



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2026 – 07:03 AM EDT

PDB ID : 9PCT / pdb_00009pct
Title : Structure of Porcine Trypsin Crystals Grown from PEG Complexed with Crystallization Additives III
Authors : McPherson, A.
Deposited on : 2025-06-29
Resolution : 1.41 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

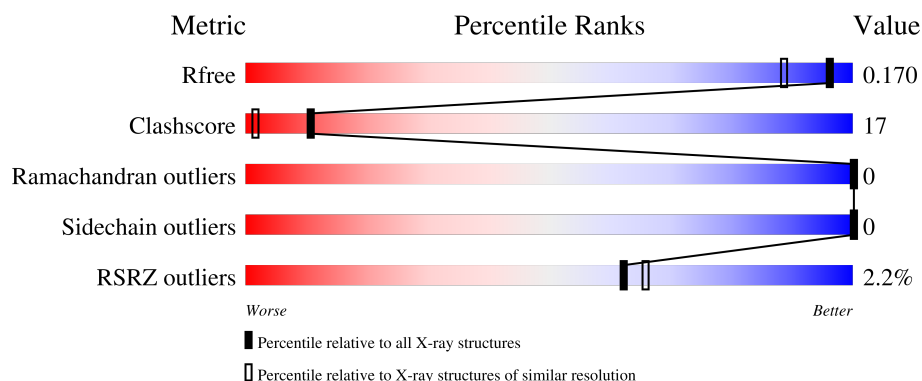
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




The reported resolution of this entry is 1.41 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (1.44-1.40)

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 $\leq 5\%$. 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	231	 2% 83% 13%
2	B	2	 100%
3	F	2	 100%

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
13	EPE	A	313[B]	-	-	X	-
2	GLC	B	1	-	-	X	-
3	FRU	F	1	-	-	X	-
7	PG4	A	307	-	-	X	-
9	GOL	A	321	-	-	X	-

2 Entry composition

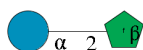
There are 17 unique types of molecules in this entry. The entry contains 4343 atoms, of which 2091 are hydrogens and 0 are deuteriums.

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 Trypsin.

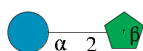
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	223	Total	C	H	N	O	S	7	18	0
			3389	1064	1676	296	338	15			

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	H	O	0	0	0
			45	12	22	11			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose.

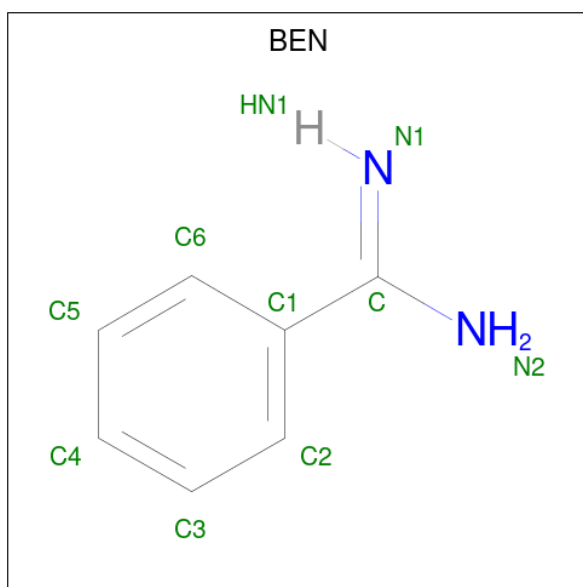


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	H	O	0	0	0
			44	12	21	11			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

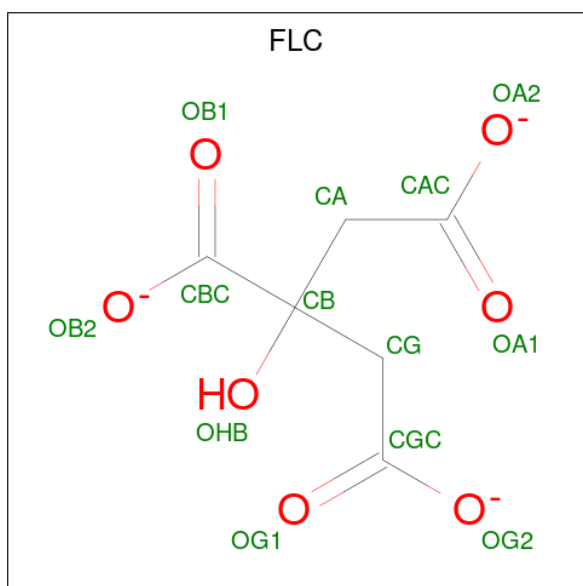
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is BENZAMIDINE (CCD ID: BEN) (formula: C₇H₈N₂).



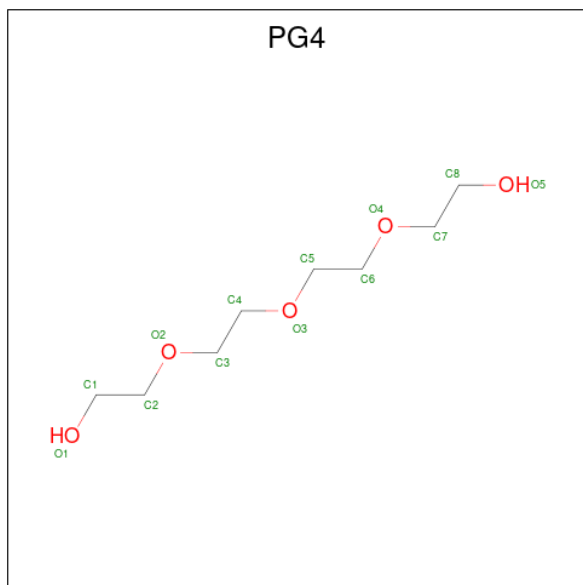
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	N	0	0
			17	7	8	2		
5	A	1	Total	C	H	N	0	0
			17	7	8	2		
5	A	1	Total	C	H	N	0	0
			17	7	8	2		

- Molecule 6 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$) (labeled as "Ligand of Interest" by depositor).



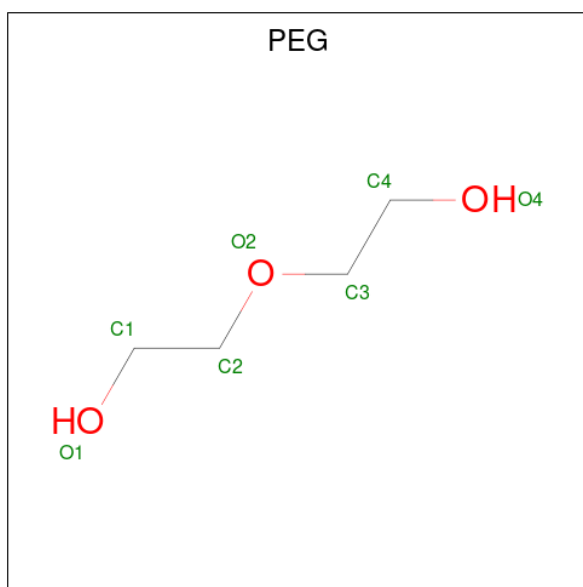
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			18	6	5	7		
6	A	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



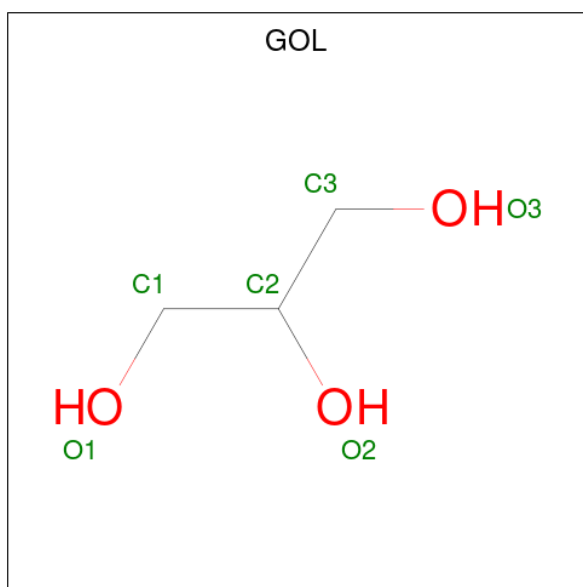
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			31	8	18	5		
7	A	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



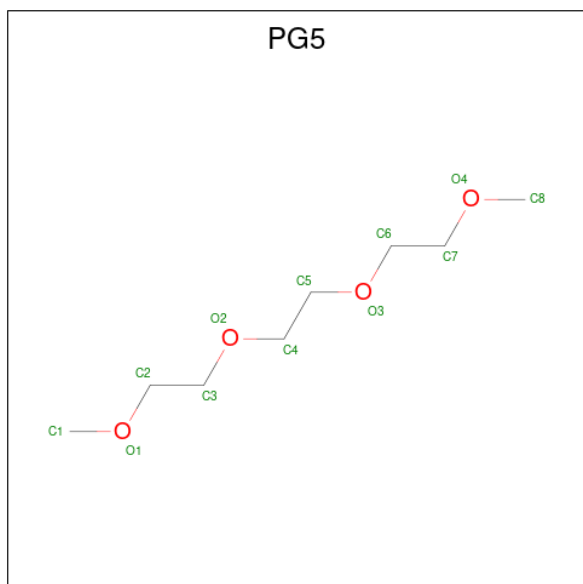
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			17	4	10	3		
8	A	1	Total	C	H	O	0	0
			17	4	10	3		
8	A	1	Total	C	H	O	0	0
			17	4	10	3		
8	A	1	Total	C	H	O	0	0
			17	4	10	3		
8	A	1	Total	C	H	O	0	0
			17	4	10	3		
8	A	1	Total	C	H	O	0	0
			15	4	9	2		
8	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			14	3	8	3		
9	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 10 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY)]-ETHANE (CCD ID: PG5) (formula: $C_8H_{18}O_4$).



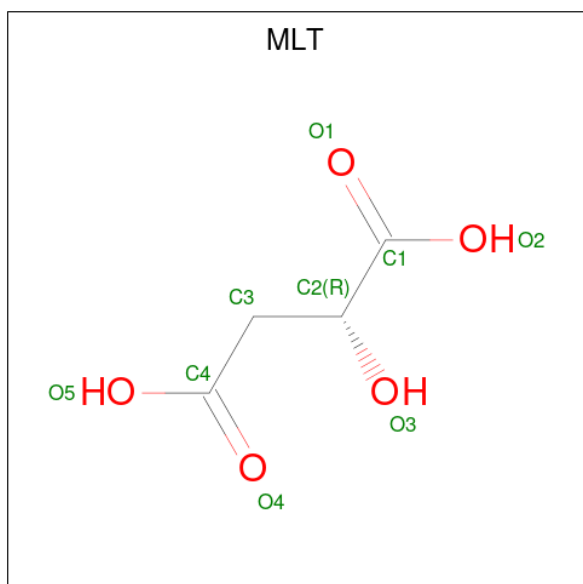
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			30	8	18	4		

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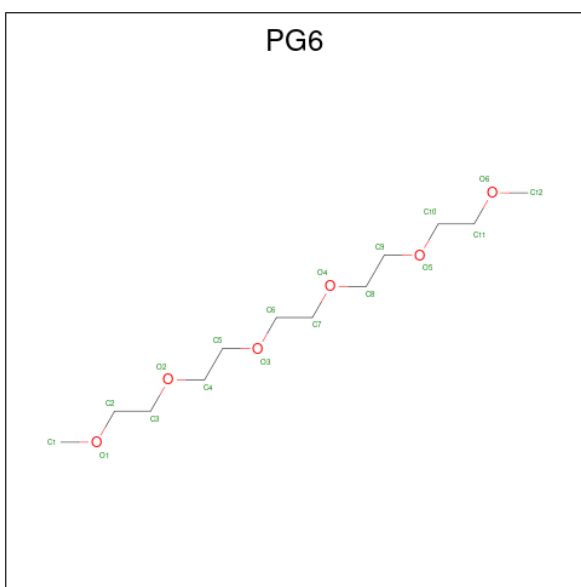
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			30	8	18	4		
10	A	1	Total	C	H	O	0	0
			29	8	17	4		
10	A	1	Total	C	H	O	0	0
			30	8	18	4		
10	A	1	Total	C	H	O	0	0
			29	8	17	4		

- Molecule 11 is D-MALATE (CCD ID: MLT) (formula: $C_4H_6O_5$) (labeled as "Ligand of Interest" by depositor).



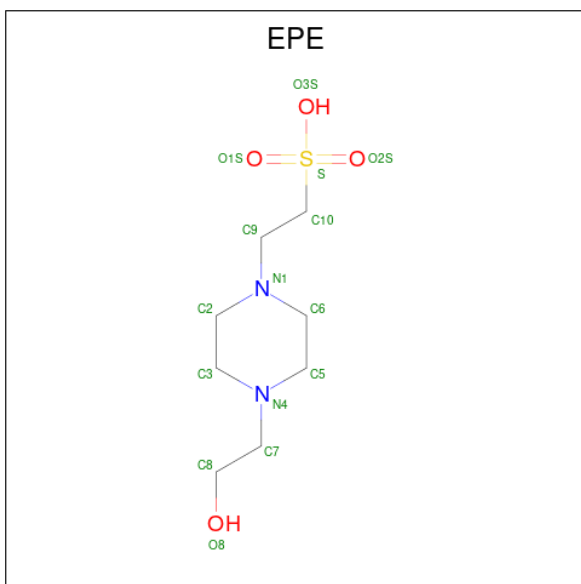
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			13	4	4	5		
11	A	1	Total	C	H	O	0	0
			13	4	4	5		
11	A	1	Total	C	H	O	0	0
			13	4	4	5		

- Molecule 12 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHANE (CCD ID: PG6) (formula: $C_{12}H_{26}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	H	O	0	0
			44	12	26	6		
12	A	1	Total	C	H	O	0	0
			42	11	25	6		

- Molecule 13 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$) (labeled as "Ligand of Interest" by depositor).



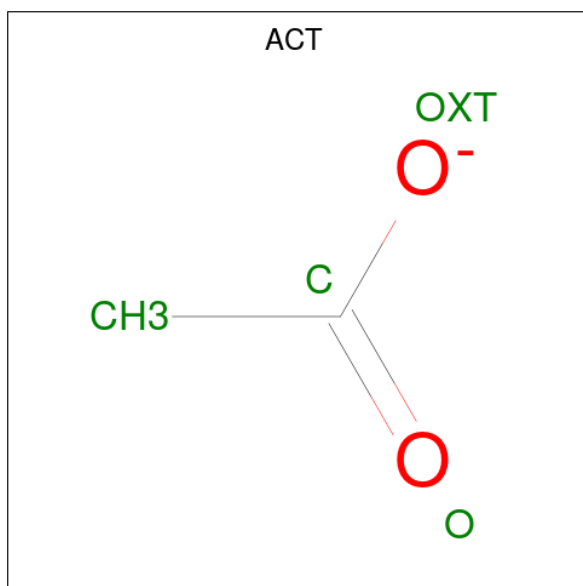
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	H	N	O	0	1
			32	8	17	2	4		

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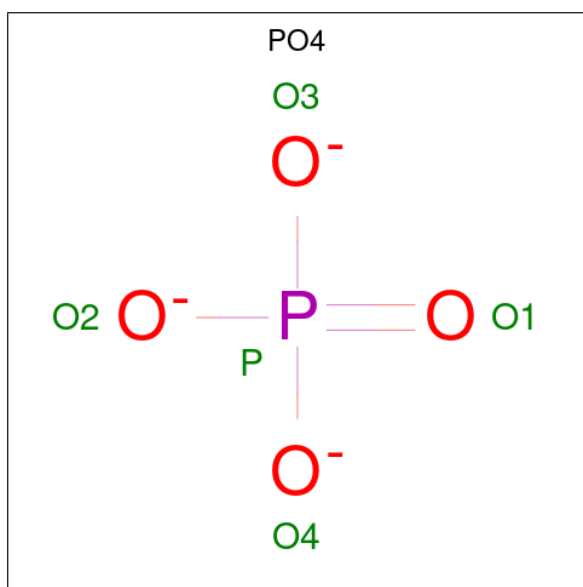
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	H	N	O	S	
			31	8	16	2	4	1	
								0	0

- Molecule 14 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



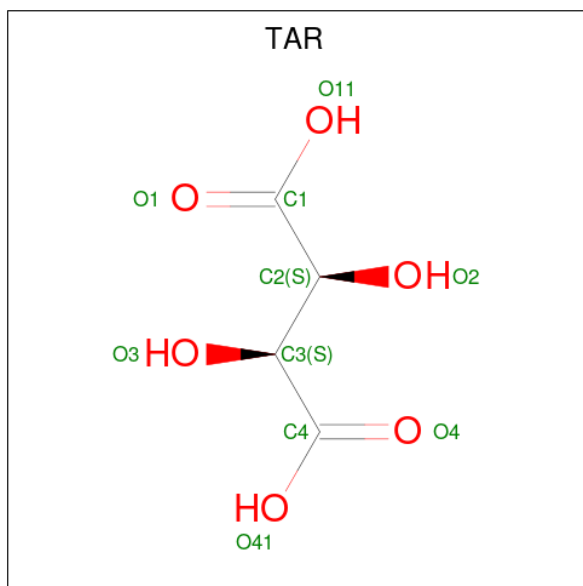
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	H	O		
			7	2	3	2	0	0
14	A	1	Total	C	H	O		
			7	2	3	2	0	0
14	A	1	Total	C	H	O		
			7	2	3	2	0	0

- Molecule 15 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 16 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: $C_4H_6O_6$) (labeled as "Ligand of Interest" by depositor).

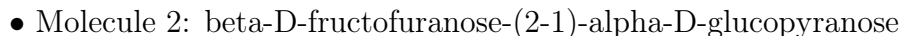


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	A	1	Total	C	H	O	0	0
			14	4	4	6		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	154	Total 160	O 160	0	19

- Molecule 1: Trypsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	58.82Å 58.82Å 135.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.31 – 1.41 26.31 – 1.41	Depositor EDS
% Data completeness (in resolution range)	77.9 (26.31-1.41) 77.9 (26.31-1.41)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.57 (at 1.41Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.131 , 0.170 0.131 , 0.170	Depositor DCC
R_{free} test set	2547 reflections (5.46%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 79.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4343	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.90% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLT, FLC, EPE, FRU, PEG, TAR, BEN, PG4, CA, GOL, PG5, ACT, PO4, PG6, GLC

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	0.35	0/1818	0.62	0/2466

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1713	1676	1659	53	2
2	B	23	22	21	13	2
3	F	23	21	21	8	0
4	A	1	0	0	0	0
5	A	27	24	21	2	0
6	A	26	10	10	2	0
7	A	26	36	36	9	0
8	A	62	89	87	3	0
9	A	12	16	16	7	0
10	A	60	88	90	6	0
11	A	27	12	12	1	0
12	A	35	51	49	0	0
13	A	30	33	35	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	12	9	9	0	0
15	A	5	0	0	0	0
16	A	10	4	4	0	0
17	A	160	0	0	18	0
All	All	2252	2091	2070	70	2

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 17.

The worst 5 of 70 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:24:PHE:O	2:B:1:GLC:O4	1.70	1.08
17:A:427:HOH:O	2:B:1:GLC:O6	1.71	1.05
13:A:314:EPE:O2S	17:A:401:HOH:O	1.90	0.88
1:A:167:GLU:OE2	17:A:402:HOH:O	1.91	0.86
17:A:450:HOH:O	3:F:2:GLC:O3	1.95	0.84

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:O	2:B:2:FRU:O1[5_655]	1.70	0.50
1:A:107:ARG:O	2:B:2:FRU:HO1[5_655]	1.18	0.42

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	241/231 (104%)	236 (98%)	5 (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	A	202/191 (106%)	202 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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](#)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLC	B	1	2	11,11,12	1.41	2 (18%)	15,15,17	3.43	8 (53%)
2	FRU	B	2	2	11,12,12	0.98	0	10,18,18	1.30	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FRU	F	1	3	11,12,12	1.04	1 (9%)	10,18,18	0.99	0
3	GLC	F	2	3	11,11,12	1.24	1 (9%)	15,15,17	1.63	4 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	B	1	2	-	2/2/19/22	0/1/1/1
2	FRU	B	2	2	-	2/5/24/24	0/1/1/1
3	FRU	F	1	3	-	0/5/24/24	0/1/1/1
3	GLC	F	2	3	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	GLC	O5-C5	-2.80	1.38	1.43
3	F	2	GLC	O5-C5	-2.68	1.38	1.43
3	F	1	FRU	O3-C3	-2.13	1.38	1.42
2	B	1	GLC	C2-C3	-2.02	1.49	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GLC	C2-C3-C4	-7.31	98.00	110.86
2	B	1	GLC	C3-C4-C5	6.30	121.66	110.23
2	B	1	GLC	C1-O5-C5	5.10	119.02	112.19
3	F	2	GLC	C1-O5-C5	4.19	117.80	112.19
2	B	1	GLC	O5-C1-C2	4.03	120.41	110.79

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

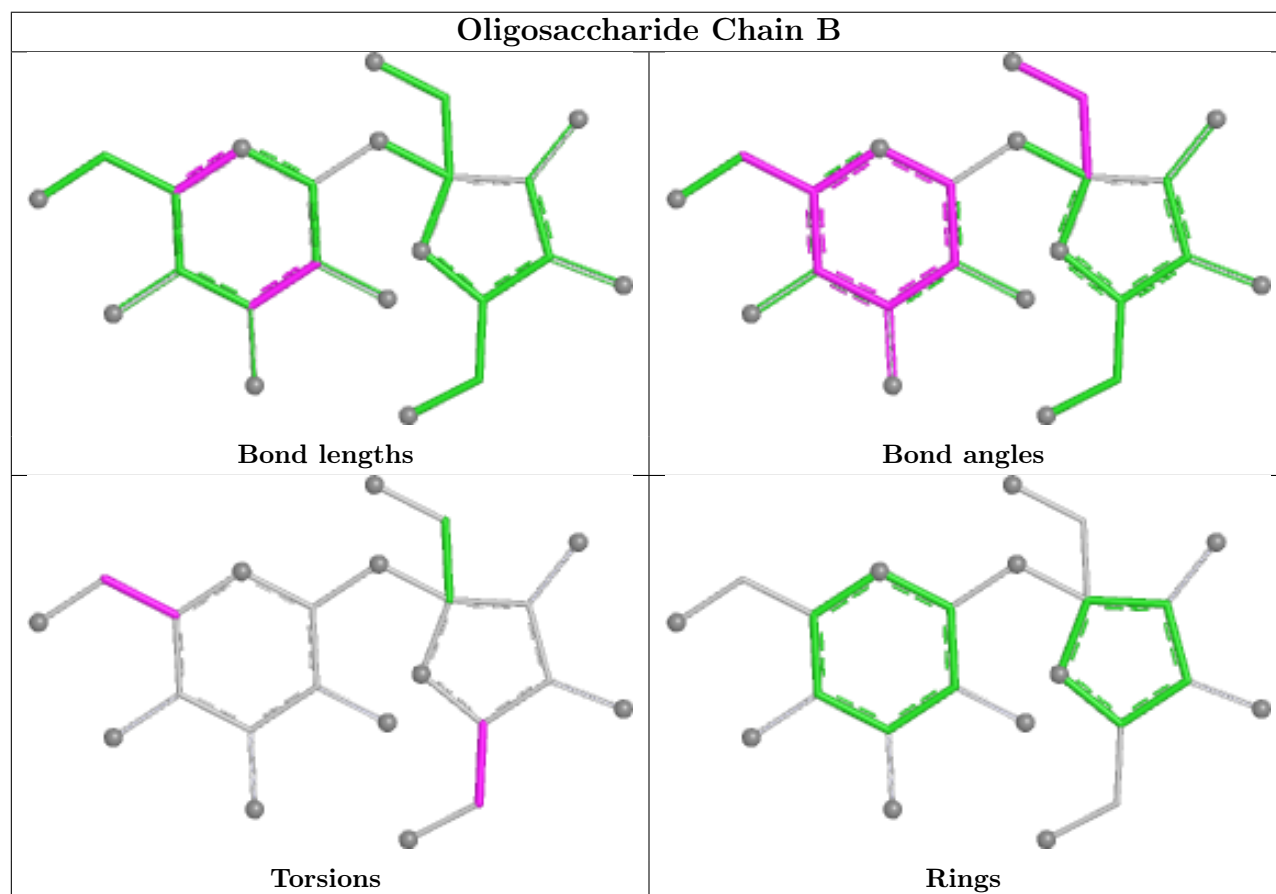
Mol	Chain	Res	Type	Atoms
2	B	2	FRU	O5-C5-C6-O6
2	B	2	FRU	C4-C5-C6-O6
2	B	1	GLC	O5-C5-C6-O6
3	F	2	GLC	O5-C5-C6-O6
3	F	2	GLC	C4-C5-C6-O6

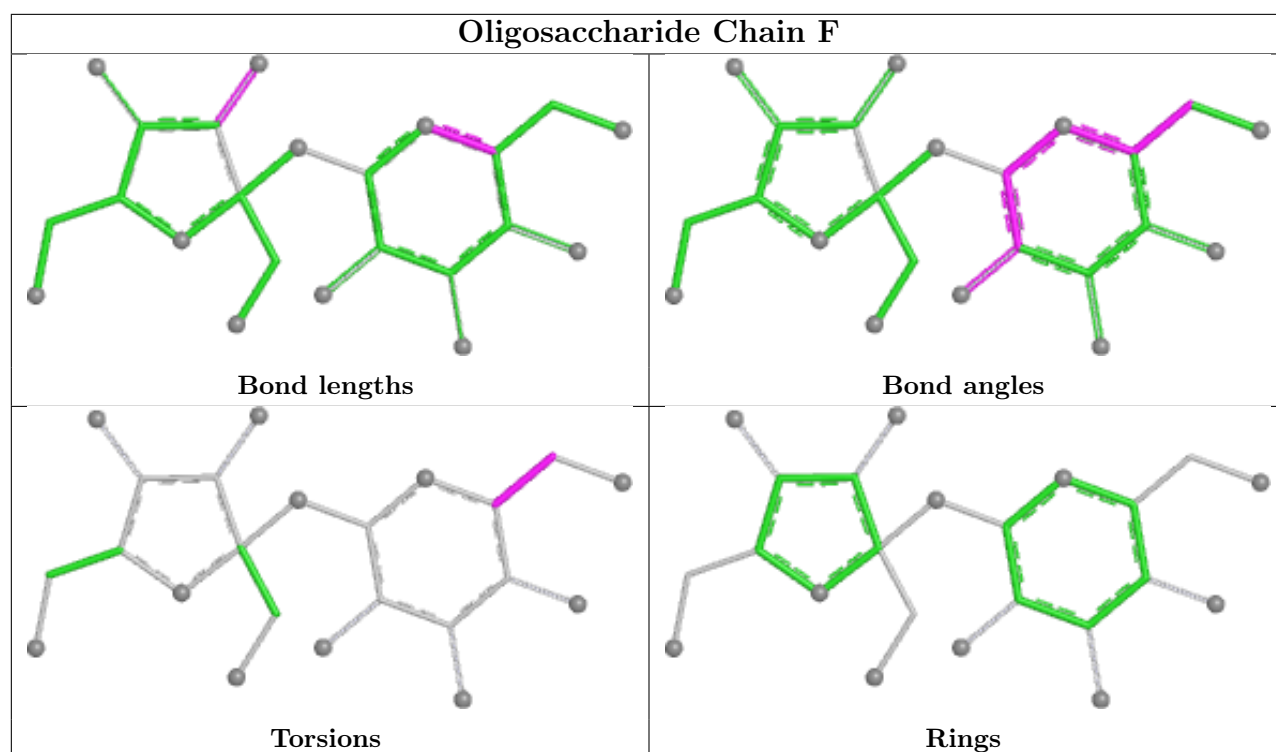
There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	GLC	2	0
2	B	2	FRU	2	2
3	F	1	FRU	7	0
2	B	1	GLC	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 1 is monoatomic - leaving 35 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	$\# Z > 2$
7	PG4	A	304	-	12,12,12	0.30	0	11,11,11	0.23	0
10	PG5	A	331	-	11,11,11	0.38	0	10,10,10	0.52	0
8	PEG	A	322	-	6,6,6	0.28	0	5,5,5	0.24	0
8	PEG	A	330	-	5,5,6	0.32	0	4,4,5	0.26	0
10	PG5	A	326	-	11,11,11	0.40	0	10,10,10	0.13	0
15	PO4	A	316	-	4,4,4	1.59	1 (25%)	6,6,6	1.62	1 (16%)
8	PEG	A	306	-	6,6,6	0.28	0	5,5,5	0.52	0
5	BEN	A	318	-	9,9,9	0.70	0	7,11,11	0.61	0
10	PG5	A	328	-	11,11,11	0.38	0	10,10,10	0.17	0
11	MLT	A	311	-	8,8,8	1.31	0	10,10,10	2.01	3 (30%)
6	FLC	A	335	-	12,12,12	1.04	0	17,17,17	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BEN	A	302	-	9,9,9	0.59	0	7,11,11	0.73	0
14	ACT	A	317	-	3,3,3	1.36	0	3,3,3	0.99	0
8	PEG	A	323	-	6,6,6	0.24	0	5,5,5	0.32	0
11	MLT	A	319	-	8,8,8	1.38	1 (12%)	10,10,10	1.86	3 (30%)
11	MLT	A	333	-	8,8,8	1.35	1 (12%)	10,10,10	1.89	2 (20%)
7	PG4	A	307	-	12,12,12	0.28	0	11,11,11	0.29	0
5	BEN	A	332	-	9,9,9	0.72	0	7,11,11	0.97	0
8	PEG	A	334	-	6,6,6	0.24	0	5,5,5	0.18	0
10	PG5	A	309	-	11,11,11	0.39	0	10,10,10	0.21	0
13	EPE	A	313[B]	-	15,15,15	0.74	1 (6%)	19,20,20	2.19	8 (42%)
10	PG5	A	320	-	11,11,11	0.41	0	10,10,10	0.30	0
16	TAR	A	336	-	9,9,9	1.30	1 (11%)	12,12,12	1.25	1 (8%)
8	PEG	A	305	-	6,6,6	0.25	0	5,5,5	0.33	0
14	ACT	A	315	-	3,3,3	1.37	0	3,3,3	1.10	0
9	GOL	A	308	-	5,5,5	0.26	0	5,5,5	0.78	0
12	PG6	A	329	-	16,16,17	0.30	0	15,15,16	0.20	0
8	PEG	A	324	-	6,6,6	0.27	0	5,5,5	0.18	0
14	ACT	A	327	-	3,3,3	1.38	0	3,3,3	1.04	0
12	PG6	A	312	-	17,17,17	0.39	0	16,16,16	0.15	0
8	PEG	A	325	-	6,6,6	0.29	0	5,5,5	0.13	0
13	EPE	A	314	-	15,15,15	0.85	1 (6%)	19,20,20	1.14	1 (5%)
9	GOL	A	321	-	5,5,5	0.55	0	5,5,5	0.85	0
6	FLC	A	303	-	12,12,12	1.04	0	17,17,17	1.22	1 (5%)
8	PEG	A	310	-	6,6,6	0.26	0	5,5,5	0.25	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
7	PG4	A	304	-	-	6/10/10/10	-
10	PG5	A	331	-	-	6/9/9/9	-
8	PEG	A	322	-	-	2/4/4/4	-
8	PEG	A	330	-	-	0/3/3/4	-
10	PG5	A	326	-	-	4/9/9/9	-
8	PEG	A	306	-	-	1/4/4/4	-
5	BEN	A	318	-	-	3/4/4/4	0/1/1/1
10	PG5	A	328	-	-	6/9/9/9	-
11	MLT	A	311	-	-	4/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FLC	A	335	-	-	0/16/16/16	-
5	BEN	A	302	-	-	4/4/4/4	0/1/1/1
8	PEG	A	323	-	-	4/4/4/4	-
11	MLT	A	319	-	-	3/8/8/8	-
11	MLT	A	333	-	-	2/8/8/8	-
7	PG4	A	307	-	-	6/10/10/10	-
5	BEN	A	332	-	-	4/4/4/4	0/1/1/1
8	PEG	A	334	-	-	1/4/4/4	-
10	PG5	A	309	-	-	6/9/9/9	-
13	EPE	A	313[B]	-	-	7/9/19/19	0/1/1/1
10	PG5	A	320	-	-	4/9/9/9	-
16	TAR	A	336	-	-	0/12/12/12	-
8	PEG	A	305	-	-	2/4/4/4	-
9	GOL	A	308	-	-	3/4/4/4	-
12	PG6	A	329	-	-	4/14/14/15	-
8	PEG	A	324	-	-	2/4/4/4	-
12	PG6	A	312	-	-	7/15/15/15	-
8	PEG	A	325	-	-	1/4/4/4	-
13	EPE	A	314	-	-	3/9/19/19	0/1/1/1
9	GOL	A	321	-	-	4/4/4/4	-
6	FLC	A	303	-	-	6/16/16/16	-
8	PEG	A	310	-	-	2/4/4/4	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	316	PO4	P-O1	2.57	1.56	1.50
11	A	319	MLT	C2-C1	2.35	1.55	1.52
13	A	314	EPE	C10-S	2.20	1.80	1.77
13	A	313[B]	EPE	C10-S	2.17	1.80	1.77
11	A	333	MLT	C2-C1	2.16	1.55	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	313[B]	EPE	O2S-S-C10	-5.58	98.30	106.73
13	A	313[B]	EPE	C9-N1-C2	4.20	122.44	111.24
11	A	311	MLT	O1-C1-C2	-4.16	114.29	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	333	MLT	O1-C1-C2	-3.83	114.95	122.60
11	A	319	MLT	O1-C1-C2	-3.58	115.45	122.60

There are no chirality outliers.

5 of 107 torsion outliers are listed below:

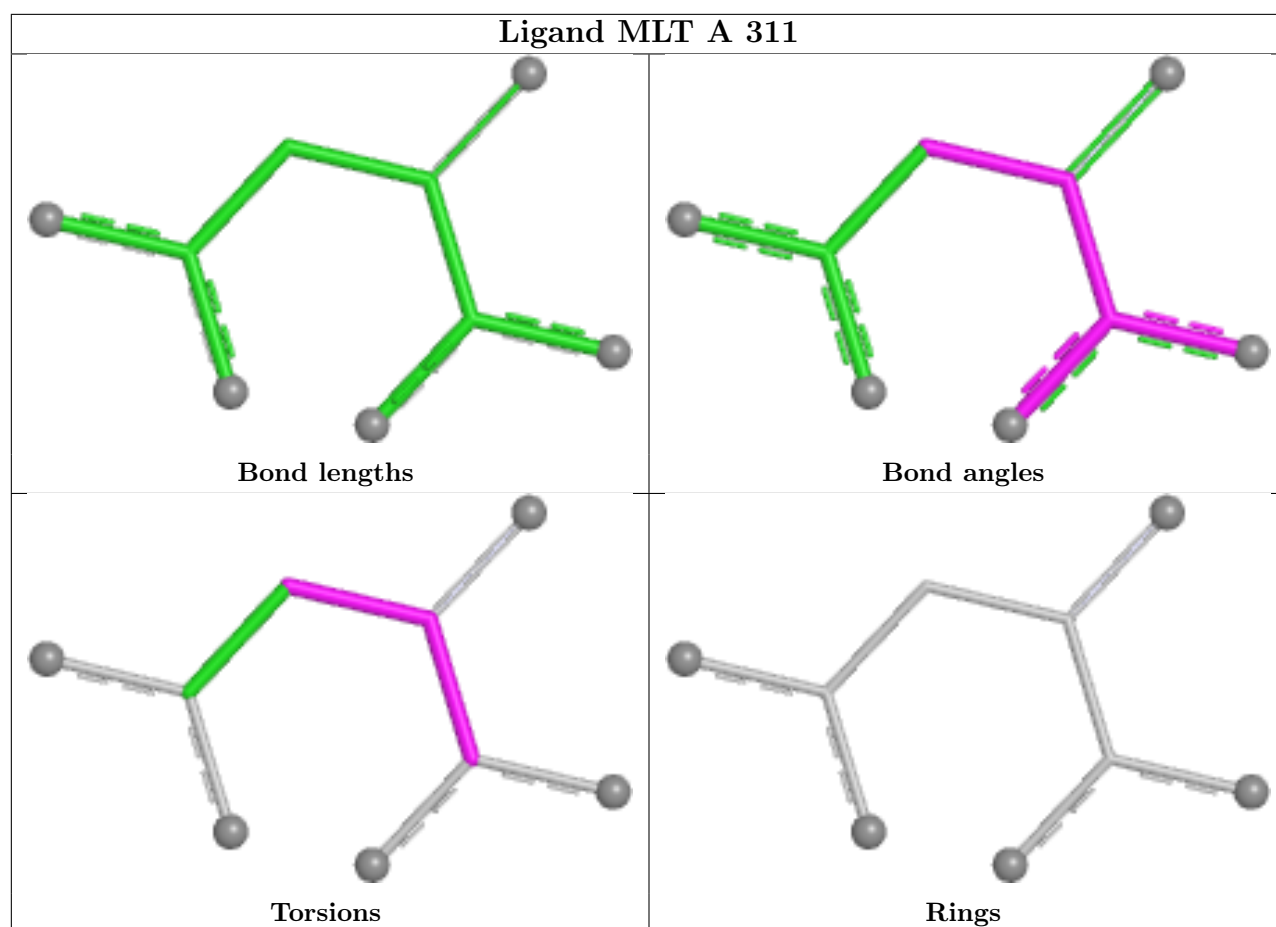
Mol	Chain	Res	Type	Atoms
6	A	303	FLC	CA-CB-CBC-OB1
6	A	303	FLC	CA-CB-CBC-OB2
6	A	303	FLC	OHB-CB-CBC-OB1
6	A	303	FLC	OHB-CB-CBC-OB2
9	A	308	GOL	O1-C1-C2-O2

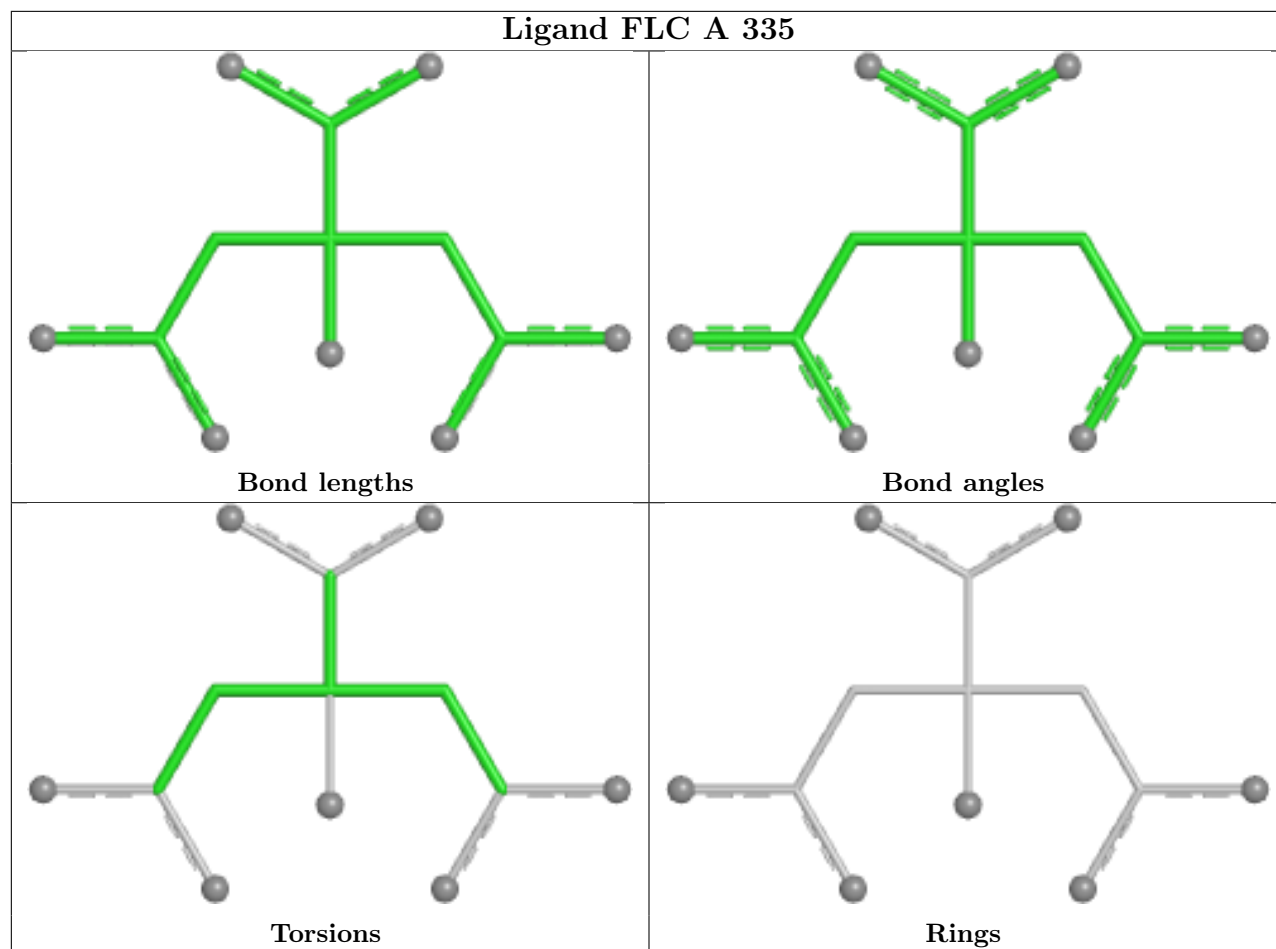
There are no ring outliers.

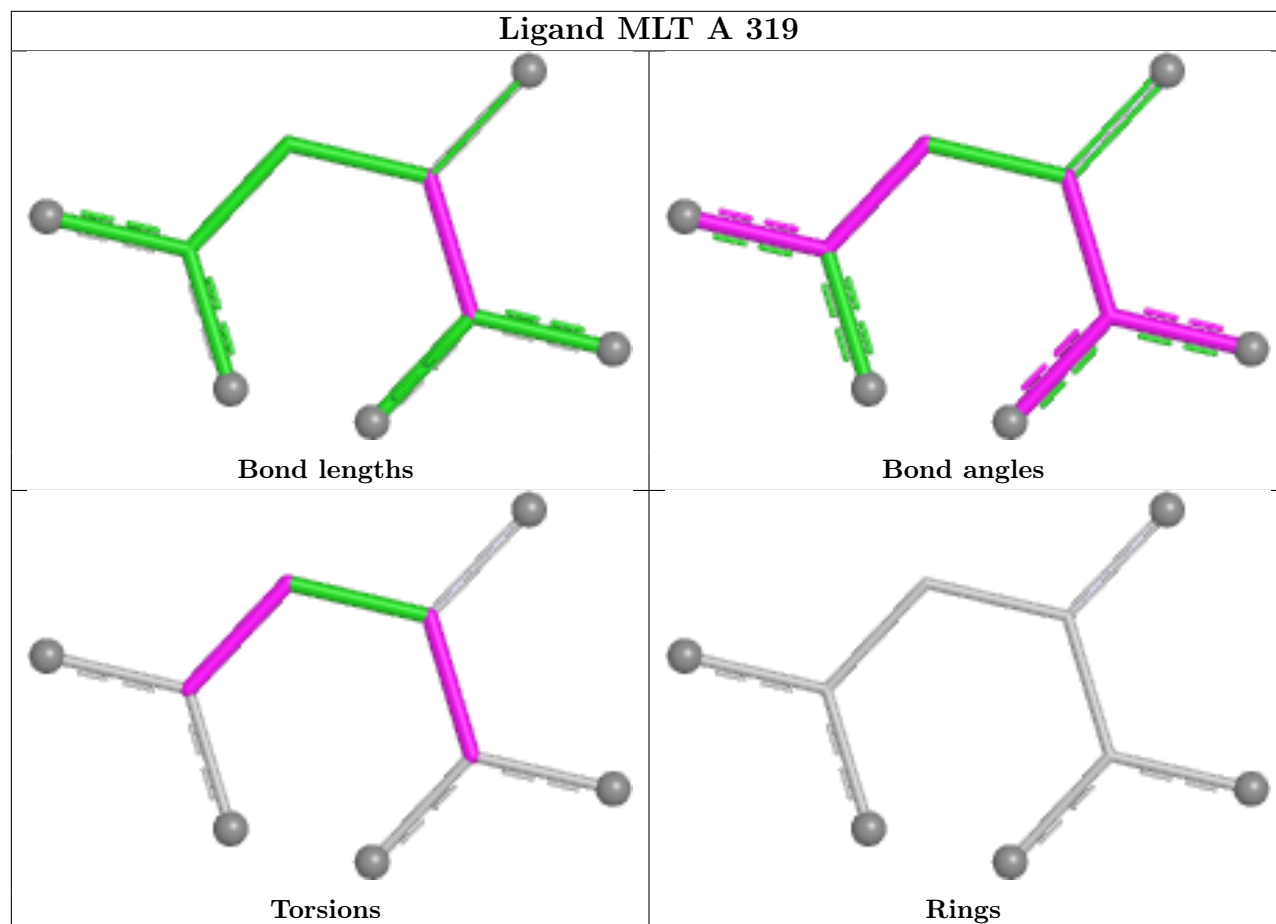
12 monomers are involved in 39 short contacts:

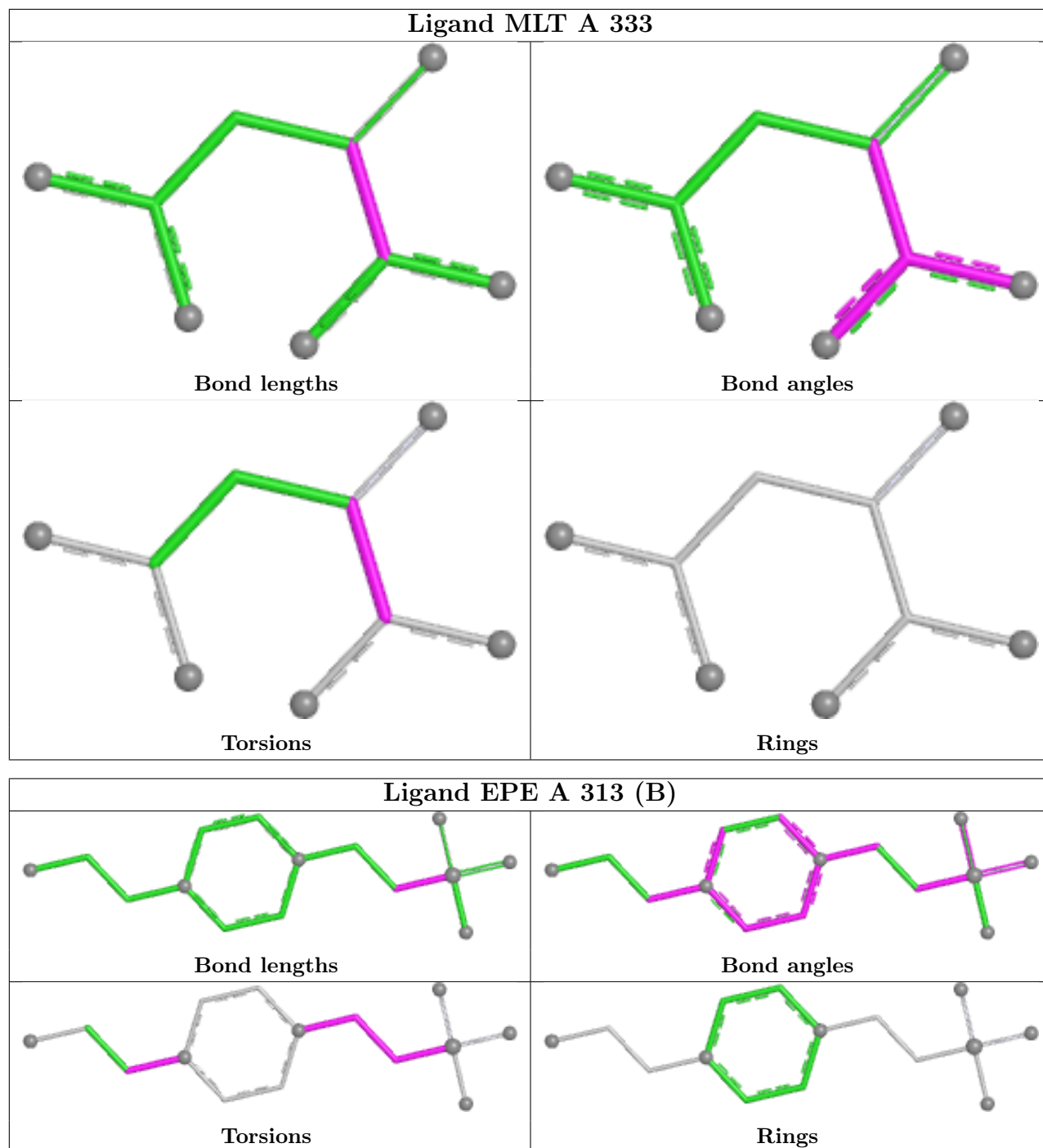
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	304	PG4	2	0
10	A	331	PG5	6	0
8	A	306	PEG	2	0
11	A	319	MLT	1	0
7	A	307	PG4	7	0
5	A	332	BEN	2	0
13	A	313[B]	EPE	8	0
9	A	308	GOL	3	0
8	A	325	PEG	1	0
13	A	314	EPE	4	0
9	A	321	GOL	4	0
6	A	303	FLC	2	0

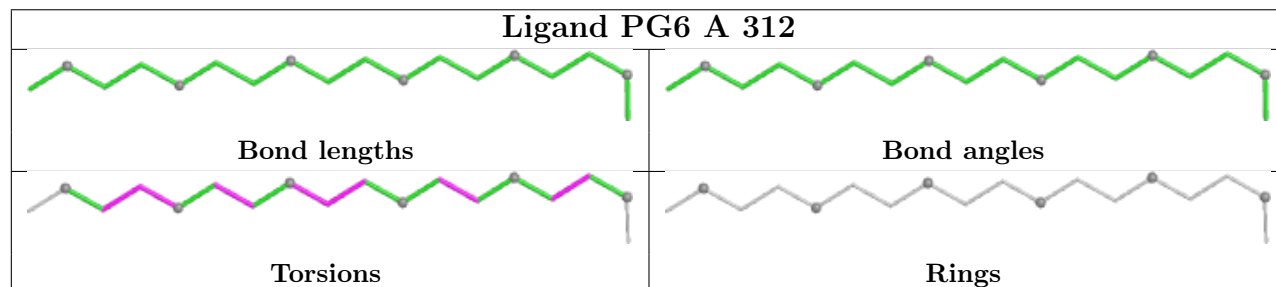
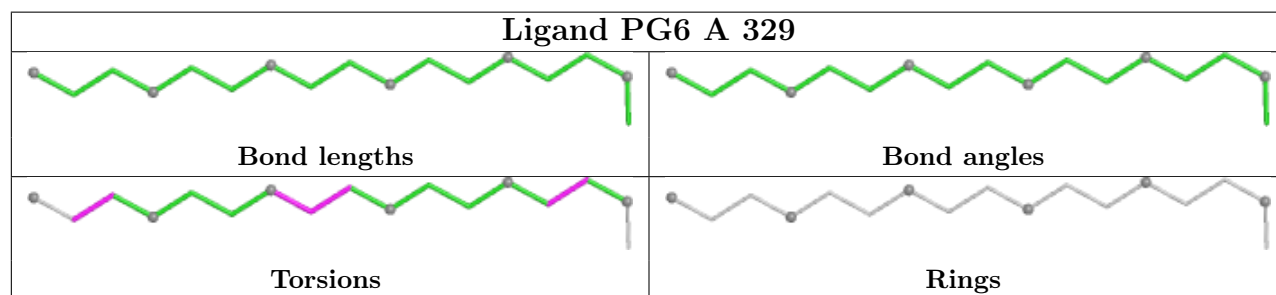
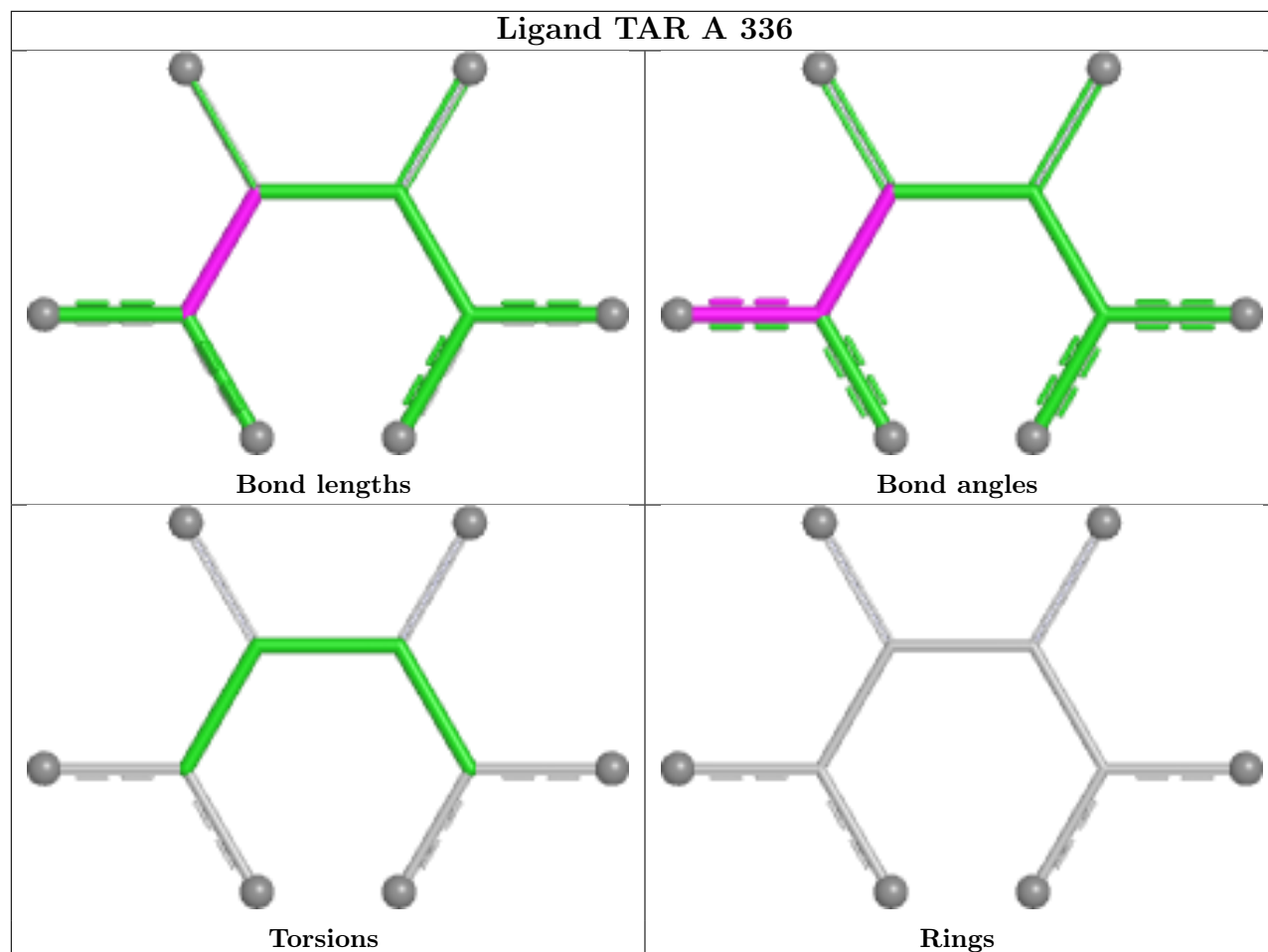
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

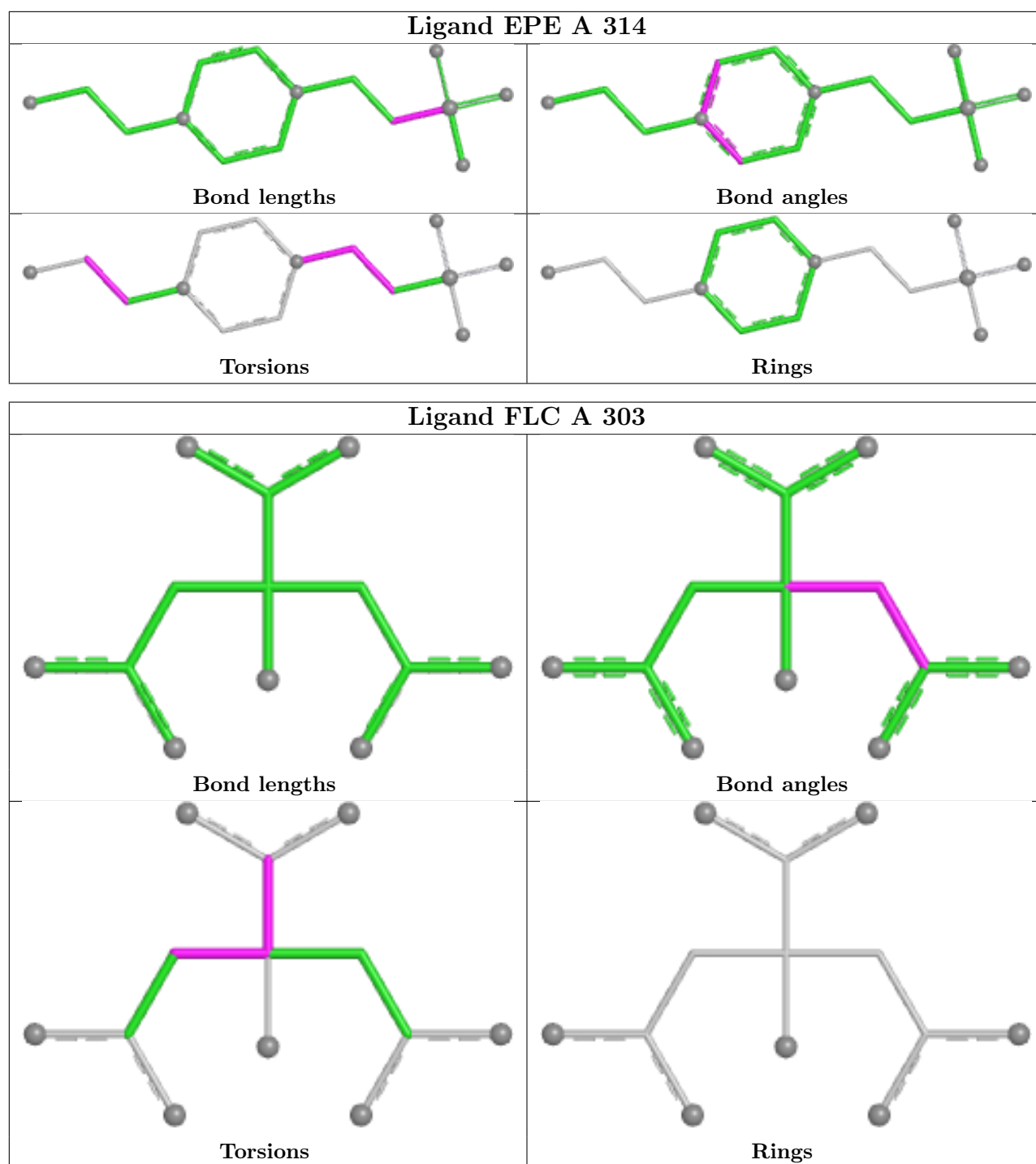












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	223/231 (96%)	-0.36	5 (2%) 62 66	13, 28, 47, 84	18 (8%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	TYR	4.3
1	A	129	SER	3.2
1	A	128	GLY	2.8
1	A	126	SER	2.5
1	A	130	SER	2.1

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

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

6.3 Carbohydrates [i](#)

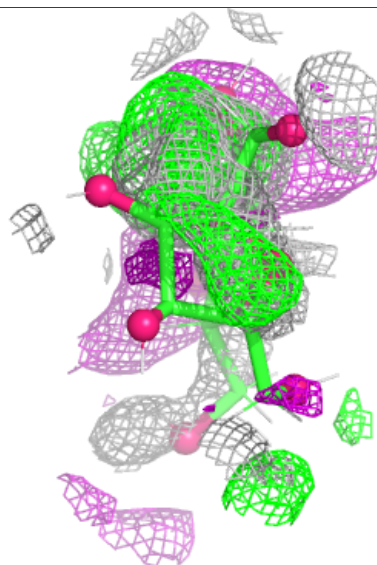
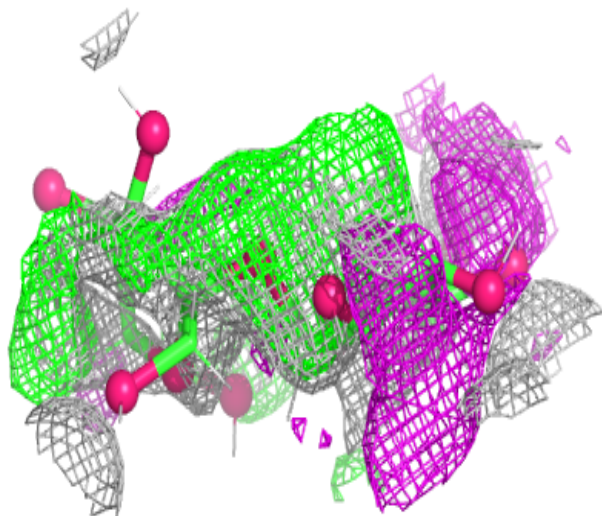
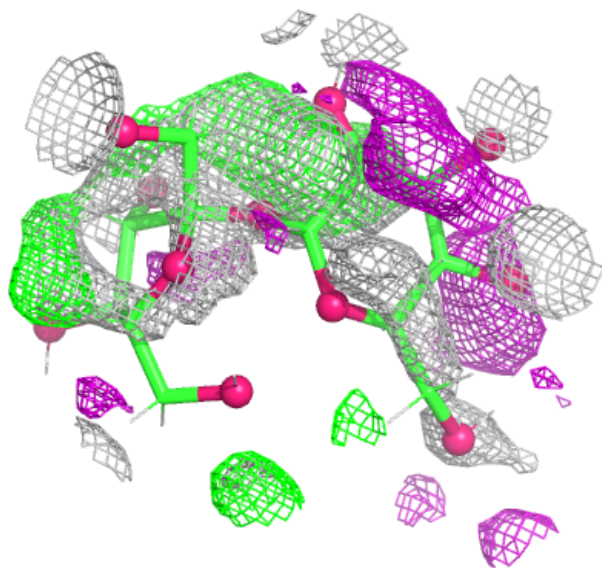
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

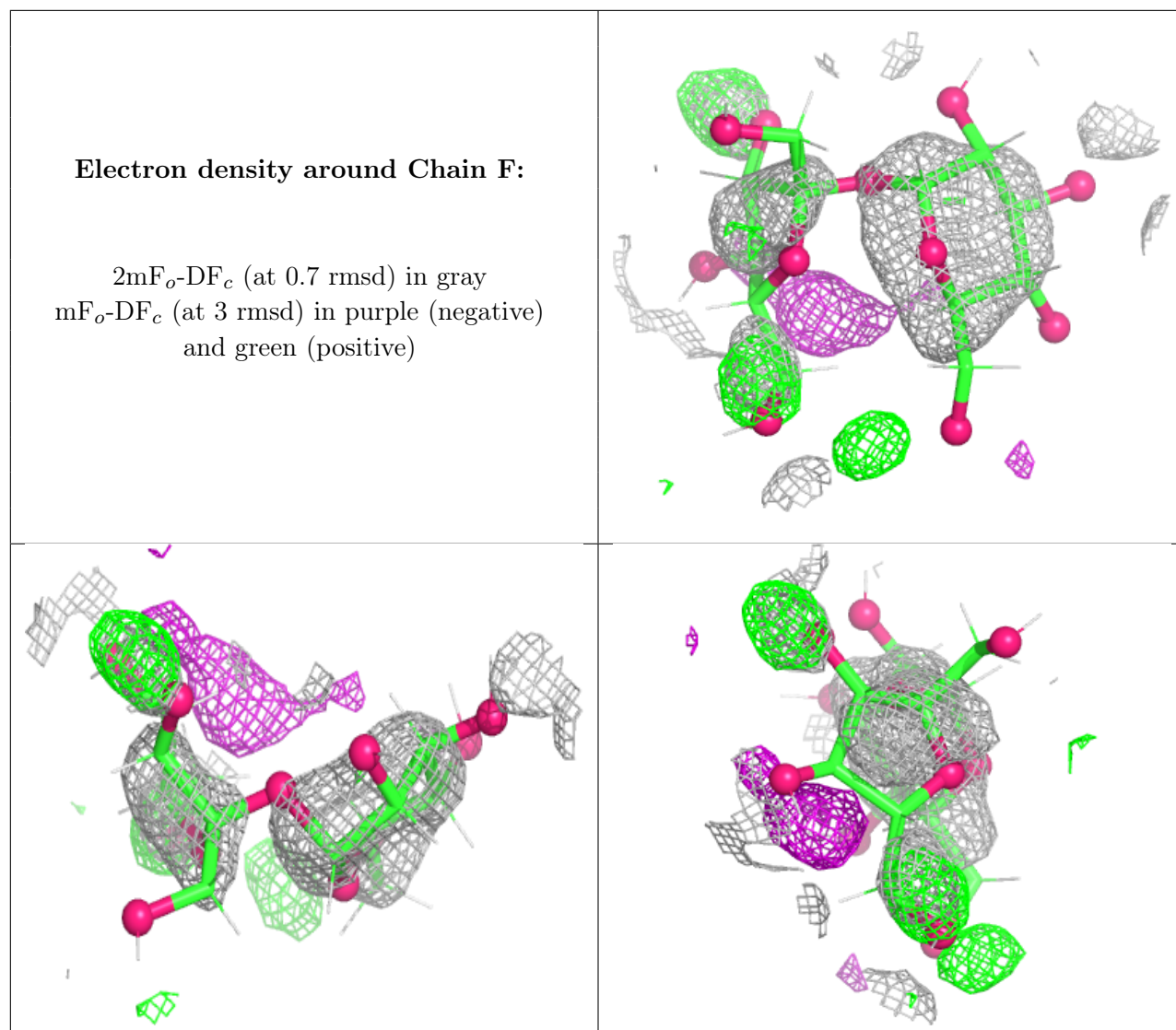
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	B	1	11/12	0.84	0.33	114,182,268,322	0
2	FRU	B	2	12/12	0.92	0.24	86,212,276,312	0
3	FRU	F	1	12/12	-	-	142,201,298,358	0
3	GLC	F	2	11/12	-	-	31,63,118,163	21

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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





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(Å ²)	Q<0.9
14	ACT	A	315	4/4	0.15	0.17	100,123,125,165	0
10	PG5	A	309	12/12	0.29	0.18	79,121,167,175	30
8	PEG	A	323	7/7	0.32	0.16	80,112,139,139	17
8	PEG	A	324	7/7	0.33	0.14	62,102,118,122	17
8	PEG	A	330	6/7	0.33	0.16	92,131,161,194	0
8	PEG	A	305	7/7	0.36	0.14	71,98,125,128	0
12	PG6	A	312	18/18	0.40	0.17	54,106,159,174	44

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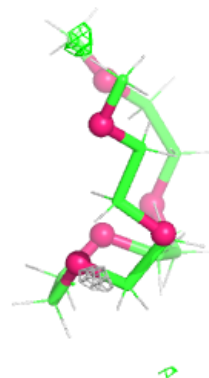
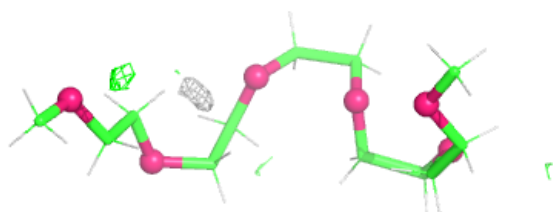
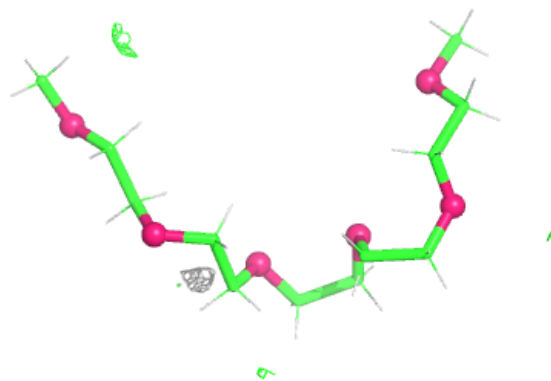
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	PEG	A	310	7/7	0.42	0.15	70,94,139,139	17
6	FLC	A	335	13/13	0.44	0.13	55,79,104,125	18
11	MLT	A	311	9/9	0.48	0.12	76,101,122,147	13
10	PG5	A	326	12/12	0.50	0.17	58,101,135,137	29
13	EPE	A	314	15/15	0.52	0.18	65,100,142,171	31
5	BEN	A	318	9/9	0.54	0.14	82,104,147,158	0
14	ACT	A	317	4/4	0.54	0.12	78,93,106,140	0
11	MLT	A	333	9/9	0.56	0.17	72,96,115,138	13
12	PG6	A	329	17/18	0.57	0.19	0,141,206,225	0
10	PG5	A	328	12/12	0.59	0.23	35,118,149,160	30
8	PEG	A	322	7/7	0.61	0.24	156,199,331,344	0
8	PEG	A	334	7/7	0.63	0.17	72,105,137,137	0
16	TAR	A	336	10/10	0.64	0.15	62,88,110,115	14
6	FLC	A	303	13/13	0.69	0.19	61,87,106,113	18
7	PG4	A	304	13/13	0.70	0.20	40,78,100,106	31
8	PEG	A	306	7/7	0.71	0.22	38,56,84,84	17
10	PG5	A	331	12/12	0.71	0.19	61,116,163,192	0
8	PEG	A	325	7/7	0.74	0.23	75,132,158,158	17
10	PG5	A	320	12/12	0.76	0.18	47,77,118,141	30
9	GOL	A	308	6/6	0.76	0.18	57,73,127,153	14
7	PG4	A	307	13/13	0.78	0.18	34,63,81,97	31
5	BEN	A	332	9/9	0.79	0.26	112,147,197,201	0
15	PO4	A	316	5/5	0.80	0.18	34,39,73,165	5
11	MLT	A	319	9/9	0.81	0.22	24,68,174,181	13
14	ACT	A	327	4/4	0.84	0.17	49,78,103,113	0
9	GOL	A	321	6/6	0.85	0.17	42,56,99,119	14
13	EPE	A	313[B]	15/15	0.87	0.22	42,59,71,72	32
5	BEN	A	302	9/9	0.97	0.06	23,28,36,40	0
4	CA	A	301	1/1	1.00	0.03	21,21,21,21	1

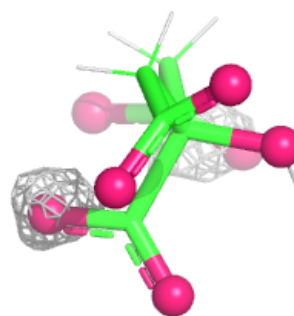
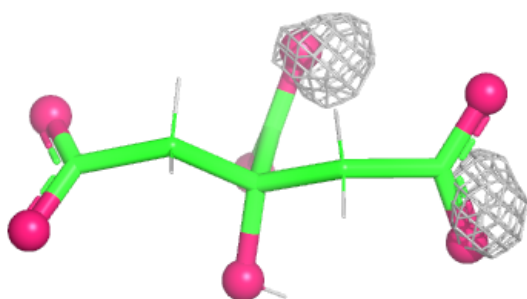
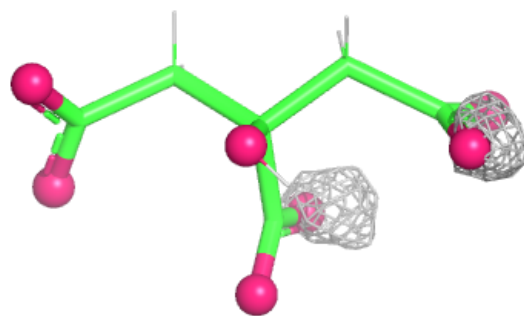
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PG6 A 312:

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

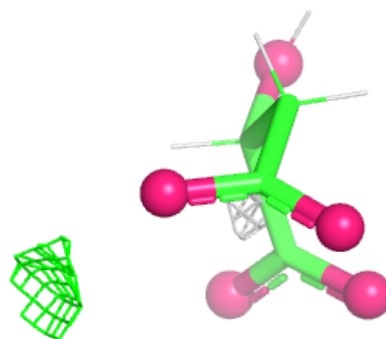
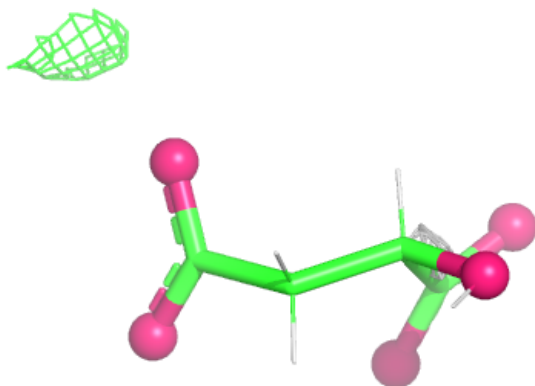
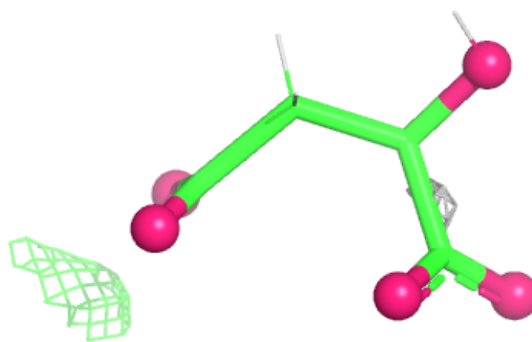
**Electron density around FLC A 335:**

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

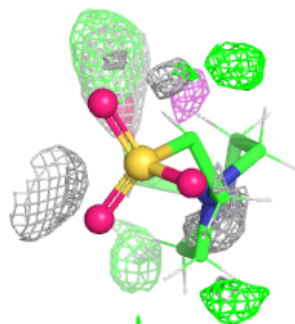
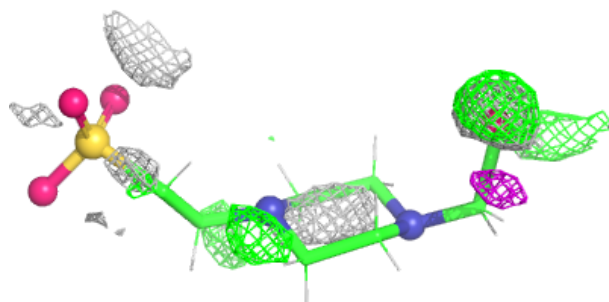
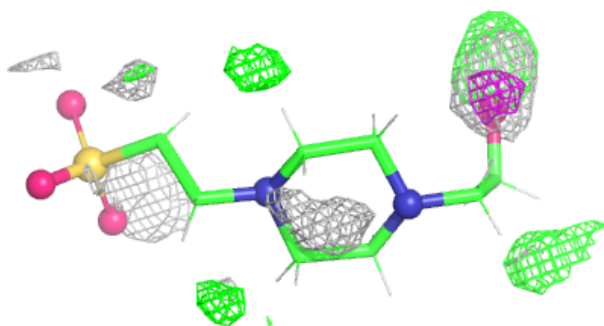


Electron density around MLT A 311:

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

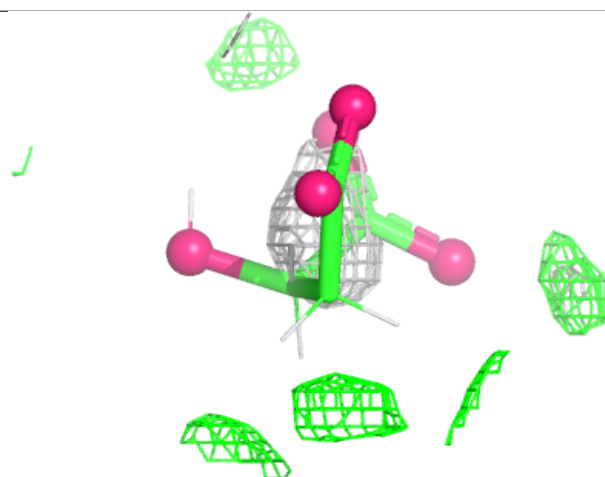
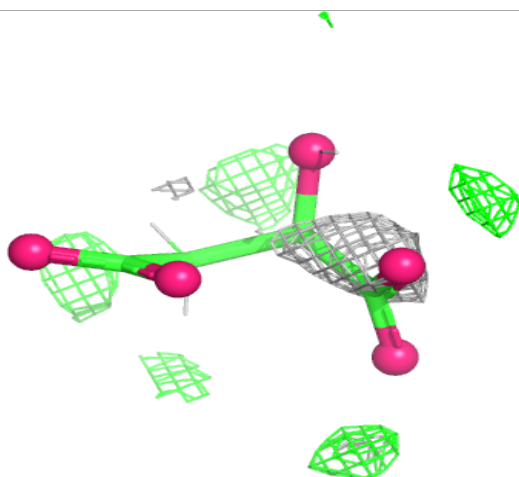
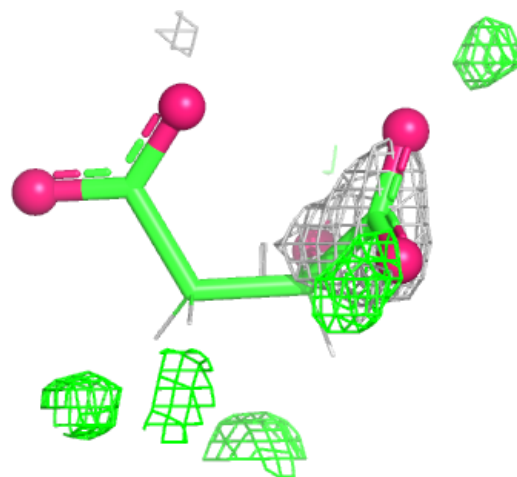
**Electron density around EPE A 314:**

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



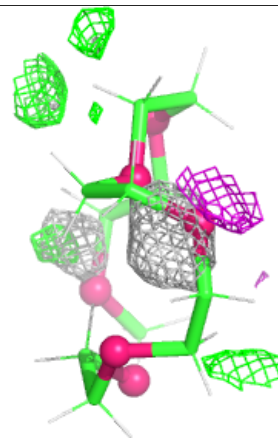
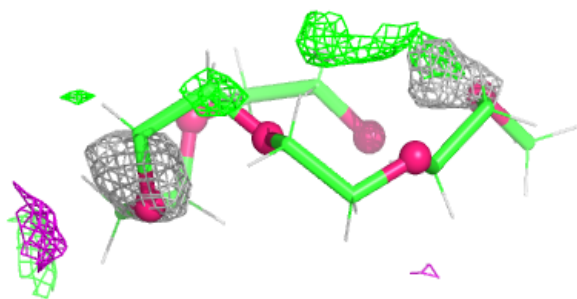
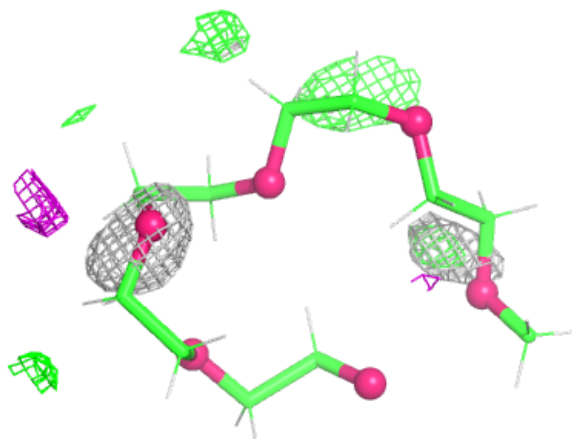
Electron density around MLT A 333:

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



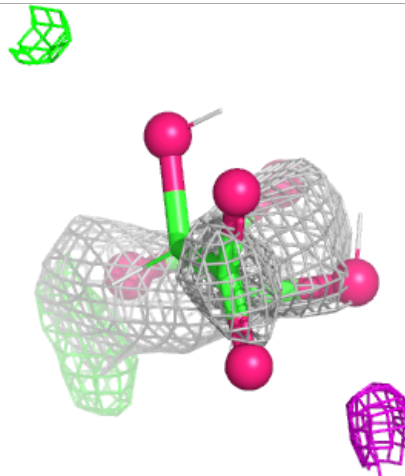
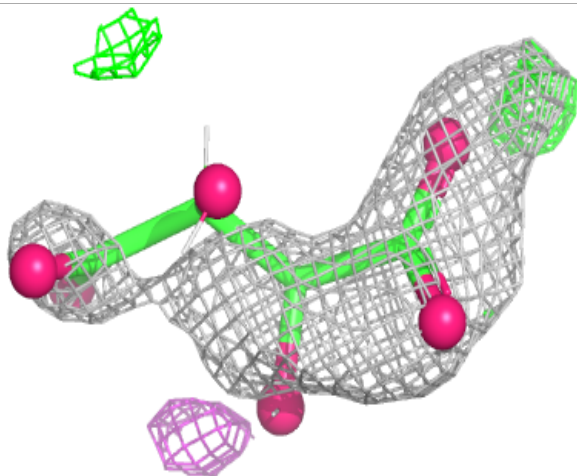
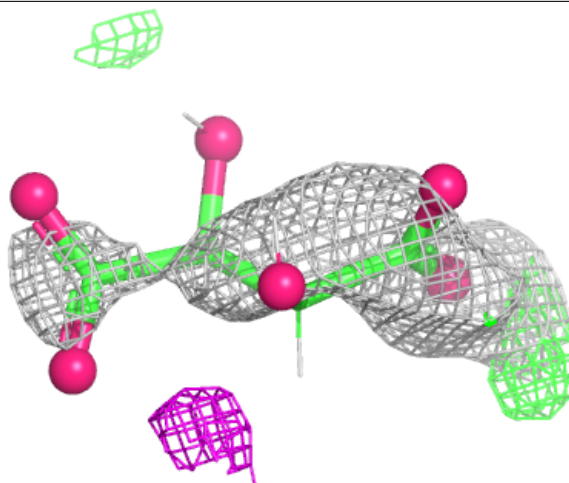
Electron density around PG6 A 329:

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



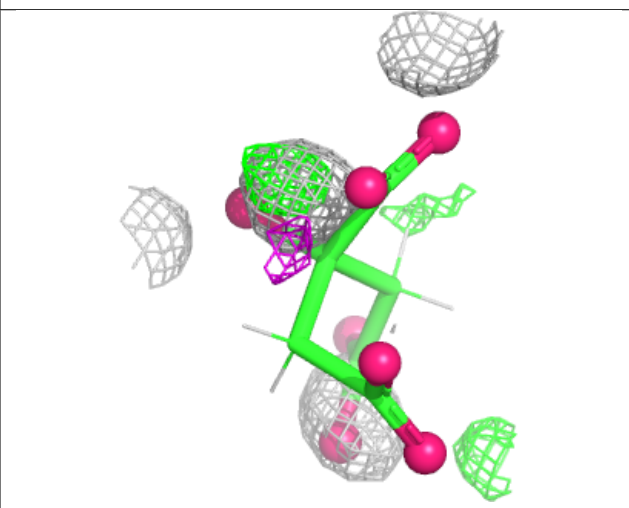
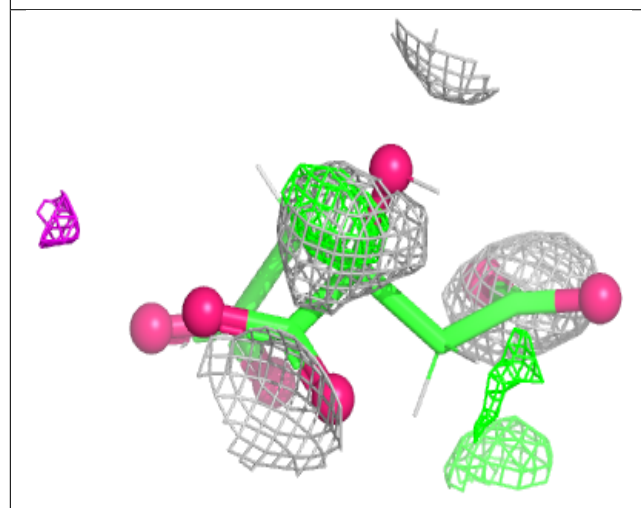
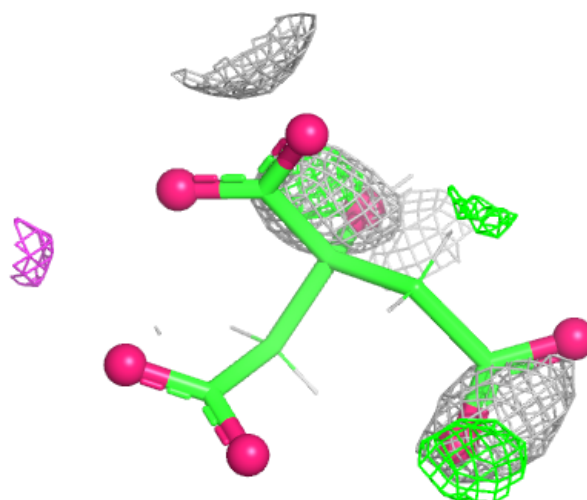
Electron density around TAR A 336:

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



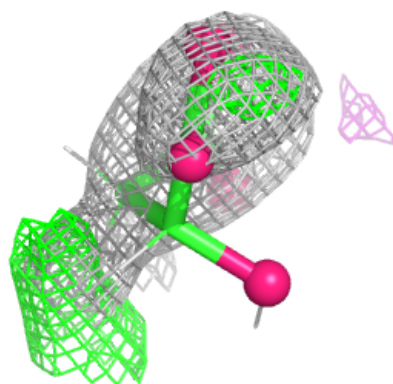
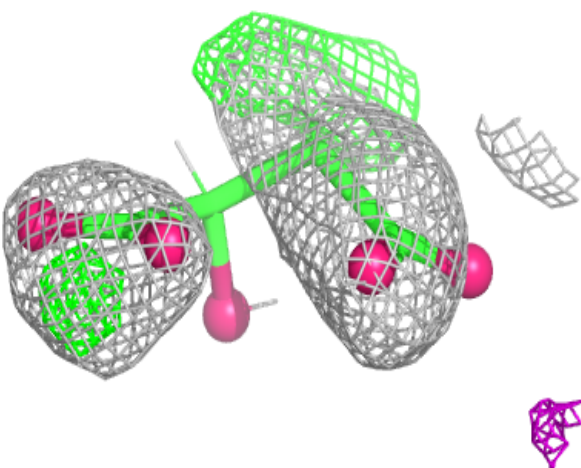
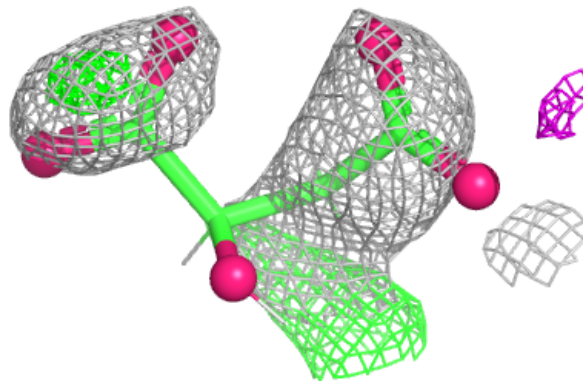
Electron density around FLC A 303:

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



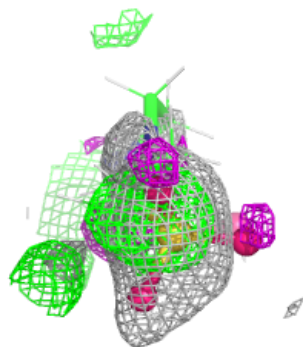
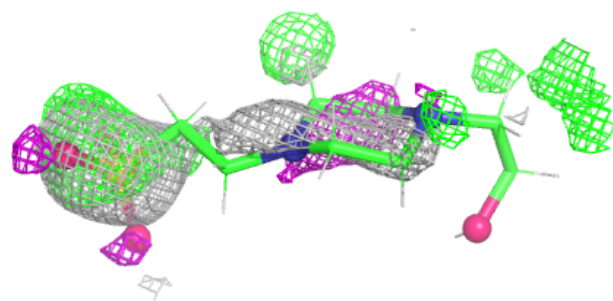
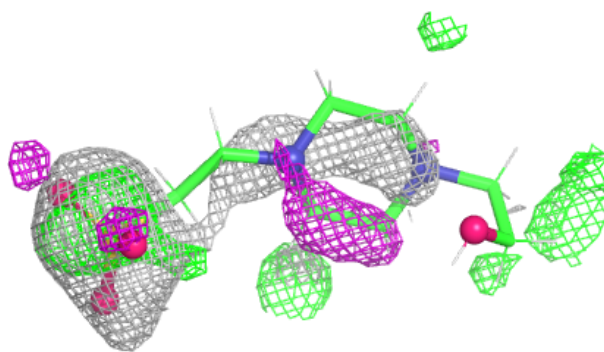
Electron density around MLT A 319:

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



Electron density around EPE A 313 (B):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.