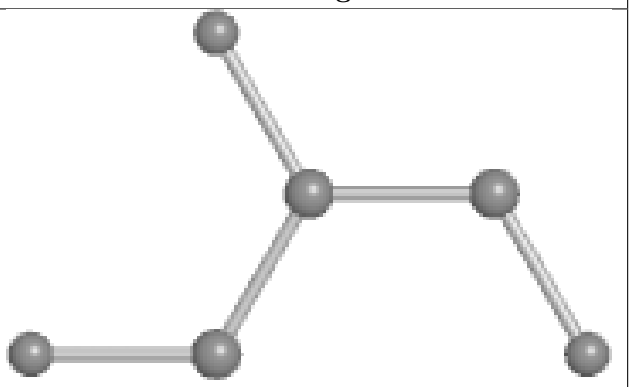
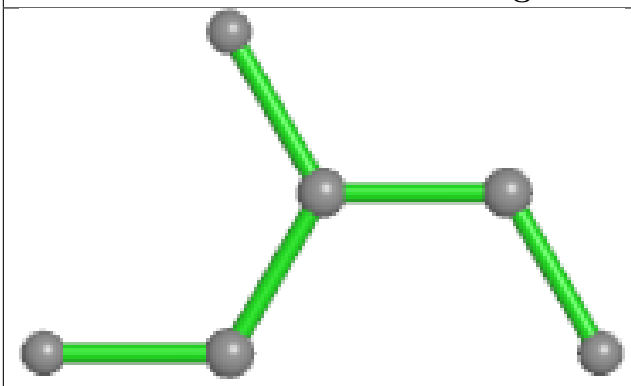


Rings

Ligand GOL D 1005



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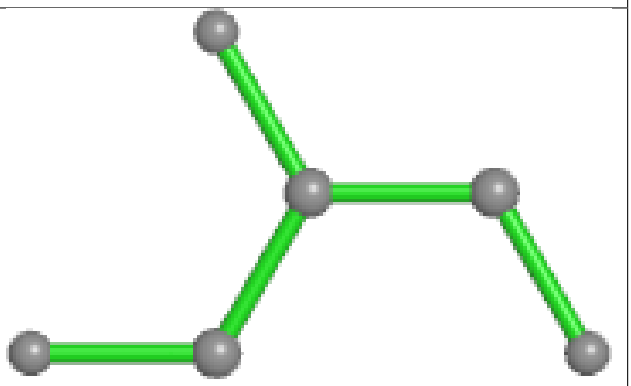

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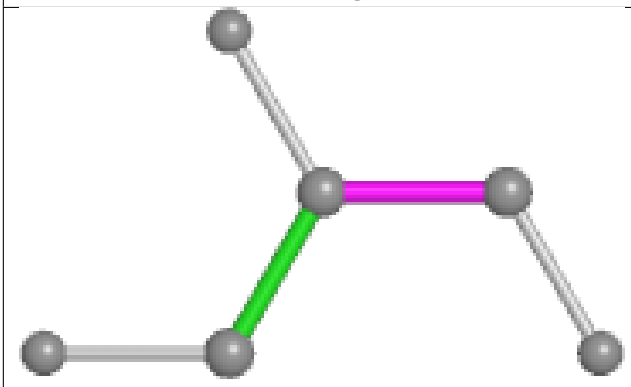

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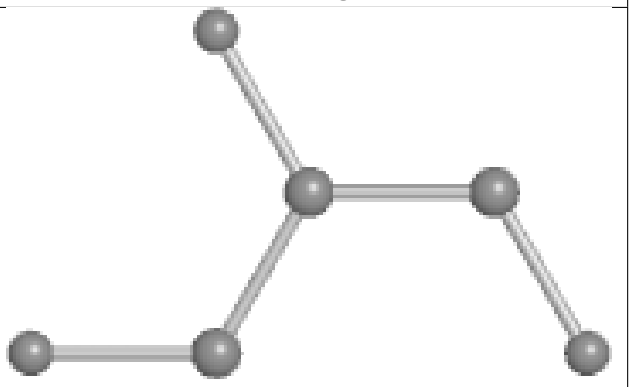
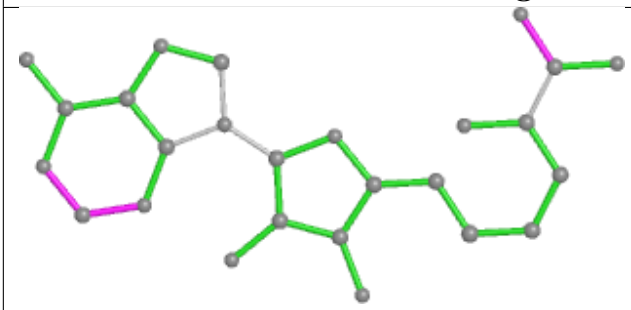
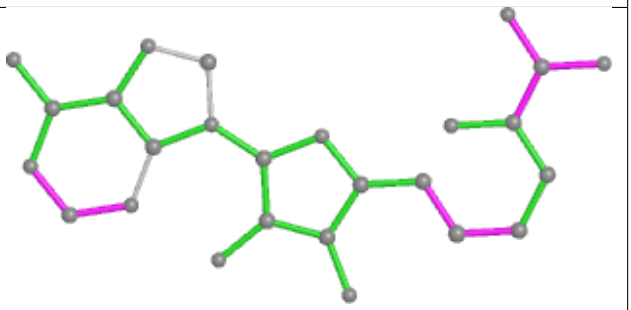


Rings

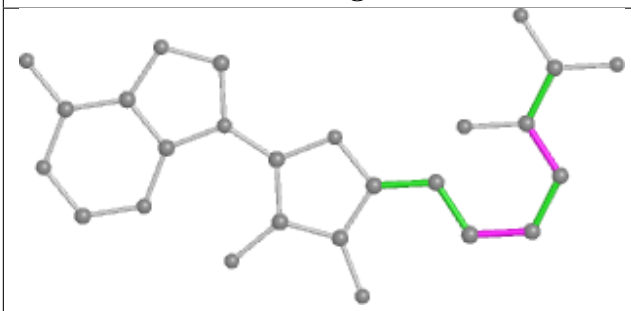
Ligand SAH C 1001



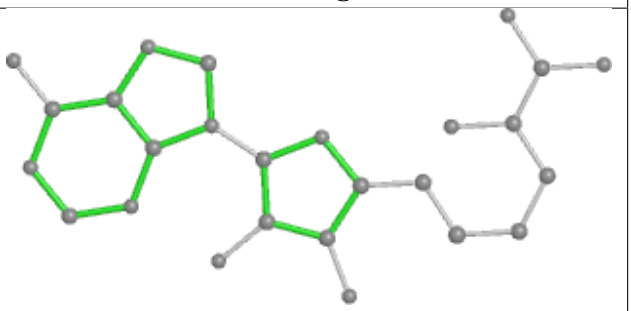
Bond lengths



Bond angles

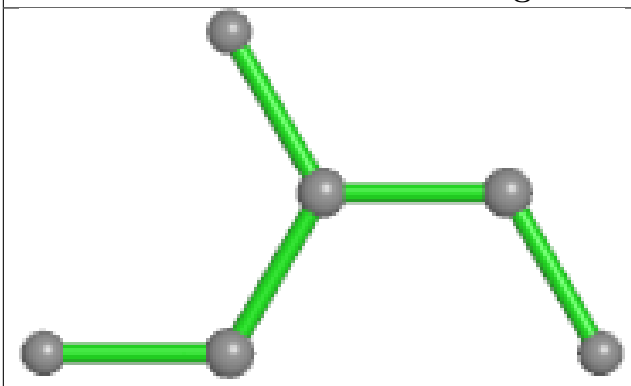


Torsions

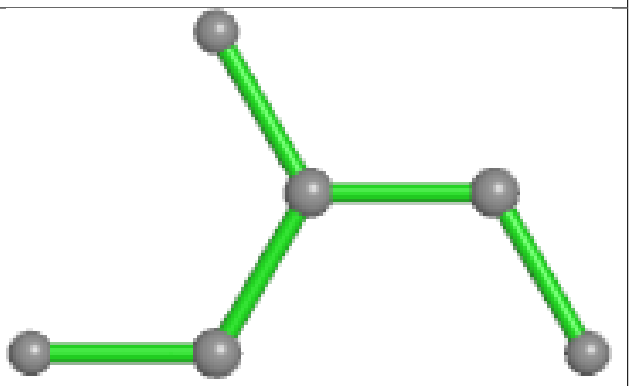


Rings

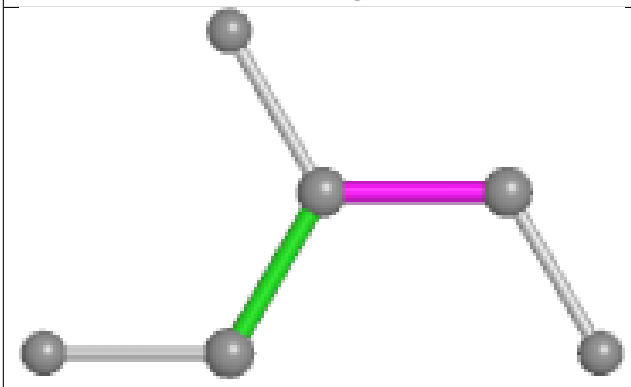
Ligand GOL A 1002



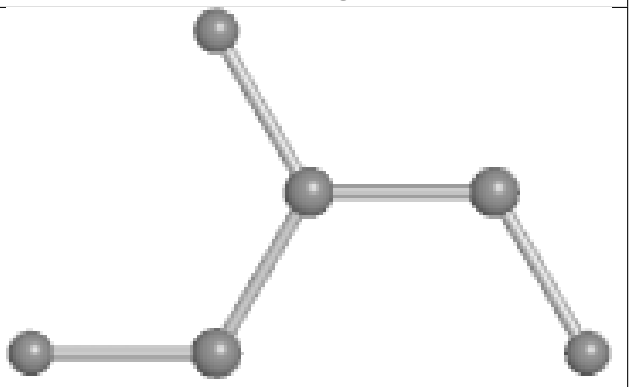
Bond lengths



Bond angles

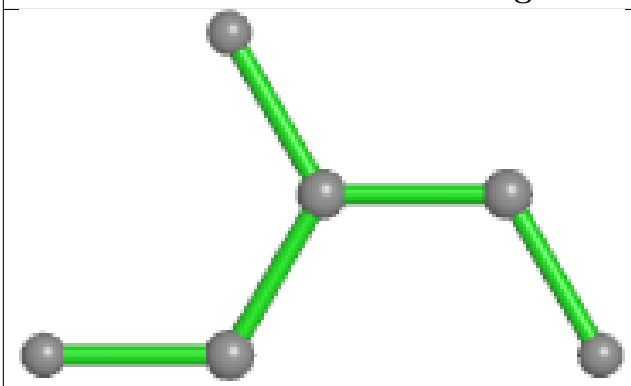


Torsions

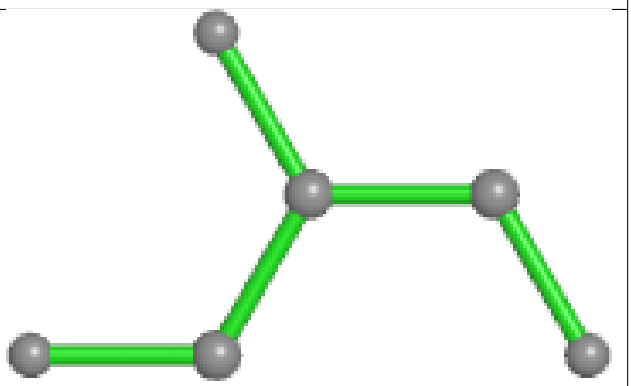


Rings

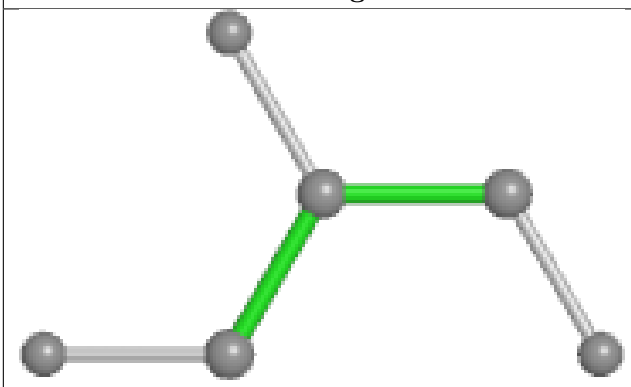
Ligand GOL C 1002



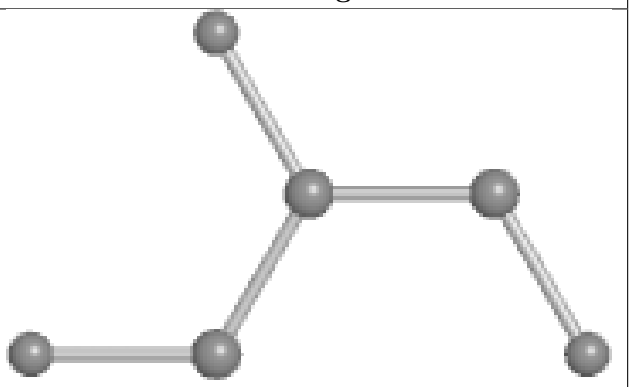
Bond lengths



Bond angles

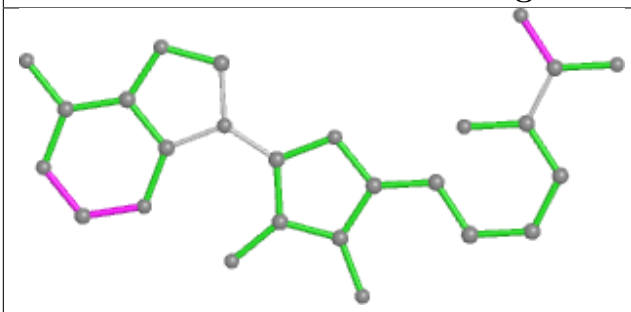


Torsions

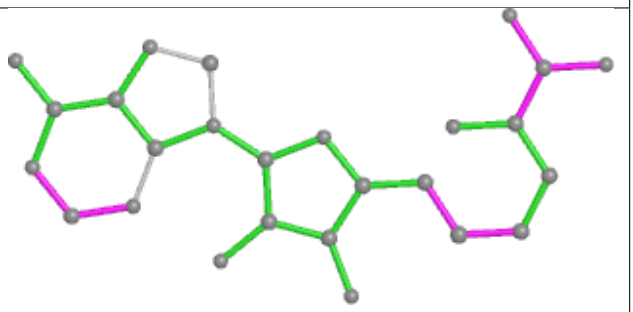


Rings

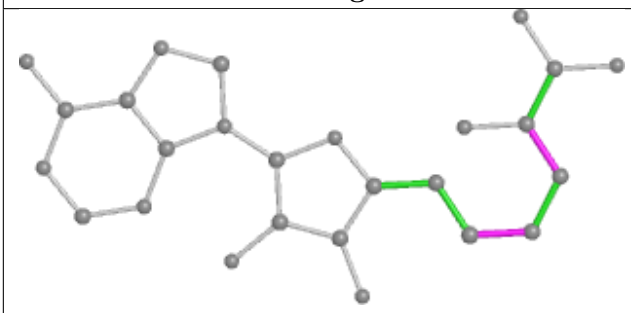
Ligand SAH B 1001



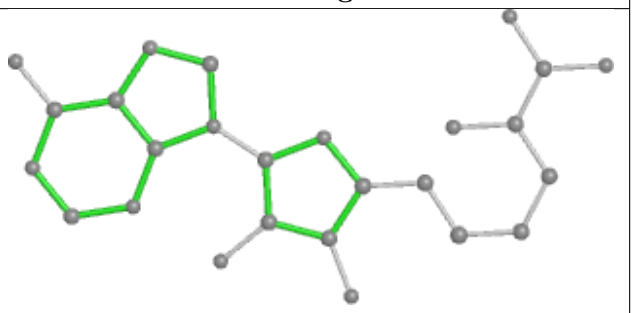
Bond lengths



Bond angles

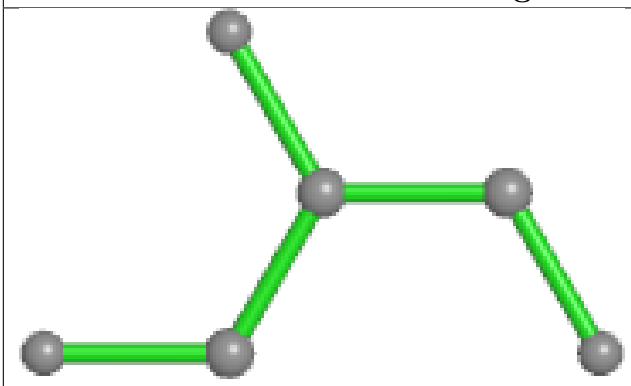


Torsions

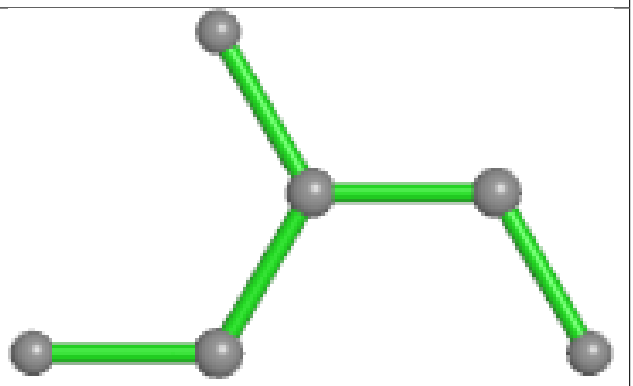


Rings

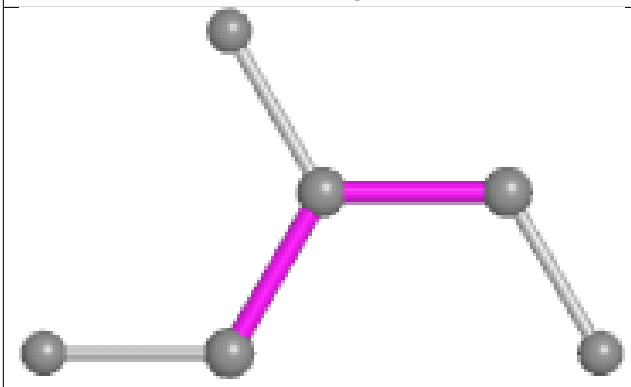
Ligand GOL A 1003



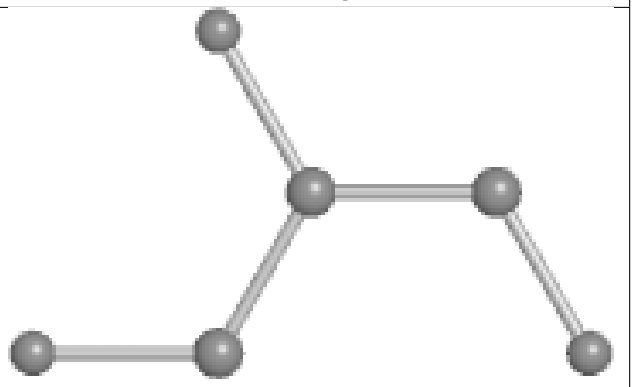
Bond lengths



Bond angles

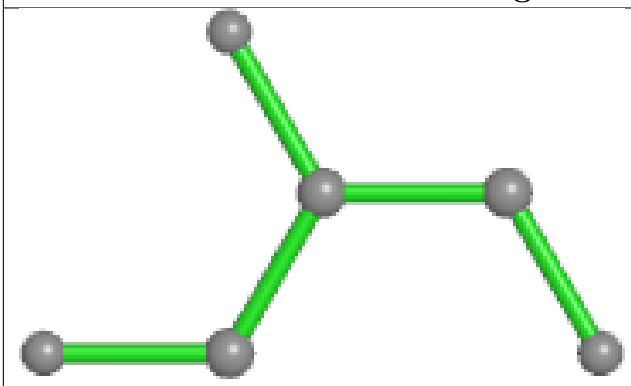


Torsions

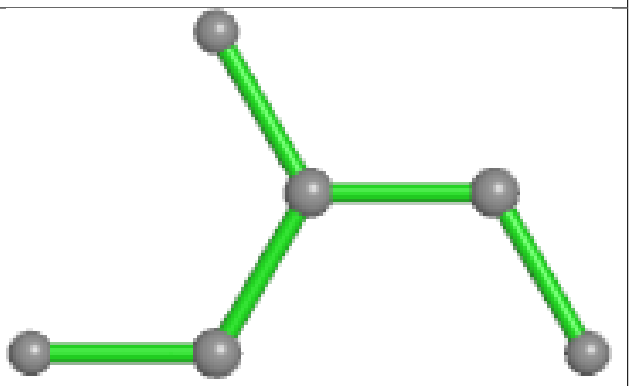


Rings

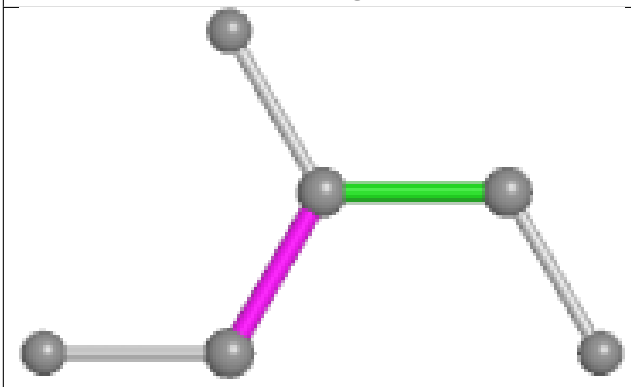
Ligand GOL A 1006



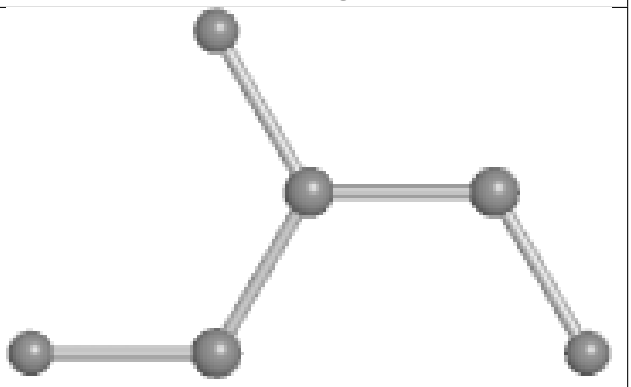
Bond lengths



Bond angles

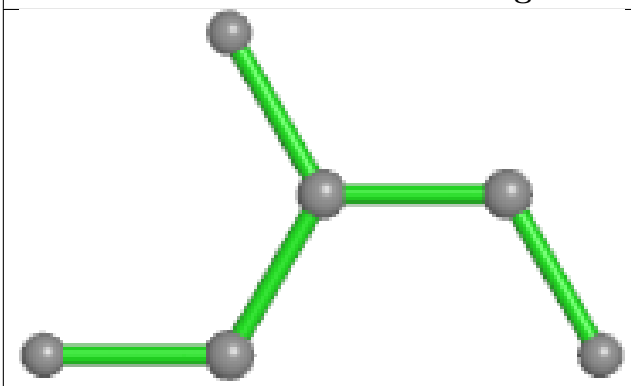


Torsions

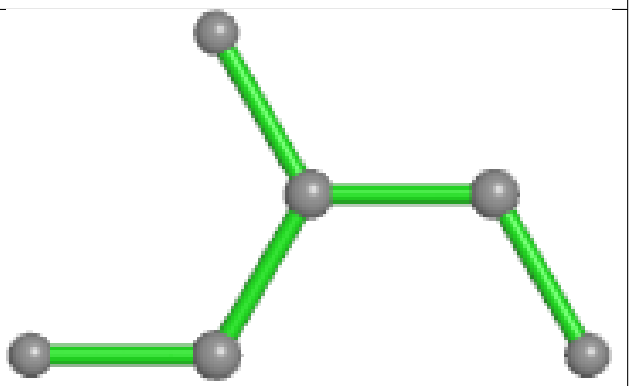


Rings

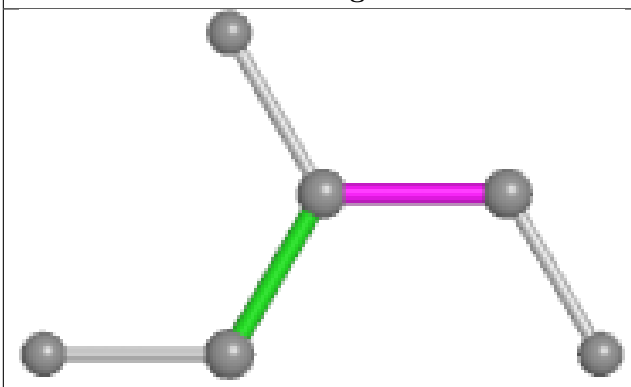
Ligand GOL B 1005



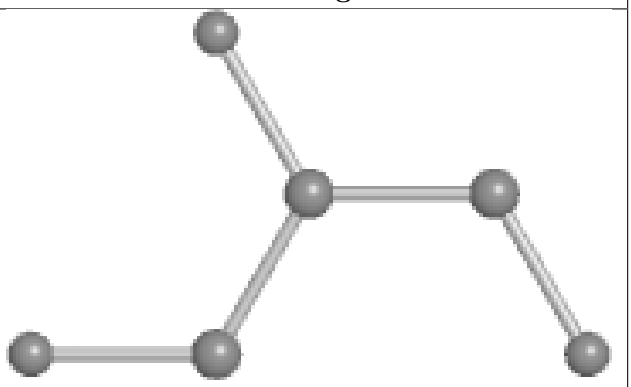
Bond lengths



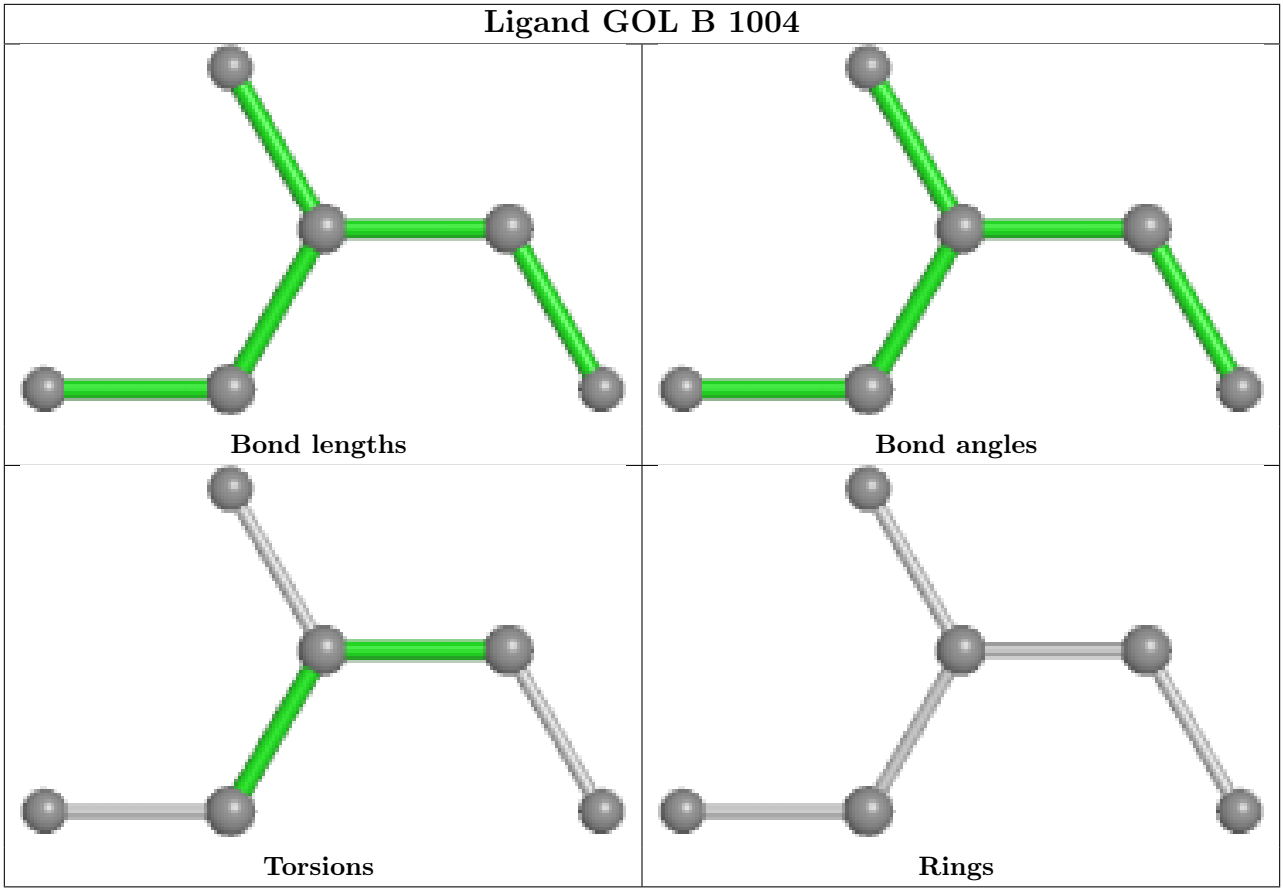
Bond angles



Torsions



Rings



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	273/287 (95%)	-0.31	0 100 100	35, 48, 82, 108	0
1	B	275/287 (95%)	-0.27	0 100 100	36, 47, 83, 125	0
1	C	275/287 (95%)	-0.27	0 100 100	36, 47, 86, 122	0
1	D	275/287 (95%)	-0.26	0 100 100	36, 48, 82, 114	0
1	E	158/287 (55%)	-0.11	2 (1%) 77 75	41, 63, 106, 133	0
1	F	161/287 (56%)	-0.09	4 (2%) 57 53	45, 65, 102, 130	0
1	G	173/287 (60%)	0.00	6 (3%) 44 40	45, 67, 138, 167	0
1	H	171/287 (59%)	-0.06	3 (1%) 68 65	41, 63, 129, 166	0
All	All	1761/2296 (76%)	-0.20	15 (0%) 84 83	35, 53, 101, 167	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	628	ALA	6.3
1	H	892	SER	5.2
1	G	629	GLU	5.0
1	F	791	ALA	4.6
1	F	760	ALA	4.4
1	H	891	ARG	3.8
1	G	890	GLY	3.7
1	G	759	VAL	3.0
1	G	791	ALA	3.0
1	F	759	VAL	2.9
1	E	791	ALA	2.7
1	F	628	ALA	2.7
1	G	760	ALA	2.7
1	H	628	ALA	2.1
1	G	891	ARG	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)

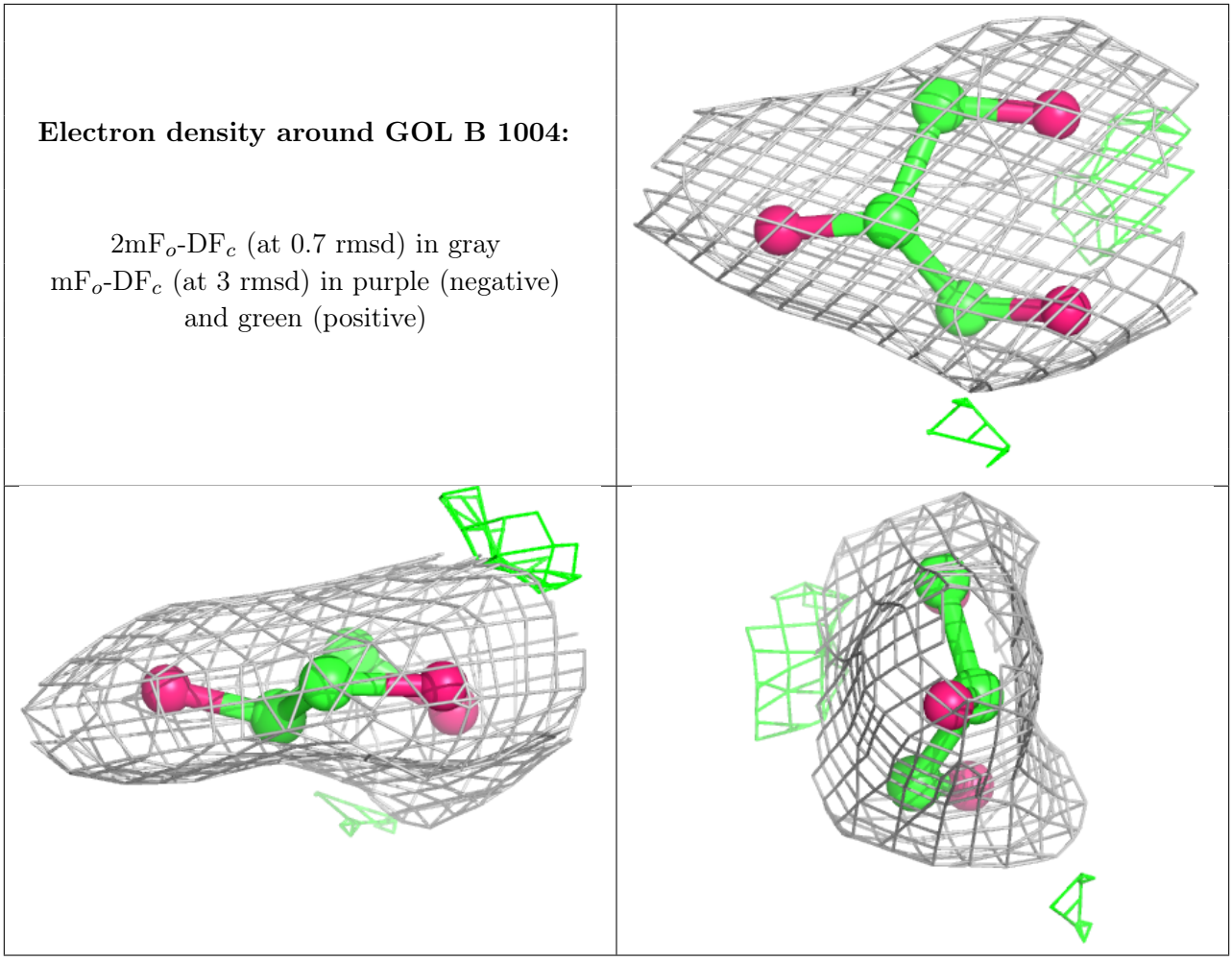
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	GOL	B	1004	6/6	0.72	0.21	91,94,98,109	0
3	GOL	C	1002	6/6	0.75	0.15	72,85,96,104	0
3	GOL	A	1004	6/6	0.77	0.16	80,86,90,97	0
3	GOL	B	1002	6/6	0.77	0.16	56,79,90,109	0
3	GOL	D	1003	6/6	0.80	0.18	43,82,95,99	0
3	GOL	C	1003	6/6	0.81	0.20	73,88,102,105	0
3	GOL	A	1002	6/6	0.83	0.20	60,75,100,102	0
3	GOL	A	1003	6/6	0.83	0.17	42,63,87,90	0
3	GOL	D	1005	6/6	0.83	0.17	78,88,105,120	0
3	GOL	A	1005	6/6	0.84	0.18	56,93,97,105	0
3	GOL	B	1005	6/6	0.84	0.15	60,79,89,91	0
3	GOL	D	1002	6/6	0.86	0.16	68,78,98,111	0
3	GOL	A	1006	6/6	0.88	0.18	46,72,81,97	0
3	GOL	D	1004	6/6	0.89	0.14	44,80,88,93	0
3	GOL	B	1006	6/6	0.91	0.20	69,93,99,100	0
3	GOL	B	1003	6/6	0.94	0.16	64,71,79,89	0
2	SAH	C	1001	26/26	0.97	0.15	40,48,58,73	0
2	SAH	D	1001	26/26	0.97	0.15	42,50,61,63	0
2	SAH	A	1001	26/26	0.97	0.14	42,51,61,65	0
2	SAH	B	1001	26/26	0.98	0.15	40,48,57,61	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.

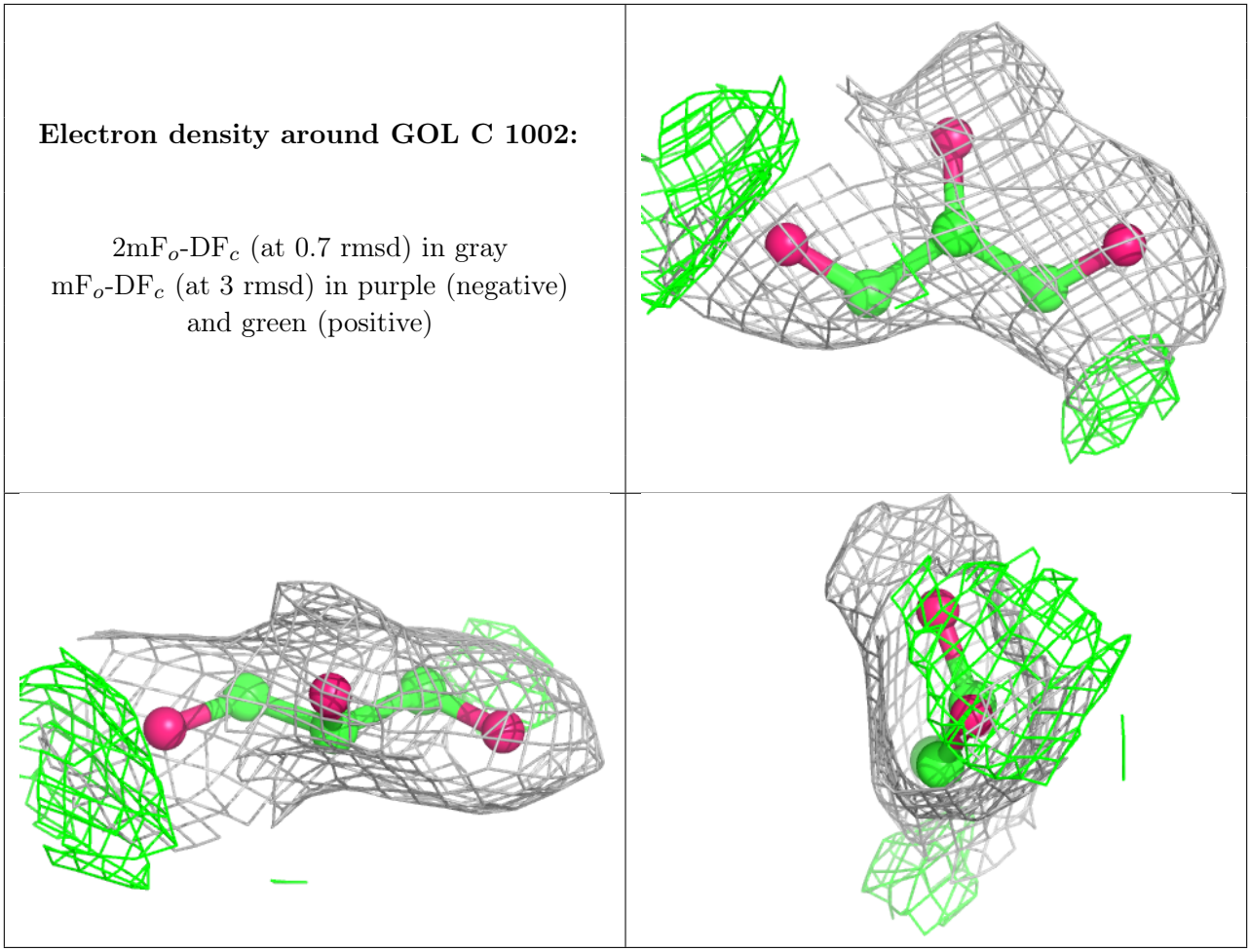
Electron density around GOL B 1004:

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



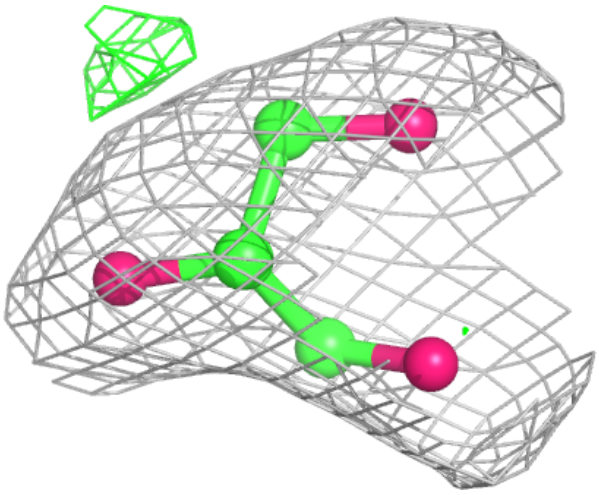
Electron density around GOL C 1002:

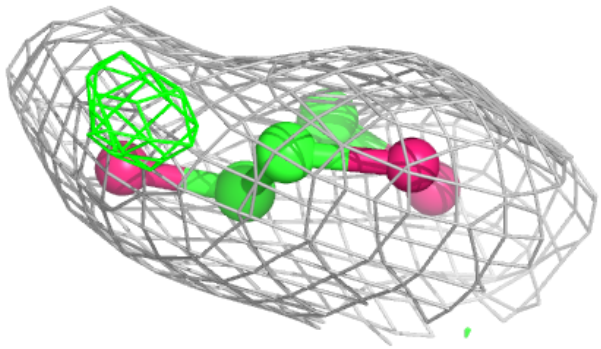
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

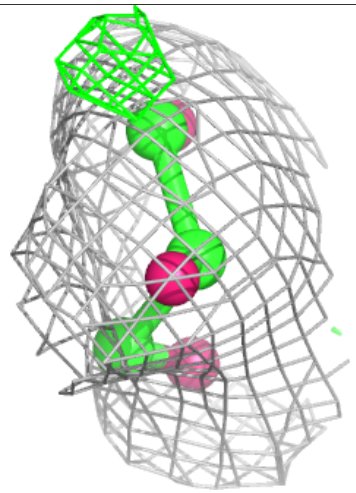


Electron density around GOL A 1004:

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

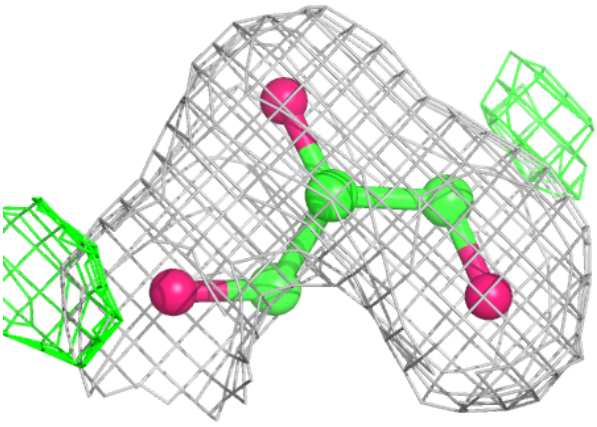


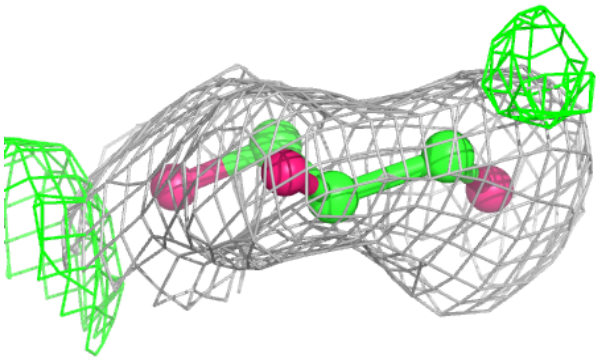


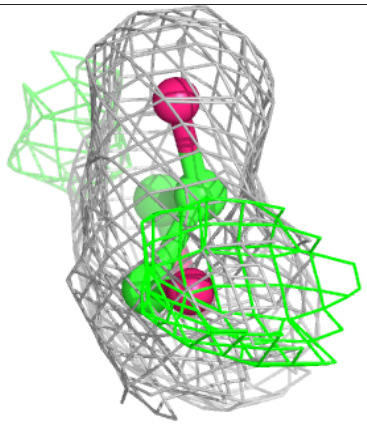


Electron density around GOL B 1002:

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

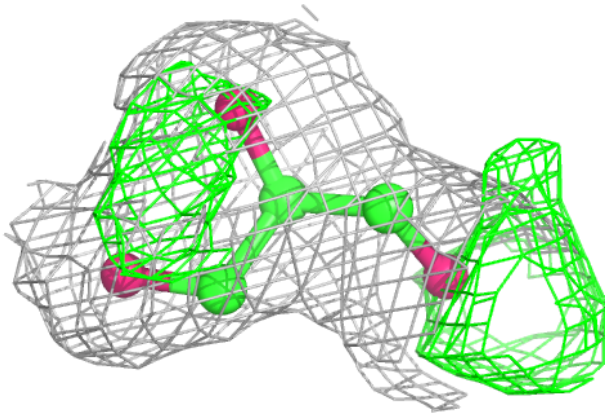


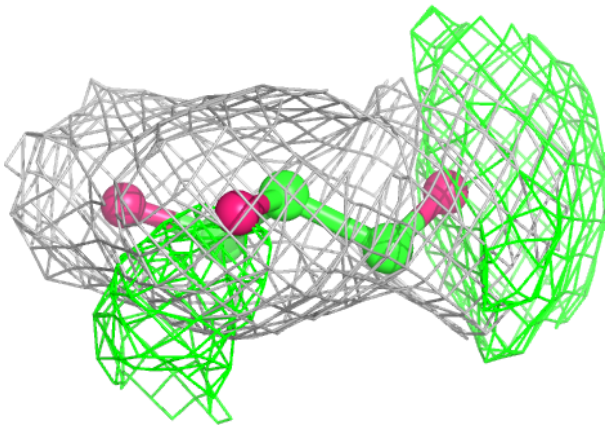


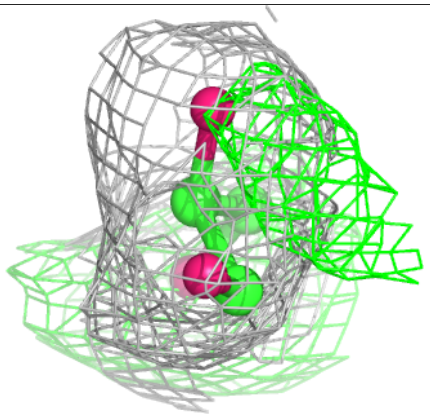


Electron density around GOL D 1003:

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

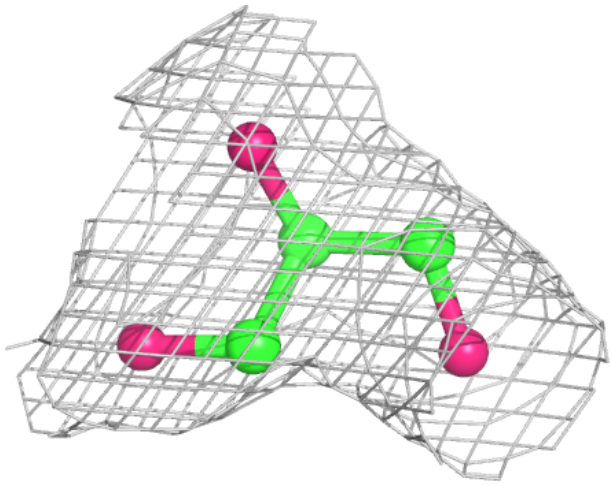


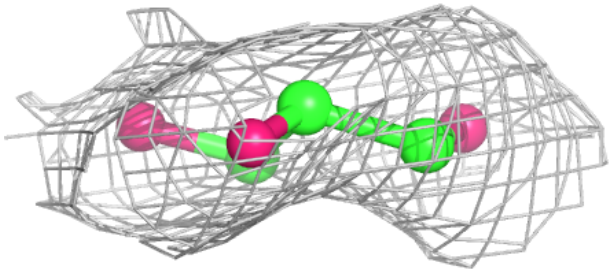


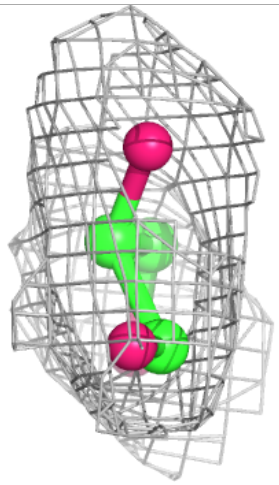


Electron density around GOL C 1003:

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

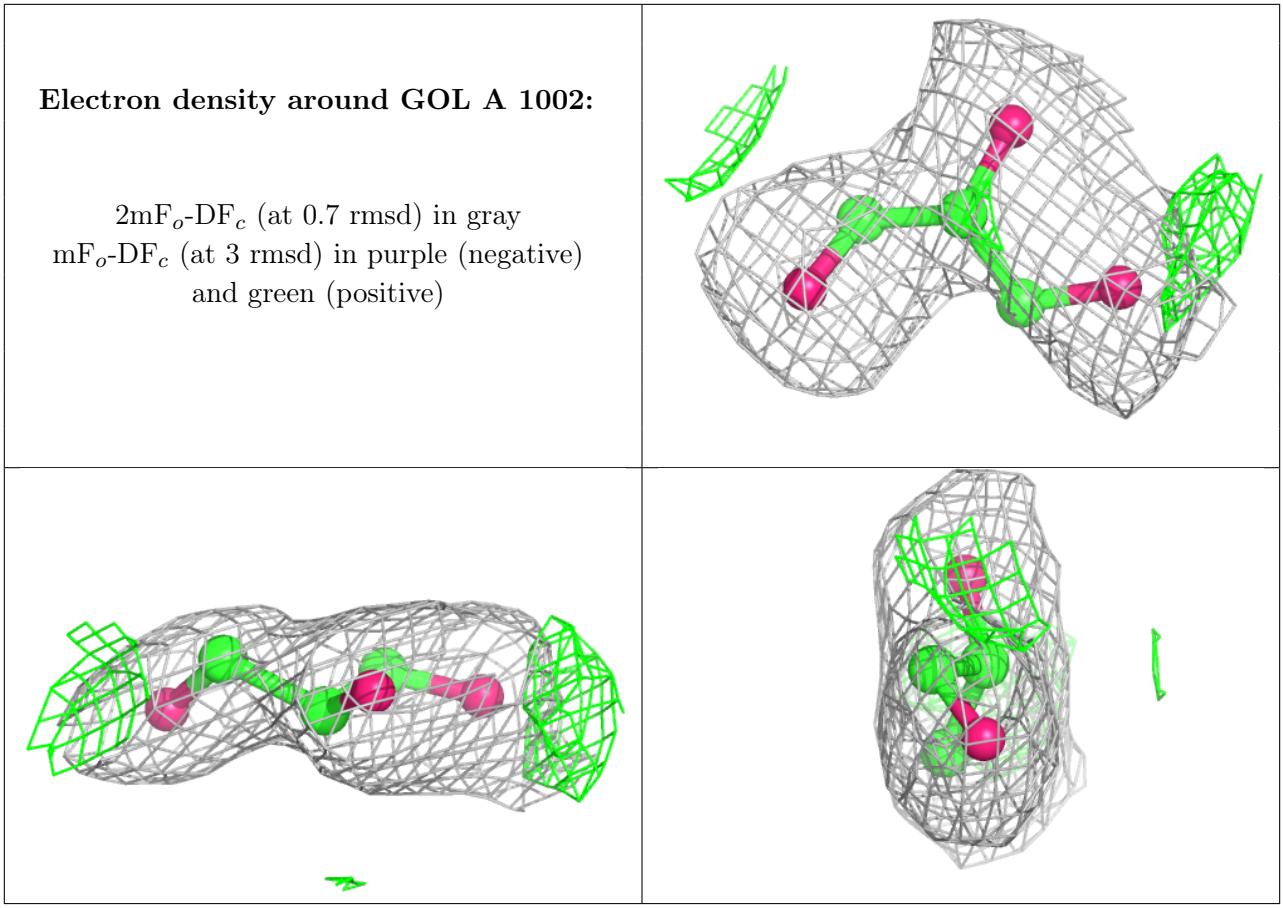






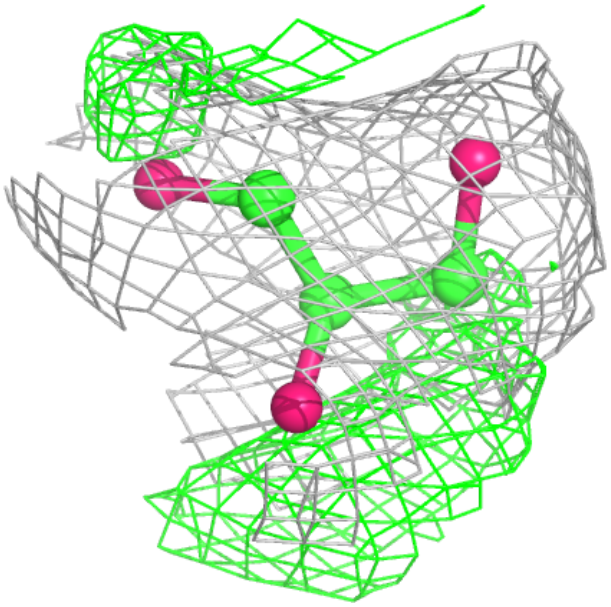
Electron density around GOL A 1002:

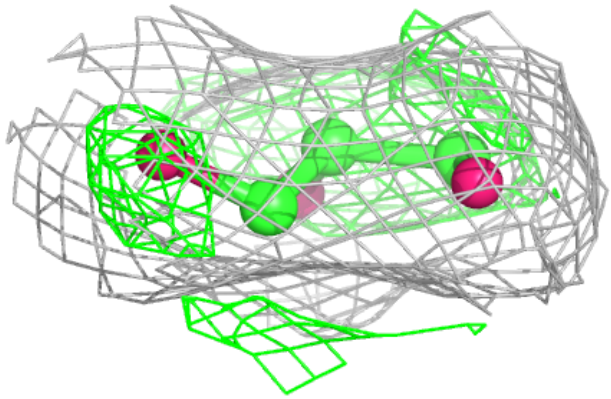
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

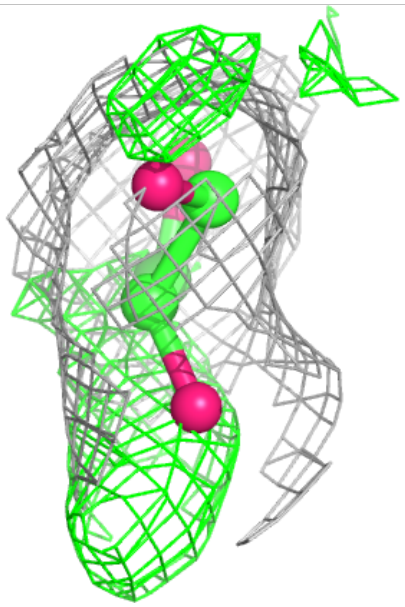


Electron density around GOL A 1003:

$2mF_o$-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 1005:

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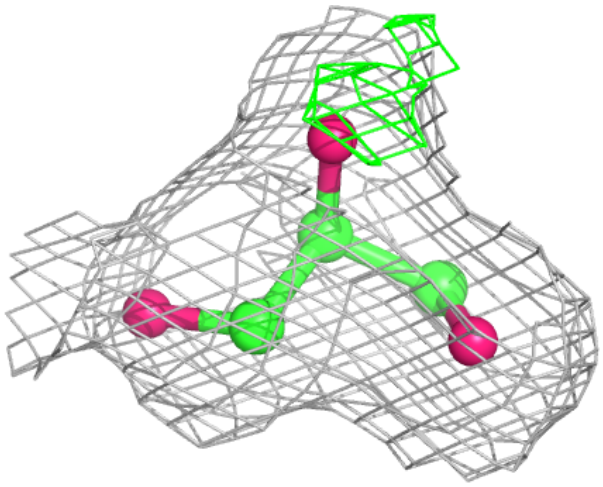
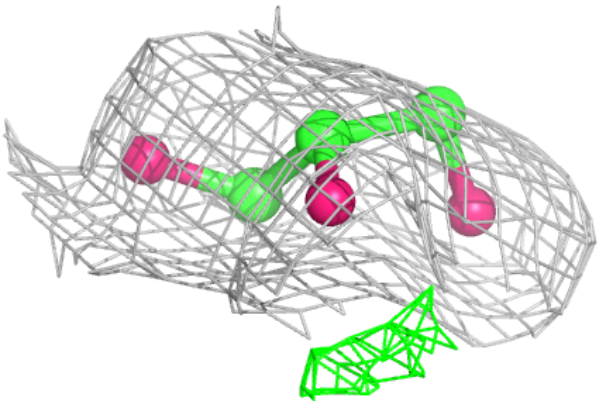
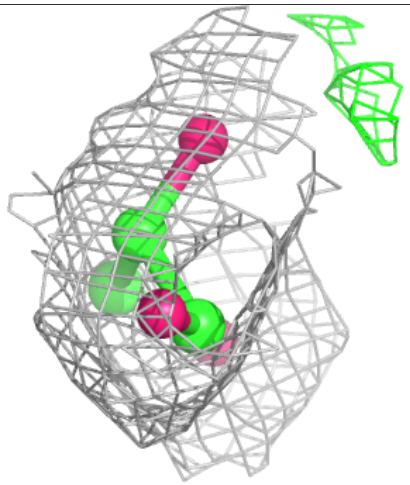
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

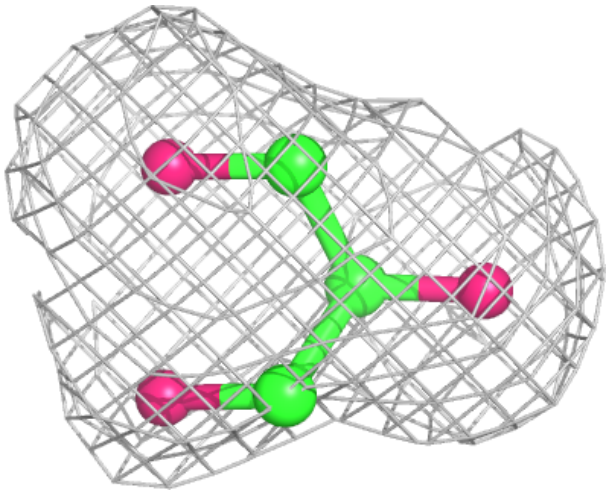


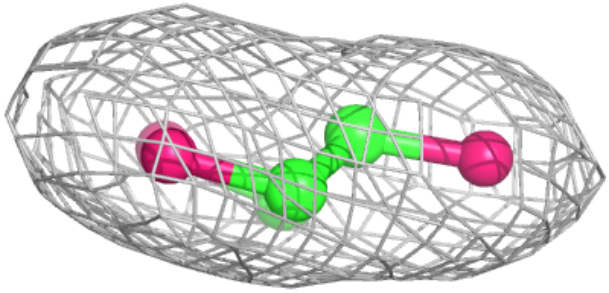


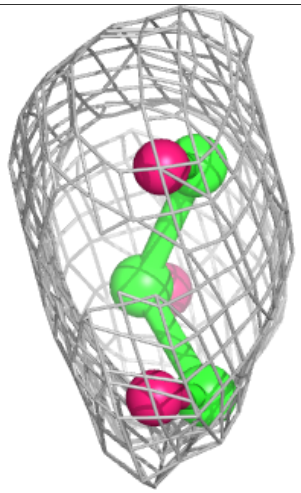


Electron density around GOL A 1005:

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

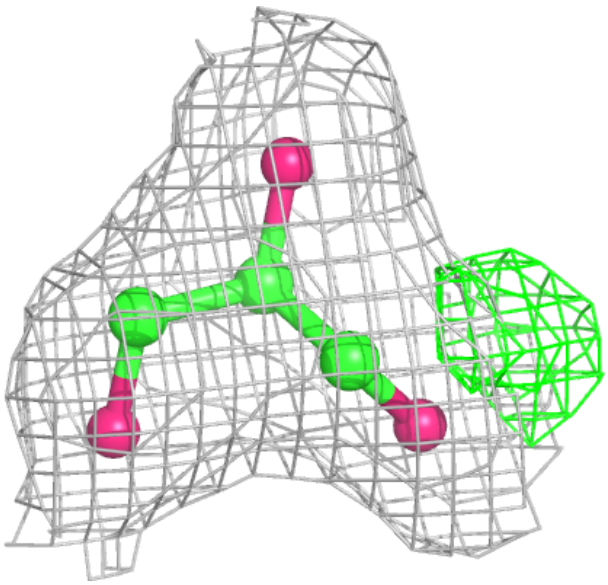


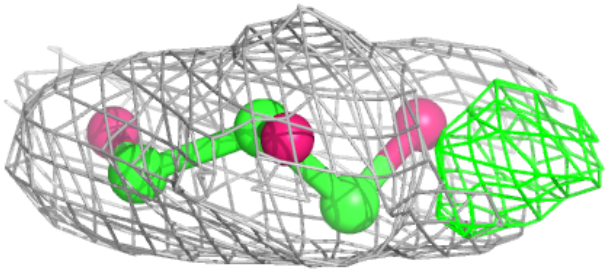


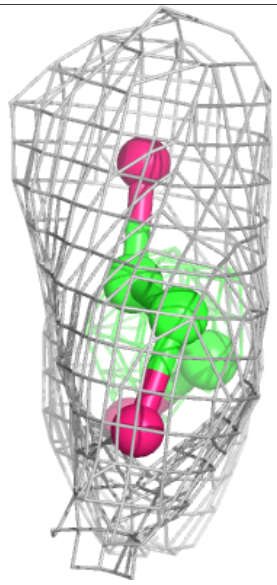


Electron density around GOL B 1005:

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

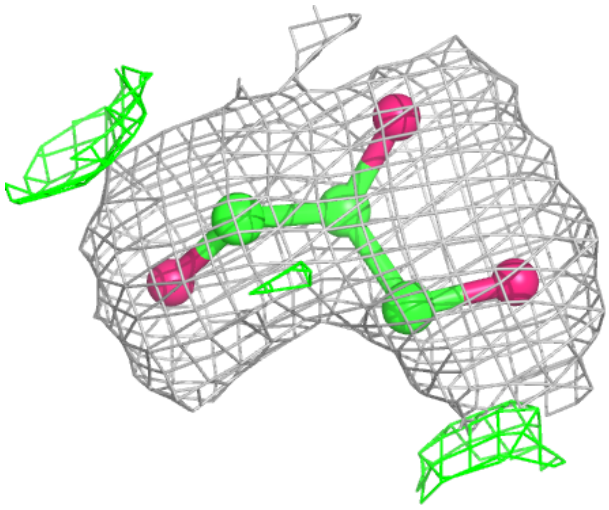


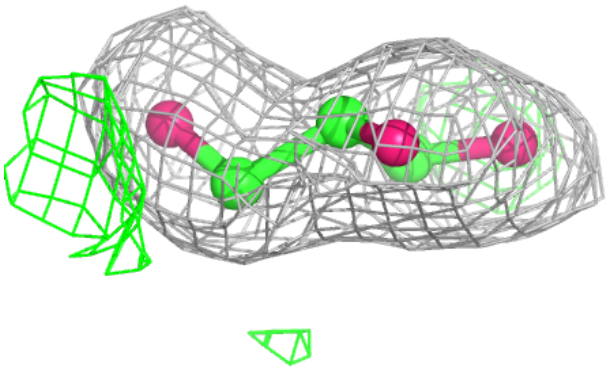


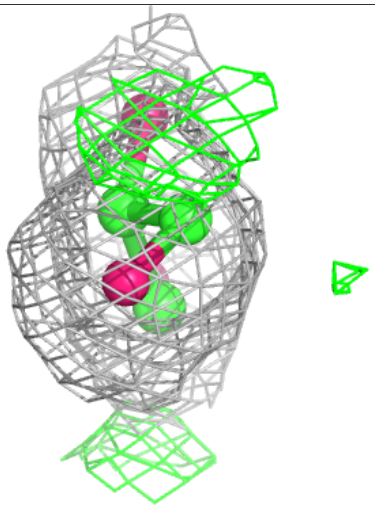


Electron density around GOL D 1002:

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

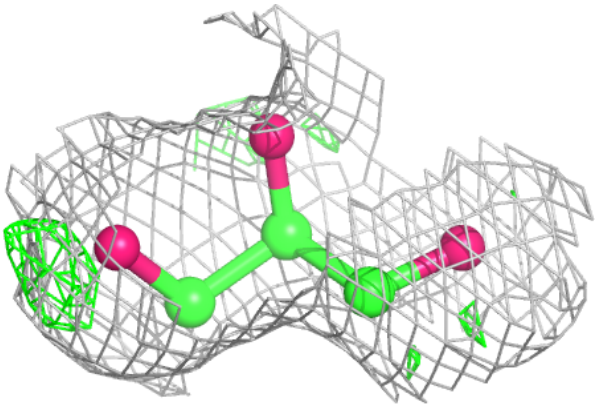


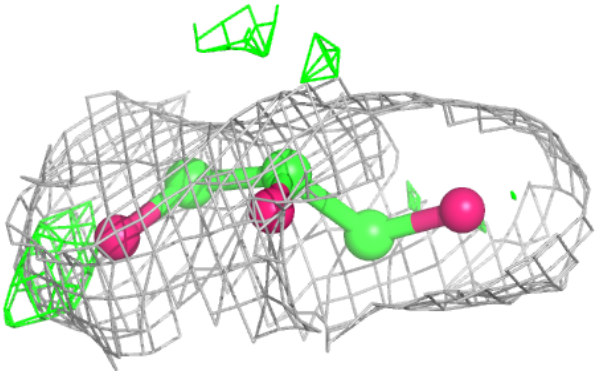


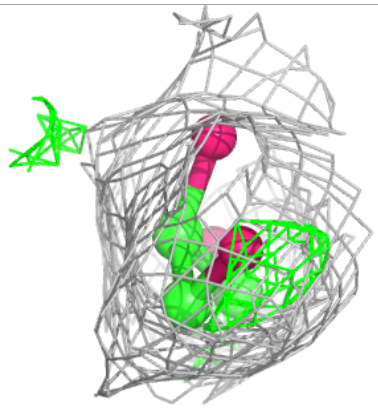


Electron density around GOL A 1006:

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

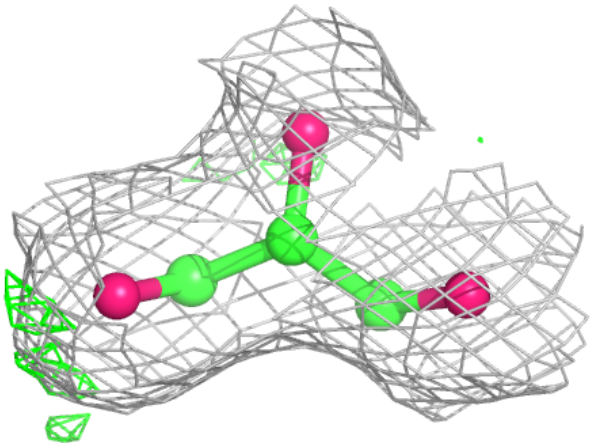


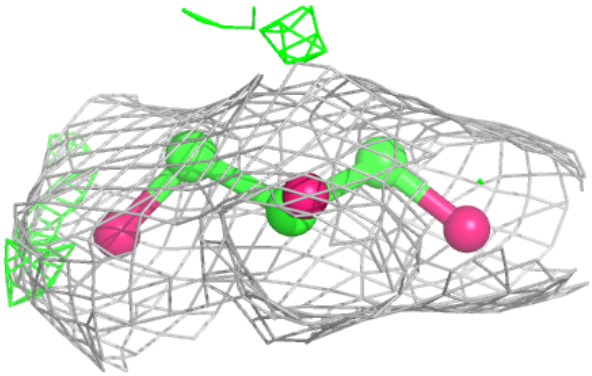


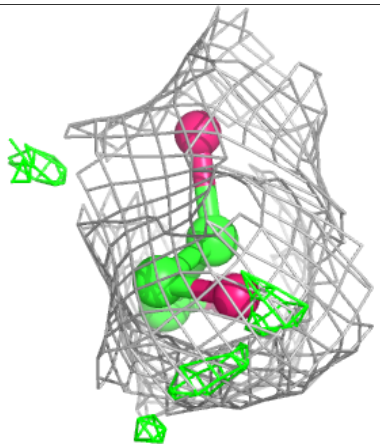


Electron density around GOL D 1004:

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

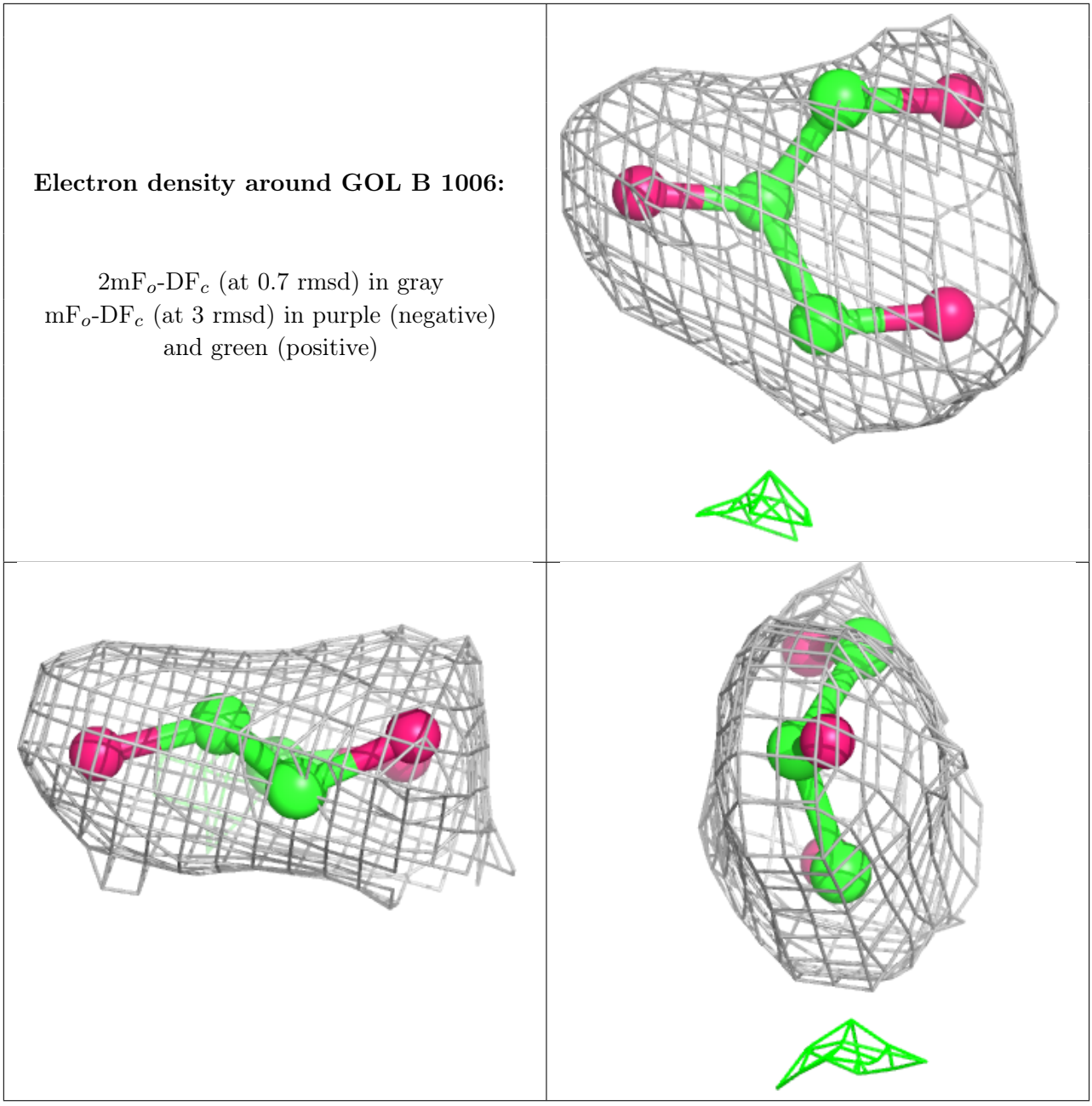






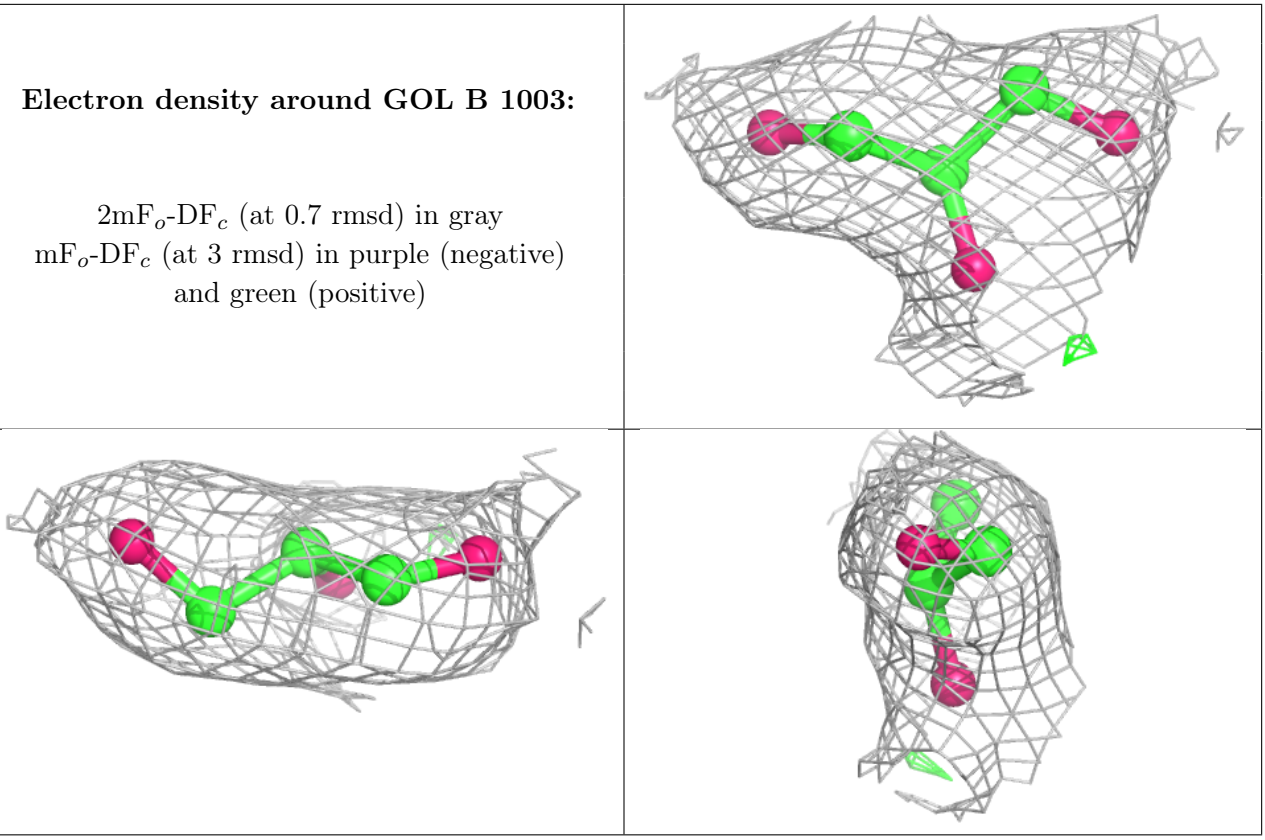
Electron density around GOL B 1006:

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



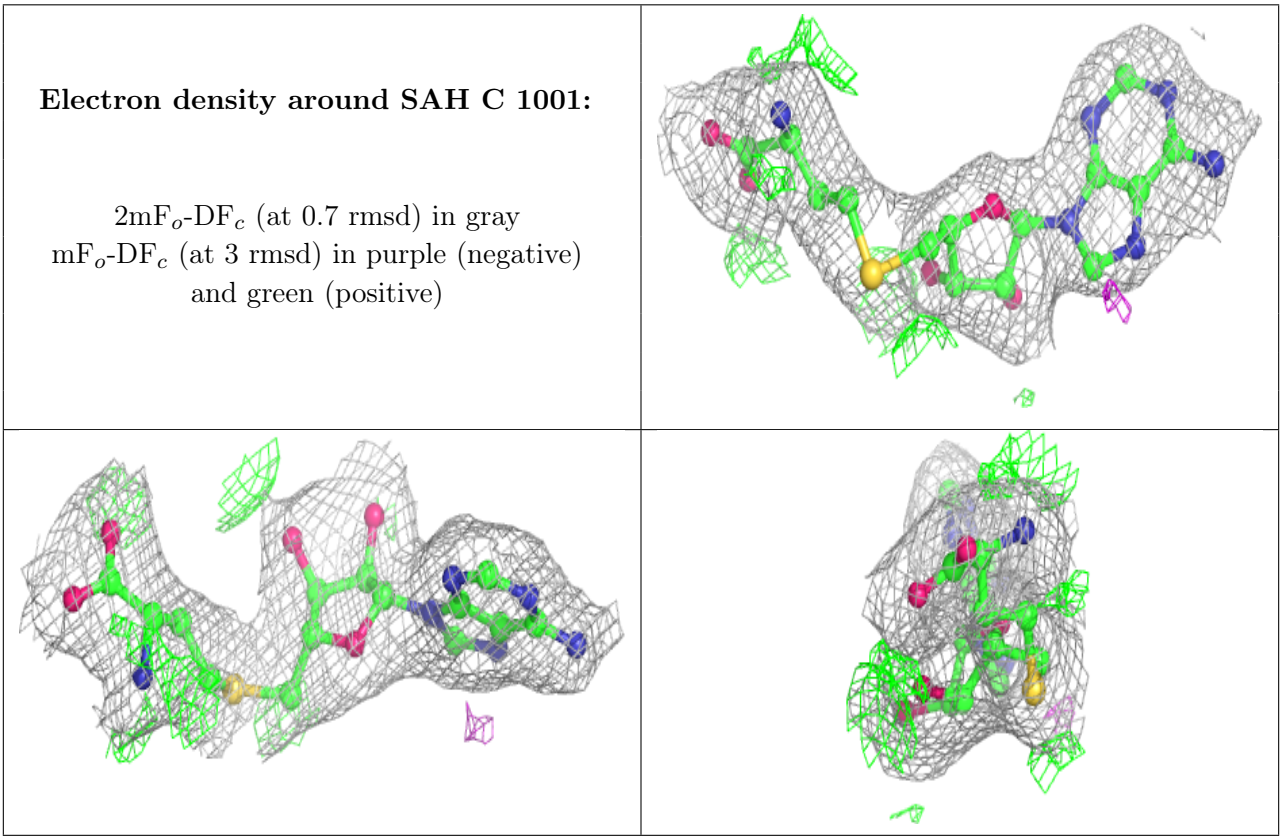
Electron density around GOL B 1003:

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



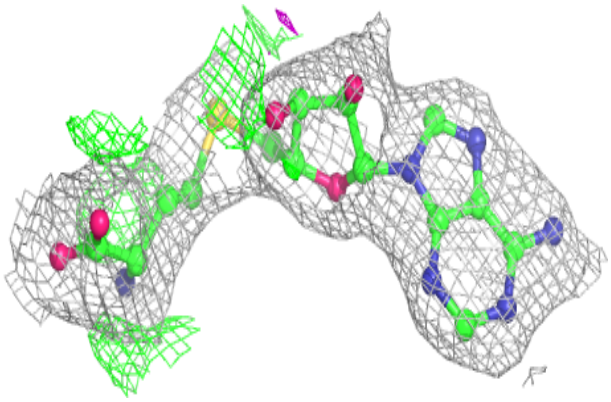
Electron density around SAH C 1001:

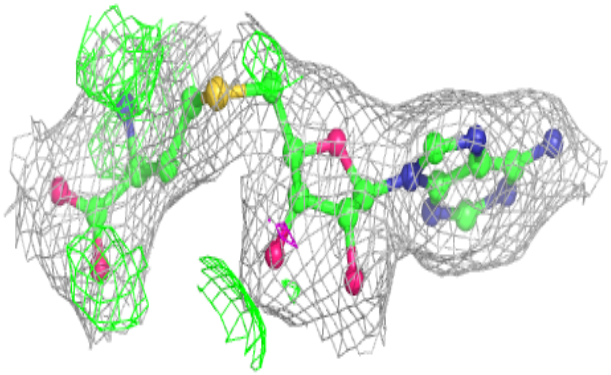
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

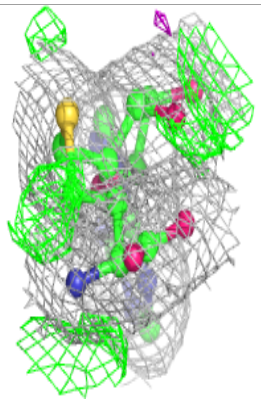


Electron density around SAH D 1001:

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

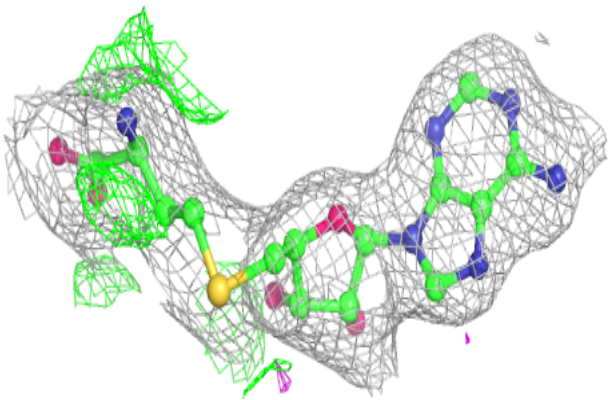


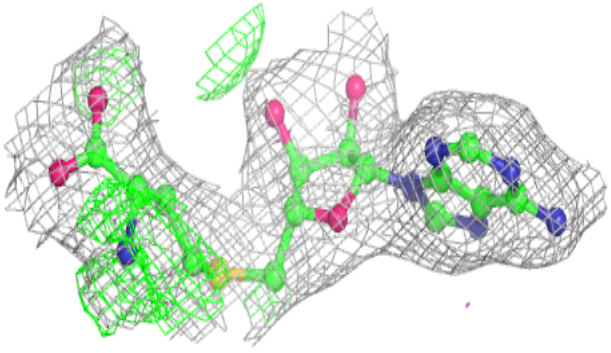


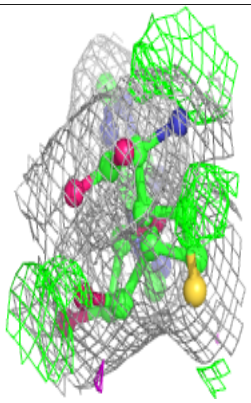


Electron density around SAH A 1001:

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

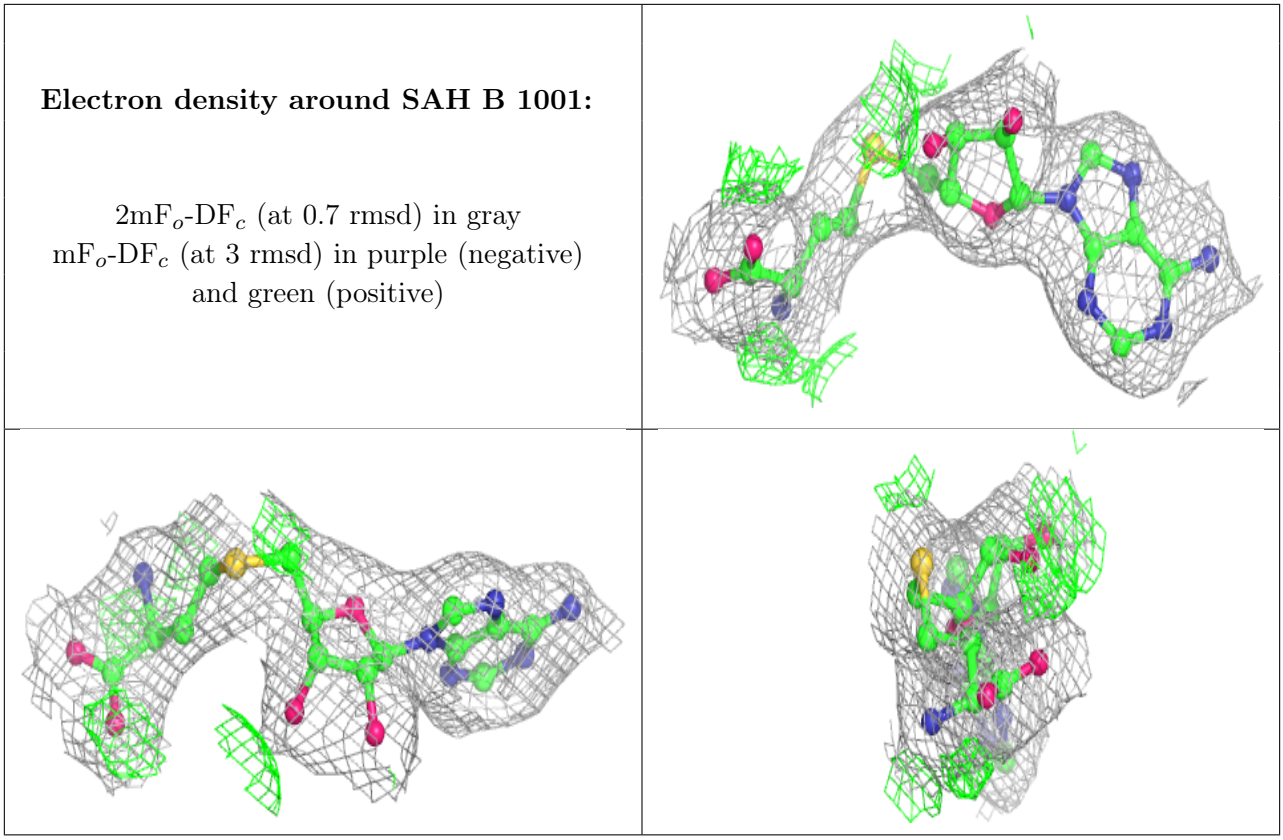






Electron density around SAH B 1001:

$2mF_o$-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.