Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2022 – 01:07 pm BST

PDB ID	:	6SLC
Title	:	Mutations in SsgB correlate to longitudinal cell division during sporulation of Streptomyces coelicolor
Authors	:	Xiao, X.S.; Willemse, J.
Deposited on	:	2019-08-19
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

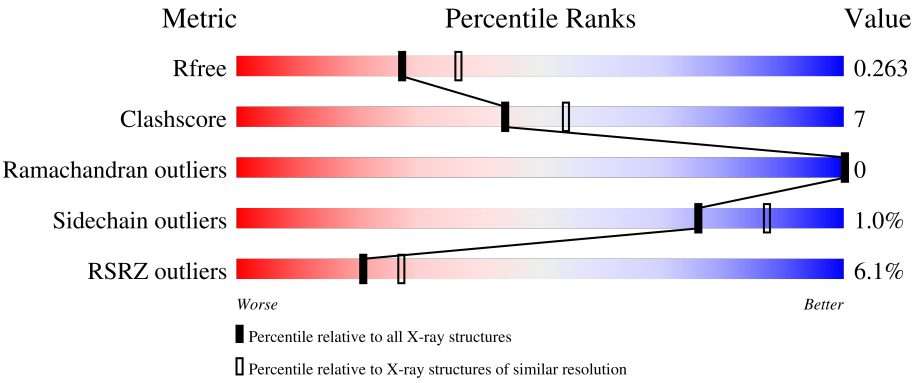
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	AAA	157	8% 75% 6% 19%
1	BBB	157	3% 71% 10% 19%
1	CCC	157	4% 68% 11% 21%

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	BBB	903	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3138 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 Sporulation and cell division protein SsgA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	127	Total	C	N	O	S	0	0	0
			965	603	175	184	3			
1	BBB	127	Total	C	N	O	S	0	0	0
			965	603	175	184	3			
1	CCC	124	Total	C	N	O	S	0	0	0
			941	587	172	179	3			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-19	MET	-	initiating methionine	UNP A0A3D9WLS9
AAA	-18	GLY	-	expression tag	UNP A0A3D9WLS9
AAA	-17	SER	-	expression tag	UNP A0A3D9WLS9
AAA	-16	SER	-	expression tag	UNP A0A3D9WLS9
AAA	-15	HIS	-	expression tag	UNP A0A3D9WLS9
AAA	-14	HIS	-	expression tag	UNP A0A3D9WLS9
AAA	-13	HIS	-	expression tag	UNP A0A3D9WLS9
AAA	-12	HIS	-	expression tag	UNP A0A3D9WLS9
AAA	-11	HIS	-	expression tag	UNP A0A3D9WLS9
AAA	-10	HIS	-	expression tag	UNP A0A3D9WLS9
AAA	-9	SER	-	expression tag	UNP A0A3D9WLS9
AAA	-8	SER	-	expression tag	UNP A0A3D9WLS9
AAA	-7	GLY	-	expression tag	UNP A0A3D9WLS9
AAA	-6	LEU	-	expression tag	UNP A0A3D9WLS9
AAA	-5	VAL	-	expression tag	UNP A0A3D9WLS9
AAA	-4	PRO	-	expression tag	UNP A0A3D9WLS9
AAA	-3	ARG	-	expression tag	UNP A0A3D9WLS9
AAA	-2	GLY	-	expression tag	UNP A0A3D9WLS9
AAA	-1	SER	-	expression tag	UNP A0A3D9WLS9
AAA	0	HIS	-	expression tag	UNP A0A3D9WLS9
BBB	-19	MET	-	initiating methionine	UNP A0A3D9WLS9
BBB	-18	GLY	-	expression tag	UNP A0A3D9WLS9
BBB	-17	SER	-	expression tag	UNP A0A3D9WLS9

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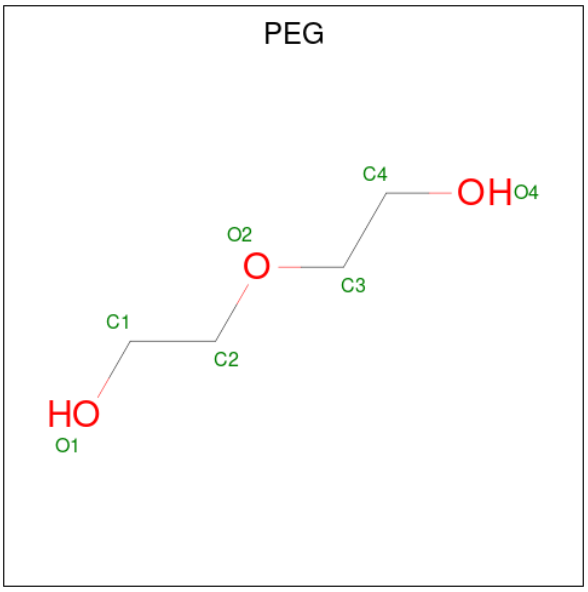
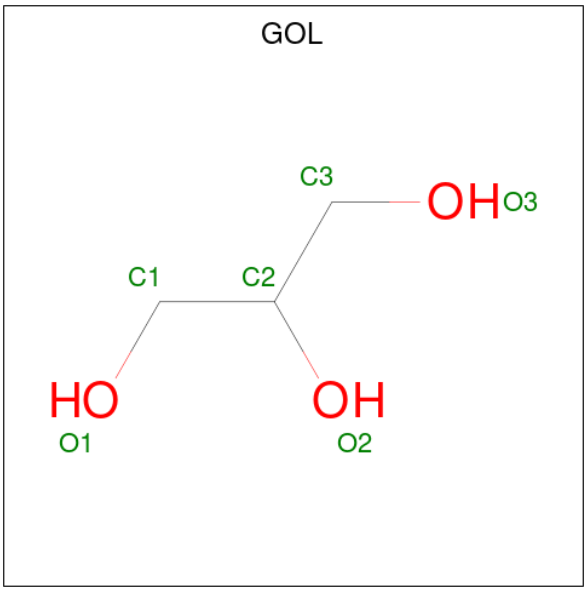
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-16	SER	-	expression tag	UNP A0A3D9WLS9
BBB	-15	HIS	-	expression tag	UNP A0A3D9WLS9
BBB	-14	HIS	-	expression tag	UNP A0A3D9WLS9
BBB	-13	HIS	-	expression tag	UNP A0A3D9WLS9
BBB	-12	HIS	-	expression tag	UNP A0A3D9WLS9
BBB	-11	HIS	-	expression tag	UNP A0A3D9WLS9
BBB	-10	HIS	-	expression tag	UNP A0A3D9WLS9
BBB	-9	SER	-	expression tag	UNP A0A3D9WLS9
BBB	-8	SER	-	expression tag	UNP A0A3D9WLS9
BBB	-7	GLY	-	expression tag	UNP A0A3D9WLS9
BBB	-6	LEU	-	expression tag	UNP A0A3D9WLS9
BBB	-5	VAL	-	expression tag	UNP A0A3D9WLS9
BBB	-4	PRO	-	expression tag	UNP A0A3D9WLS9
BBB	-3	ARG	-	expression tag	UNP A0A3D9WLS9
BBB	-2	GLY	-	expression tag	UNP A0A3D9WLS9
BBB	-1	SER	-	expression tag	UNP A0A3D9WLS9
BBB	0	HIS	-	expression tag	UNP A0A3D9WLS9
CCC	-19	MET	-	initiating methionine	UNP A0A3D9WLS9
CCC	-18	GLY	-	expression tag	UNP A0A3D9WLS9
CCC	-17	SER	-	expression tag	UNP A0A3D9WLS9
CCC	-16	SER	-	expression tag	UNP A0A3D9WLS9
CCC	-15	HIS	-	expression tag	UNP A0A3D9WLS9
CCC	-14	HIS	-	expression tag	UNP A0A3D9WLS9
CCC	-13	HIS	-	expression tag	UNP A0A3D9WLS9
CCC	-12	HIS	-	expression tag	UNP A0A3D9WLS9
CCC	-11	HIS	-	expression tag	UNP A0A3D9WLS9
CCC	-10	HIS	-	expression tag	UNP A0A3D9WLS9
CCC	-9	SER	-	expression tag	UNP A0A3D9WLS9
CCC	-8	SER	-	expression tag	UNP A0A3D9WLS9
CCC	-7	GLY	-	expression tag	UNP A0A3D9WLS9
CCC	-6	LEU	-	expression tag	UNP A0A3D9WLS9
CCC	-5	VAL	-	expression tag	UNP A0A3D9WLS9
CCC	-4	PRO	-	expression tag	UNP A0A3D9WLS9
CCC	-3	ARG	-	expression tag	UNP A0A3D9WLS9
CCC	-2	GLY	-	expression tag	UNP A0A3D9WLS9
CCC	-1	SER	-	expression tag	UNP A0A3D9WLS9
CCC	0	HIS	-	expression tag	UNP A0A3D9WLS9

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



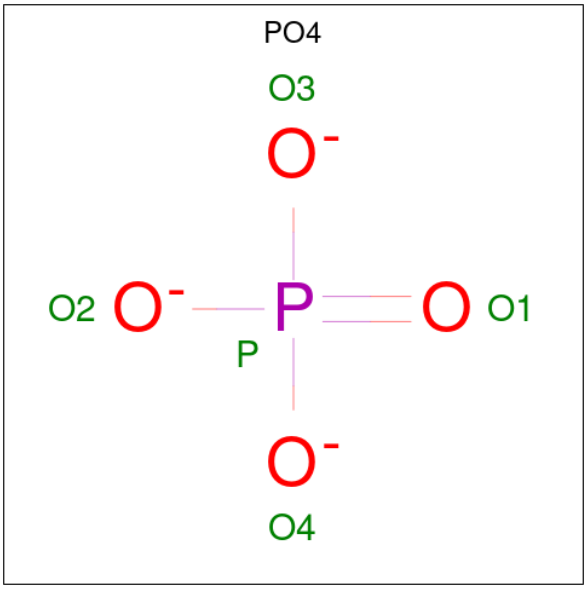
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	0
			7	4	3		
2	AAA	1	Total	C	O	0	0
			7	4	3		
2	BBB	1	Total	C	O	0	0
			7	4	3		
2	BBB	1	Total	C	O	0	0
			7	4	3		
2	CCC	1	Total	C	O	0	0
			7	4	3		
2	CCC	1	Total	C	O	0	0
			7	4	3		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	BBB	1	Total	C	O	0	0
			6	3	3		
3	BBB	1	Total	C	O	0	0
			6	3	3		
3	BBB	1	Total	C	O	0	0
			6	3	3		
3	BBB	1	Total	C	O	0	0
			6	3	3		
3	BBB	1	Total	C	O	0	0
			6	3	3		
3	CCC	1	Total	C	O	0	0
			6	3	3		
3	CCC	1	Total	C	O	0	0
			6	3	3		
3	CCC	1	Total	C	O	0	0
			6	3	3		
3	CCC	1	Total	C	O	0	0
			6	3	3		
3	CCC	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	BBB	1	Total O P 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	47	Total O 47 47	0	0
5	BBB	44	Total O 44 44	0	0
5	CCC	45	Total O 45 45	0	0

3 Residue-property plots (i)

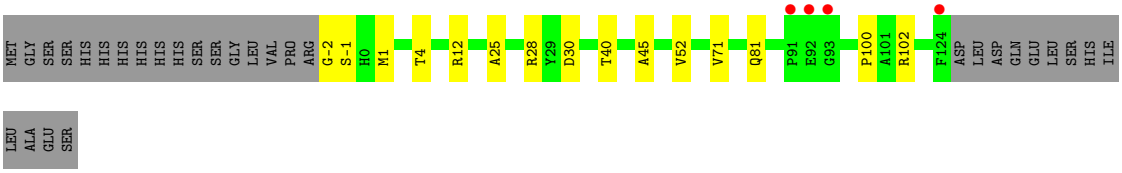
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Sporulation and cell division protein SsgA

Chain AAA:

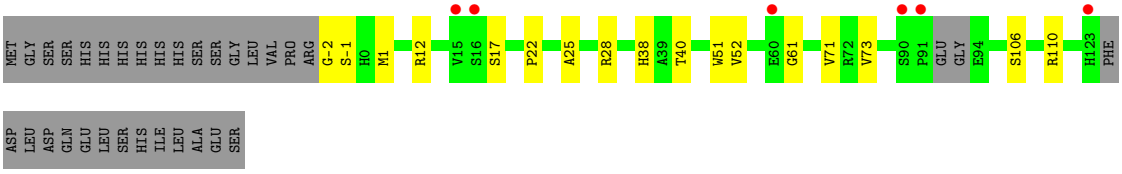
• Molecule 1: Sporulation and cell division protein SsgA

Chain BBB:



• Molecule 1: Sporulation and cell division protein SsgA

Chain CCC:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	155.47Å 155.47Å 53.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 2.30 49.16 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.9 (49.21-2.30) 94.9 (49.16-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.208 , 0.256 0.216 , 0.263	Depositor DCC
R_{free} test set	1349 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	53.5	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3138	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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, PO4, PEG

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	AAA	0.65	0/991	0.80	0/1354
1	BBB	0.66	0/991	0.81	0/1354
1	CCC	0.65	0/965	0.80	0/1318
All	All	0.66	0/2947	0.80	0/4026

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	965	0	931	15	0
1	BBB	965	0	931	19	0
1	CCC	941	0	912	16	0
2	AAA	14	0	20	0	0
2	BBB	14	0	20	5	0
2	CCC	14	0	20	0	0
3	AAA	24	0	32	3	0
3	BBB	30	0	40	5	0
3	CCC	30	0	40	0	0
4	BBB	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AAA	47	0	0	0	0
5	BBB	44	0	0	0	0
5	CCC	45	0	0	2	0
All	All	3138	0	2946	39	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (39) 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:BBB:100:PRO:HB2	2:BBB:902:PEG:H31	1.54	0.87
1:BBB:71:VAL:HG21	1:CCC:-2:GLY:HA3	1.70	0.74
1:AAA:-2:GLY:HA2	1:CCC:52:VAL:O	1.90	0.71
1:AAA:1:MET:HG2	1:CCC:52:VAL:HG23	1.72	0.69
1:AAA:59:ALA:HB1	3:AAA:204:GOL:H2	1.79	0.64
1:BBB:28:ARG:HB2	3:BBB:903:GOL:H11	1.83	0.59
1:AAA:52:VAL:HG23	1:BBB:1:MET:HG2	1.85	0.59
1:BBB:4:THR:HG22	1:BBB:30:ASP:OD1	2.03	0.59
1:AAA:0:HIS:HB2	1:CCC:51:TRP:CZ2	2.39	0.58
1:BBB:81:GLN:HE22	2:BBB:904:PEG:H21	1.70	0.57
1:CCC:-1:SER:HB3	1:CCC:1:MET:HE1	1.87	0.56
1:BBB:102:ARG:HB3	2:BBB:902:PEG:H21	1.86	0.55
1:BBB:102:ARG:HB3	2:BBB:902:PEG:H32	1.88	0.54
1:BBB:40:THR:OG1	3:BBB:903:GOL:H2	2.08	0.54
1:BBB:45:ALA:N	3:BBB:905:GOL:H12	2.23	0.53
1:AAA:1:MET:HA	1:AAA:1:MET:CE	2.39	0.52
1:AAA:48:THR:HG1	1:BBB:4:THR:HG1	1.50	0.50
1:BBB:52:VAL:O	1:CCC:-2:GLY:HA2	2.12	0.49
1:CCC:-1:SER:HB3	1:CCC:1:MET:CE	2.42	0.49
1:BBB:12:ARG:HG2	2:BBB:904:PEG:H32	1.94	0.49
1:AAA:-2:GLY:HA3	1:CCC:71:VAL:HG21	1.95	0.49
1:AAA:108:LEU:HB3	3:AAA:204:GOL:H31	1.96	0.48
1:AAA:52:VAL:O	1:BBB:-2:GLY:HA2	2.14	0.48
1:BBB:25:ALA:HA	1:BBB:40:THR:O	2.16	0.46
1:CCC:25:ALA:HA	1:CCC:40:THR:O	2.16	0.46
1:CCC:28:ARG:HG3	1:CCC:38:HIS:HB2	1.97	0.46
1:AAA:0:HIS:C	1:AAA:0:HIS:CD2	2.89	0.45
1:CCC:12:ARG:HG3	5:CCC:722:HOH:O	2.17	0.44
1:AAA:25:ALA:HA	1:AAA:40:THR:O	2.17	0.44
1:CCC:28:ARG:CG	1:CCC:38:HIS:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:0:HIS:HB2	1:CCC:51:TRP:CE2	2.53	0.43
1:CCC:61:GLY:HA3	1:CCC:73:VAL:HG12	2.01	0.42
1:BBB:28:ARG:CB	3:BBB:903:GOL:H11	2.49	0.42
1:CCC:110:ARG:HD3	5:CCC:701:HOH:O	2.19	0.42
1:BBB:28:ARG:HB3	1:BBB:28:ARG:NH1	2.35	0.42
1:CCC:12:ARG:NH1	1:CCC:22:PRO:HB3	2.35	0.42
1:AAA:52:VAL:HG23	1:BBB:1:MET:CG	2.50	0.41
1:BBB:28:ARG:NH1	3:BBB:903:GOL:H32	2.34	0.41
1:AAA:108:LEU:HB3	3:AAA:204:GOL:C3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	125/157 (80%)	123 (98%)	2 (2%)	0	100	100
1	BBB	125/157 (80%)	122 (98%)	3 (2%)	0	100	100
1	CCC	120/157 (76%)	118 (98%)	2 (2%)	0	100	100
All	All	370/471 (79%)	363 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	103/130 (79%)	103 (100%)	0	100	100
1	BBB	103/130 (79%)	102 (99%)	1 (1%)	76	87
1	CCC	101/130 (78%)	99 (98%)	2 (2%)	55	72
All	All	307/390 (79%)	304 (99%)	3 (1%)	76	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	-1	SER
1	CCC	17	SER
1	CCC	106	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	CCC	607	-	5,5,5	0.11	0	5,5,5	0.26	0
3	GOL	AAA	202	-	5,5,5	0.12	0	5,5,5	0.33	0
2	PEG	CCC	606	-	6,6,6	0.33	0	5,5,5	0.24	0
3	GOL	CCC	604	-	5,5,5	0.13	0	5,5,5	0.29	0
2	PEG	BBB	902	-	6,6,6	0.37	0	5,5,5	0.33	0
2	PEG	AAA	201	-	6,6,6	0.22	0	5,5,5	0.16	0
3	GOL	AAA	204	-	5,5,5	0.20	0	5,5,5	0.51	0
2	PEG	AAA	205	-	6,6,6	0.19	0	5,5,5	0.11	0
3	GOL	CCC	603	-	5,5,5	0.10	0	5,5,5	0.26	0
3	GOL	BBB	907	-	5,5,5	0.18	0	5,5,5	0.52	0
3	GOL	CCC	605	-	5,5,5	0.14	0	5,5,5	0.37	0
2	PEG	BBB	904	-	6,6,6	0.31	0	5,5,5	0.17	0
3	GOL	AAA	203	-	5,5,5	0.07	0	5,5,5	0.24	0
2	PEG	CCC	602	-	6,6,6	0.22	0	5,5,5	0.14	0
3	GOL	BBB	901	-	5,5,5	0.15	0	5,5,5	0.40	0
3	GOL	BBB	903	-	5,5,5	0.16	0	5,5,5	0.51	0
3	GOL	AAA	206	-	5,5,5	0.12	0	5,5,5	0.31	0
3	GOL	CCC	601	-	5,5,5	0.10	0	5,5,5	0.30	0
3	GOL	BBB	905	-	5,5,5	0.13	0	5,5,5	0.47	0
3	GOL	BBB	906	-	5,5,5	0.10	0	5,5,5	0.37	0
4	PO4	BBB	908	-	4,4,4	0.93	0	6,6,6	0.46	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	CCC	607	-	-	0/4/4/4	-
3	GOL	AAA	202	-	-	2/4/4/4	-
2	PEG	CCC	606	-	-	0/4/4/4	-
3	GOL	CCC	604	-	-	0/4/4/4	-
2	PEG	BBB	902	-	-	3/4/4/4	-
2	PEG	AAA	201	-	-	2/4/4/4	-
3	GOL	AAA	204	-	-	0/4/4/4	-
2	PEG	AAA	205	-	-	0/4/4/4	-
3	GOL	CCC	603	-	-	0/4/4/4	-
3	GOL	BBB	907	-	-	0/4/4/4	-
3	GOL	CCC	605	-	-	0/4/4/4	-
2	PEG	BBB	904	-	-	3/4/4/4	-
3	GOL	AAA	203	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	CCC	602	-	-	1/4/4/4	-
3	GOL	BBB	901	-	-	0/4/4/4	-
3	GOL	BBB	903	-	-	2/4/4/4	-
3	GOL	AAA	206	-	-	2/4/4/4	-
3	GOL	CCC	601	-	-	0/4/4/4	-
3	GOL	BBB	905	-	-	2/4/4/4	-
3	GOL	BBB	906	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	202	GOL	C1-C2-C3-O3
3	BBB	903	GOL	C1-C2-C3-O3
2	BBB	902	PEG	O1-C1-C2-O2
2	BBB	904	PEG	O1-C1-C2-O2
3	BBB	903	GOL	O2-C2-C3-O3
2	BBB	904	PEG	O2-C3-C4-O4
2	CCC	602	PEG	O1-C1-C2-O2
2	AAA	201	PEG	C1-C2-O2-C3
2	BBB	902	PEG	O2-C3-C4-O4
2	BBB	902	PEG	C4-C3-O2-C2
3	AAA	202	GOL	O2-C2-C3-O3
3	AAA	203	GOL	O2-C2-C3-O3
3	AAA	203	GOL	O1-C1-C2-O2
3	AAA	206	GOL	O2-C2-C3-O3
3	BBB	905	GOL	O2-C2-C3-O3
2	AAA	201	PEG	O2-C3-C4-O4
2	BBB	904	PEG	C4-C3-O2-C2
3	AAA	203	GOL	O1-C1-C2-C3
3	AAA	206	GOL	C1-C2-C3-O3
3	BBB	905	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	902	PEG	3	0

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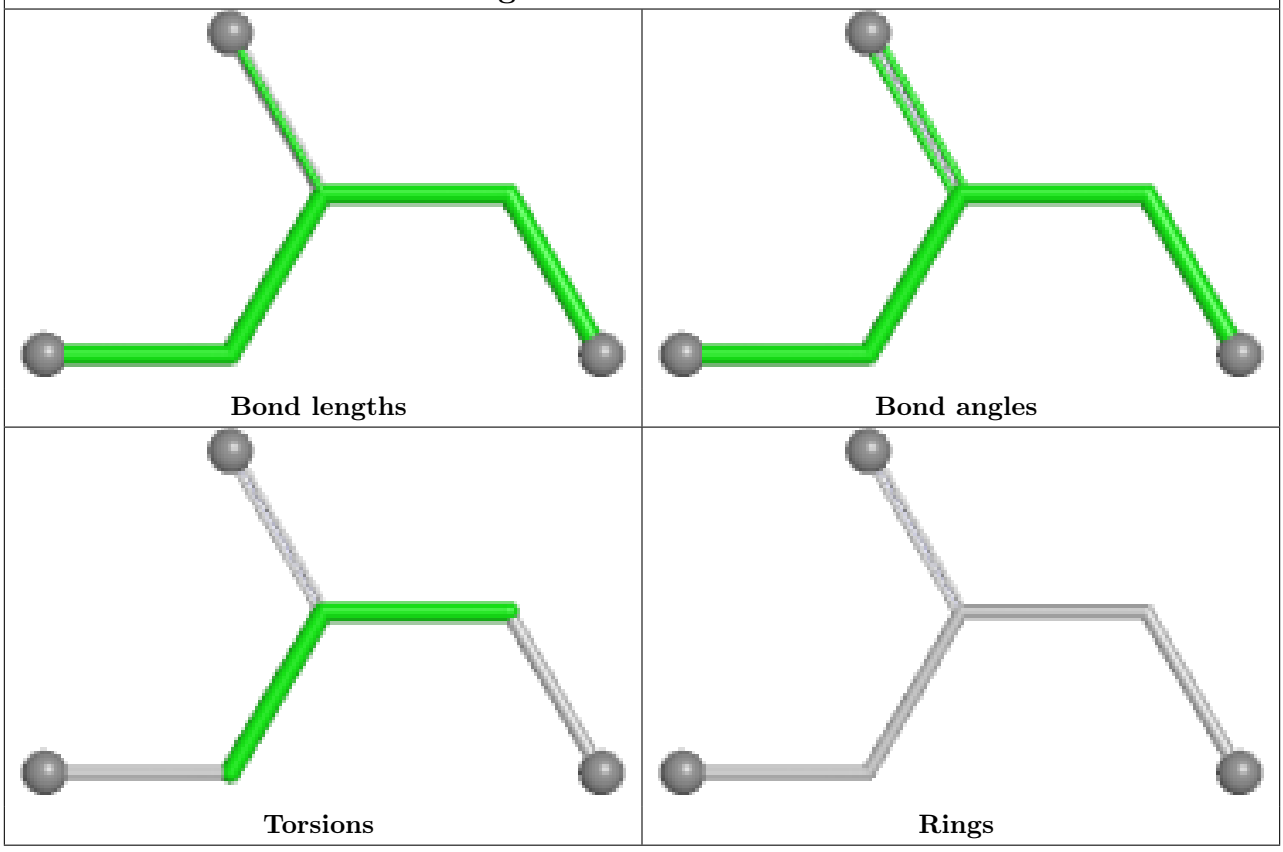
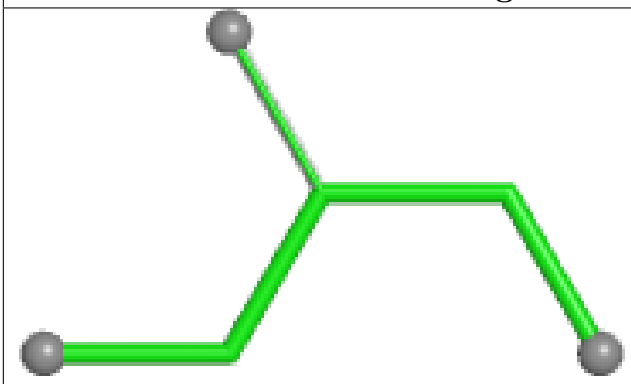
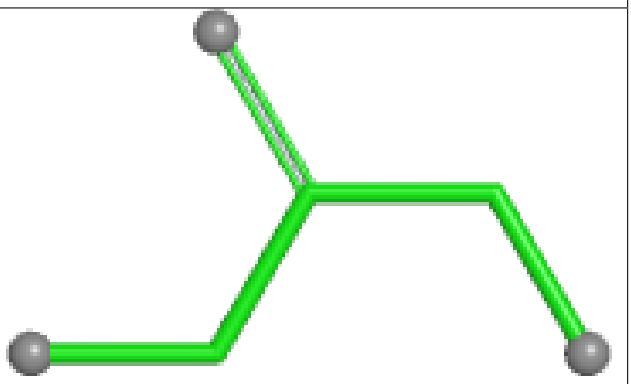
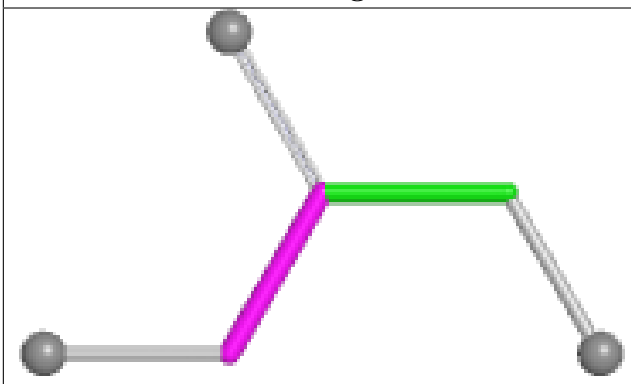
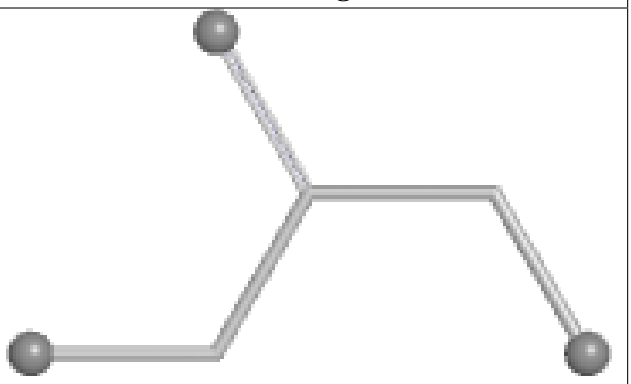
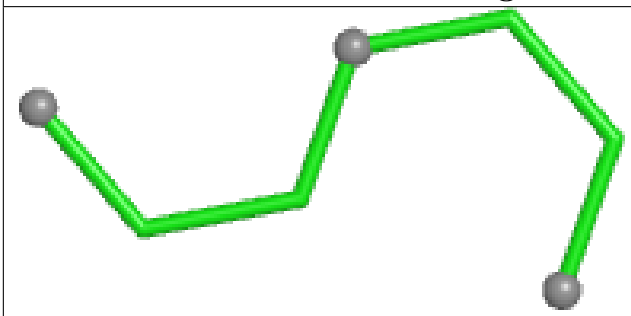
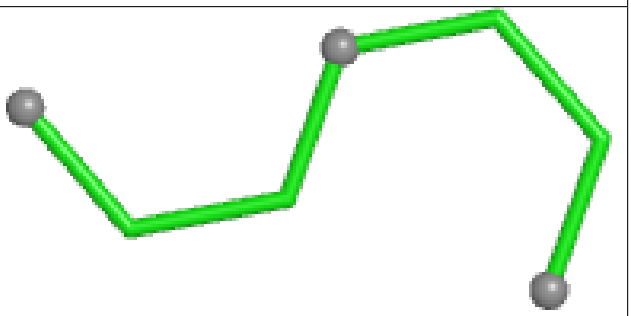
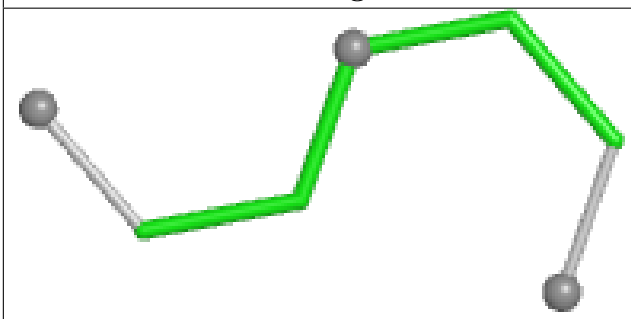
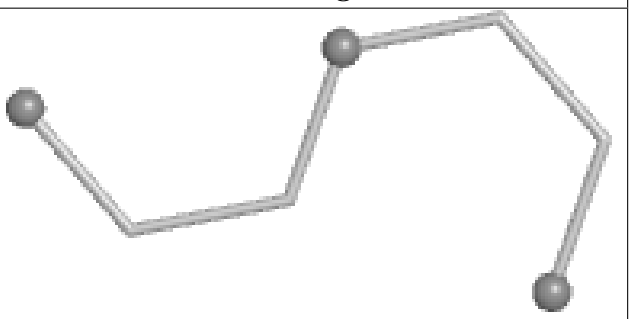
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	204	GOL	3	0
2	BBB	904	PEG	2	0
3	BBB	903	GOL	4	0
3	BBB	905	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

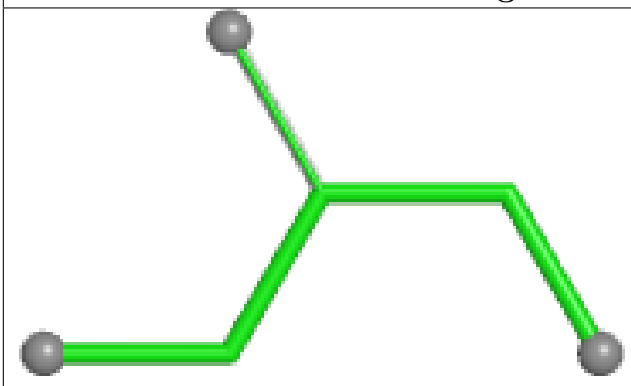
Ligand GOL CCC 607



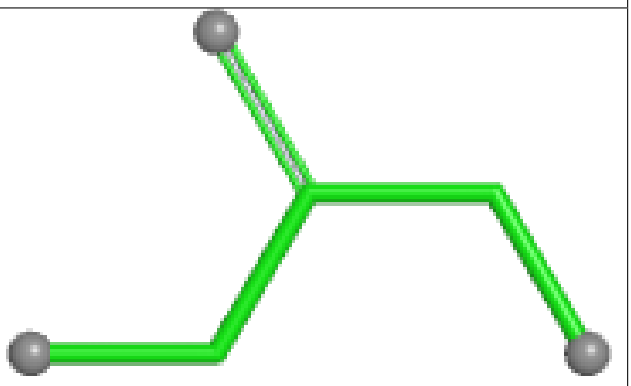
Ligand GOL AAA 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEG CCC 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

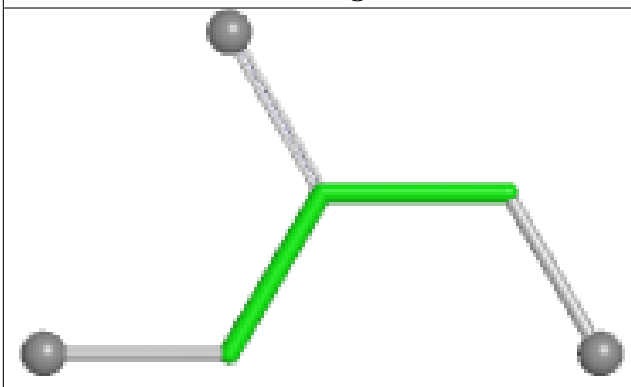
Ligand GOL CCC 604



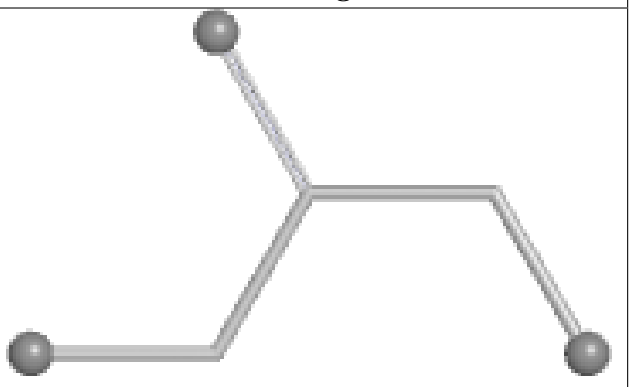
Bond lengths



Bond angles

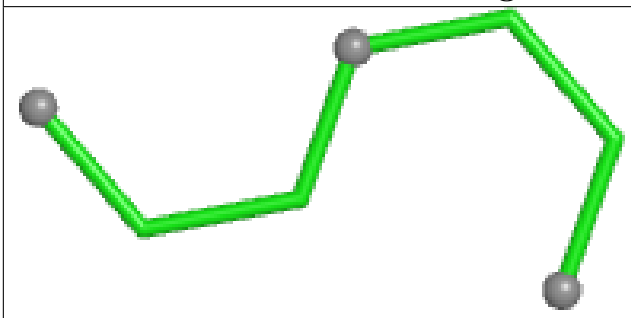


Torsions

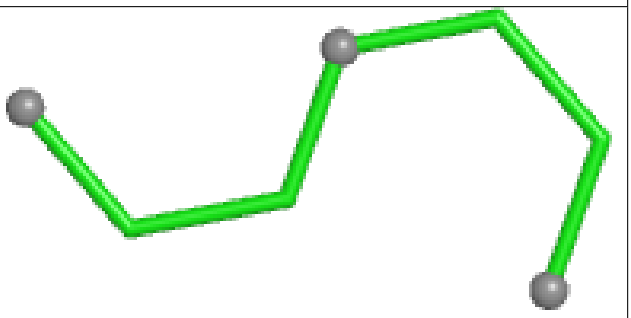


Rings

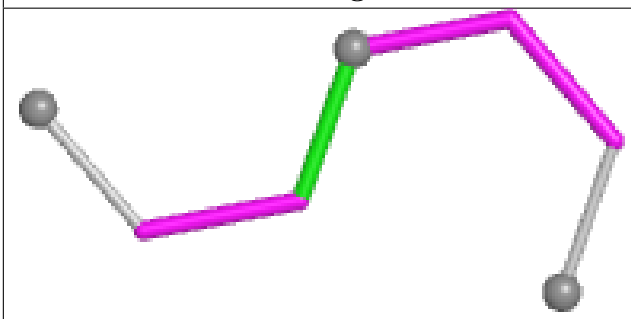
Ligand PEG BBB 902



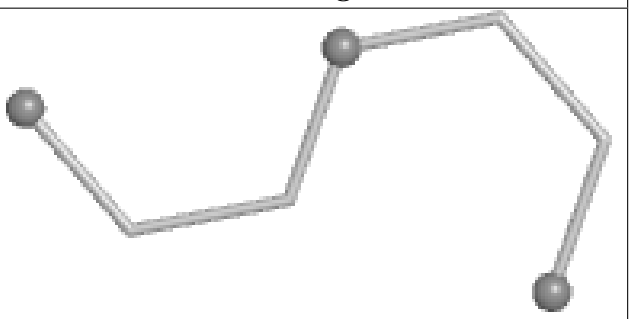
Bond lengths



Bond angles

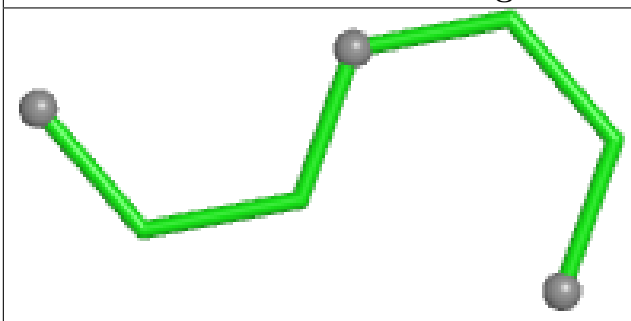


Torsions

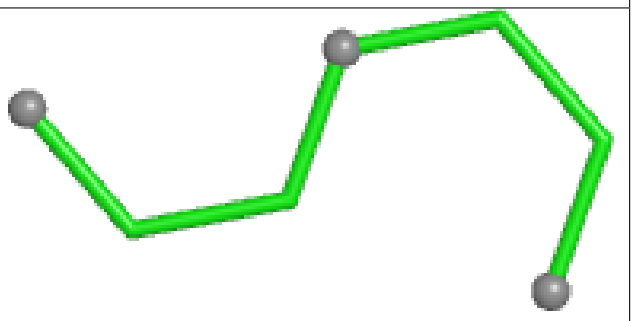


Rings

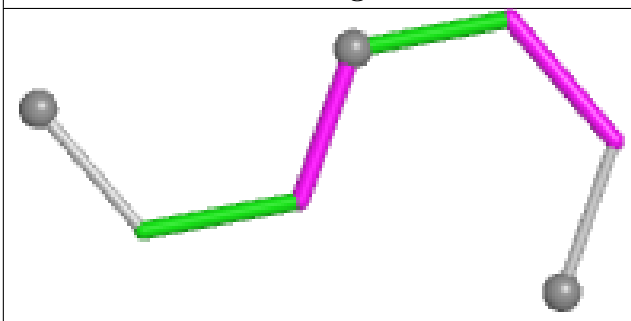
Ligand PEG AAA 201



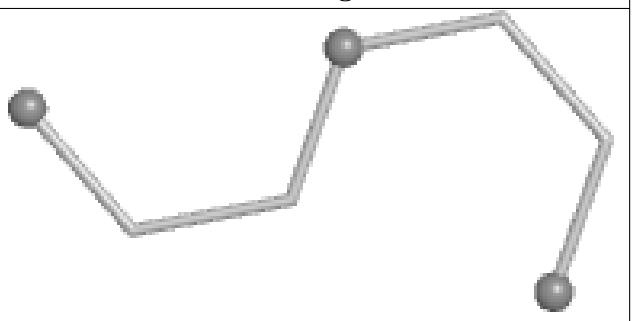
Bond lengths



Bond angles



Torsions



Rings

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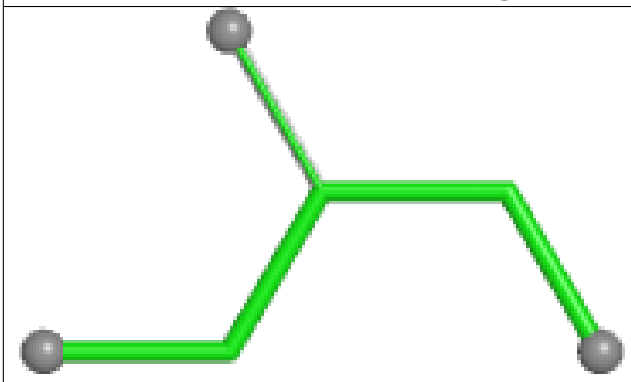

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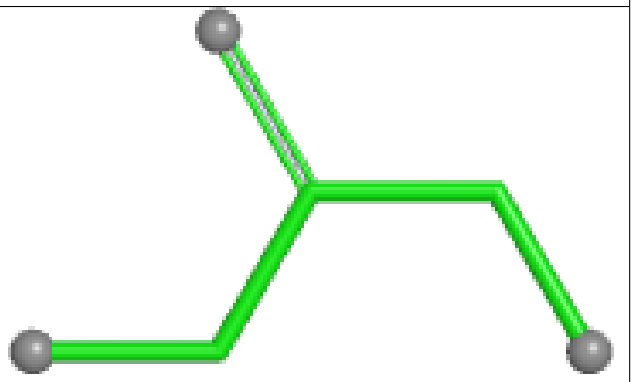
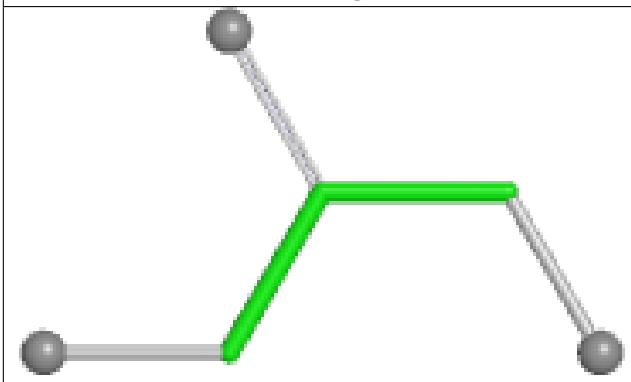


Bond angles



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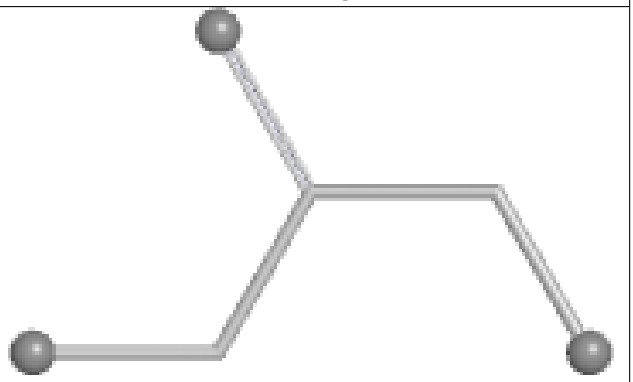
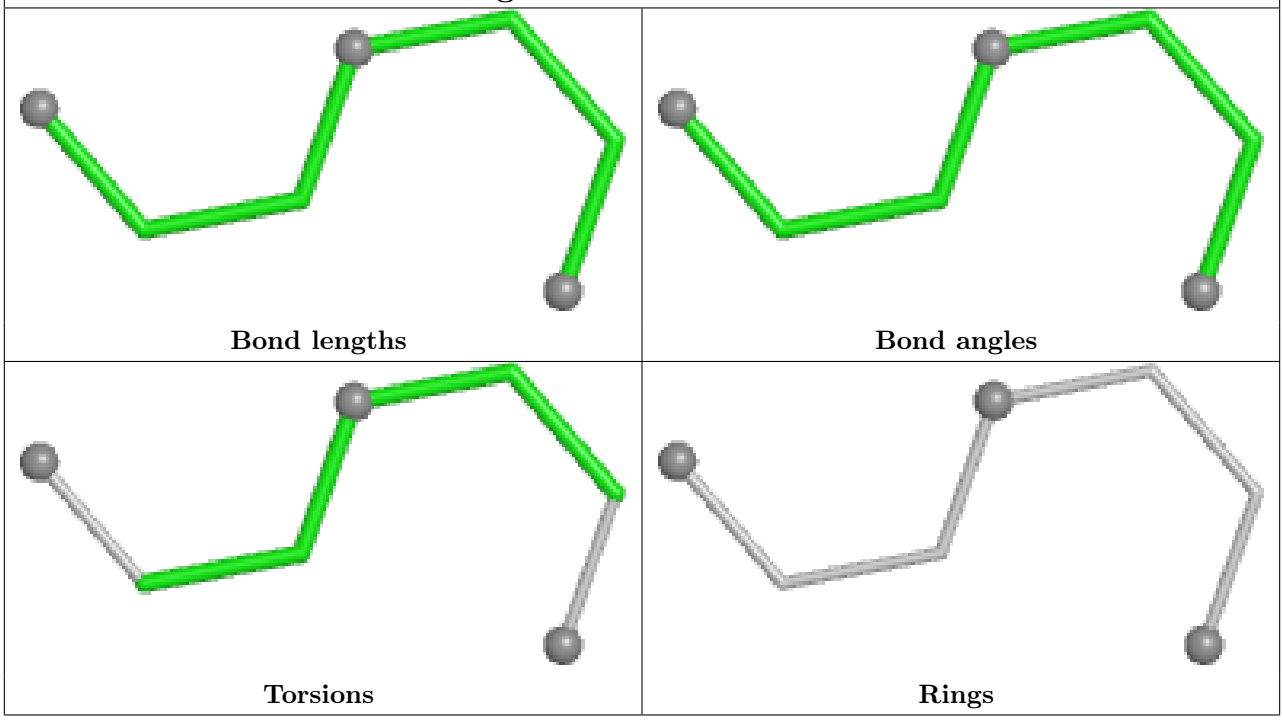
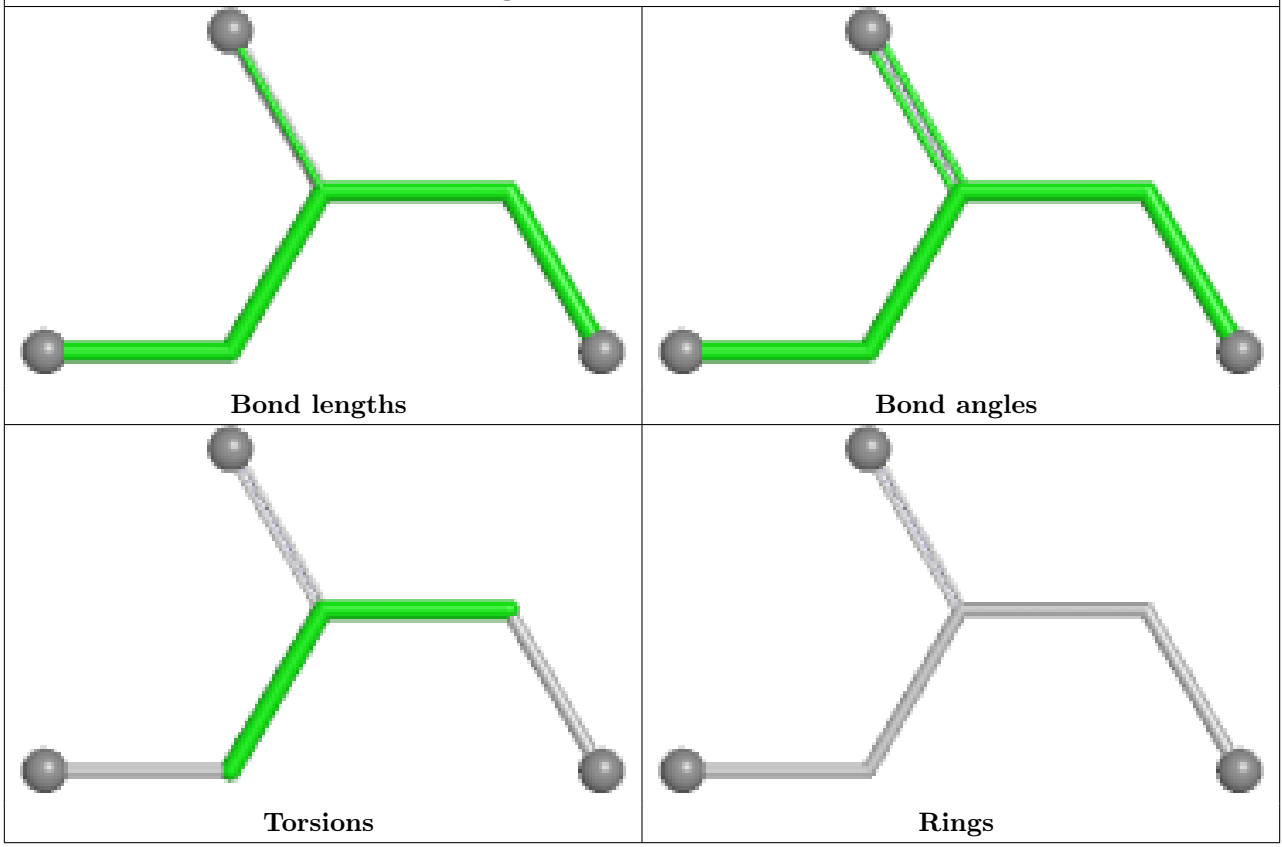


Rings

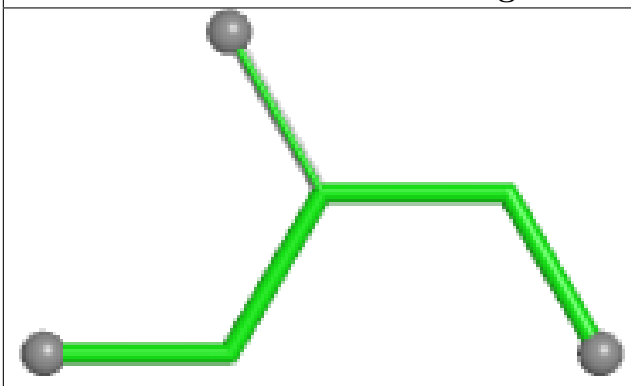
Ligand PEG AAA 205



Ligand GOL CCC 603



Ligand GOL BBB 907



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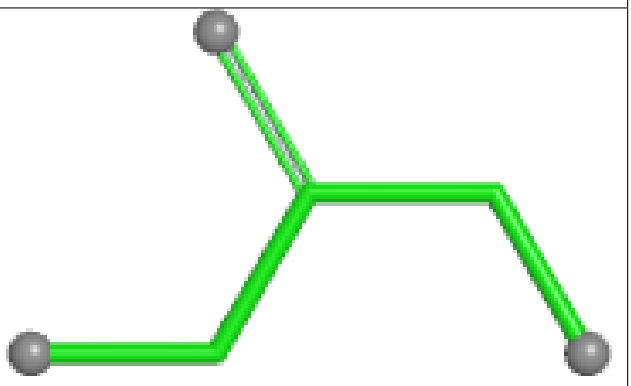
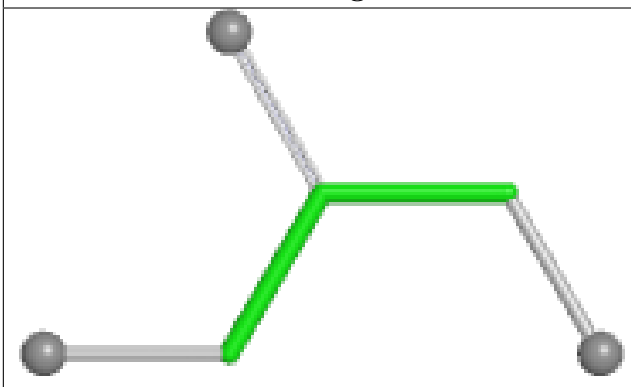
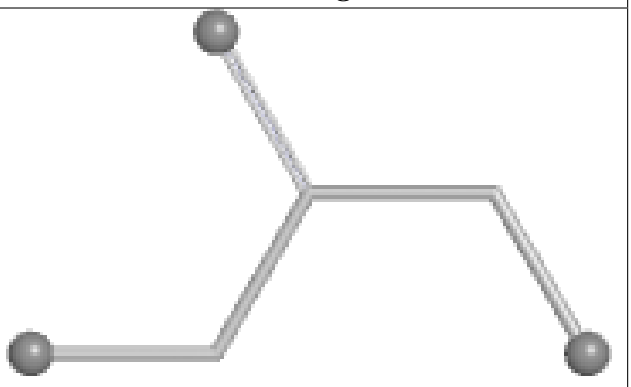


Bond angles

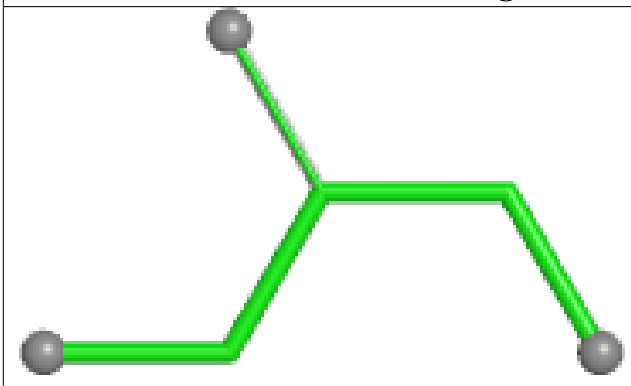


Torsions

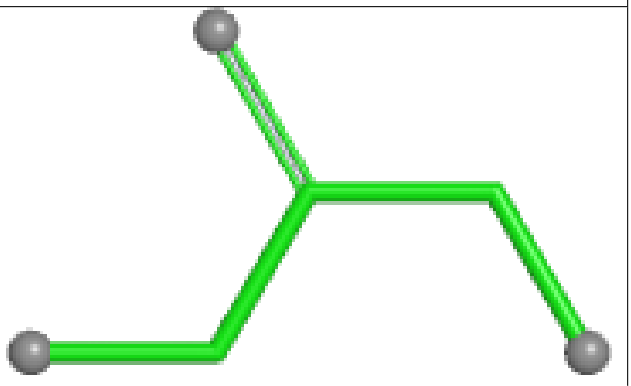


Rings

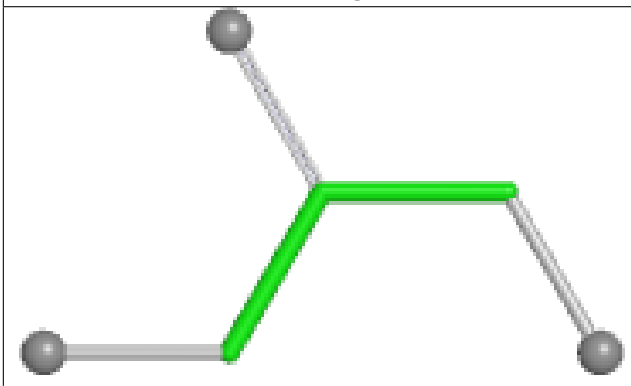
Ligand GOL CCC 605



Bond lengths



Bond angles



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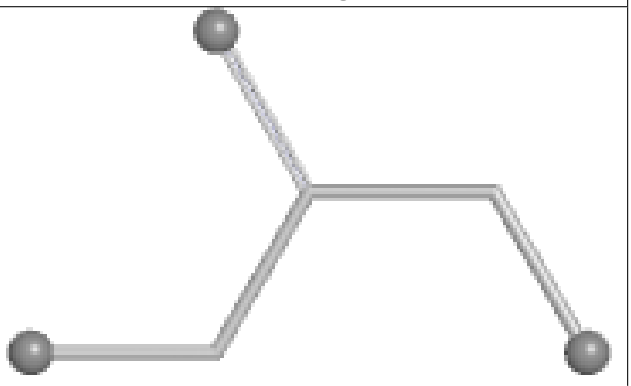
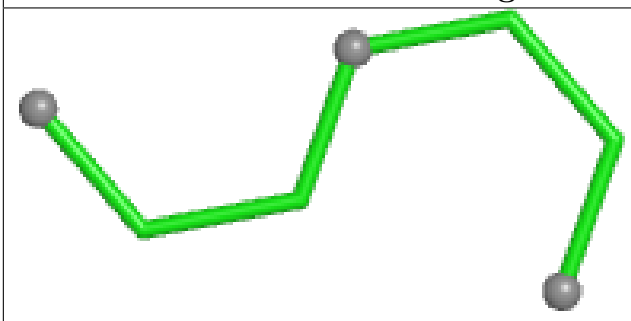
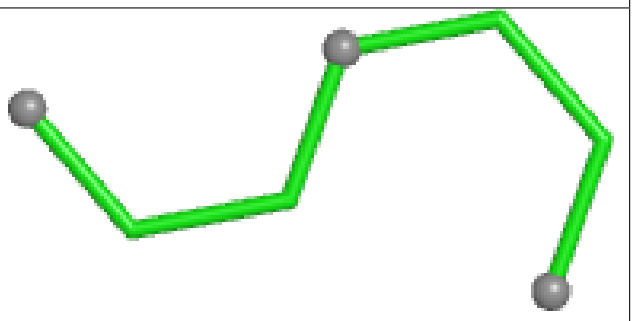


Rings

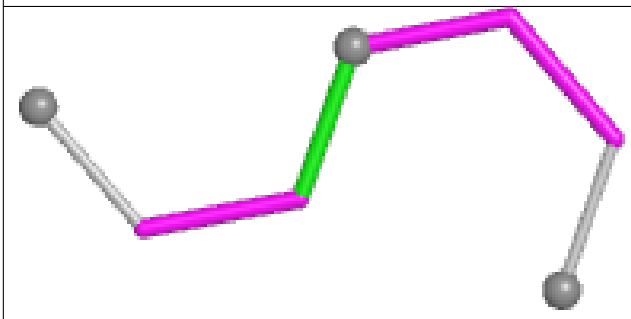
Ligand PEG BBB 904



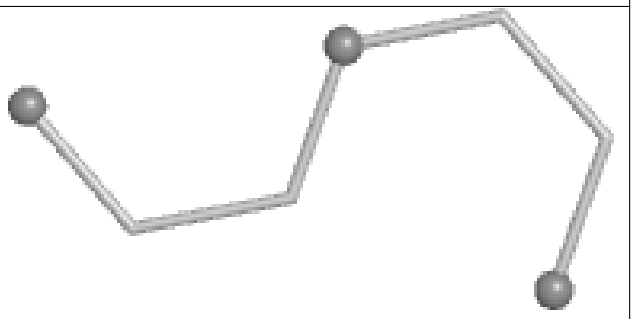
Bond lengths



Bond angles

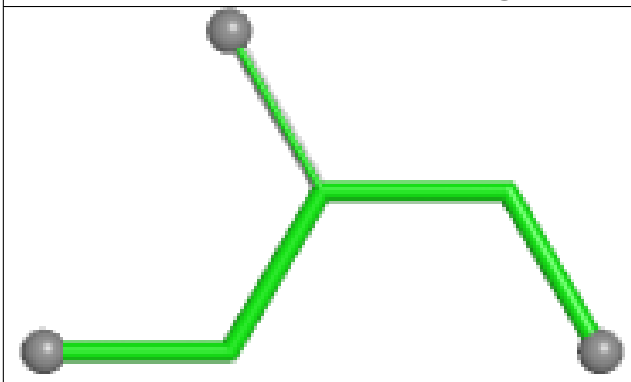


Torsions

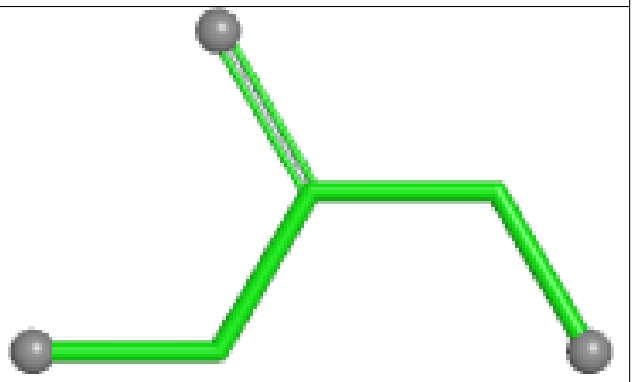


Rings

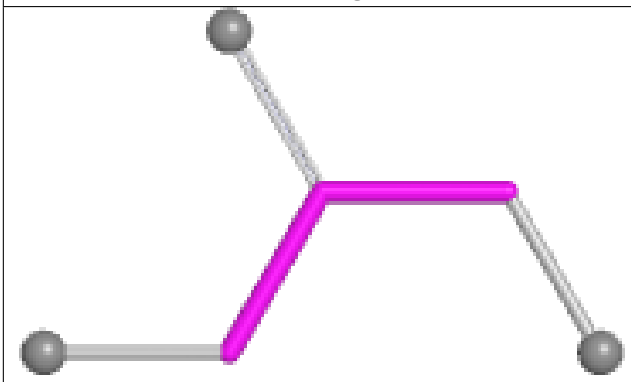
Ligand GOL AAA 203



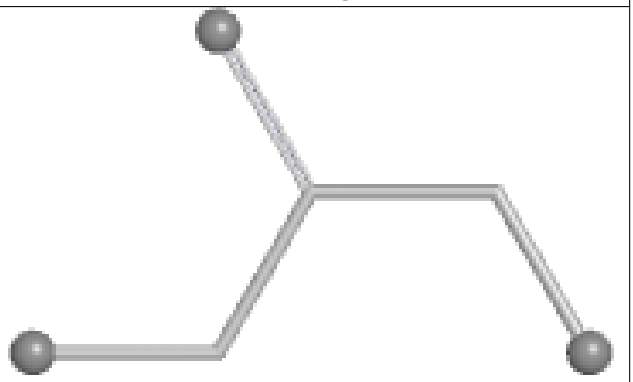
Bond lengths



Bond angles

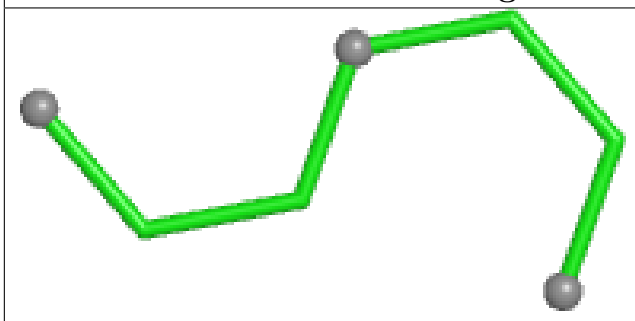


Torsions

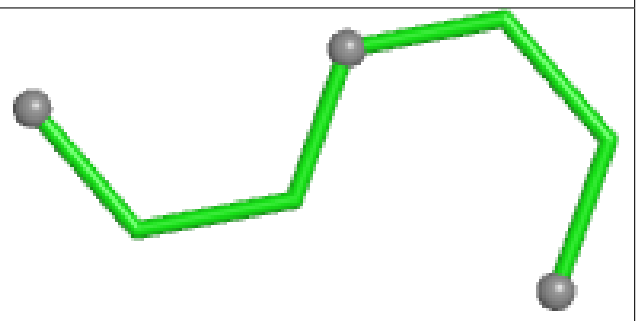


Rings

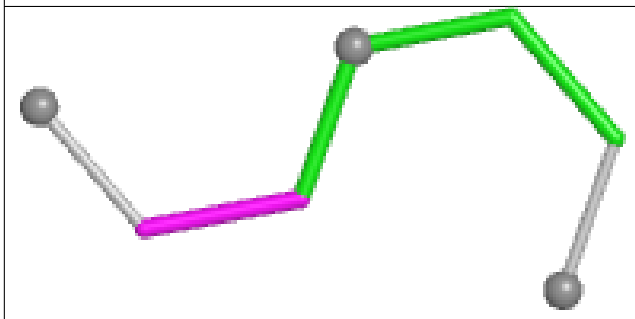
Ligand PEG CCC 602



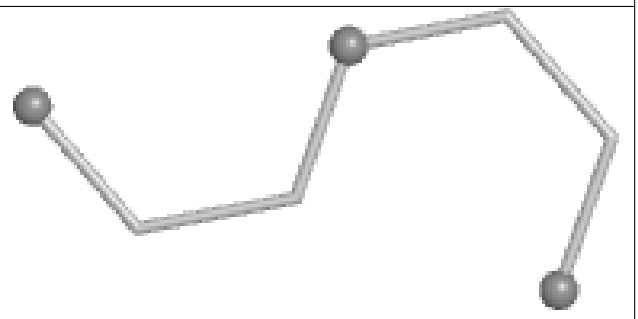
Bond lengths



Bond angles

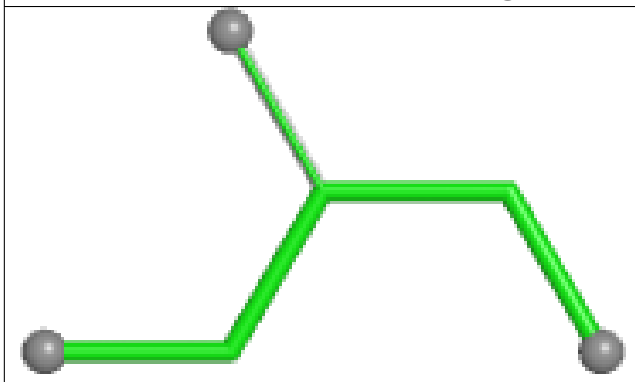


Torsions

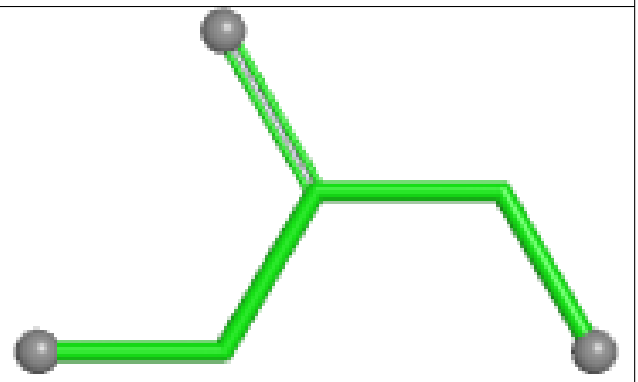


Rings

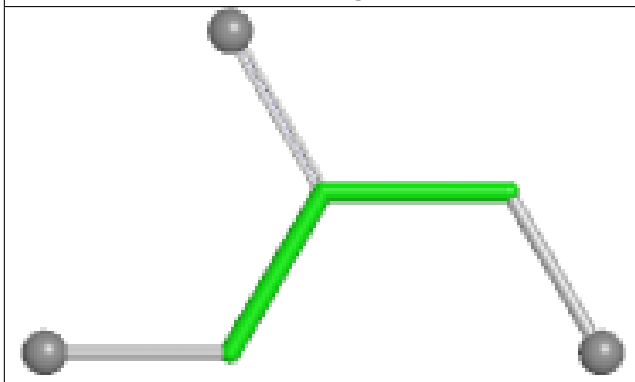
Ligand GOL BBB 901



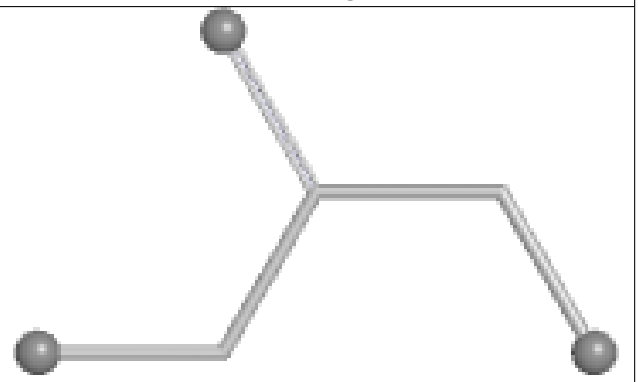
Bond lengths



Bond angles

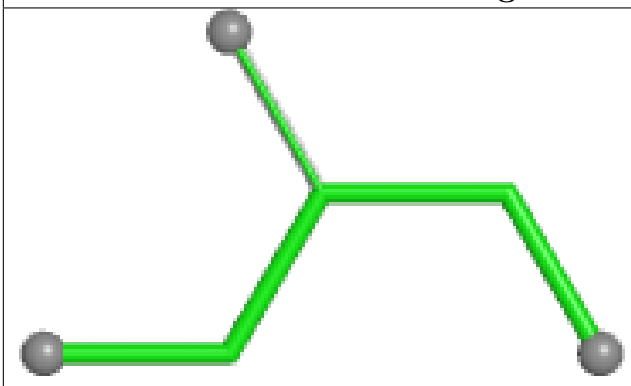


Torsions

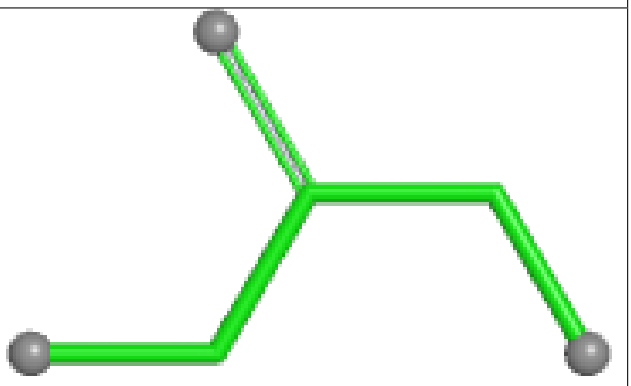


Rings

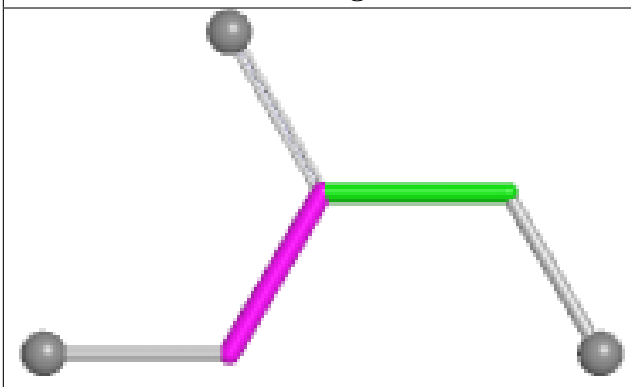
Ligand GOL BBB 903



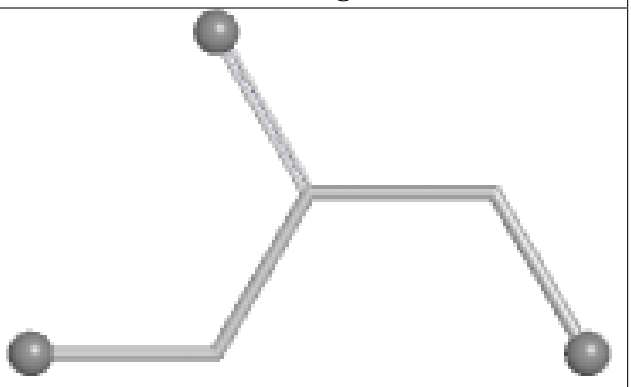
Bond lengths



Bond angles

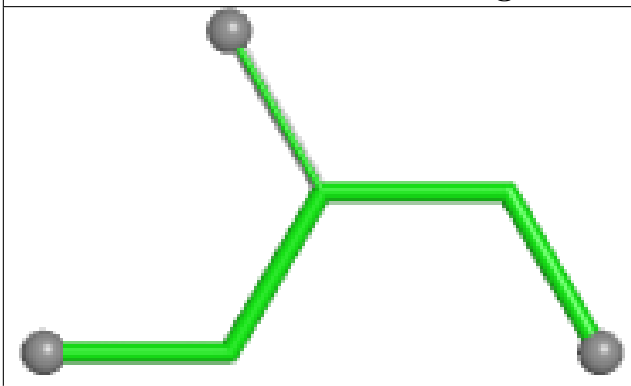


Torsions

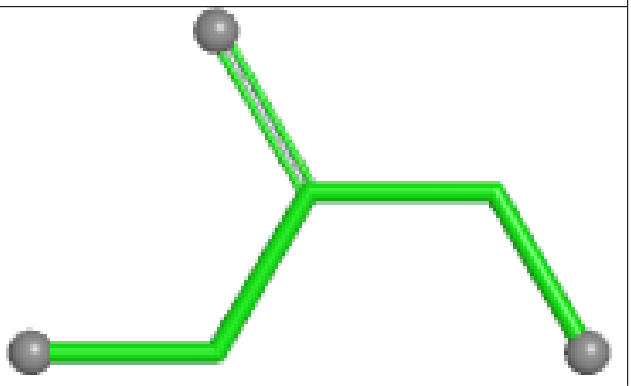


Rings

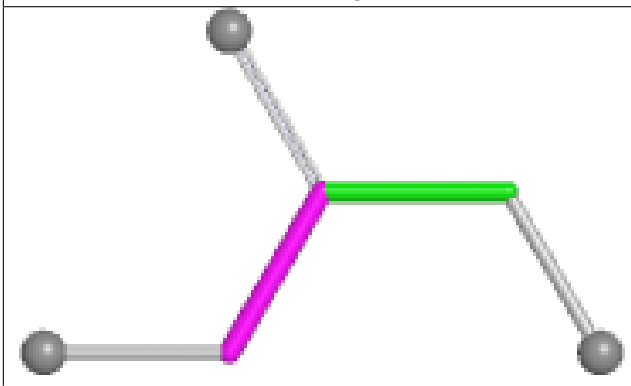
Ligand GOL AAA 206



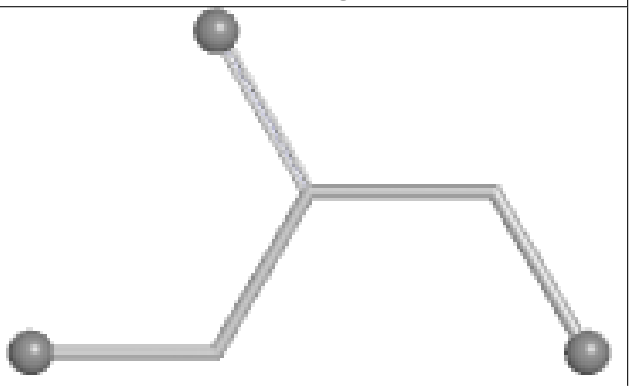
Bond lengths



Bond angles

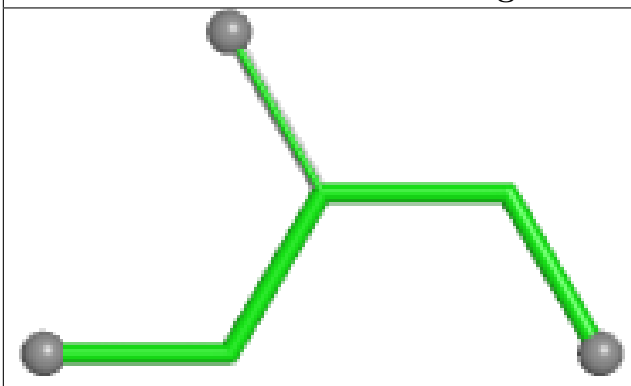


Torsions

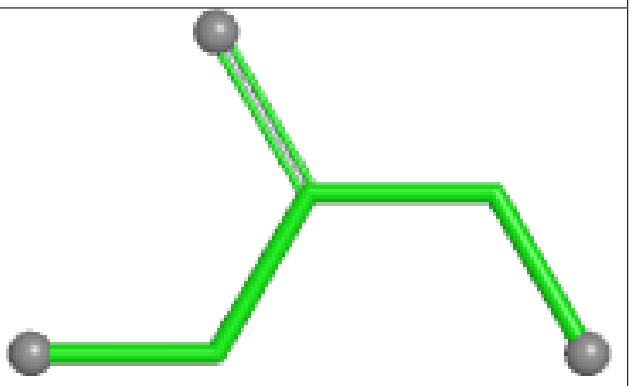


Rings

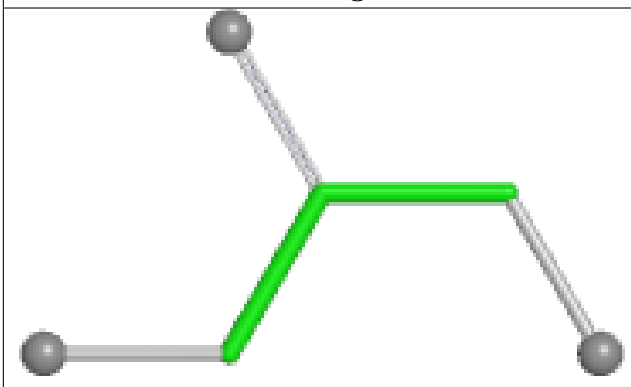
Ligand GOL CCC 601



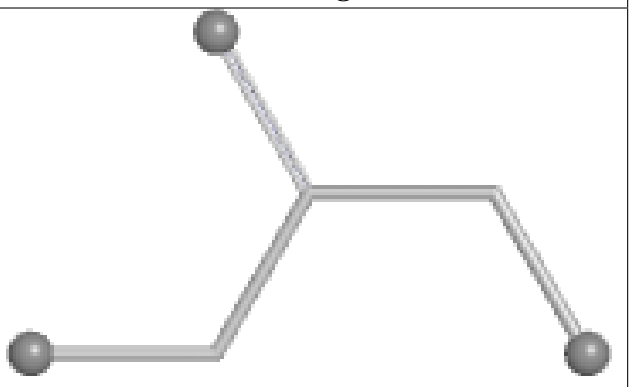
Bond lengths



Bond angles

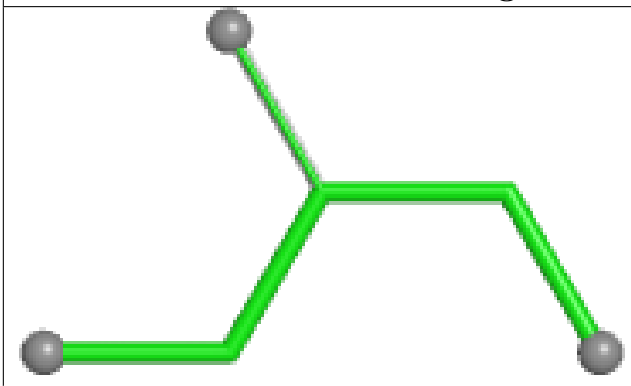


Torsions

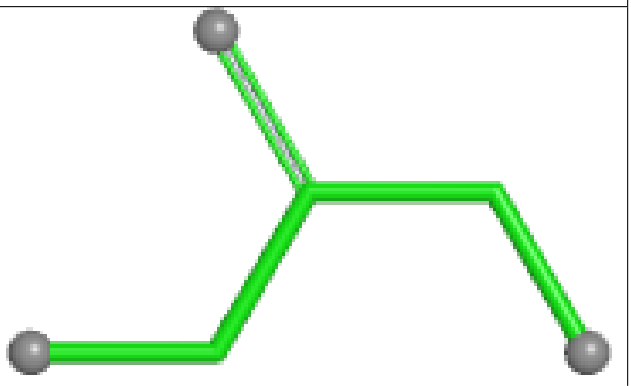


Rings

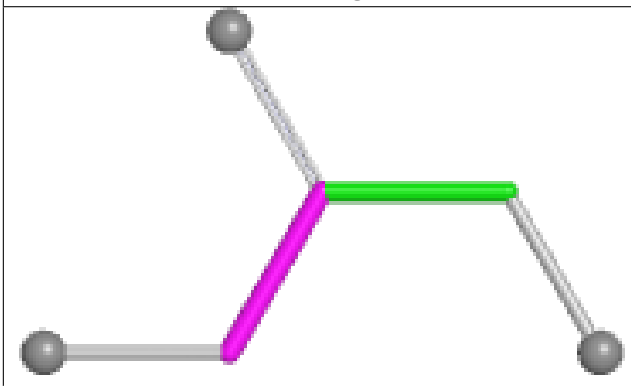
Ligand GOL BBB 905



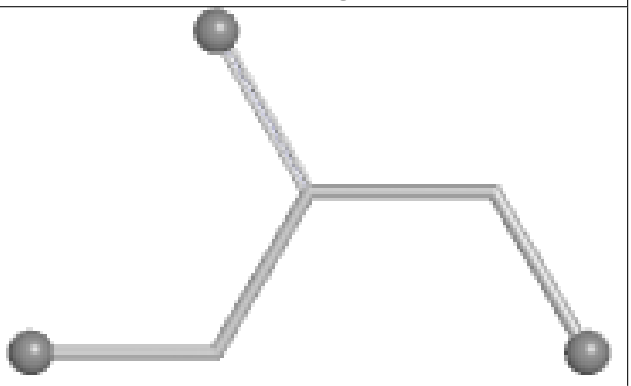
Bond lengths



Bond angles

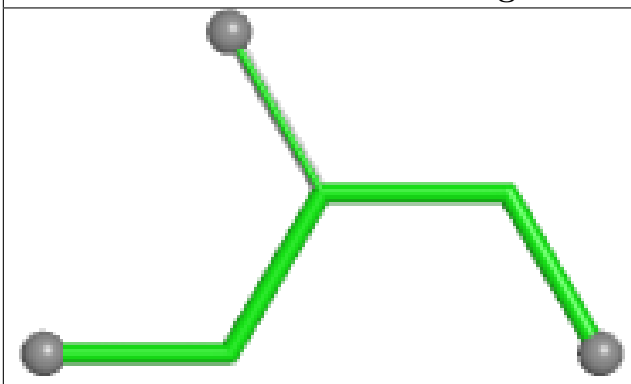


Torsions

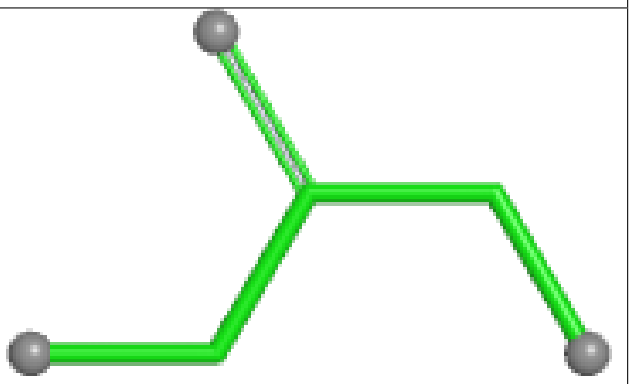


Rings

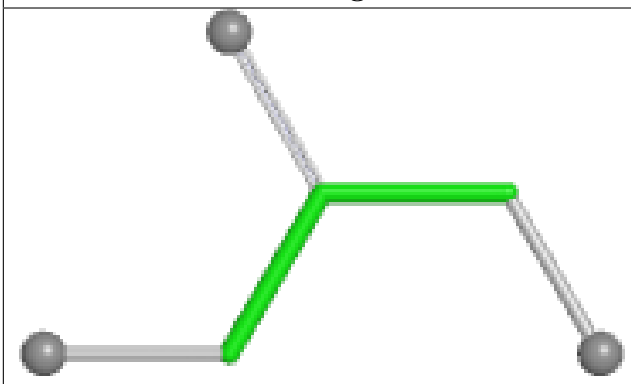
Ligand GOL BBB 906



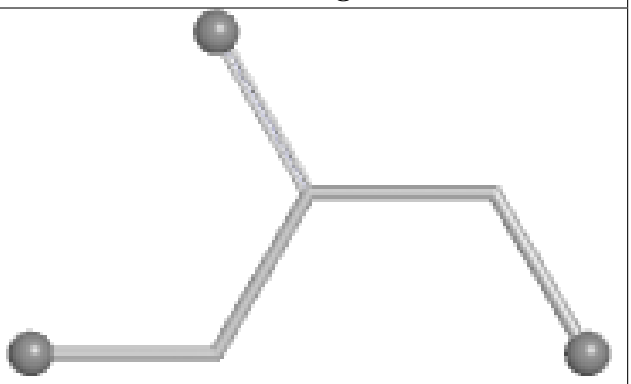
Bond lengths



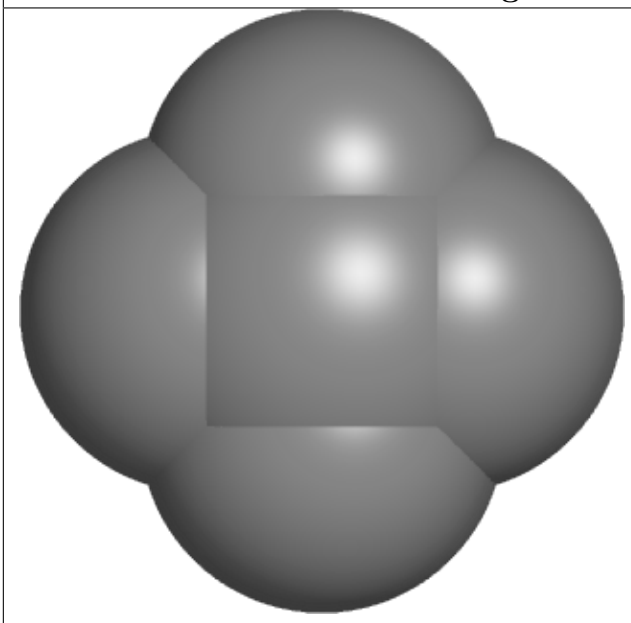
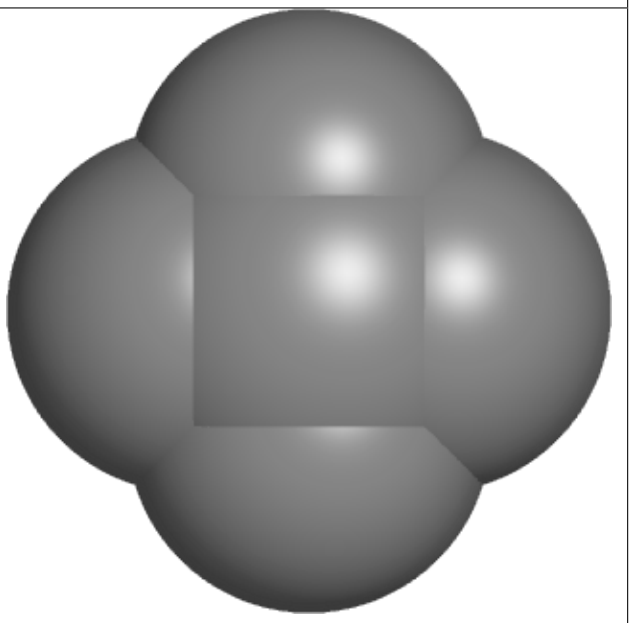
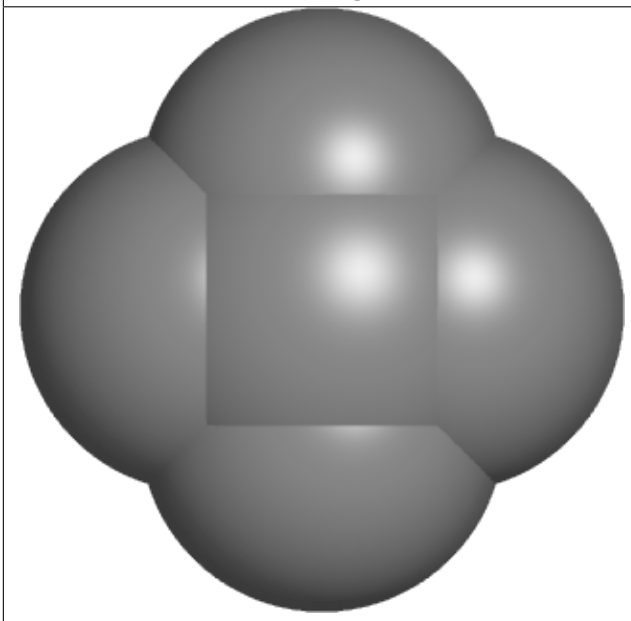
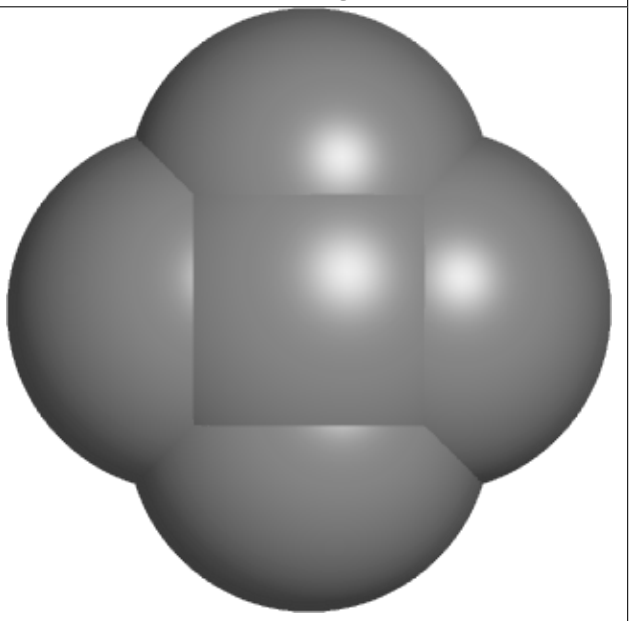
Bond angles



Torsions



Rings

Ligand PO4 BBB 908	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AAA	127/157 (80%)	0.67	13 (10%) 6 9	42, 62, 113, 138	0
1	BBB	127/157 (80%)	0.49	4 (3%) 49 56	39, 55, 109, 130	0
1	CCC	124/157 (78%)	0.41	6 (4%) 30 37	45, 63, 110, 152	0
All	All	378/471 (80%)	0.53	23 (6%) 21 27	39, 62, 113, 152	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	15	VAL	4.7
1	CCC	15	VAL	4.6
1	BBB	93	GLY	4.3
1	AAA	1	MET	4.0
1	AAA	17	SER	4.0
1	BBB	92	GLU	3.9
1	BBB	124	PHE	3.6
1	AAA	-2	GLY	3.5
1	AAA	124	PHE	3.4
1	AAA	78	SER	3.4
1	BBB	91	PRO	3.2
1	AAA	19	SER	3.1
1	AAA	-1	SER	2.9
1	AAA	16	SER	2.8
1	CCC	123	HIS	2.7
1	CCC	91	PRO	2.7
1	AAA	80	GLY	2.5
1	AAA	93	GLY	2.5
1	AAA	79	HIS	2.5
1	CCC	90	SER	2.5
1	AAA	18	GLU	2.4
1	CCC	16	SER	2.2
1	CCC	60	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

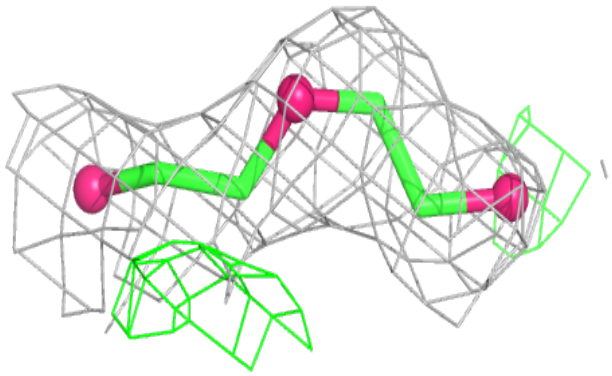
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

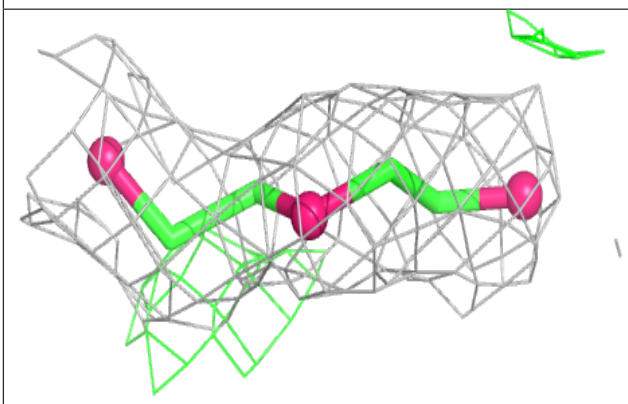
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PEG	BBB	902	7/7	0.65	0.20	73,81,92,93	0
3	GOL	AAA	204	6/6	0.70	0.32	77,82,89,89	0
3	GOL	BBB	905	6/6	0.71	0.19	91,103,105,108	0
2	PEG	CCC	602	7/7	0.72	0.15	88,99,110,114	0
3	GOL	BBB	903	6/6	0.75	0.27	79,83,98,103	0
3	GOL	AAA	202	6/6	0.75	0.18	76,86,94,97	0
3	GOL	CCC	601	6/6	0.78	0.19	77,87,94,101	0
3	GOL	CCC	604	6/6	0.78	0.15	71,85,93,94	0
2	PEG	CCC	606	7/7	0.80	0.23	72,86,95,97	0
3	GOL	BBB	901	6/6	0.80	0.26	75,88,95,100	0
3	GOL	CCC	605	6/6	0.80	0.22	88,94,100,103	0
2	PEG	AAA	205	7/7	0.82	0.25	80,95,99,105	0
3	GOL	CCC	603	6/6	0.82	0.51	97,105,107,117	0
3	GOL	AAA	203	6/6	0.83	0.38	107,118,120,128	0
3	GOL	AAA	206	6/6	0.84	0.24	84,105,109,110	0
3	GOL	CCC	607	6/6	0.85	0.19	91,99,104,105	0
2	PEG	AAA	201	7/7	0.86	0.20	83,84,87,93	0
2	PEG	BBB	904	7/7	0.89	0.15	80,84,88,89	0
3	GOL	BBB	907	6/6	0.90	0.19	72,78,82,82	0
3	GOL	BBB	906	6/6	0.94	0.19	76,79,83,90	0
4	PO4	BBB	908	5/5	0.99	0.18	52,54,72,86	0

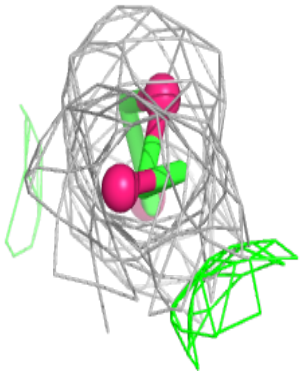
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PEG BBB 902:

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

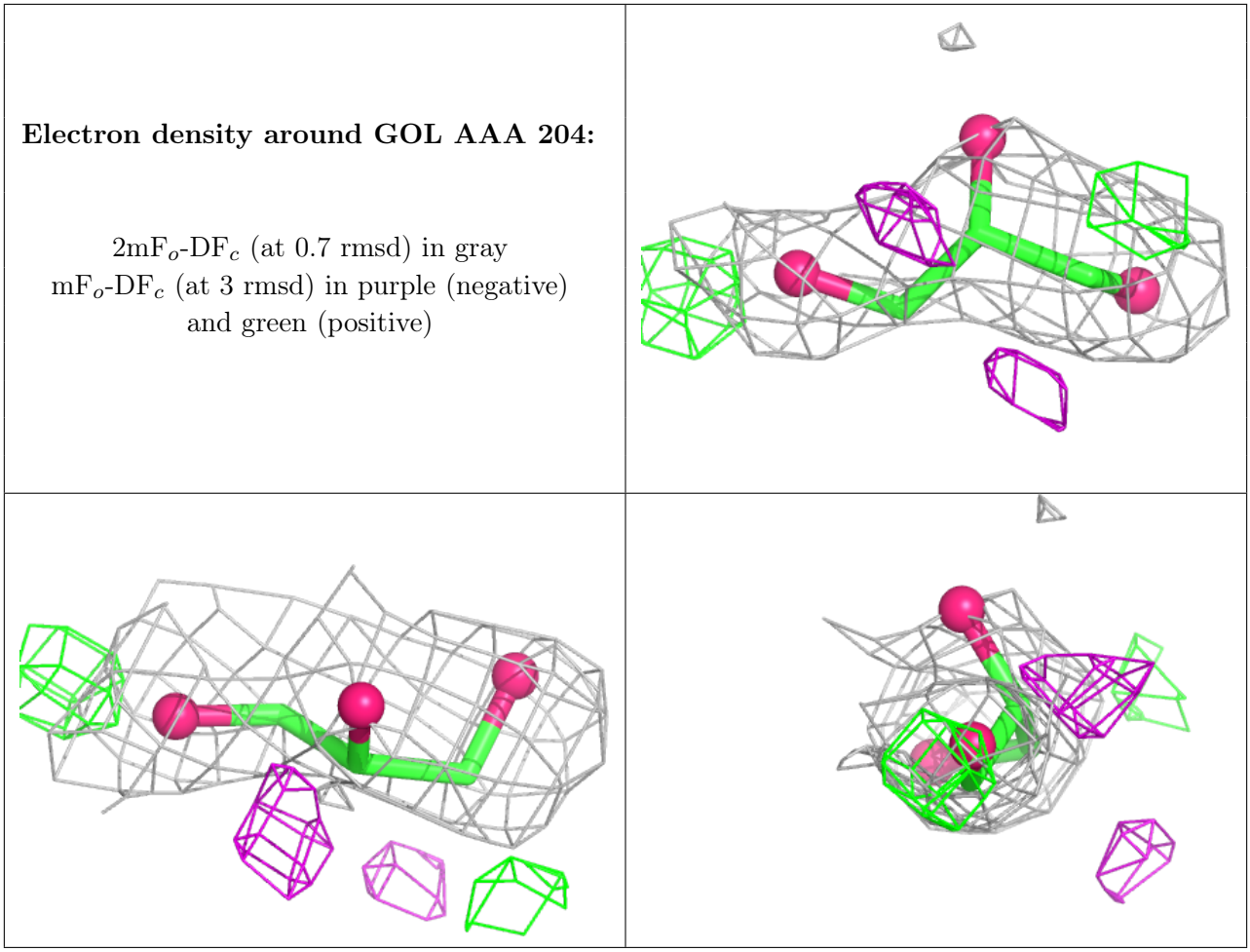






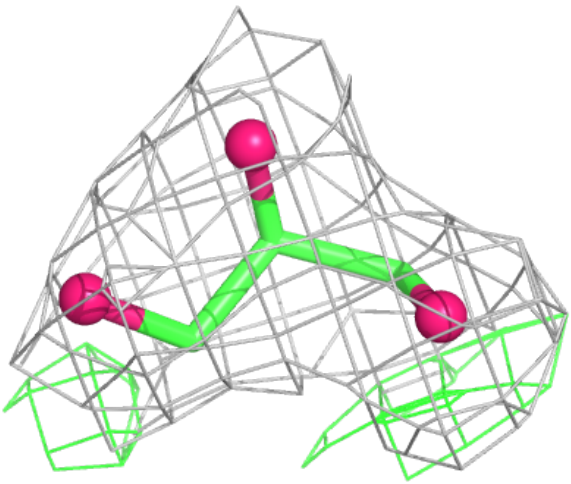
Electron density around GOL AAA 204:

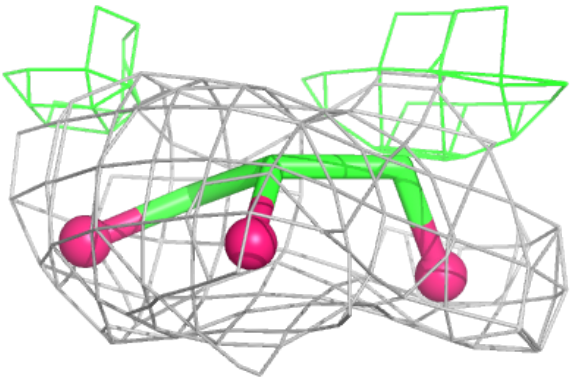
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

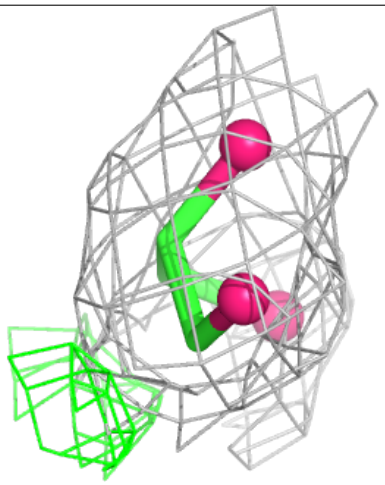


Electron density around GOL BBB 905:

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

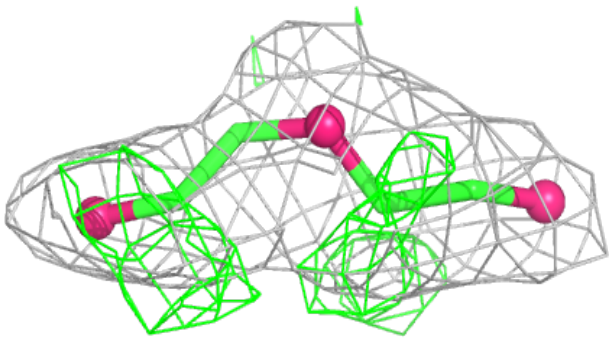


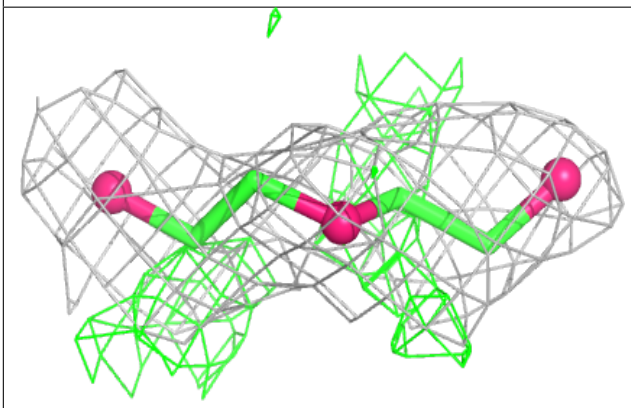


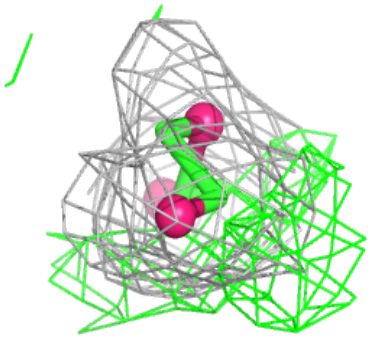


Electron density around PEG CCC 602:

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

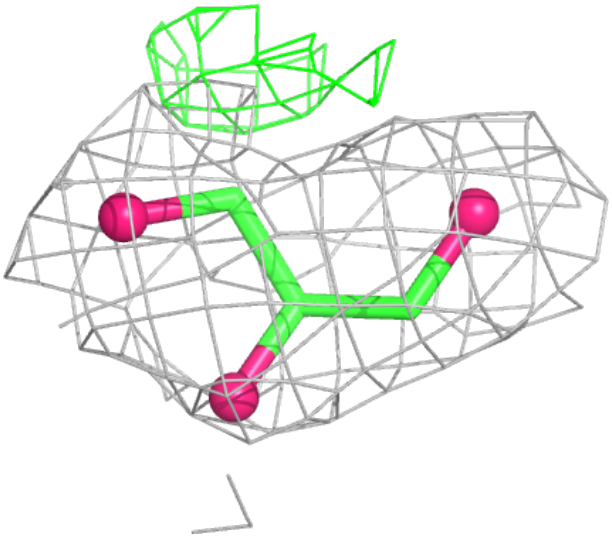


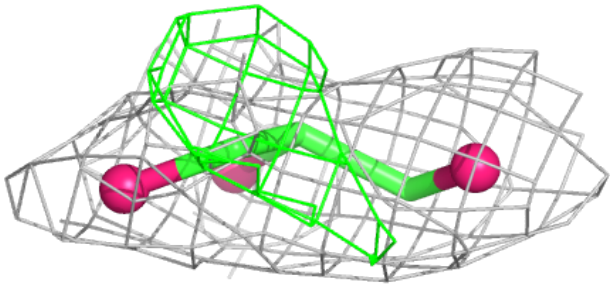


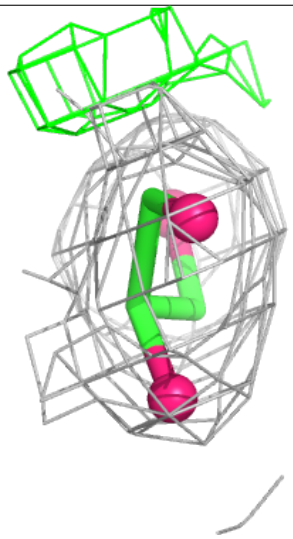


Electron density around GOL BBB 903:

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

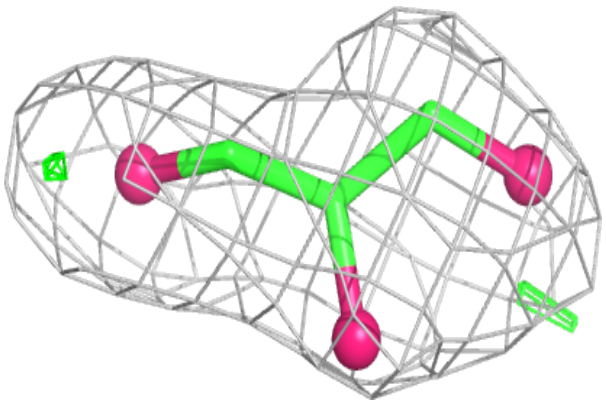


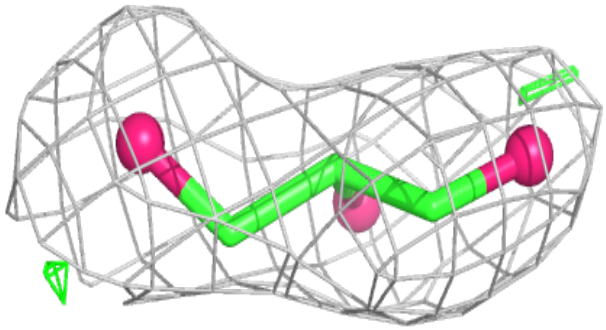


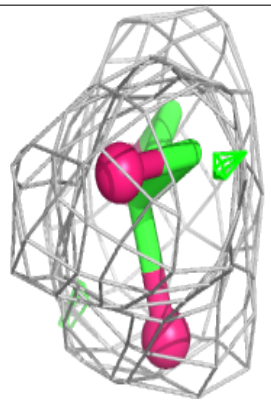


Electron density around GOL AAA 202:

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

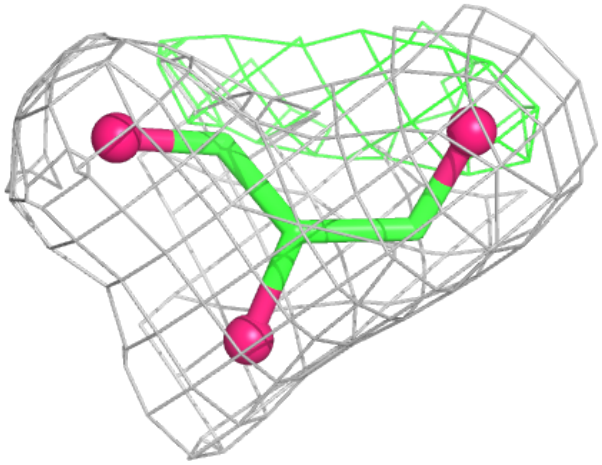


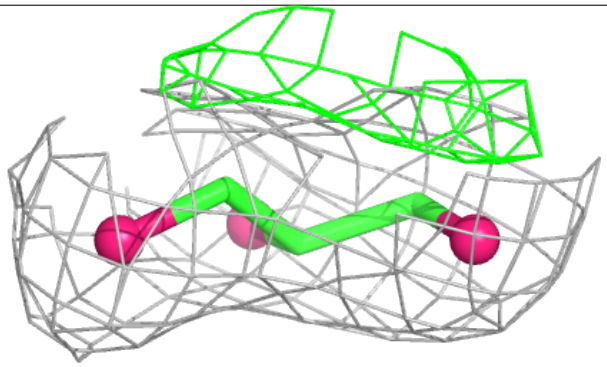


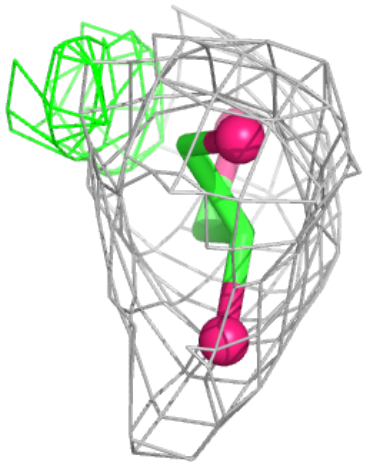


Electron density around GOL CCC 601:

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

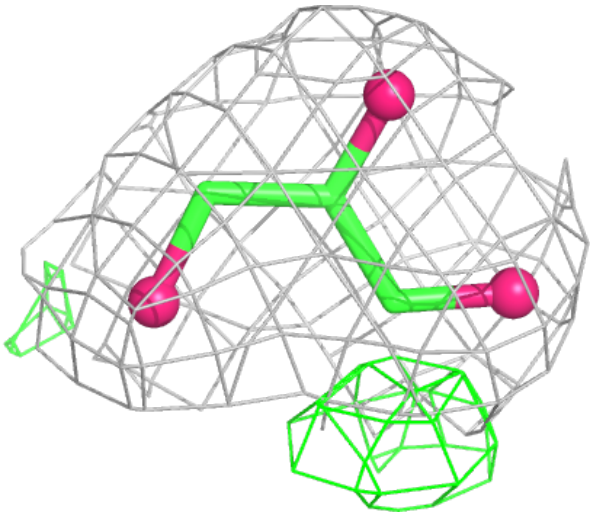


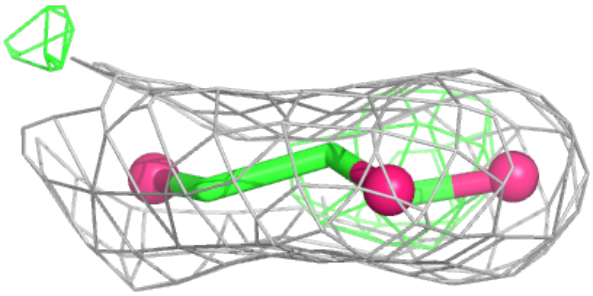


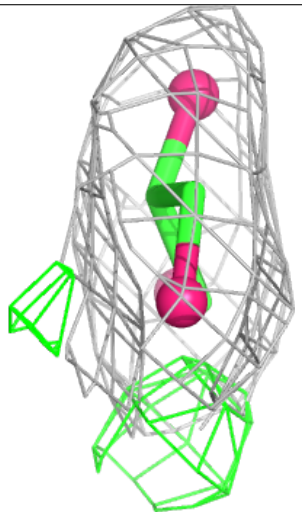


Electron density around GOL CCC 604:

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

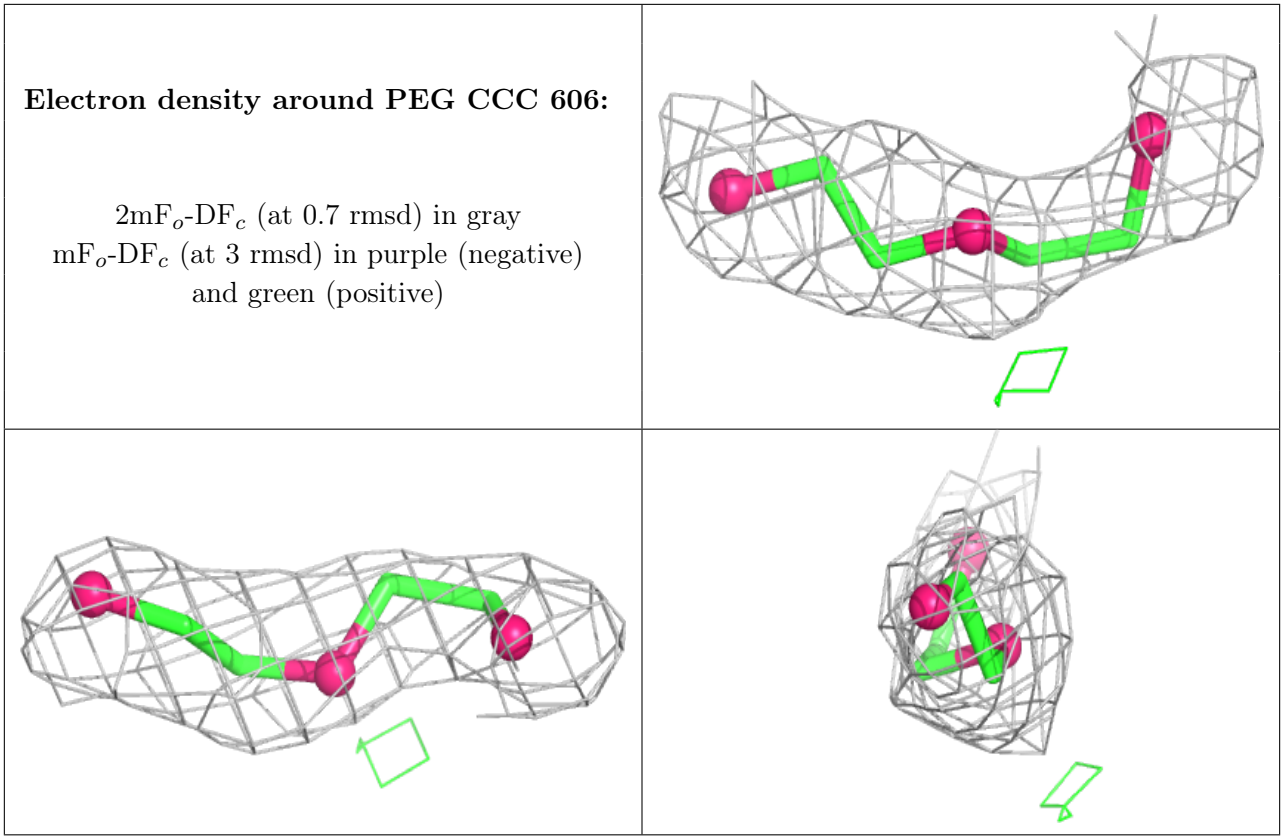






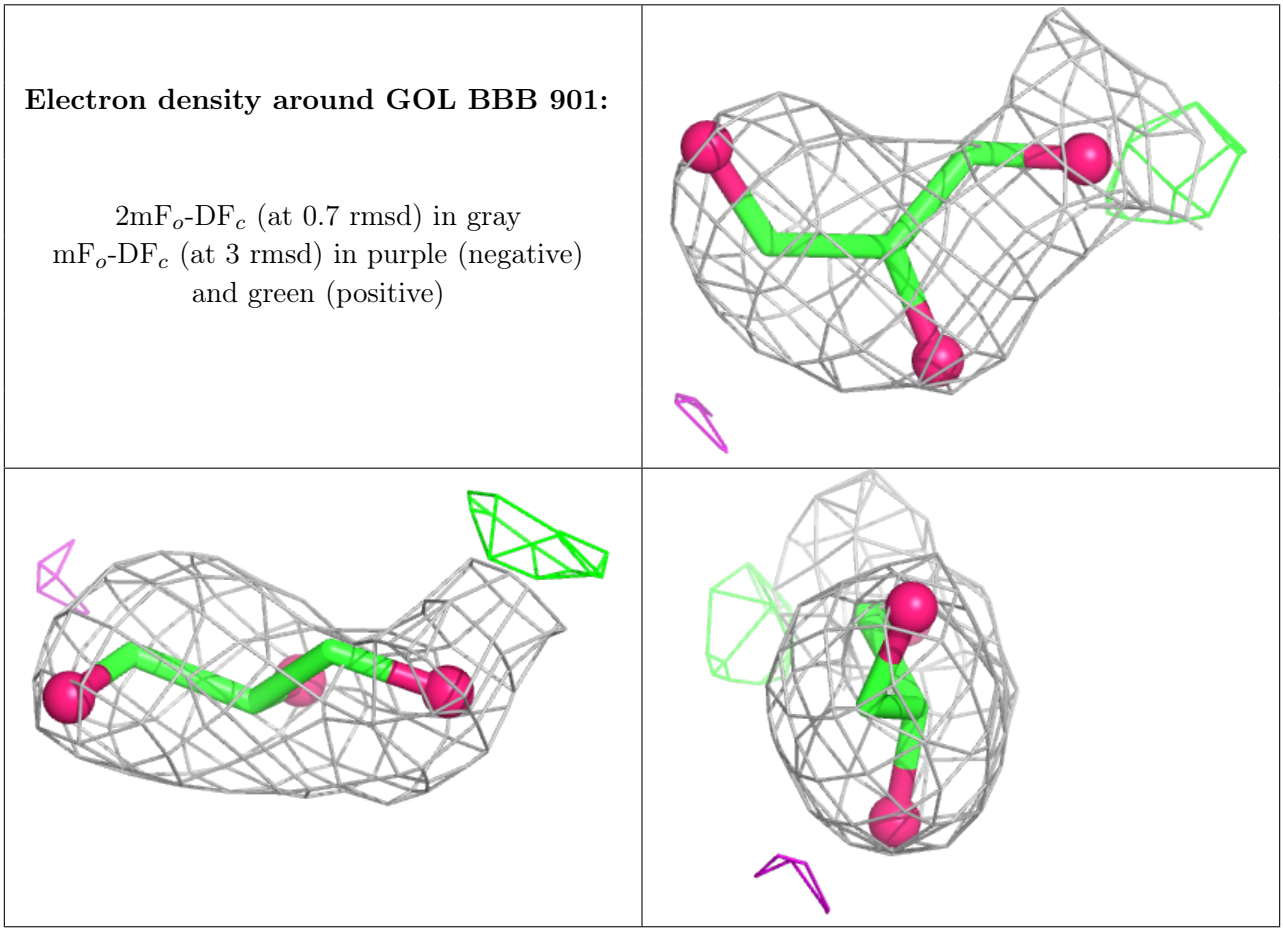
Electron density around PEG CCC 606:

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



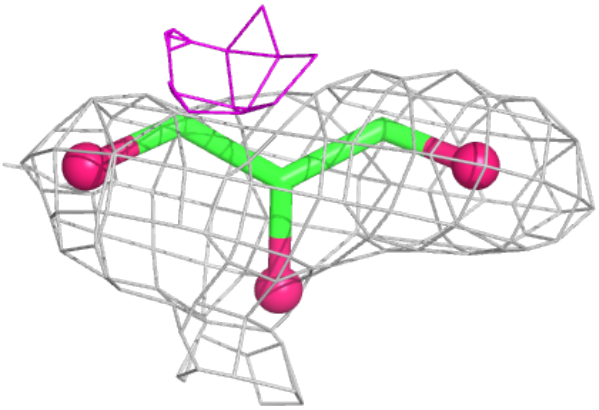
Electron density around GOL BBB 901:

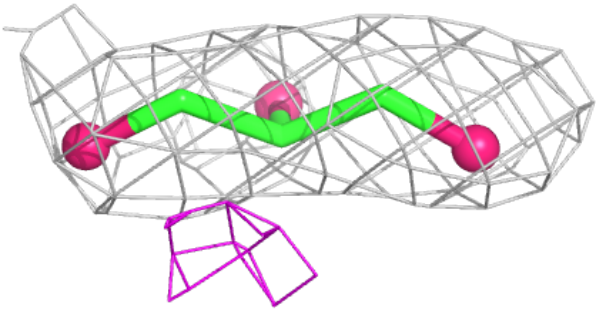
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

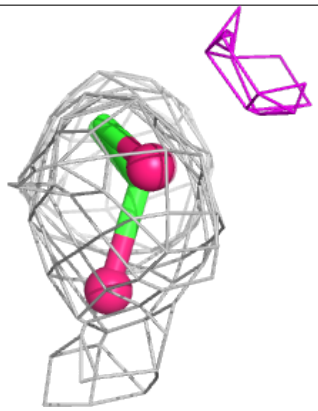


Electron density around GOL CCC 605:

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

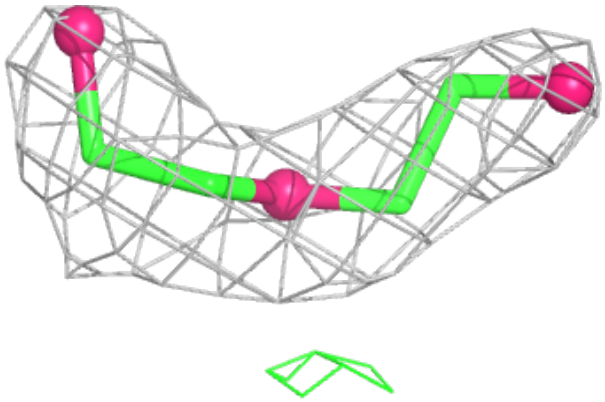


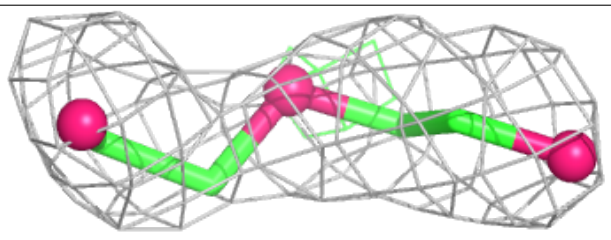


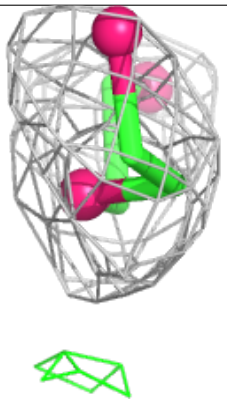


Electron density around PEG AAA 205:

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

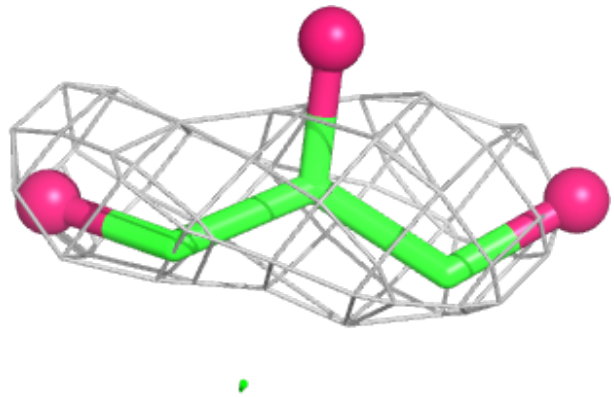


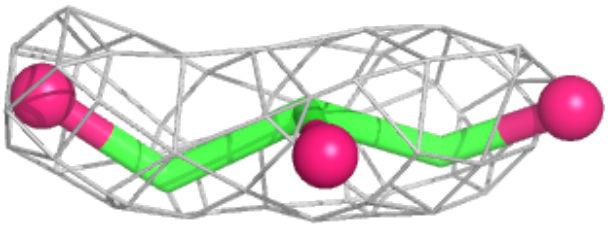


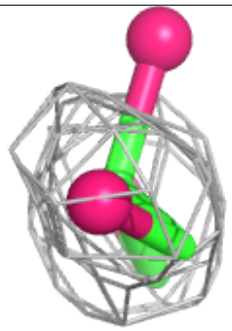


Electron density around GOL CCC 603:

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

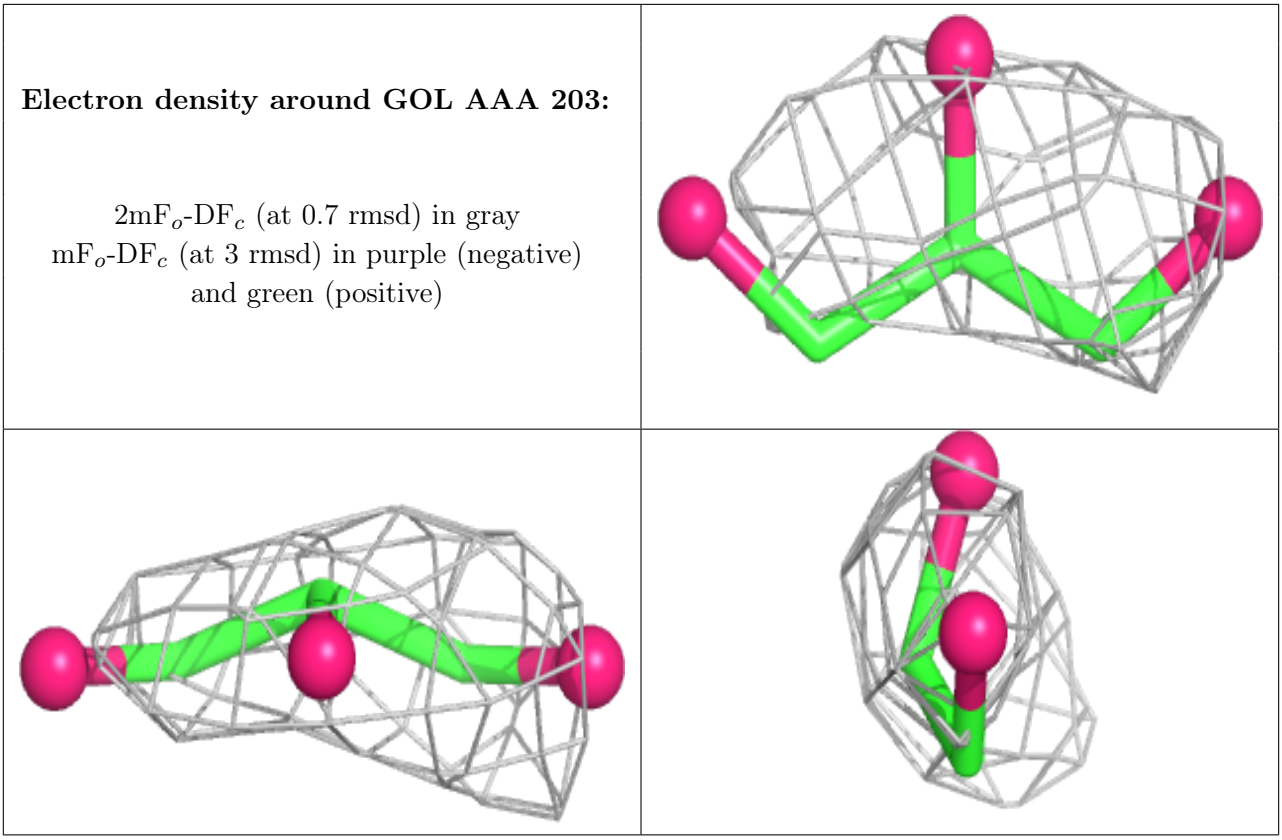






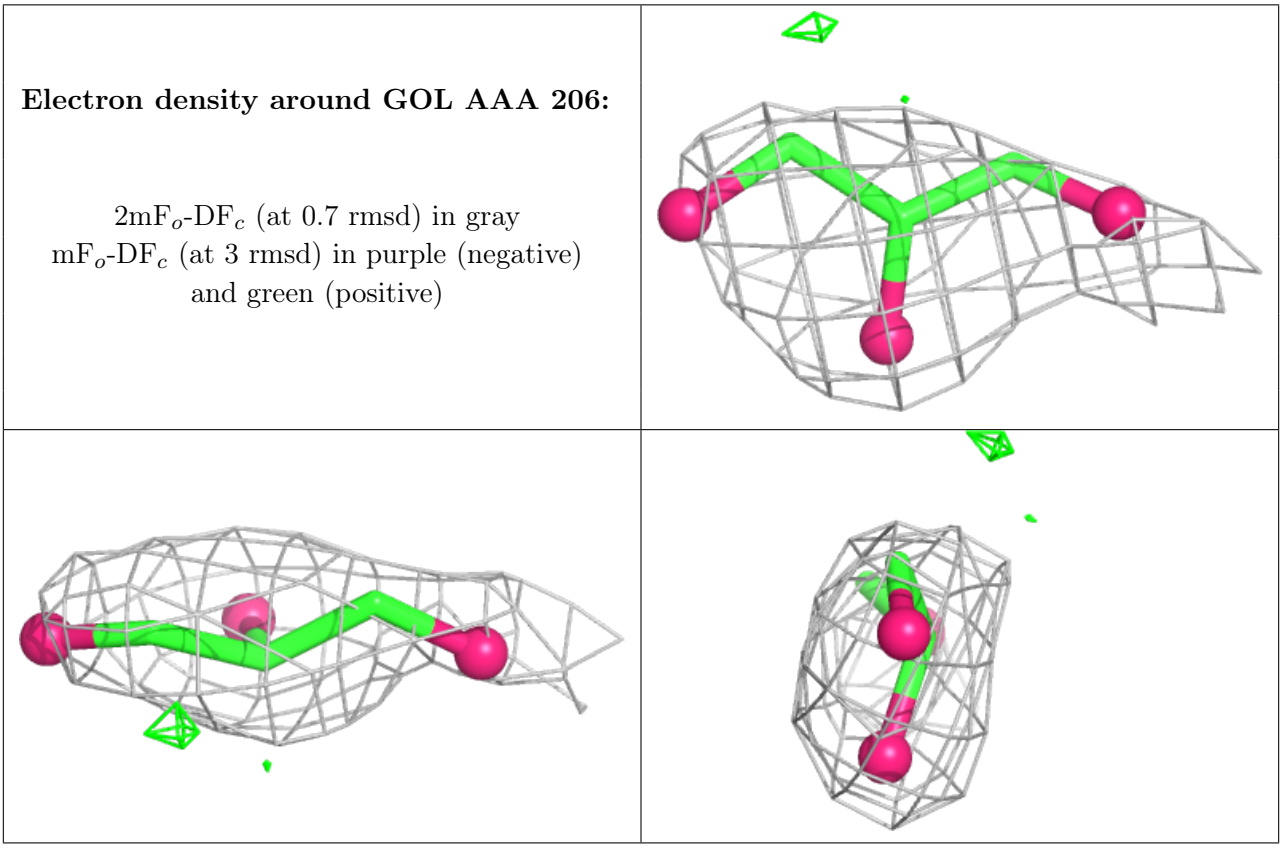
Electron density around GOL AAA 203:

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



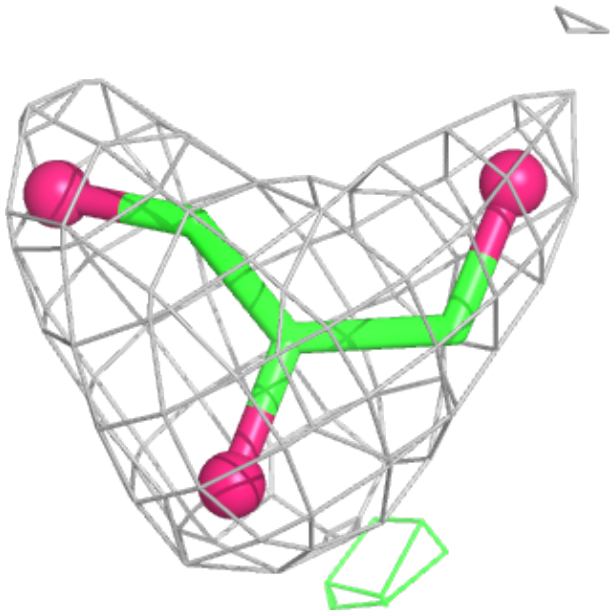
Electron density around GOL AAA 206:

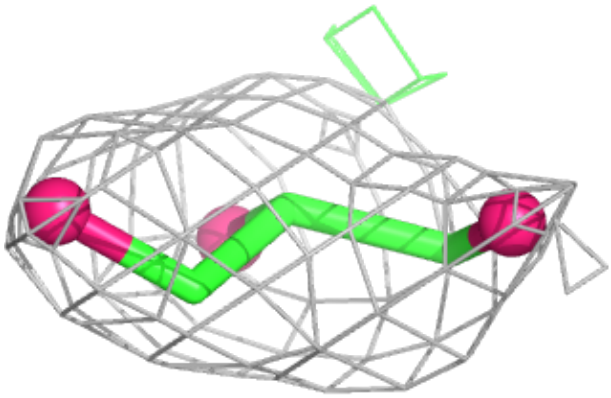
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

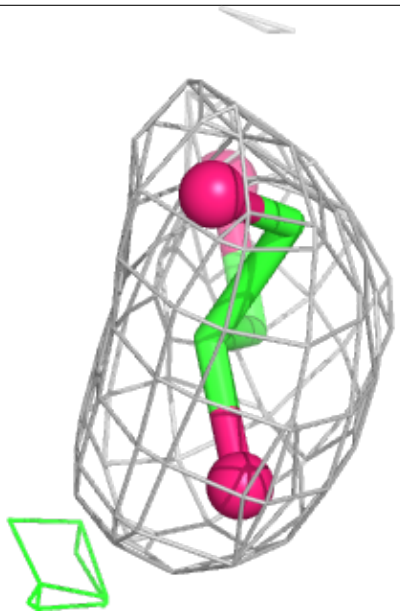


Electron density around GOL CCC 607:

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

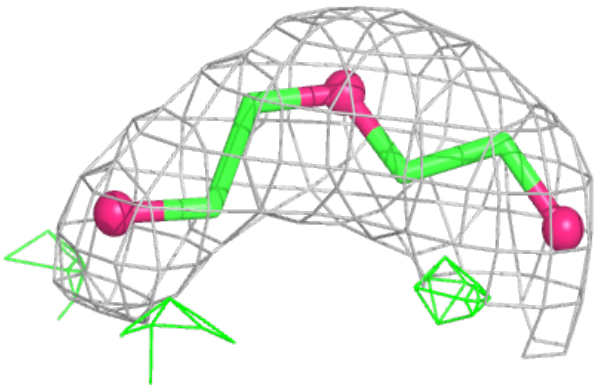


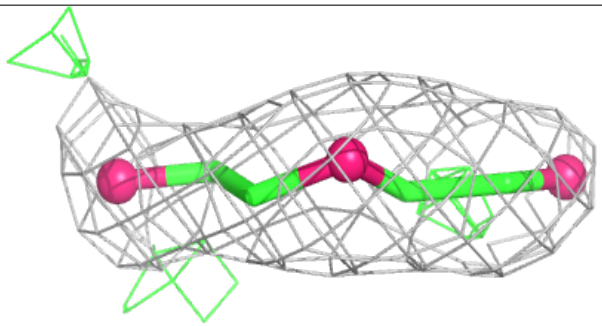


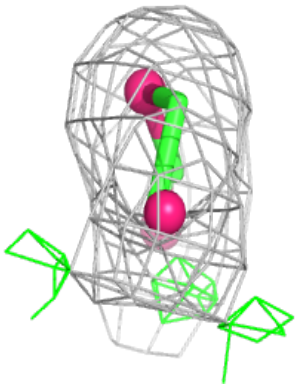


Electron density around PEG AAA 201:

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

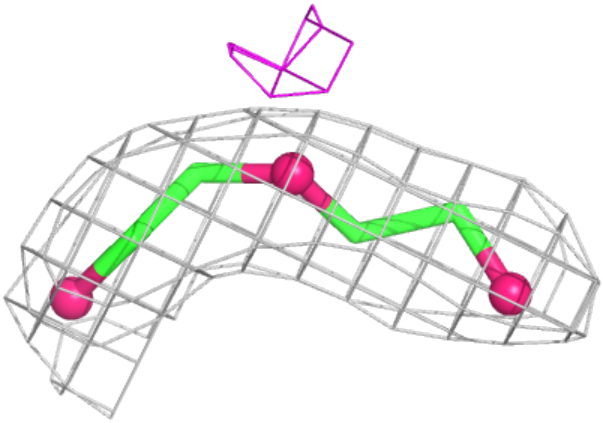


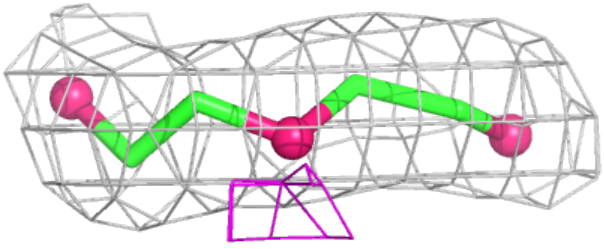


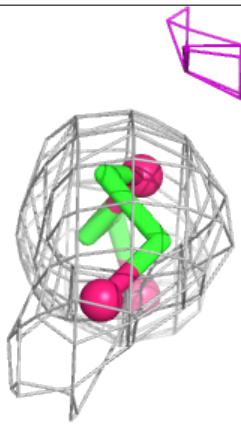


Electron density around PEG BBB 904:

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

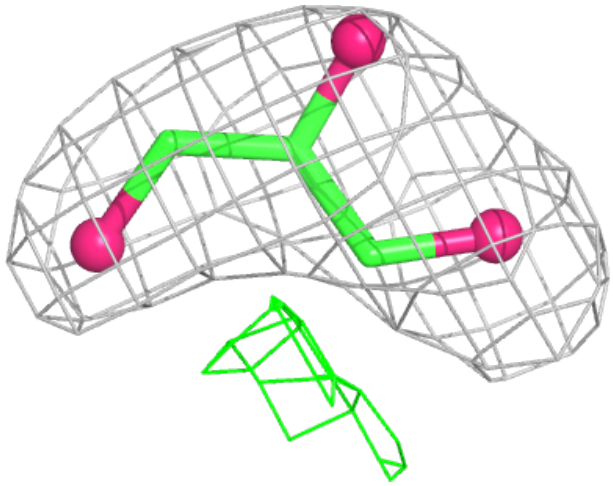


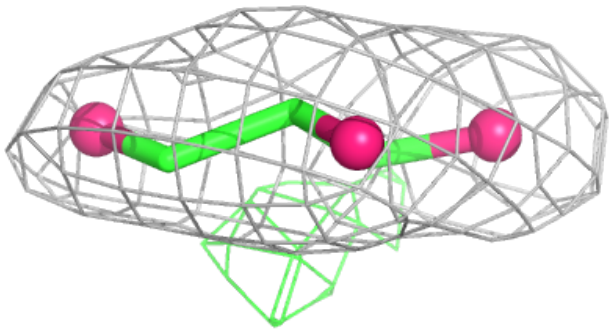


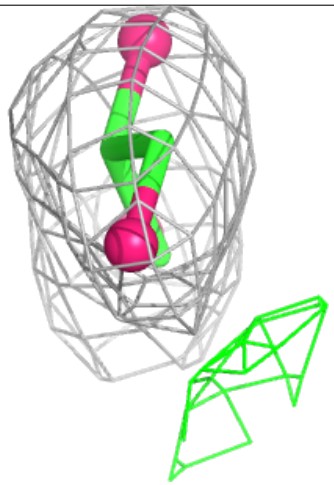


Electron density around GOL BBB 907:

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

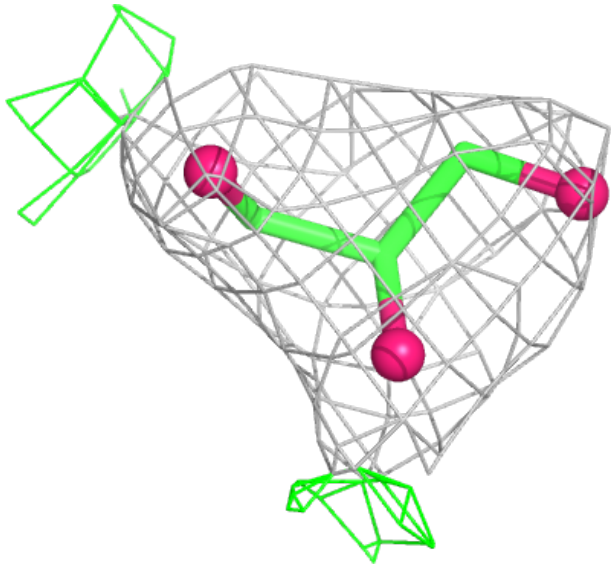


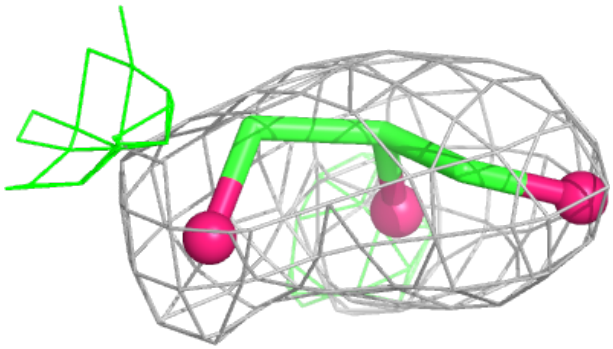


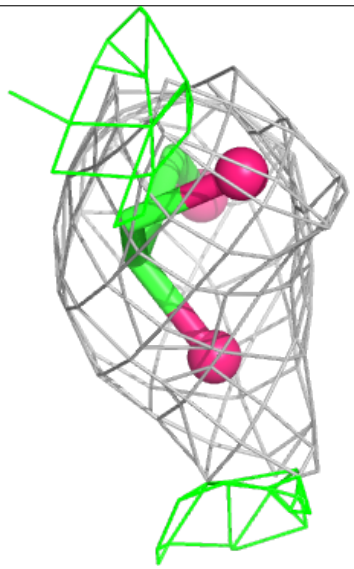


Electron density around GOL BBB 906:

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

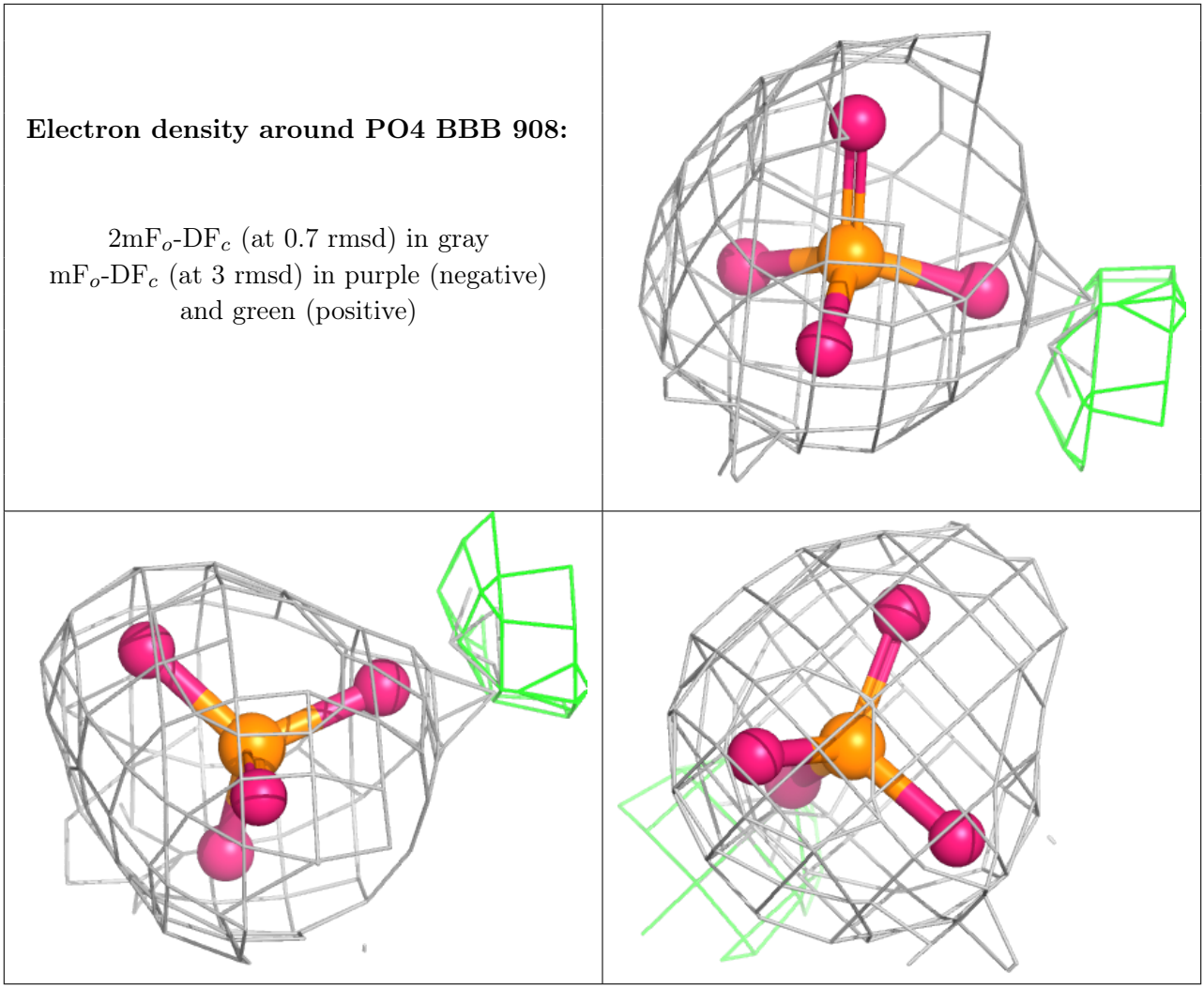






Electron density around PO4 BBB 908:

$2mF_o$-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

There are no such residues in this entry.