Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2024 – 02:13 PM JST

PDB ID	:	8IQE
Title	:	Crystal structure of tetrameric K2-2 TSP
Authors	:	Ye, T.J.; Huang, K.F.; Tu, I.F.; Lee, I.M.; Chang, Y.P.; Wu, S.H.
Deposited on	:	2023-03-16
Resolution	:	2.17 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 (i) symbol.

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

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

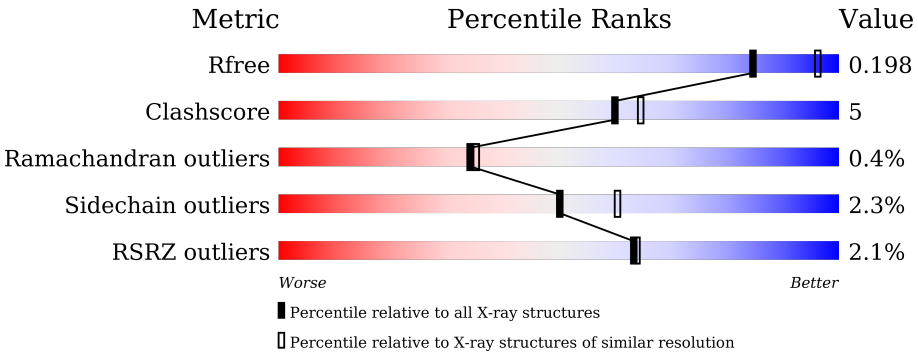
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.17 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	586	87% 9% •
1	B	586	2% 81% 11% 8%
1	C	586	3% 83% 13% • •
1	D	586	82% 10% • 7%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	D	602	-	-	X	-

2 Entry composition

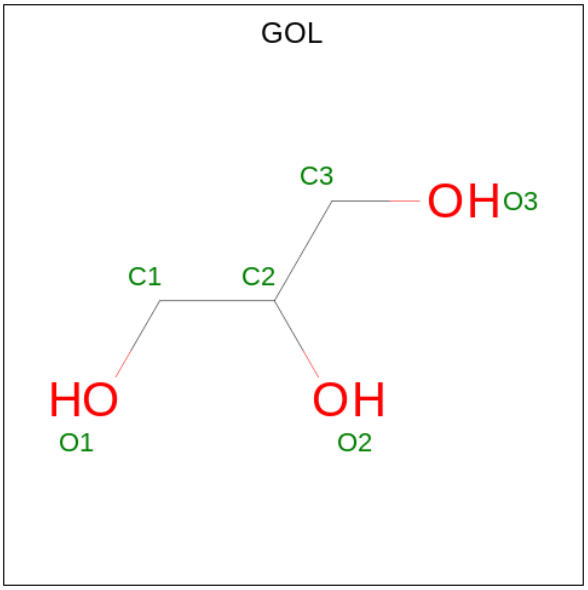
There are 3 unique types of molecules in this entry. The entry contains 18702 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 K2-VCL6 TSP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4218	2659	718	821	20			
1	B	540	Total	C	N	O	S	0	1	0
			4001	2524	688	769	20			
1	C	568	Total	C	N	O	S	0	1	0
			4219	2659	718	821	21			
1	D	546	Total	C	N	O	S	0	2	0
			4051	2553	693	785	20			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	1
			12	6	6			
2	A	1	Total	C	O		0	0
			6	3	3			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 12 6 6	0	1
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	593	Total O 594 594	0	1

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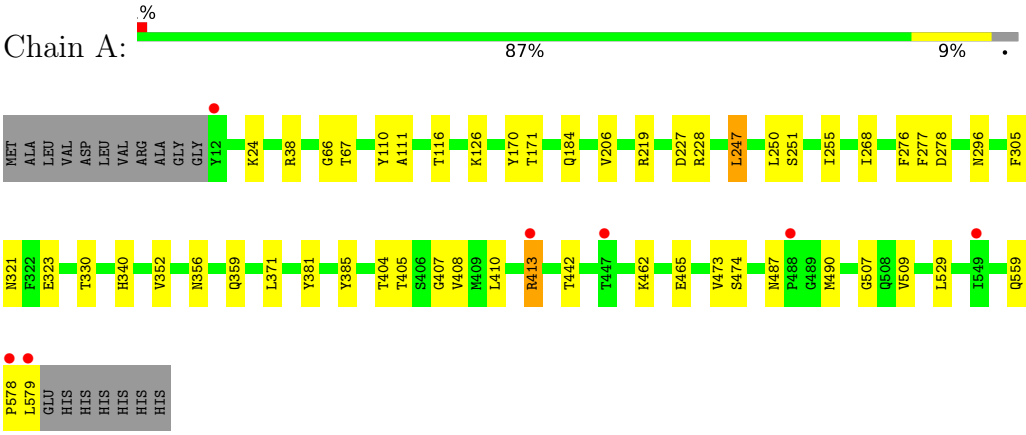
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	435	Total O 439 439	0	4
3	C	457	Total O 459 459	0	2
3	D	585	Total O 589 589	0	4

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.

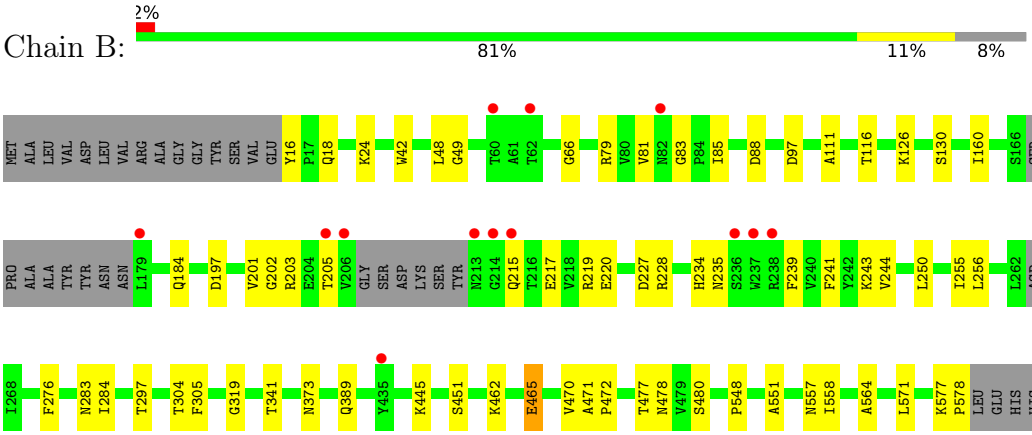
• Molecule 1: K2-VCL6 TSP

Chain A:



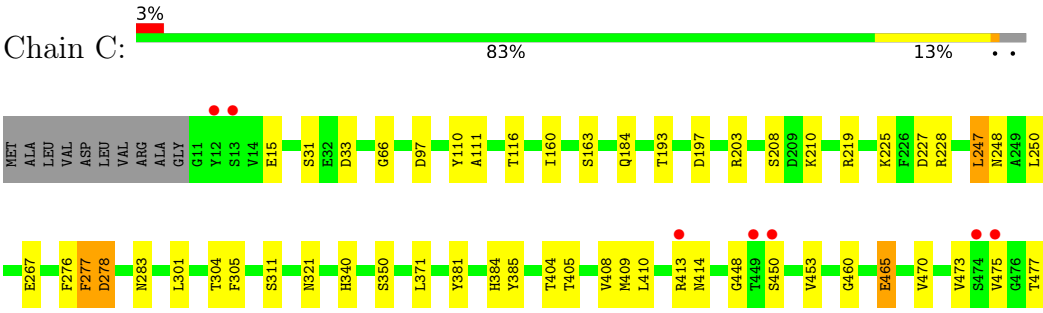
• Molecule 1: K2-VCL6 TSP

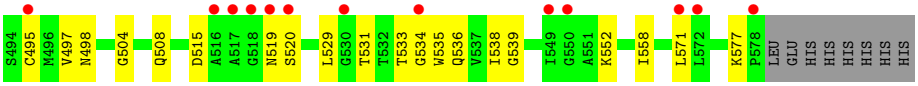
Chain B:



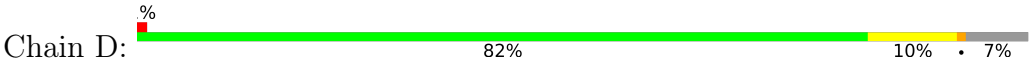
• Molecule 1: K2-VCL6 TSP

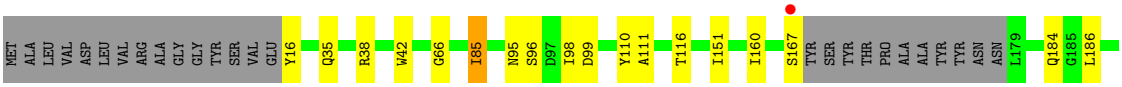
Chain C:

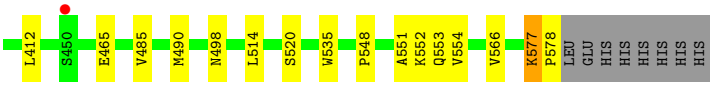




• Molecule 1: K2-VCL6 TSP







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	232.88Å 232.88Å 102.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.56 – 2.17 29.56 – 2.17	Depositor EDS
% Data completeness (in resolution range)	95.4 (29.56-2.17) 95.4 (29.56-2.17)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.168 , 0.198 0.169 , 0.198	Depositor DCC
R_{free} test set	7985 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18702	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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: 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	0.26	0/4311	0.52	0/5871
1	B	0.26	0/4087	0.50	0/5560
1	C	0.27	0/4315	0.53	2/5875 (0.0%)
1	D	0.26	0/4142	0.51	0/5636
All	All	0.26	0/16855	0.52	2/22942 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	552	LYS	CB-CG-CD	8.29	133.17	111.60
1	C	552	LYS	CA-CB-CG	5.30	125.05	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	448	GLY	Peptide

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	4218	0	4097	30	0
1	B	4001	0	3917	35	0
1	C	4219	0	4098	46	0
1	D	4051	0	3952	40	0
2	A	54	0	72	2	0
2	B	18	0	24	0	0
2	C	24	0	32	3	0
2	D	36	0	48	9	0
3	A	594	0	0	5	0
3	B	439	0	0	2	0
3	C	459	0	0	7	0
3	D	589	0	0	3	0
All	All	18702	0	16240	150	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 5.

All (150) 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:C:495:CYS:N	1:C:538:ILE:O	2.17	0.77
1:C:536:GLN:NE2	3:C:704:HOH:O	2.19	0.76
1:C:577:LYS:O	3:C:701:HOH:O	2.04	0.75
1:B:470:VAL:HG12	1:B:472:PRO:HD3	1.69	0.74
1:D:96:SER:OG	1:D:98:ILE:HG22	1.89	0.72
1:A:407:GLY:HA2	1:A:579:LEU:H	1.57	0.69
1:B:445:LYS:HA	1:B:477:THR:HG23	1.75	0.69
1:C:321:ASN:ND2	1:C:350:SER:OG	2.26	0.68
1:D:412:LEU:HD11	1:D:490:MET:HG2	1.76	0.66
1:C:15:GLU:OE1	1:D:38:ARG:NH2	2.30	0.64
1:C:371:LEU:HD11	1:C:404:THR:HG23	1.79	0.64
1:D:389:GLN:NE2	3:D:706:HOH:O	2.31	0.64
1:D:220:GLU:HG2	1:D:243:LYS:HE2	1.81	0.63
1:C:405:THR:HG23	1:C:408:VAL:HB	1.82	0.62
1:D:167:SER:OG	1:D:203:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:TYR:HB3	1:C:414:ASN:HD22	1.65	0.61
1:C:267:GLU:HB2	2:D:601[B]:GOL:H31	1.83	0.60
1:A:296:ASN:HD21	1:A:318:ASN:HD22	1.50	0.60
1:D:202:GLY:HA2	1:D:235:ASN:HD22	1.66	0.60
1:A:407:GLY:HA2	1:A:578:PRO:HA	1.83	0.60
1:D:514:LEU:HB2	1:D:553:GLN:HG3	1.84	0.59
1:A:371:LEU:HD11	1:A:404:THR:HG23	1.84	0.59
1:C:31:SER:O	3:C:702:HOH:O	2.16	0.59
1:B:49:GLY:O	1:B:79:ARG:NH2	2.28	0.58
1:D:485:VAL:HG11	1:D:554:VAL:HB	1.86	0.58
1:C:203:ARG:NH1	3:C:708:HOH:O	2.38	0.57
2:C:602:GOL:H32	2:D:604:GOL:H32	1.85	0.57
1:B:160:ILE:HG22	1:B:197:ASP:HB2	1.88	0.56
1:B:202:GLY:HA2	1:B:235:ASN:HD22	1.70	0.55
1:C:381:TYR:HA	1:C:385:TYR:CE2	2.42	0.55
1:B:220:GLU:HG2	1:B:243:LYS:HE2	1.88	0.55
1:A:509:VAL:HG23	1:A:529:LEU:HD21	1.89	0.55
1:D:331:ARG:HB2	2:D:602:GOL:H31	1.88	0.54
1:D:16:TYR:N	3:D:708:HOH:O	2.40	0.54
1:C:97:ASP:OD2	3:C:703:HOH:O	2.19	0.53
1:A:251:SER:HB2	2:A:607:GOL:H12	1.89	0.53
1:A:126:LYS:NZ	3:A:710:HOH:O	2.41	0.53
1:C:450:SER:OG	1:C:473:VAL:HG21	2.09	0.53
1:D:98:ILE:HD12	1:D:99:ASP:H	1.73	0.53
1:A:462:LYS:NZ	3:A:708:HOH:O	2.40	0.53
1:B:373[A]:ASN:OD1	3:B:701:HOH:O	2.19	0.52
1:D:329:SER:CB	2:D:602:GOL:H11	2.40	0.52
1:B:203:ARG:HG2	1:B:234:HIS:O	2.10	0.52
1:C:33:ASP:N	3:C:702:HOH:O	2.43	0.51
1:B:462:LYS:HB2	1:B:465:GLU:OE2	2.11	0.51
1:C:453:VAL:HG21	1:C:477:THR:HG21	1.92	0.51
1:C:384:HIS:H	1:C:384:HIS:CD2	2.28	0.51
1:A:356:ASN:HD21	1:A:359:GLN:HE21	1.58	0.50
1:B:16:TYR:N	3:B:709:HOH:O	2.43	0.50
1:C:255:ILE:HG21	1:C:276:PHE:HB3	1.93	0.50
1:A:296:ASN:ND2	1:A:318:ASN:HD22	2.09	0.50
2:A:603:GOL:H32	3:A:888:HOH:O	2.11	0.49
1:D:85:ILE:HD12	1:D:110:TYR:HD2	1.78	0.49
1:A:184:GLN:HA	1:A:219:ARG:O	2.13	0.49
1:D:260:ALA:HA	1:D:288:CYS:HA	1.95	0.48
1:C:184:GLN:HA	1:C:219:ARG:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:PHE:HA	1:D:301:LEU:O	2.14	0.48
1:A:413:ARG:HA	1:A:413:ARG:HE	1.79	0.48
1:D:352:VAL:HG11	2:D:601[A]:GOL:H32	1.95	0.48
1:A:67:THR:HG21	1:A:110:TYR:CE2	2.49	0.48
1:B:577:LYS:HE3	1:B:577:LYS:HB2	1.43	0.47
1:B:97:ASP:HA	1:B:126:LYS:HE3	1.95	0.47
1:B:184:GLN:HA	1:B:219:ARG:O	2.14	0.47
1:B:48:LEU:HD12	1:B:88:ASP:OD2	2.14	0.47
1:B:558:ILE:HD11	1:B:571:LEU:HD13	1.97	0.47
1:C:277:PHE:CD1	1:C:278:ASP:N	2.83	0.47
1:C:515:ASP:OD1	1:C:519:ASN:HB2	2.15	0.47
1:D:35:GLN:NE2	3:D:709:HOH:O	2.43	0.47
1:A:405:THR:HG21	1:A:576:VAL:HG12	1.96	0.47
1:C:160:ILE:HG22	1:C:197:ASP:HB2	1.97	0.47
1:C:453:VAL:HG22	1:C:470:VAL:HG13	1.97	0.47
1:D:184:GLN:HA	1:D:219:ARG:O	2.15	0.47
1:A:405:THR:HG23	1:A:408:VAL:HB	1.97	0.47
1:A:38:ARG:NH1	3:A:716:HOH:O	2.46	0.46
1:D:228:ARG:HH22	2:D:603:GOL:H11	1.80	0.46
1:B:227:ASP:HA	1:B:250:LEU:HB3	1.96	0.46
1:B:577:LYS:HB2	1:B:578:PRO:HD2	1.98	0.46
1:D:203:ARG:HH21	1:D:206:VAL:C	2.19	0.46
1:C:111:ALA:HB1	1:C:116:THR:O	2.15	0.45
1:A:410:LEU:H	1:A:490:MET:HE2	1.79	0.45
1:A:170:TYR:CD2	1:A:171:THR:HG23	2.52	0.45
1:D:329:SER:HB3	2:D:602:GOL:H11	1.98	0.45
1:A:255:ILE:HG21	1:A:276:PHE:HB3	1.99	0.45
1:C:110:TYR:HB2	2:C:603:GOL:H11	2.00	0.44
1:C:247:LEU:HA	1:C:277:PHE:O	2.17	0.44
1:C:311:SER:HA	1:C:340:HIS:O	2.18	0.44
1:D:255:ILE:HG21	1:D:276:PHE:HB3	1.99	0.44
1:D:283:ASN:HB3	1:D:304:THR:O	2.18	0.44
1:D:548:PRO:HG2	1:D:551:ALA:HB2	1.99	0.44
1:B:255:ILE:HG21	1:B:276:PHE:HB3	1.99	0.44
1:C:210:LYS:HD2	1:C:264:ASP:CG	2.38	0.44
1:C:534:GLY:O	1:C:536:GLN:NE2	2.50	0.44
1:D:373:ASN:OD1	1:D:404:THR:OG1	2.30	0.44
1:A:442:THR:HG23	3:A:714:HOH:O	2.17	0.44
1:C:460:GLY:HA3	1:C:465:GLU:HG2	2.00	0.44
1:B:297:THR:HA	1:B:319:GLY:O	2.18	0.43
1:B:241:PHE:HD2	1:B:244:VAL:HG21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:VAL:O	1:C:475:VAL:N	2.47	0.43
1:B:478:ASN:HB3	1:B:557:ASN:HD21	1.84	0.43
1:D:202:GLY:HA2	1:D:235:ASN:ND2	2.31	0.43
1:C:558:ILE:HD11	1:C:571:LEU:HD13	2.00	0.43
1:B:201:VAL:HG13	1:B:239:PHE:CZ	2.54	0.43
1:B:480:SER:HB3	1:B:557:ASN:HD22	1.83	0.43
1:C:498:ASN:HB2	1:C:535:TRP:CD2	2.53	0.43
1:D:111:ALA:HB1	1:D:116:THR:O	2.19	0.43
1:B:81:VAL:HG12	1:B:83:GLY:H	1.84	0.43
1:B:217:GLU:HG2	1:B:219:ARG:CG	2.49	0.43
1:B:451:SER:HB3	1:B:472:PRO:HA	1.99	0.42
1:D:577:LYS:HB2	1:D:578:PRO:HD2	2.01	0.42
1:C:160:ILE:CD1	1:C:163:SER:HB3	2.50	0.42
1:C:405:THR:HG22	3:C:701:HOH:O	2.19	0.42
1:A:111:ALA:HB1	1:A:116:THR:O	2.18	0.42
1:B:24:LYS:HB3	1:B:24:LYS:HE3	1.84	0.42
1:B:111:ALA:HB1	1:B:116:THR:O	2.19	0.42
1:C:504:GLY:O	1:C:531:THR:HG22	2.19	0.42
1:D:328:ALA:O	1:D:356:ASN:HB3	2.19	0.42
1:D:514:LEU:HD23	1:D:520:SER:HA	2.01	0.42
1:D:552:LYS:HA	1:D:552:LYS:HD3	1.78	0.42
1:B:203:ARG:HG3	1:B:205:THR:O	2.19	0.42
1:B:389:GLN:OE1	1:D:329:SER:HA	2.18	0.42
1:B:283:ASN:HB3	1:B:304:THR:O	2.20	0.42
1:C:110:TYR:HA	2:C:603:GOL:H32	2.01	0.42
1:C:283:ASN:HB3	1:C:304:THR:O	2.19	0.42
1:A:381:TYR:HA	1:A:385:TYR:CE2	2.55	0.42
1:C:225:LYS:HA	1:C:248:ASN:O	2.19	0.42
1:D:356:ASN:HB2	1:D:357:PRO:HD2	2.01	0.42
1:C:277:PHE:HA	1:C:301:LEU:O	2.20	0.41
1:A:227:ASP:HA	1:A:250:LEU:HB3	2.01	0.41
1:A:206:VAL:O	1:D:95:ASN:HB3	2.20	0.41
1:C:538:ILE:HA	1:C:539:GLY:HA2	1.84	0.41
1:A:323:GLU:HG3	1:A:352:VAL:HB	2.02	0.41
1:A:330:THR:HA	1:A:359:GLN:HE22	1.86	0.41
1:A:465:GLU:OE1	1:A:465:GLU:N	2.49	0.41
1:B:85:ILE:HD13	1:B:111:ALA:HA	2.02	0.41
1:D:498:ASN:HB2	1:D:535:TRP:CD2	2.55	0.41
1:C:497:VAL:HG11	1:C:529:LEU:HD22	2.02	0.41
1:A:311:SER:HA	1:A:340:HIS:O	2.20	0.41
1:B:471:ALA:HA	1:B:564:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:ASN:O	2:D:602:GOL:H2	2.21	0.41
1:D:331:ARG:NH1	2:D:602:GOL:O2	2.54	0.41
1:B:548:PRO:HG2	1:B:551:ALA:HB2	2.02	0.41
1:C:227:ASP:HA	1:C:250:LEU:HB3	2.03	0.40
1:D:151:ILE:HD11	1:D:186:LEU:HD22	2.03	0.40
1:D:264:ASP:N	1:D:264:ASP:OD1	2.52	0.40
1:A:247:LEU:HA	1:A:277:PHE:O	2.22	0.40
1:A:507:GLY:HA3	1:A:559:GLN:O	2.22	0.40
1:B:256:LEU:HB3	1:B:284:ILE:HG12	2.03	0.40
1:C:493:MET:HB2	1:C:493:MET:HE2	1.92	0.40
1:C:410:LEU:H	1:C:490:MET:HE2	1.87	0.40
1:C:413:ARG:HD2	1:C:413:ARG:HA	1.69	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	566/586 (97%)	549 (97%)	14 (2%)	3 (0%)	29	28
1	B	533/586 (91%)	518 (97%)	14 (3%)	1 (0%)	47	52
1	C	567/586 (97%)	550 (97%)	15 (3%)	2 (0%)	34	35
1	D	542/586 (92%)	526 (97%)	14 (3%)	2 (0%)	34	35
All	All	2208/2344 (94%)	2143 (97%)	57 (3%)	8 (0%)	34	35

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	ASP
1	A	66	GLY
1	C	66	GLY

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Mol	Chain	Res	Type
1	B	66	GLY
1	C	278	ASP
1	D	577	LYS
1	D	66	GLY
1	A	268	ILE

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	455/469 (97%)	446 (98%)	9 (2%)	55	66
1	B	432/469 (92%)	424 (98%)	8 (2%)	57	68
1	C	455/469 (97%)	443 (97%)	12 (3%)	46	55
1	D	438/469 (93%)	427 (98%)	11 (2%)	47	57
All	All	1780/1876 (95%)	1740 (98%)	40 (2%)	50	62

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	228	ARG
1	A	247	LEU
1	A	305	PHE
1	A	321	ASN
1	A	413	ARG
1	A	473	VAL
1	A	474	SER
1	A	487	ASN
1	B	18	GLN
1	B	42	TRP
1	B	130	SER
1	B	215	GLN
1	B	228	ARG
1	B	305	PHE
1	B	341	THR

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Mol	Chain	Res	Type
1	B	465	GLU
1	C	193	THR
1	C	208	SER
1	C	228	ARG
1	C	247	LEU
1	C	277	PHE
1	C	305	PHE
1	C	409	MET
1	C	465	GLU
1	C	493	MET
1	C	508	GLN
1	C	520	SER
1	C	533	THR
1	D	42	TRP
1	D	85	ILE
1	D	160	ILE
1	D	201	VAL
1	D	228	ARG
1	D	264	ASP
1	D	305	PHE
1	D	311	SER
1	D	341	THR
1	D	465	GLU
1	D	566	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	296	ASN
1	A	321	ASN
1	A	359	GLN
1	B	213	ASN
1	B	478	ASN
1	B	557	ASN
1	C	321	ASN
1	C	384	HIS
1	C	508	GLN
1	C	536	GLN
1	D	18	GLN
1	D	35	GLN
1	D	165	ASN

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Mol	Chain	Res	Type
1	D	389	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	A	602	-	5,5,5	0.90	0	5,5,5	0.97	0
2	GOL	A	601[A]	-	5,5,5	0.92	0	5,5,5	1.00	0
2	GOL	A	606	-	5,5,5	0.87	0	5,5,5	0.98	0
2	GOL	B	603	-	5,5,5	0.90	0	5,5,5	0.99	0
2	GOL	C	603	-	5,5,5	0.90	0	5,5,5	0.99	0
2	GOL	A	608	-	5,5,5	0.92	0	5,5,5	0.90	0
2	GOL	D	601[A]	-	5,5,5	0.87	0	5,5,5	1.02	0
2	GOL	A	601[B]	-	5,5,5	0.89	0	5,5,5	1.01	0
2	GOL	C	602	-	5,5,5	0.88	0	5,5,5	1.02	0
2	GOL	C	604	-	5,5,5	0.89	0	5,5,5	1.00	0
2	GOL	D	601[B]	-	5,5,5	0.90	0	5,5,5	1.01	0
2	GOL	B	602	-	5,5,5	0.91	0	5,5,5	0.99	0
2	GOL	C	601	-	5,5,5	0.92	0	5,5,5	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	D	604	-	5,5,5	0.90	0	5,5,5	1.02	0
2	GOL	A	605	-	5,5,5	0.91	0	5,5,5	1.00	0
2	GOL	D	605	-	5,5,5	0.88	0	5,5,5	1.03	0
2	GOL	D	603	-	5,5,5	0.91	0	5,5,5	0.94	0
2	GOL	B	601	-	5,5,5	0.94	0	5,5,5	0.91	0
2	GOL	A	603	-	5,5,5	0.87	0	5,5,5	1.04	0
2	GOL	A	604	-	5,5,5	0.93	0	5,5,5	0.99	0
2	GOL	A	607	-	5,5,5	0.94	0	5,5,5	0.99	0
2	GOL	D	602	-	5,5,5	0.94	0	5,5,5	1.06	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	602	-	-	2/4/4/4	-
2	GOL	A	601[A]	-	-	0/4/4/4	-
2	GOL	A	606	-	-	0/4/4/4	-
2	GOL	B	603	-	-	1/4/4/4	-
2	GOL	C	603	-	-	2/4/4/4	-
2	GOL	A	608	-	-	3/4/4/4	-
2	GOL	D	601[A]	-	-	2/4/4/4	-
2	GOL	A	601[B]	-	-	0/4/4/4	-
2	GOL	C	602	-	-	0/4/4/4	-
2	GOL	C	604	-	-	0/4/4/4	-
2	GOL	D	601[B]	-	-	4/4/4/4	-
2	GOL	B	602	-	-	0/4/4/4	-
2	GOL	C	601	-	-	0/4/4/4	-
2	GOL	D	604	-	-	0/4/4/4	-
2	GOL	A	605	-	-	0/4/4/4	-
2	GOL	D	605	-	-	0/4/4/4	-
2	GOL	D	603	-	-	2/4/4/4	-
2	GOL	B	601	-	-	3/4/4/4	-
2	GOL	A	603	-	-	3/4/4/4	-
2	GOL	A	604	-	-	2/4/4/4	-
2	GOL	A	607	-	-	2/4/4/4	-
2	GOL	D	602	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	603	GOL	C1-C2-C3-O3
2	A	603	GOL	O2-C2-C3-O3
2	A	607	GOL	O1-C1-C2-C3
2	A	608	GOL	O1-C1-C2-C3
2	D	601[B]	GOL	O1-C1-C2-C3
2	A	608	GOL	O1-C1-C2-O2
2	C	603	GOL	O1-C1-C2-O2
2	A	602	GOL	C1-C2-C3-O3
2	A	603	GOL	O1-C1-C2-C3
2	A	604	GOL	O1-C1-C2-C3
2	B	601	GOL	O1-C1-C2-C3
2	B	603	GOL	O1-C1-C2-C3
2	C	603	GOL	O1-C1-C2-C3
2	D	601[A]	GOL	C1-C2-C3-O3
2	D	601[B]	GOL	C1-C2-C3-O3
2	D	603	GOL	O1-C1-C2-C3
2	A	602	GOL	O2-C2-C3-O3
2	A	604	GOL	O1-C1-C2-O2
2	D	601[B]	GOL	O1-C1-C2-O2
2	A	607	GOL	O1-C1-C2-O2
2	D	601[B]	GOL	O2-C2-C3-O3
2	A	608	GOL	O2-C2-C3-O3
2	D	603	GOL	O1-C1-C2-O2
2	B	601	GOL	O1-C1-C2-O2
2	D	601[A]	GOL	O2-C2-C3-O3
2	B	601	GOL	C1-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	603	GOL	2	0
2	D	601[A]	GOL	1	0
2	C	602	GOL	1	0
2	D	601[B]	GOL	1	0
2	D	604	GOL	1	0
2	D	603	GOL	1	0
2	A	603	GOL	1	0

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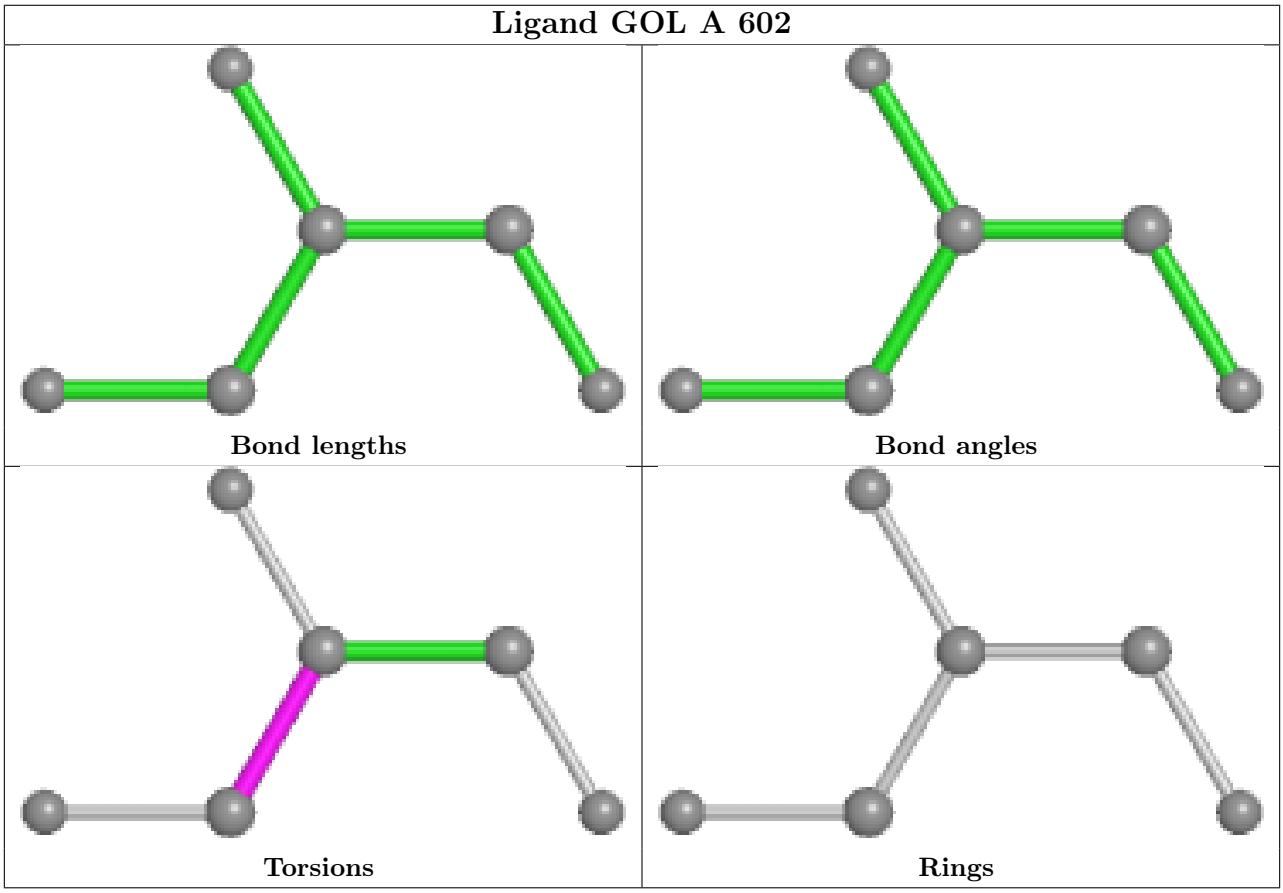
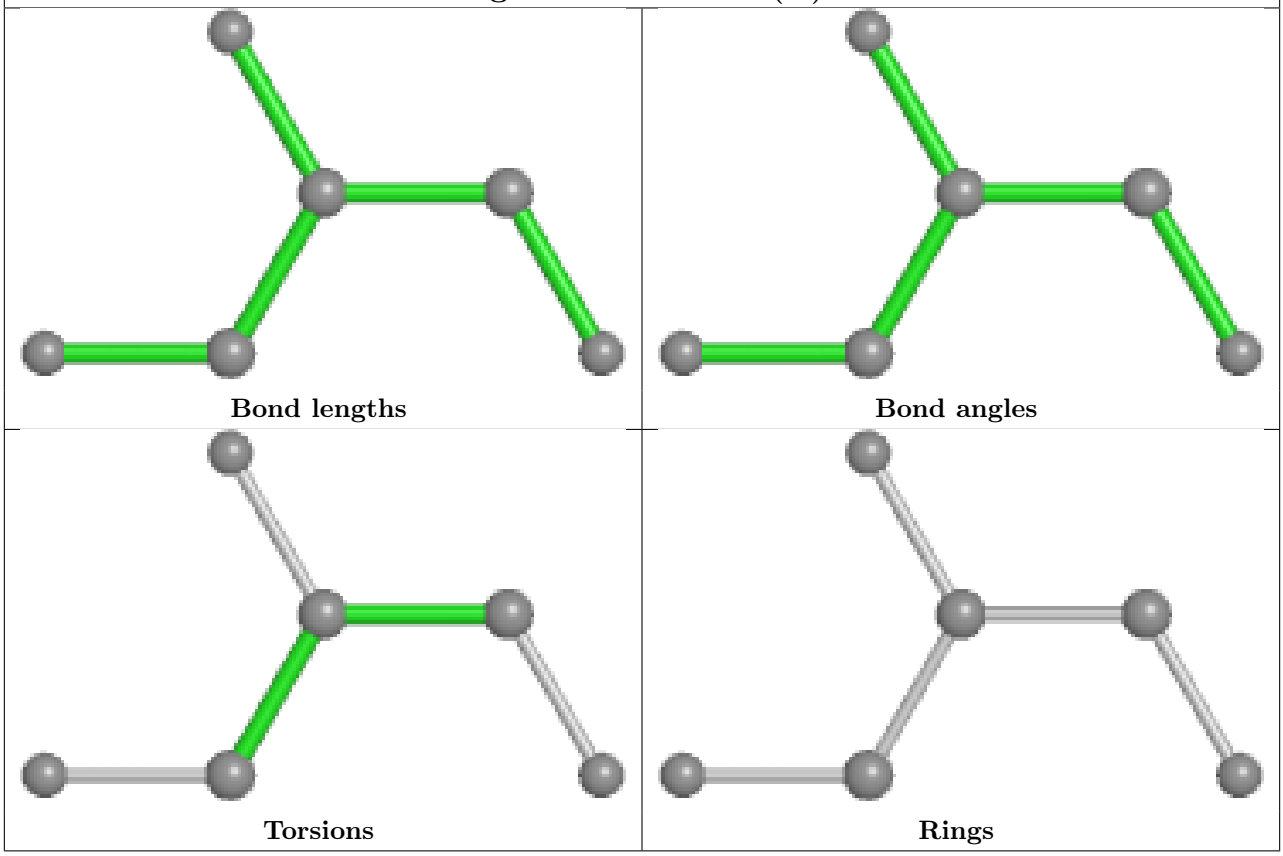
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	607	GOL	1	0
2	D	602	GOL	5	0

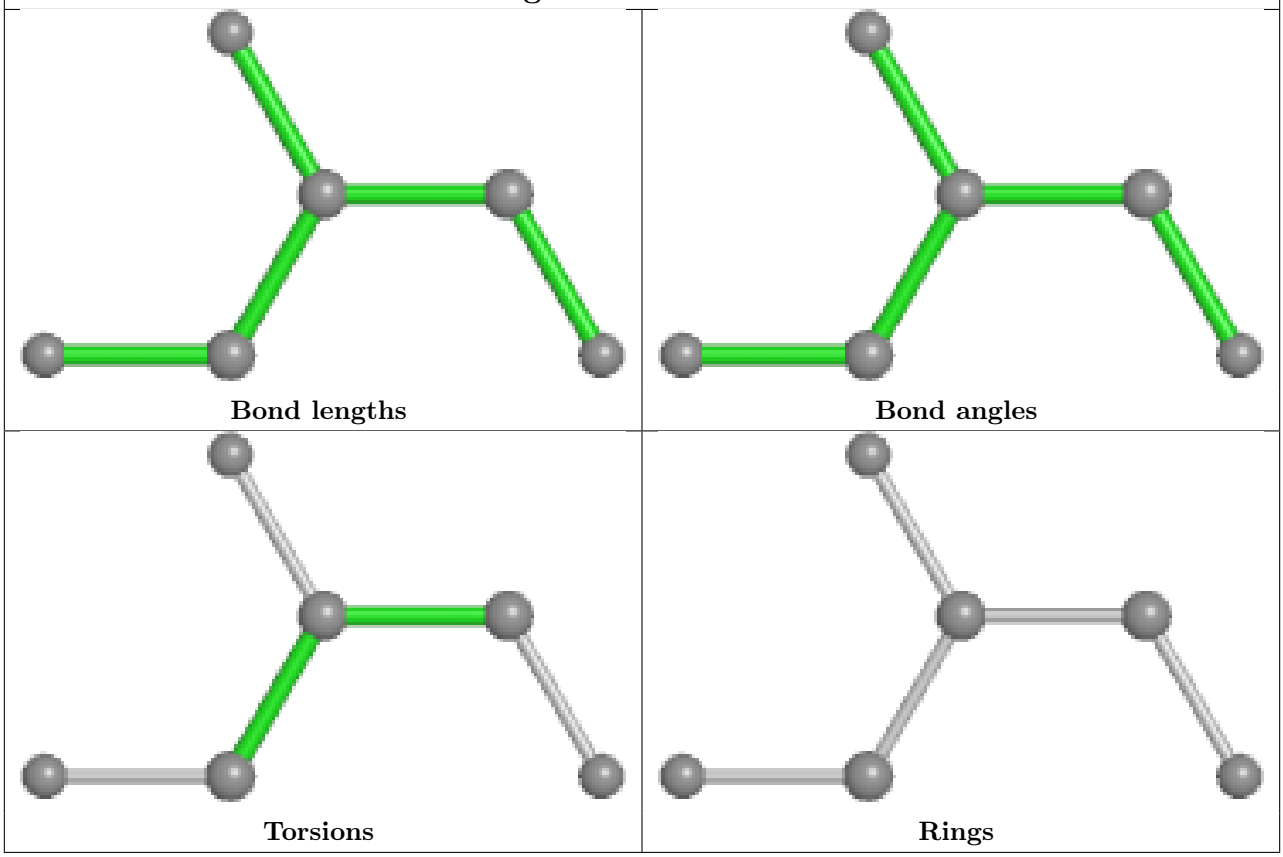
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



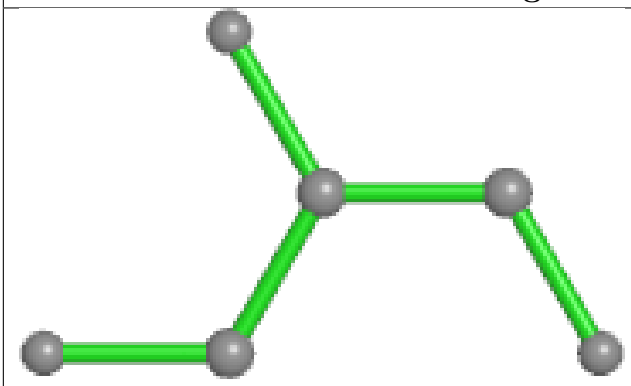
Ligand GOL A 601 (A)



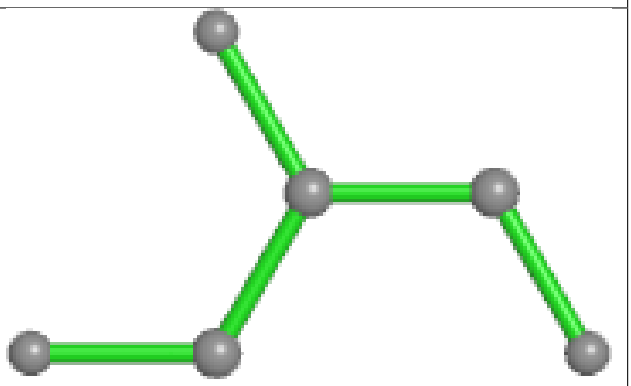
Ligand GOL A 606



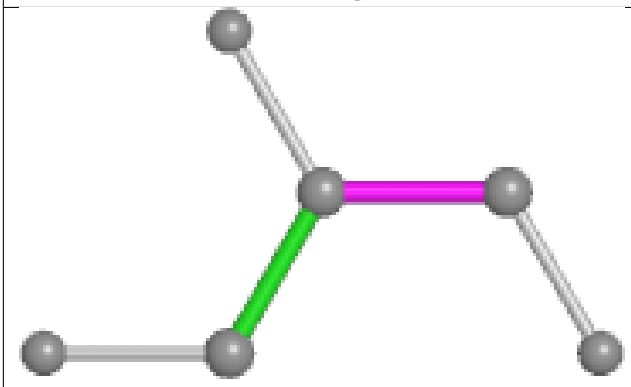
Ligand GOL B 603



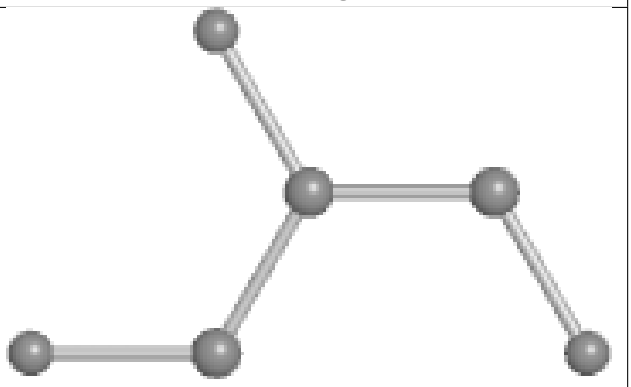
Bond lengths



Bond angles

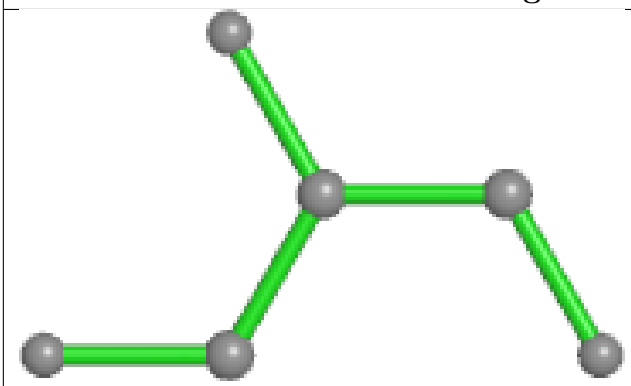


Torsions

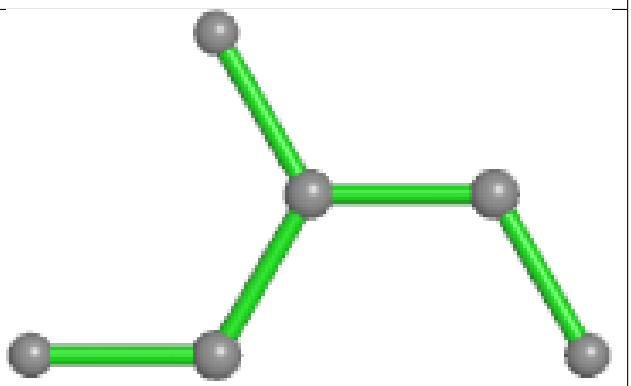


Rings

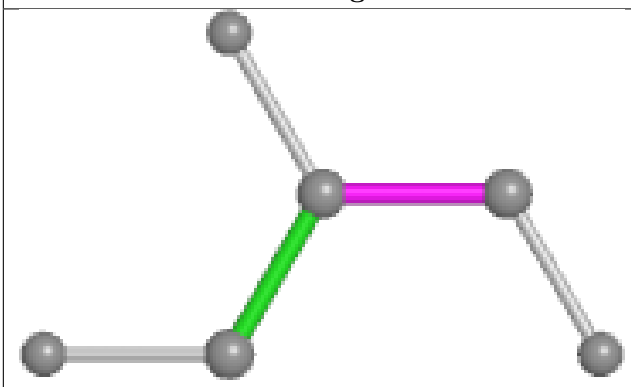
Ligand GOL C 603



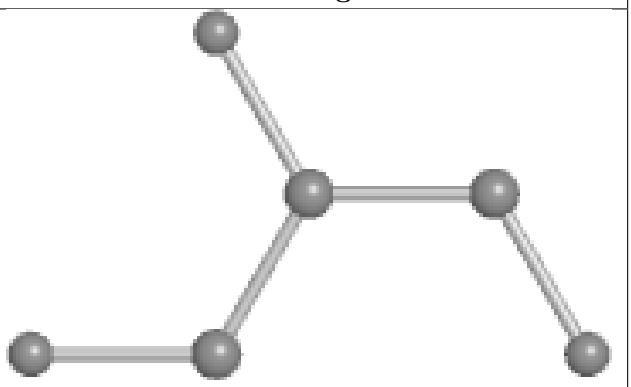
Bond lengths



Bond angles

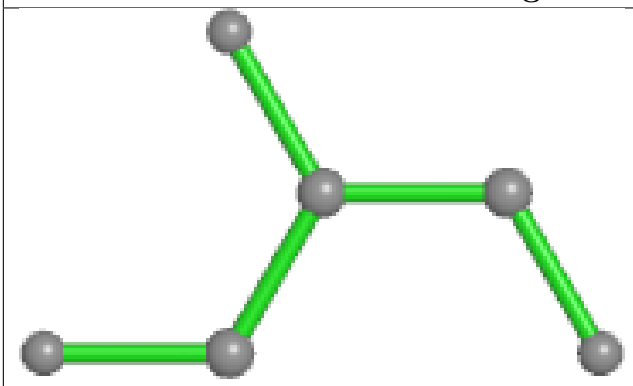


Torsions

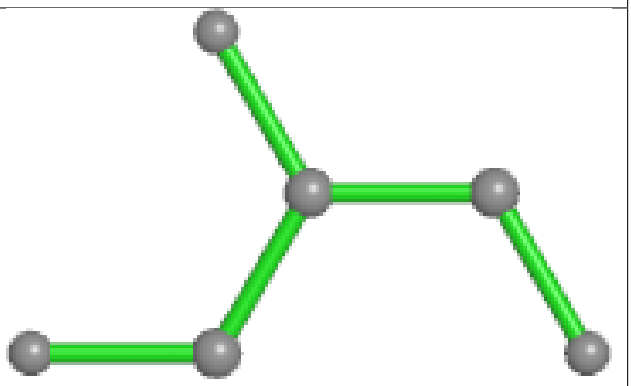


Rings

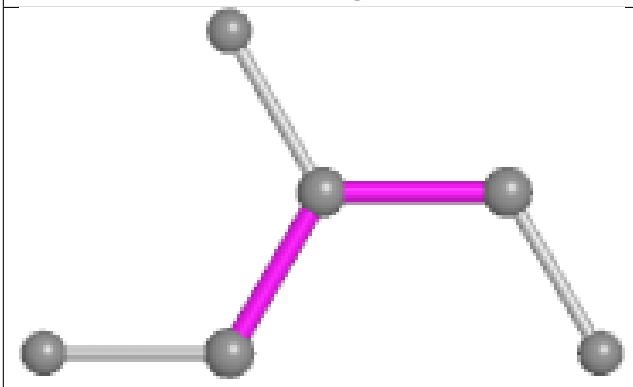
Ligand GOL A 608



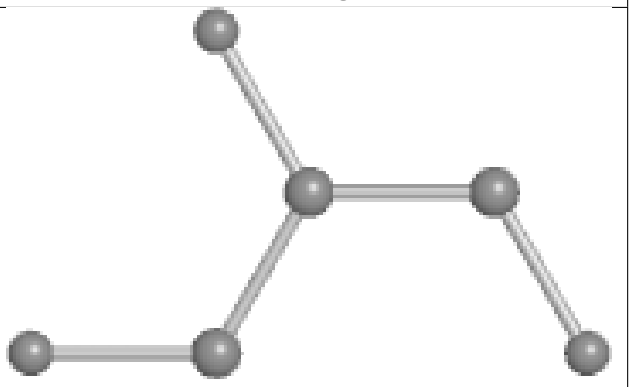
Bond lengths



Bond angles

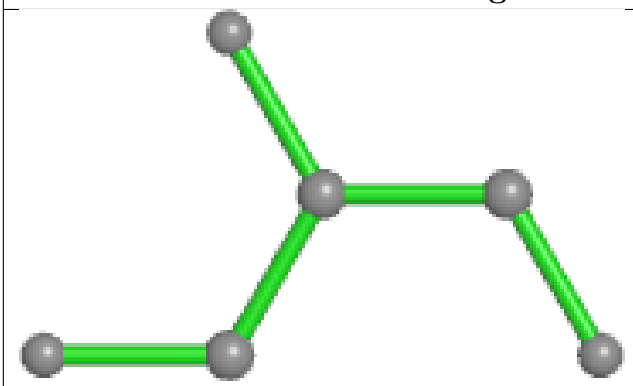


Torsions

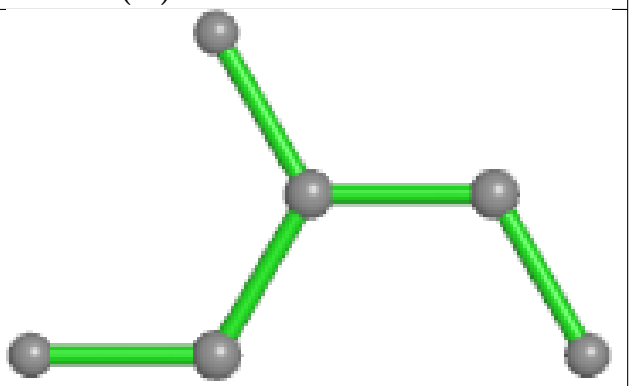


Rings

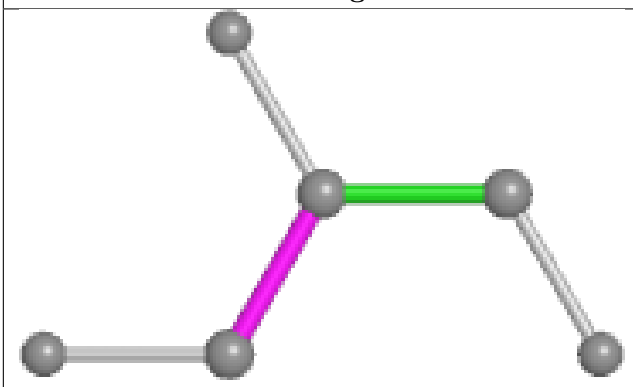
Ligand GOL D 601 (A)



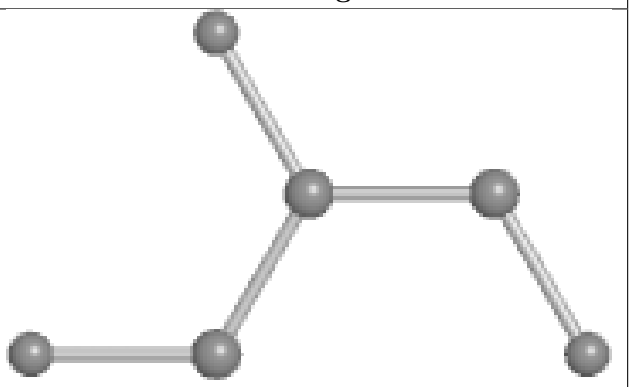
Bond lengths



Bond angles

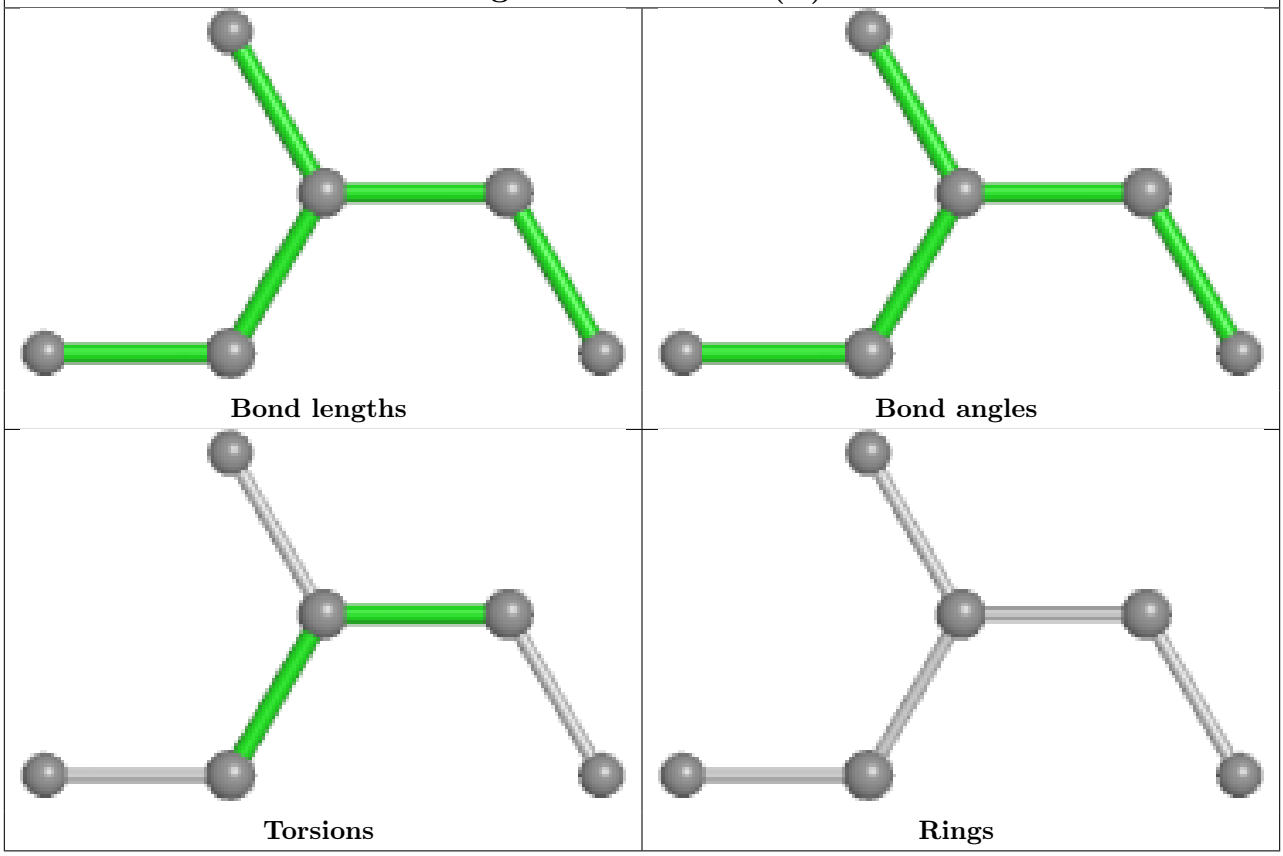


Torsions

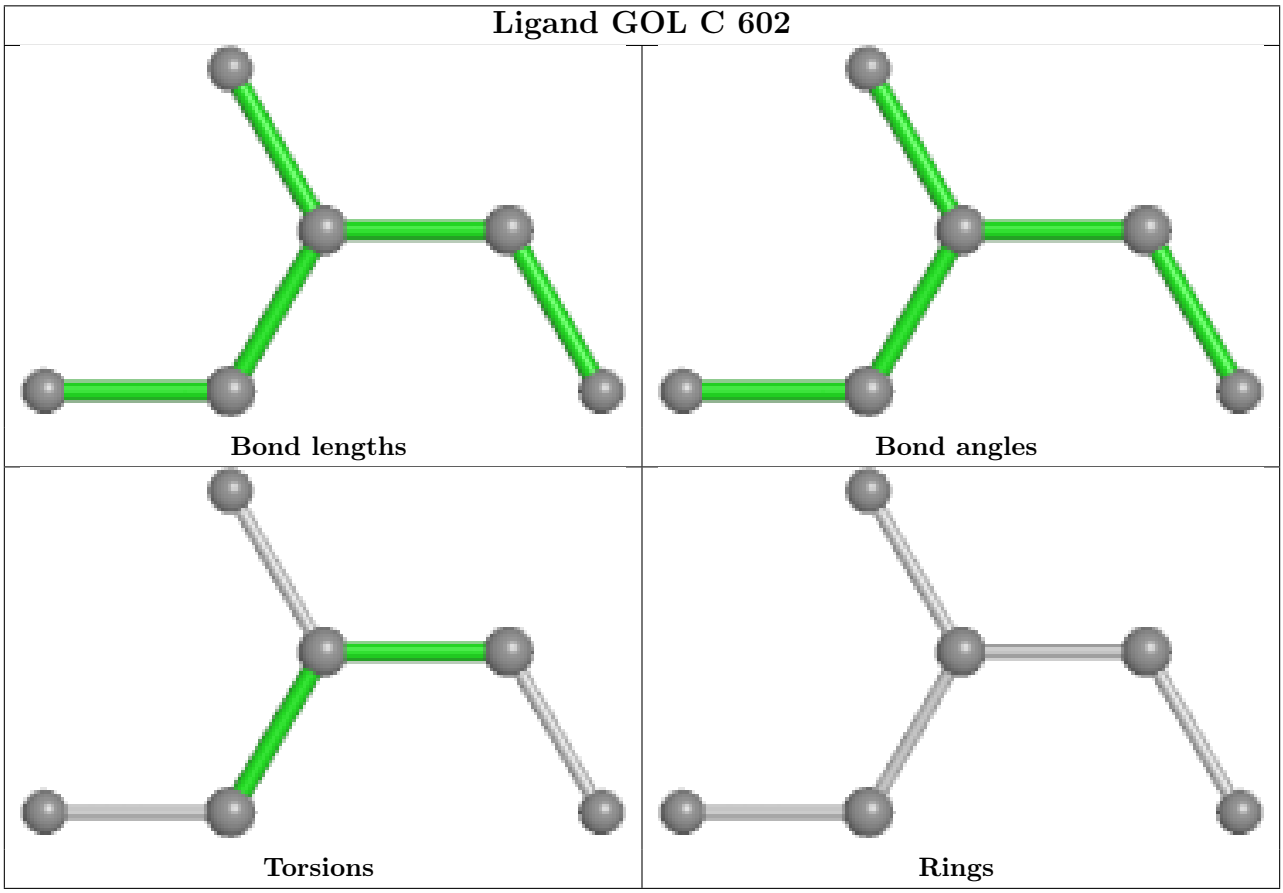


Rings

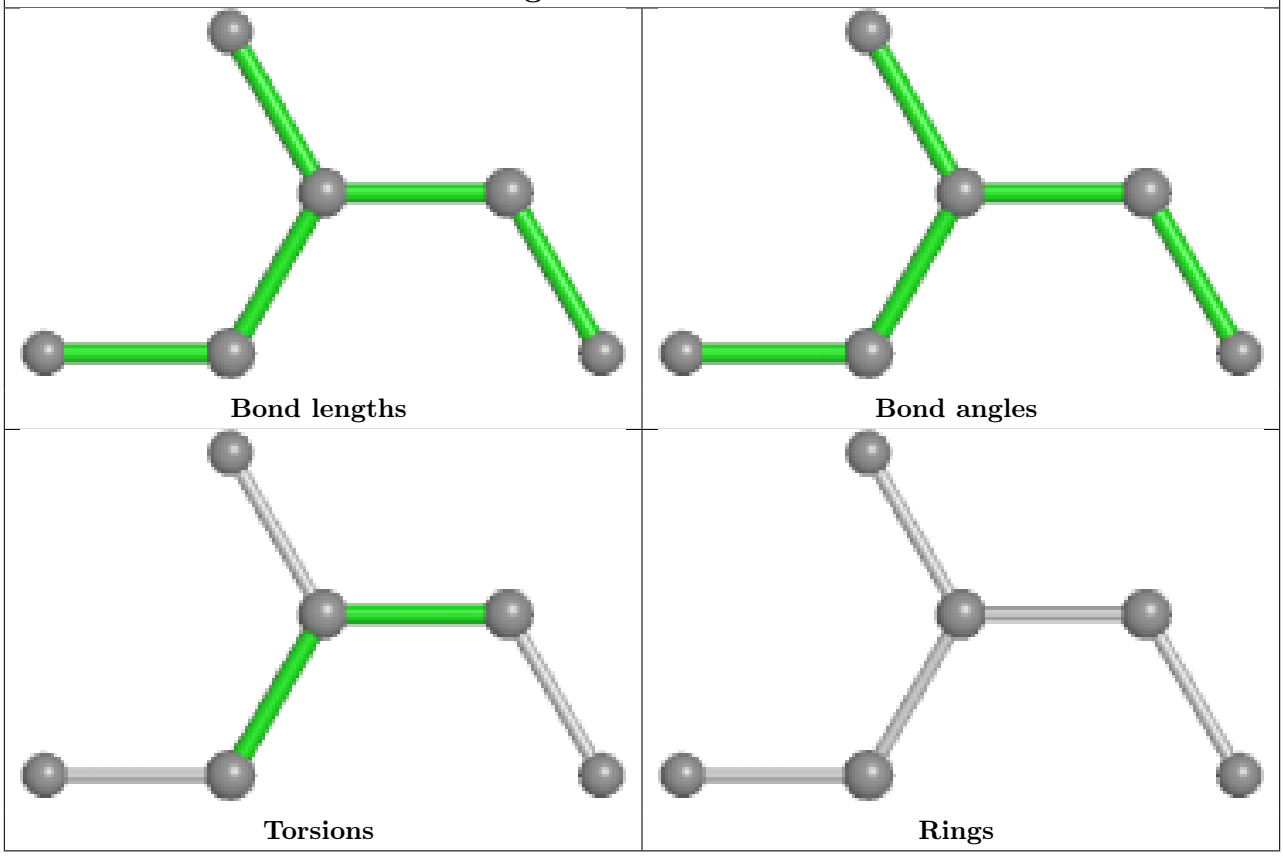
Ligand GOL A 601 (B)



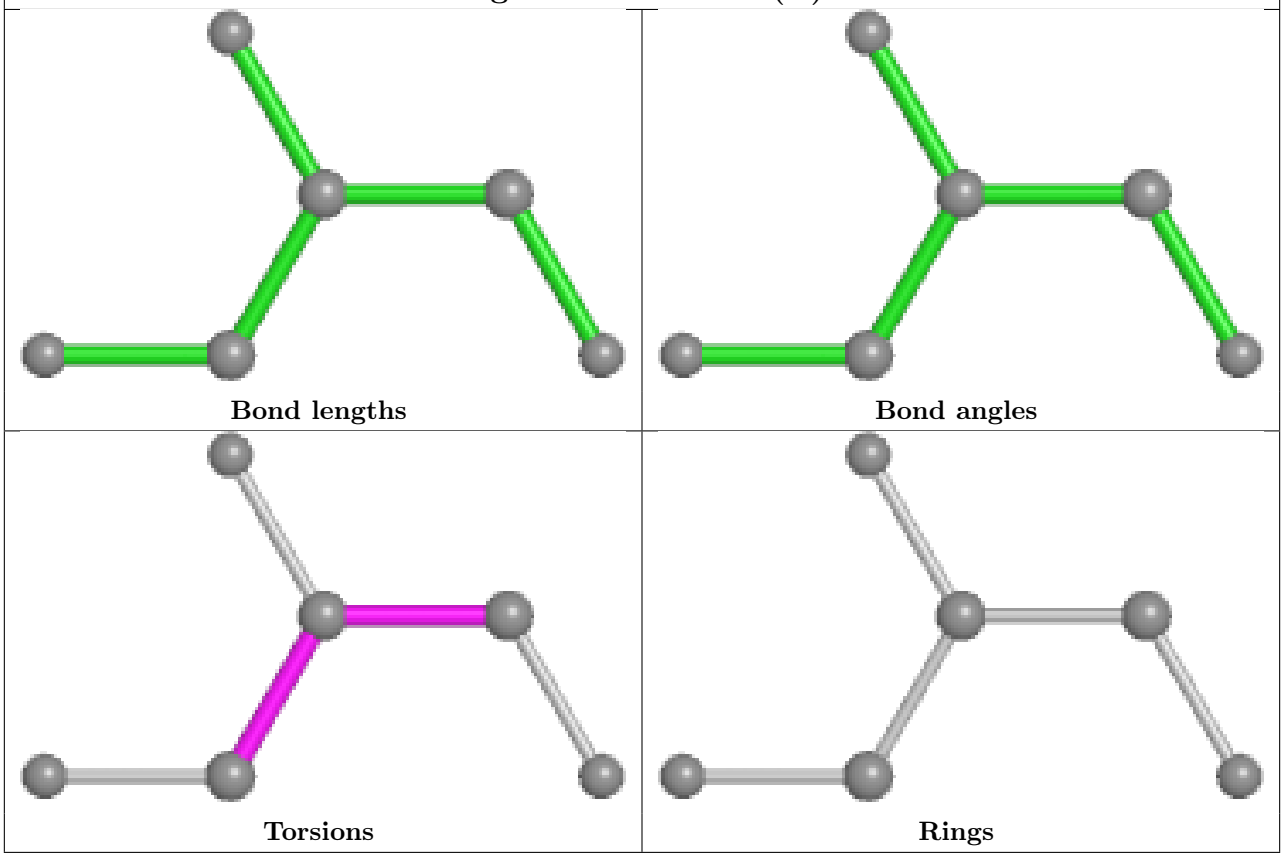
Ligand GOL C 602



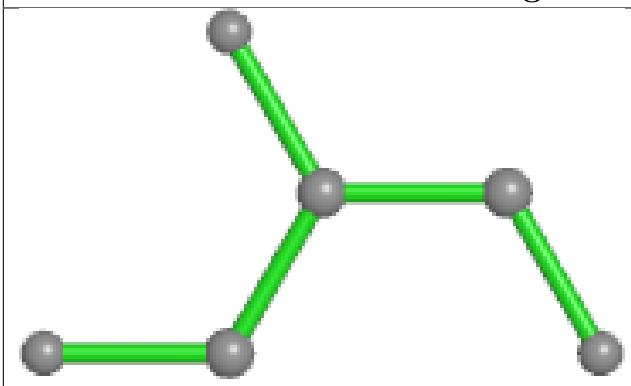
Ligand GOL C 604



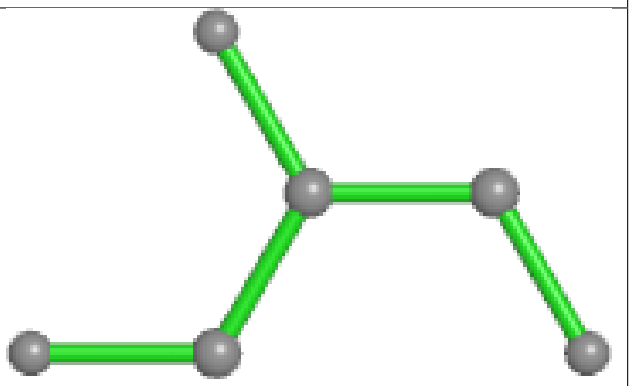
Ligand GOL D 601 (B)



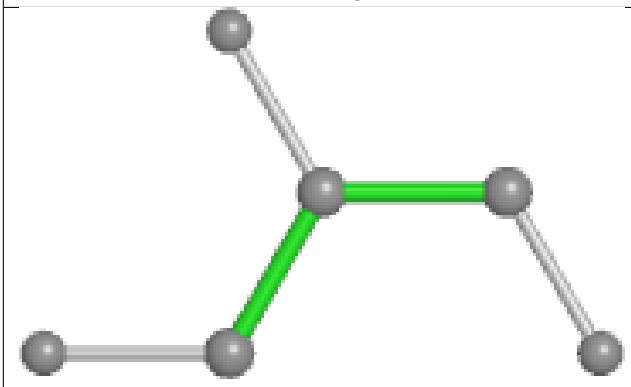
Ligand GOL B 602



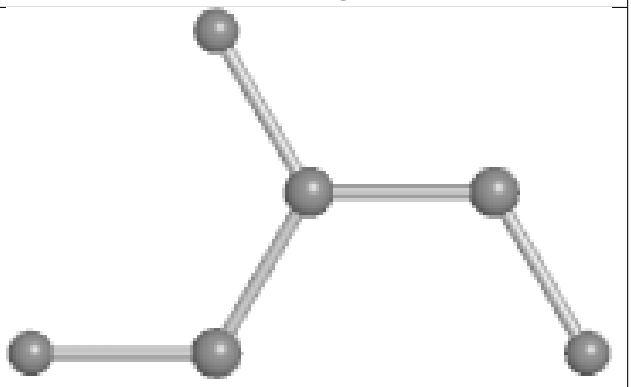
Bond lengths



Bond angles

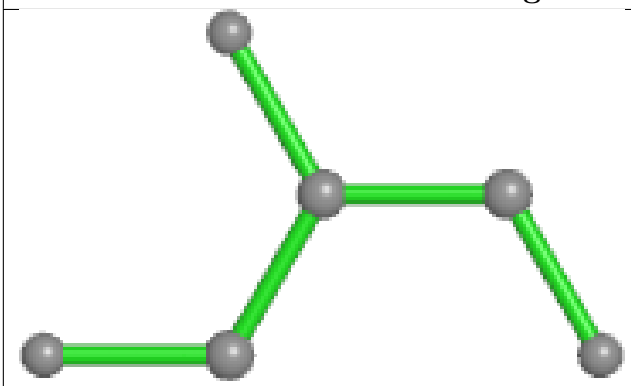


Torsions

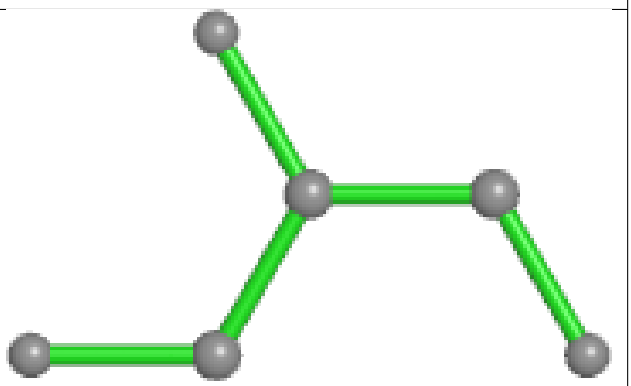


Rings

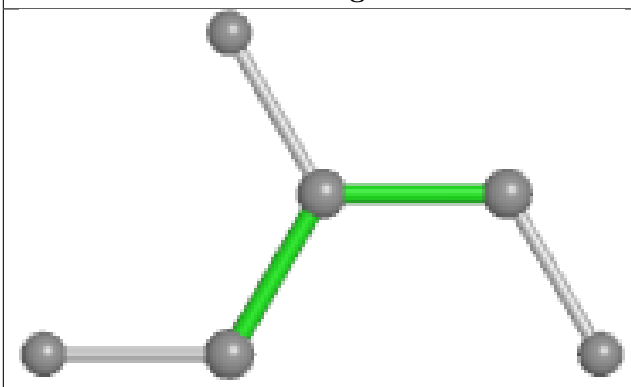
Ligand GOL C 601



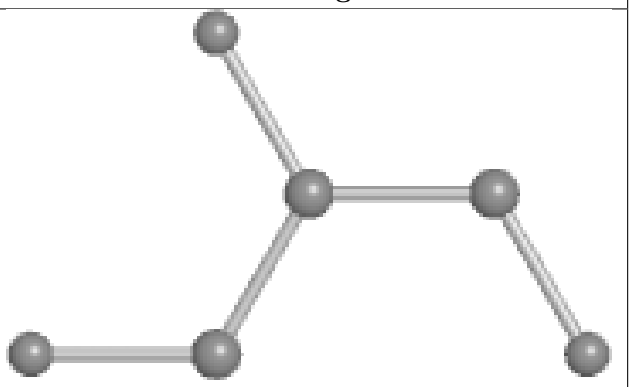
Bond lengths



Bond angles

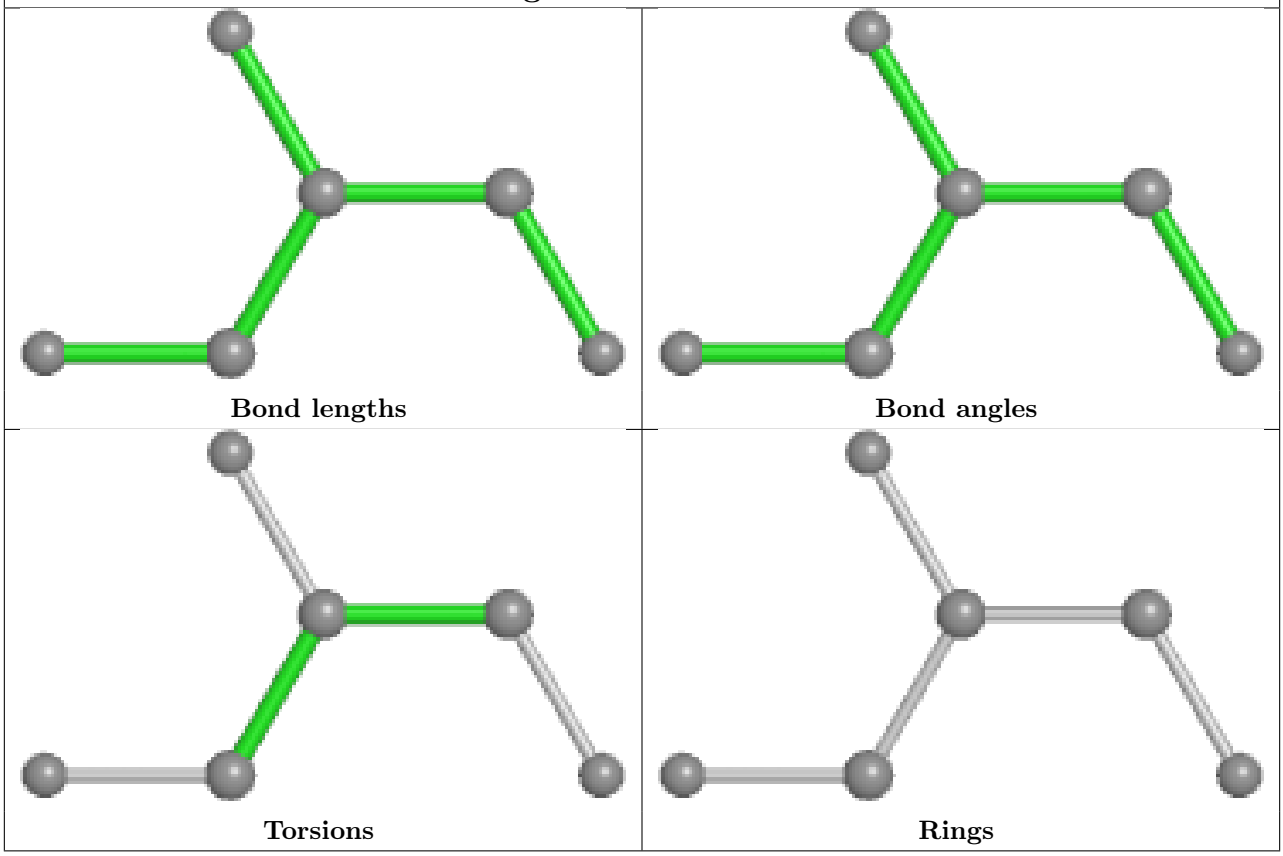


Torsions

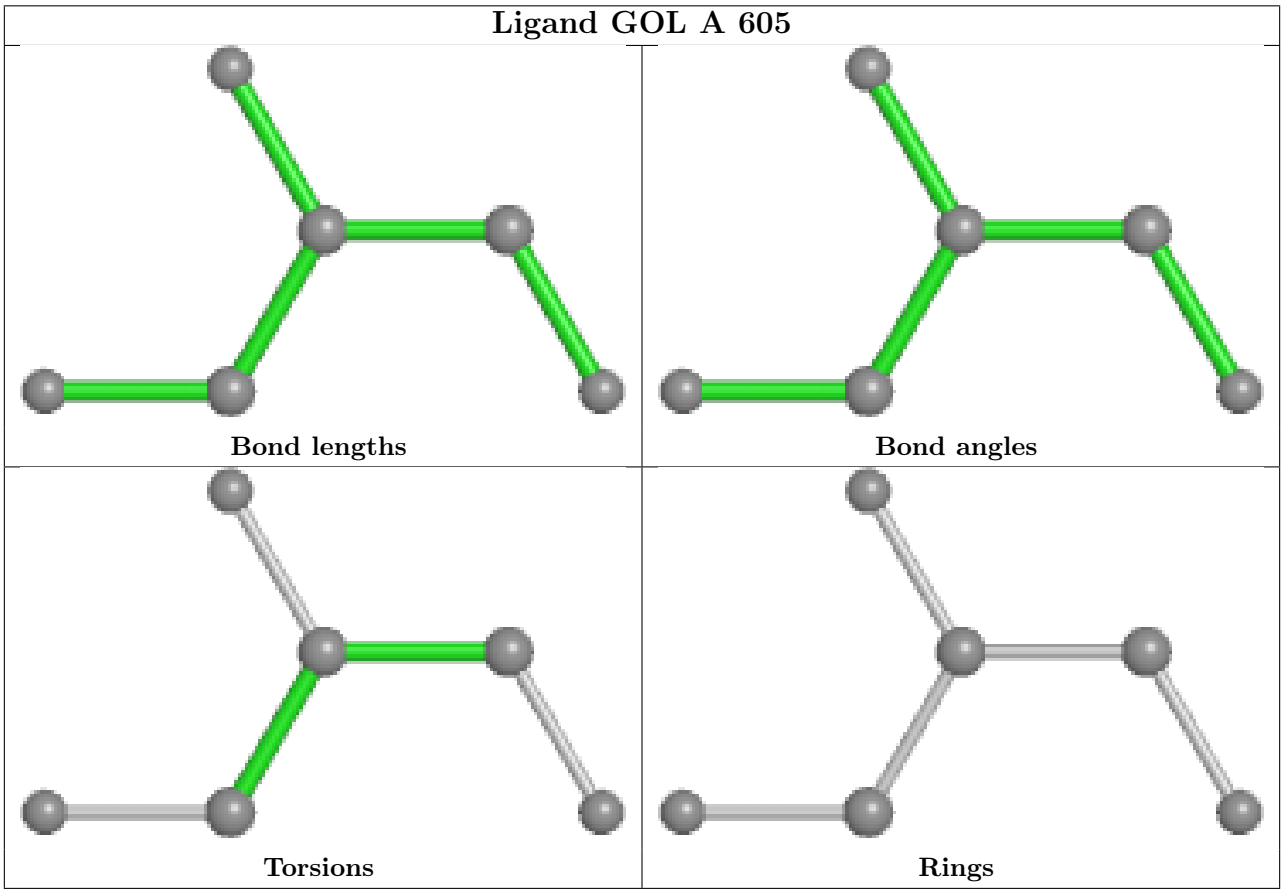


Rings

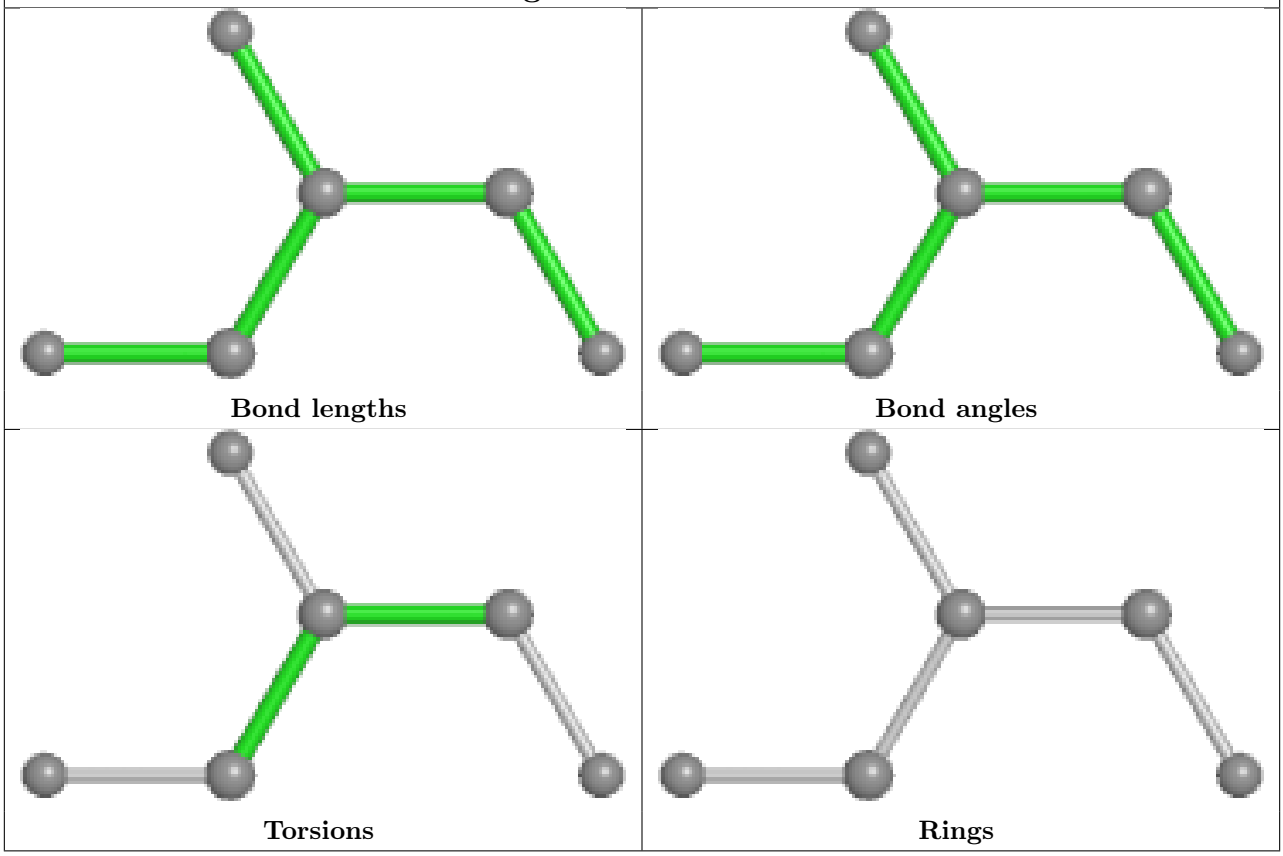
Ligand GOL D 604



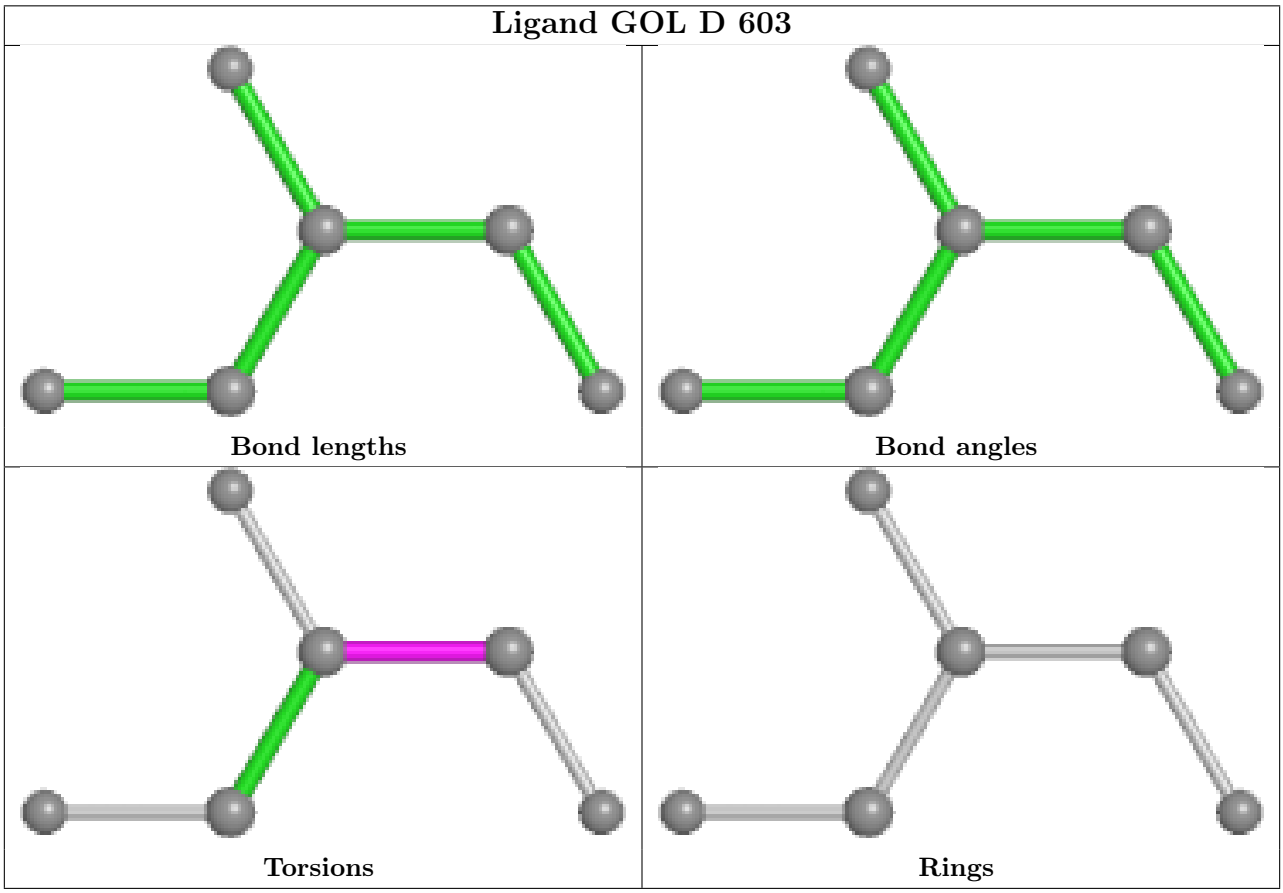
Ligand GOL A 605



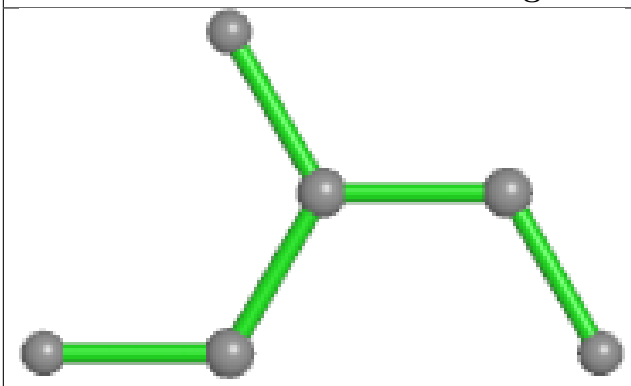
Ligand GOL D 605



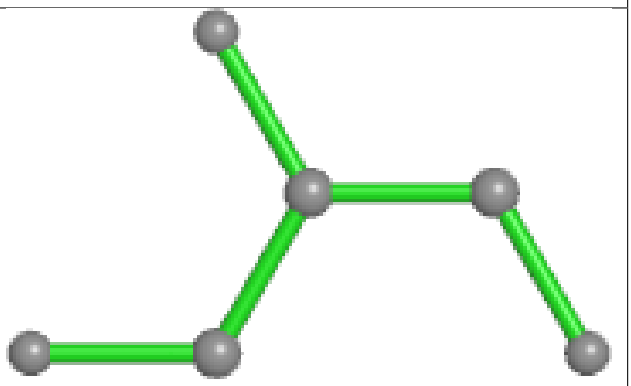
Ligand GOL D 603



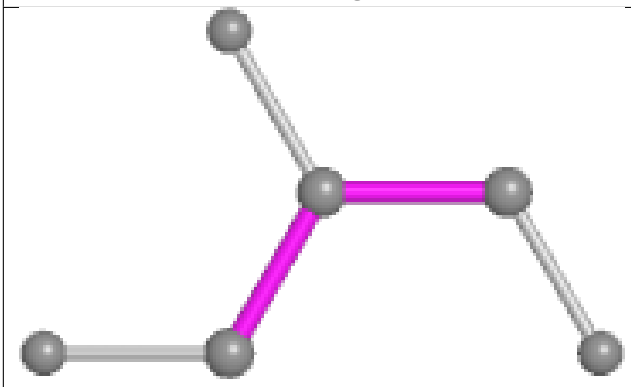
Ligand GOL B 601



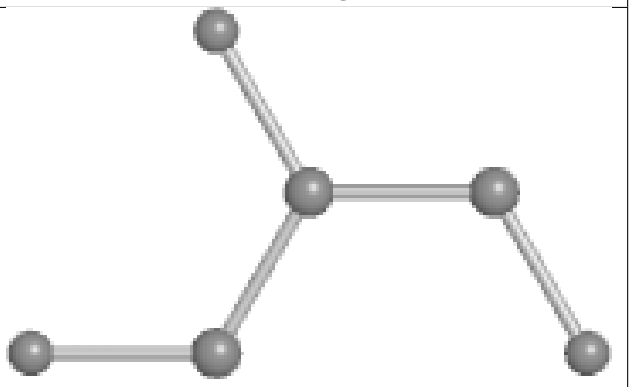
Bond lengths



Bond angles

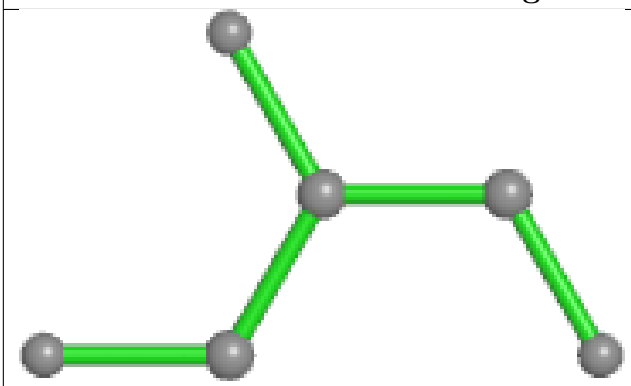


Torsions

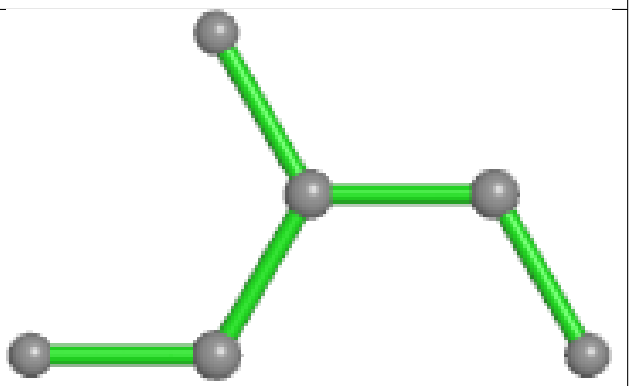


Rings

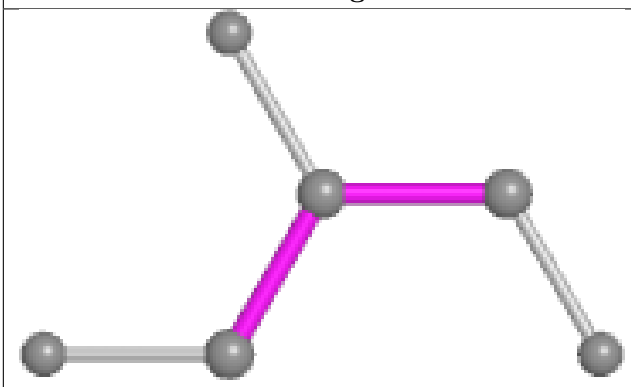
Ligand GOL A 603



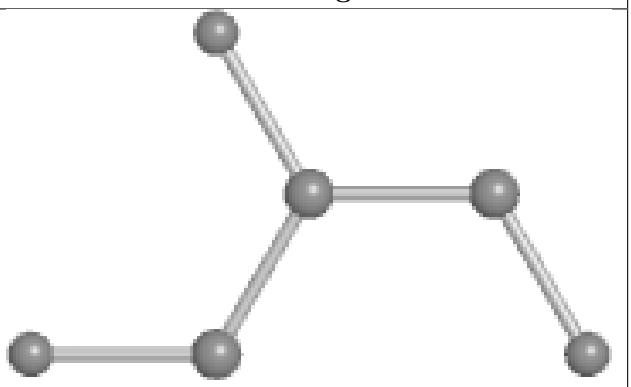
Bond lengths



Bond angles

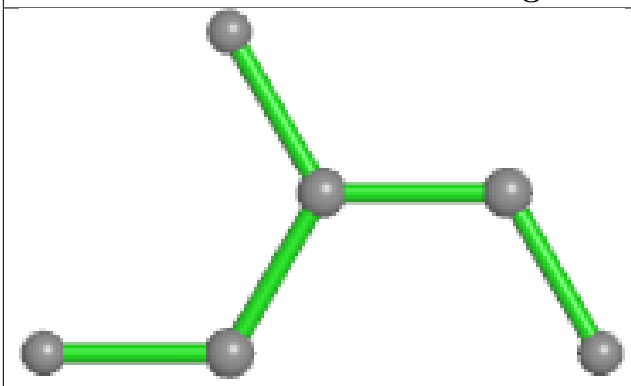


Torsions

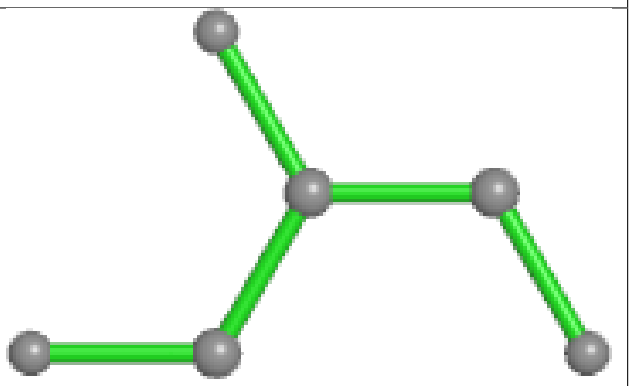


Rings

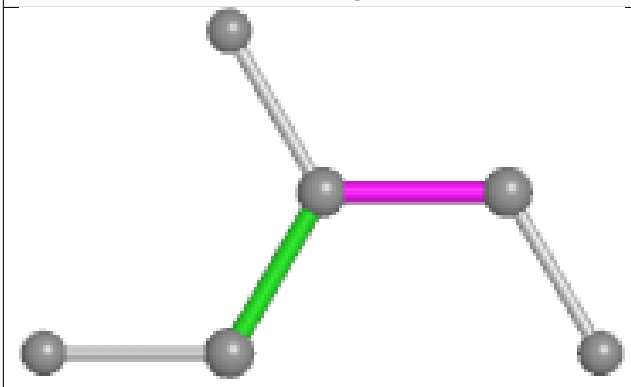
Ligand GOL A 604



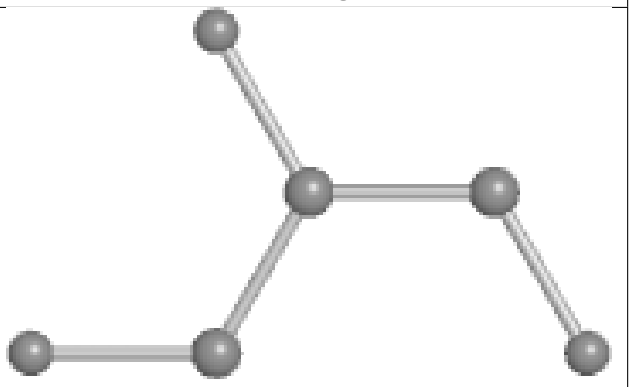
Bond lengths



Bond angles

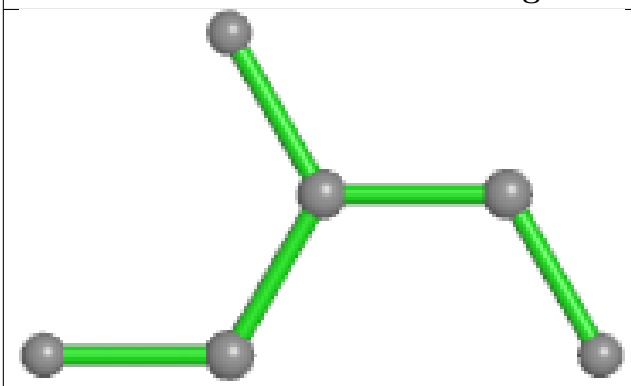


Torsions

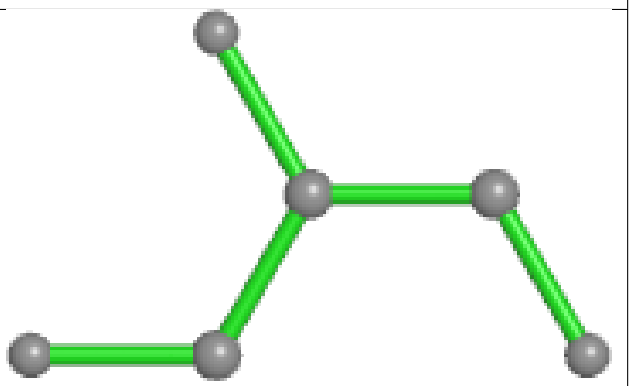


Rings

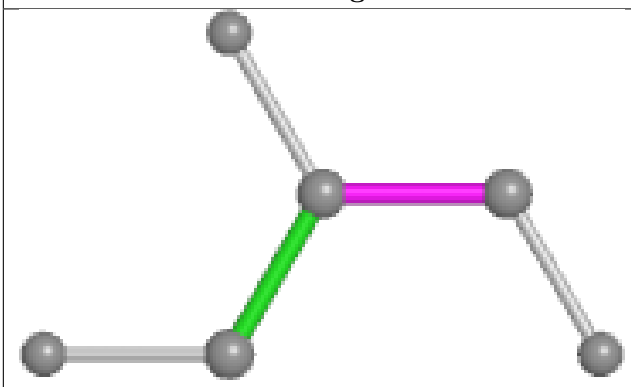
Ligand GOL A 607



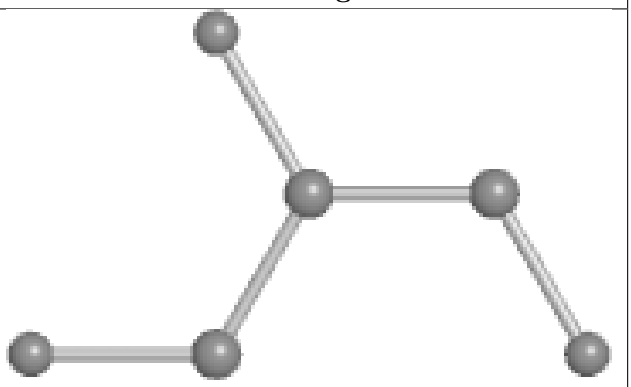
Bond lengths



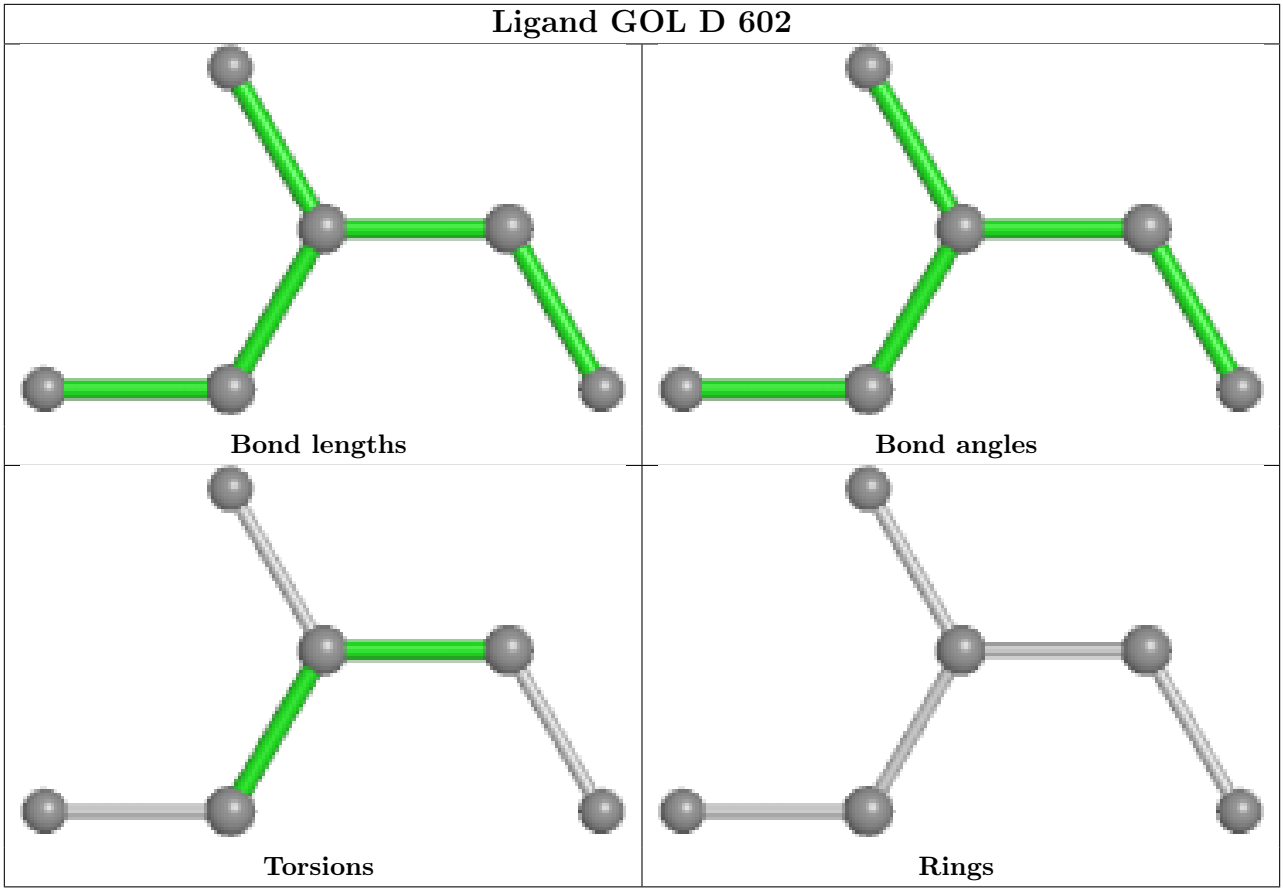
Bond angles



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	568/586 (96%)	-0.38	8 (1%)	75	75	17, 33, 59, 106	0
1	B	540/586 (92%)	-0.29	13 (2%)	59	59	20, 39, 61, 115	0
1	C	568/586 (96%)	-0.14	20 (3%)	44	44	18, 41, 74, 91	0
1	D	546/586 (93%)	-0.37	5 (0%)	84	84	17, 33, 57, 96	0
All	All	2222/2344 (94%)	-0.30	46 (2%)	63	64	17, 37, 65, 115	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	TRP	6.6
1	A	579	LEU	6.1
1	D	167	SER	5.7
1	B	179	LEU	4.6
1	B	213	ASN	4.6
1	C	12	TYR	4.0
1	A	413	ARG	3.9
1	A	12	TYR	3.7
1	B	205	THR	3.5
1	B	236	SER	3.5
1	B	82	ASN	3.5
1	A	549	ILE	3.4
1	C	517	ALA	3.4
1	B	215	GLN	3.2
1	C	578	PRO	3.1
1	B	238	ARG	3.0
1	A	572	LEU	2.9
1	B	60	THR	2.9
1	C	534	GLY	2.8
1	B	214	GLY	2.7
1	C	449	THR	2.7

Continued on next page...

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Mol	Chain	Res	Type	RSRZ
1	C	571	LEU	2.7
1	D	450	SER	2.6
1	B	206	VAL	2.6
1	C	474	SER	2.6
1	C	572	LEU	2.6
1	C	475	VAL	2.6
1	C	13	SER	2.5
1	C	550	GLY	2.5
1	C	518	GLY	2.5
1	C	516	ALA	2.5
1	C	519	ASN	2.4
1	C	530	GLY	2.4
1	D	213	ASN	2.3
1	C	413	ARG	2.3
1	C	450	SER	2.3
1	C	520	SER	2.2
1	C	495	CYS	2.2
1	D	264	ASP	2.2
1	A	488	PRO	2.2
1	D	206	VAL	2.2
1	B	435	TYR	2.1
1	B	62	THR	2.1
1	C	549	ILE	2.1
1	A	578	PRO	2.1
1	A	447	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

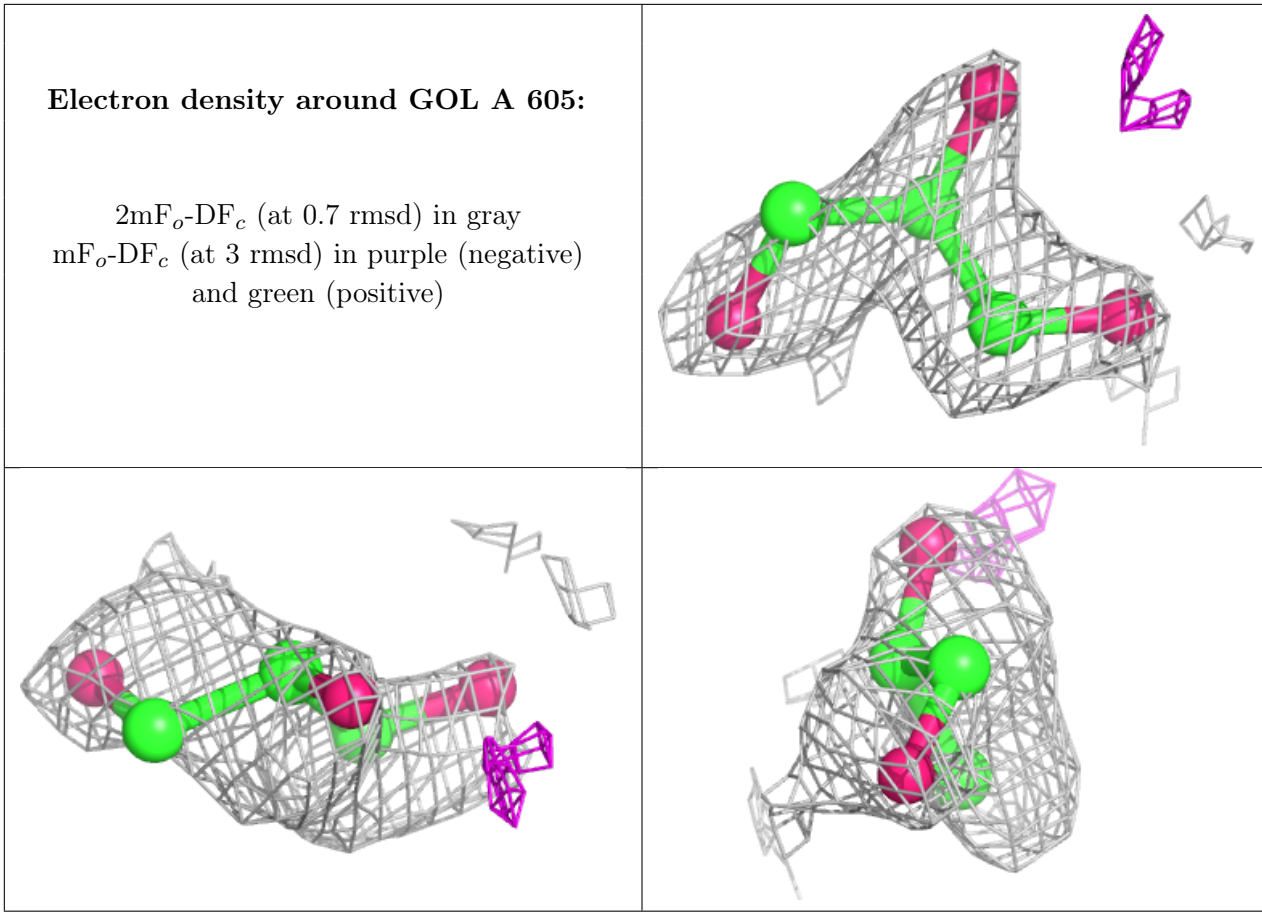
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	605	6/6	0.70	0.30	86,91,96,98	0
2	GOL	A	607	6/6	0.72	0.26	70,73,89,93	0
2	GOL	A	608	6/6	0.72	0.23	63,71,72,78	0
2	GOL	D	602	6/6	0.78	0.17	34,37,41,42	0
2	GOL	D	601[A]	6/6	0.81	0.21	47,49,52,56	6
2	GOL	D	601[B]	6/6	0.81	0.21	43,49,53,53	6
2	GOL	C	603	6/6	0.81	0.22	40,54,57,64	0
2	GOL	A	602	6/6	0.83	0.17	52,57,72,73	0
2	GOL	B	602	6/6	0.83	0.22	66,71,73,75	0
2	GOL	D	604	6/6	0.85	0.19	23,36,49,63	0
2	GOL	A	604	6/6	0.87	0.31	55,56,57,60	0
2	GOL	D	605	6/6	0.87	0.19	55,58,69,77	0
2	GOL	A	603	6/6	0.89	0.22	37,62,66,69	0
2	GOL	C	601	6/6	0.90	0.27	50,55,59,60	0
2	GOL	D	603	6/6	0.90	0.22	54,61,68,69	0
2	GOL	C	602	6/6	0.93	0.10	30,39,44,46	0
2	GOL	A	606	6/6	0.93	0.10	27,31,37,47	0
2	GOL	A	601[A]	6/6	0.94	0.13	23,28,31,31	6
2	GOL	A	601[B]	6/6	0.94	0.13	23,28,30,34	6
2	GOL	B	603	6/6	0.94	0.22	38,52,73,78	0
2	GOL	B	601	6/6	0.95	0.12	26,36,47,56	0
2	GOL	C	604	6/6	0.96	0.10	34,39,44,62	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.

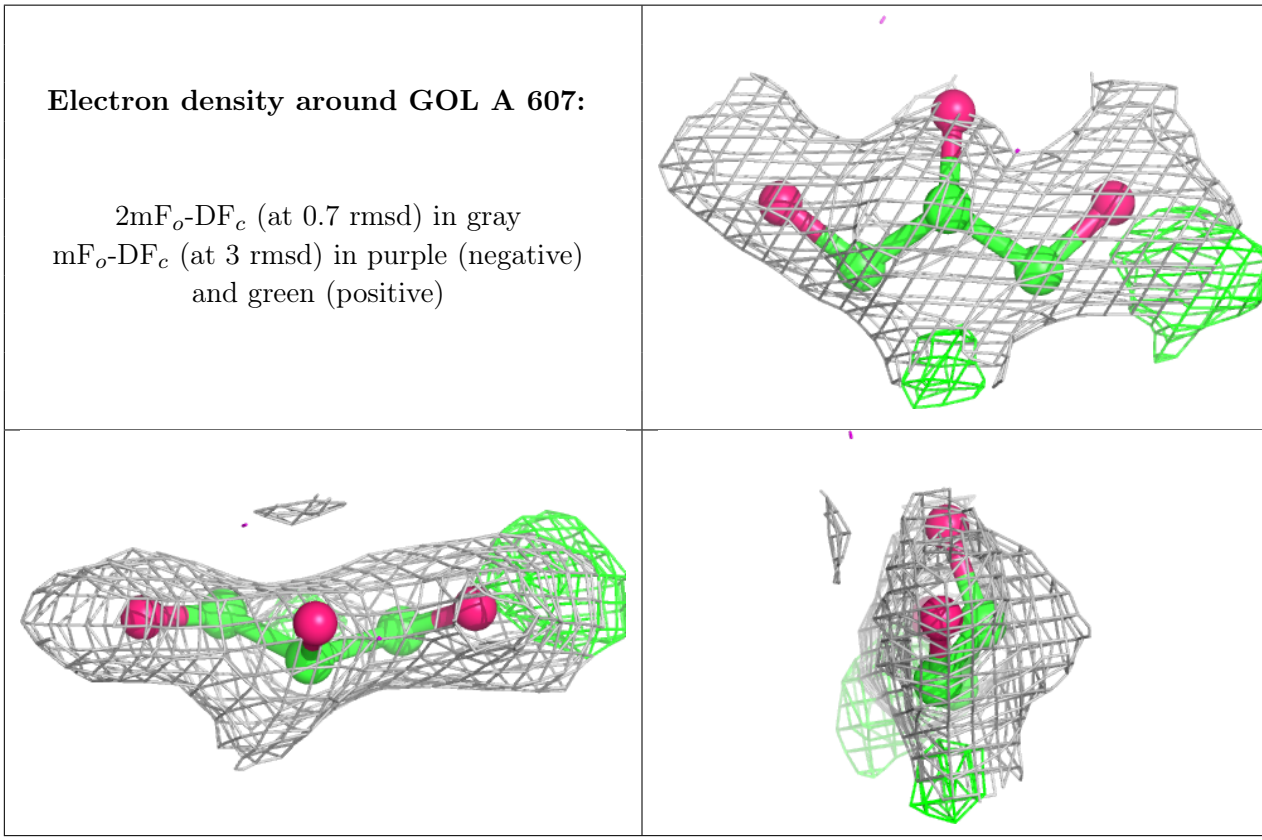
Electron density around GOL A 605:

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



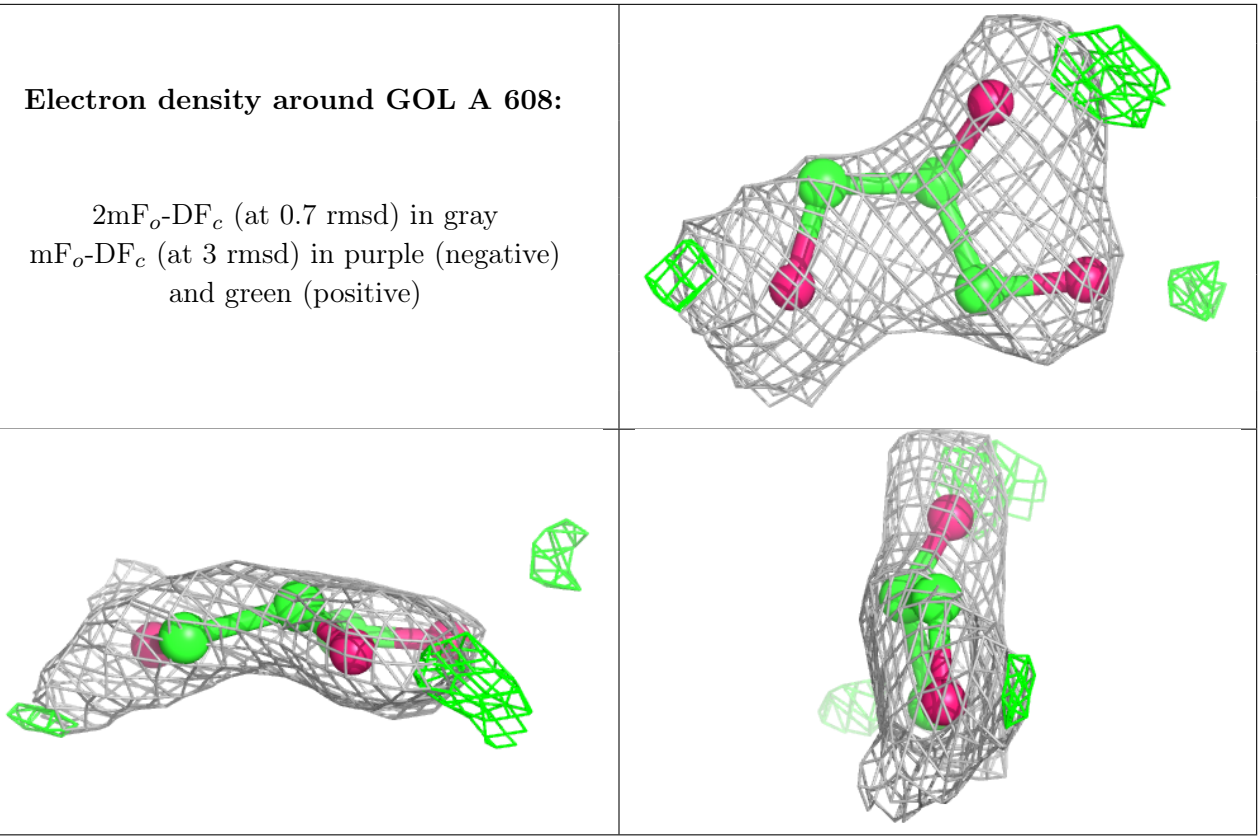
Electron density around GOL A 607:

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



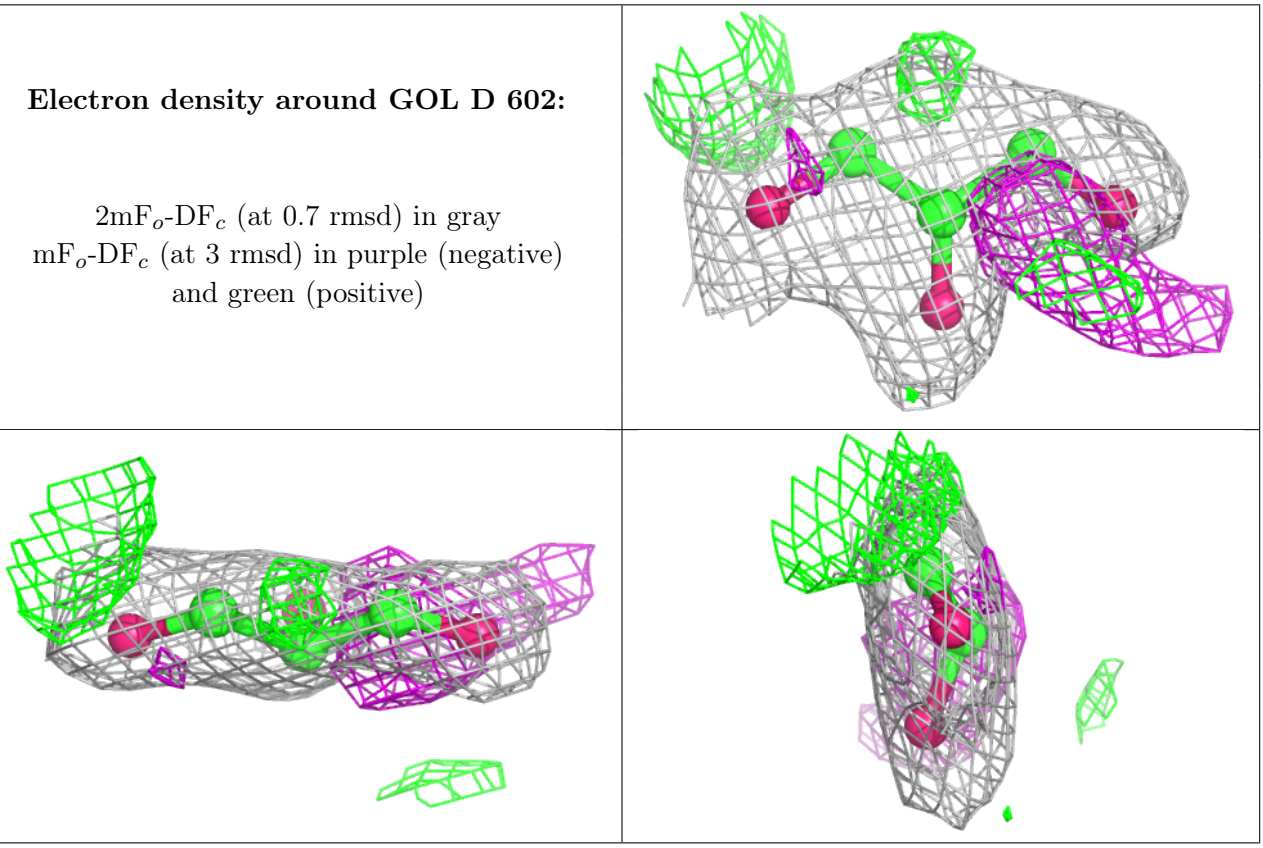
Electron density around GOL A 608:

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



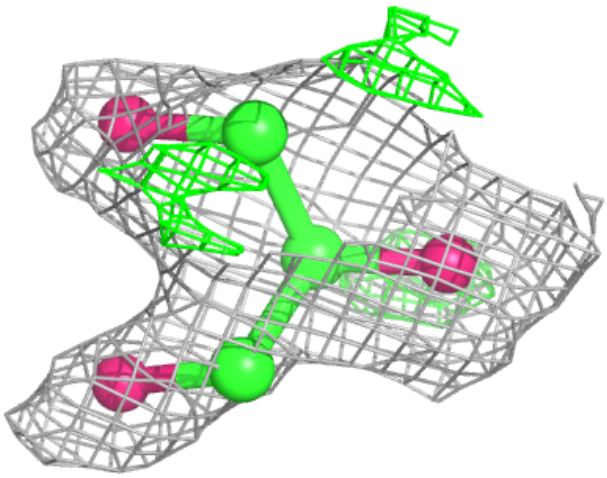
Electron density around GOL D 602:

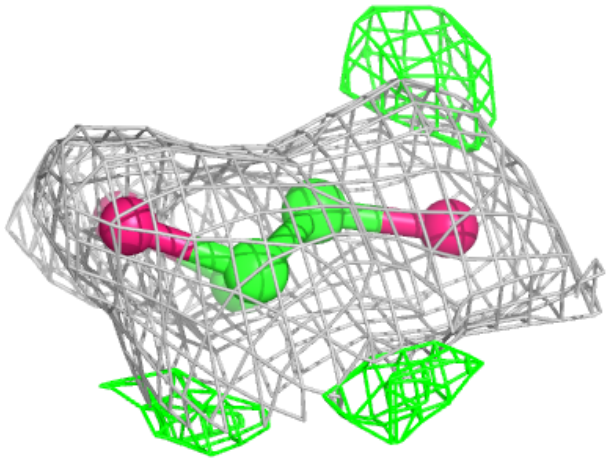
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

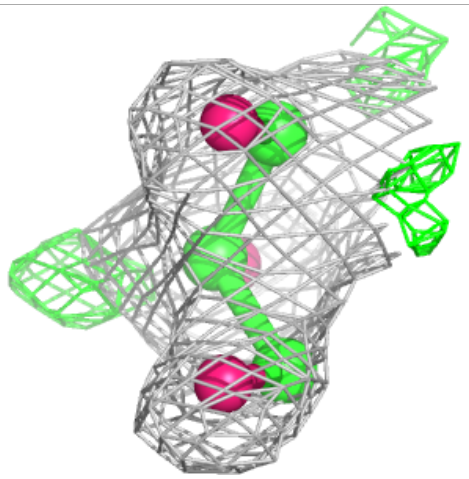


Electron density around GOL D 601 (A):

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

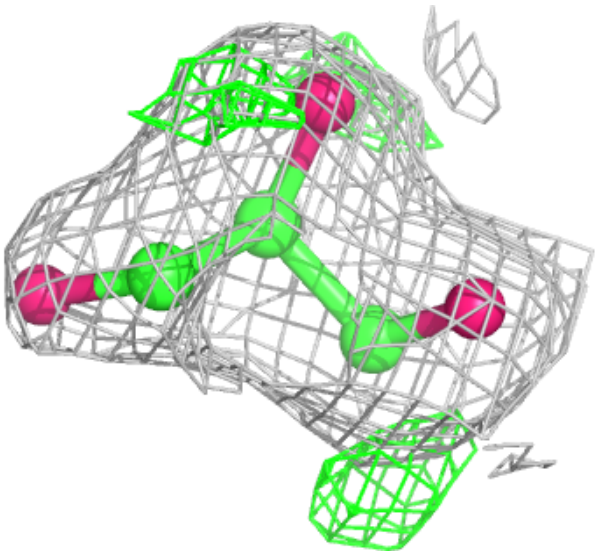


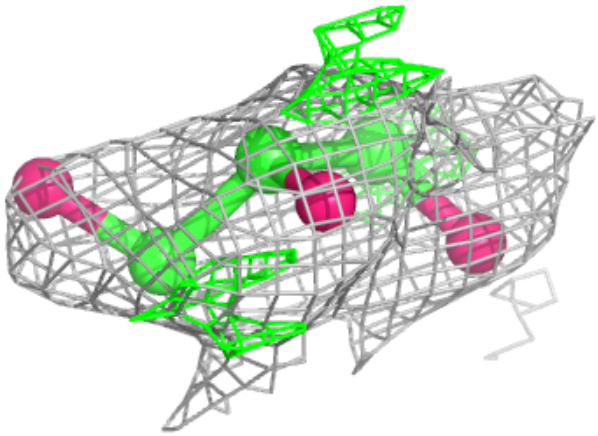


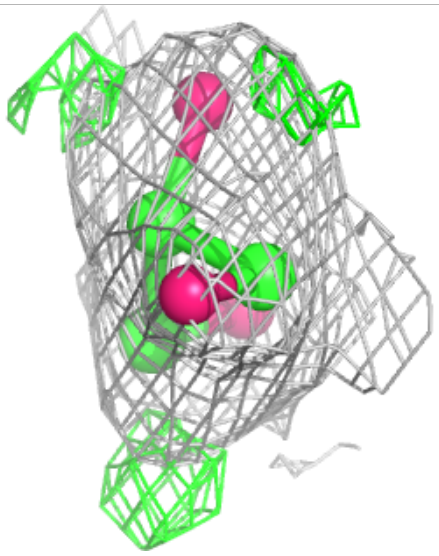


Electron density around GOL D 601 (B):

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

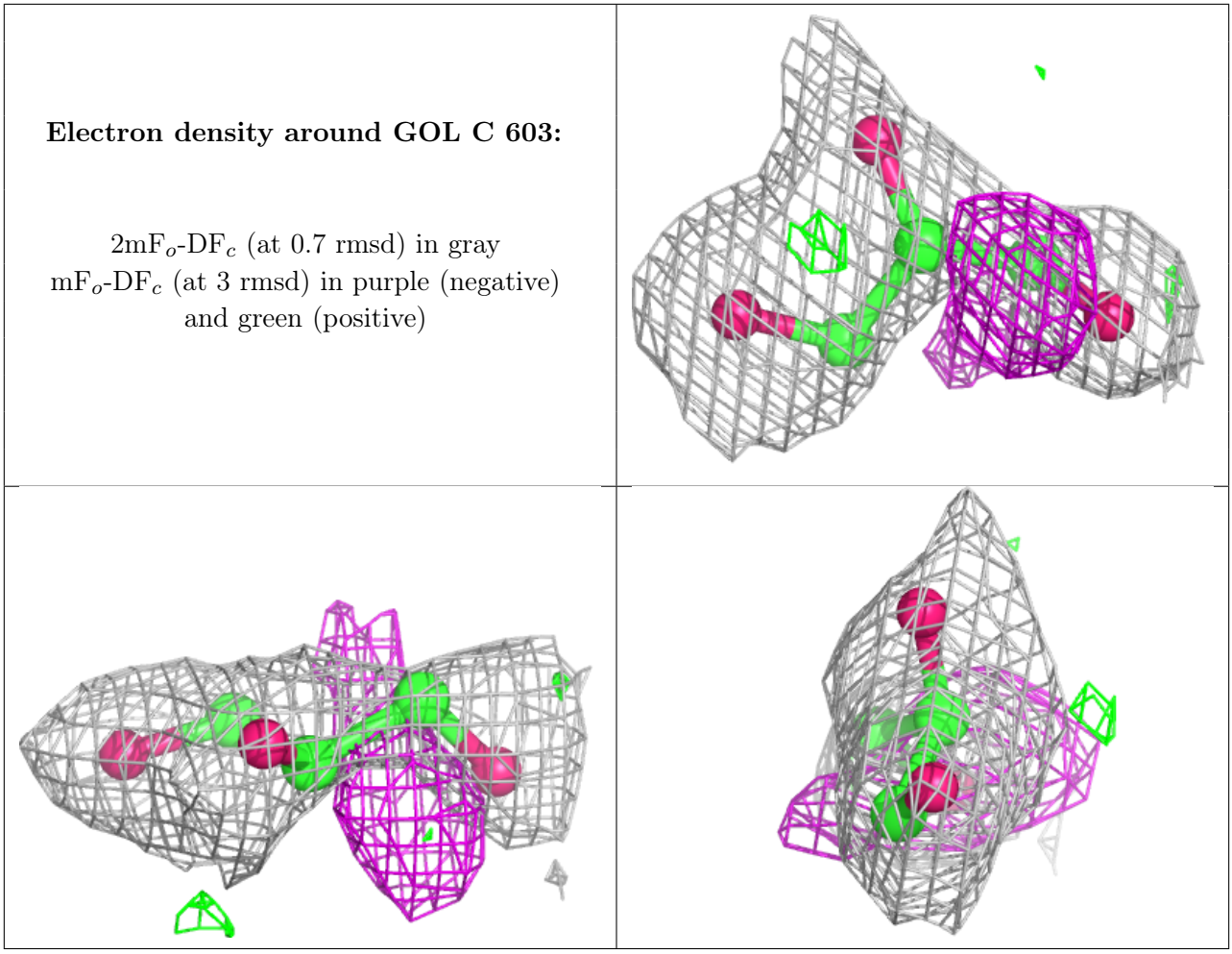






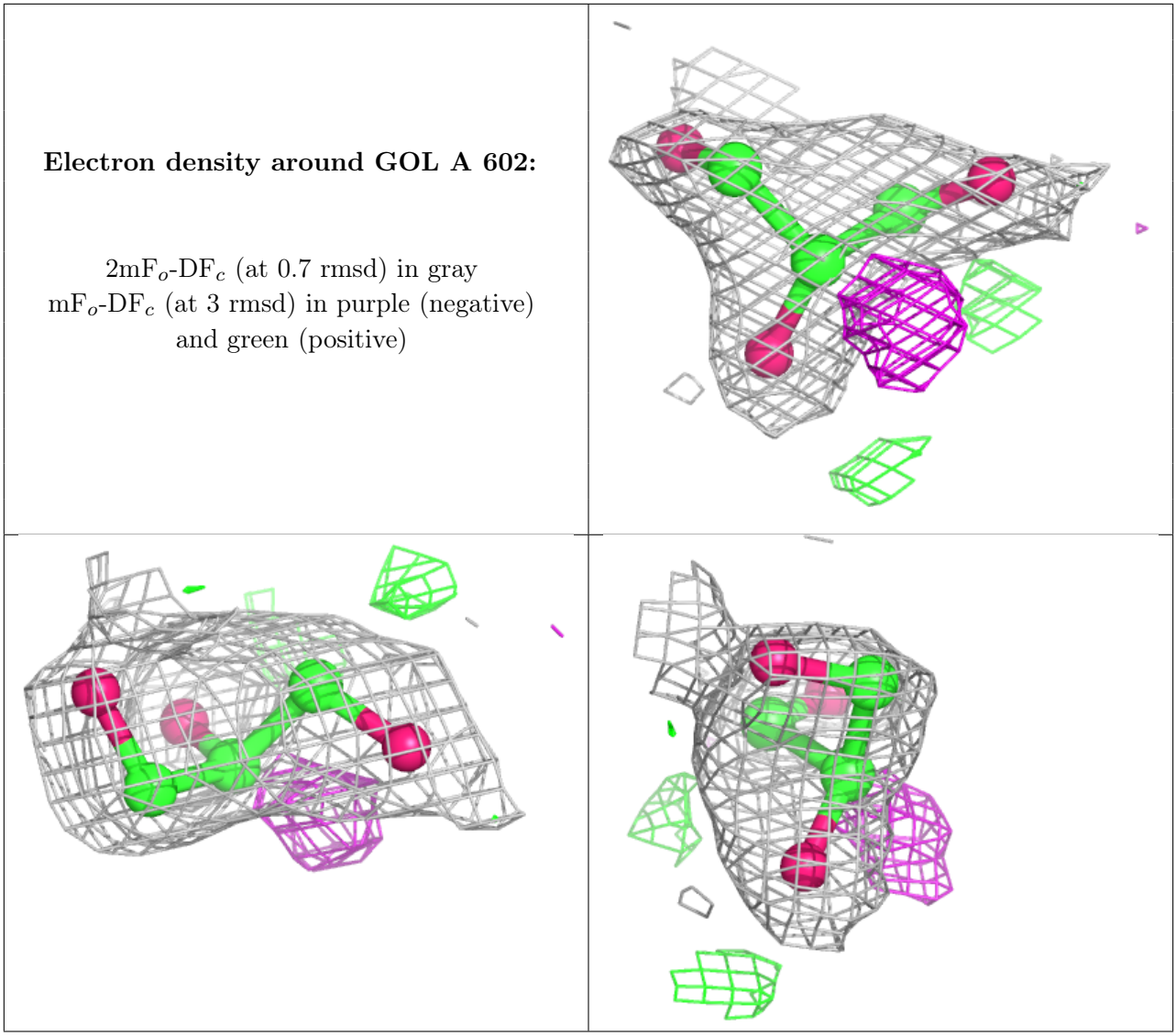
Electron density around GOL C 603:

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



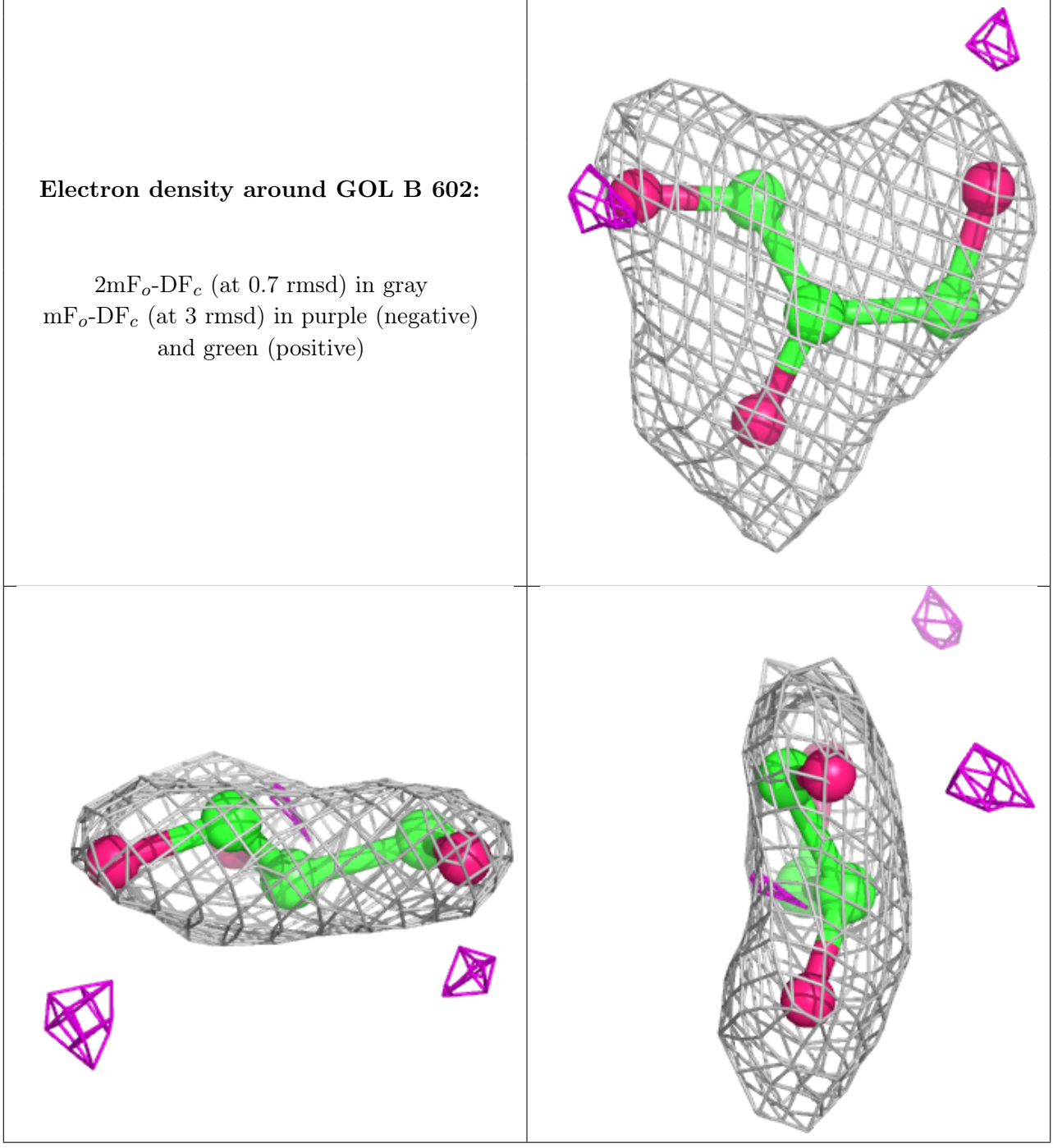
Electron density around GOL A 602:

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



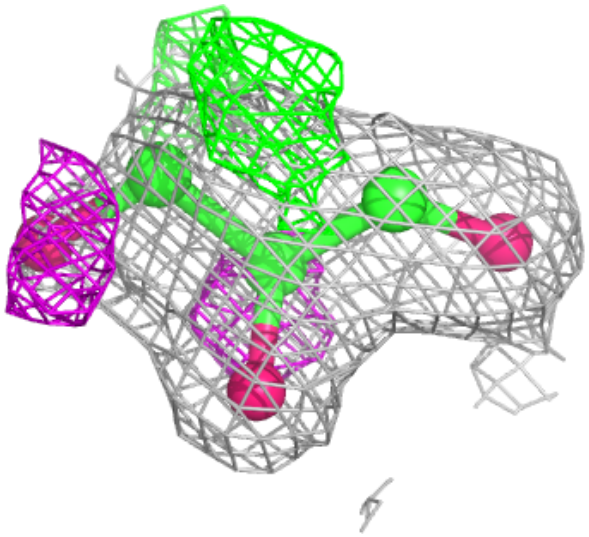
Electron density around GOL B 602:

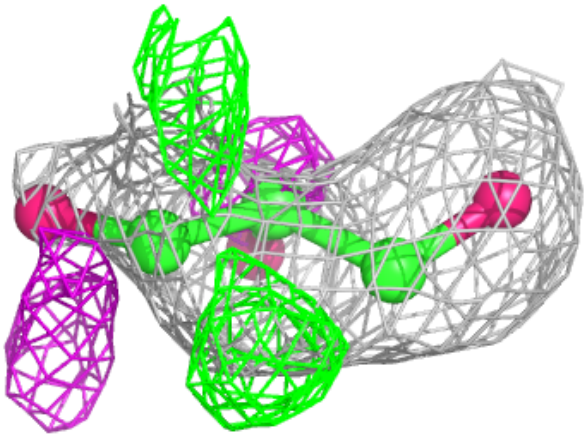
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

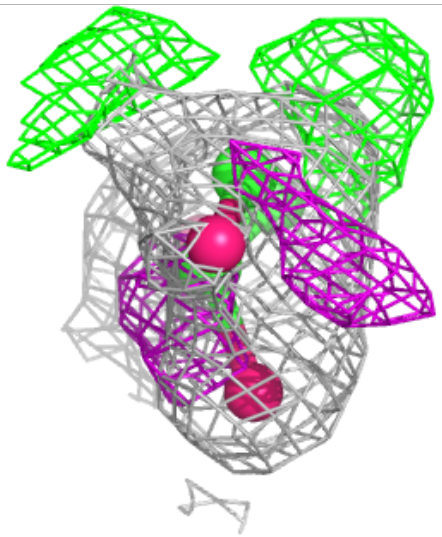


Electron density around GOL D 604:

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

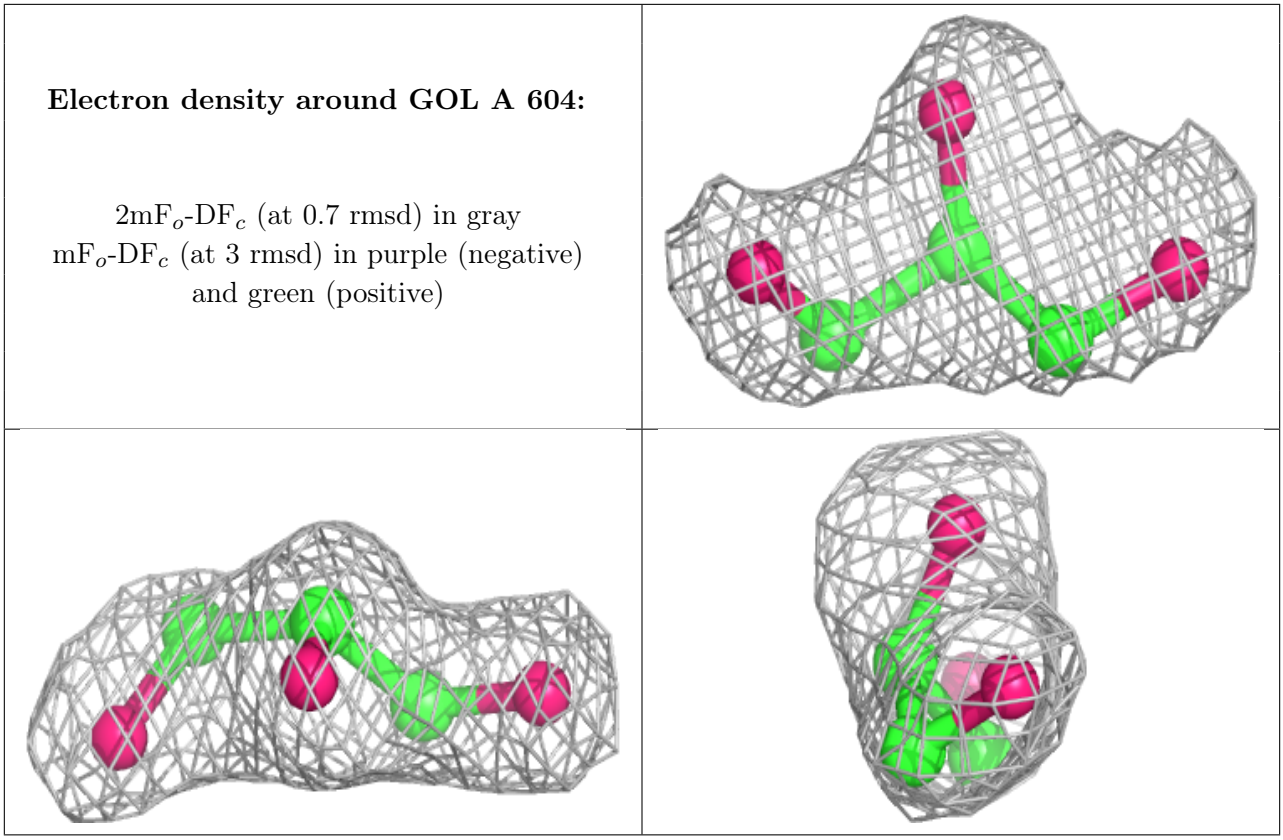






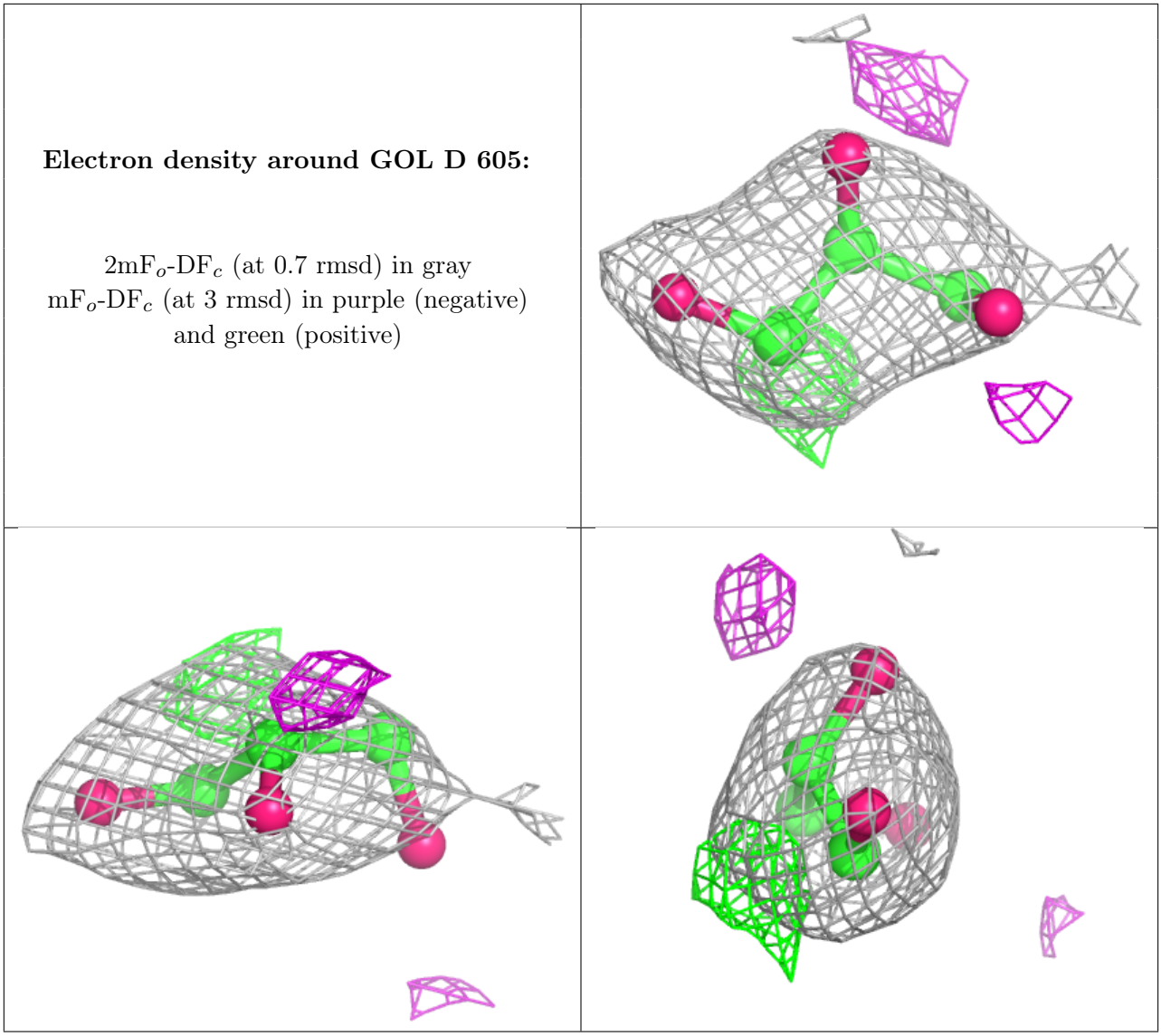
Electron density around GOL A 604:

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



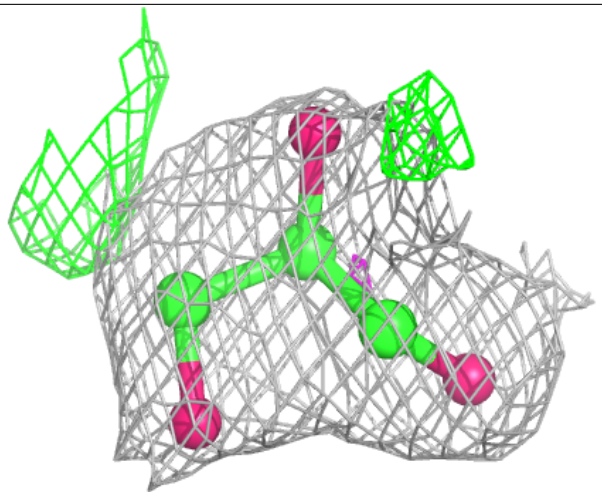
Electron density around GOL D 605:

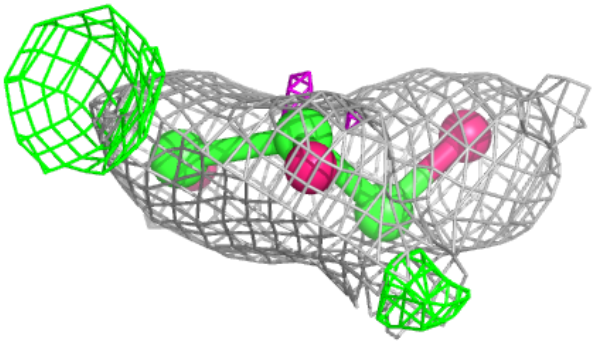
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

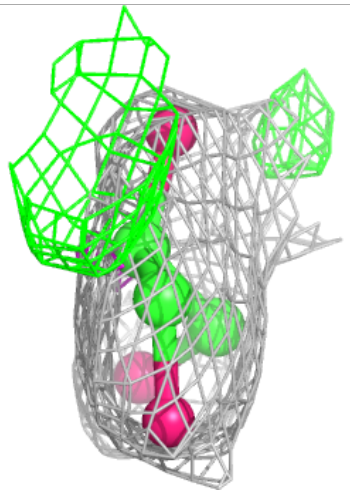


Electron density around GOL A 603:

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

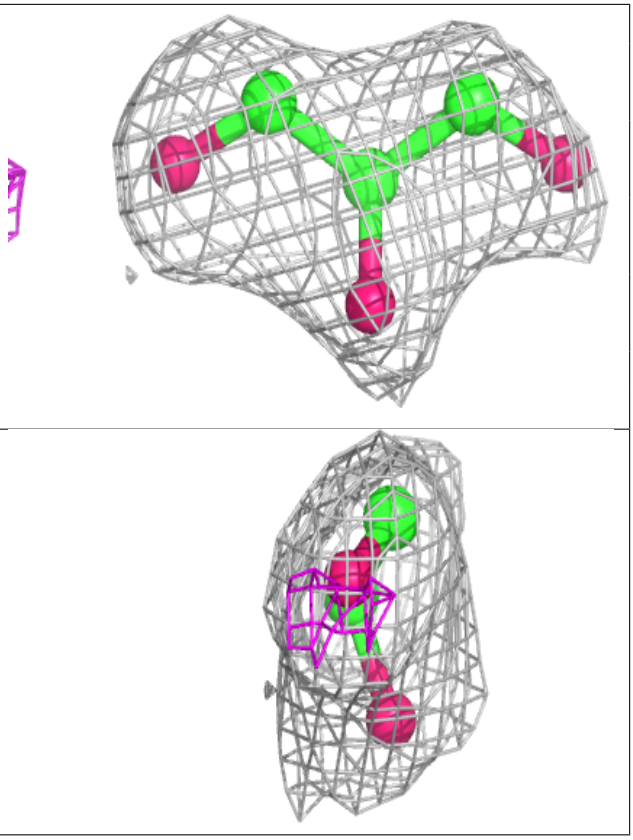


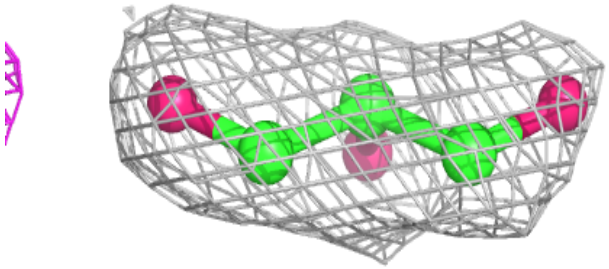




Electron density around GOL C 601:

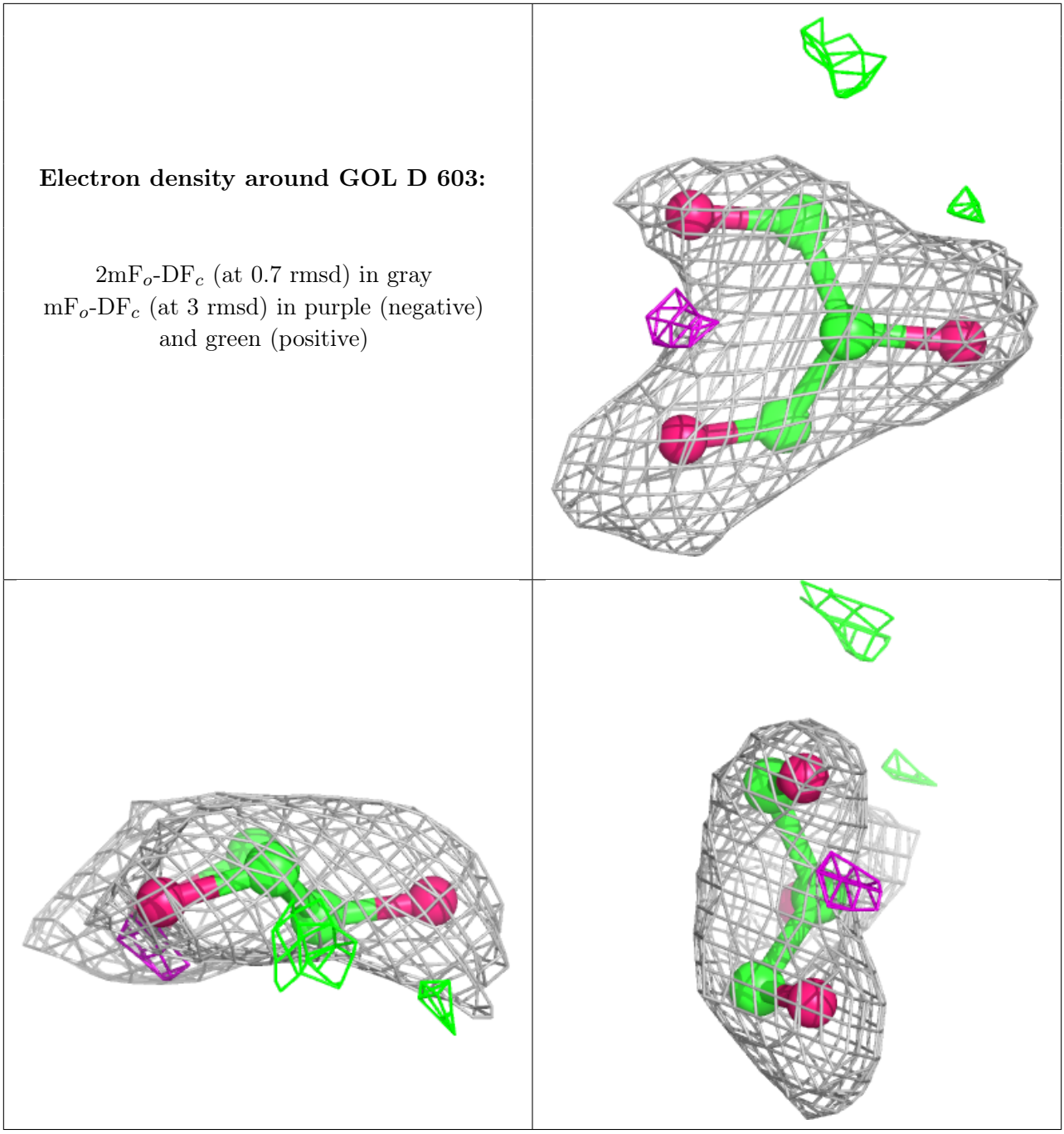
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





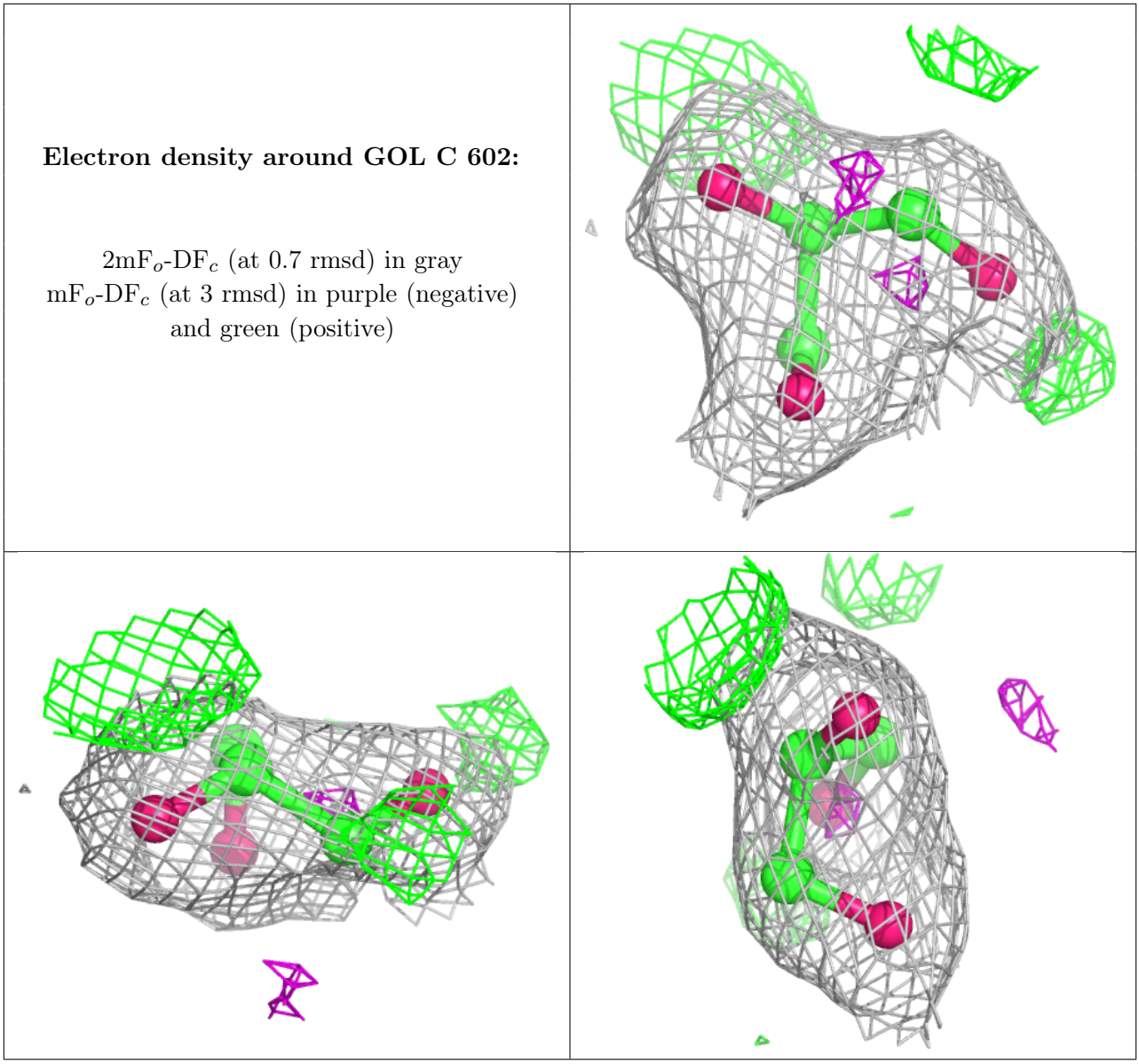
Electron density around GOL D 603:

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



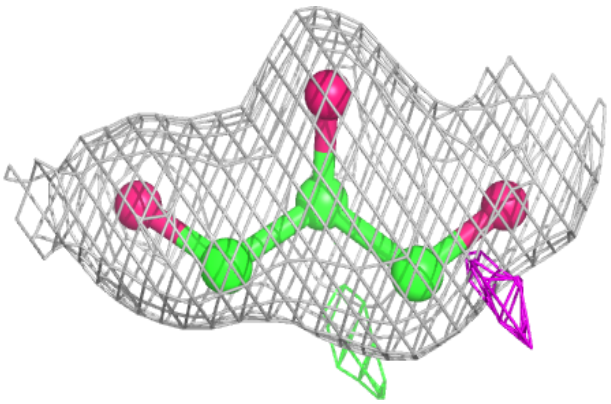
Electron density around GOL C 602:

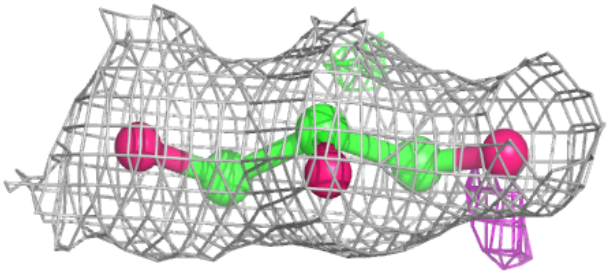
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

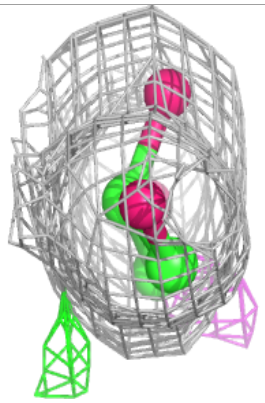


Electron density around GOL A 606:

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

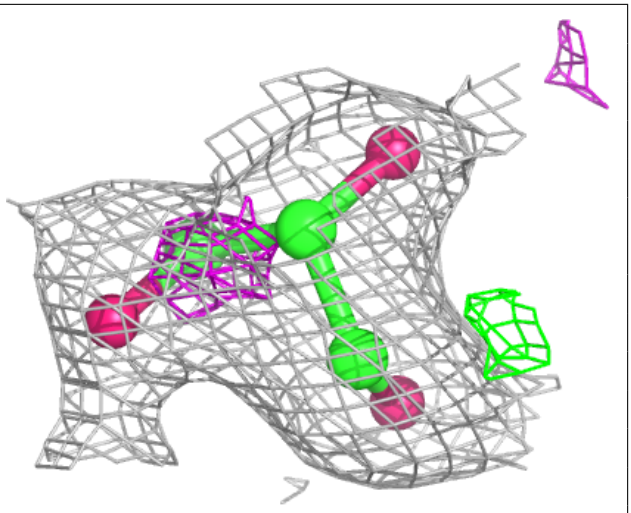


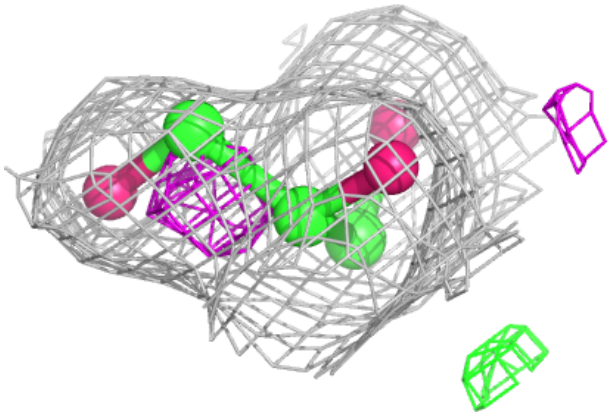


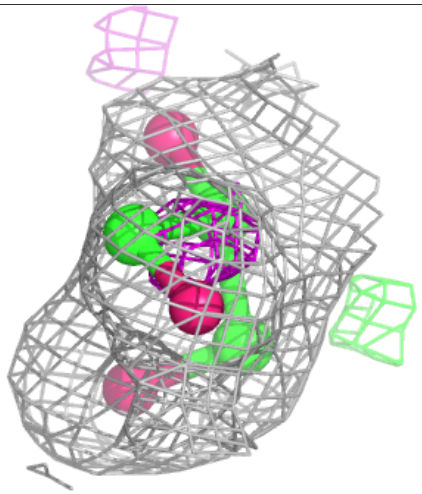


Electron density around GOL A 601 (A):

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

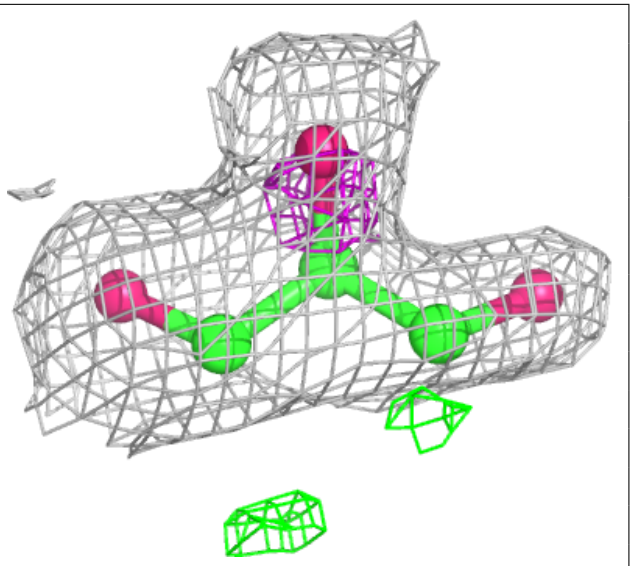


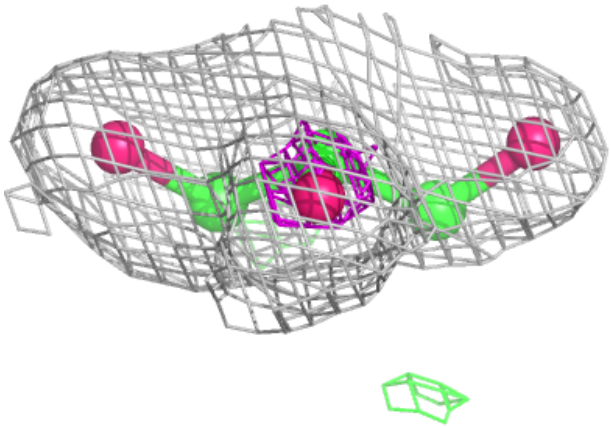


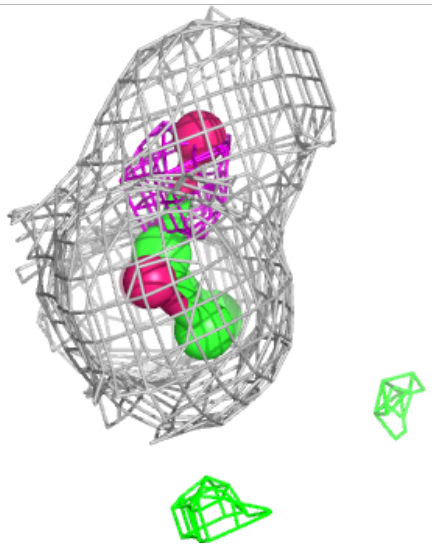


Electron density around GOL A 601 (B):

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

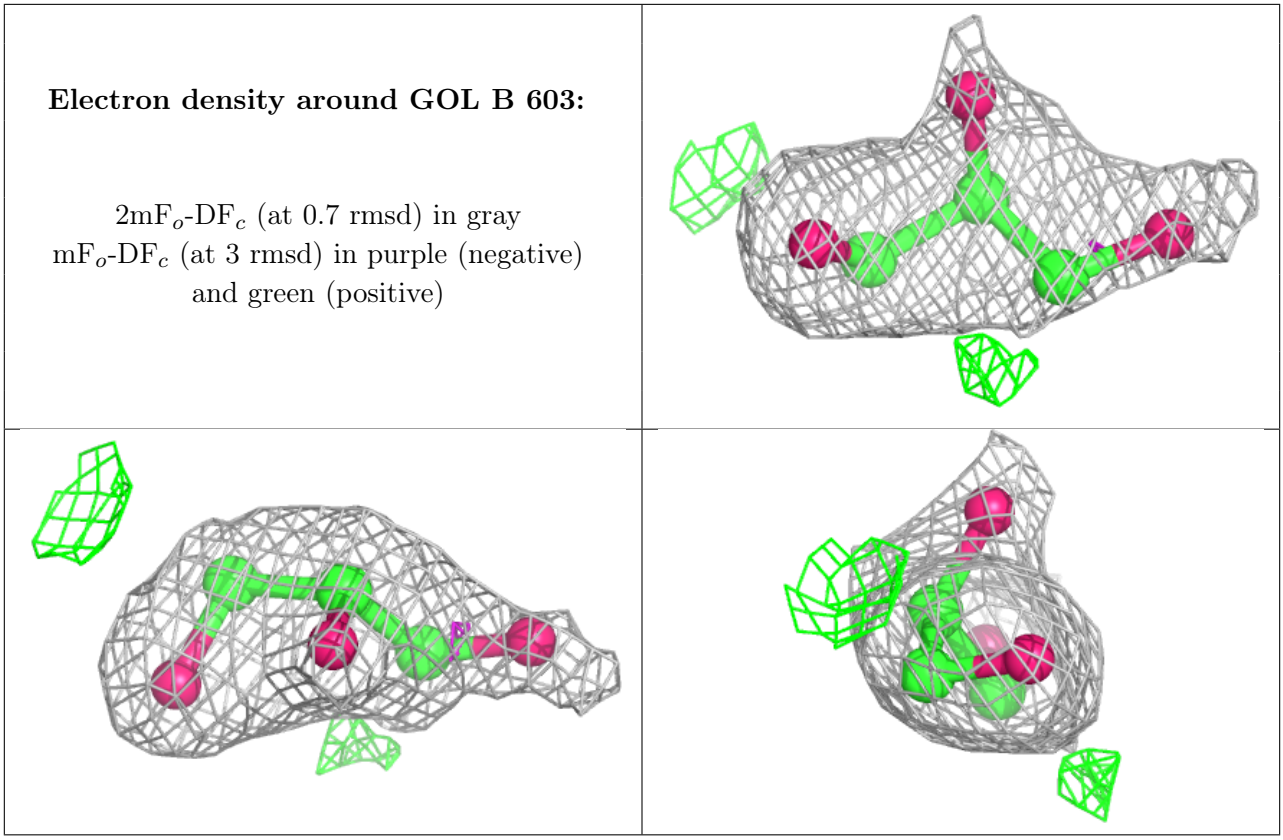






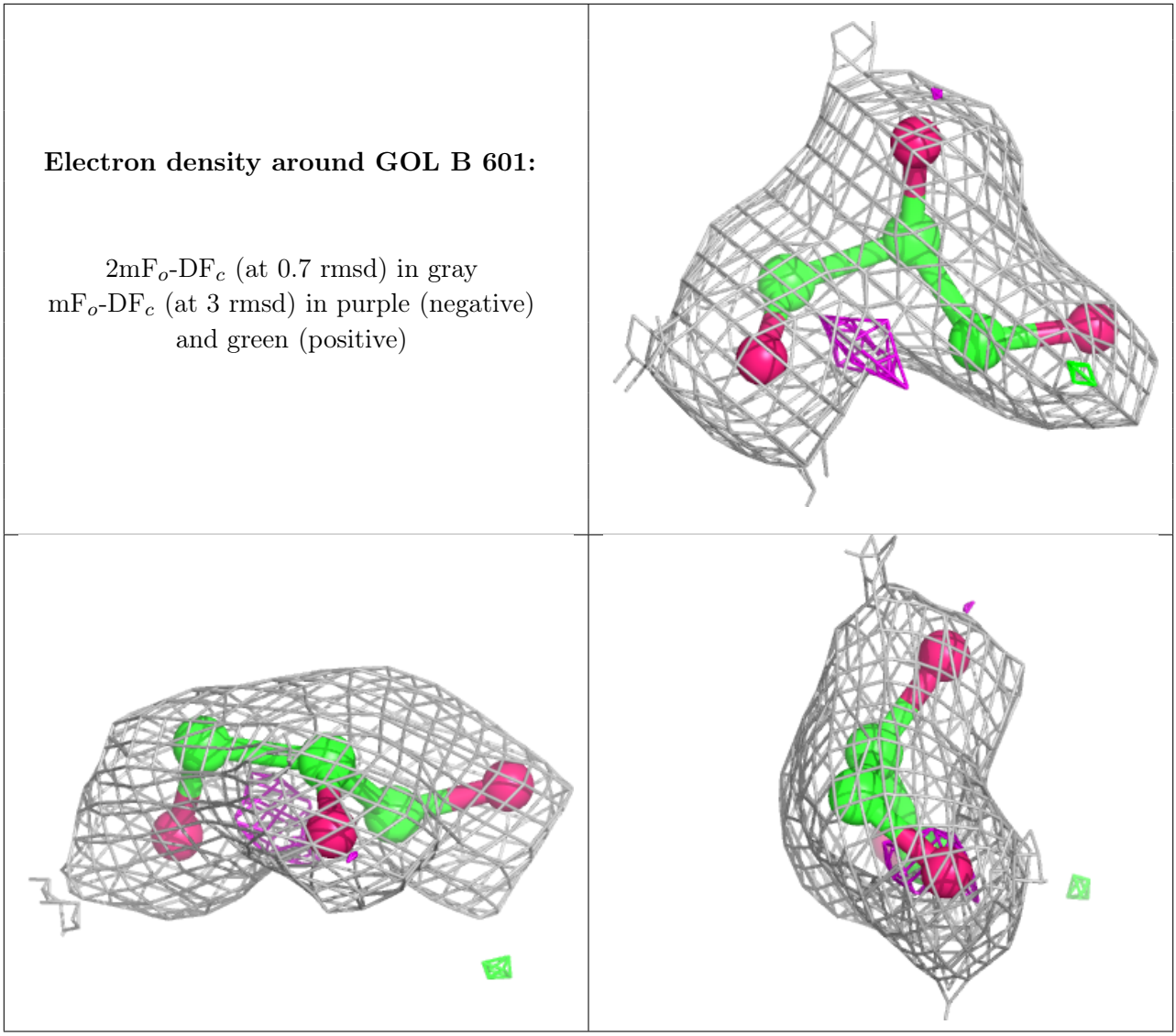
Electron density around GOL B 603:

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



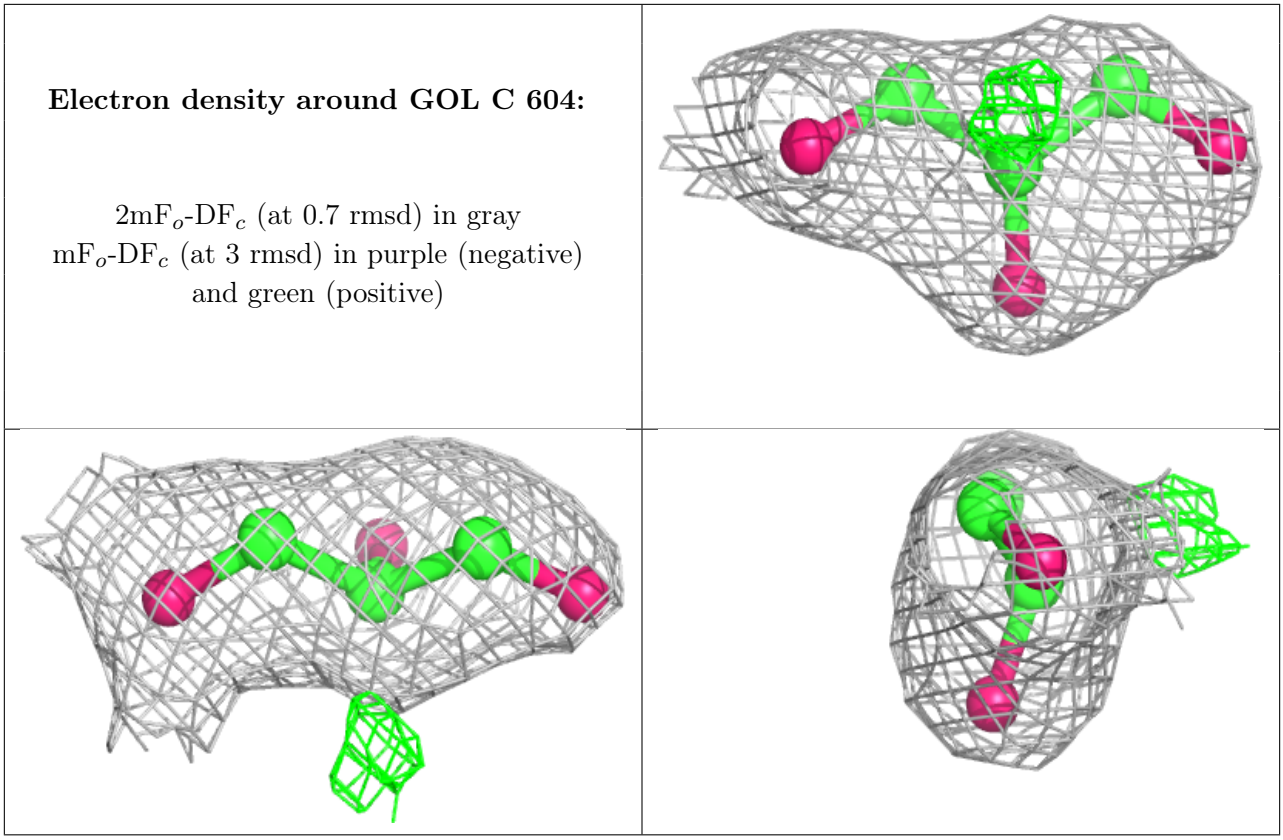
Electron density around GOL B 601:

$2mF_o$-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 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)



6.5 Other polymers (i)

There are no such residues in this entry.