Full wwPDB X-ray Structure Validation Report (i)

Mar 30, 2026 – 03:02 PM UTC

PDB ID	:	8IQ5 / pdb_00008iq5
Title	:	Crystal structure of trimeric K2-2 TSP
Authors	:	Ye, T.J.; Huang, K.F.; Ko, T.P.
Deposited on	:	2023-03-15
Resolution	:	1.38 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:

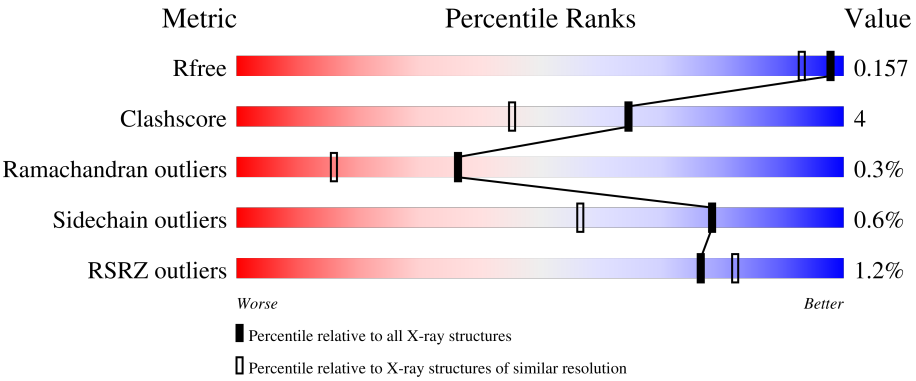
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.38 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}	180053	4403 (1.40-1.36)
Clashscore	190562	4528 (1.40-1.36)
Ramachandran outliers	187476	4459 (1.40-1.36)
Sidechain outliers	187428	4458 (1.40-1.36)
RSRZ outliers	180081	4399 (1.40-1.36)

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	612	85% 7% 8%
1	B	612	85% 7% 8%
1	C	612	85% 7% 8%
1	D	612	87% 5% 8%
1	E	612	85% 7% 8%

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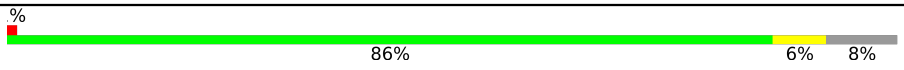
Mol	Chain	Length	Quality of chain
1	F	612	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	602	-	X	-	-
3	GOL	C	601	-	X	-	-
3	GOL	E	602	-	X	-	-

2 Entry composition (i)

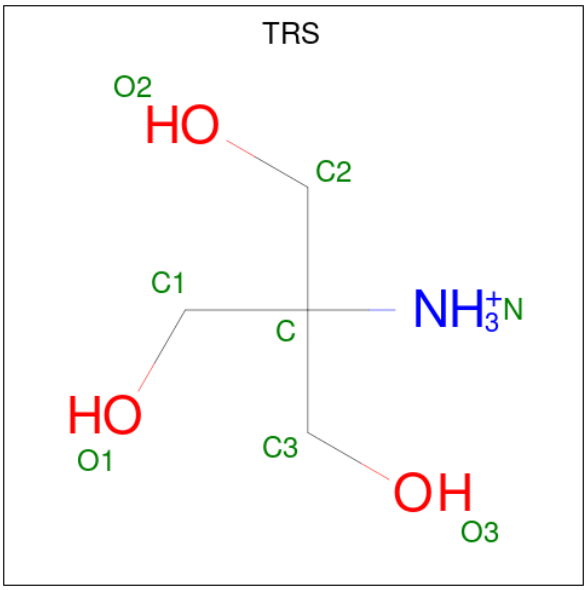
There are 5 unique types of molecules in this entry. The entry contains 30892 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 K2-2 TSP.

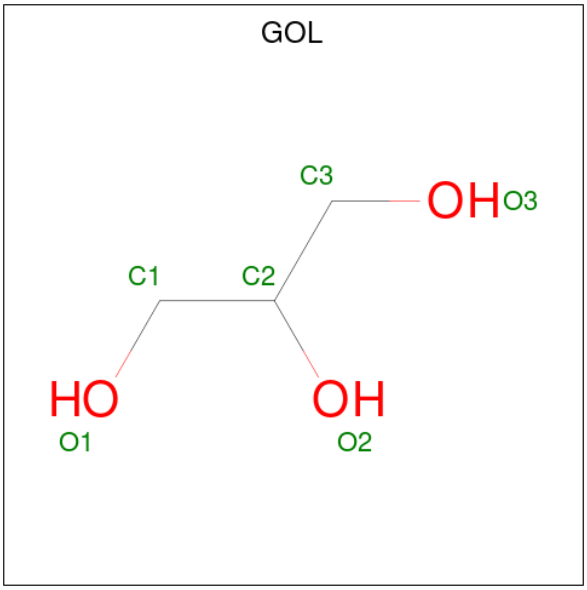
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	563	Total	C	N	O	S	0	25	0
			4267	2686	728	830	23			
1	B	563	Total	C	N	O	S	0	25	0
			4244	2669	721	831	23			
1	C	563	Total	C	N	O	S	0	31	0
			4274	2688	729	835	22			
1	D	564	Total	C	N	O	S	0	29	0
			4258	2678	723	834	23			
1	E	563	Total	C	N	O	S	0	19	0
			4244	2671	724	827	22			
1	F	563	Total	C	N	O	S	0	19	0
			4246	2668	726	830	22			

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 8 4 1 3	0	0
2	D	1	Total C N O 8 4 1 3	0	0

- Molecule 3 is GLYCEROL (CCD ID: 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	B	1	Total C O 12 6 6	0	1
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
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

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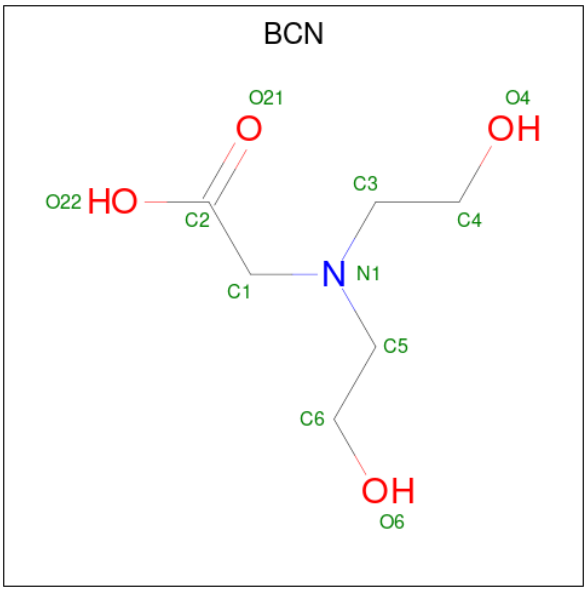
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	1
			12	6	6		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	1
			7	3	4		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	1
			7	3	4		

- Molecule 4 is BICINE (CCD ID: BCN) (formula: $C_6H_{13}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C N O 11 6 1 4	0	0

- Molecule 5 is water.

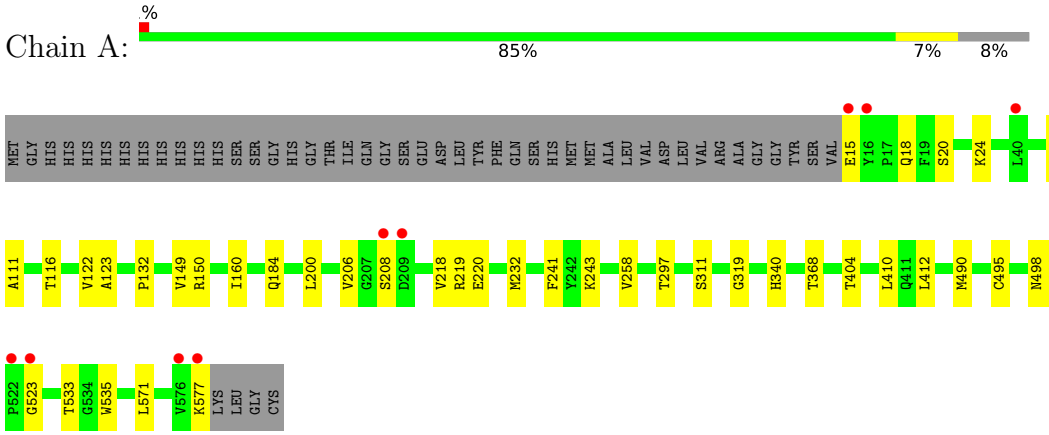
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	879	Total O 879 879	0	0
5	B	864	Total O 864 864	0	0
5	C	821	Total O 821 821	0	0
5	D	880	Total O 882 882	0	2
5	E	835	Total O 835 835	0	0
5	F	886	Total O 887 887	0	1

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.

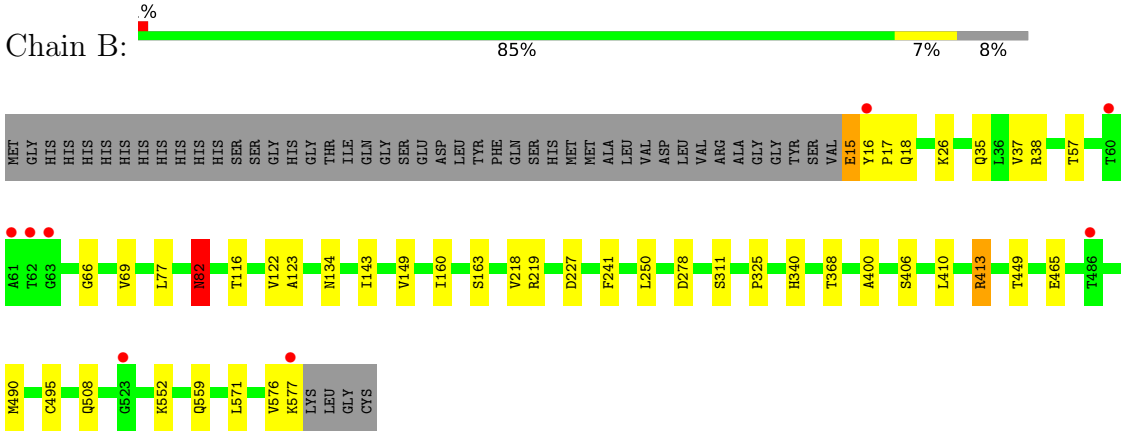
• Molecule 1: K2-2 TSP

Chain A:



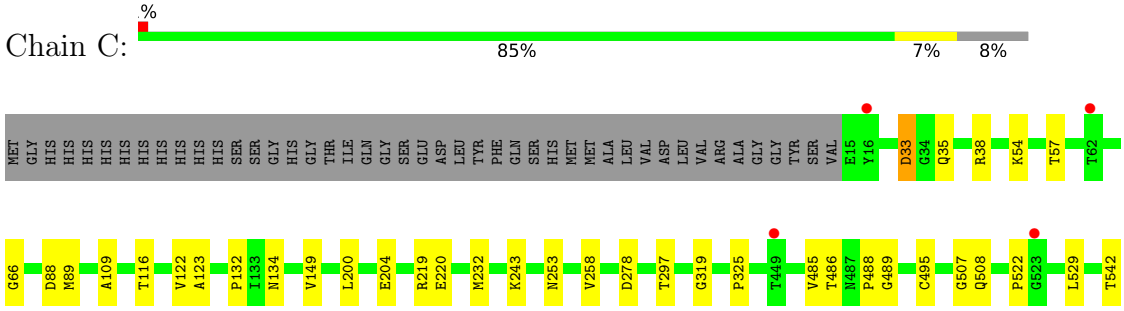
• Molecule 1: K2-2 TSP

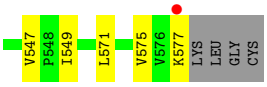
Chain B:



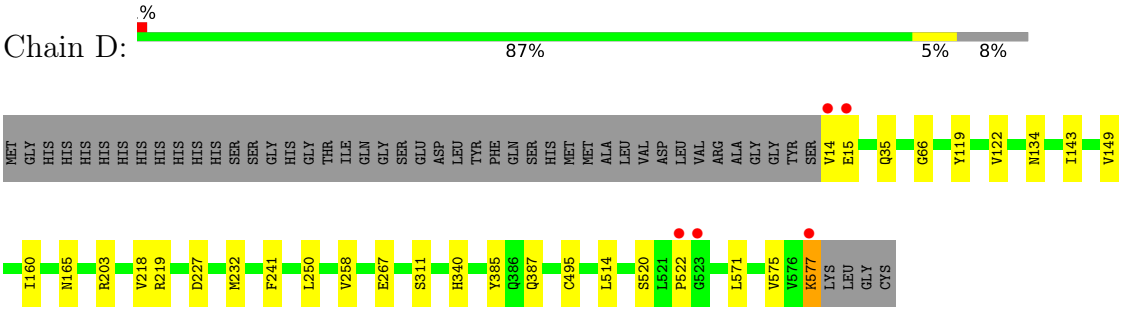
• Molecule 1: K2-2 TSP

Chain C:

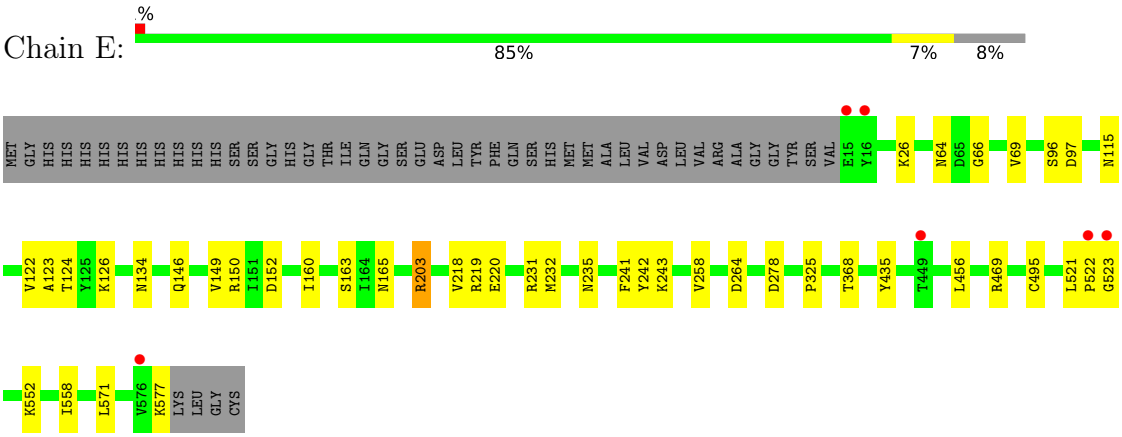




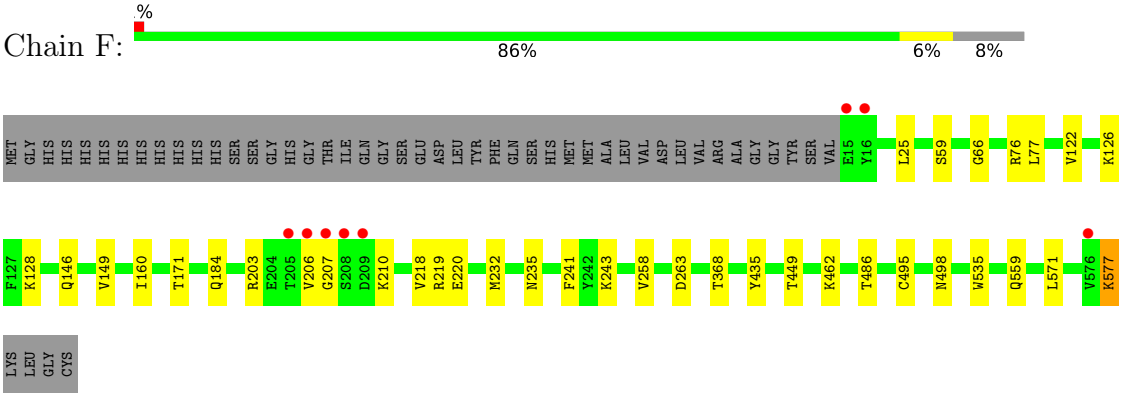
• Molecule 1: K2-2 TSP



• Molecule 1: K2-2 TSP



• Molecule 1: K2-2 TSP



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.81Å 82.84Å 196.14Å 90.00° 98.37° 90.00°	Depositor
Resolution (Å)	25.42 – 1.38 25.42 – 1.38	Depositor EDS
% Data completeness (in resolution range)	98.1 (25.42-1.38) 98.0 (25.42-1.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 1.38Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.134 , 0.158 0.134 , 0.157	Depositor DCC
R_{free} test set	2000 reflections (0.30%)	wwPDB-VP
Wilson B-factor (Å^2)	13.0	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	30892	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.40% 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, BCN, TRS

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	0.55	0/4462	0.72	0/6068
1	B	0.56	0/4451	0.72	2/6058 (0.0%)
1	C	0.53	0/4508	0.71	0/6133
1	D	0.56	0/4487	0.73	0/6104
1	E	0.53	0/4409	0.71	0/5998
1	F	0.53	0/4411	0.71	1/6002 (0.0%)
All	All	0.54	0/26728	0.72	3/36363 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	462	LYS	CG-CD-CE	5.93	124.94	111.30
1	B	82[A]	ASN	N-CA-C	5.30	119.74	113.12
1	B	82[B]	ASN	N-CA-C	5.30	119.74	113.12

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	4267	0	4167	33	0
1	B	4244	0	4142	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4274	0	4167	51	0
1	D	4258	0	4137	23	0
1	E	4244	0	4144	36	0
1	F	4246	0	4120	26	0
2	A	8	0	12	1	0
2	D	8	0	12	2	0
3	A	18	0	24	0	0
3	B	36	0	48	2	0
3	C	24	0	32	3	0
3	D	43	0	54	3	0
3	E	24	0	30	6	0
3	F	19	0	22	3	0
4	E	11	0	12	1	0
5	A	879	0	0	8	13
5	B	864	0	0	16	12
5	C	821	0	0	13	9
5	D	882	0	0	5	15
5	E	835	0	0	10	16
5	F	887	0	0	11	10
All	All	30892	0	25123	201	40

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 4.

All (201) 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:489:GLY:HA3	1:C:577:LYS:NZ	1.62	1.14
1:C:489:GLY:HA3	1:C:577:LYS:HZ1	1.00	1.10
1:B:508[A]:GLN:OE1	1:B:559:GLN:NE2	1.98	0.97
1:D:134[A]:ASN:ND2	5:D:701:HOH:O	2.06	0.87
1:C:89:MET:SD	5:C:1428:HOH:O	2.35	0.85
1:E:134[A]:ASN:ND2	5:E:702:HOH:O	2.08	0.85
1:C:489:GLY:CA	1:C:577:LYS:HZ1	1.87	0.84
1:A:523:GLY:O	5:A:701:HOH:O	1.95	0.84
1:C:232[B]:MET:HG2	1:C:258:VAL:HG22	1.61	0.81
1:A:412:LEU:HD11	1:A:490[B]:MET:HG3	1.61	0.80
1:B:368[B]:THR:HG23	5:B:1223:HOH:O	1.82	0.80
1:E:115:ASN:ND2	5:E:703:HOH:O	2.14	0.80
1:A:232[B]:MET:HG2	1:A:258:VAL:HG22	1.62	0.79
1:D:35:GLN:NE2	5:D:702:HOH:O	2.07	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134[B]:ASN:OD1	5:C:701:HOH:O	2.02	0.78
1:B:368[B]:THR:HG22	1:B:400:ALA:HB3	1.66	0.77
1:B:577:LYS:NZ	5:B:704:HOH:O	2.17	0.77
1:E:203[A]:ARG:HG3	1:E:235:ASN:HD22	1.50	0.76
1:E:96:SER:OG	5:E:701:HOH:O	2.05	0.74
1:F:495[B]:CYS:HB2	1:F:571:LEU:HD23	1.70	0.73
1:B:559:GLN:NE2	5:B:707:HOH:O	2.22	0.72
1:C:486:THR:O	1:C:577:LYS:HE3	1.88	0.72
1:C:132:PRO:HG3	5:C:961:HOH:O	1.91	0.71
1:D:267:GLU:HA	3:D:603:GOL:H2	1.71	0.71
1:E:220:GLU:HG2	1:E:243:LYS:HE2	1.73	0.69
1:E:64:ASN:HD22	3:E:603:GOL:H12	1.58	0.69
1:A:495[B]:CYS:HB2	1:A:571:LEU:HD23	1.76	0.68
3:C:601:GOL:O1	5:C:702:HOH:O	2.11	0.68
1:D:495[B]:CYS:HB2	1:D:571:LEU:HD23	1.74	0.68
1:E:278:ASP:OD1	3:E:602:GOL:H32	1.94	0.68
3:F:602:GOL:H12	5:F:1271:HOH:O	1.92	0.68
1:C:575:VAL:CG1	1:C:577:LYS:HZ3	2.07	0.67
1:C:547:VAL:HG21	1:C:577:LYS:NZ	2.11	0.66
1:B:278:ASP:OD1	3:B:602:GOL:H11	1.95	0.66
1:C:220:GLU:HG2	1:C:243[A]:LYS:HE3	1.79	0.64
1:C:33:ASP:OD1	1:C:57:THR:N	2.25	0.64
1:A:160[B]:ILE:HD13	1:A:200:LEU:HB2	1.80	0.64
1:C:495[B]:CYS:HB2	1:C:571:LEU:HD23	1.80	0.63
1:C:325:PRO:HG2	3:C:601:GOL:H12	1.80	0.63
1:C:508[A]:GLN:NE2	5:C:708:HOH:O	2.31	0.63
1:F:203[A]:ARG:NE	1:F:235:ASN:HD21	1.97	0.63
1:B:35[A]:GLN:OE1	5:B:702:HOH:O	2.15	0.62
1:C:522[B]:PRO:HD2	5:C:1311:HOH:O	1.98	0.62
1:E:495[B]:CYS:HB2	1:E:571:LEU:HD23	1.81	0.62
1:B:449:THR:O	5:B:703:HOH:O	2.15	0.61
5:B:753:HOH:O	1:C:549[B]:ILE:HD11	2.00	0.61
1:B:495[B]:CYS:HB2	1:B:571:LEU:HD23	1.82	0.61
1:A:220:GLU:HG2	1:A:243[A]:LYS:HE3	1.83	0.61
1:C:278:ASP:OD1	3:C:601:GOL:H11	2.00	0.61
1:F:486:THR:H	1:F:577:LYS:HZ1	1.48	0.60
1:D:15:GLU:OE2	5:D:704:HOH:O	2.16	0.60
1:A:410:LEU:HD12	1:A:490[B]:MET:HG2	1.84	0.59
1:A:20:SER:OG	1:A:24:LYS:HD2	2.03	0.59
1:E:552:LYS:NZ	5:E:707:HOH:O	2.35	0.59
1:E:325:PRO:HG2	3:E:602:GOL:H31	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:ASP:N	5:E:701:HOH:O	2.36	0.58
1:C:575:VAL:CG1	1:C:577:LYS:NZ	2.67	0.57
5:B:1247:HOH:O	1:C:549[B]:ILE:HD12	2.04	0.57
1:D:165:ASN:CG	1:D:203[B]:ARG:HG3	2.29	0.57
1:E:124[B]:THR:HG21	5:E:1256:HOH:O	2.06	0.56
1:A:150[B]:ARG:NH2	5:A:713:HOH:O	2.37	0.56
1:B:413:ARG:NH2	5:B:705:HOH:O	2.18	0.56
1:F:449:THR:HB	5:F:1334:HOH:O	2.05	0.56
1:F:206:VAL:HG21	1:F:263[B]:ASP:OD2	2.05	0.56
1:C:486:THR:O	1:C:577:LYS:CE	2.53	0.56
1:E:456:LEU:HD11	1:E:469:ARG:HB2	1.88	0.55
1:E:124[B]:THR:HG23	5:E:1224:HOH:O	2.07	0.55
1:E:232[B]:MET:HG3	1:E:258:VAL:HG22	1.89	0.55
1:C:547:VAL:HG21	1:C:577:LYS:HZ3	1.72	0.55
1:E:242:TYR:CE2	1:E:243:LYS:HD3	2.42	0.54
1:B:508[A]:GLN:NE2	5:B:707:HOH:O	2.41	0.54
1:A:18:GLN:NE2	1:C:38[B]:ARG:HH22	2.06	0.54
1:B:325:PRO:HG2	3:B:602:GOL:H12	1.90	0.54
1:B:552:LYS:NZ	5:B:714:HOH:O	2.40	0.54
1:B:134:ASN:HB2	5:B:839:HOH:O	2.06	0.54
1:E:521:LEU:HB3	1:E:522[A]:PRO:HD2	1.90	0.54
1:F:559:GLN:NE2	5:F:720:HOH:O	2.40	0.54
1:A:132:PRO:HG3	5:A:956:HOH:O	2.08	0.53
1:F:171:THR:HG21	5:F:791:HOH:O	2.08	0.53
1:C:575:VAL:HG12	1:C:577:LYS:HG3	1.91	0.53
1:D:143[B]:ILE:CD1	1:E:146:GLN:NE2	2.72	0.53
1:A:499:ILE:O	1:A:533[B]:THR:HG23	2.09	0.52
3:F:603[B]:GOL:O1	5:F:702:HOH:O	2.19	0.52
1:C:109:ALA:HB3	5:C:1051:HOH:O	2.10	0.52
1:F:232[B]:MET:HG3	1:F:258:VAL:HG22	1.91	0.52
1:B:160:ILE:HD12	1:B:163:SER:HB3	1.92	0.52
1:C:489:GLY:HA3	1:C:577:LYS:HZ2	1.67	0.52
1:D:232[B]:MET:HG3	1:D:258:VAL:HG22	1.91	0.52
1:A:150[B]:ARG:NH2	5:A:716:HOH:O	2.43	0.51
1:C:253:ASN:ND2	5:C:717:HOH:O	2.42	0.51
1:C:485:VAL:HG22	1:C:577:LYS:HE2	1.93	0.51
1:F:146[B]:GLN:OE1	5:F:703:HOH:O	2.19	0.50
1:F:210:LYS:HB2	5:F:785:HOH:O	2.11	0.50
1:B:15:GLU:HG2	1:B:16:TYR:H	1.77	0.50
1:E:264:ASP:OD1	4:E:600:BCN:H61	2.12	0.49
1:F:128:LYS:NZ	5:F:706:HOH:O	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26[A]:LYS:HG2	1:E:69:VAL:CG1	2.43	0.49
1:A:410:LEU:HB2	1:A:490[B]:MET:SD	2.53	0.49
1:B:35[B]:GLN:NE2	5:B:720:HOH:O	2.46	0.49
1:E:126:LYS:HD3	1:E:152:ASP:HB3	1.95	0.49
1:D:575:VAL:HG12	1:D:577:LYS:HG2	1.94	0.49
1:E:368[A]:THR:HG23	5:E:1235:HOH:O	2.12	0.49
1:F:207:GLY:HA2	5:F:716:HOH:O	2.13	0.49
1:D:122:VAL:HA	1:D:149:VAL:HG22	1.95	0.48
1:D:143[B]:ILE:CD1	1:E:146:GLN:HE22	2.26	0.48
1:E:435:TYR:CD2	3:E:601:GOL:H12	2.48	0.48
1:A:122:VAL:HA	1:A:149:VAL:HG22	1.95	0.48
1:B:406:SER:HA	5:B:718:HOH:O	2.14	0.48
1:F:220:GLU:HG2	1:F:243:LYS:HE3	1.94	0.48
1:A:18:GLN:HE22	1:C:38[B]:ARG:CZ	2.27	0.48
1:B:82[A]:ASN:O	5:B:706:HOH:O	2.20	0.48
1:E:122:VAL:HA	1:E:149:VAL:HG22	1.96	0.48
1:A:18:GLN:HE22	1:C:38[B]:ARG:NH2	2.11	0.48
1:C:577:LYS:HD3	5:C:1240:HOH:O	2.13	0.48
1:C:122:VAL:HA	1:C:149:VAL:HG22	1.96	0.48
1:A:206:VAL:HG23	5:A:1093:HOH:O	2.13	0.48
5:B:753:HOH:O	1:C:549[B]:ILE:CD1	2.60	0.47
1:E:523[A]:GLY:N	5:E:718:HOH:O	2.46	0.47
1:A:184[A]:GLN:HA	1:A:219:ARG:O	2.14	0.47
1:F:184[B]:GLN:HA	1:F:219:ARG:O	2.15	0.47
1:A:184[B]:GLN:HA	1:A:219:ARG:O	2.15	0.47
1:A:490[B]:MET:HB2	1:A:490[B]:MET:HE3	1.79	0.47
1:D:134[B]:ASN:ND2	5:D:721:HOH:O	2.48	0.47
1:A:18:GLN:NE2	1:C:38[B]:ARG:NH2	2.63	0.46
1:A:368[A]:THR:HG23	5:A:1288:HOH:O	2.14	0.46
1:C:507:GLY:C	1:C:508[B]:GLN:HG3	2.40	0.46
1:F:59:SER:HB3	1:F:76:ARG:HB2	1.96	0.46
1:F:184[A]:GLN:HA	1:F:219:ARG:O	2.15	0.46
2:D:600:TRS:O3	2:D:600:TRS:O2	2.32	0.46
1:A:517:ALA:O	5:A:704:HOH:O	2.21	0.46
1:E:64:ASN:ND2	3:E:603:GOL:H12	2.29	0.46
1:C:575:VAL:HG13	1:C:577:LYS:HZ3	1.79	0.45
1:A:18:GLN:HE22	1:C:38[B]:ARG:NH1	2.14	0.45
1:B:18:GLN:HG2	1:B:38:ARG:HB3	1.97	0.45
1:D:119:TYR:HE1	1:D:143[B]:ILE:HD12	1.81	0.45
1:B:26[A]:LYS:HG2	1:B:69:VAL:CG1	2.46	0.45
1:B:15:GLU:O	1:B:17:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522[A]:PRO:HG2	5:C:1311:HOH:O	2.16	0.44
1:F:203[A]:ARG:NE	1:F:235:ASN:ND2	2.64	0.44
1:B:122:VAL:HA	1:B:149:VAL:HG22	1.99	0.44
1:E:218:VAL:O	1:E:241:PHE:HA	2.18	0.44
1:D:514[B]:LEU:HD23	1:D:520:SER:HA	1.99	0.44
1:F:126:LYS:HD3	5:F:1272:HOH:O	2.16	0.44
1:F:232[B]:MET:CG	1:F:258:VAL:HG22	2.48	0.44
1:B:577:LYS:HD2	5:B:718:HOH:O	2.18	0.44
1:E:165:ASN:CG	1:E:203[A]:ARG:HG2	2.42	0.44
1:A:111:ALA:HB1	1:A:116:THR:O	2.18	0.44
1:F:368[A]:THR:HG23	5:F:1265:HOH:O	2.17	0.44
1:B:410:LEU:HD12	1:B:490[B]:MET:HG3	2.00	0.44
1:E:124[B]:THR:HG22	1:E:150:ARG:HB3	2.00	0.44
1:C:200:LEU:CD2	1:C:204[A]:GLU:HG2	2.48	0.43
1:E:64:ASN:HD22	3:E:603:GOL:C1	2.27	0.43
1:C:54:LYS:NZ	5:C:703:HOH:O	2.18	0.43
1:E:231:ARG:NH2	5:E:724:HOH:O	2.51	0.43
1:B:82[B]:ASN:HD21	1:C:88[B]:ASP:CG	2.26	0.43
1:D:165:ASN:ND2	1:D:203[B]:ARG:HG3	2.34	0.43
1:B:490[B]:MET:HG2	1:B:576:VAL:CG2	2.49	0.43
1:C:488:PRO:O	1:C:577:LYS:HG2	2.19	0.43
1:C:495[B]:CYS:CB	1:C:571:LEU:HD23	2.48	0.43
1:F:122:VAL:HA	1:F:149:VAL:HG22	2.00	0.43
1:D:267:GLU:HG3	3:D:603:GOL:H11	2.01	0.42
1:C:297:THR:HA	1:C:319:GLY:O	2.20	0.42
1:B:227:ASP:HA	1:B:250:LEU:HB3	2.01	0.42
1:D:218:VAL:O	1:D:241:PHE:HA	2.20	0.42
1:F:218:VAL:O	1:F:241:PHE:HA	2.19	0.42
1:A:81[B]:VAL:HG21	5:A:875:HOH:O	2.19	0.42
1:B:311:SER:HA	1:B:340:HIS:O	2.20	0.42
1:D:267:GLU:HA	3:D:603:GOL:C2	2.46	0.42
1:A:404:THR:CG2	1:B:577:LYS:HD3	2.50	0.42
1:A:311:SER:HA	1:A:340:HIS:O	2.20	0.41
1:D:311:SER:HA	1:D:340:HIS:O	2.20	0.41
1:F:25:LEU:HD11	1:F:77:LEU:HD22	2.01	0.41
1:A:498:ASN:HB2	1:A:535:TRP:CD2	2.55	0.41
2:A:600:TRS:O3	2:A:600:TRS:O1	2.38	0.41
1:A:122:VAL:HG11	1:C:116:THR:HG23	2.02	0.41
1:A:297:THR:HA	1:A:319:GLY:O	2.21	0.41
1:B:37[B]:VAL:HG21	1:B:77:LEU:HD23	2.01	0.41
1:F:435:TYR:CG	3:F:601:GOL:H32	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:VAL:O	1:A:241:PHE:HA	2.21	0.41
1:B:15:GLU:C	1:B:17:PRO:HD3	2.45	0.41
1:B:116:THR:HG23	1:C:122:VAL:HG11	2.01	0.41
1:C:35[B]:GLN:NE2	5:C:713:HOH:O	2.37	0.41
1:B:218:VAL:O	1:B:241:PHE:HA	2.20	0.41
1:D:522[A]:PRO:HD2	5:D:1452:HOH:O	2.21	0.41
1:F:220:GLU:HG2	1:F:243:LYS:CE	2.51	0.41
1:C:577:LYS:HA	5:C:1257:HOH:O	2.20	0.41
1:D:227:ASP:HA	1:D:250:LEU:HB3	2.03	0.41
2:D:600:TRS:O3	2:D:600:TRS:O1	2.36	0.41
1:E:160:ILE:HD12	1:E:163:SER:HB3	2.03	0.41
1:F:498:ASN:HB2	1:F:535:TRP:CD2	2.56	0.40
1:E:124[B]:THR:HG22	1:E:150:ARG:HD3	2.03	0.40
1:D:385:TYR:HB3	1:D:387:GLN:OE1	2.22	0.40
1:E:558:ILE:HD11	1:E:571:LEU:HD13	2.03	0.40

All (40) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:994:HOH:O	5:E:1128:HOH:O[2_455]	1.68	0.52
5:A:1315:HOH:O	5:D:1169:HOH:O[2_445]	1.76	0.44
5:D:859:HOH:O	5:E:854:HOH:O[2_455]	1.79	0.41
5:B:1369:HOH:O	5:F:1376:HOH:O[1_455]	1.81	0.39
5:E:1028:HOH:O	5:F:980:HOH:O[2_455]	1.81	0.39
5:A:966:HOH:O	5:E:896:HOH:O[2_546]	1.92	0.28
5:A:1482:HOH:O	5:D:1217:HOH:O[1_455]	1.94	0.26
5:B:738:HOH:O	5:D:730:HOH:O[1_455]	1.94	0.26
5:C:804:HOH:O	5:F:768:HOH:O[1_455]	1.94	0.26
5:C:1291:HOH:O	5:E:1150:HOH:O[1_455]	1.94	0.26
5:A:1266:HOH:O	5:E:1152:HOH:O[2_546]	1.96	0.24
5:B:871:HOH:O	5:F:988:HOH:O[1_455]	1.96	0.24
5:C:739:HOH:O	5:E:1213:HOH:O[1_455]	1.97	0.23
5:D:805:HOH:O	5:F:717:HOH:O[2_555]	1.97	0.23
5:D:779:HOH:O	5:D:1109:HOH:O[2_555]	1.98	0.22
5:D:1403:HOH:O	5:E:1353:HOH:O[2_455]	1.99	0.21
5:D:1403:HOH:O	5:E:739:HOH:O[2_455]	2.00	0.20
5:E:912:HOH:O	5:F:804:HOH:O[2_455]	2.01	0.19
5:A:862:HOH:O	5:B:1357:HOH:O[2_446]	2.02	0.18
5:B:818:HOH:O	5:C:774:HOH:O[1_455]	2.02	0.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1323:HOH:O	5:F:1457:HOH:O[2_455]	2.02	0.18
5:B:1110:HOH:O	5:F:1424:HOH:O[1_455]	2.04	0.16
5:A:725:HOH:O	5:E:791:HOH:O[1_455]	2.06	0.14
5:A:980:HOH:O	5:B:1357:HOH:O[2_446]	2.07	0.13
5:A:1093:HOH:O	5:B:1428:HOH:O[2_446]	2.10	0.10
5:C:978:HOH:O	5:E:1232:HOH:O[1_455]	2.11	0.09
5:A:704:HOH:O	5:D:1255:HOH:O[1_455]	2.12	0.08
5:B:1122:HOH:O	5:F:1281:HOH:O[1_455]	2.13	0.07
5:D:1351:HOH:O	5:D:1468:HOH:O[2_545]	2.13	0.07
5:E:1108:HOH:O	5:F:994:HOH:O[2_455]	2.13	0.07
5:A:868:HOH:O	5:B:1425:HOH:O[2_446]	2.14	0.06
5:B:1431:HOH:O	5:E:706:HOH:O[1_455]	2.14	0.06
5:D:851:HOH:O	5:D:1443:HOH:O[2_555]	2.14	0.06
5:A:1325:HOH:O	5:D:1467:HOH:O[1_455]	2.15	0.05
5:A:712:HOH:O	5:C:710:HOH:O[2_546]	2.16	0.04
5:B:1511:HOH:O	5:C:1304:HOH:O[2_556]	2.16	0.04
5:C:815:HOH:O	5:E:862:HOH:O[1_455]	2.16	0.04
5:D:1553:HOH:O	5:D:1573:HOH:O[2_555]	2.17	0.03
5:A:1335:HOH:O	5:C:1322:HOH:O[2_546]	2.19	0.01
5:D:851:HOH:O	5:D:1513:HOH:O[2_555]	2.19	0.01

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	586/612 (96%)	568 (97%)	16 (3%)	2 (0%)	36	16
1	B	586/612 (96%)	564 (96%)	20 (3%)	2 (0%)	36	16
1	C	592/612 (97%)	569 (96%)	21 (4%)	2 (0%)	36	16
1	D	591/612 (97%)	571 (97%)	19 (3%)	1 (0%)	43	19
1	E	580/612 (95%)	557 (96%)	21 (4%)	2 (0%)	36	16
1	F	580/612 (95%)	562 (97%)	17 (3%)	1 (0%)	43	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3515/3672 (96%)	3391 (96%)	114 (3%)	10 (0%)	36 16

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	GLY
1	D	66	GLY
1	F	66	GLY
1	B	66	GLY
1	E	66	GLY
1	A	123	ALA
1	C	66	GLY
1	E	123	ALA
1	B	123	ALA
1	C	123	ALA

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	474/490 (97%)	470 (99%)	4 (1%)	73 48
1	B	474/490 (97%)	467 (98%)	7 (2%)	57 25
1	C	479/490 (98%)	476 (99%)	3 (1%)	78 56
1	D	478/490 (98%)	475 (99%)	3 (1%)	78 56
1	E	467/490 (95%)	464 (99%)	3 (1%)	78 56
1	F	467/490 (95%)	465 (100%)	2 (0%)	84 68
All	All	2839/2940 (97%)	2817 (99%)	22 (1%)	78 48

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	208[A]	SER

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Mol	Chain	Res	Type
1	A	208[B]	SER
1	A	577	LYS
1	B	15	GLU
1	B	57[A]	THR
1	B	57[B]	THR
1	B	82[A]	ASN
1	B	82[B]	ASN
1	B	413	ARG
1	B	465	GLU
1	C	33	ASP
1	C	529[A]	LEU
1	C	529[B]	LEU
1	D	14	VAL
1	D	160	ILE
1	D	577	LYS
1	E	203[A]	ARG
1	E	203[B]	ARG
1	E	577	LYS
1	F	160	ILE
1	F	577	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	115	ASN
1	A	296	ASN
1	A	386	GLN
1	A	519	ASN
1	A	553	GLN
1	B	18	GLN
1	B	115	ASN
1	B	296	ASN
1	B	386	GLN
1	B	458	ASN
1	B	541	ASN
1	B	559	GLN
1	C	18	GLN
1	C	115	ASN
1	C	386	GLN
1	D	115	ASN
1	D	235	ASN

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Mol	Chain	Res	Type
1	D	296	ASN
1	D	386	GLN
1	D	483	GLN
1	D	553	GLN
1	E	115	ASN
1	E	146	GLN
1	E	235	ASN
1	E	296	ASN
1	E	386	GLN
1	E	559	GLN
1	F	18	GLN
1	F	115	ASN
1	F	235	ASN
1	F	296	ASN
1	F	386	GLN
1	F	553	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 oligosaccharides in this entry.

5.6 Ligand geometry

32 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	B	601[B]	-	5,5,5	0.95	0	5,5,5	0.96	0
3	GOL	D	602[A]	-	5,5,5	1.08	0	5,5,5	0.89	0
3	GOL	F	603[B]	-	5,5,5	0.89	0	5,5,5	1.27	0
3	GOL	D	605	-	5,5,5	0.91	0	5,5,5	1.08	0
3	GOL	D	604	-	5,5,5	0.94	0	5,5,5	0.88	0
3	GOL	D	606[A]	-	5,5,5	1.00	0	5,5,5	0.97	0
3	GOL	B	602	-	5,5,5	1.56	2 (40%)	5,5,5	1.96	1 (20%)
2	TRS	D	600	-	7,7,7	0.34	0	9,9,9	1.22	0
3	GOL	E	601	-	5,5,5	1.13	0	5,5,5	1.24	1 (20%)
3	GOL	B	603	-	5,5,5	1.19	0	5,5,5	0.61	0
3	GOL	C	601	-	5,5,5	1.77	2 (40%)	5,5,5	1.83	1 (20%)
3	GOL	E	603	-	5,5,5	1.08	0	5,5,5	1.72	1 (20%)
3	GOL	E	602	-	5,5,5	1.84	2 (40%)	5,5,5	1.89	2 (40%)
3	GOL	D	601	-	5,5,5	0.77	0	5,5,5	1.18	0
3	GOL	D	602[B]	-	5,5,5	0.90	0	5,5,5	0.94	0
3	GOL	D	606[B]	-	5,5,5	1.00	0	5,5,5	1.03	0
3	GOL	B	601[A]	-	5,5,5	1.05	0	5,5,5	1.16	0
3	GOL	F	603[A]	-	5,5,5	0.93	0	5,5,5	1.23	0
3	GOL	D	603	-	5,5,5	0.98	0	5,5,5	1.75	1 (20%)
3	GOL	C	603	-	5,5,5	1.03	0	5,5,5	0.97	0
3	GOL	B	605	-	5,5,5	1.13	1 (20%)	5,5,5	1.25	1 (20%)
3	GOL	F	601	-	5,5,5	0.99	0	5,5,5	1.22	0
3	GOL	C	604	-	5,5,5	0.82	0	5,5,5	0.71	0
3	GOL	F	602	-	5,5,5	1.02	0	5,5,5	1.25	0
3	GOL	A	602	-	5,5,5	0.54	0	5,5,5	1.37	1 (20%)
3	GOL	B	604	-	5,5,5	1.06	1 (20%)	5,5,5	0.94	0
3	GOL	A	601	-	5,5,5	0.61	0	5,5,5	1.42	1 (20%)
3	GOL	A	603	-	5,5,5	0.90	0	5,5,5	1.14	1 (20%)
3	GOL	C	602	-	5,5,5	1.02	0	5,5,5	1.26	1 (20%)
3	GOL	E	604	-	5,5,5	0.78	0	5,5,5	0.93	0
4	BCN	E	600	-	10,10,10	1.00	0	11,11,11	1.52	2 (18%)
2	TRS	A	600	-	7,7,7	0.45	0	9,9,9	1.10	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	B	601[B]	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	602[A]	-	-	0/4/4/4	-
3	GOL	F	603[B]	-	-	2/4/4/4	-
3	GOL	D	605	-	-	0/4/4/4	-
3	GOL	D	604	-	-	0/4/4/4	-
3	GOL	D	606[A]	-	-	2/4/4/4	-
3	GOL	B	602	-	-	3/4/4/4	-
2	TRS	D	600	-	-	0/9/9/9	-
3	GOL	E	601	-	-	2/4/4/4	-
3	GOL	B	603	-	-	0/4/4/4	-
3	GOL	C	601	-	-	4/4/4/4	-
3	GOL	E	603	-	-	0/4/4/4	-
3	GOL	E	602	-	-	2/4/4/4	-
3	GOL	D	601	-	-	0/4/4/4	-
3	GOL	D	602[B]	-	-	0/4/4/4	-
3	GOL	D	606[B]	-	-	0/4/4/4	-
3	GOL	B	601[A]	-	-	0/4/4/4	-
3	GOL	F	603[A]	-	-	0/4/4/4	-
3	GOL	D	603	-	-	3/4/4/4	-
3	GOL	C	603	-	-	0/4/4/4	-
3	GOL	B	605	-	-	2/4/4/4	-
3	GOL	F	601	-	-	3/4/4/4	-
3	GOL	C	604	-	-	2/4/4/4	-
3	GOL	F	602	-	-	2/4/4/4	-
3	GOL	A	602	-	-	0/4/4/4	-
3	GOL	B	604	-	-	2/4/4/4	-
3	GOL	A	601	-	-	0/4/4/4	-
3	GOL	A	603	-	-	0/4/4/4	-
3	GOL	C	602	-	-	0/4/4/4	-
3	GOL	E	604	-	-	2/4/4/4	-
4	BCN	E	600	-	-	4/10/10/10	-
2	TRS	A	600	-	-	0/9/9/9	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	GOL	C3-C2	2.79	1.62	1.51
3	C	601	GOL	O2-C2	2.77	1.51	1.43
3	E	602	GOL	O2-C2	2.55	1.50	1.43
3	C	601	GOL	C1-C2	2.49	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	GOL	O2-C2	2.34	1.50	1.43
3	B	602	GOL	C1-C2	2.28	1.60	1.51
3	B	605	GOL	O2-C2	-2.15	1.37	1.43
3	B	604	GOL	C1-C2	2.02	1.59	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	GOL	C3-C2-C1	-3.96	97.26	111.80
3	C	601	GOL	C3-C2-C1	-3.45	99.14	111.80
3	E	602	GOL	C3-C2-C1	-3.43	99.20	111.80
4	E	600	BCN	C4-C3-N1	-3.37	101.61	113.44
3	E	603	GOL	C3-C2-C1	-3.19	100.11	111.80
3	D	603	GOL	O2-C2-C3	2.68	120.28	109.18
3	E	601	GOL	C3-C2-C1	-2.44	102.86	111.80
3	A	601	GOL	C3-C2-C1	-2.26	103.53	111.80
3	A	603	GOL	C3-C2-C1	-2.23	103.62	111.80
3	B	605	GOL	C3-C2-C1	-2.11	104.08	111.80
3	C	602	GOL	C3-C2-C1	-2.10	104.09	111.80
4	E	600	BCN	O22-C2-C1	2.07	121.55	113.38
3	E	602	GOL	O2-C2-C3	2.07	117.73	109.18
3	A	602	GOL	C3-C2-C1	-2.06	104.23	111.80

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	604	GOL	O2-C2-C3-O3
3	C	601	GOL	C1-C2-C3-O3
3	D	603	GOL	C1-C2-C3-O3
3	E	601	GOL	C1-C2-C3-O3
3	E	604	GOL	O1-C1-C2-C3
3	F	601	GOL	O1-C1-C2-C3
3	F	602	GOL	O1-C1-C2-C3
4	E	600	BCN	N1-C1-C2-O22
4	E	600	BCN	N1-C5-C6-O6
4	E	600	BCN	N1-C1-C2-O21
3	B	602	GOL	C1-C2-C3-O3
3	B	604	GOL	C1-C2-C3-O3
3	B	605	GOL	C1-C2-C3-O3
3	C	601	GOL	O1-C1-C2-C3
3	C	604	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	D	606[A]	GOL	C1-C2-C3-O3
3	E	602	GOL	O1-C1-C2-C3
3	F	603[B]	GOL	O1-C1-C2-C3
4	E	600	BCN	C2-C1-N1-C3
3	C	601	GOL	O1-C1-C2-O2
3	C	601	GOL	O2-C2-C3-O3
3	D	603	GOL	O2-C2-C3-O3
3	E	604	GOL	O1-C1-C2-O2
3	F	601	GOL	O1-C1-C2-O2
3	F	602	GOL	O1-C1-C2-O2
3	C	604	GOL	O2-C2-C3-O3
3	D	606[A]	GOL	O2-C2-C3-O3
3	E	601	GOL	O2-C2-C3-O3
3	B	605	GOL	O2-C2-C3-O3
3	D	603	GOL	O1-C1-C2-O2
3	F	601	GOL	O2-C2-C3-O3
3	F	603[B]	GOL	O1-C1-C2-O2
3	B	602	GOL	O1-C1-C2-C3
3	B	602	GOL	O2-C2-C3-O3
3	E	602	GOL	C1-C2-C3-O3

There are no ring outliers.

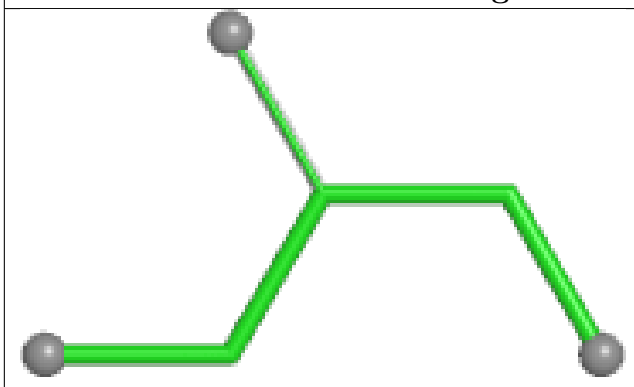
12 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	603[B]	GOL	1	0
3	B	602	GOL	2	0
2	D	600	TRS	2	0
3	E	601	GOL	1	0
3	C	601	GOL	3	0
3	E	603	GOL	3	0
3	E	602	GOL	2	0
3	D	603	GOL	3	0
3	F	601	GOL	1	0
3	F	602	GOL	1	0
4	E	600	BCN	1	0
2	A	600	TRS	1	0

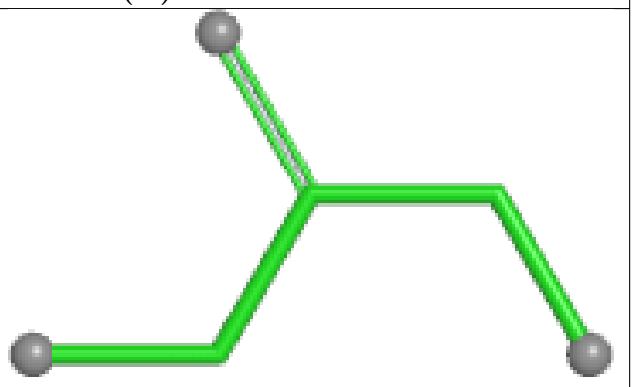
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

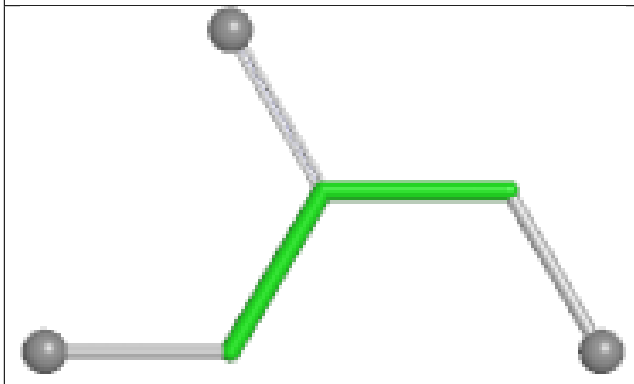
Ligand GOL B 601 (B)



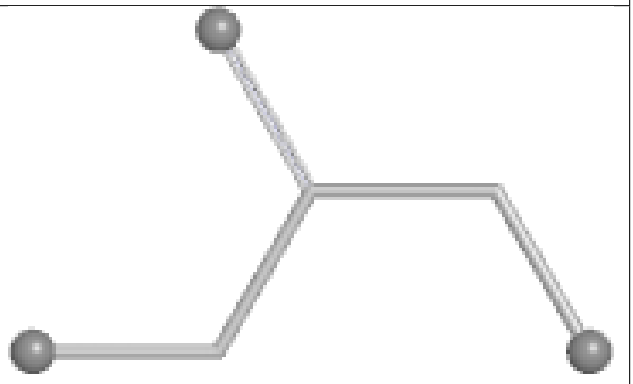
Bond lengths



Bond angles

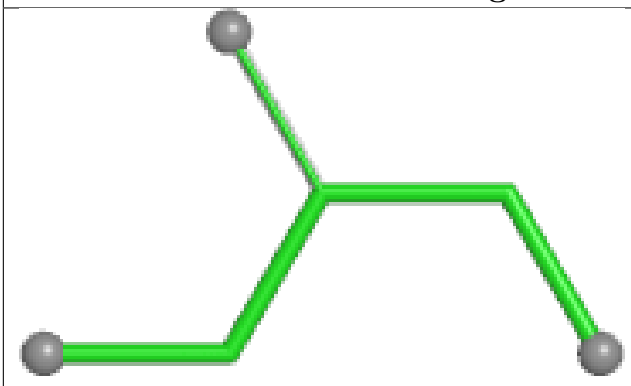


Torsions

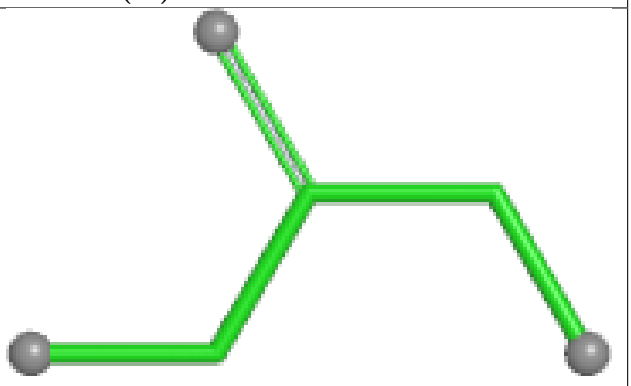


Rings

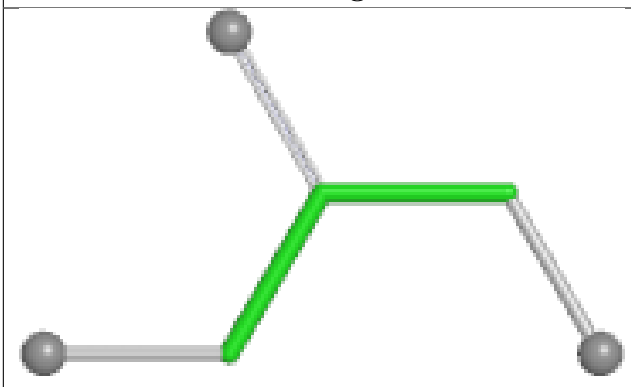
Ligand GOL D 602 (A)



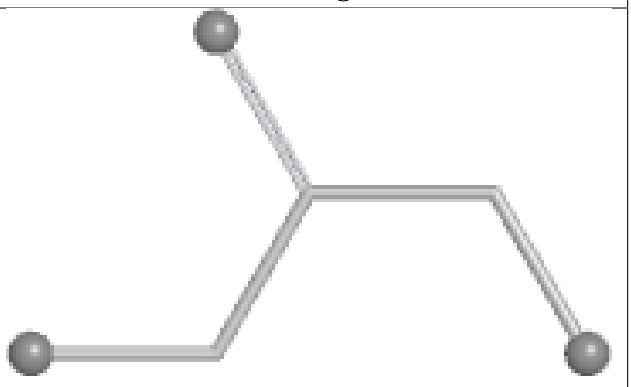
Bond lengths



Bond angles

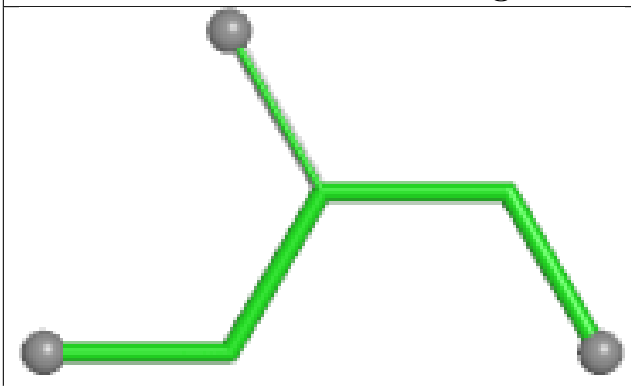


Torsions

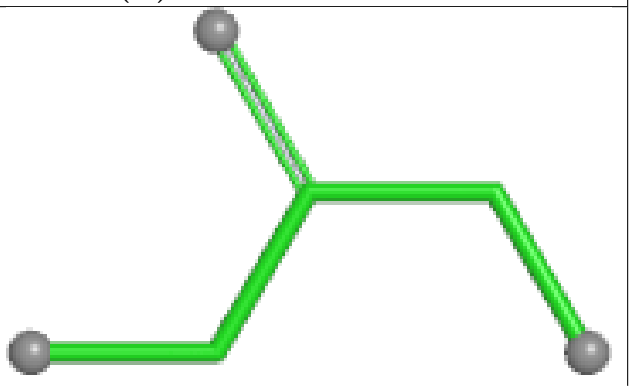


Rings

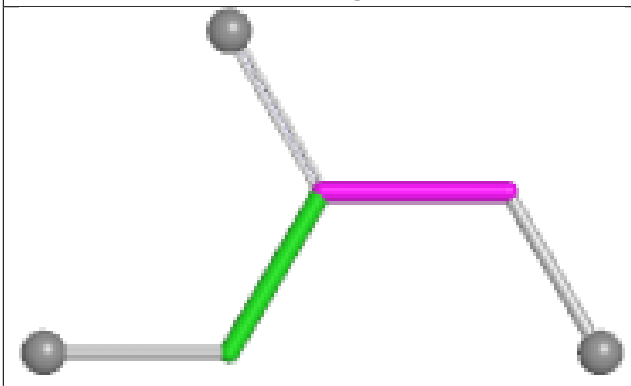
Ligand GOL F 603 (B)



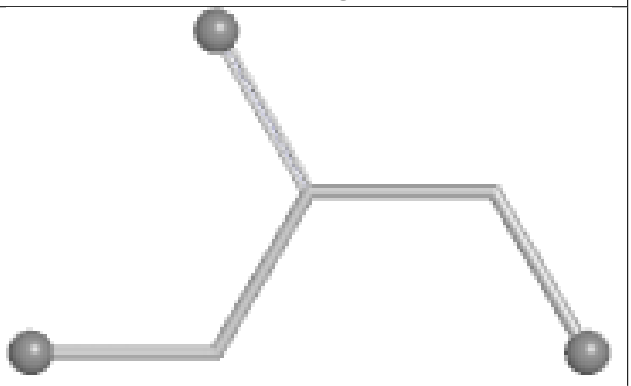
Bond lengths



Bond angles

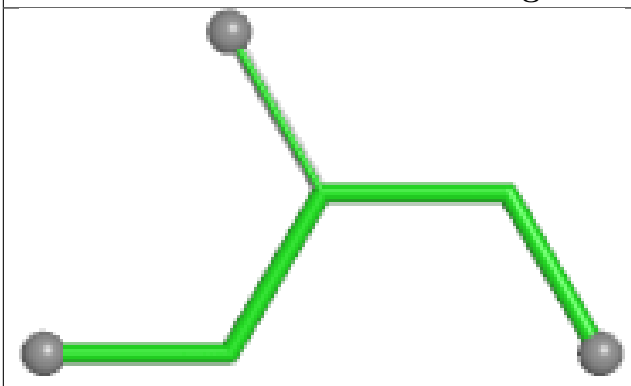


Torsions

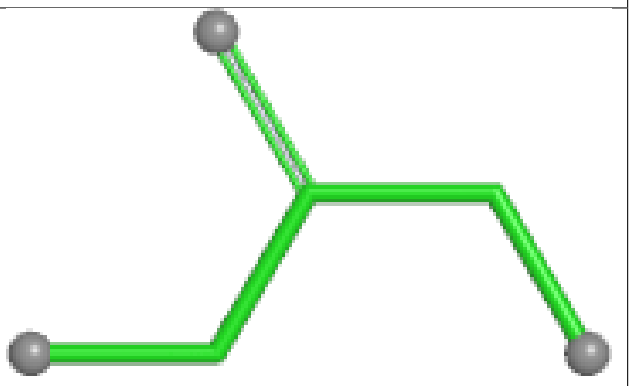


Rings

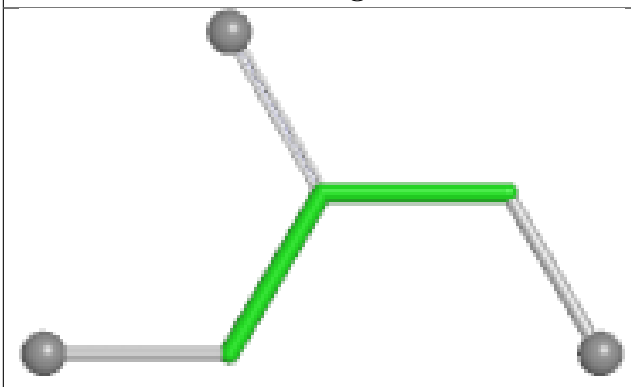
Ligand GOL D 605



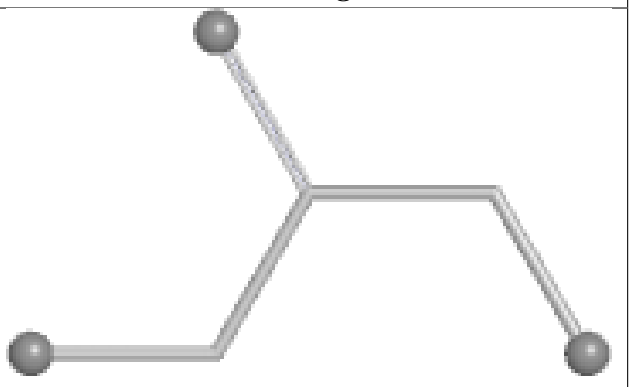
Bond lengths



Bond angles

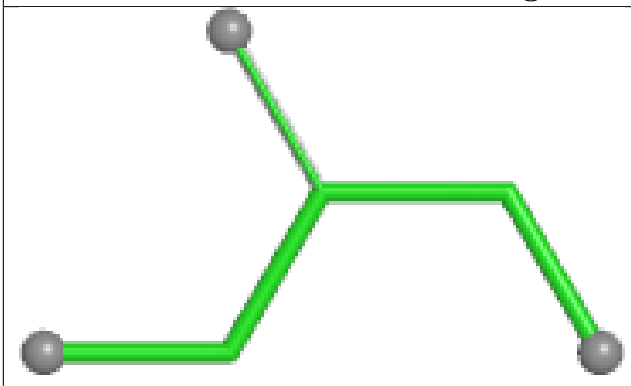


Torsions

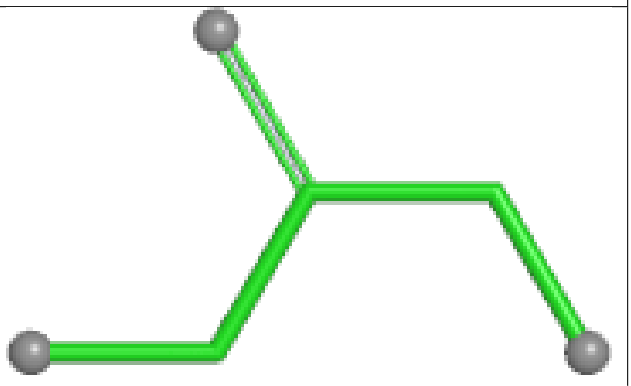


Rings

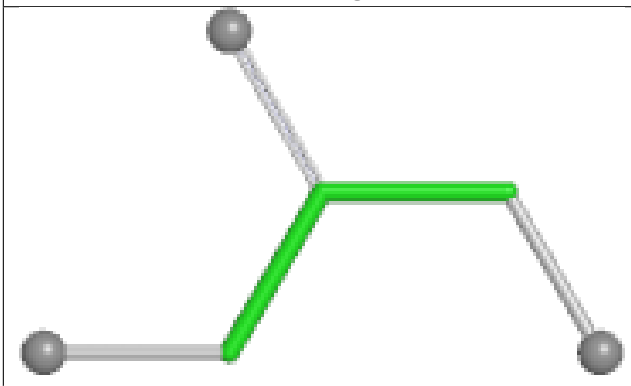
Ligand GOL D 604



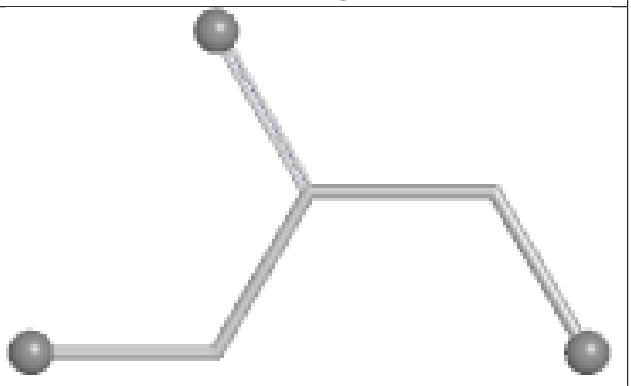
Bond lengths



Bond angles

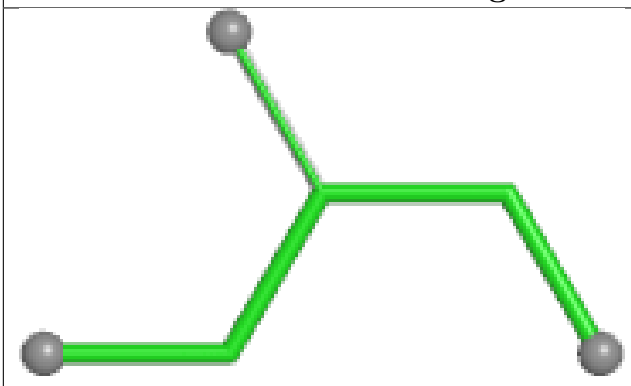


Torsions

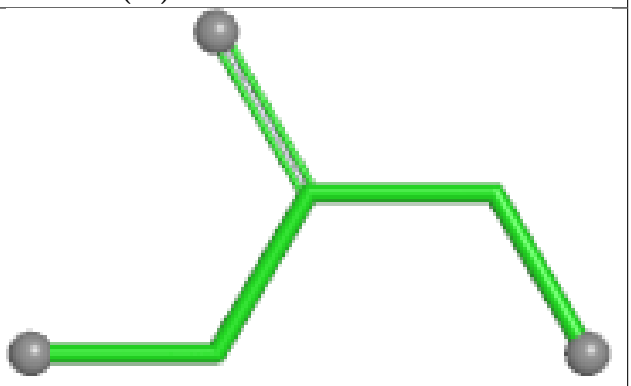


Rings

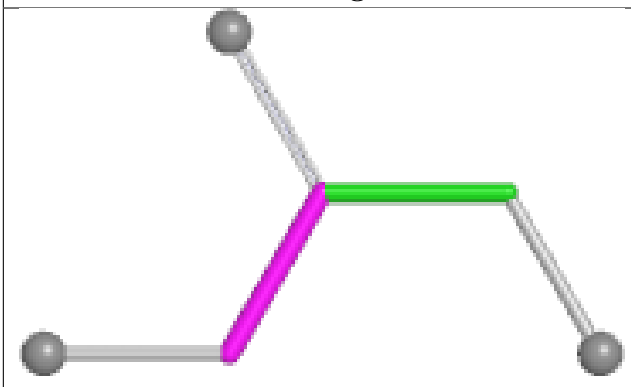
Ligand GOL D 606 (A)



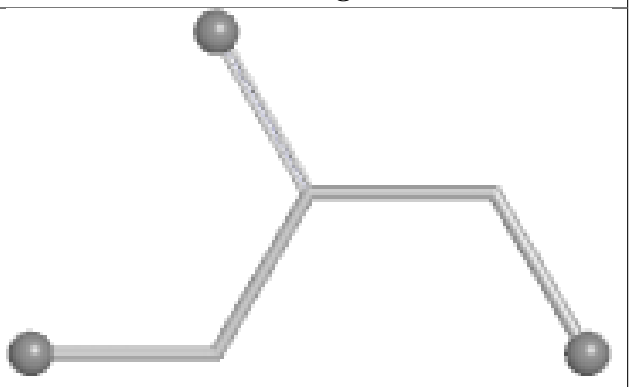
Bond lengths



Bond angles

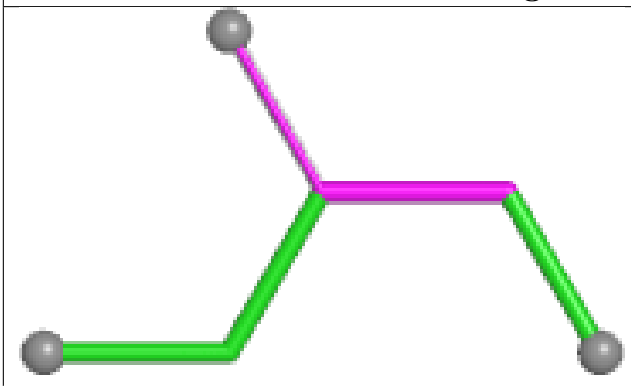


Torsions

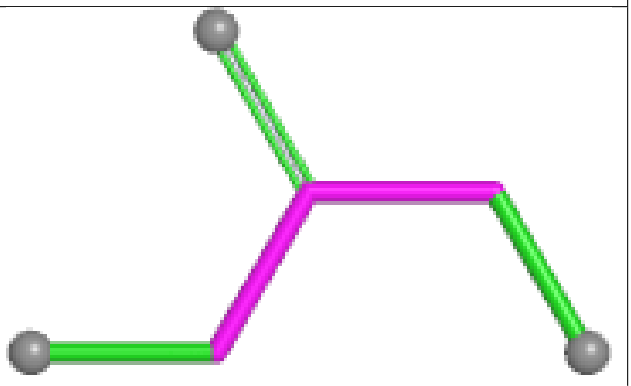


Rings

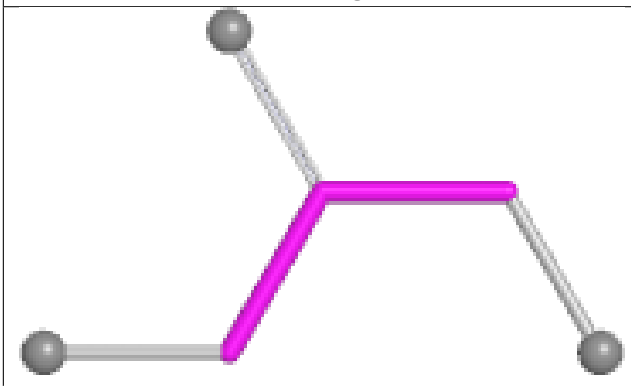
Ligand GOL B 602



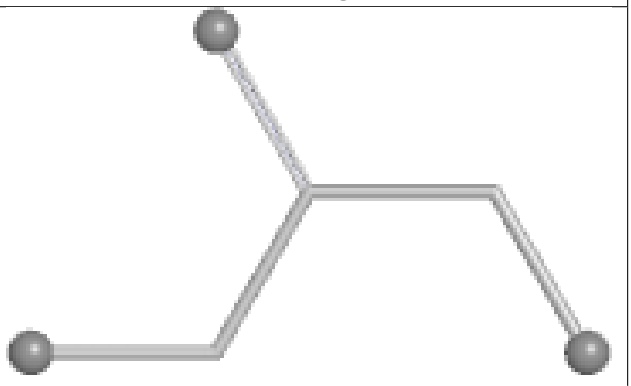
Bond lengths



Bond angles

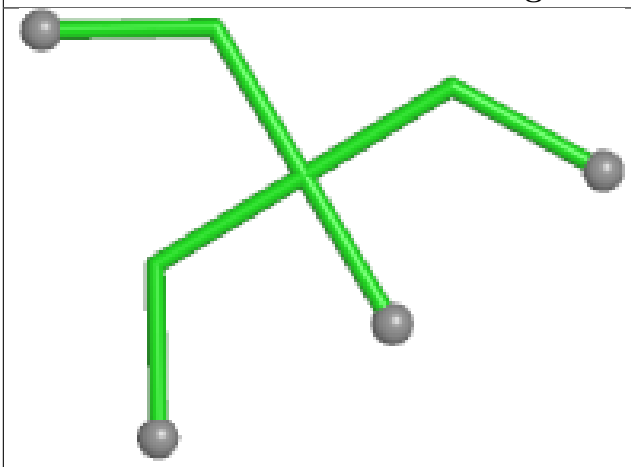


Torsions

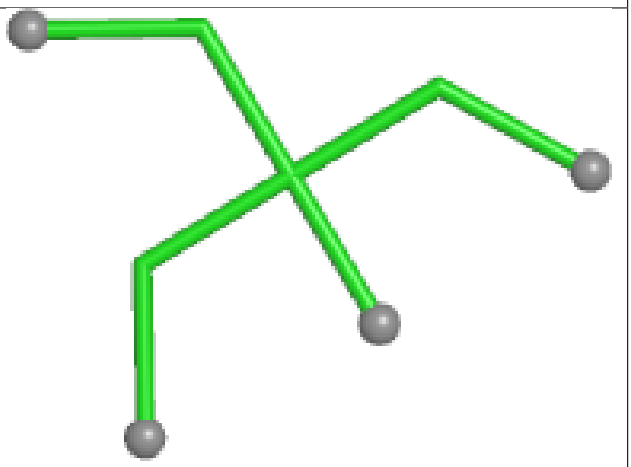


Rings

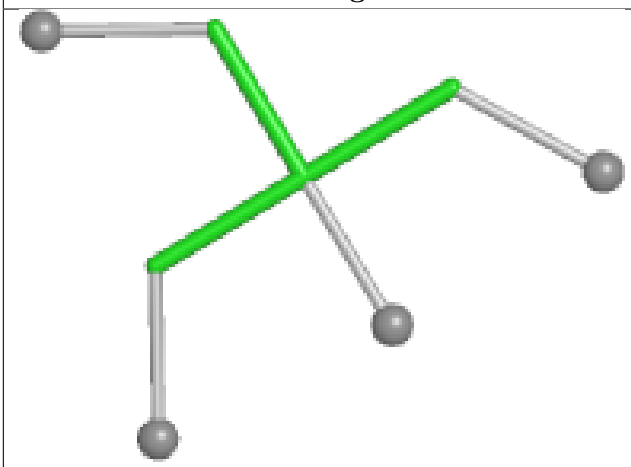
Ligand TRS D 600



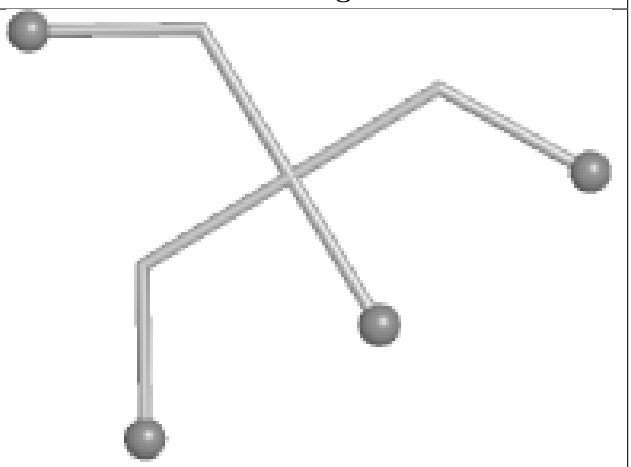
Bond lengths



Bond angles

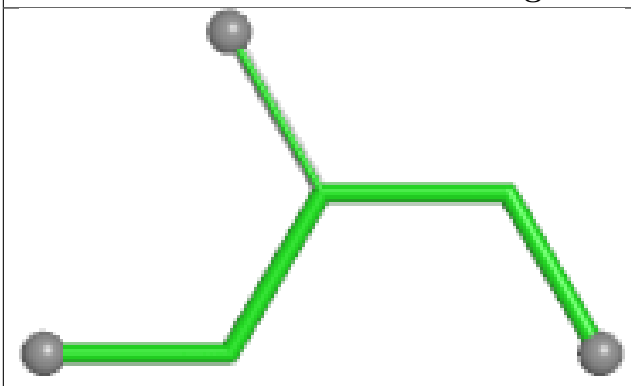


Torsions



Rings

Ligand GOL E 601



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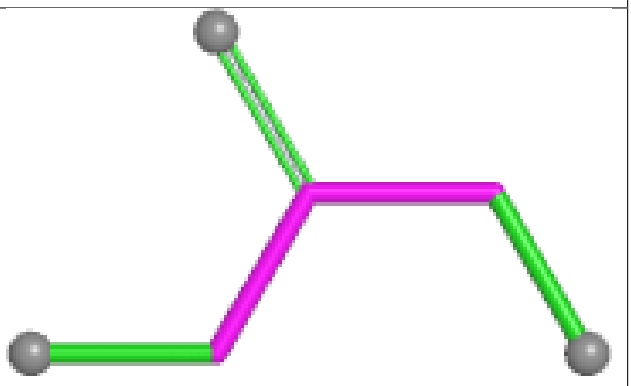
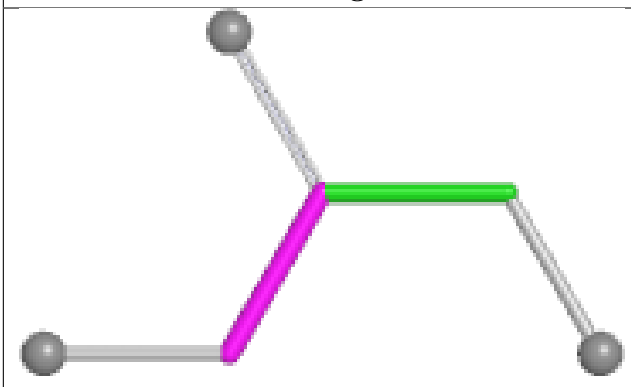


Bond angles



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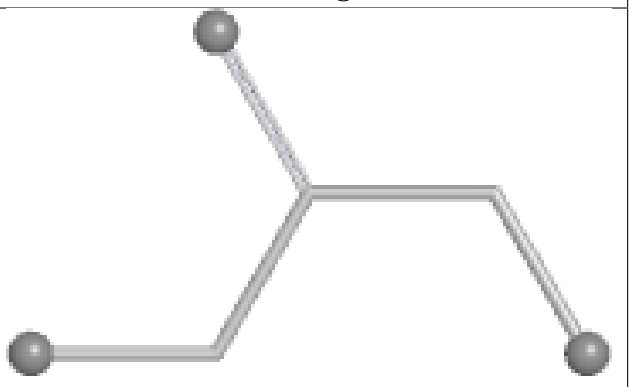
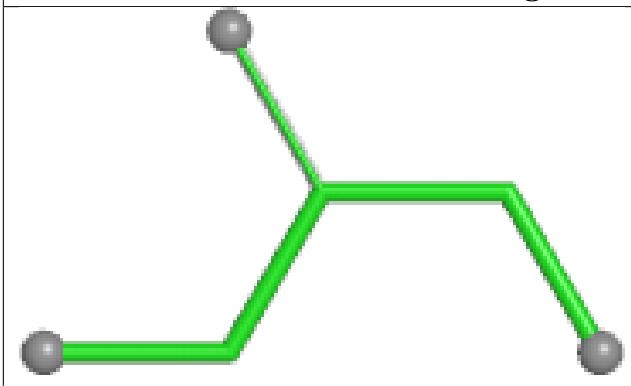


Rings

Ligand GOL B 603



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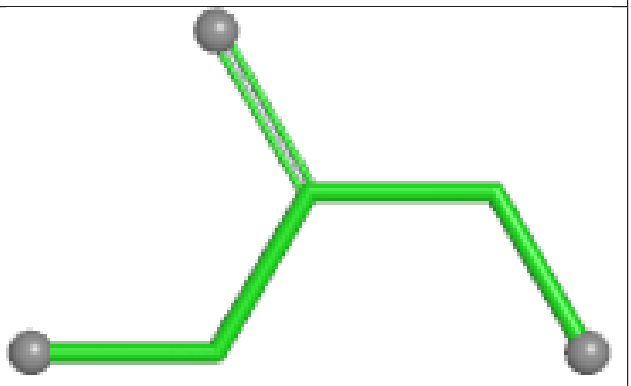
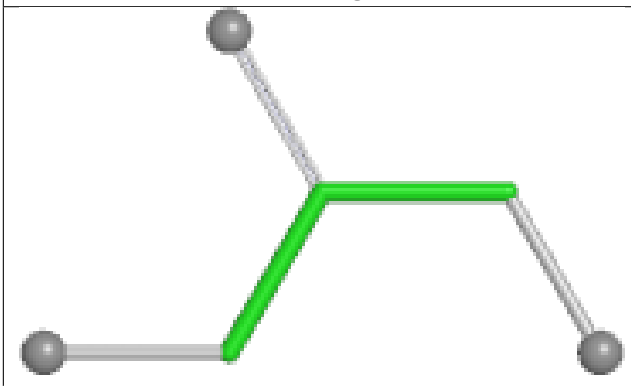


Bond angles



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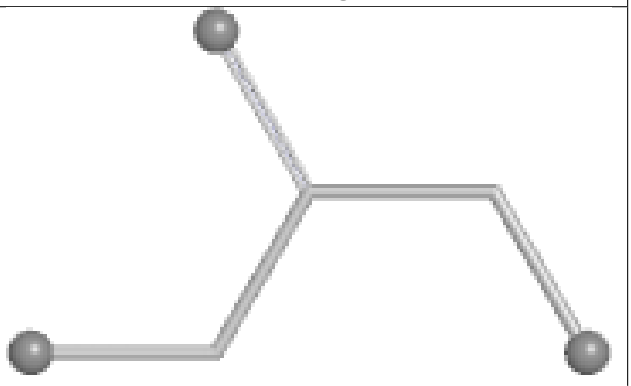
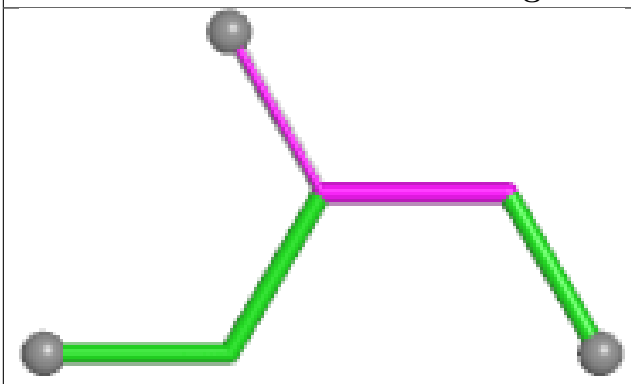


Rings

Ligand GOL C 601



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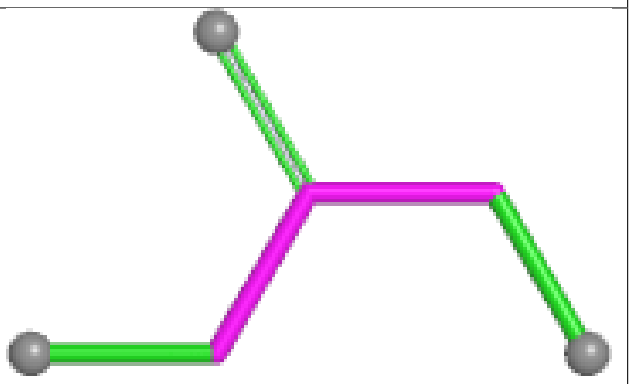
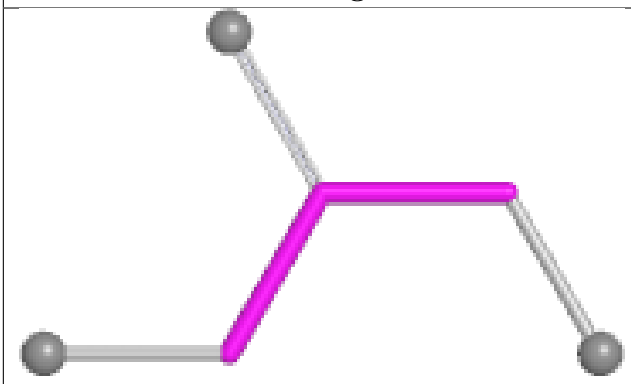


Bond angles



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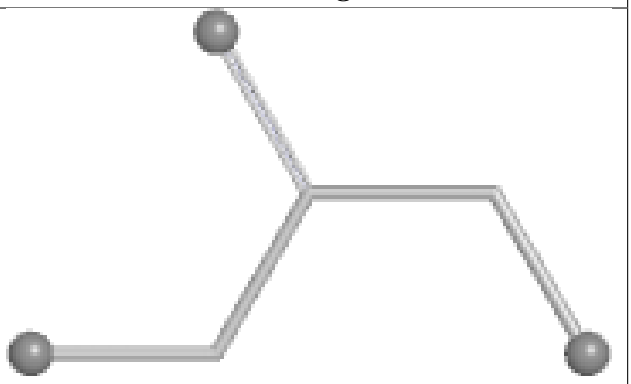
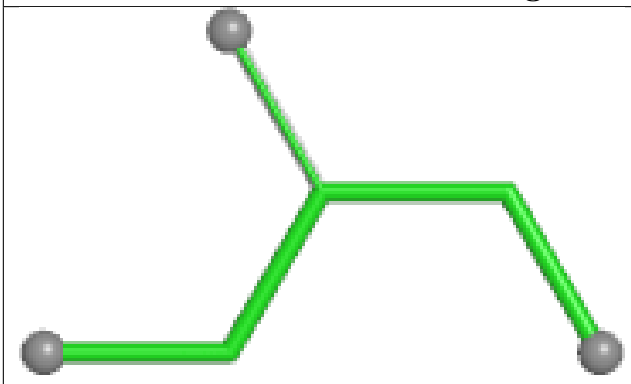


Rings

Ligand GOL E 603



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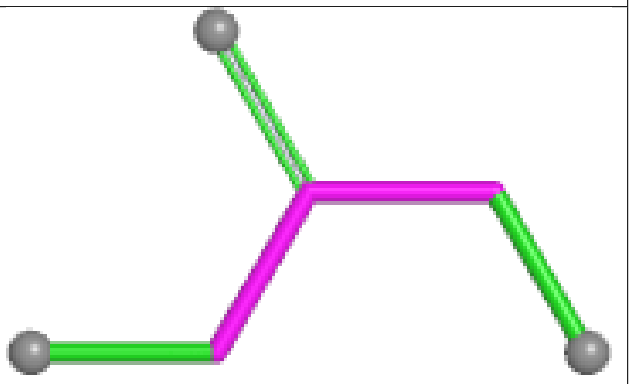
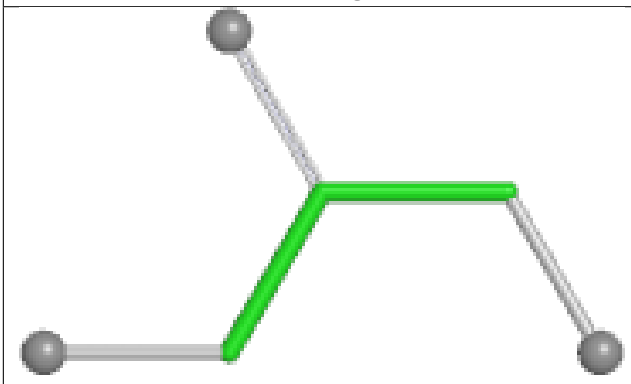


Bond angles



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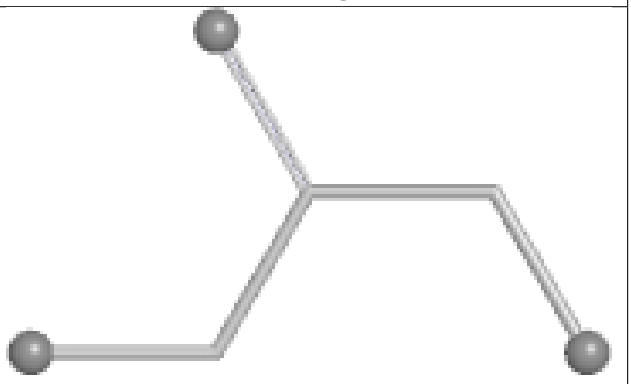
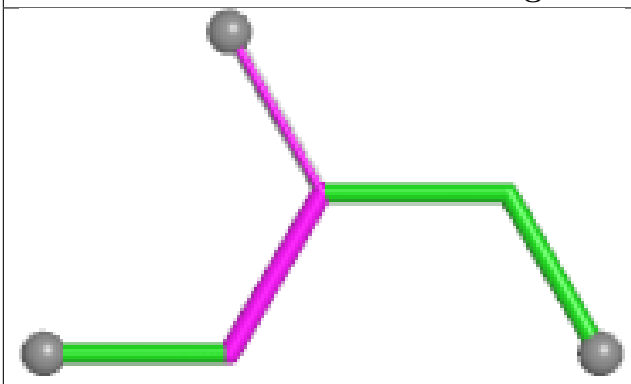


Rings

Ligand GOL E 602



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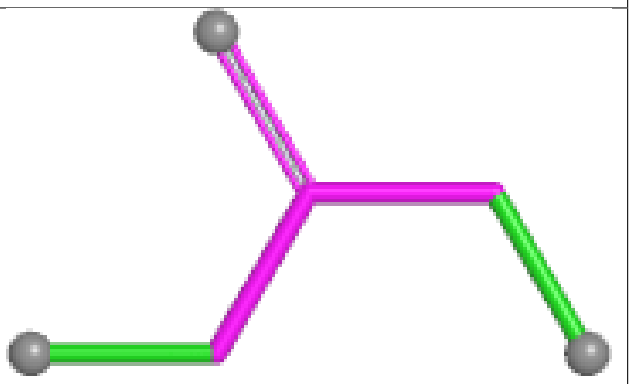
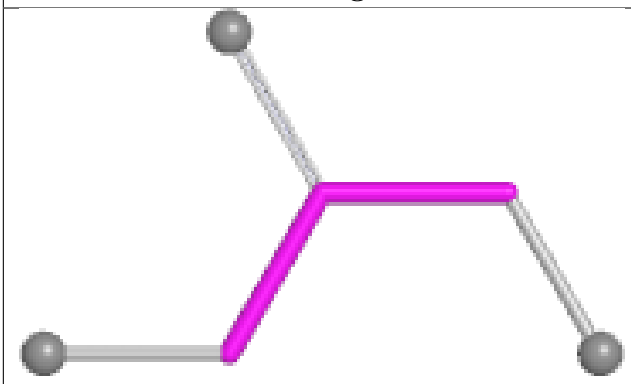


Bond angles



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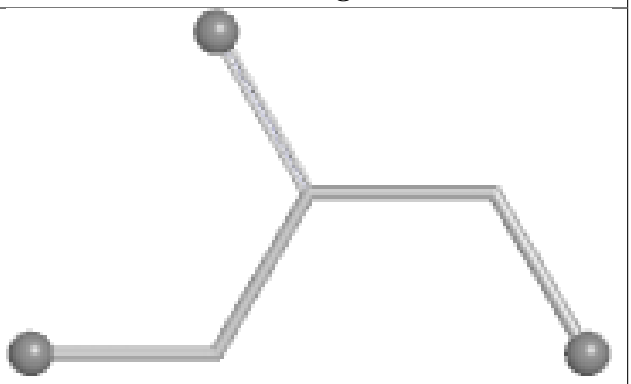
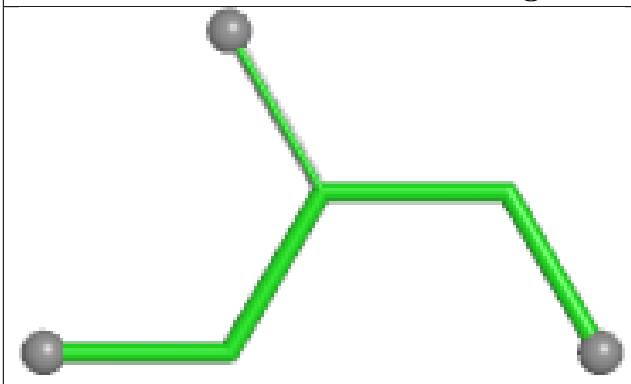


Rings

Ligand GOL D 601



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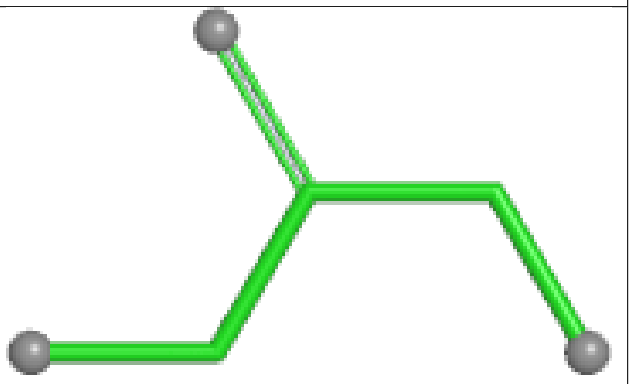
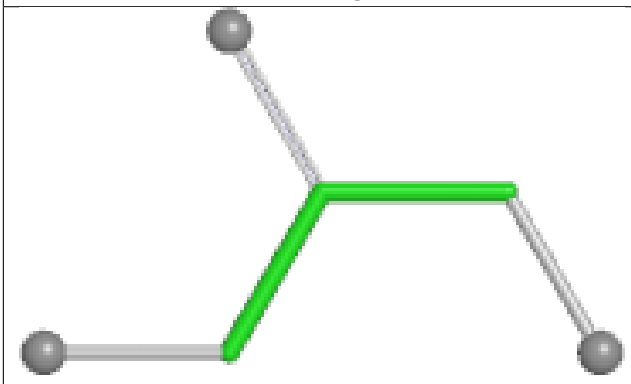


Bond angles



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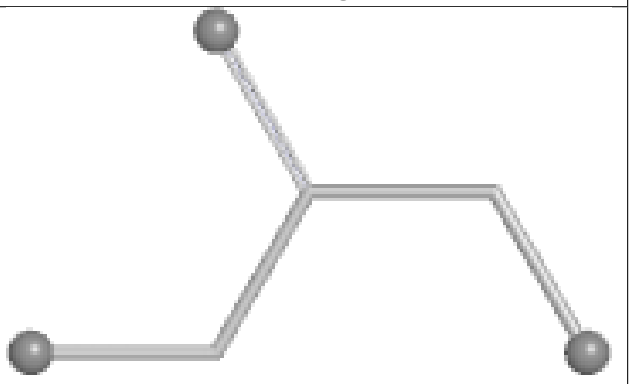
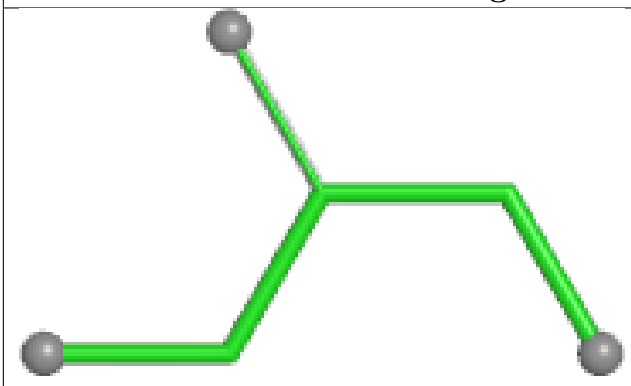


Rings

Ligand GOL D 602 (B)



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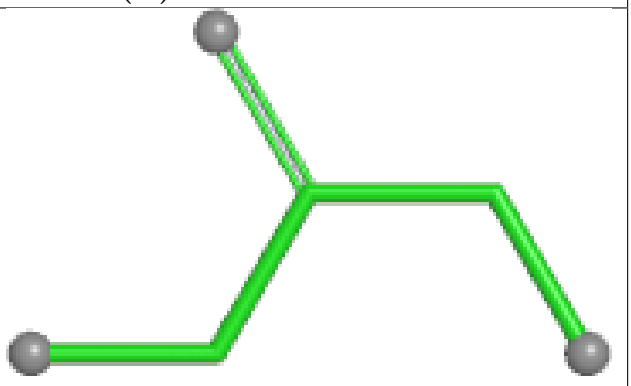
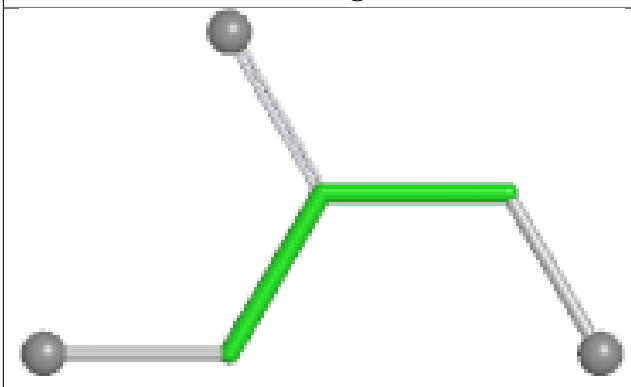
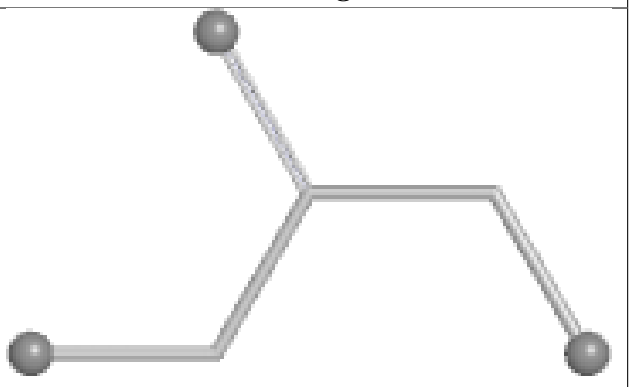


Bond angles

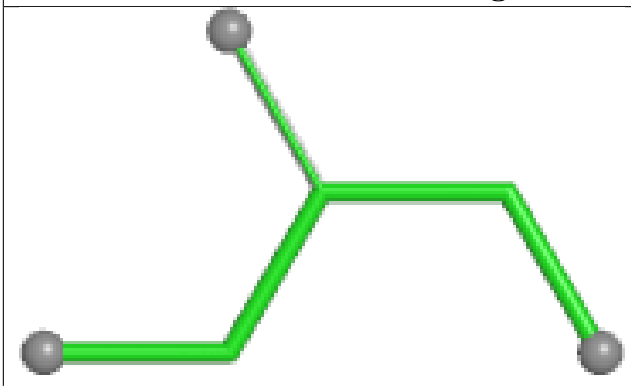


Torsions



Rings

Ligand GOL D 606 (B)



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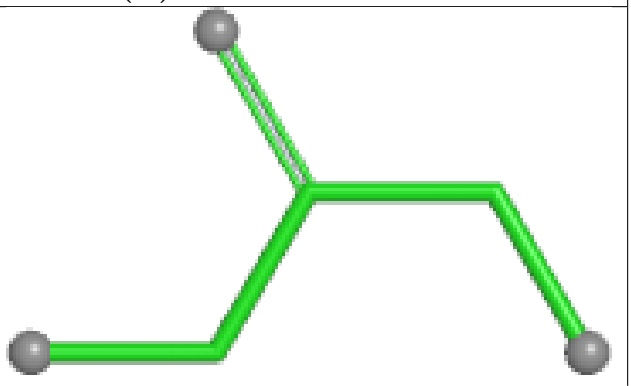
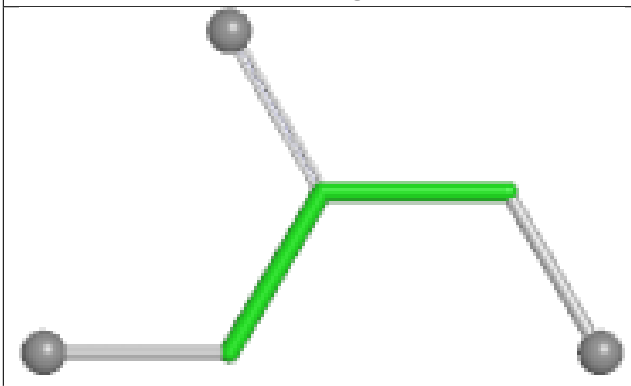
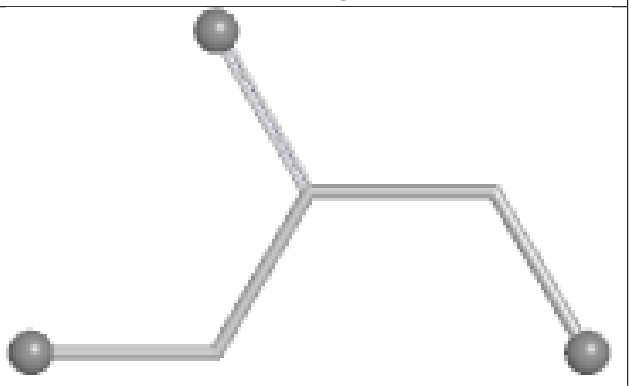


Bond angles

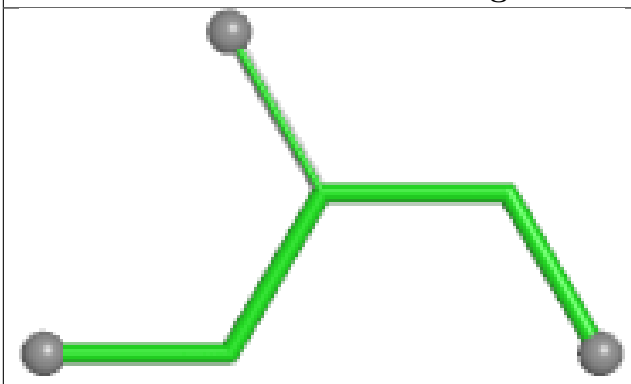


Torsions



Rings

Ligand GOL B 601 (A)



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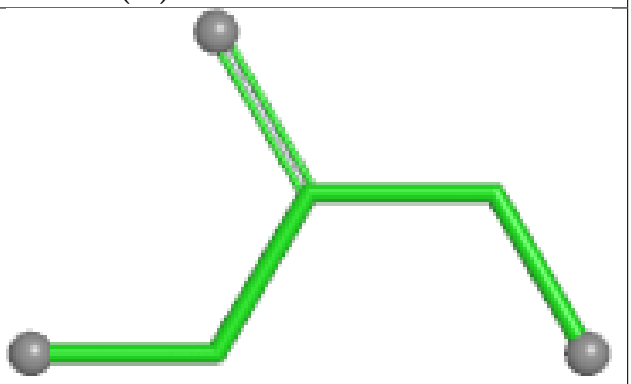
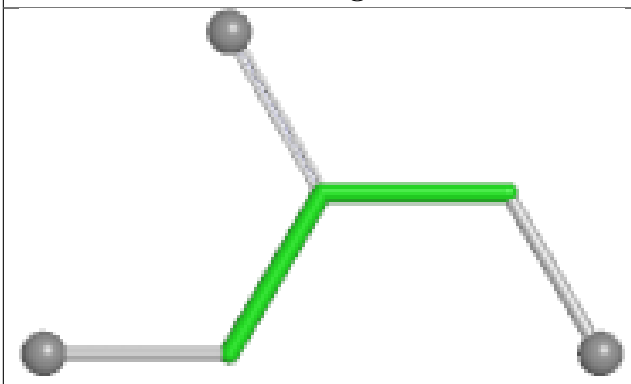


Bond angles



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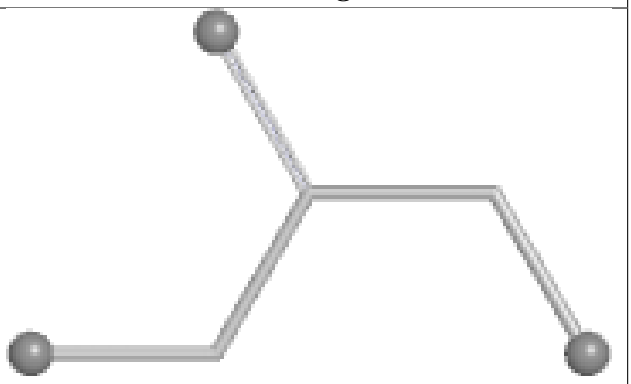
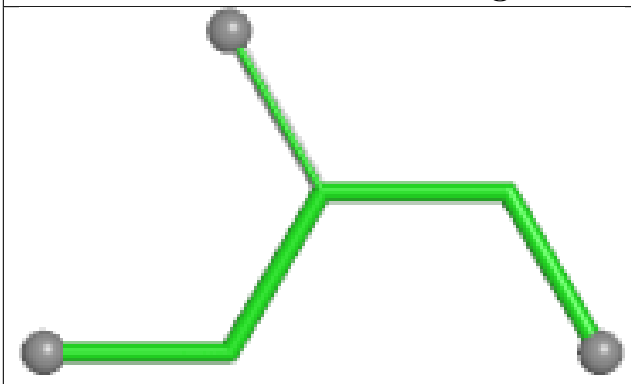
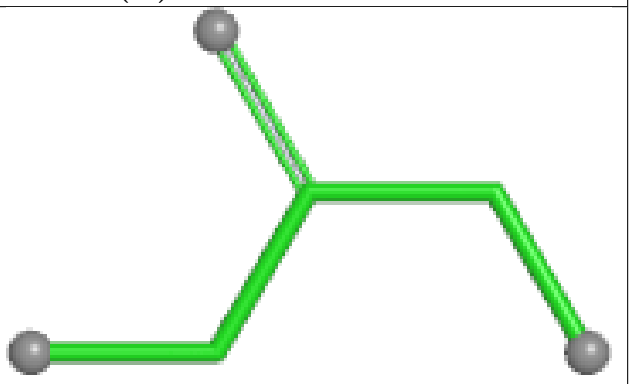


Rings

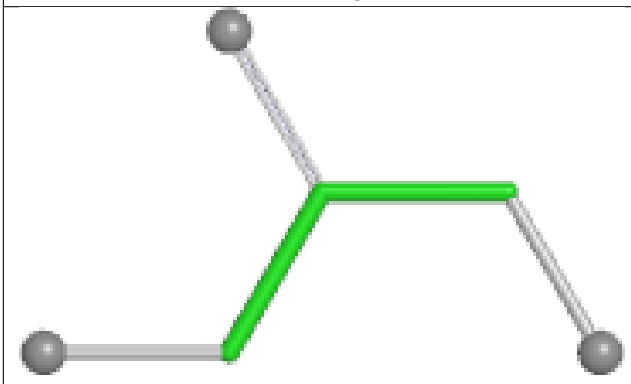
Ligand GOL F 603 (A)



Bond lengths



Bond angles



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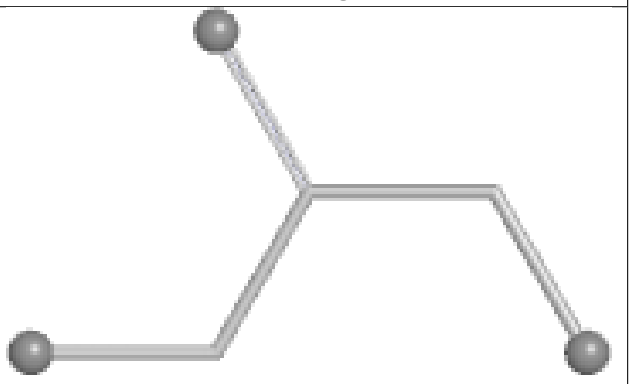
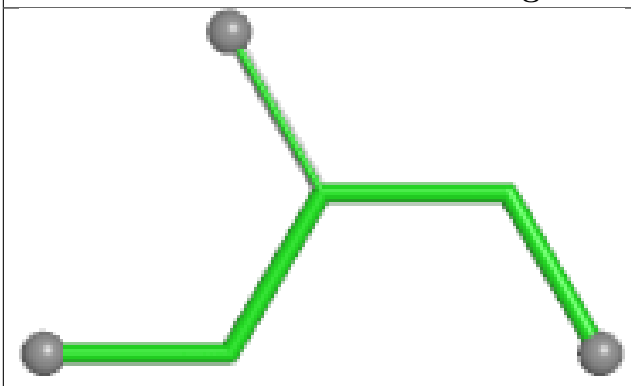


Rings

Ligand GOL D 603



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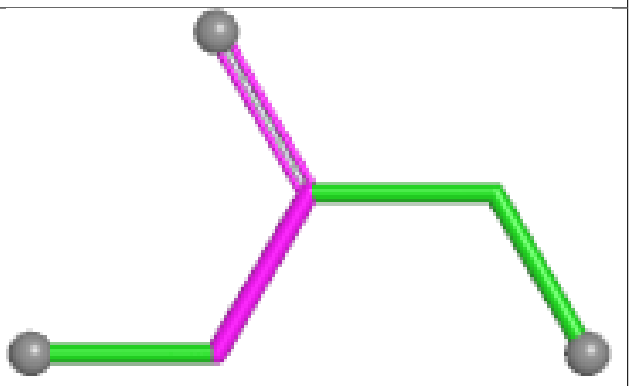
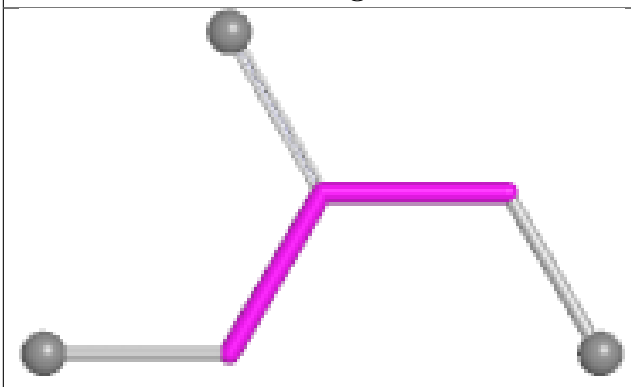
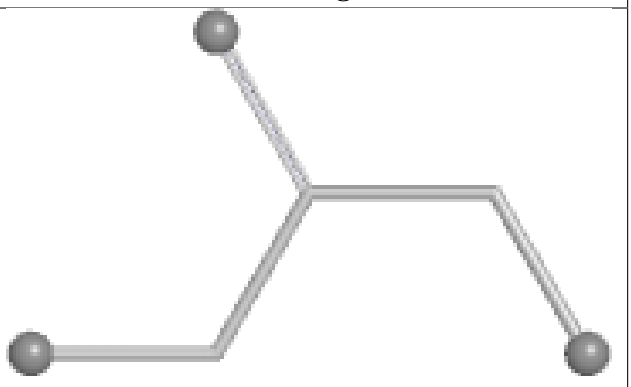


Bond angles

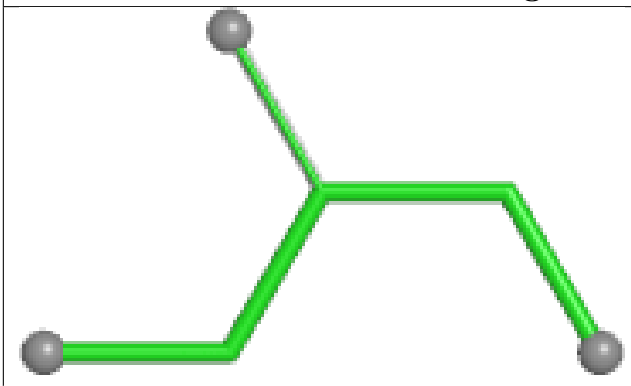


Torsions

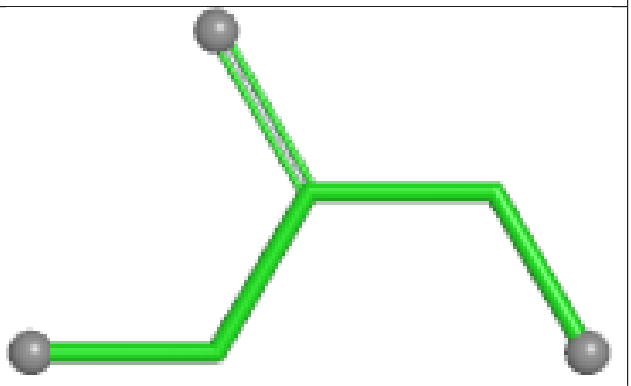


Rings

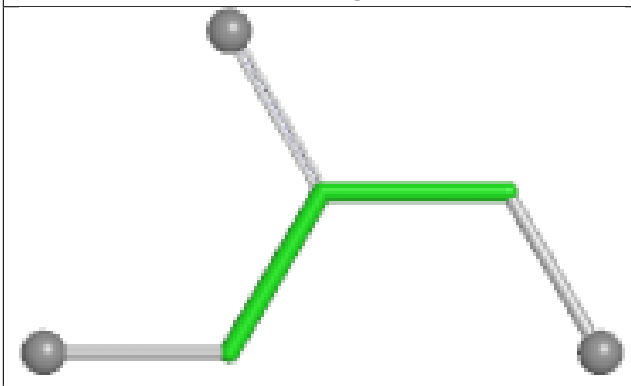
Ligand GOL C 603



Bond lengths



Bond angles



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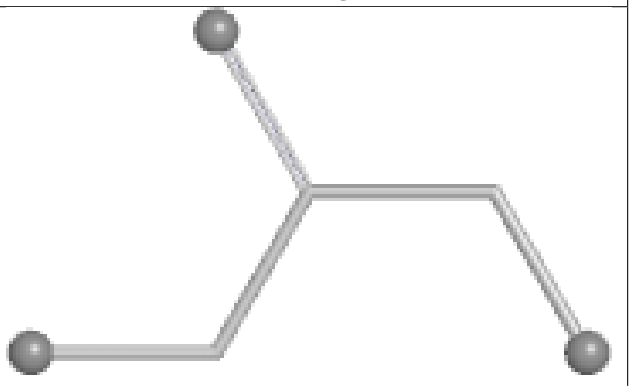
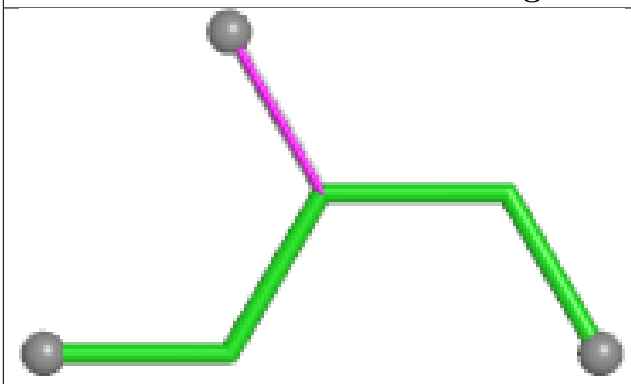
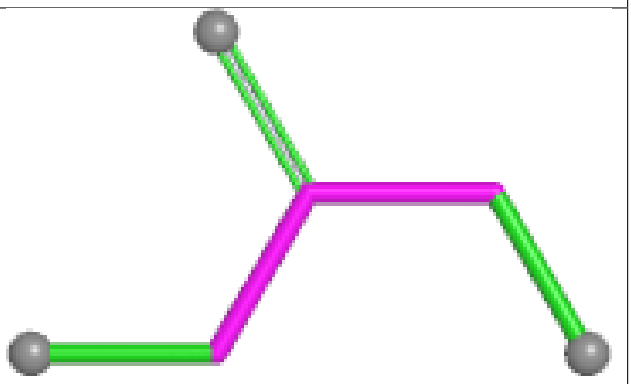


Rings

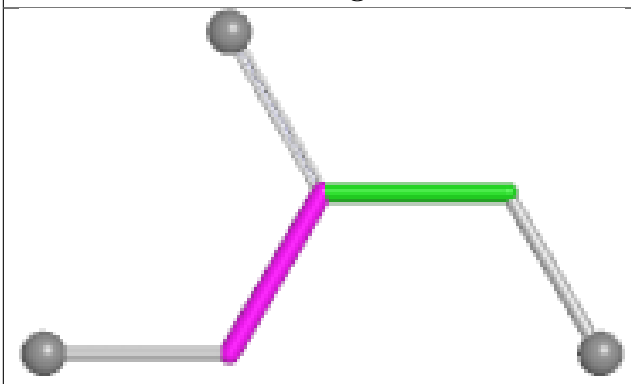
Ligand GOL B 605



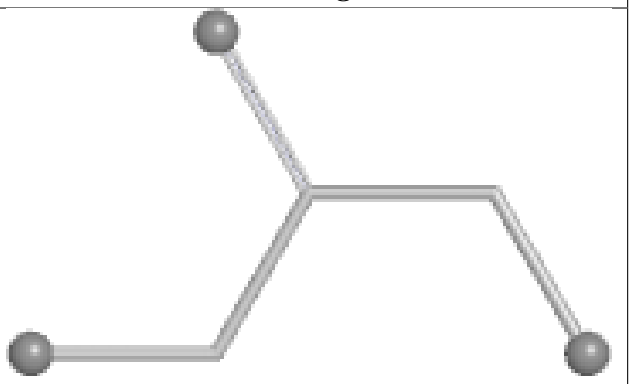
Bond lengths



Bond angles

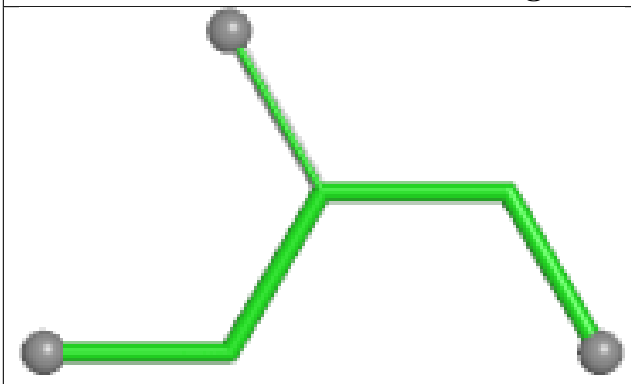


Torsions



Rings

Ligand GOL F 601



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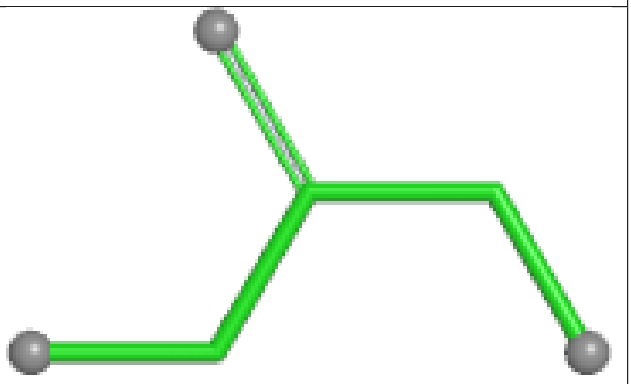
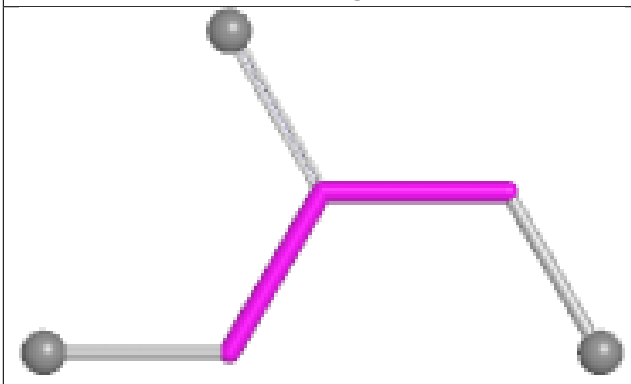
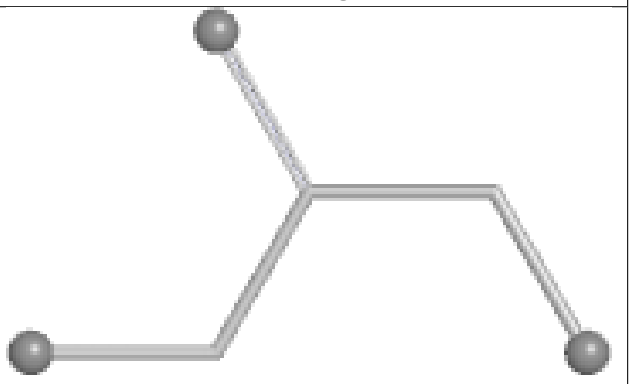


Bond angles

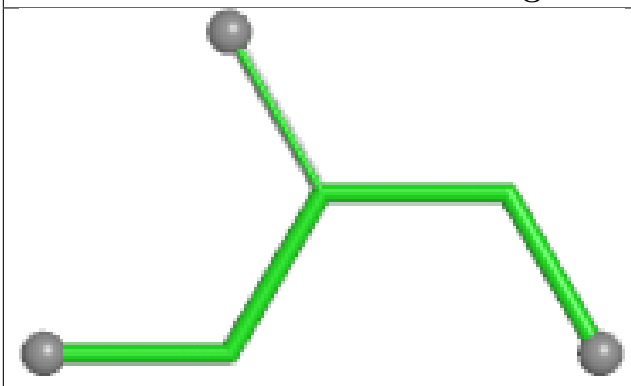


Torsions



Rings

Ligand GOL C 604



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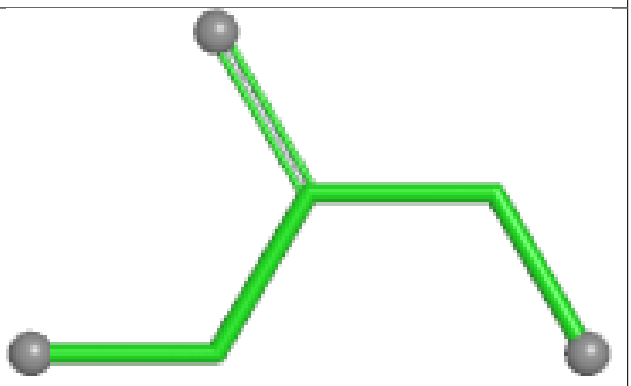

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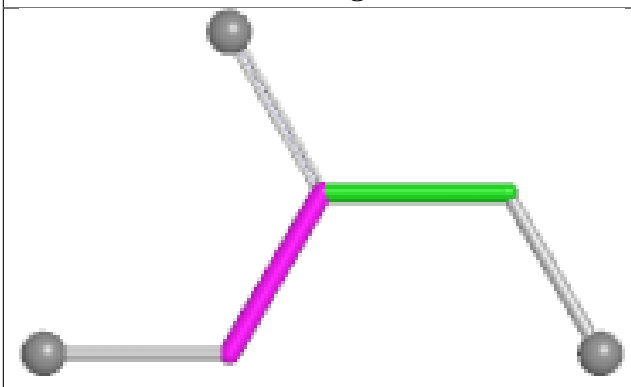
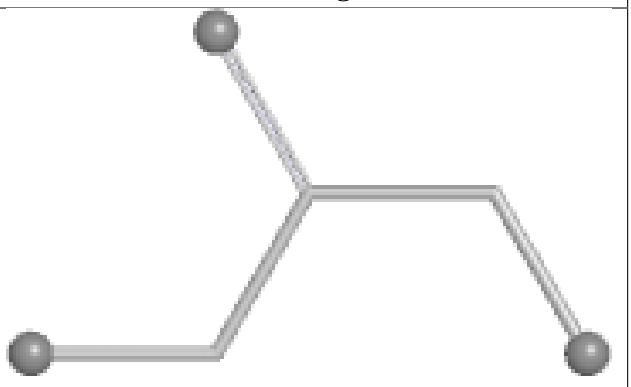


Torsions



Rings

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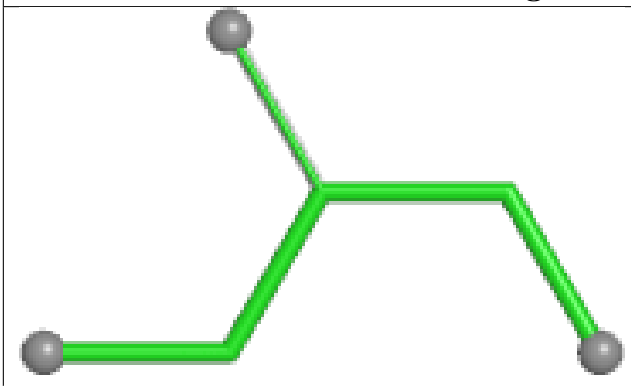
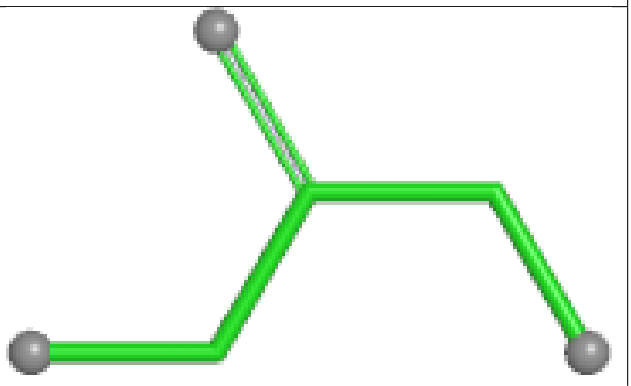
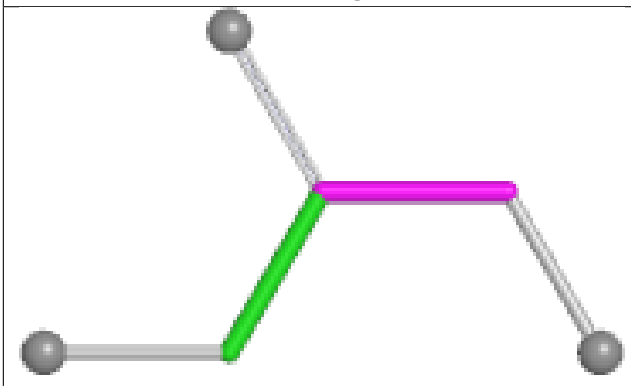


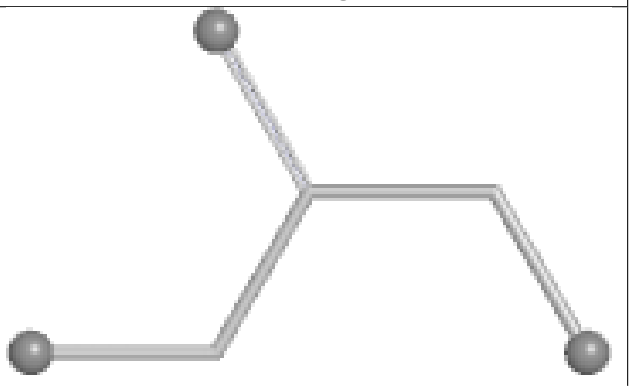
Bond lengths



Bond angles

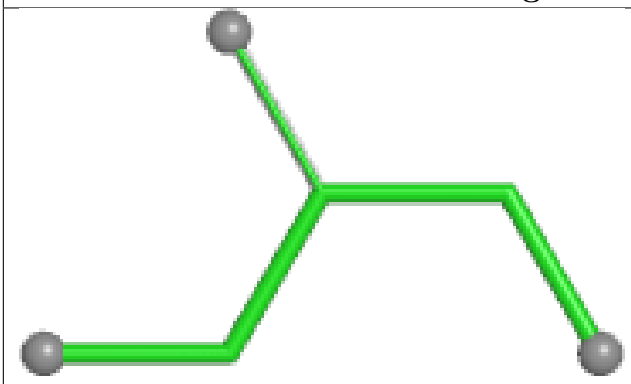


Torsions

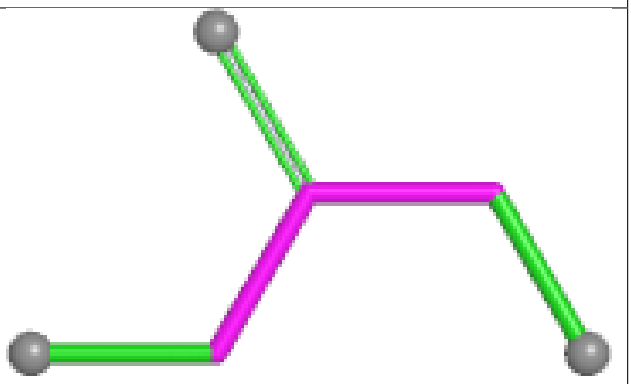


Rings

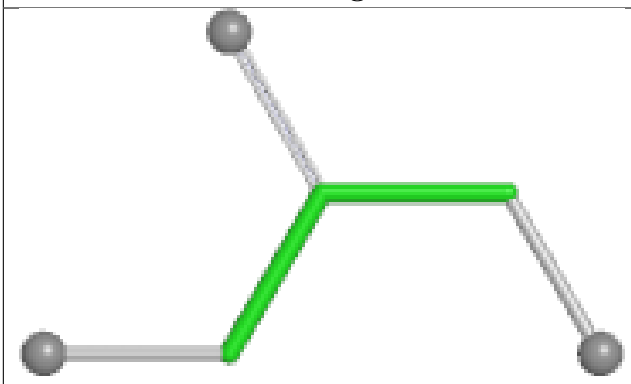
Ligand GOL A 602



Bond lengths



Bond angles



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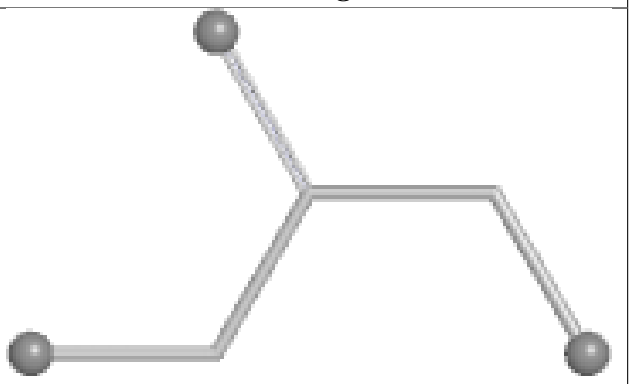
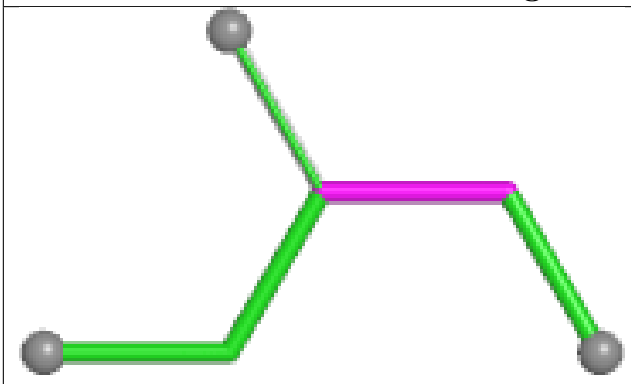


Rings

Ligand GOL B 604



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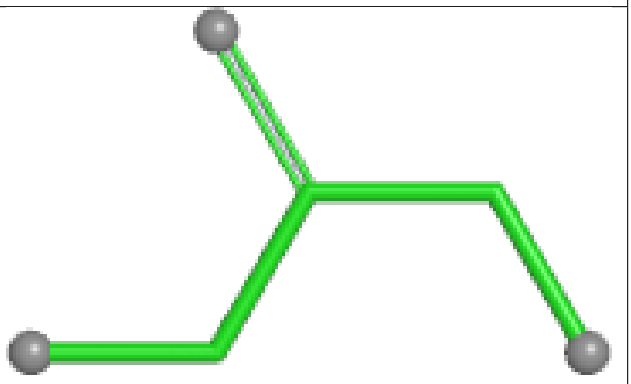
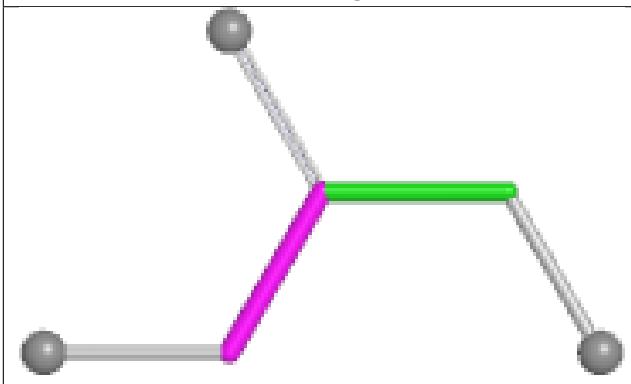
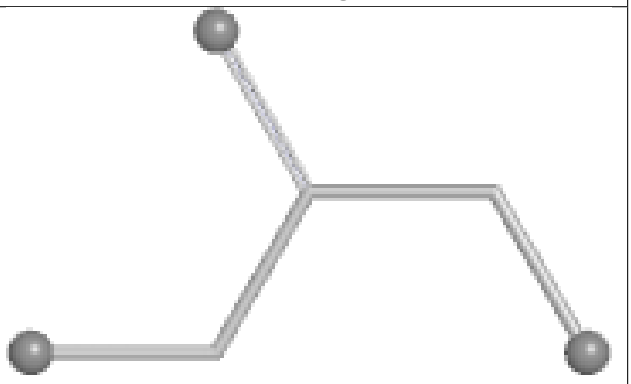


Bond angles

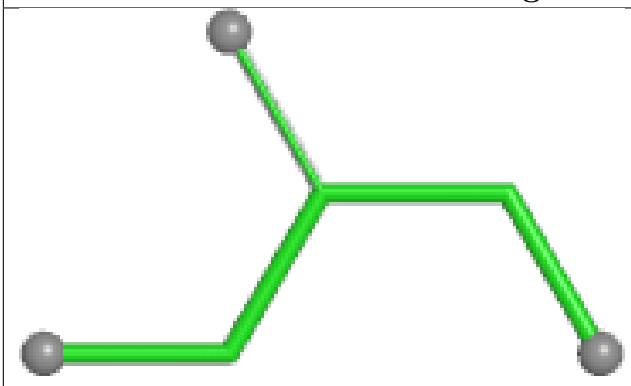


Torsions

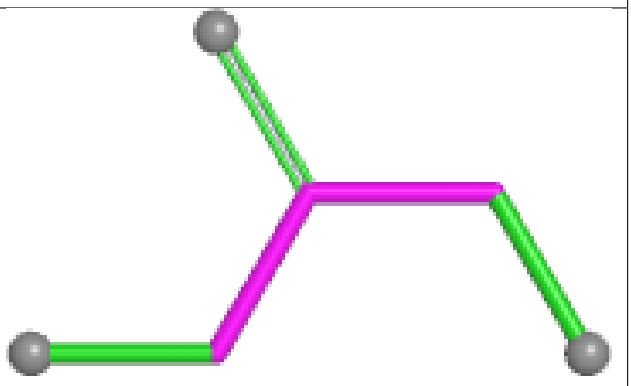


Rings

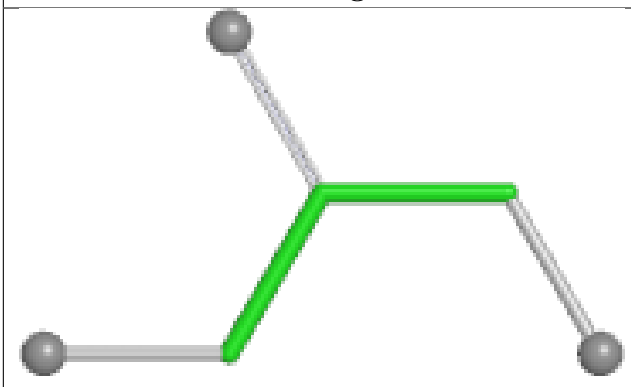
Ligand GOL A 601



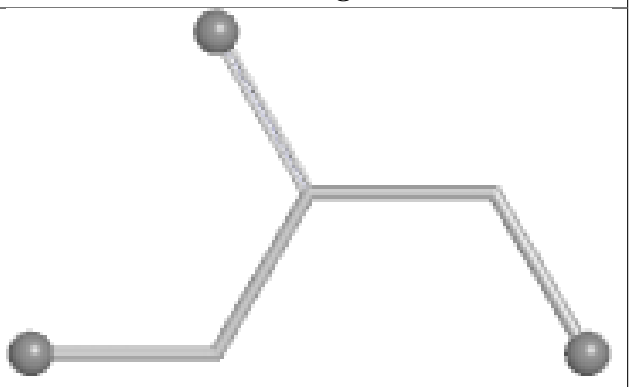
Bond lengths



Bond angles

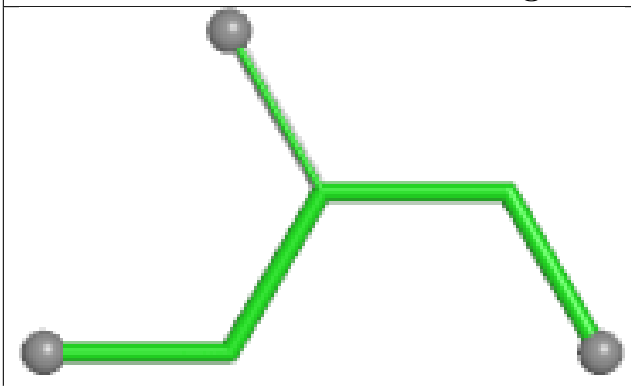


Torsions



Rings

Ligand GOL A 603



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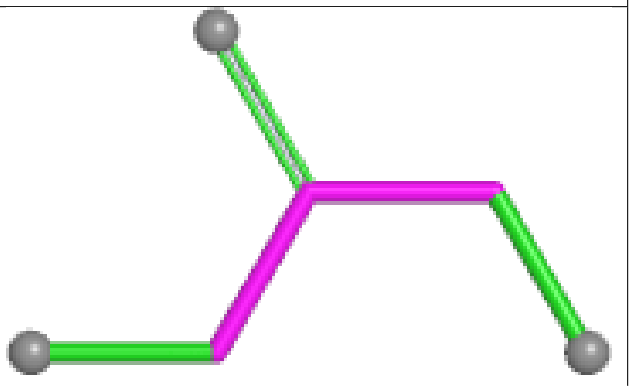
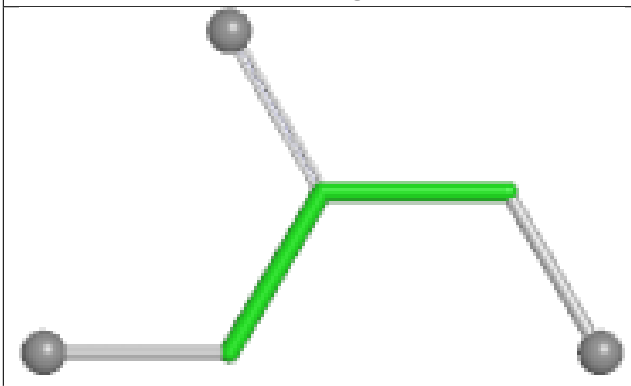
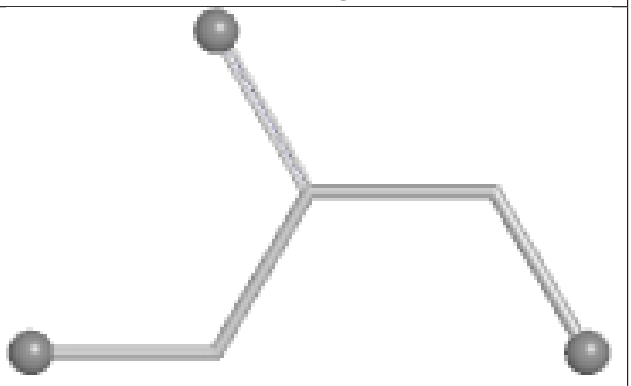


Bond angles

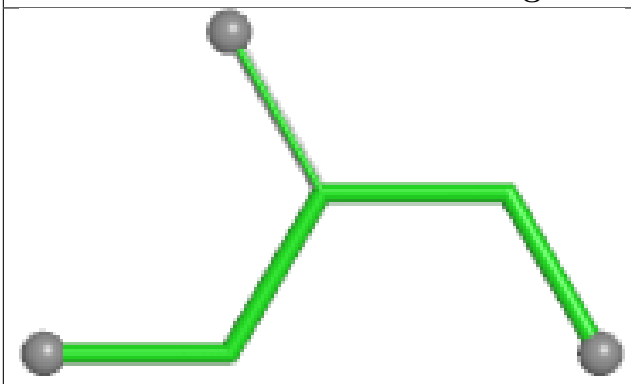


Torsions



Rings

Ligand GOL C 602



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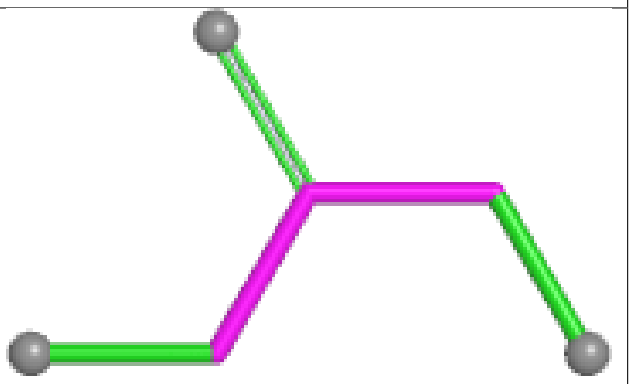
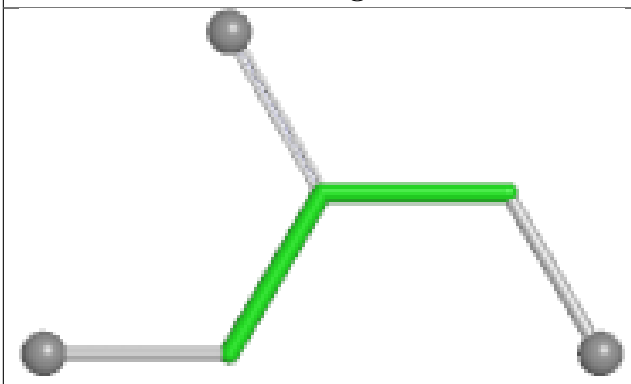


Bond angles



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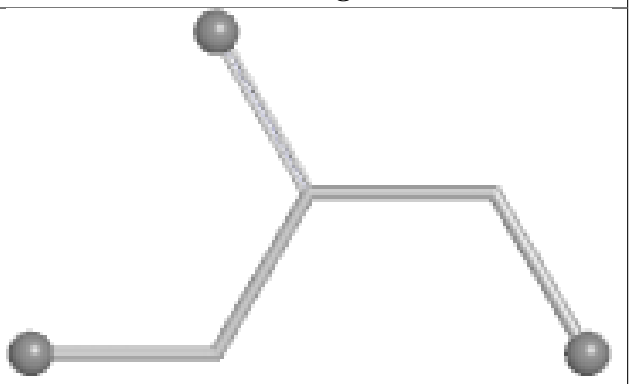

Rings

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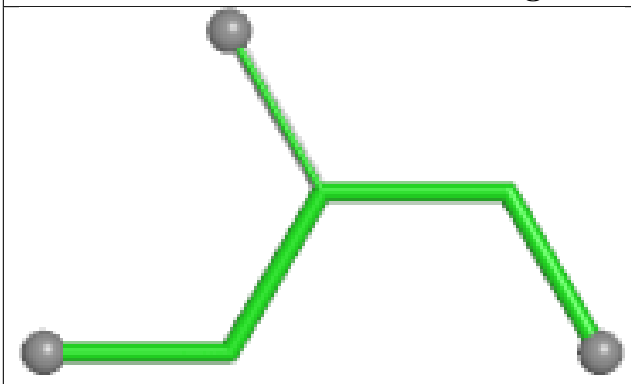
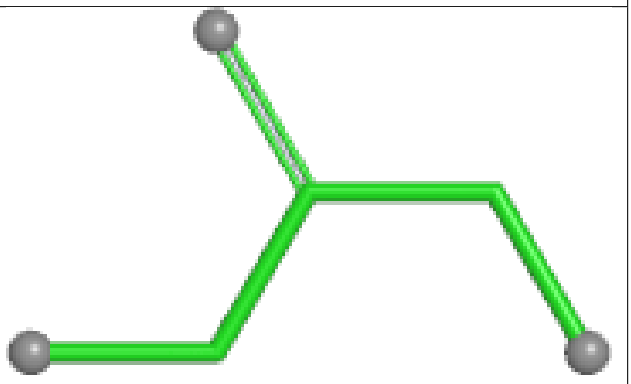
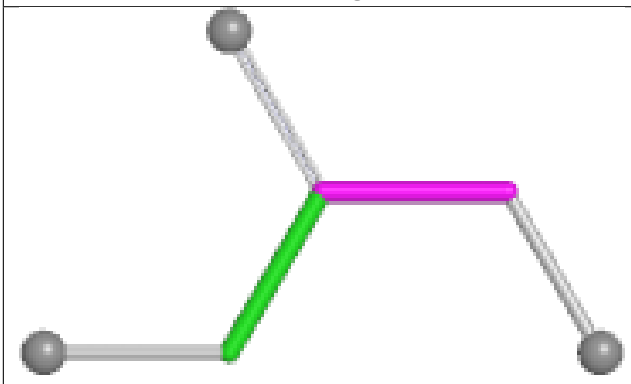


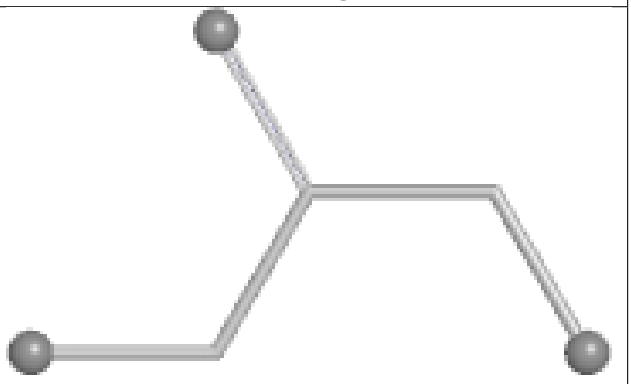
Bond lengths



Bond angles

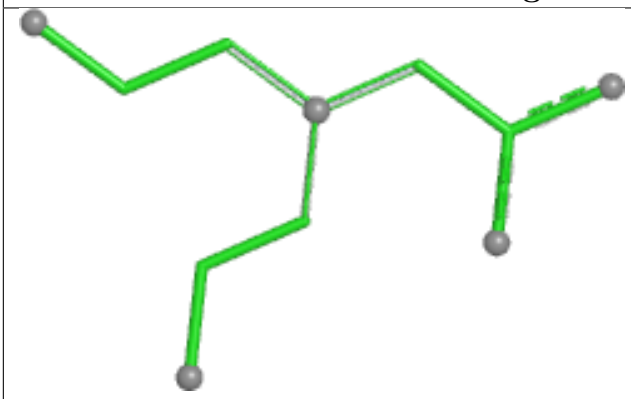


Torsions

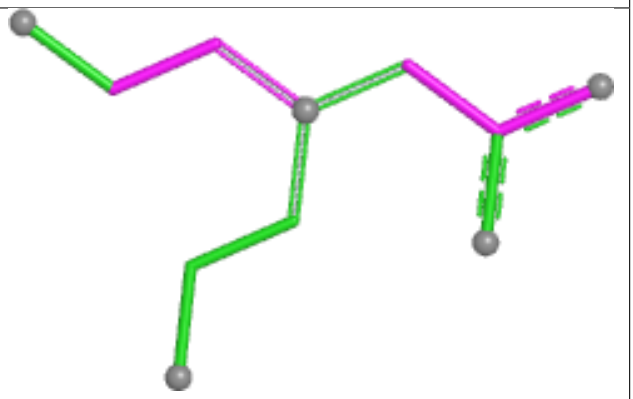


Rings

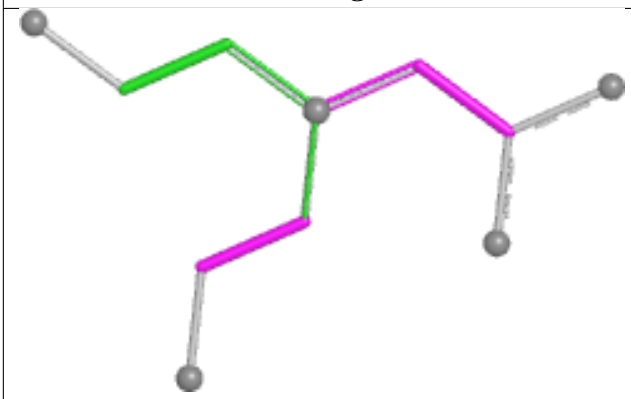
Ligand BCN E 600



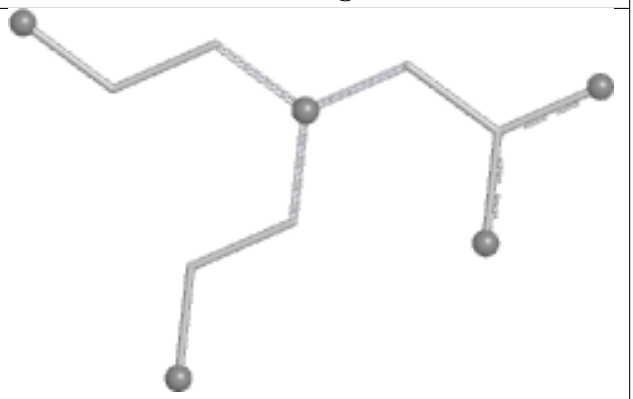
Bond lengths



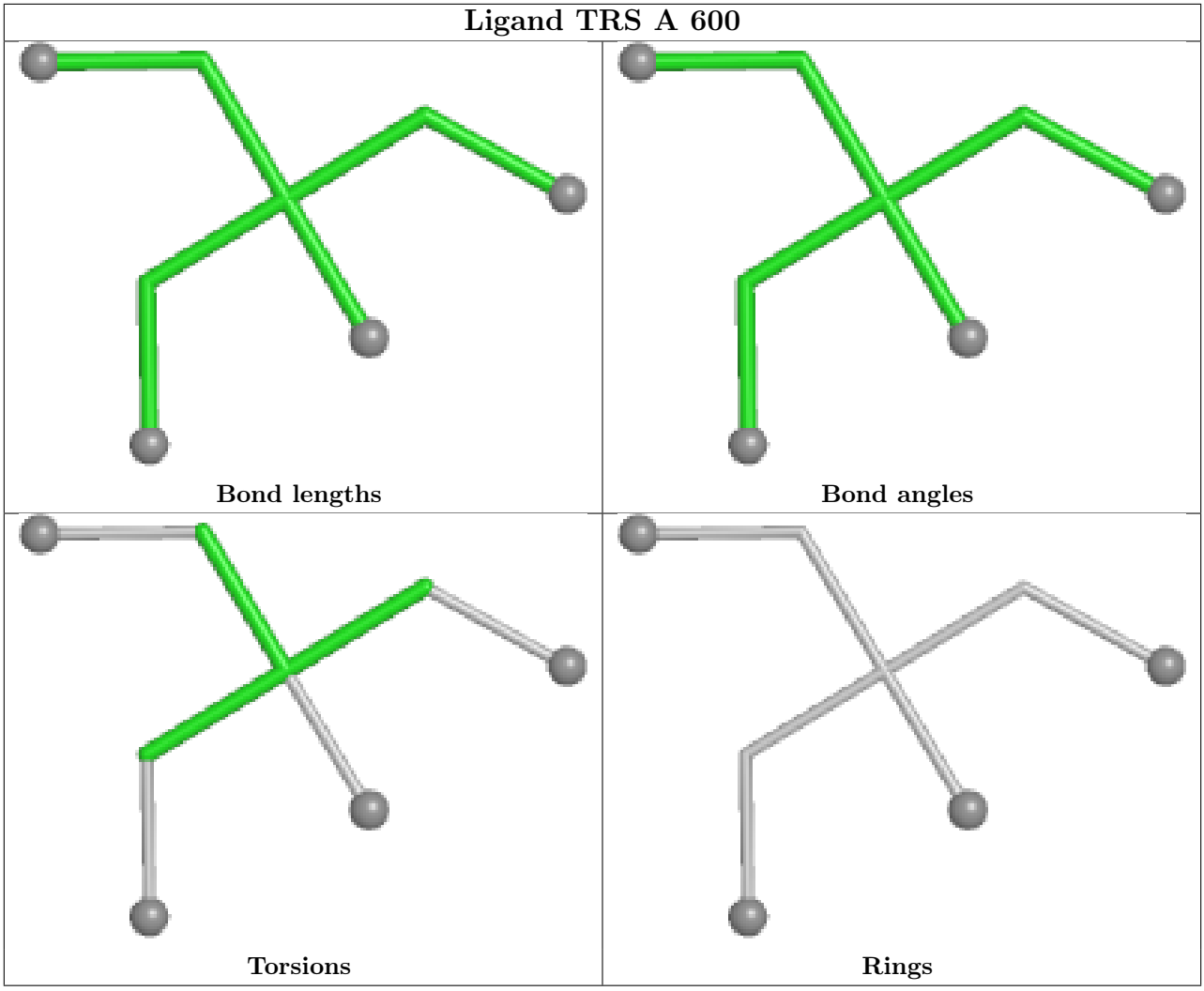
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	563/612 (91%)	-0.35	9 (1%)	70	76	7, 13, 23, 59	25 (4%)
1	B	563/612 (91%)	-0.37	8 (1%)	73	79	7, 12, 24, 55	25 (4%)
1	C	563/612 (91%)	-0.33	5 (0%)	81	86	8, 13, 23, 55	31 (5%)
1	D	564/612 (92%)	-0.47	5 (0%)	81	86	7, 12, 18, 60	28 (4%)
1	E	563/612 (91%)	-0.36	6 (1%)	78	83	7, 13, 23, 66	19 (3%)
1	F	563/612 (91%)	-0.36	8 (1%)	73	79	7, 13, 24, 63	19 (3%)
All	All	3379/3672 (92%)	-0.37	41 (1%)	76	82	7, 13, 23, 66	147 (4%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	16	TYR	9.1
1	C	16	TYR	6.8
1	A	16	TYR	6.4
1	F	206	VAL	5.7
1	C	577	LYS	5.5
1	B	577	LYS	5.4
1	D	14	VAL	5.1
1	B	62	THR	4.4
1	B	16	TYR	4.3
1	E	15	GLU	3.8
1	A	523	GLY	3.8
1	F	207	GLY	3.7
1	B	61	ALA	3.7
1	D	15	GLU	3.5
1	A	208[A]	SER	3.3
1	F	208	SER	3.2
1	A	15	GLU	3.1
1	E	576	VAL	3.1
1	B	523	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	16	TYR	2.9
1	B	63	GLY	2.8
1	D	523[A]	GLY	2.8
1	F	209	ASP	2.7
1	A	522	PRO	2.6
1	C	523[A]	GLY	2.6
1	B	60	THR	2.5
1	F	205	THR	2.4
1	A	577	LYS	2.4
1	D	522[A]	PRO	2.4
1	D	577	LYS	2.4
1	F	15	GLU	2.4
1	B	486	THR	2.3
1	A	576	VAL	2.3
1	A	40	LEU	2.3
1	C	449	THR	2.2
1	F	576	VAL	2.2
1	E	523[A]	GLY	2.2
1	E	522[A]	PRO	2.2
1	A	209[A]	ASP	2.2
1	C	62	THR	2.2
1	E	449	THR	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 oligosaccharides 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	TRS	A	600	8/8	0.72	0.15	20,25,35,36	0

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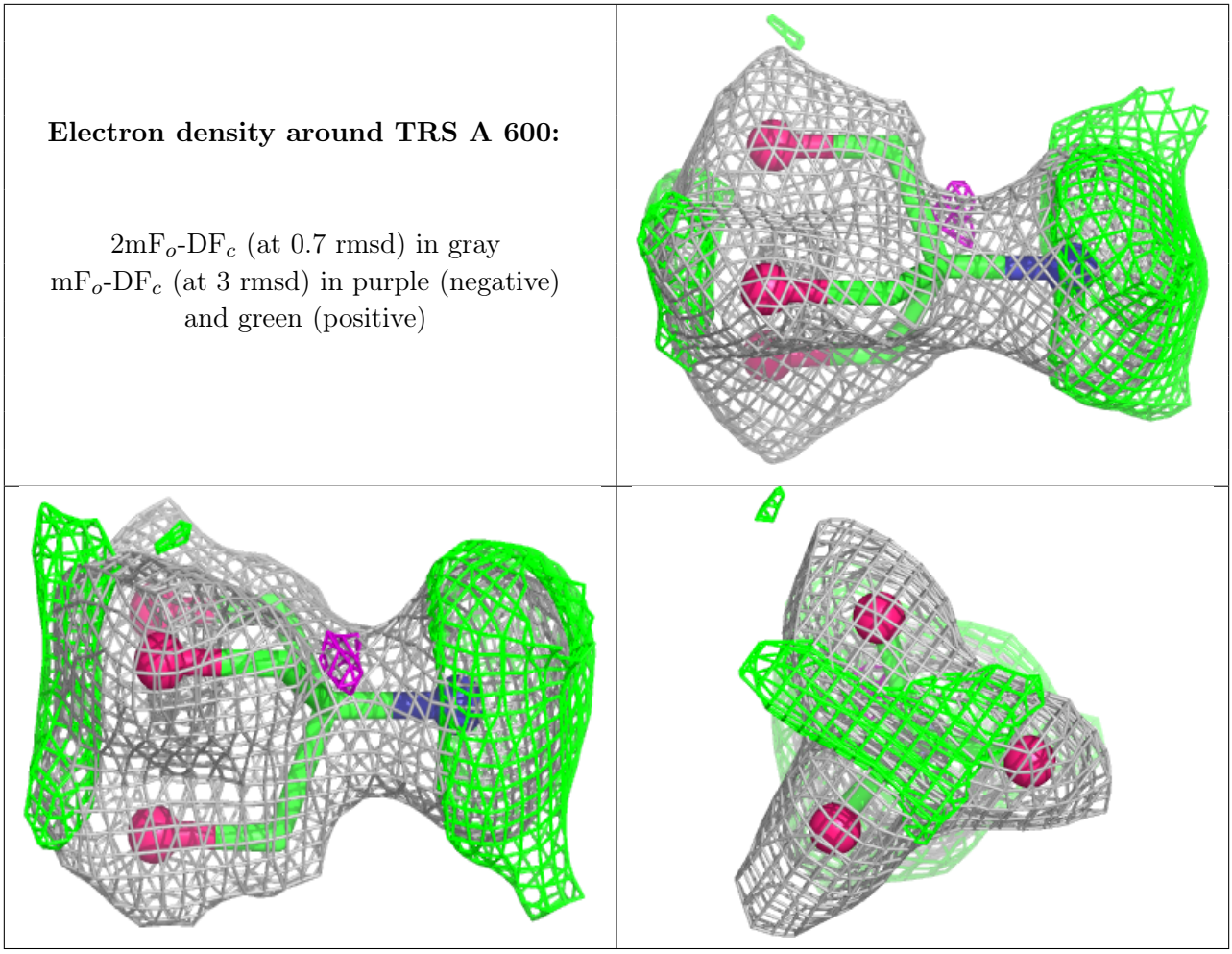
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TRS	D	600	8/8	0.72	0.16	22,28,37,40	0
3	GOL	E	603	6/6	0.76	0.16	24,27,41,44	0
3	GOL	F	602	6/6	0.79	0.17	19,28,48,49	0
3	GOL	C	604	6/6	0.83	0.15	28,31,39,42	0
3	GOL	B	604	6/6	0.84	0.15	27,34,36,37	0
4	BCN	E	600	11/11	0.84	0.14	19,31,44,53	0
3	GOL	E	601	6/6	0.86	0.11	26,35,43,48	0
3	GOL	C	603	6/6	0.86	0.10	30,31,43,44	0
3	GOL	D	604	6/6	0.86	0.14	27,28,36,39	0
3	GOL	D	605	6/6	0.86	0.10	26,35,38,41	0
3	GOL	E	602	6/6	0.87	0.16	15,23,38,43	0
3	GOL	F	601	6/6	0.88	0.11	19,30,43,47	0
3	GOL	A	603	6/6	0.89	0.09	23,28,32,38	0
3	GOL	C	601	6/6	0.89	0.13	16,25,36,48	0
3	GOL	B	601[A]	6/6	0.90	0.09	17,18,20,20	6
3	GOL	B	601[B]	6/6	0.90	0.09	13,18,20,20	6
3	GOL	D	602[A]	6/6	0.90	0.09	11,17,18,20	6
3	GOL	D	602[B]	6/6	0.90	0.09	13,16,18,20	6
3	GOL	D	603	6/6	0.91	0.10	19,25,35,41	0
3	GOL	A	601	6/6	0.91	0.11	16,31,33,33	0
3	GOL	B	602	6/6	0.91	0.11	15,26,31,43	0
3	GOL	D	606[A]	6/6	0.93	0.10	16,27,31,31	1
3	GOL	D	606[B]	6/6	0.93	0.10	16,24,29,31	1
3	GOL	B	603	6/6	0.93	0.08	19,22,23,24	0
3	GOL	B	605	6/6	0.93	0.10	17,28,38,40	0
3	GOL	F	603[B]	6/6	0.94	0.10	15,27,28,32	1
3	GOL	F	603[A]	6/6	0.94	0.10	15,24,27,28	1
3	GOL	E	604	6/6	0.96	0.08	17,22,27,41	0
3	GOL	A	602	6/6	0.96	0.06	17,20,25,29	0
3	GOL	C	602	6/6	0.96	0.07	16,21,29,34	0
3	GOL	D	601	6/6	0.97	0.06	13,20,25,27	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.

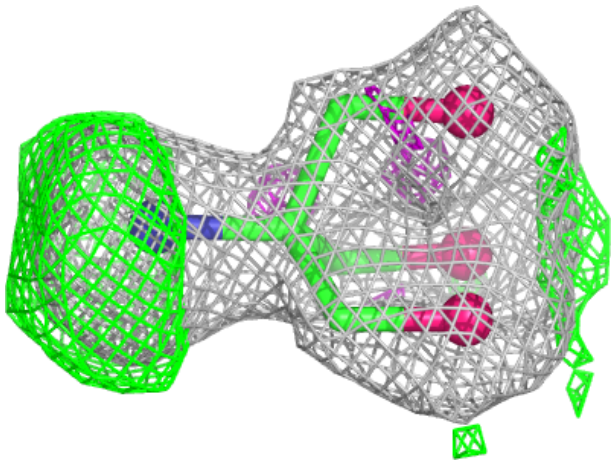
Electron density around TRS A 600:

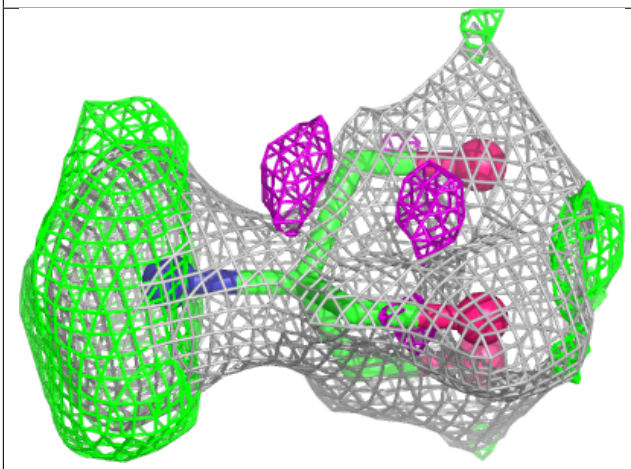
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

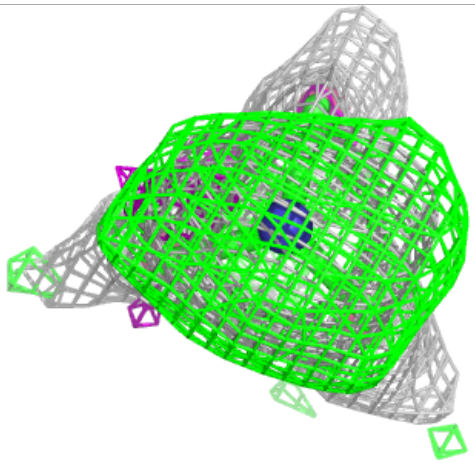


Electron density around TRS D 600:

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

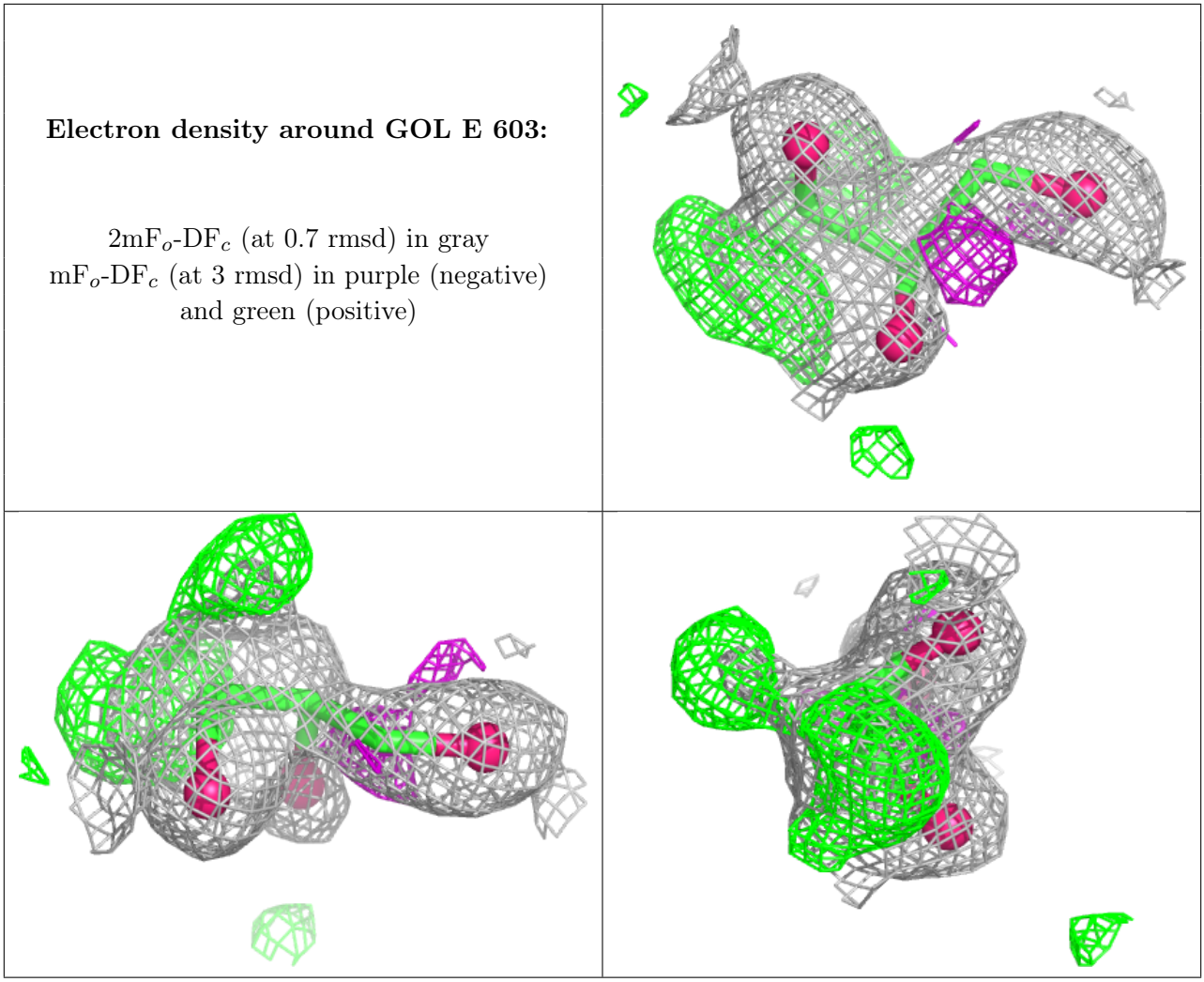






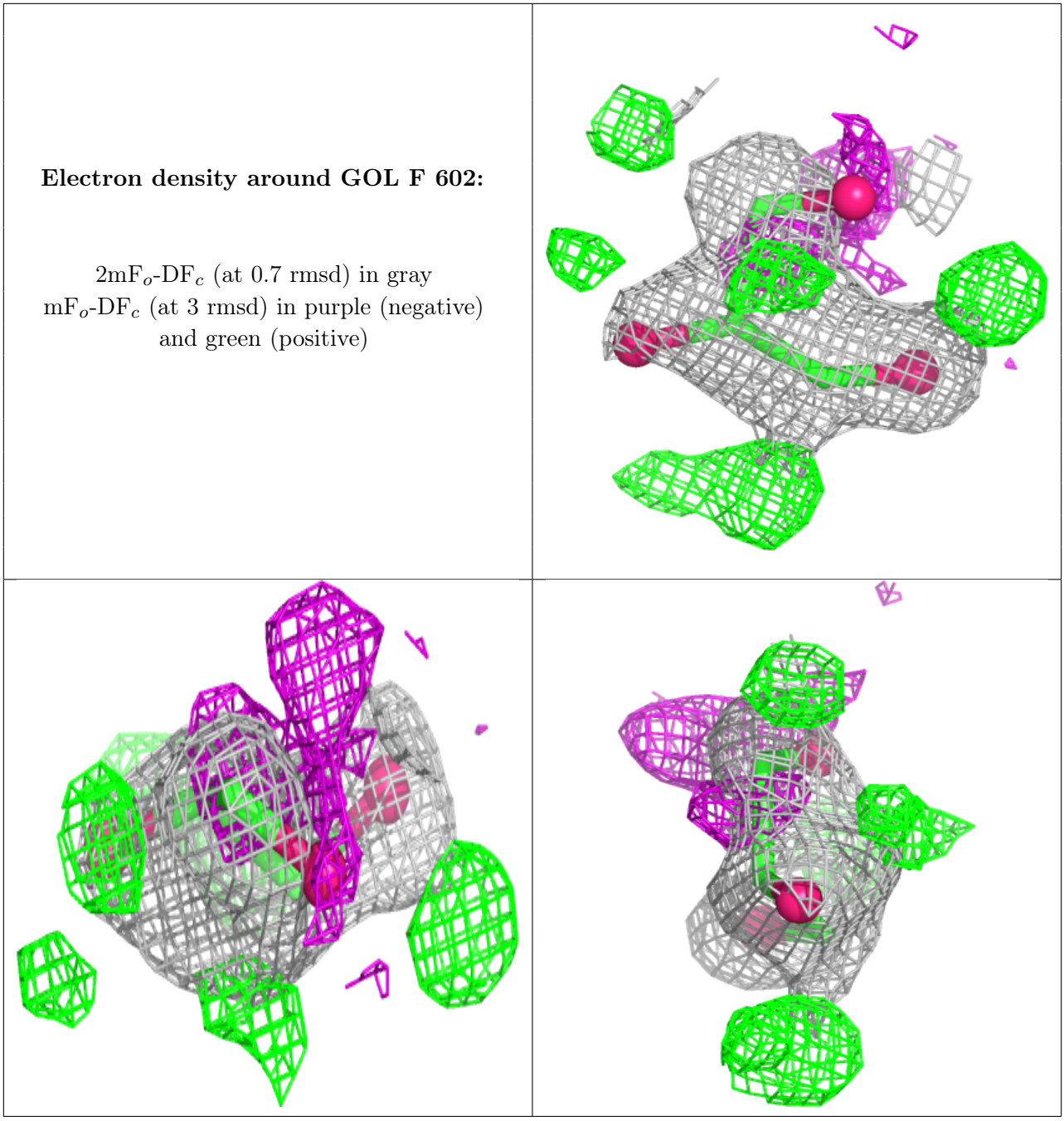
Electron density around GOL E 603:

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



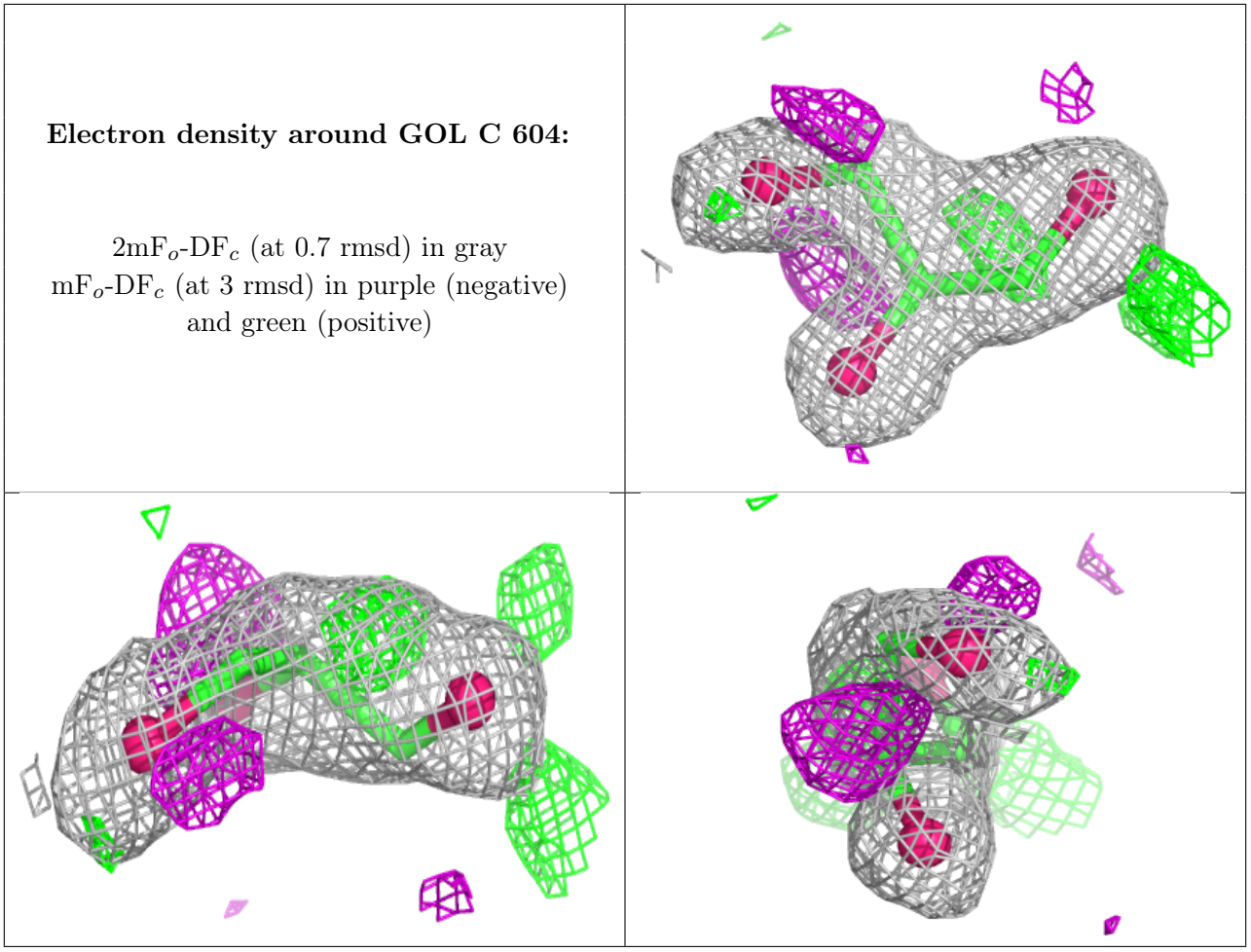
Electron density around GOL F 602:

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



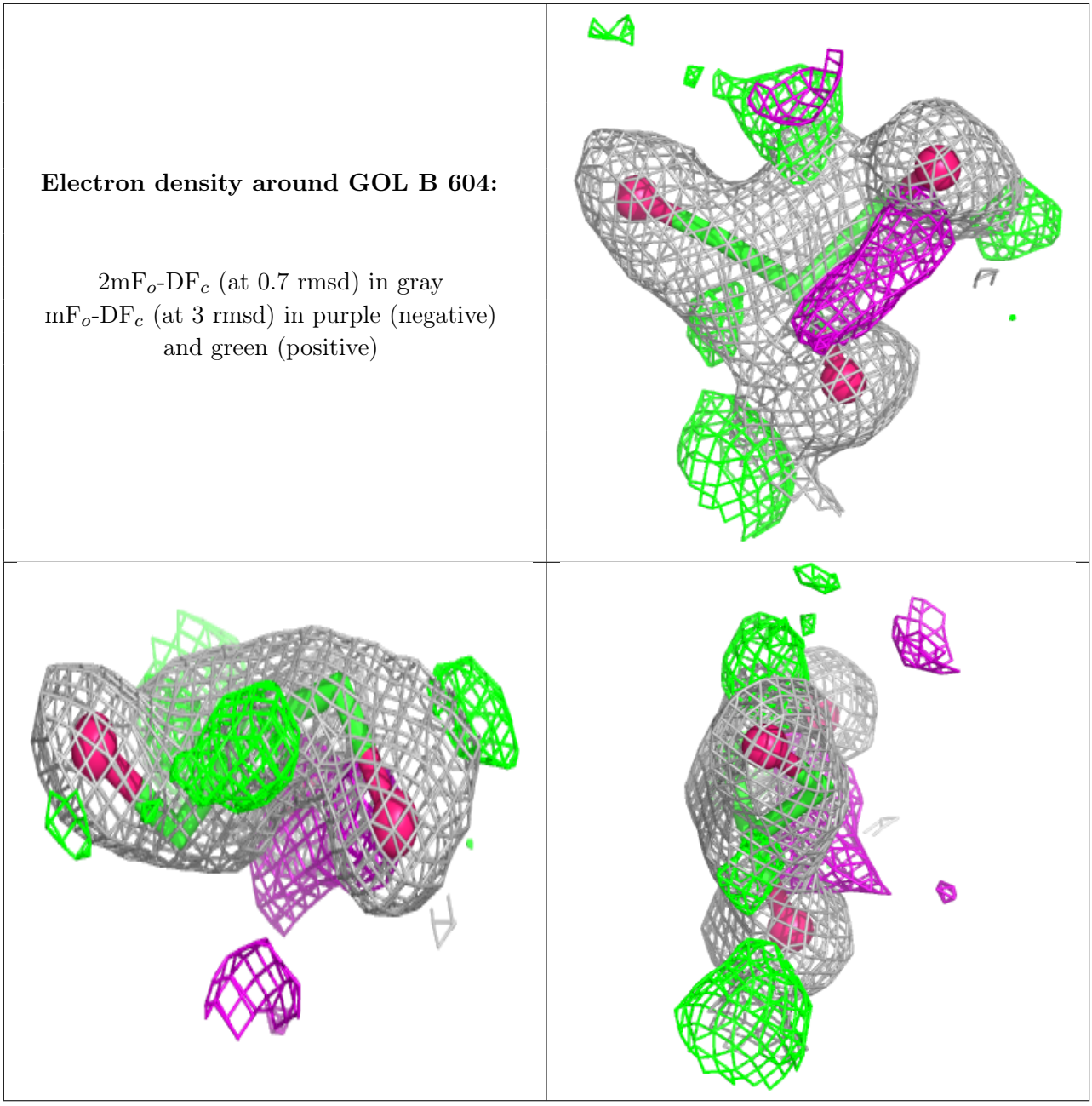
Electron density around GOL C 604:

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



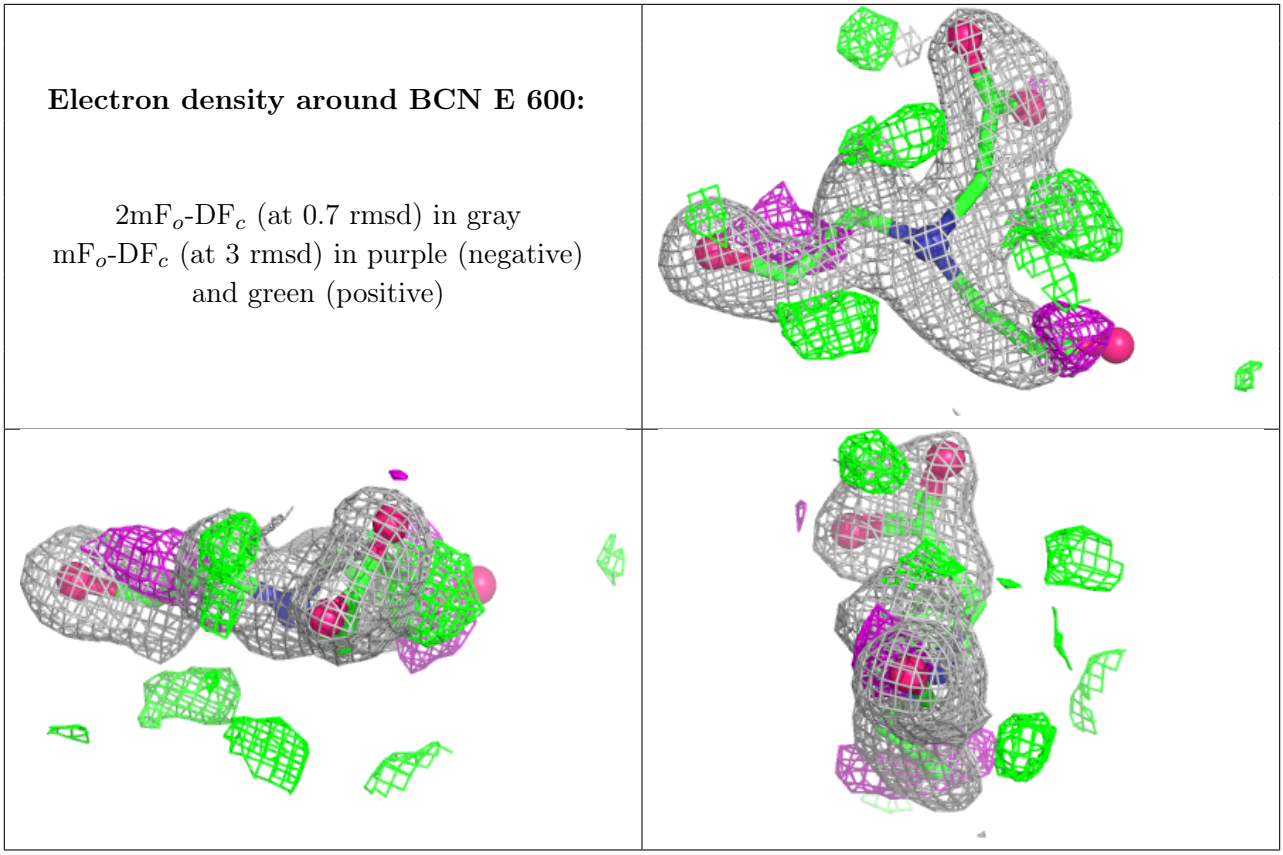
Electron density around GOL B 604:

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



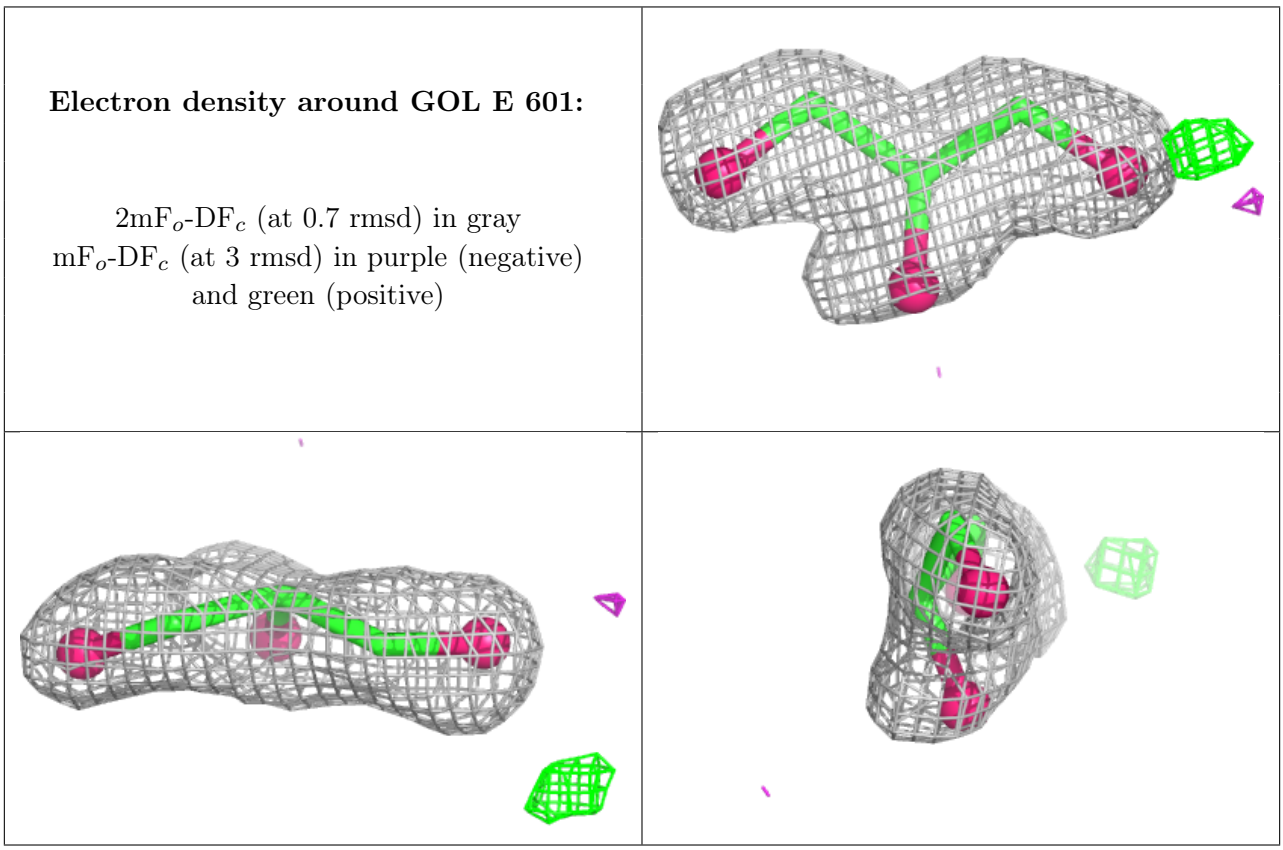
Electron density around BCN E 600:

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



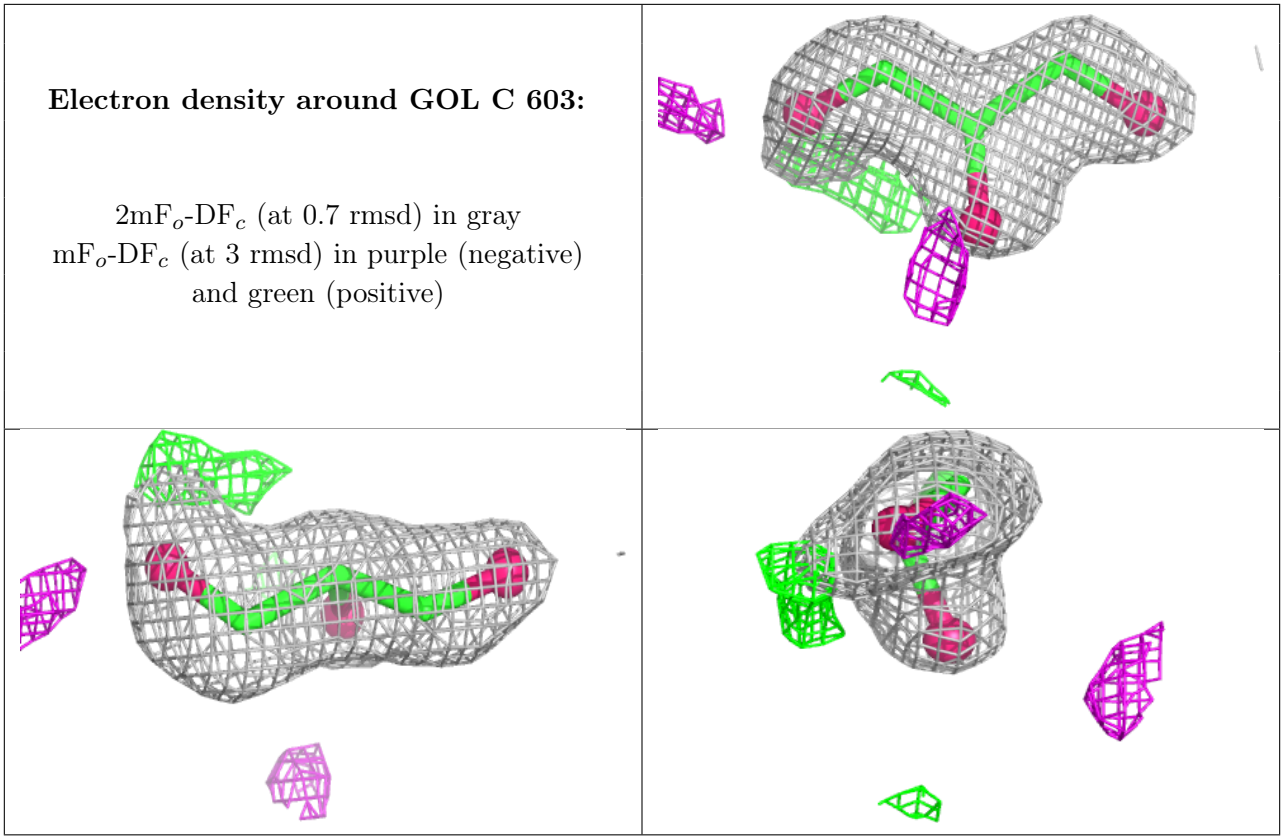
Electron density around GOL E 601:

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



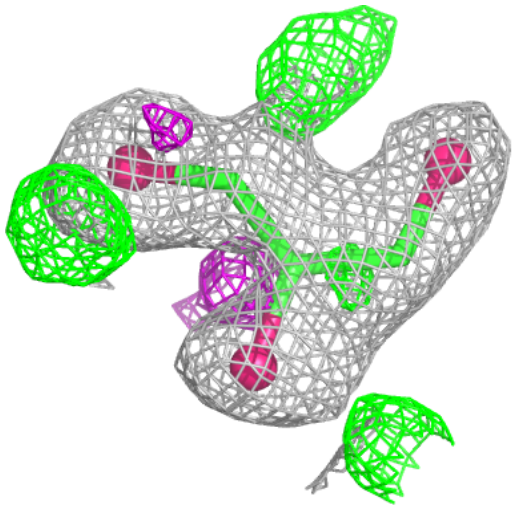
Electron density around GOL C 603:

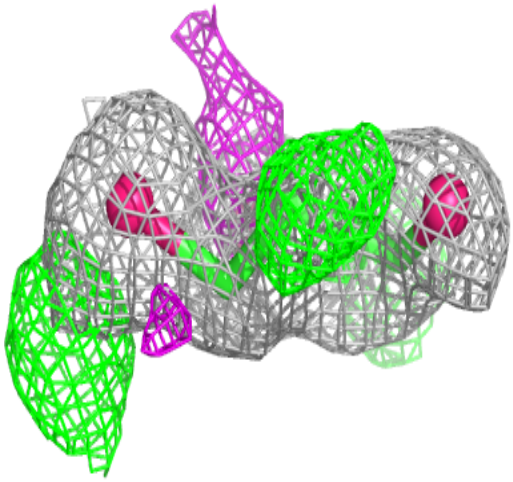
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

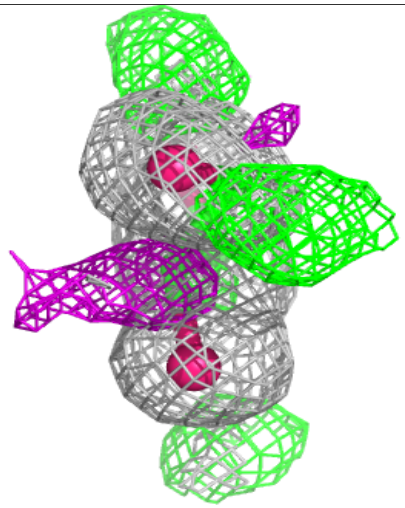


Electron density around GOL D 604:

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

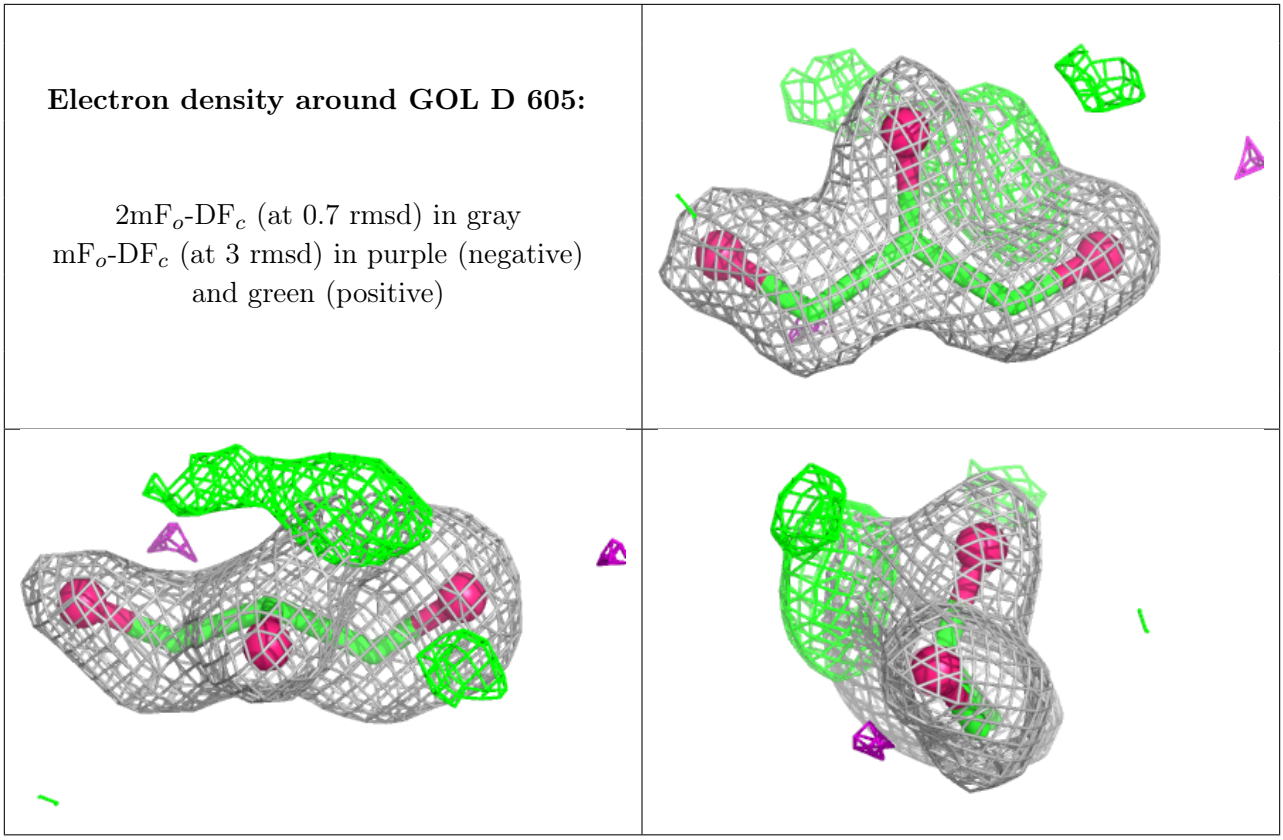






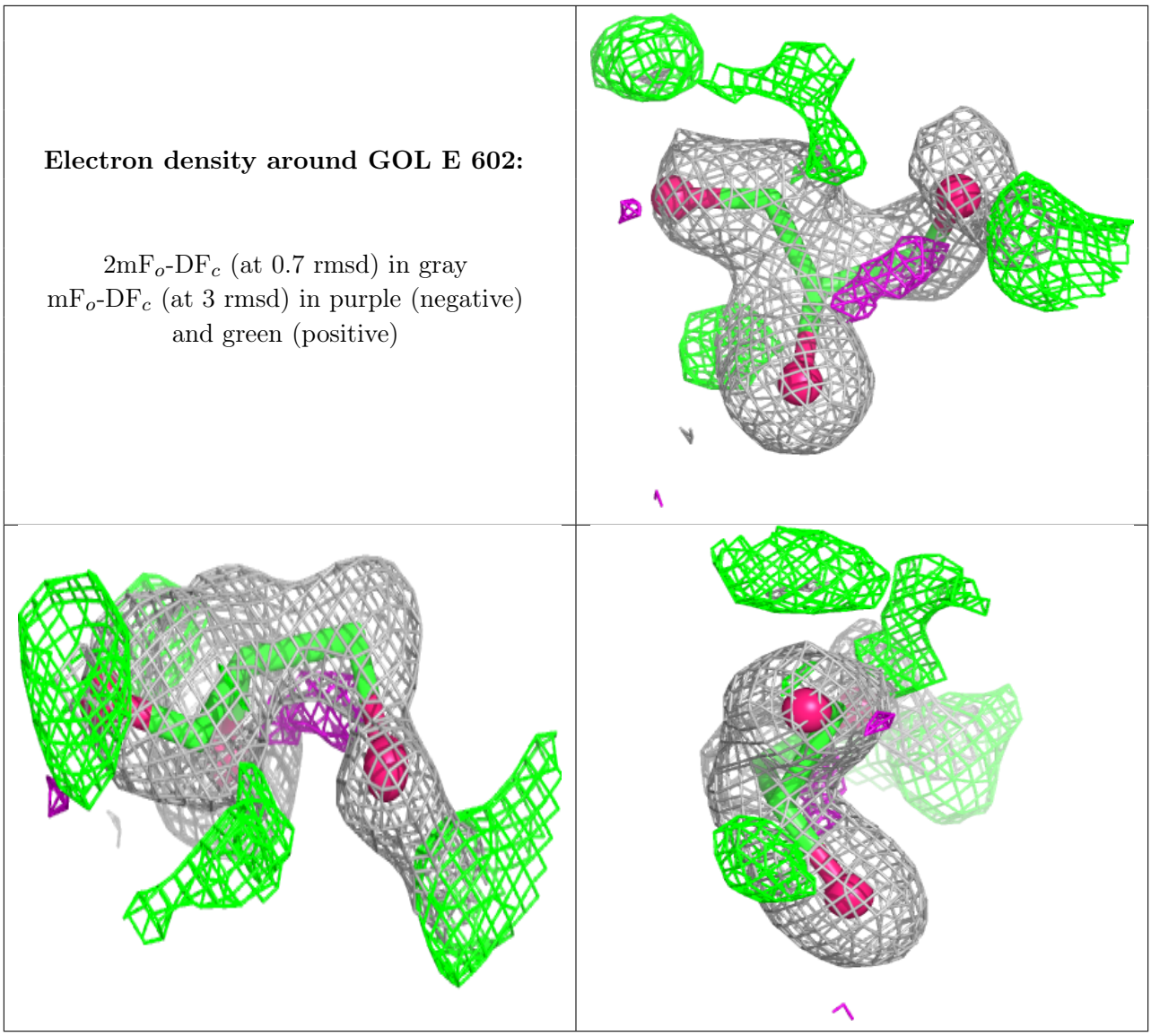
Electron density around GOL D 605:

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



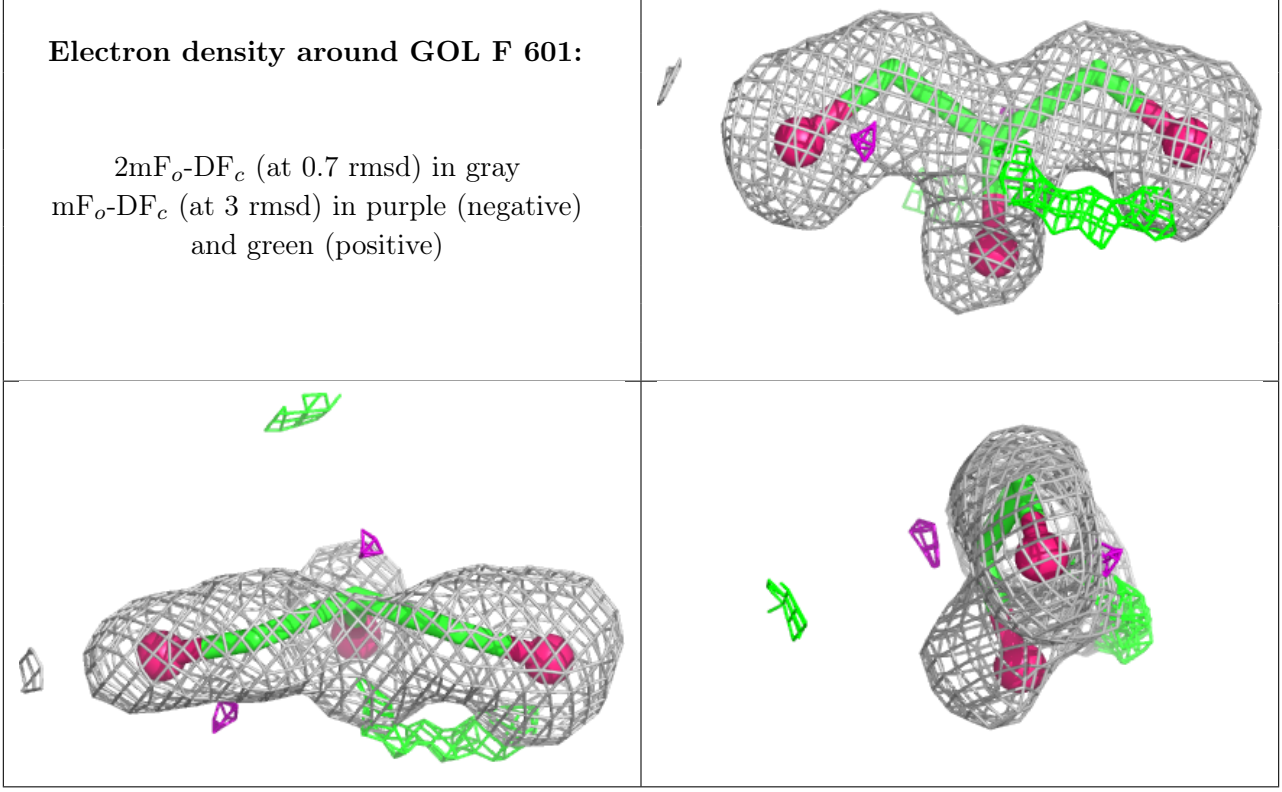
Electron density around GOL E 602:

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



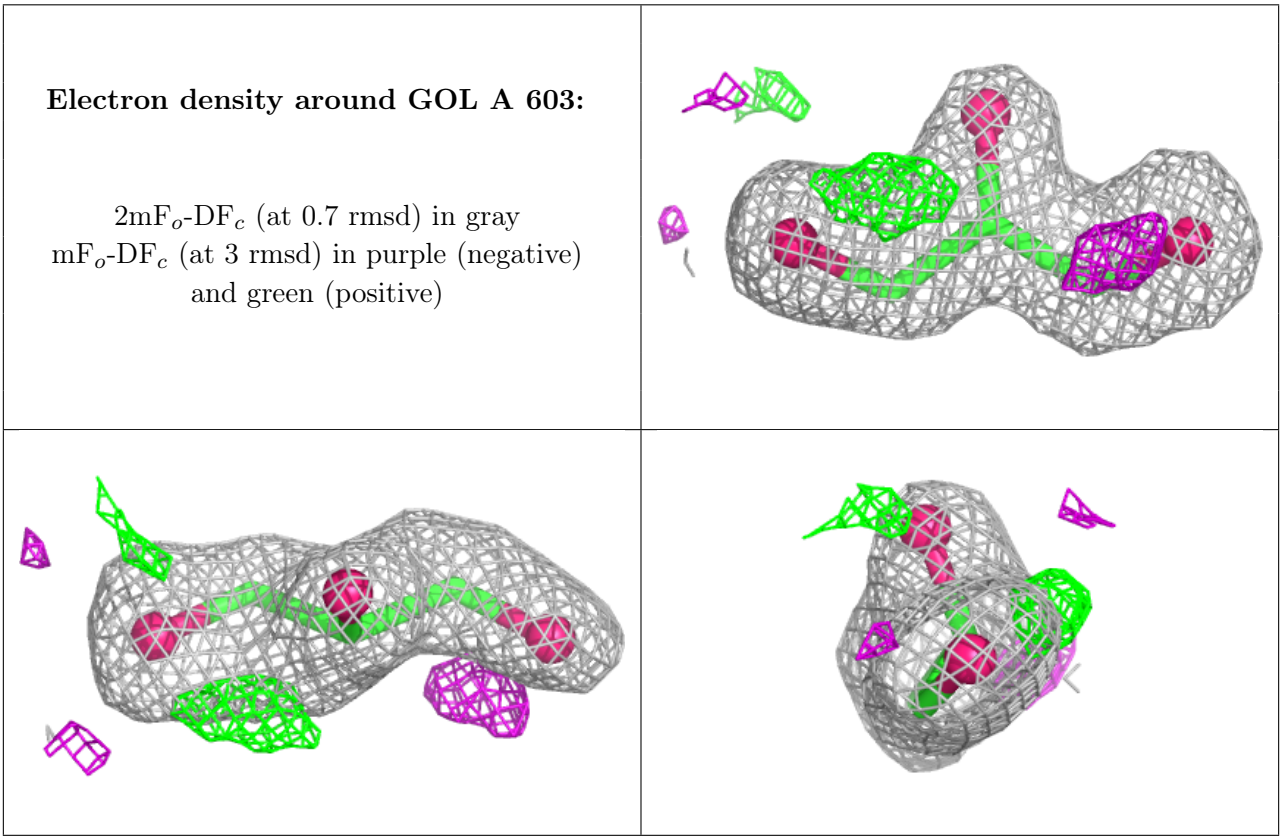
Electron density around GOL F 601:

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



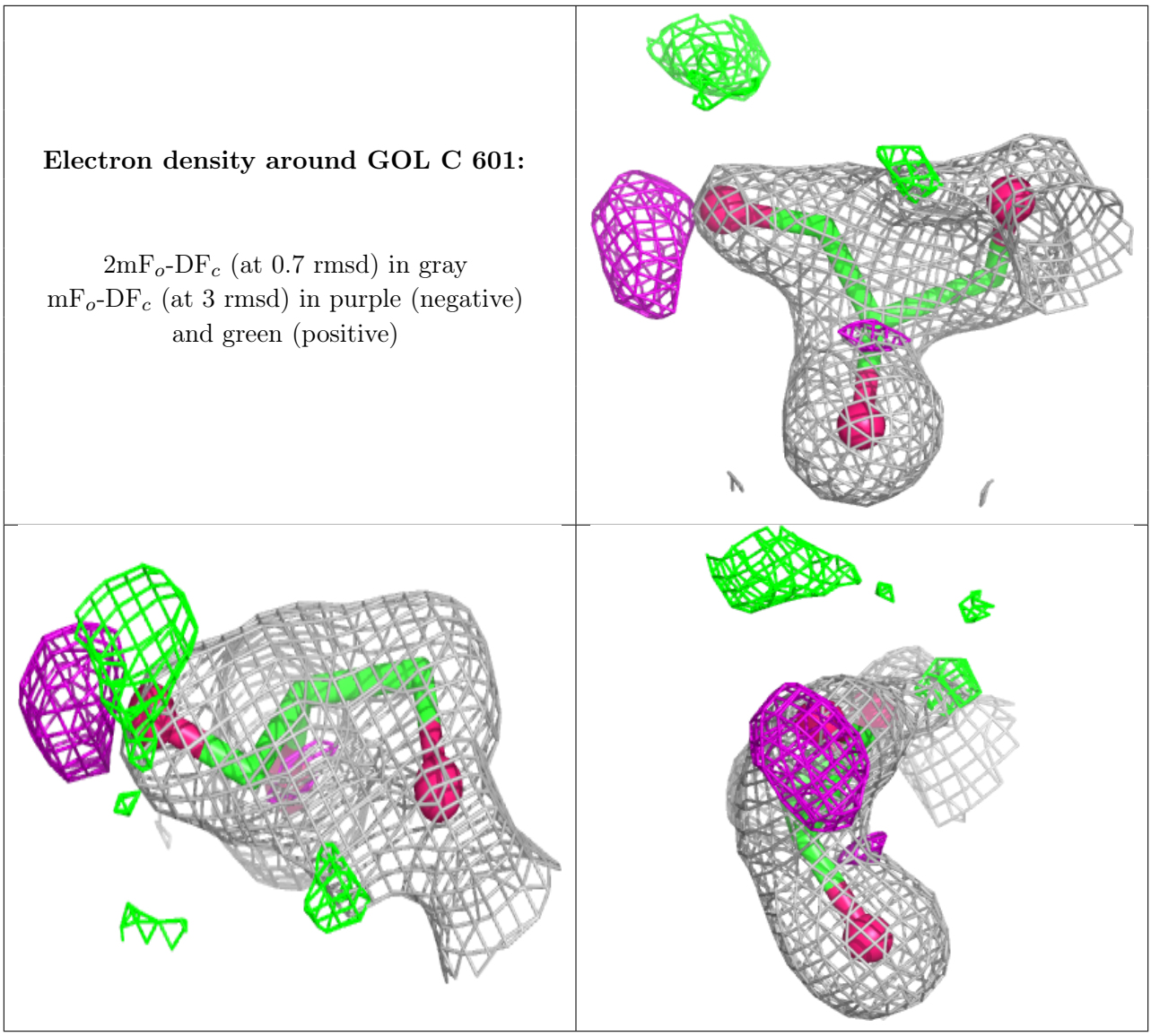
Electron density around GOL A 603:

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



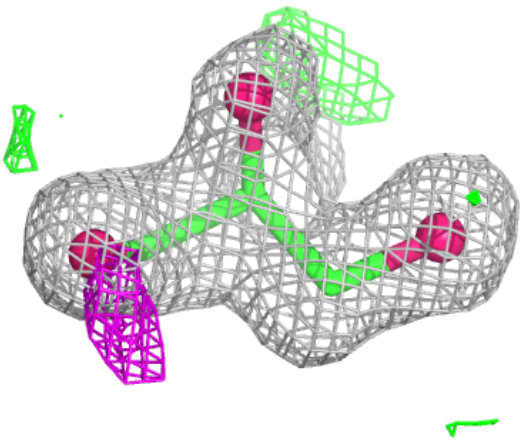
Electron density around GOL C 601:

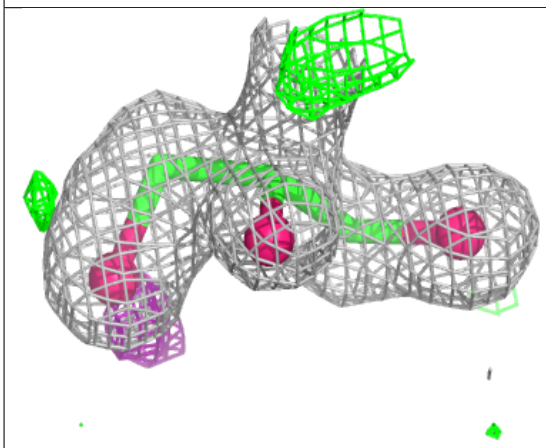
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

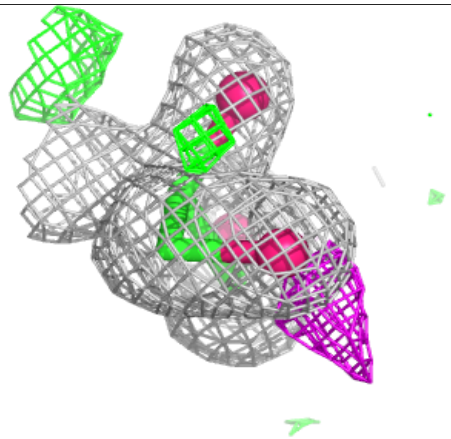


Electron density around GOL B 601 (A):

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

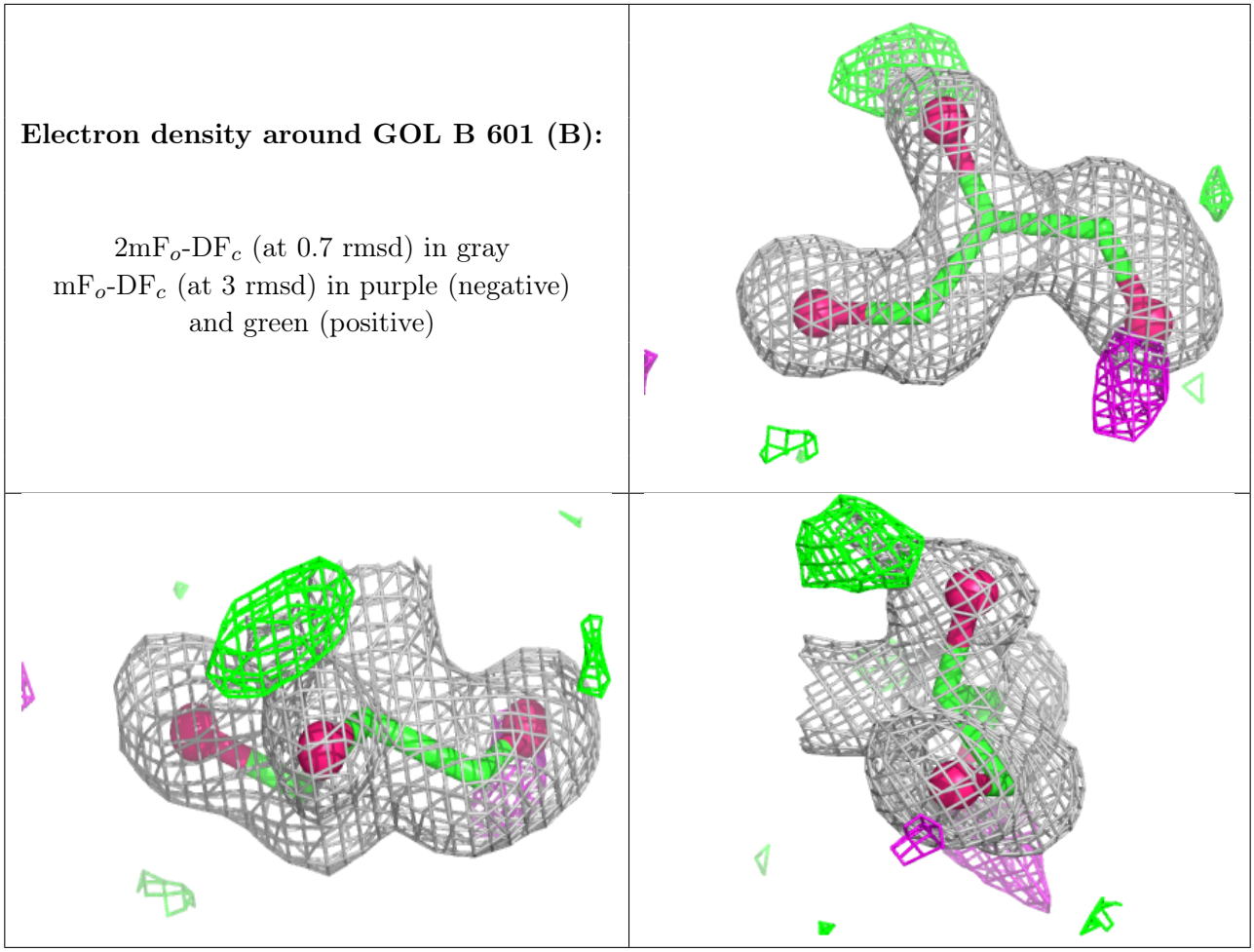






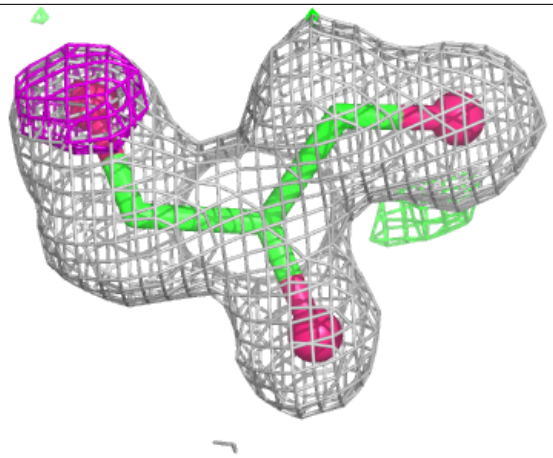
Electron density around GOL B 601 (B):

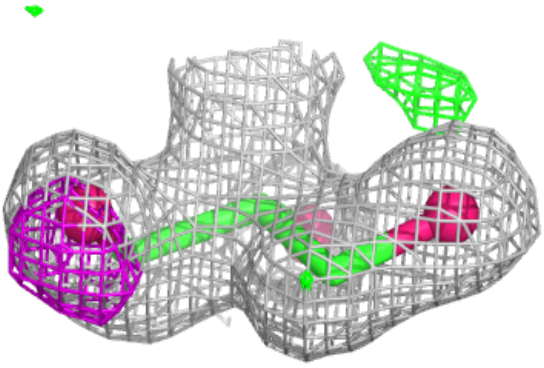
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

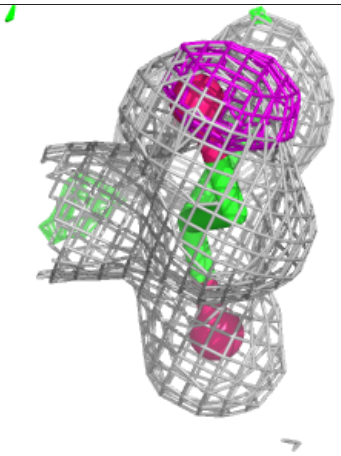


Electron density around GOL D 602 (A):

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

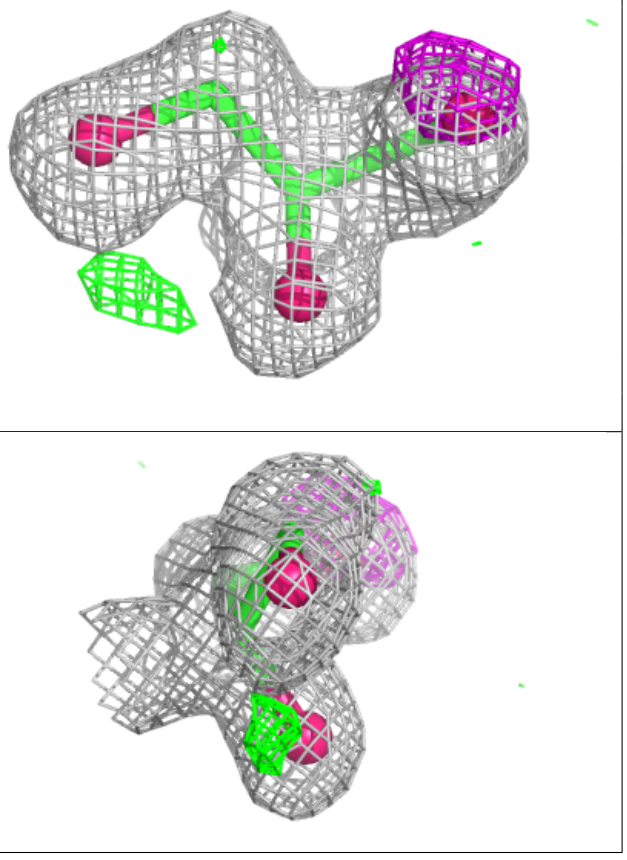






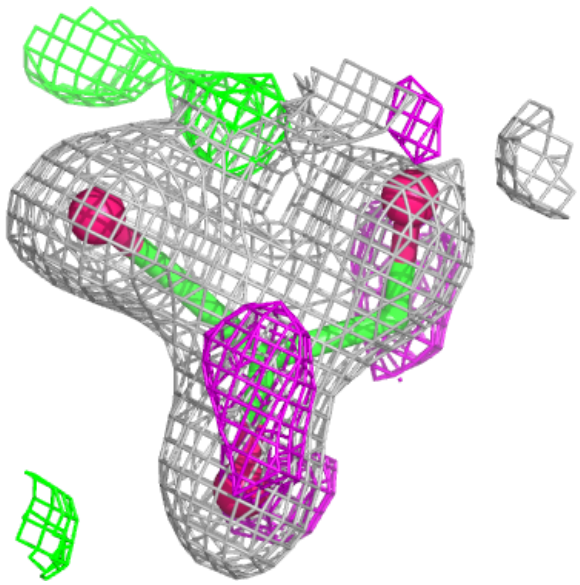
Electron density around GOL D 602 (B):

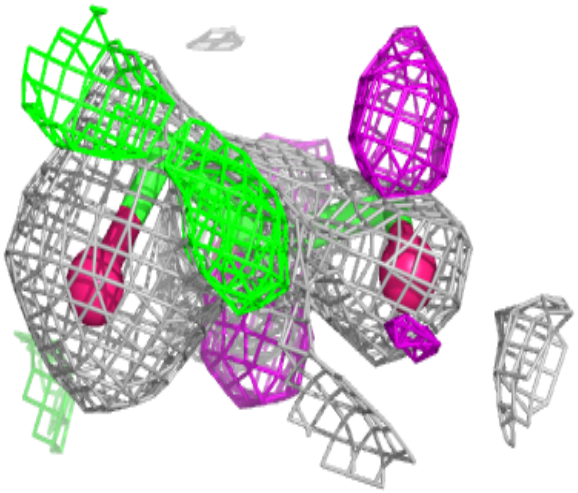
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

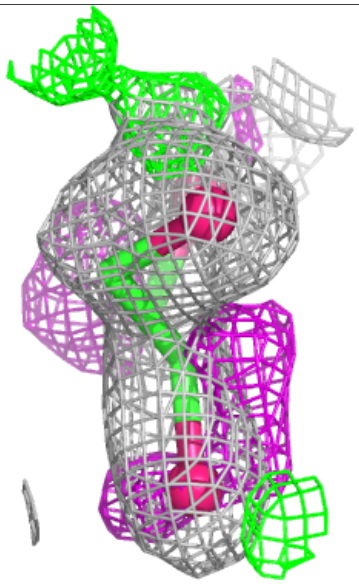


Electron density around GOL D 603:

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

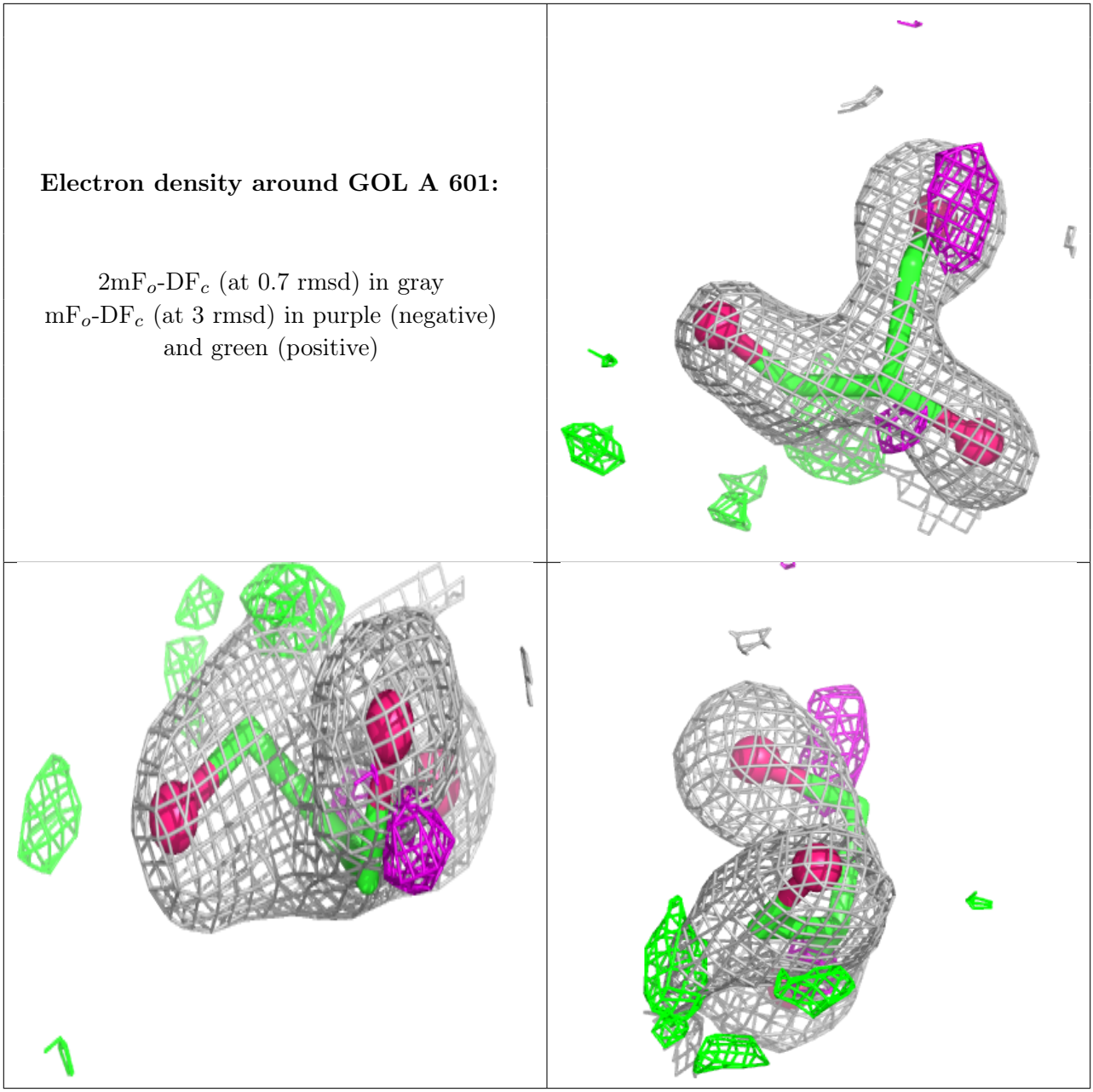






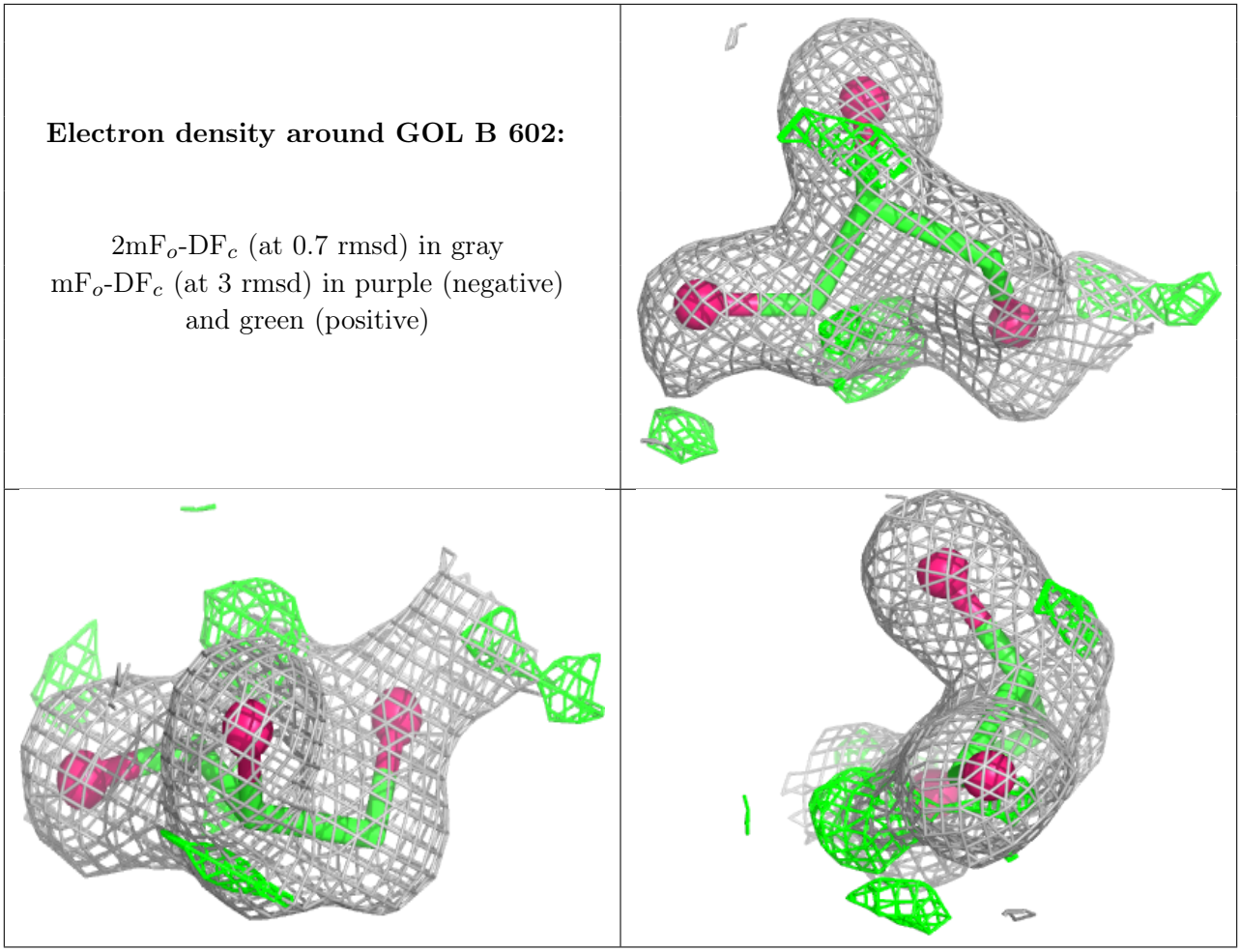
Electron density around GOL A 601:

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



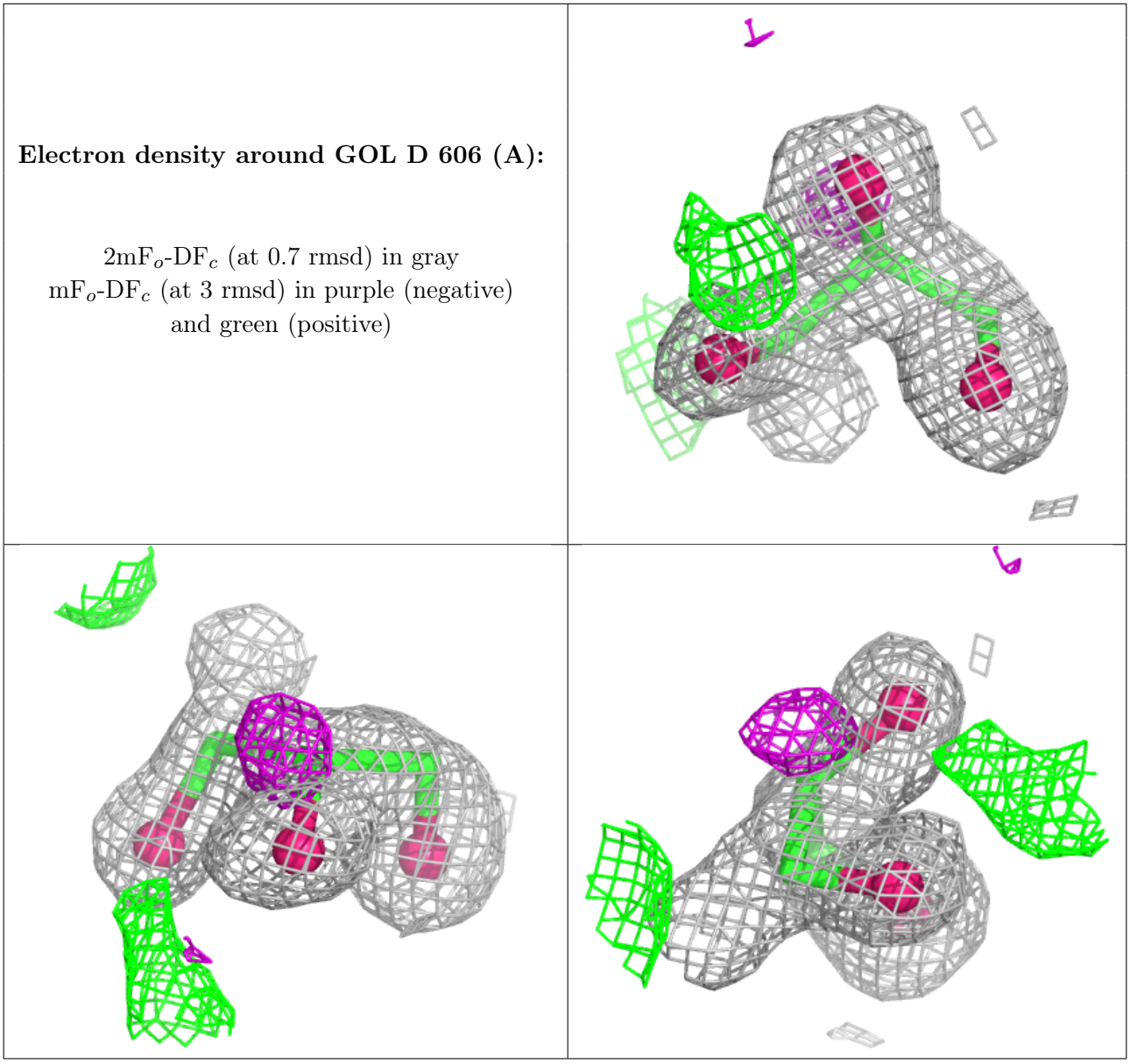
Electron density around GOL B 602:

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



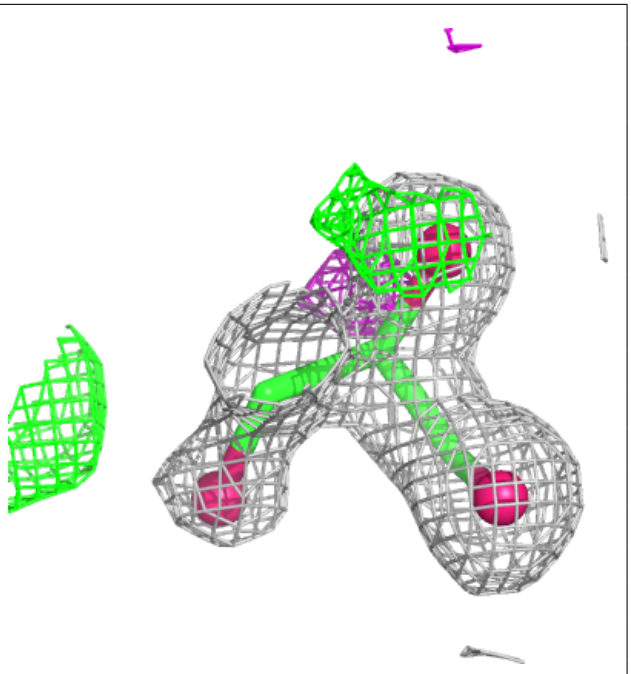
Electron density around GOL D 606 (A):

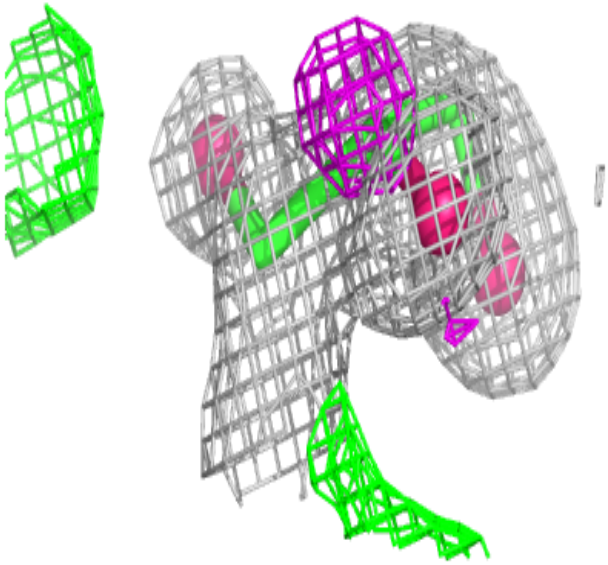
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

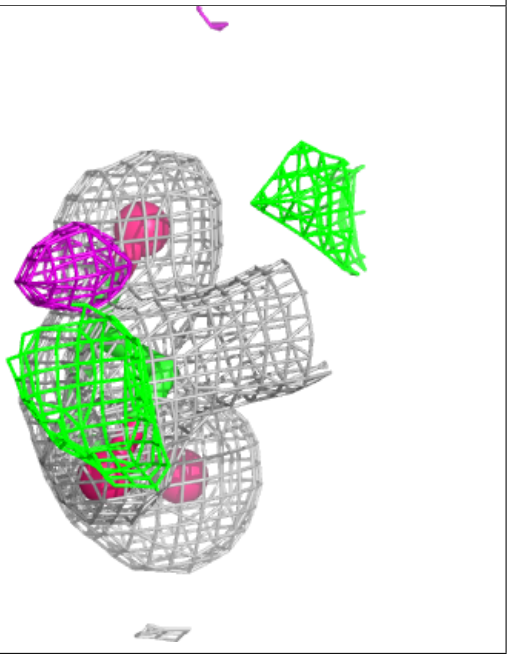


Electron density around GOL D 606 (B):

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

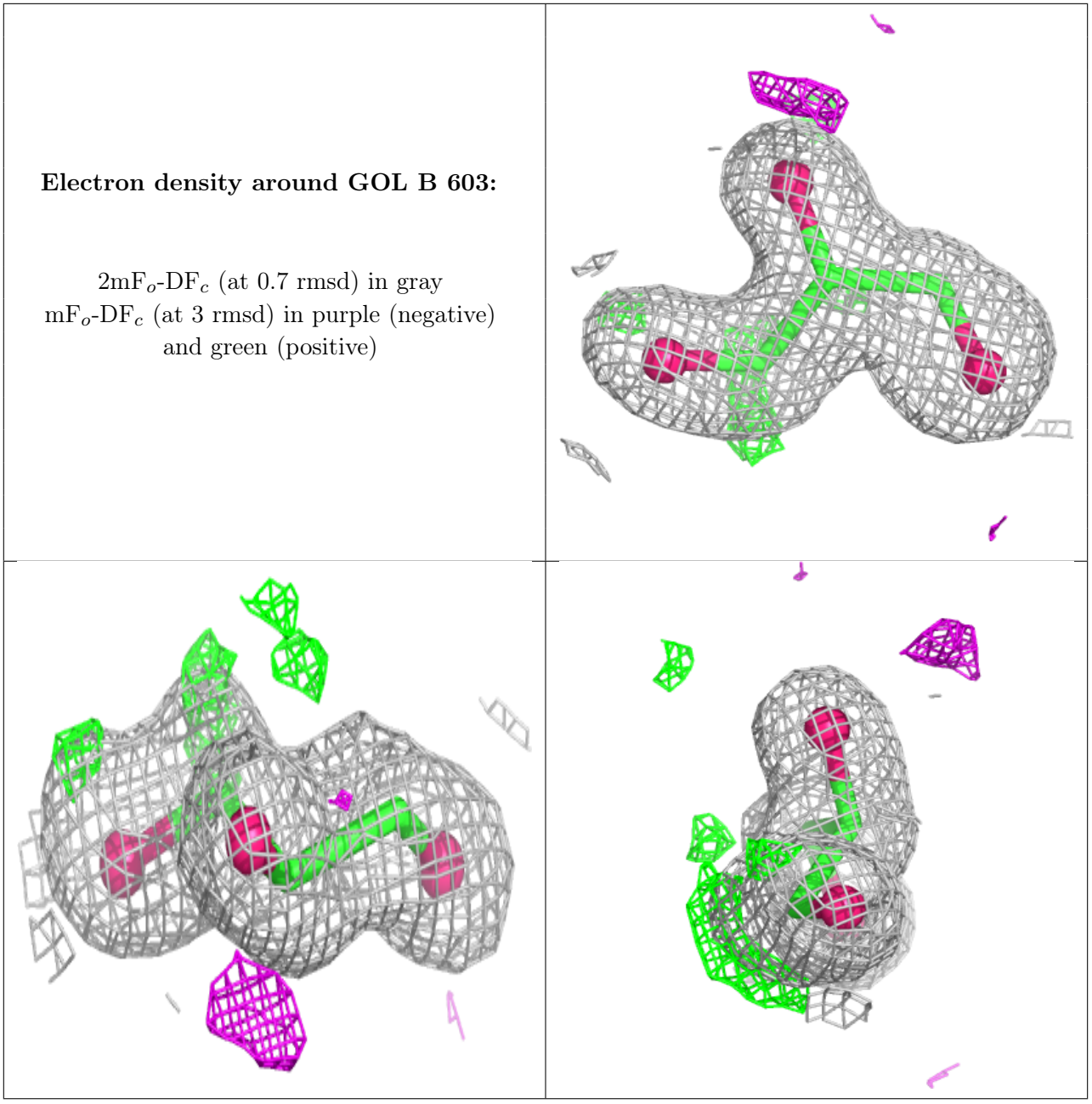






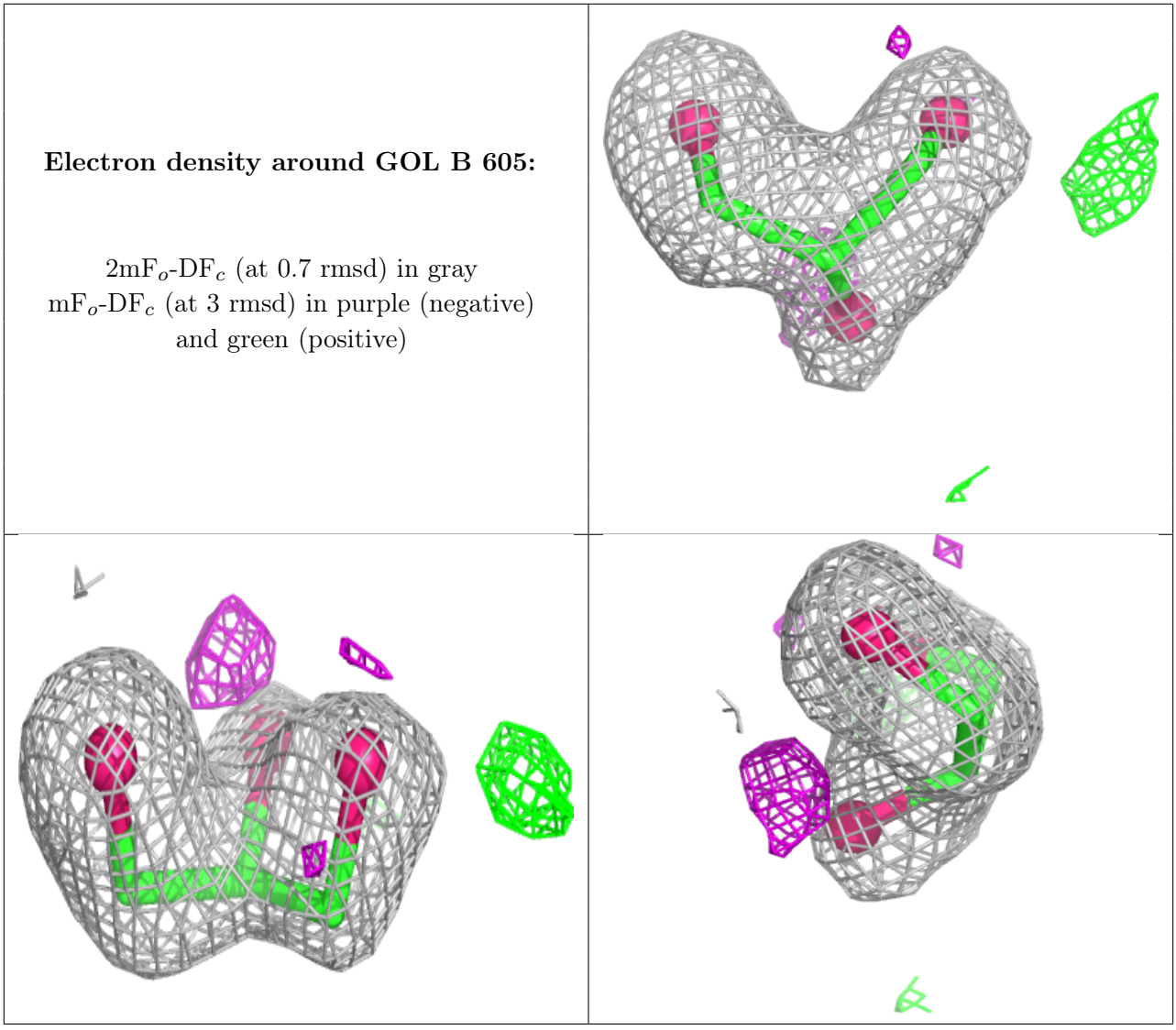
Electron density around GOL B 603:

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



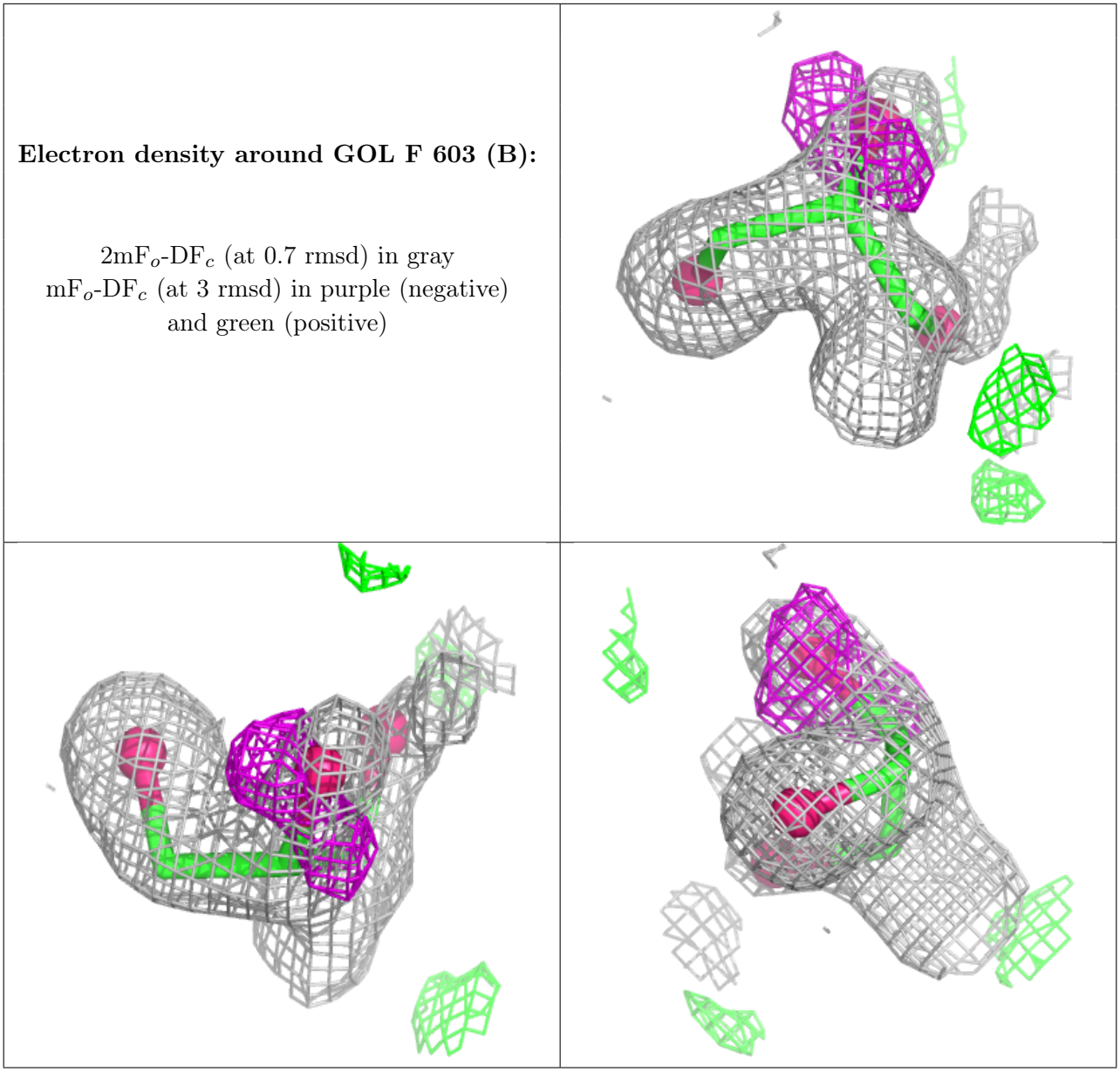
Electron density around GOL B 605:

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



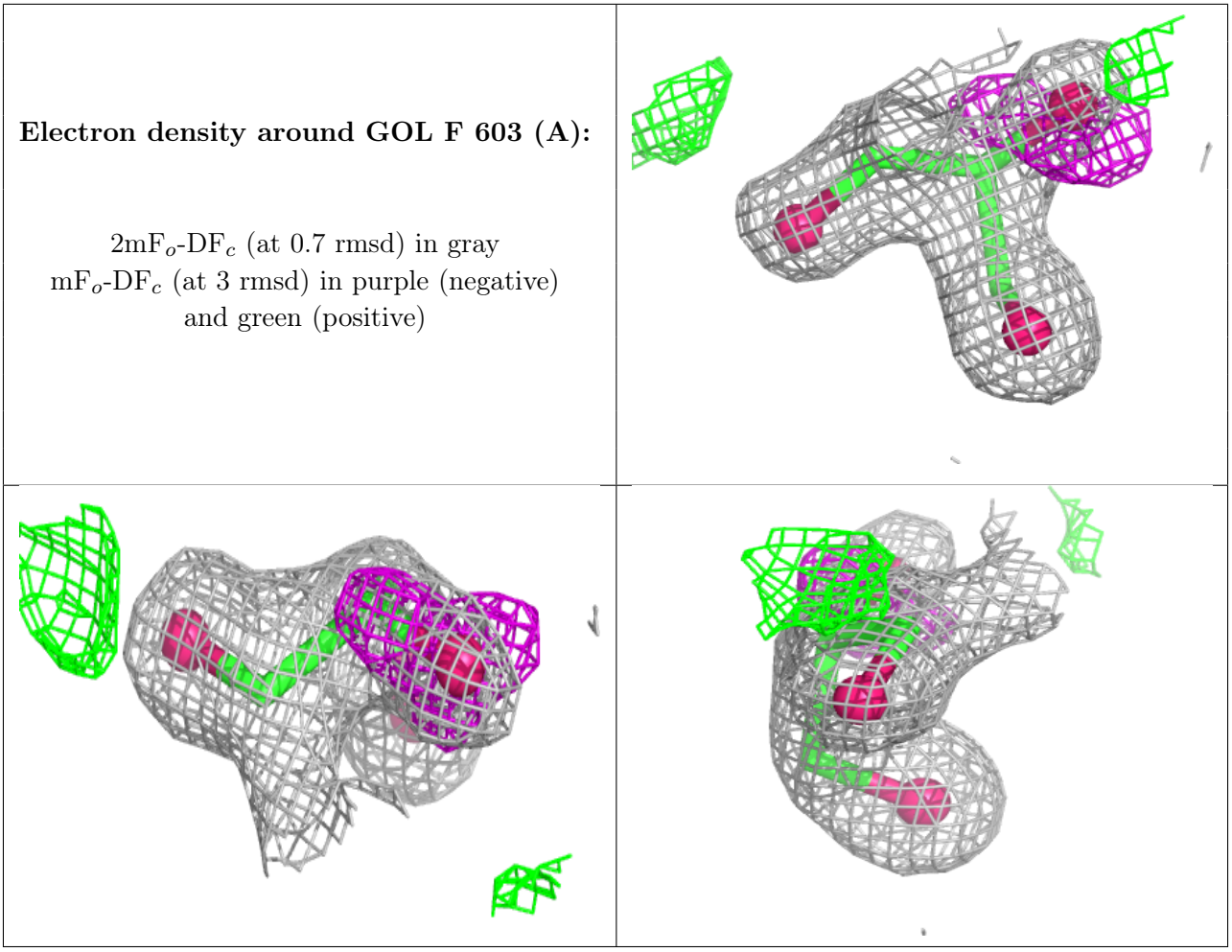
Electron density around GOL F 603 (B):

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



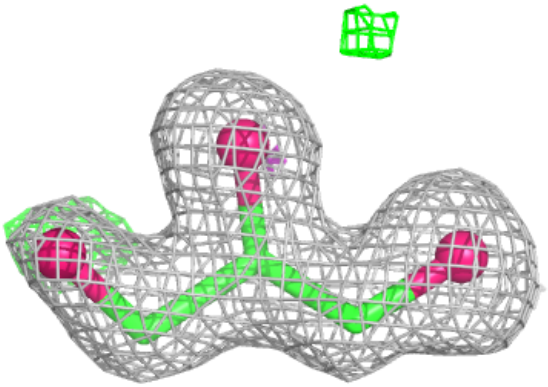
Electron density around GOL F 603 (A):

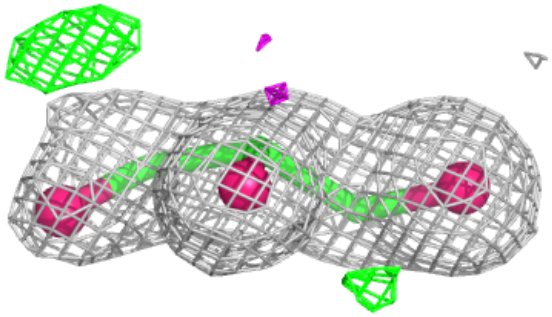
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

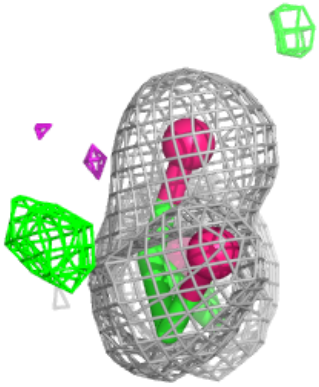


Electron density around GOL E 604:

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

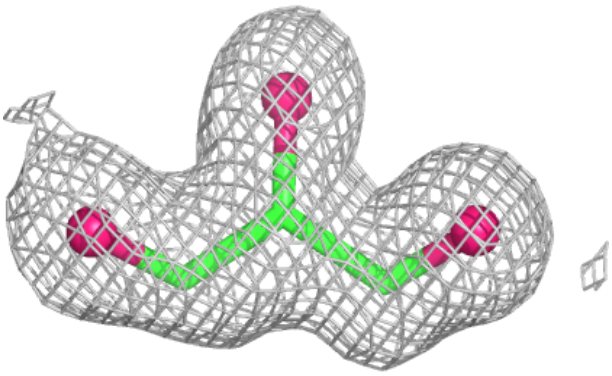


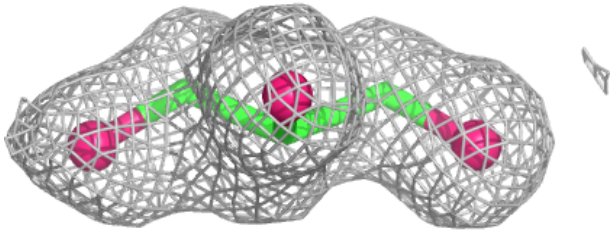


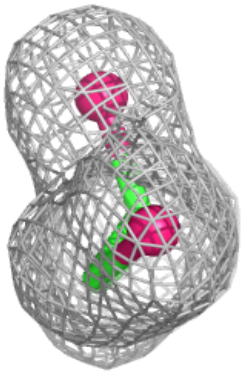


Electron density around GOL A 602:

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

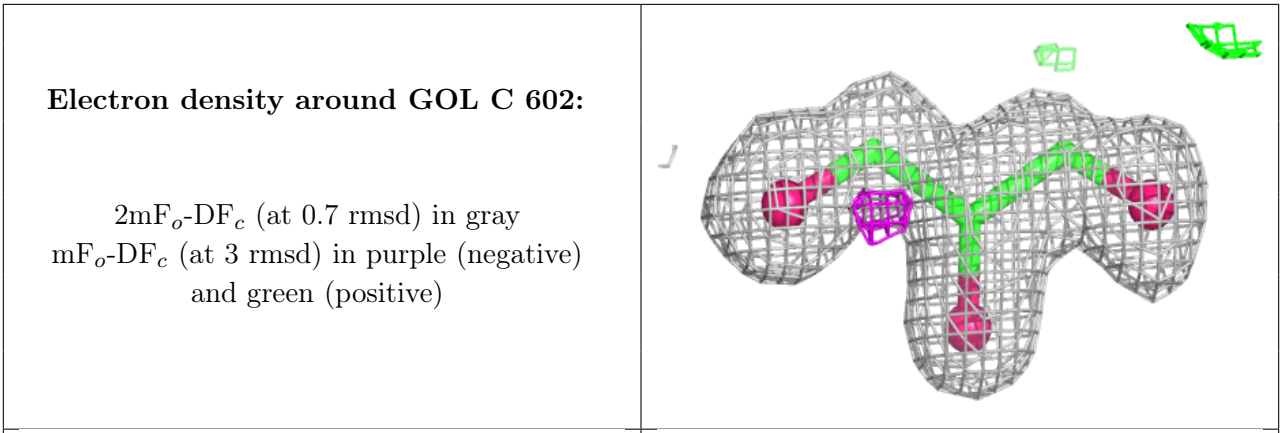






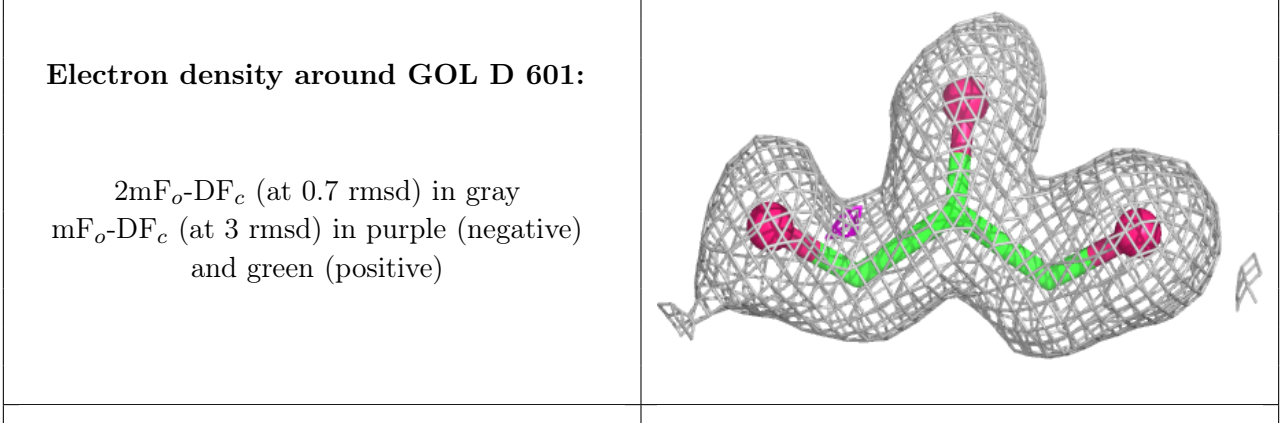
Electron density around GOL C 602:

$2mF_o$-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 D 601:

$2mF_o$-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.