



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:43 am BST

PDB ID : 6HOS
Title : Structure of the KpFlo2 adhesin domain in complex with glycerol
Authors : Essen, L.-O.; Kock, M.; Veelders, M.
Deposited on : 2018-09-18
Resolution : 2.15 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

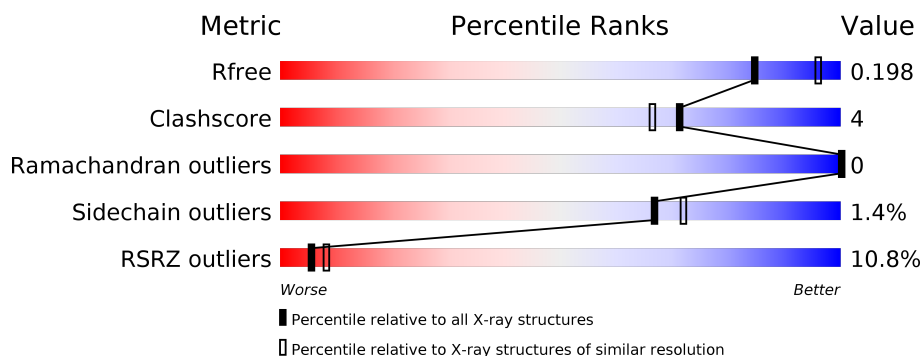
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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 $\leq 5\%$. 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	242	<div> <div>10%</div> <div>79%</div> <div>8%</div> <div>12%</div> </div>
1	B	242	<div> <div>9%</div> <div>83%</div> <div>5%</div> <div>13%</div> </div>
2	C	11	<div> <div>27%</div> <div>45%</div> <div>55%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3899 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 BA75_04148T0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	5	0
			1725	1096	271	350	8			
1	B	211	Total	C	N	O	S	0	7	0
			1710	1089	271	342	8			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP A0A1B2JGH2
A	13	GLY	-	expression tag	UNP A0A1B2JGH2
A	14	SER	-	expression tag	UNP A0A1B2JGH2
A	15	SER	-	expression tag	UNP A0A1B2JGH2
A	16	HIS	-	expression tag	UNP A0A1B2JGH2
A	17	HIS	-	expression tag	UNP A0A1B2JGH2
A	18	HIS	-	expression tag	UNP A0A1B2JGH2
A	19	HIS	-	expression tag	UNP A0A1B2JGH2
A	20	HIS	-	expression tag	UNP A0A1B2JGH2
A	21	HIS	-	expression tag	UNP A0A1B2JGH2
A	22	SER	-	expression tag	UNP A0A1B2JGH2
A	23	SER	-	expression tag	UNP A0A1B2JGH2
A	24	GLY	-	expression tag	UNP A0A1B2JGH2
A	25	LEU	-	expression tag	UNP A0A1B2JGH2
A	26	VAL	-	expression tag	UNP A0A1B2JGH2
A	27	PRO	-	expression tag	UNP A0A1B2JGH2
A	28	ARG	-	expression tag	UNP A0A1B2JGH2
A	29	GLY	-	expression tag	UNP A0A1B2JGH2
A	30	SER	-	expression tag	UNP A0A1B2JGH2
A	31	HIS	-	expression tag	UNP A0A1B2JGH2
A	32	MET	-	expression tag	UNP A0A1B2JGH2
B	12	MET	-	initiating methionine	UNP A0A1B2JGH2
B	13	GLY	-	expression tag	UNP A0A1B2JGH2
B	14	SER	-	expression tag	UNP A0A1B2JGH2
B	15	SER	-	expression tag	UNP A0A1B2JGH2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	16	HIS	-	expression tag	UNP A0A1B2JGH2
B	17	HIS	-	expression tag	UNP A0A1B2JGH2
B	18	HIS	-	expression tag	UNP A0A1B2JGH2
B	19	HIS	-	expression tag	UNP A0A1B2JGH2
B	20	HIS	-	expression tag	UNP A0A1B2JGH2
B	21	HIS	-	expression tag	UNP A0A1B2JGH2
B	22	SER	-	expression tag	UNP A0A1B2JGH2
B	23	SER	-	expression tag	UNP A0A1B2JGH2
B	24	GLY	-	expression tag	UNP A0A1B2JGH2
B	25	LEU	-	expression tag	UNP A0A1B2JGH2
B	26	VAL	-	expression tag	UNP A0A1B2JGH2
B	27	PRO	-	expression tag	UNP A0A1B2JGH2
B	28	ARG	-	expression tag	UNP A0A1B2JGH2
B	29	GLY	-	expression tag	UNP A0A1B2JGH2
B	30	SER	-	expression tag	UNP A0A1B2JGH2
B	31	HIS	-	expression tag	UNP A0A1B2JGH2
B	32	MET	-	expression tag	UNP A0A1B2JGH2

- Molecule 2 is a protein called Expression tag from chain B, or symmetry related chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	0	2	0
			106	62	29	15			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

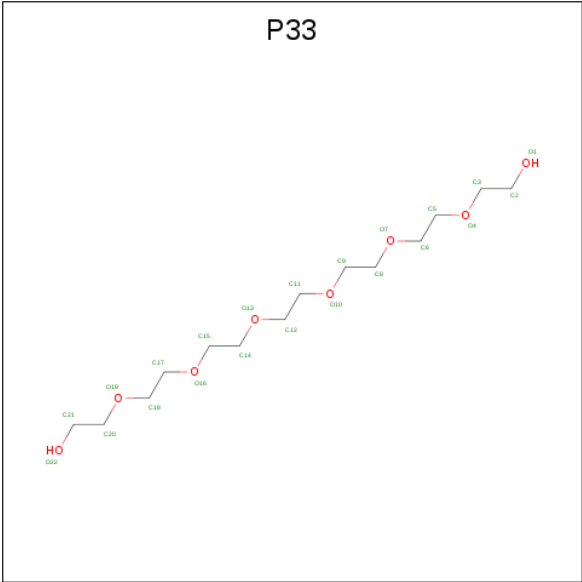
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by author).



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

- Molecule 5 is 3,6,9,12,15,18-HEXAOSAICOSANE-1,20-DIOL (three-letter code: P33) (formula: C₁₄H₃₀O₈).

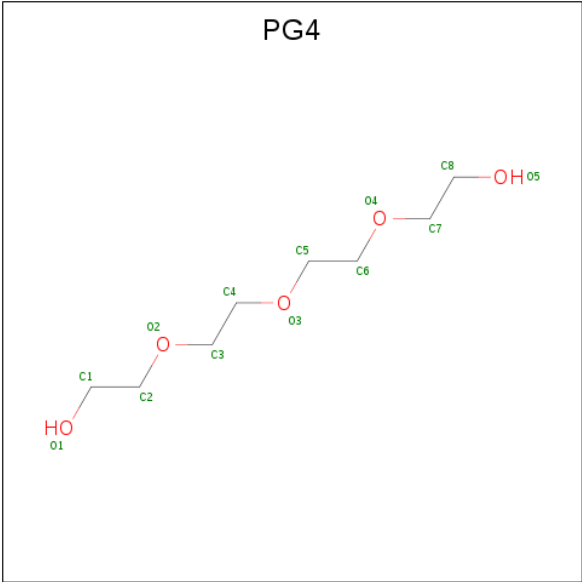


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			22	14	8		
5	A	1	Total	C	O	0	0
			22	14	8		
5	B	1	Total	C	O	0	0
			22	14	8		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Mg	0	0
			2	2		
6	A	2	Total	Mg	0	0
			2	2		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).

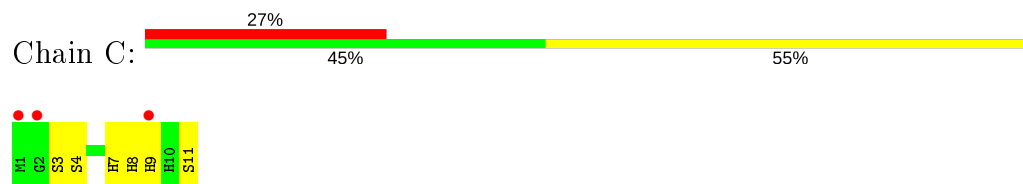
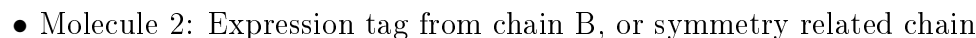


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	101	Total	O	0	1
			102	102		
8	B	107	Total	O	0	1
			108	108		
8	C	3	Total	O	0	0
			3	3		

- Molecule 1: BA75_04148T0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	79.94Å 103.19Å 72.10Å 90.00° 113.51° 90.00°	Depositor
Resolution (Å)	39.41 – 2.15 39.41 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.41-2.15) 100.0 (39.41-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.172 , 0.199 0.172 , 0.198	Depositor DCC
R_{free} test set	1005 reflections (3.44%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 69.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3899	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, GOL, MG, CA, P33

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	0.29	0/1778	0.50	0/2422
1	B	0.29	0/1769	0.51	0/2409
2	C	0.20	0/113	0.40	0/152
All	All	0.29	0/3660	0.50	0/4983

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1725	0	1582	16	0
1	B	1710	0	1578	7	0
2	C	106	0	73	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	24	0	31	2	0
4	B	36	0	47	1	0
5	A	44	0	60	3	0
5	B	22	0	30	1	0
6	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	2	0	0	0	0
7	B	13	0	18	0	0
8	A	102	0	0	2	0
8	B	108	0	0	1	0
8	C	3	0	0	1	0
All	All	3899	0	3419	25	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 4.

All (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLU:H	4:A:305:GOL:H11	1.39	0.86
1:A:161[B]:CYS:SG	8:A:476[B]:HOH:O	2.39	0.79
1:B:161[B]:CYS:SG	8:B:458[B]:HOH:O	2.42	0.77
1:A:41:SER:N	1:A:253:ALA:O	2.30	0.64
1:A:244:GLY:O	4:A:305:GOL:O2	2.19	0.59
1:A:111:LEU:HA	5:A:307:P33:H121	1.86	0.57
1:A:162[B]:CYS:SG	8:A:476[B]:HOH:O	2.58	0.57
1:A:99:PHE:HA	5:A:307:P33:H201	1.89	0.54
1:A:47:CYS:SG	1:A:161[B]:CYS:HB3	2.49	0.52
1:B:91:ILE:HD11	1:B:112:TYR:HB3	1.92	0.51
2:C:3:SER:N	8:C:101:HOH:O	2.45	0.49
1:B:47:CYS:SG	1:B:161[B]:CYS:HB3	2.53	0.48
1:A:98:GLY:O	5:A:307:P33:H172	2.16	0.46
1:A:91:ILE:HD11	1:A:112:TYR:HB3	1.95	0.46
2:C:7[A]:HIS:CE1	2:C:9:HIS:HB2	2.52	0.45
1:A:192:ASP:OD1	2:C:11:SER:HA	2.18	0.43
1:A:177:LEU:HD22	1:A:194:PHE:HB3	1.99	0.43
1:B:216:GLU:OE2	4:B:302:GOL:O2	2.13	0.43
1:B:167:ILE:H	5:B:307:P33:H21	1.84	0.42
1:A:218:HIS:CD2	1:A:218:HIS:H	2.38	0.42
1:A:151:LEU:HB3	1:A:177:LEU:HB2	2.02	0.42
1:B:77:PHE:HA	1:B:81:GLY:HA3	2.02	0.41
1:A:204:LYS:HD3	1:A:204:LYS:HA	1.90	0.41
1:A:146:ASP:HA	1:A:147:ASP:HA	1.81	0.40
1:B:192:ASP:HA	2:C:4:SER:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	216/242 (89%)	206 (95%)	10 (5%)	0	100	100
1	B	216/242 (89%)	207 (96%)	9 (4%)	0	100	100
2	C	11/11 (100%)	9 (82%)	2 (18%)	0	100	100
All	All	443/495 (90%)	422 (95%)	21 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	188/209 (90%)	186 (99%)	2 (1%)	73	78
1	B	186/209 (89%)	184 (99%)	2 (1%)	73	78
2	C	10/10 (100%)	9 (90%)	1 (10%)	7	4
All	All	384/428 (90%)	379 (99%)	5 (1%)	67	74

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	ASP
1	A	183	GLN
1	B	147	ASP
1	B	252	GLN
2	C	8	HIS

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

Mol	Chain	Res	Type
1	A	218	HIS
1	A	237	HIS
1	B	237	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	B	305	-	5,5,5	0.85	0	5,5,5	1.05	0
4	GOL	B	306	-	5,5,5	0.91	0	5,5,5	0.98	0
5	P33	A	307	-	21,21,21	0.55	0	20,20,20	0.21	0
4	GOL	A	304	-	5,5,5	0.89	0	5,5,5	1.04	0
4	GOL	B	302	3	5,5,5	0.86	0	5,5,5	1.00	0
4	GOL	B	303[A]	-	5,5,5	0.91	0	5,5,5	0.98	0
4	GOL	B	303[B]	-	5,5,5	0.88	0	5,5,5	0.99	0
5	P33	A	306	-	21,21,21	0.55	0	20,20,20	0.22	0
4	GOL	A	303	-	5,5,5	0.96	0	5,5,5	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	304	-	5,5,5	0.89	0	5,5,5	1.03	0
5	P33	B	307	-	21,21,21	0.54	0	20,20,20	0.19	0
7	PG4	B	310	-	12,12,12	0.52	0	11,11,11	0.21	0
4	GOL	A	305	-	5,5,5	1.00	0	5,5,5	0.95	0
4	GOL	A	302	3	5,5,5	0.87	0	5,5,5	1.03	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
4	GOL	B	305	-	-	0/4/4/4	-
4	GOL	B	306	-	-	1/4/4/4	-
5	P33	A	307	-	-	11/19/19/19	-
4	GOL	A	304	-	-	2/4/4/4	-
4	GOL	B	302	3	-	1/4/4/4	-
4	GOL	B	303[A]	-	-	4/4/4/4	-
4	GOL	B	303[B]	-	-	1/4/4/4	-
5	P33	A	306	-	-	11/19/19/19	-
4	GOL	A	303	-	-	4/4/4/4	-
4	GOL	B	304	-	-	4/4/4/4	-
5	P33	B	307	-	-	10/19/19/19	-
7	PG4	B	310	-	-	4/10/10/10	-
4	GOL	A	305	-	-	0/4/4/4	-
4	GOL	A	302	3	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	304	GOL	O1-C1-C2-C3
4	A	303	GOL	O2-C2-C3-O3
4	B	303[A]	GOL	O1-C1-C2-C3
4	B	303[A]	GOL	C1-C2-C3-O3
4	B	304	GOL	O1-C1-C2-C3
4	B	304	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	302	GOL	O1-C1-C2-C3
5	A	307	P33	O7-C8-C9-O10
5	A	306	P33	O7-C8-C9-O10
5	B	307	P33	O13-C14-C15-O16
5	A	307	P33	C5-C6-O7-C8
5	A	307	P33	O4-C5-C6-O7
5	A	306	P33	O13-C14-C15-O16
4	B	306	GOL	O1-C1-C2-C3
4	B	302	GOL	C1-C2-C3-O3
4	A	303	GOL	C1-C2-C3-O3
5	B	307	P33	O19-C20-C21-O22
4	B	303[A]	GOL	O1-C1-C2-O2
4	B	304	GOL	O1-C1-C2-O2
4	A	302	GOL	O1-C1-C2-O2
5	B	307	P33	O10-C11-C12-O13
5	A	306	P33	O16-C17-C18-O19
5	A	306	P33	O10-C11-C12-O13
5	A	306	P33	O19-C20-C21-O22
4	A	304	GOL	O1-C1-C2-O2
5	A	307	P33	O13-C14-C15-O16
5	B	307	P33	C9-C8-O7-C6
7	B	310	PG4	O3-C5-C6-O4
4	A	303	GOL	O1-C1-C2-O2
4	B	304	GOL	O2-C2-C3-O3
5	A	306	P33	C9-C8-O7-C6
5	A	307	P33	C9-C8-O7-C6
5	A	307	P33	C18-C17-O16-C15
4	B	303[A]	GOL	O2-C2-C3-O3
5	B	307	P33	C17-C18-O19-C20
5	A	307	P33	C12-C11-O10-C9
5	B	307	P33	C5-C6-O7-C8
5	B	307	P33	C6-C5-O4-C3
5	A	307	P33	C14-C15-O16-C17
5	A	306	P33	C18-C17-O16-C15
5	B	307	P33	O4-C5-C6-O7
5	A	306	P33	C6-C5-O4-C3
5	A	306	P33	C2-C3-O4-C5
5	A	306	P33	C17-C18-O19-C20
5	A	307	P33	O16-C17-C18-O19
5	A	306	P33	C14-C15-O16-C17
5	B	307	P33	C2-C3-O4-C5
5	B	307	P33	C18-C17-O16-C15

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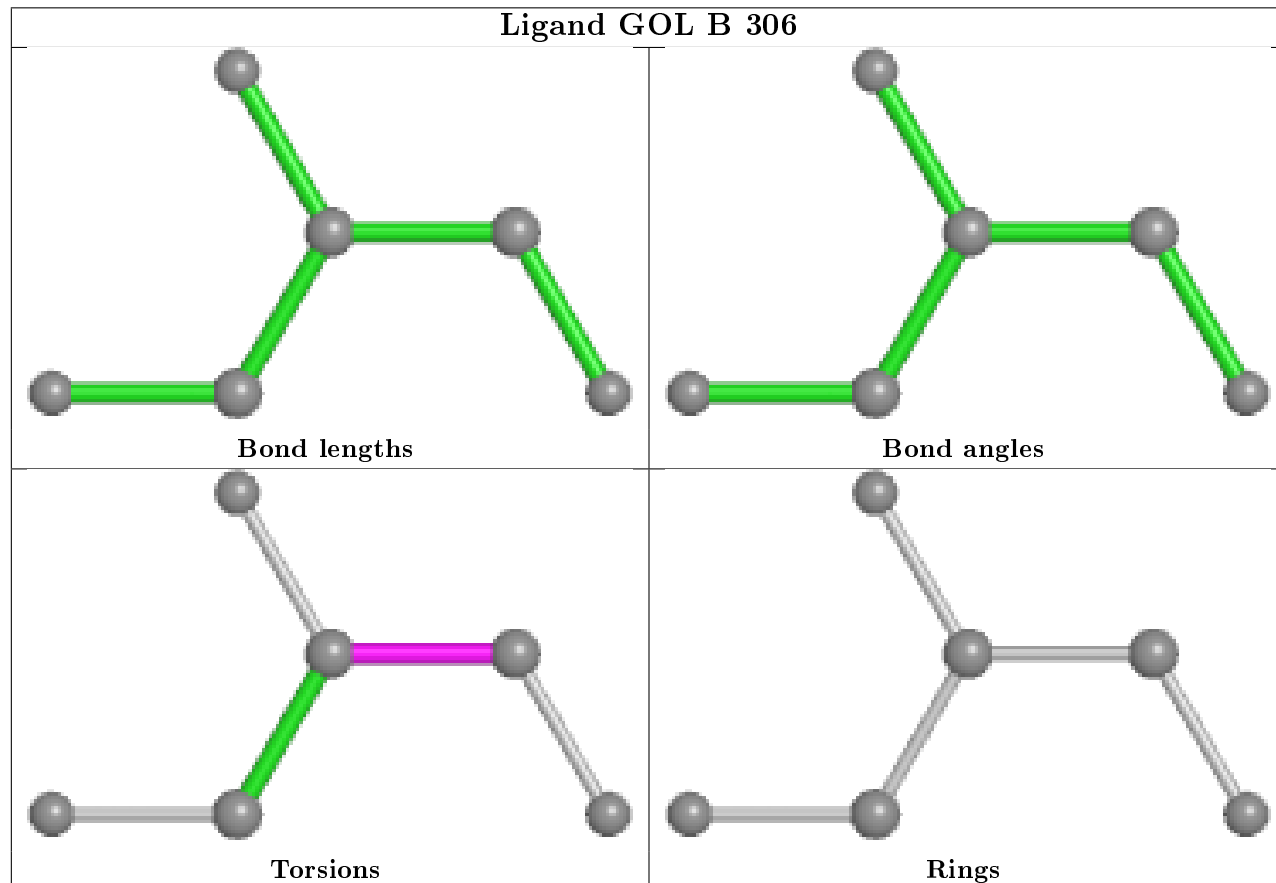
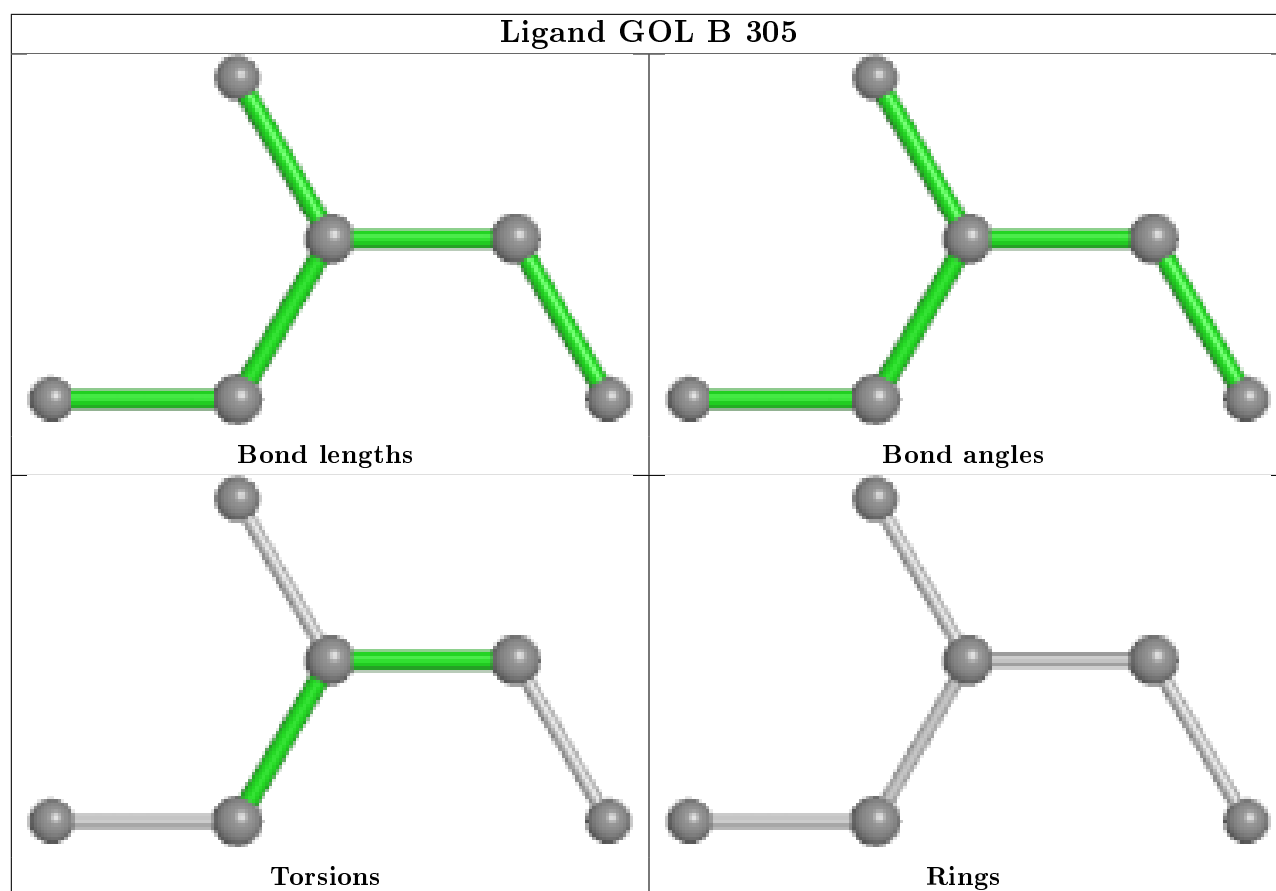
Mol	Chain	Res	Type	Atoms
7	B	310	PG4	C1-C2-O2-C3
7	B	310	PG4	C3-C4-O3-C5
7	B	310	PG4	O4-C7-C8-O5
4	B	303[B]	GOL	O1-C1-C2-C3
4	A	303	GOL	O1-C1-C2-C3
5	A	307	P33	C17-C18-O19-C20
5	A	307	P33	O10-C11-C12-O13

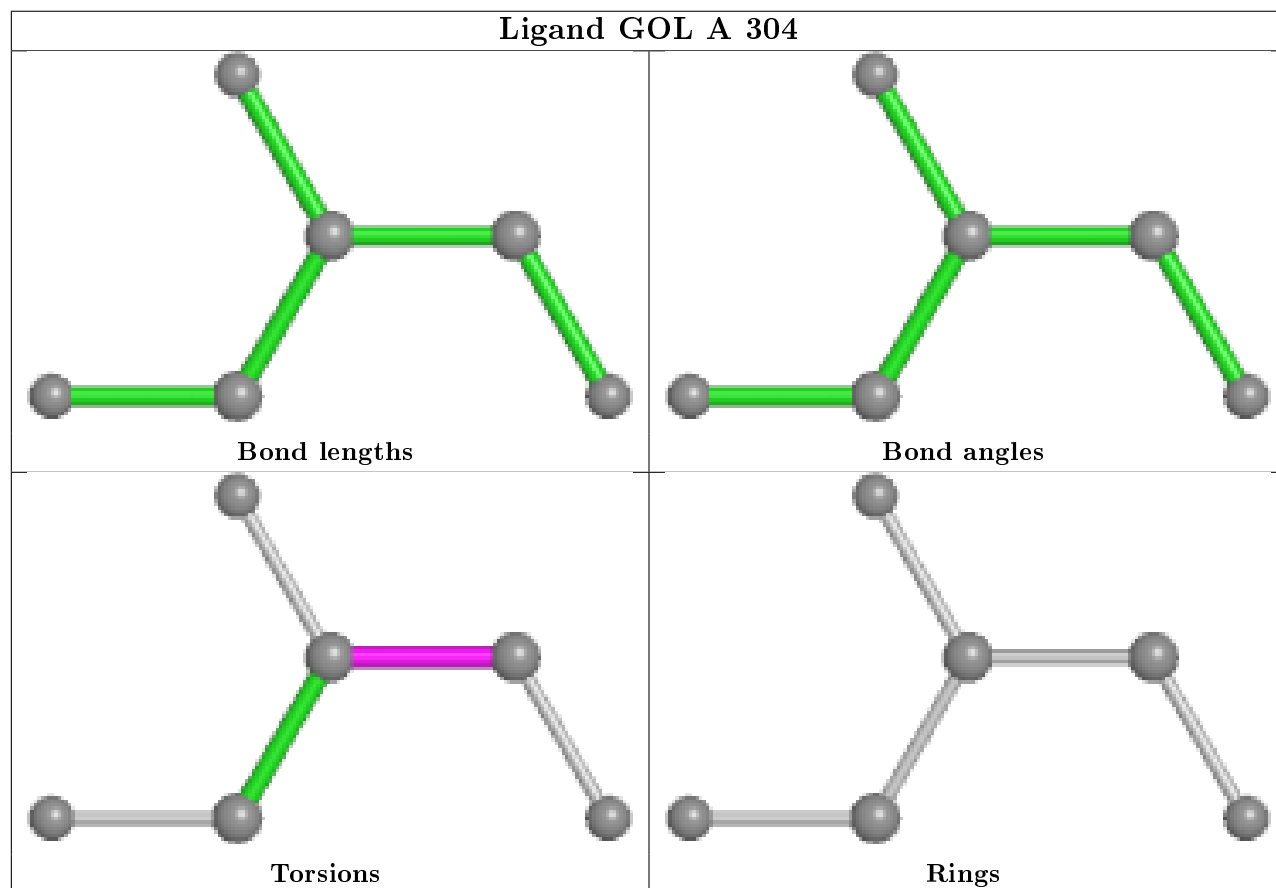
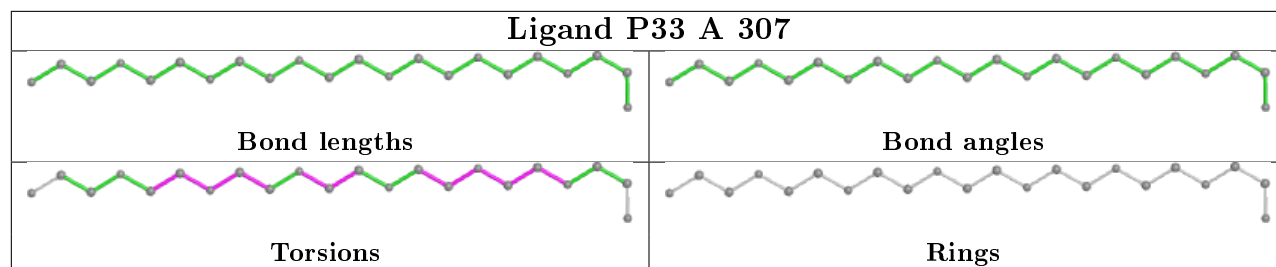
There are no ring outliers.

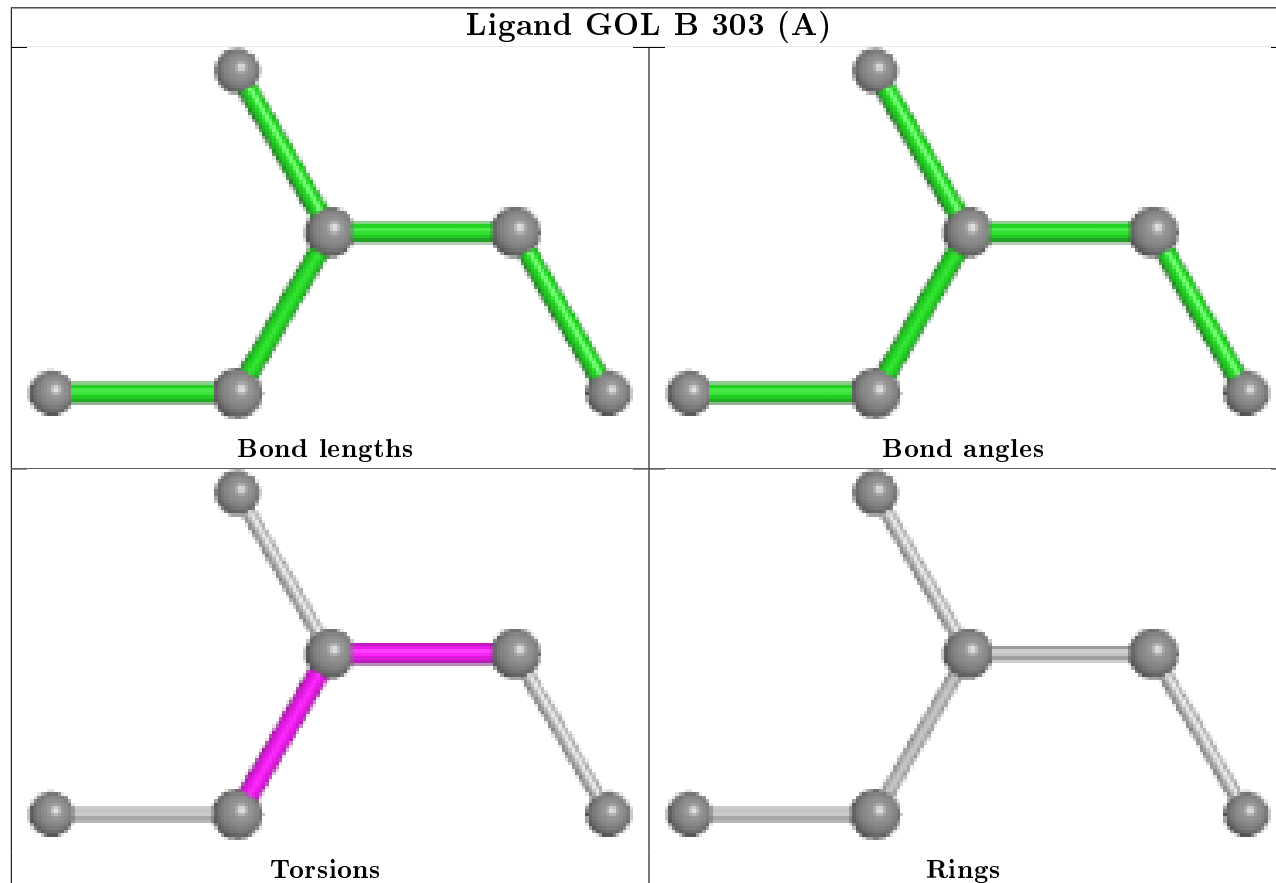
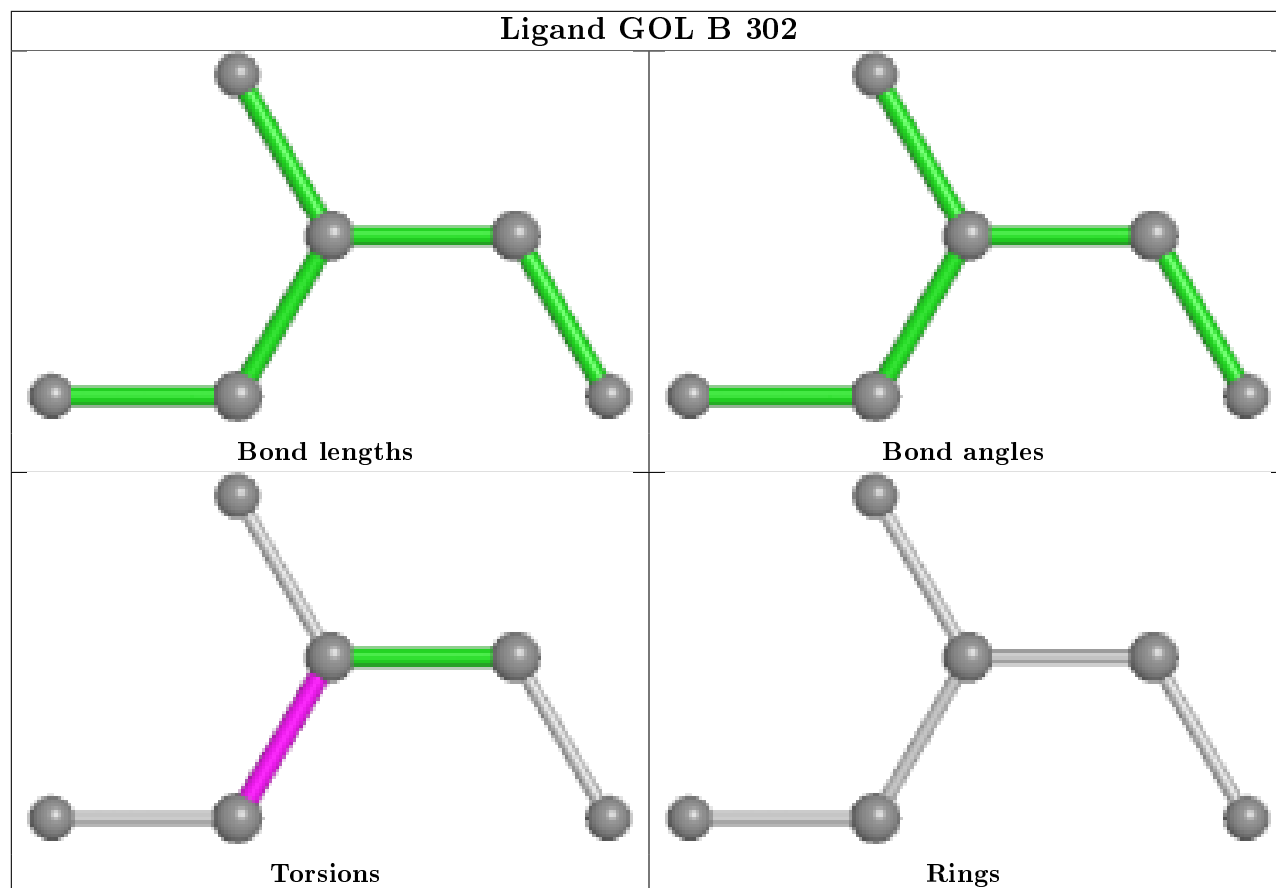
4 monomers are involved in 7 short contacts:

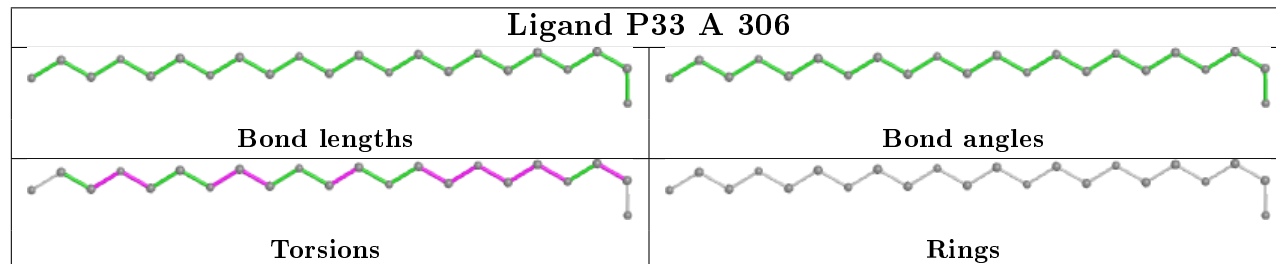
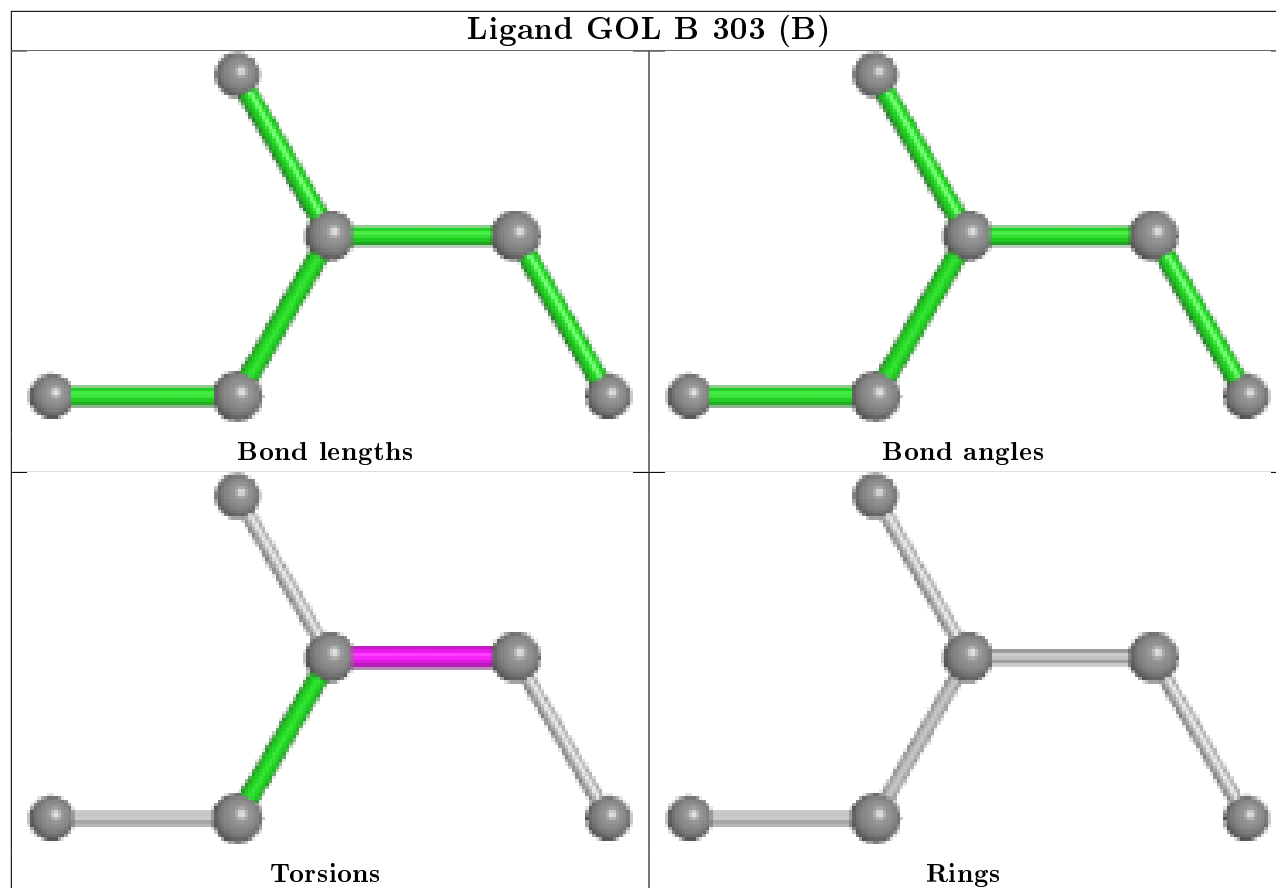
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	307	P33	3	0
4	B	302	GOL	1	0
5	B	307	P33	1	0
4	A	305	GOL	2	0

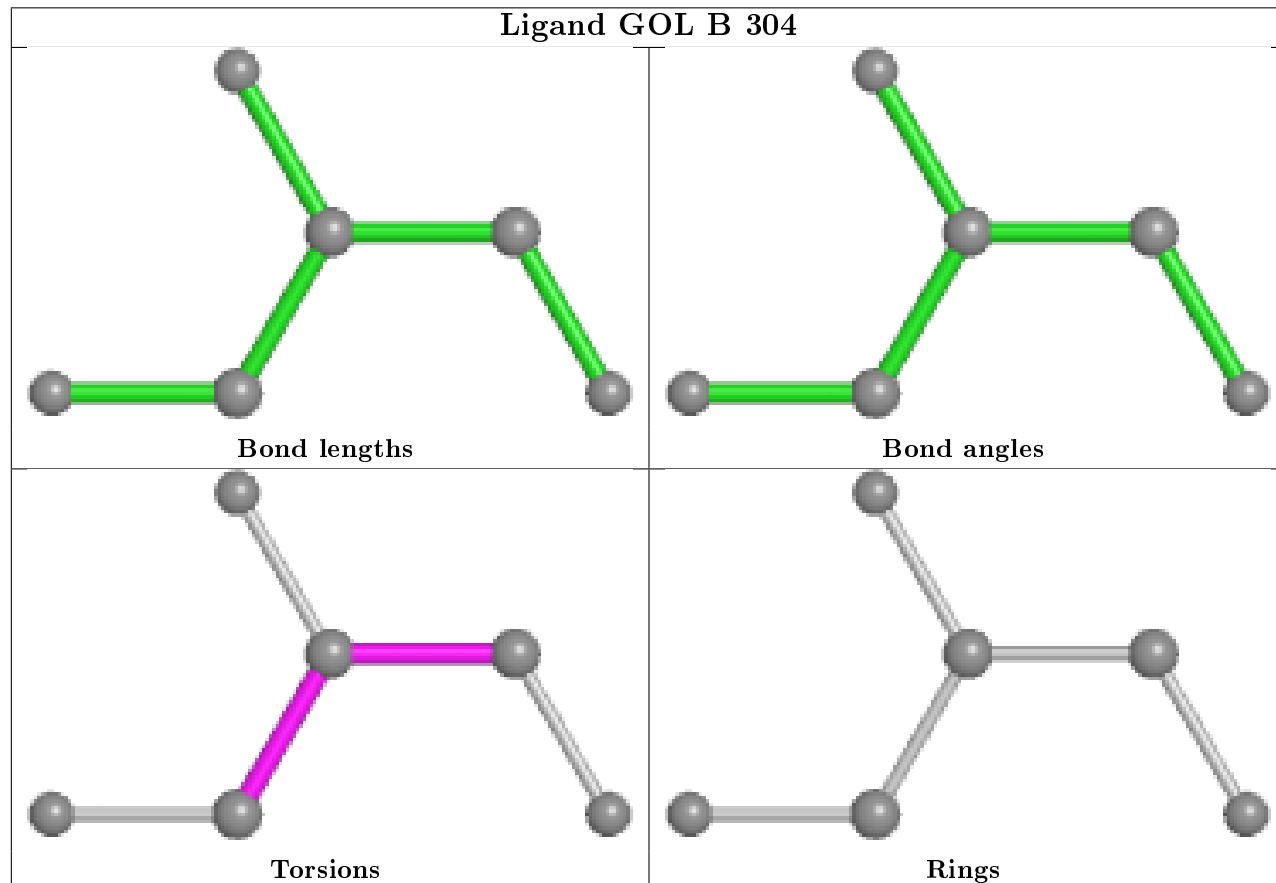
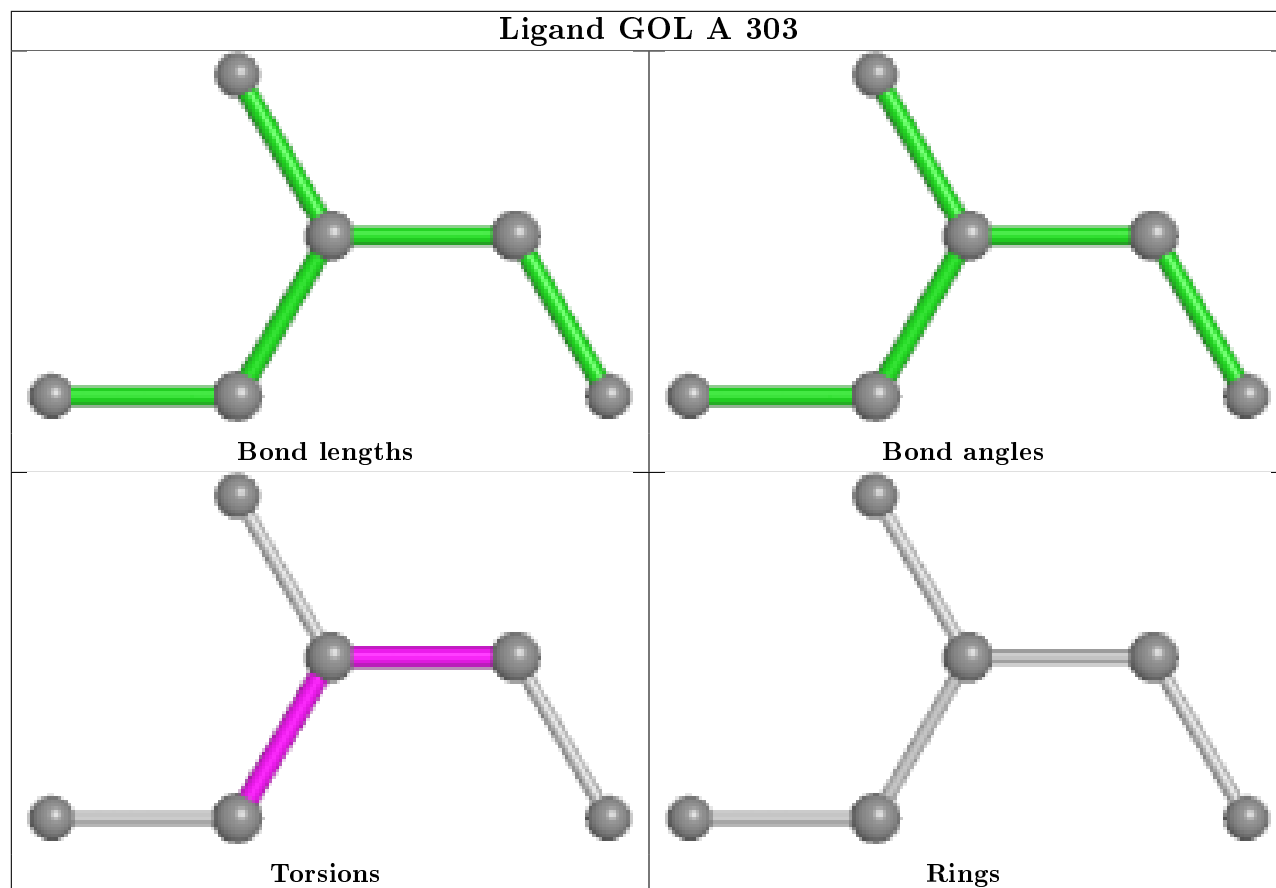
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

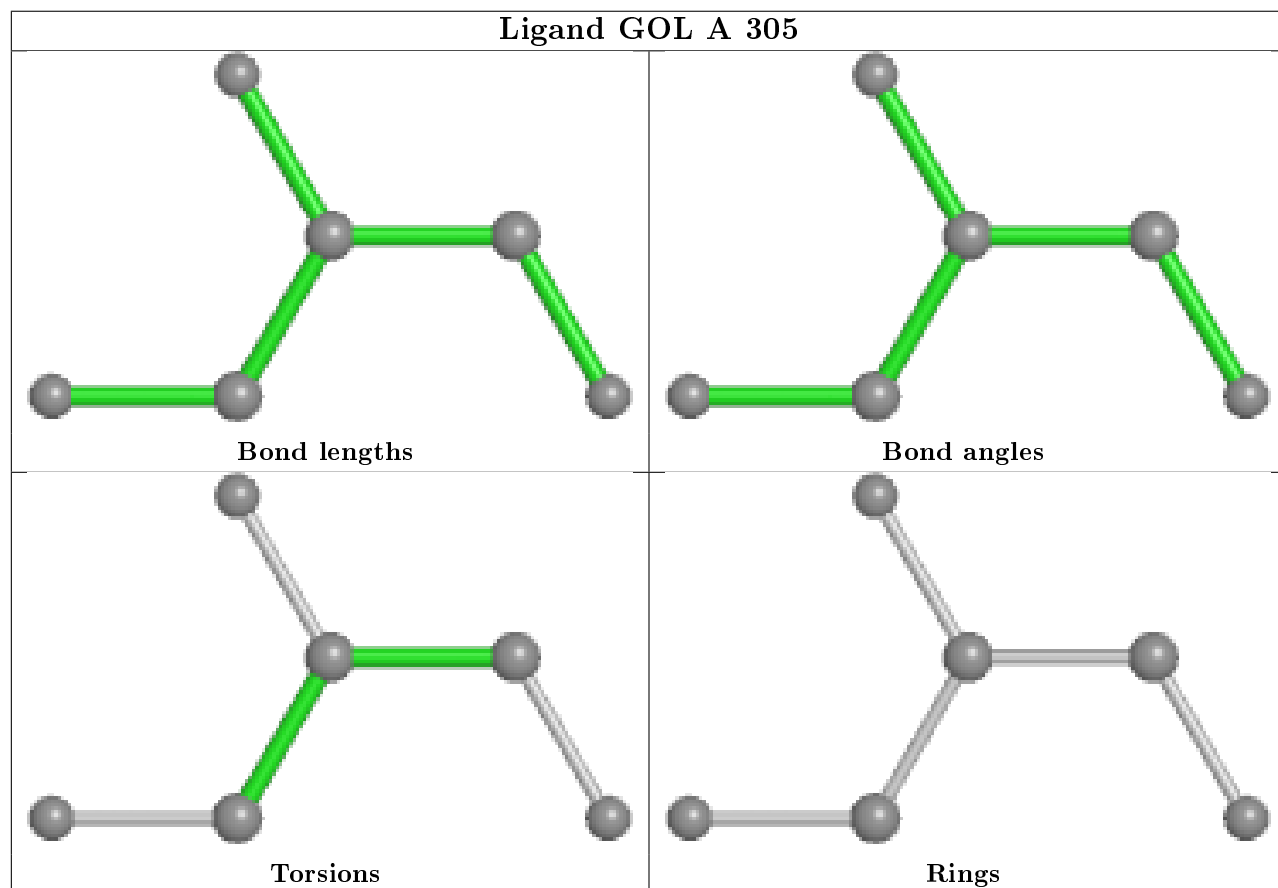
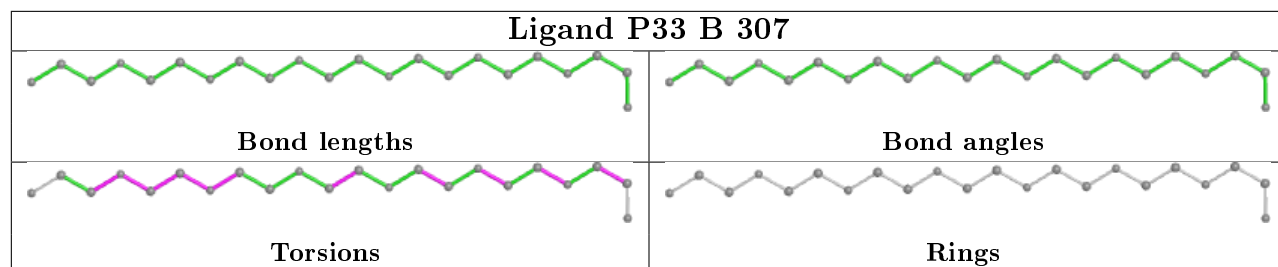


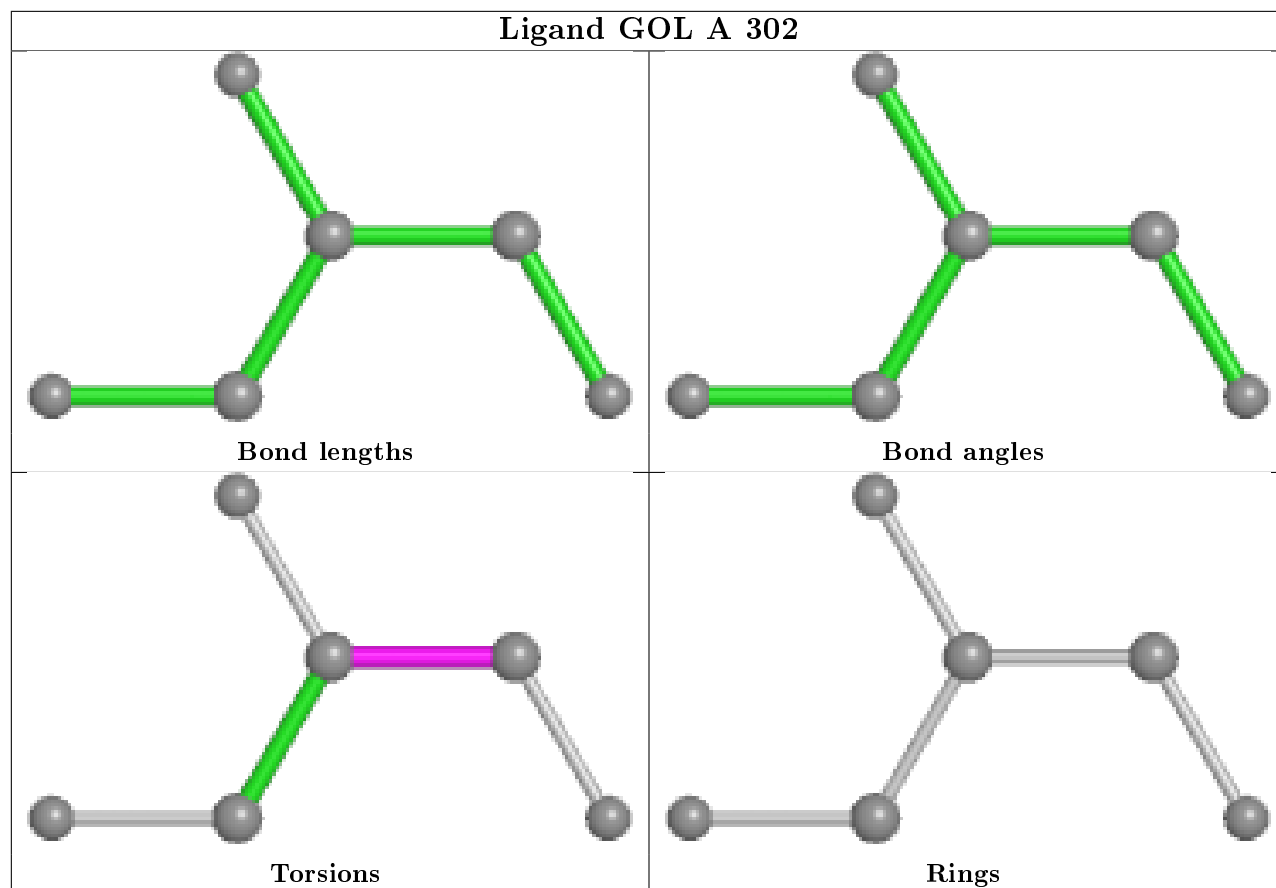












5.7 Other polymers [i](#)

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, 95th 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	213/242 (88%)	0.44	23 (10%) 5 8	22, 40, 95, 127	0
1	B	211/242 (87%)	0.45	21 (9%) 7 11	22, 39, 78, 153	0
2	C	11/11 (100%)	1.68	3 (27%) 0 0	39, 50, 87, 108	0
All	All	435/495 (87%)	0.47	47 (10%) 5 8	22, 40, 87, 153	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	185	GLY	7.7
1	B	186	ASP	7.1
1	A	186	ASP	7.1
2	C	1	MET	6.6
1	B	253	ALA	5.9
1	A	253	ALA	5.6
1	A	42	ASP	5.5
1	A	185	GLY	4.4
1	B	247	ASP	4.2
1	A	247	ASP	4.1
1	B	252	GLN	4.1
1	A	249	GLU	4.0
1	A	252	GLN	3.5
1	A	105	GLY	3.5
1	B	249	GLU	3.4
1	A	246	LEU	3.3
1	A	187	GLU	3.2
1	A	107	PRO	3.2
1	B	104	PRO	3.2
1	A	248	GLU	3.2
1	B	76	VAL	3.2
1	A	184	GLU	3.1
1	B	105	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	162[A]	CYS	3.0
1	A	104	PRO	2.9
1	A	41	SER	2.8
1	A	44	ALA	2.7
1	B	246	LEU	2.7
1	B	188	THR	2.7
1	B	248	GLU	2.6
1	A	251	CYS	2.6
1	B	187	GLU	2.6
1	B	75	PRO	2.6
1	B	162[A]	CYS	2.6
1	B	250	GLN	2.4
1	B	135	SER	2.4
2	C	2	GLY	2.4
1	B	73[A]	ARG	2.3
1	A	188	THR	2.3
1	B	107	PRO	2.2
1	B	172[A]	SER	2.2
1	A	250	GLN	2.1
1	A	245	ALA	2.1
1	B	251	CYS	2.1
1	A	75	PRO	2.1
1	A	73	ARG	2.0
2	C	9	HIS	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 carbohydrates in this entry.

6.4 Ligands [i](#)

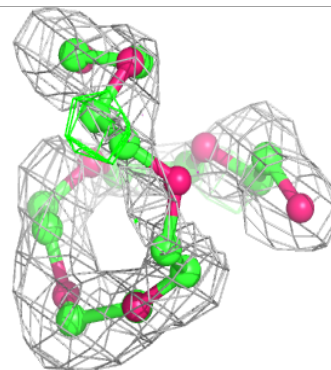
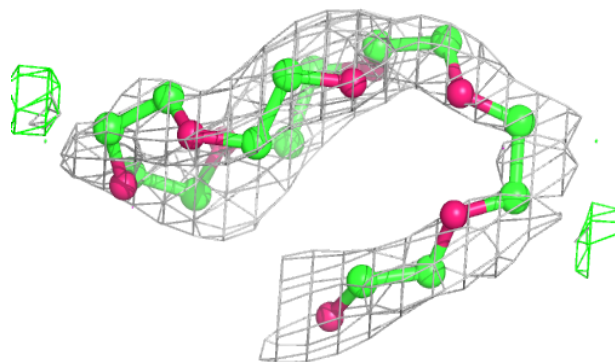
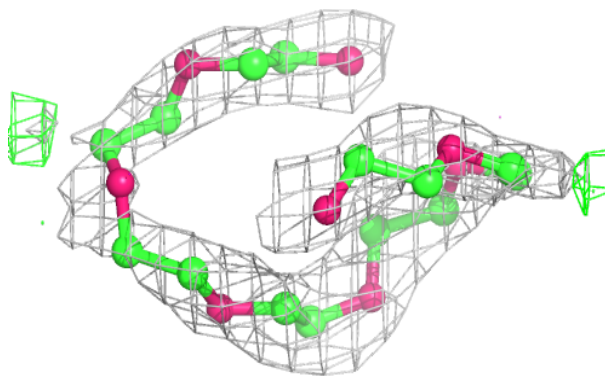
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	P33	A	306	22/22	0.58	0.29	81,82,83,84	22
5	P33	B	307	22/22	0.60	0.26	76,81,83,84	22
4	GOL	B	305	6/6	0.65	0.24	71,76,79,84	0
7	PG4	B	310	13/13	0.71	0.19	68,74,89,90	0
5	P33	A	307	22/22	0.72	0.28	81,89,95,96	0
6	MG	A	309	1/1	0.74	0.11	82,82,82,82	0
4	GOL	A	305	6/6	0.77	0.30	68,72,72,74	6
6	MG	B	308	1/1	0.81	0.06	76,76,76,76	0
4	GOL	A	302	6/6	0.81	0.23	74,79,81,84	0
4	GOL	B	306	6/6	0.82	0.28	83,83,84,86	0
4	GOL	B	304	6/6	0.83	0.38	66,68,72,75	0
4	GOL	A	303	6/6	0.85	0.16	63,66,67,72	0
4	GOL	B	302	6/6	0.85	0.20	48,62,69,74	6
4	GOL	B	303[B]	6/6	0.88	0.47	75,77,77,78	6
4	GOL	B	303[A]	6/6	0.88	0.47	74,77,77,77	6
4	GOL	A	304	6/6	0.89	0.15	85,88,90,91	0
6	MG	A	308	1/1	0.93	0.06	54,54,54,54	0
6	MG	B	309	1/1	0.95	0.11	81,81,81,81	0
3	CA	A	301	1/1	0.98	0.05	40,40,40,40	0
3	CA	B	301	1/1	0.98	0.05	36,36,36,36	1

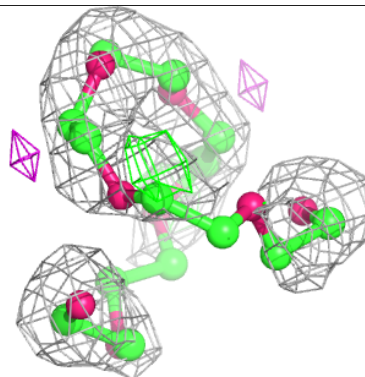
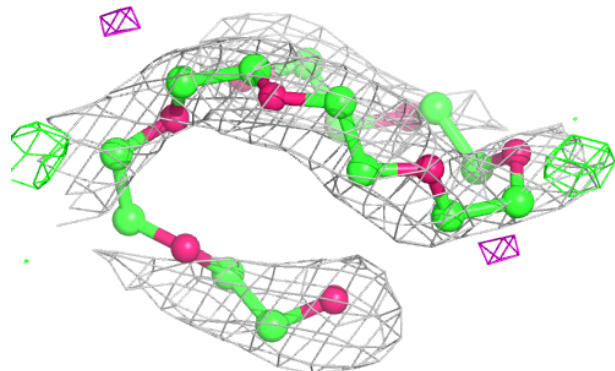
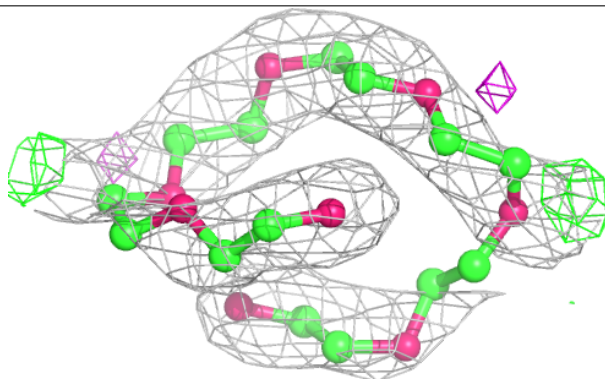
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P33 A 306:

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

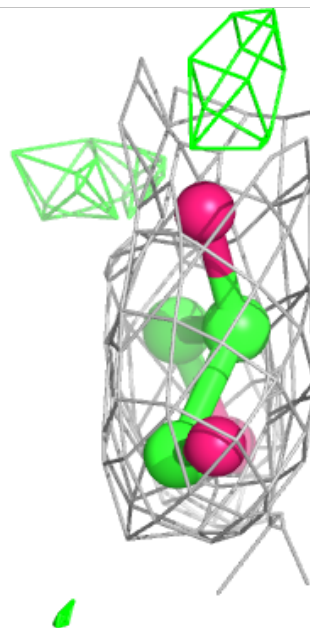
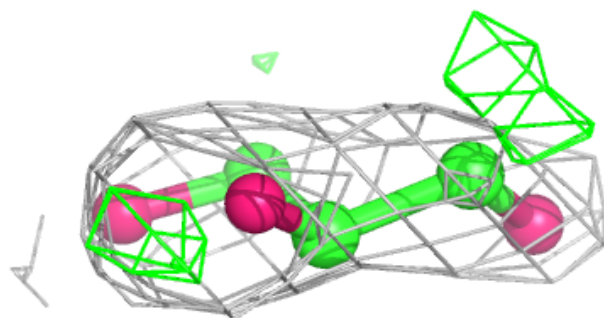
**Electron density around P33 B 307:**

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



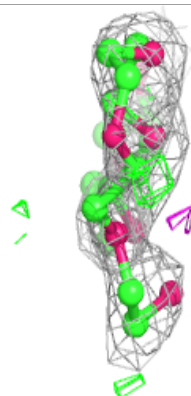
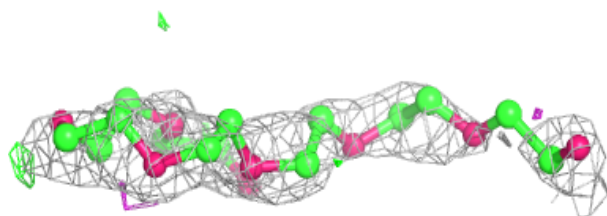
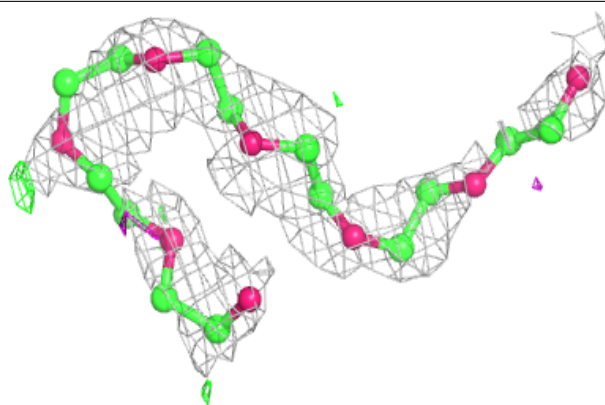
Electron density around GOL B 305:

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

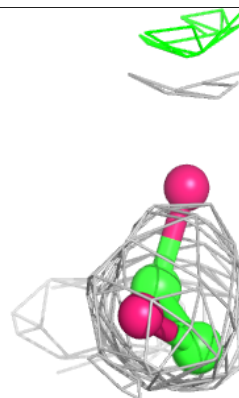
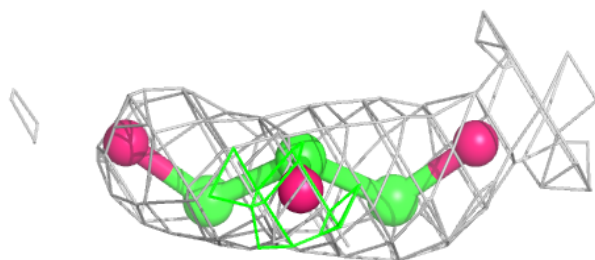
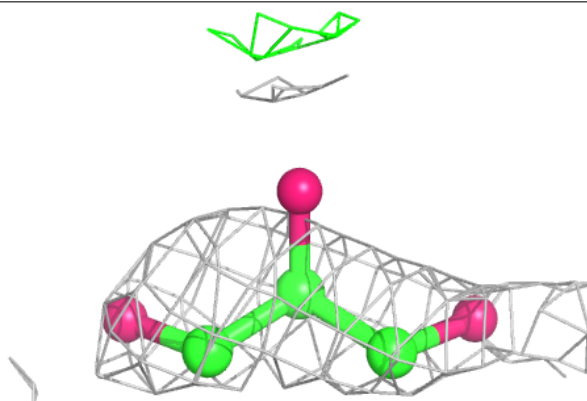


Electron density around P33 A 307:

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

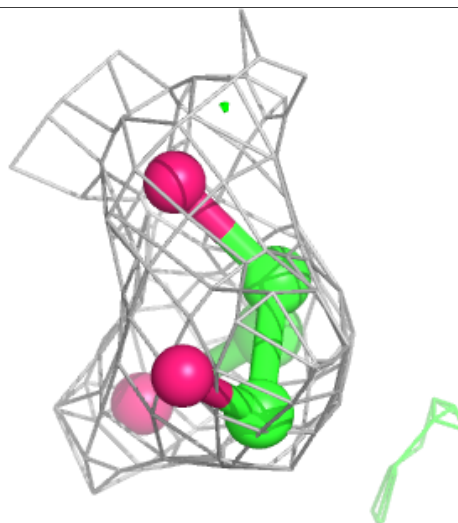
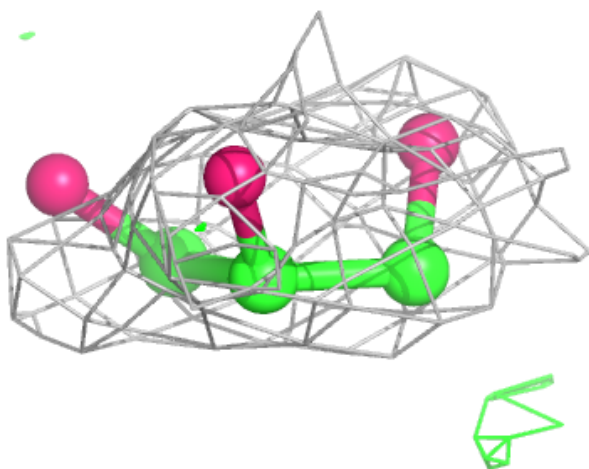
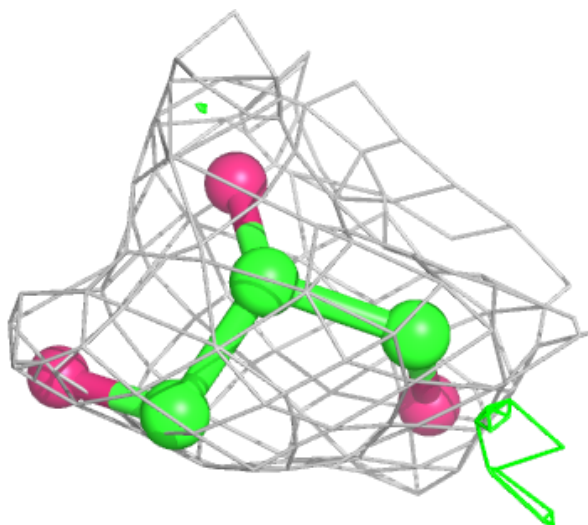
**Electron density around GOL A 305:**

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



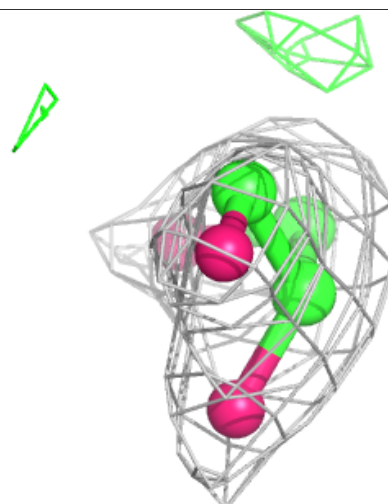
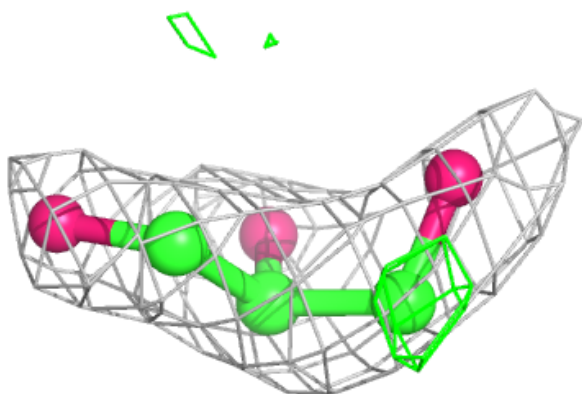
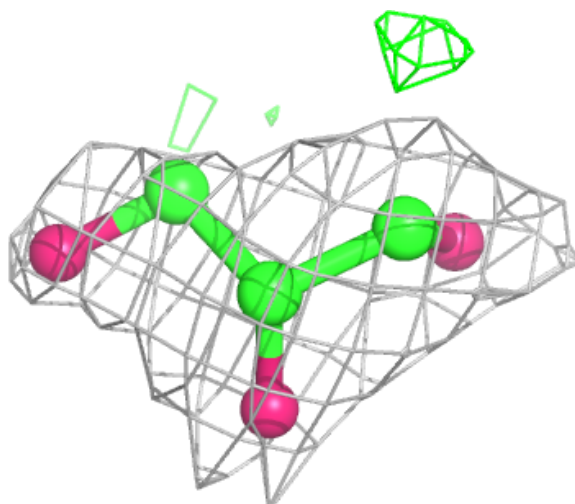
Electron density around GOL A 302:

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



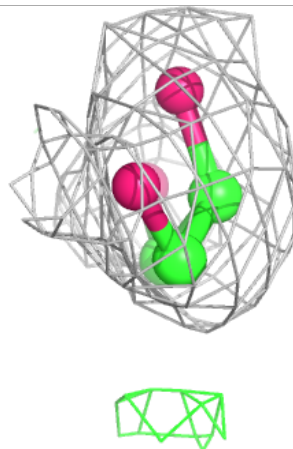
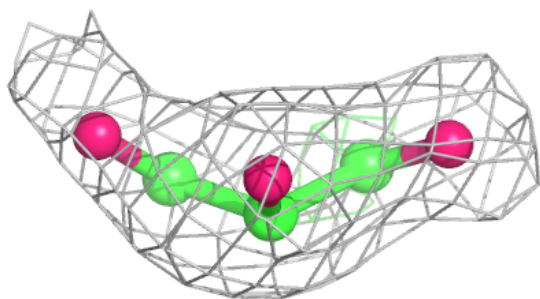
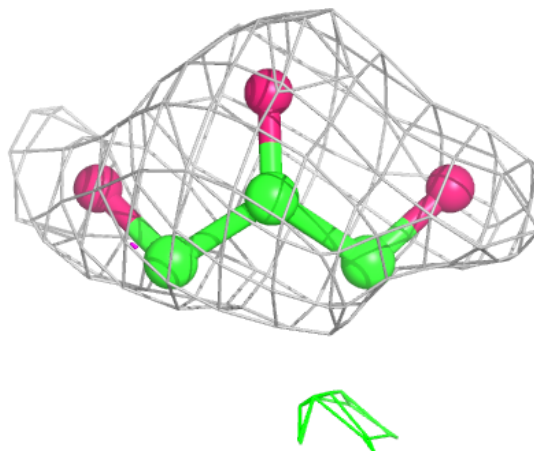
Electron density around GOL B 306:

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



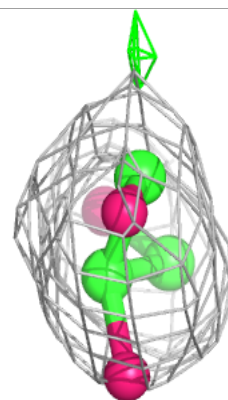
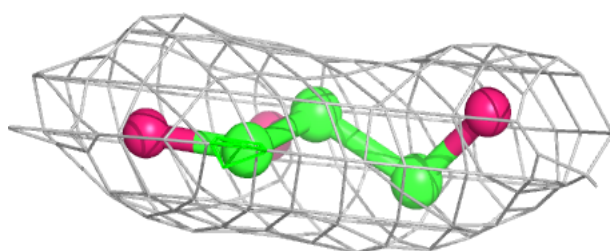
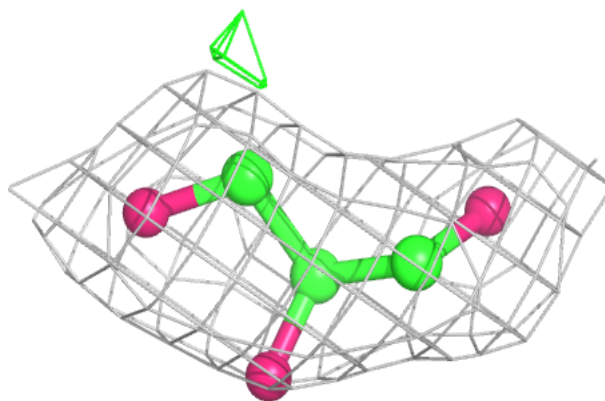
Electron density around GOL B 304:

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



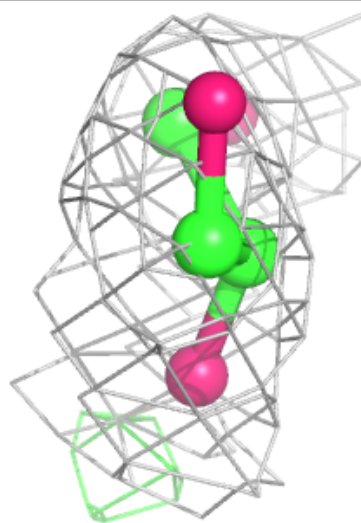
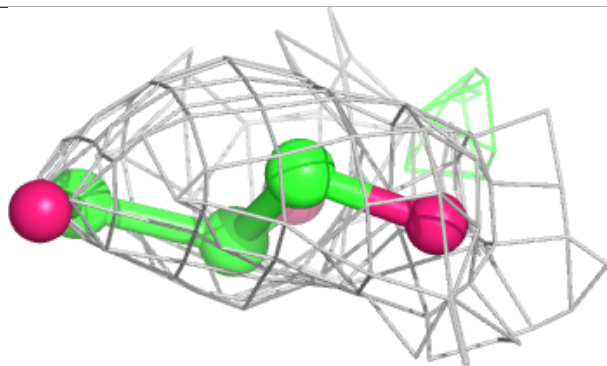
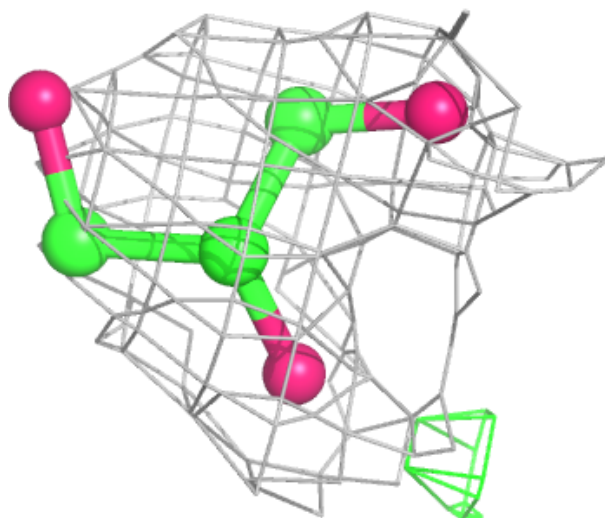
Electron density around GOL A 303:

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



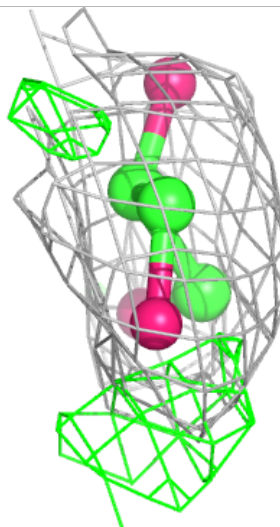
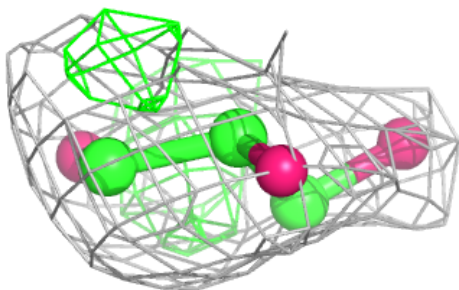
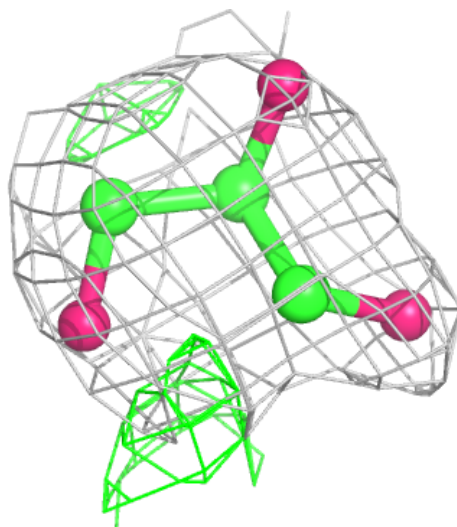
Electron density around GOL B 302:

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



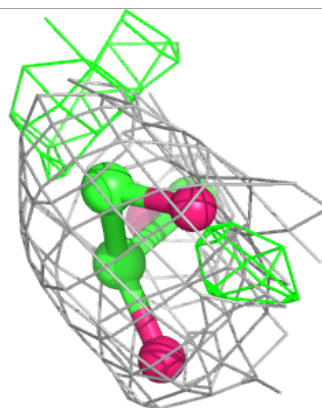
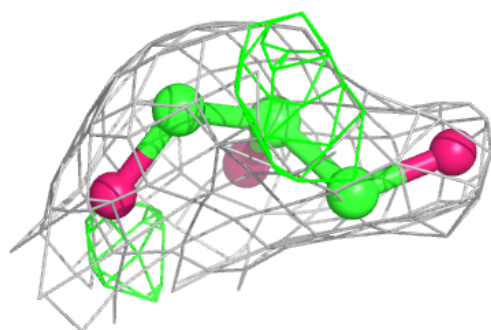
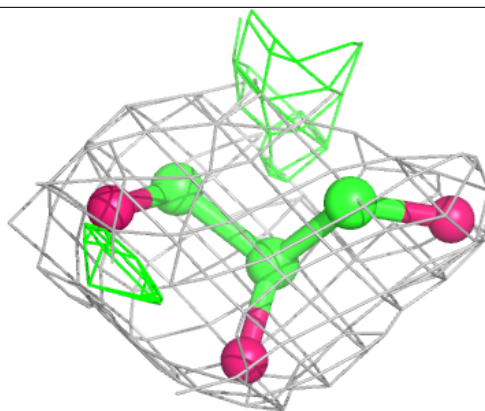
Electron density around GOL B 303 (B):

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



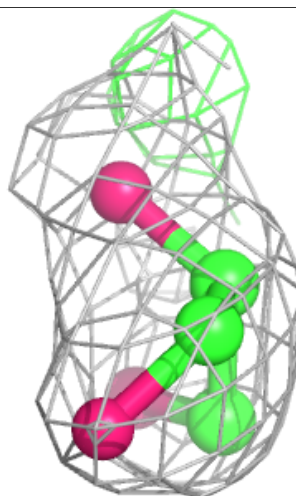
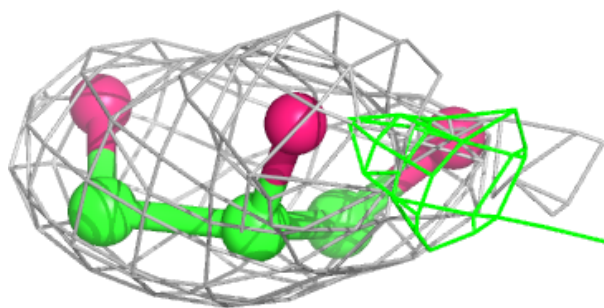
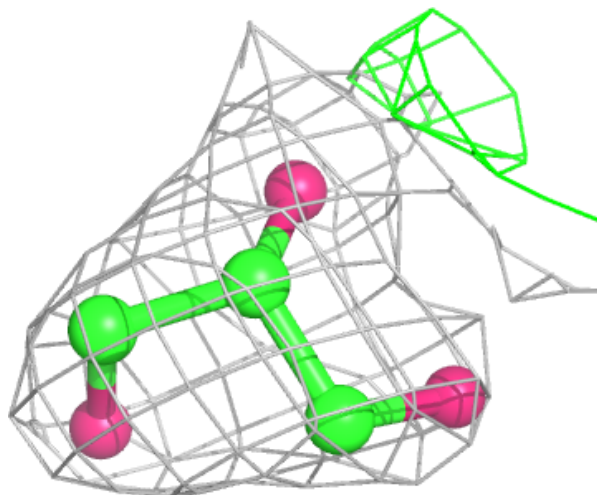
Electron density around GOL B 303 (A):

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



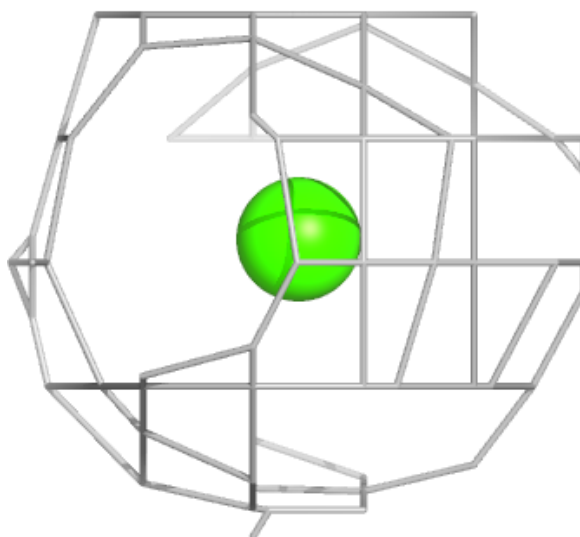
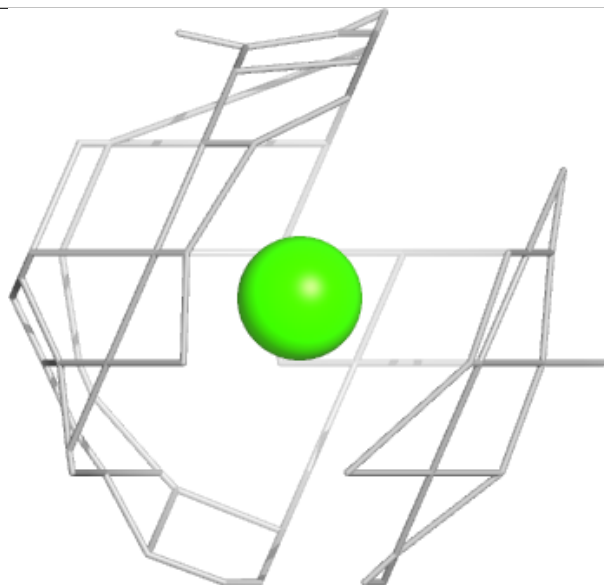
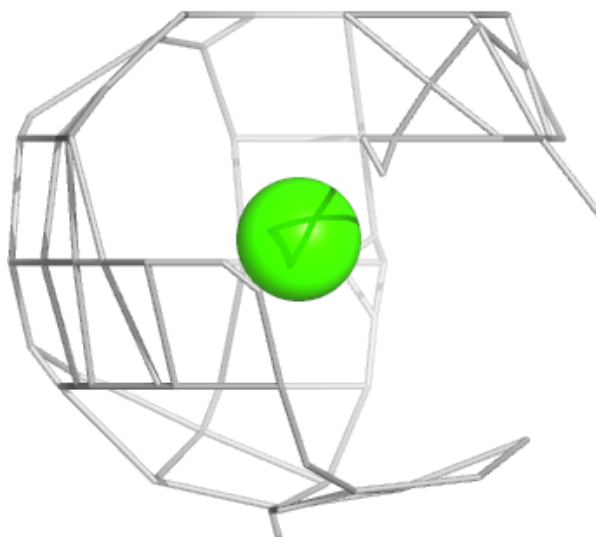
Electron density around GOL A 304:

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



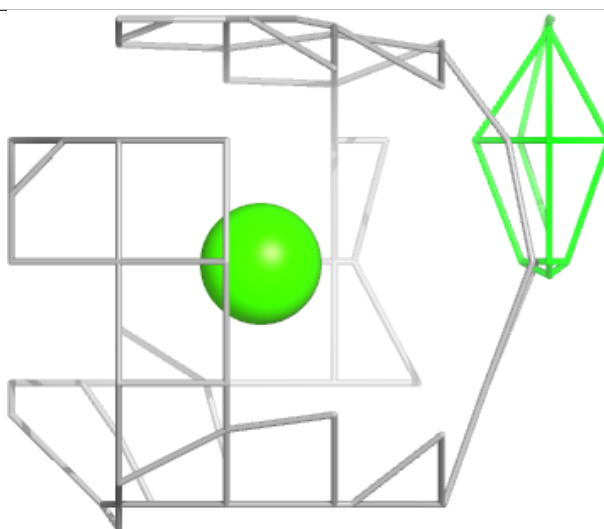
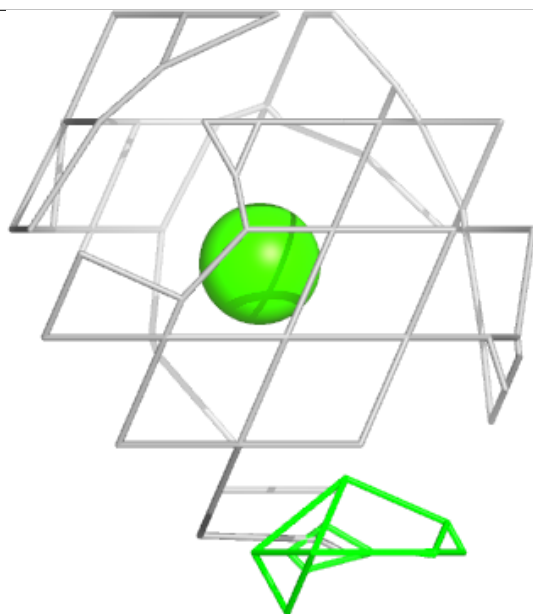
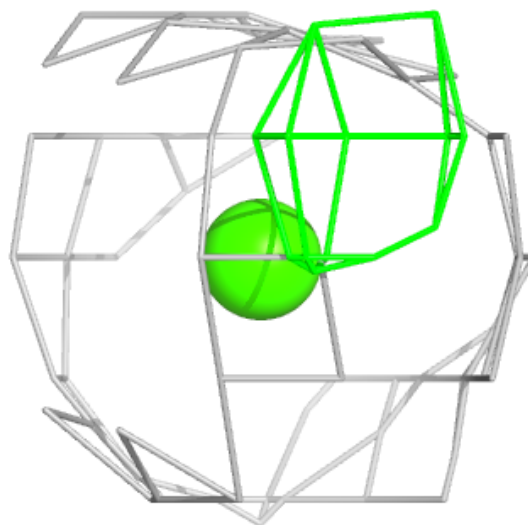
Electron density around CA A 301:

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



Electron density around CA B 301:

$2mF_o-DF_c$ (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.