Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2025 – 09:57 PM JST

PDB ID	:	8ZX9 / pdb_00008zx9
Title	:	Structure-Based Mechanism and Specificity of Human Galactosyltransferase B3GalT5
Authors	:	Lo, J.M.; Ma, C.
Deposited on	:	2024-06-14
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 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:

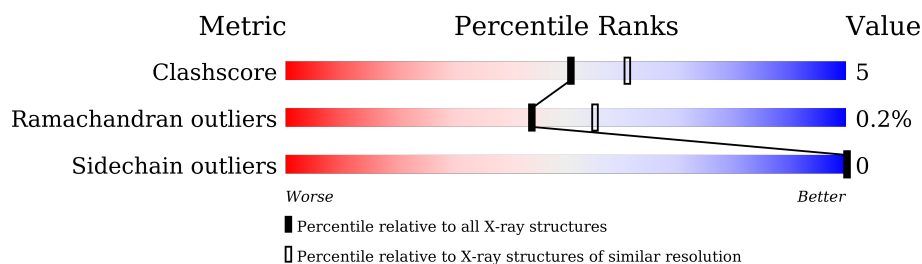|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.30 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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		0

Worse   *Better*

▮ Percentile relative to all X-ray structures
❑ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	278	84% 12% •
1	B	278	84% 12% •
2	E	2	100%
2	G	2	50% 50%
3	F	6	67% 33%
4	D	2	50% 50%

WORLDWIDE
wwPDB
PROTEIN DATA BANK

2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 4946 atoms, of which 56 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 Beta-1,3-galactosyltransferase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total 2193	C 1420	N 371	O 389	S 13	0	0	0
1	B	267	Total 2193	C 1420	N 371	O 389	S 13	0	0	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total 28	C 16	N 2	O 10	0	0	0
2	G	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.
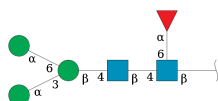
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	6	Total 127	C 40	H 56	N 2	O 29	0	0	0

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total 24	C 14	N 1	O 9	0	0	0

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mn 1	0	0
5	B	1	Total 1	Mn 1	0	0

- Molecule 6 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).

UDP
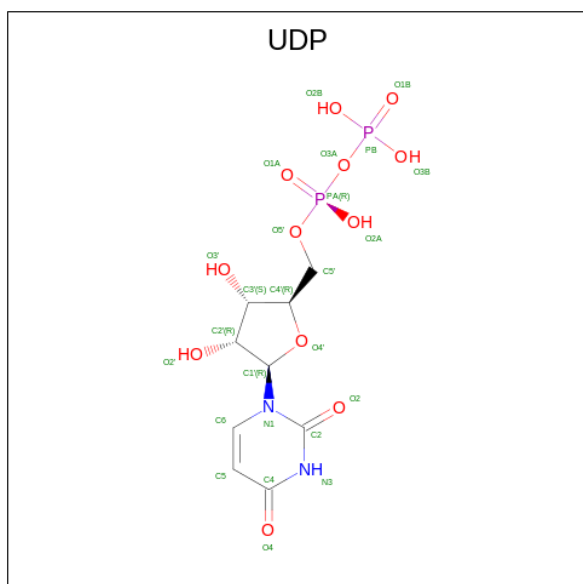
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 25	C 9	N 2	O 12	P 2	0	0
6	B	1	Total 25	C 9	N 2	O 12	P 2	0	0

- Molecule 7 is beta-D-galactopyranose (CCD ID: GAL) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).

GAL
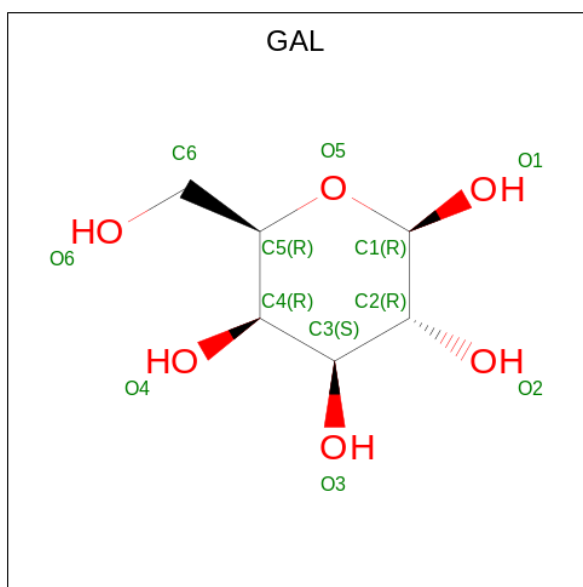
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 11	C 6	O 5	0	0
7	B	1	Total 11	C 6	O 5	0	0

- Molecule 8 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PRO PYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: $C_{11}H_{26}N_2O_6$).

B3P
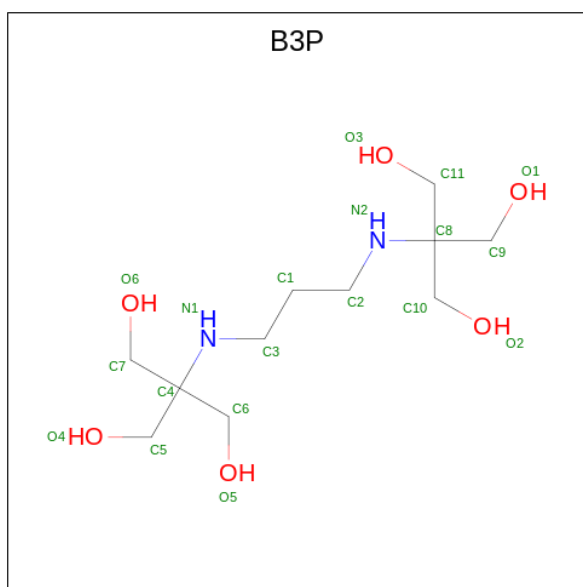
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total 19	C 11	N 2	O 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total 19	C 11	N 2	O 6	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

PEG
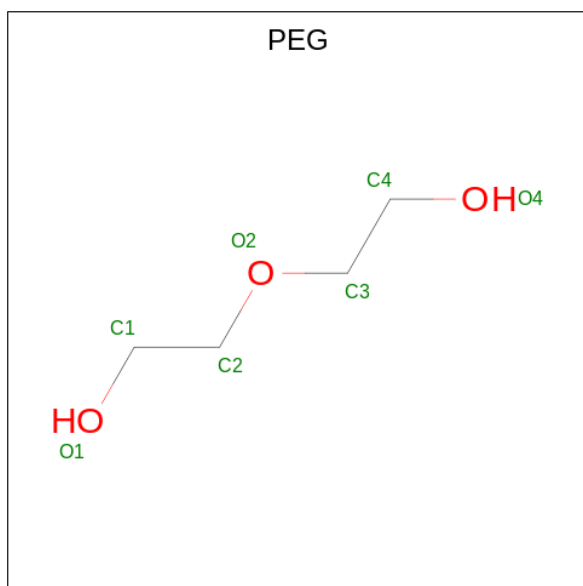
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 7	C 4	O 3	0	0
9	A	1	Total 7	C 4	O 3	0	0
9	A	1	Total 7	C 4	O 3	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	152	Total 152	O 152	0	0
10	B	68	Total 68	O 68	0	0

3 Residue-property plots ⓘ

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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: Beta-1,3-galactosyltransferase 5
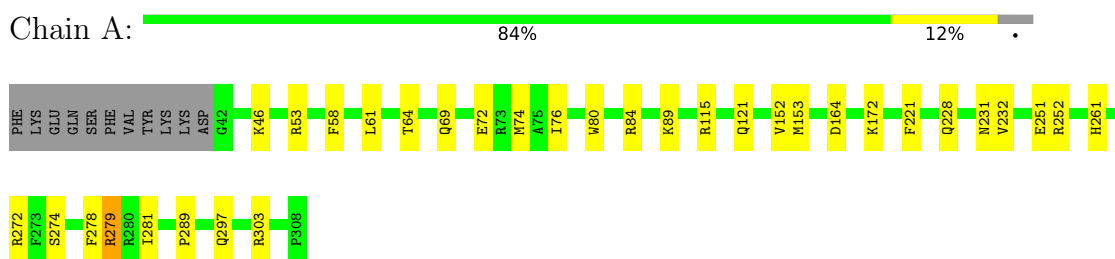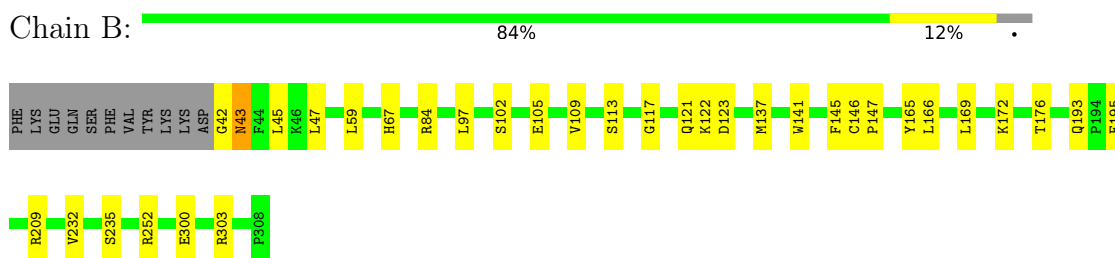
Chain A:

- Molecule 1: Beta-1,3-galactosyltransferase 5

Chain B:

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:
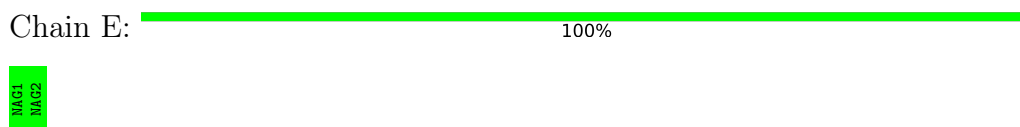
- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamid

o-2-deoxy-beta-D-glucopyranose

Chain F:

NAG1 NAG2 BMA3 MAN4 MAN5 FUC6

• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

NAG1 FUC2

4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	47.98Å 86.34Å 87.51Å 90.00° 95.48° 90.00°	Depositor
Resolution (Å)	26.63 – 2.30	Depositor
% Data completeness (in resolution range)	90.6 (26.63-2.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.83 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.180 , 0.212	Depositor
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.138	Xtriage
L-test for twinning[2]	$< \lvert L \rvert > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4946	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: BMA, B3P, MN, FUC, PEG, MAN, GAL, UDP, NAG

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	0.51	0/2252	0.75	0/3045
1	B	0.43	0/2252	0.66	0/3045
All	All	0.47	0/4504	0.70	0/6090

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	2
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ARG	Sidechain
1	A	272	ARG	Sidechain
1	A	279	ARG	Sidechain
1	A	303	ARG	Sidechain
1	A	53	ARG	Sidechain
1	B	209	ARG	Sidechain
1	B	84	ARG	Sidechain

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	2193	0	2178	23	0
1	B	2193	0	2178	19	0
2	E	28	0	25	0	0
2	G	28	0	25	0	0
3	F	71	56	61	2	0
4	D	24	0	22	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	25	0	11	0	0
6	B	25	0	11	0	0
7	A	11	0	10	0	0
7	B	11	0	10	0	0
8	A	19	0	26	1	0
8	B	19	0	26	1	0
9	A	21	0	30	3	0
10	A	152	0	0	8	0
10	B	68	0	0	3	0
All	All	4890	56	4613	47	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (47) 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)
10:B:561:HOH:O	3:F:6:FUC:H3	1.82	0.78
1:B:67:HIS:ND1	1:B:109:VAL:HG21	2.02	0.74
1:A:251:GLU:HG3	9:A:406:PEG:H32	1.80	0.64
10:B:561:HOH:O	3:F:6:FUC:C3	2.42	0.61
1:A:278:PHE:HA	1:A:281:ILE:HG12	1.82	0.61
1:A:232:VAL:CG2	1:A:252:ARG:HG2	2.32	0.59
1:A:61:LEU:HD23	1:A:153:MET:HB3	1.84	0.59
1:B:232:VAL:HG21	1:B:252:ARG:HG2	1.85	0.58
1:A:232:VAL:HG21	1:A:252:ARG:HG2	1.86	0.57
1:A:72:GLU:HG3	1:A:289:PRO:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:MET:HE2	10:A:546:HOH:O	2.04	0.55
1:B:176:THR:HB	10:B:557:HOH:O	2.05	0.55
1:B:232:VAL:CG2	1:B:252:ARG:HG2	2.37	0.55
1:A:64:THR:HG21	10:A:533:HOH:O	2.07	0.54
1:A:274:SER:HB3	10:A:589:HOH:O	2.08	0.54
1:B:300:GLU:O	1:B:303:ARG:HG2	2.08	0.54
1:A:69:GLN:NE2	10:A:503:HOH:O	2.39	0.54
1:B:42:GLY:O	1:B:43:ASN:HB2	2.08	0.53
1:A:231:ASN:ND2	10:A:504:HOH:O	2.41	0.53
1:B:97:LEU:O	1:B:121:GLN:HA	2.09	0.53
1:A:74:MET:CE	10:A:546:HOH:O	2.56	0.51
1:A:228:GLN:O	1:A:232:VAL:HG12	2.10	0.51
1:B:165:TYR:CE2	1:B:169:LEU:HD11	2.48	0.49
1:A:46:LYS:HA	9:A:405:PEG:H12	1.93	0.49
8:B:404:B3P:H32	8:B:404:B3P:H52	1.58	0.49
1:B:141:TRP:CD1	1:B:145:PHE:HD2	2.32	0.48
1:B:59:LEU:HD21	1:B:166:LEU:HD23	1.95	0.48
8:A:404:B3P:H32	8:A:404:B3P:H52	1.55	0.48
1:B:235:SER:OG	1:B:252:ARG:NH1	2.48	0.46
1:B:122:LYS:HD2	1:B:137:MET:HG3	1.99	0.45
1:A:84:ARG:HH22	1:A:164:ASP:CG	2.21	0.44
1:A:297:GLN:HB2	10:A:569:HOH:O	2.17	0.44
1:B:113:SER:O	1:B:117:GLY:N	2.40	0.44
1:A:76:ILE:HG12	1:A:80:TRP:CZ2	2.52	0.44
1:A:152:VAL:HB	1:A:221:PHE:CE2	2.53	0.43
1:A:279:ARG:NE	10:A:511:HOH:O	2.51	0.43
1:B:45:LEU:HD21	1:B:123:ASP:HB2	2.00	0.43
1:B:47:LEU:HD23	1:B:47:LEU:HA	1.85	0.42
9:A:407:PEG:H42	9:A:407:PEG:H21	1.78	0.41
1:B:172:LYS:HE3	1:B:172:LYS:HB2	1.71	0.41
1:A:232:VAL:HG21	1:A:252:ARG:CG	2.50	0.41
1:A:58:PHE:CB	1:A:89:LYS:HB3	2.51	0.41
1:A:172:LYS:HE2	1:A:261:HIS:HD2	1.86	0.41
1:A:46:LYS:HB2	1:A:121:GLN:HB3	2.03	0.41
1:B:193:GLN:HB3	1:B:195:PHE:CE2	2.56	0.41
1:B:146:CYS:N	1:B:147:PRO:CD	2.84	0.40
1:B:102:SER:HB3	1:B:105:GLU:HB2	2.03	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	265/278 (95%)	255 (96%)	10 (4%)	0	100	100
1	B	265/278 (95%)	257 (97%)	7 (3%)	1 (0%)	30	39
All	All	530/556 (95%)	512 (97%)	17 (3%)	1 (0%)	44	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	43	ASN

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	244/255 (96%)	244 (100%)	0	100	100
1	B	244/255 (96%)	244 (100%)	0	100	100
All	All	488/510 (96%)	488 (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. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	B	231	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 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	$\#|Z| > 2$
4	NAG	D	1	4,1	14,14,15	0.42	0	17,19,21	0.52	0
4	FUC	D	2	4	10,10,11	0.29	0	14,14,16	1.24	2 (14%)
2	NAG	E	1	2,1	14,14,15	0.46	0	17,19,21	0.63	0
2	NAG	E	2	2	14,14,15	0.43	0	17,19,21	0.62	0
3	NAG	F	1	3,1	14,14,15	0.43	0	17,19,21	1.11	1 (5%)
3	NAG	F	2	3	14,14,15	0.47	0	17,19,21	0.68	0
3	BMA	F	3	3	11,11,12	0.55	0	15,15,17	0.65	0
3	MAN	F	4	3	11,11,12	0.37	0	15,15,17	0.62	0
3	MAN	F	5	3	11,11,12	0.30	0	15,15,17	0.65	0
3	FUC	F	6	3	10,10,11	0.37	0	14,14,16	0.46	0
2	NAG	G	1	2,1	14,14,15	0.45	0	17,19,21	0.70	0
2	NAG	G	2	2	14,14,15	0.40	0	17,19,21	1.02	1 (5%)

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	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	FUC	D	2	4	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	FUC	F	6	3	-	-	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	2	FUC	C1-C2-C3	3.05	113.42	109.67
3	F	1	NAG	C2-N2-C7	3.02	127.20	122.90
2	G	2	NAG	C1-O5-C5	2.97	116.21	112.19
4	D	2	FUC	O5-C1-C2	2.77	115.05	110.77

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	G	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
2	G	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
4	D	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	6	FUC	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 oligosaccharide.

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings
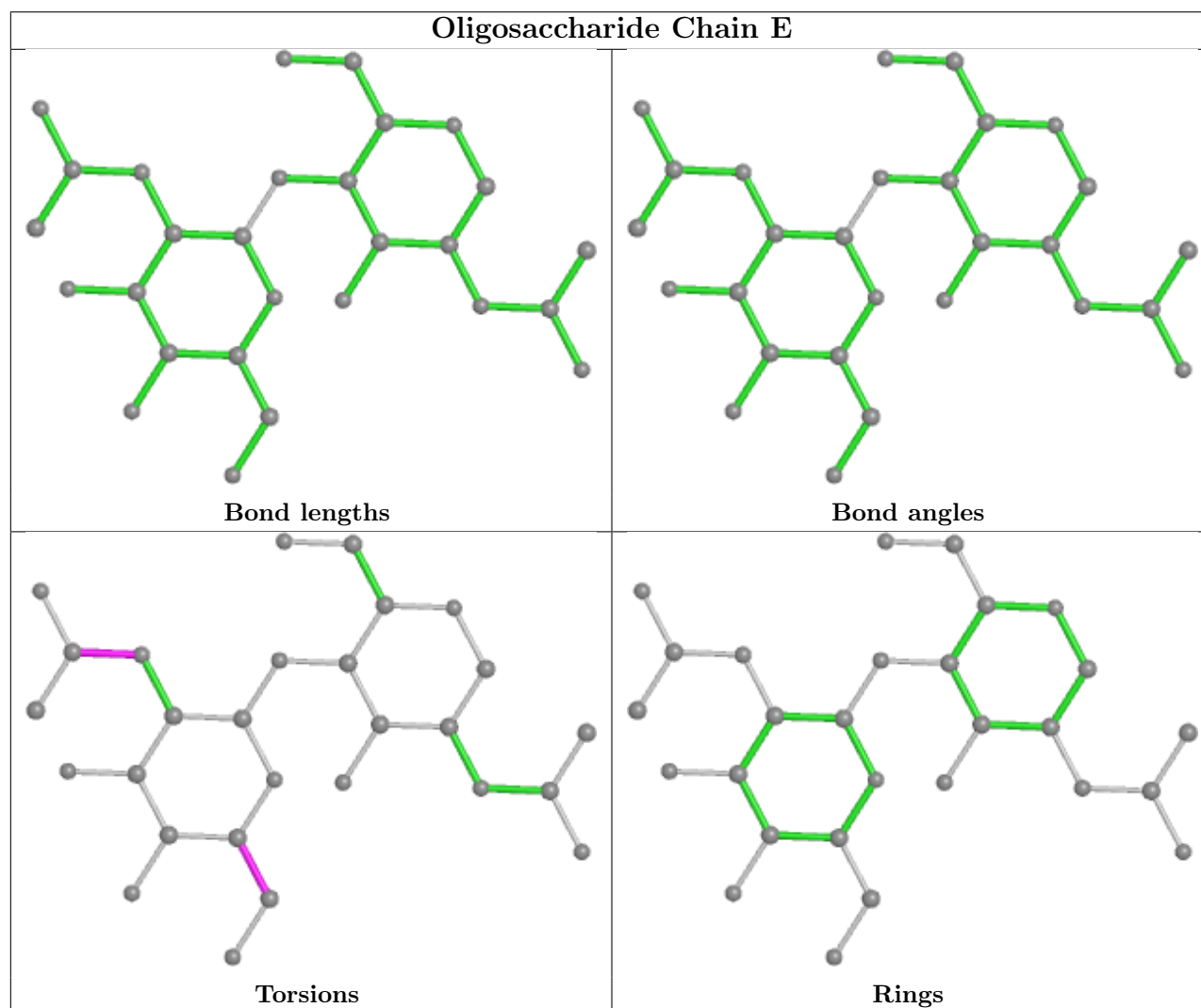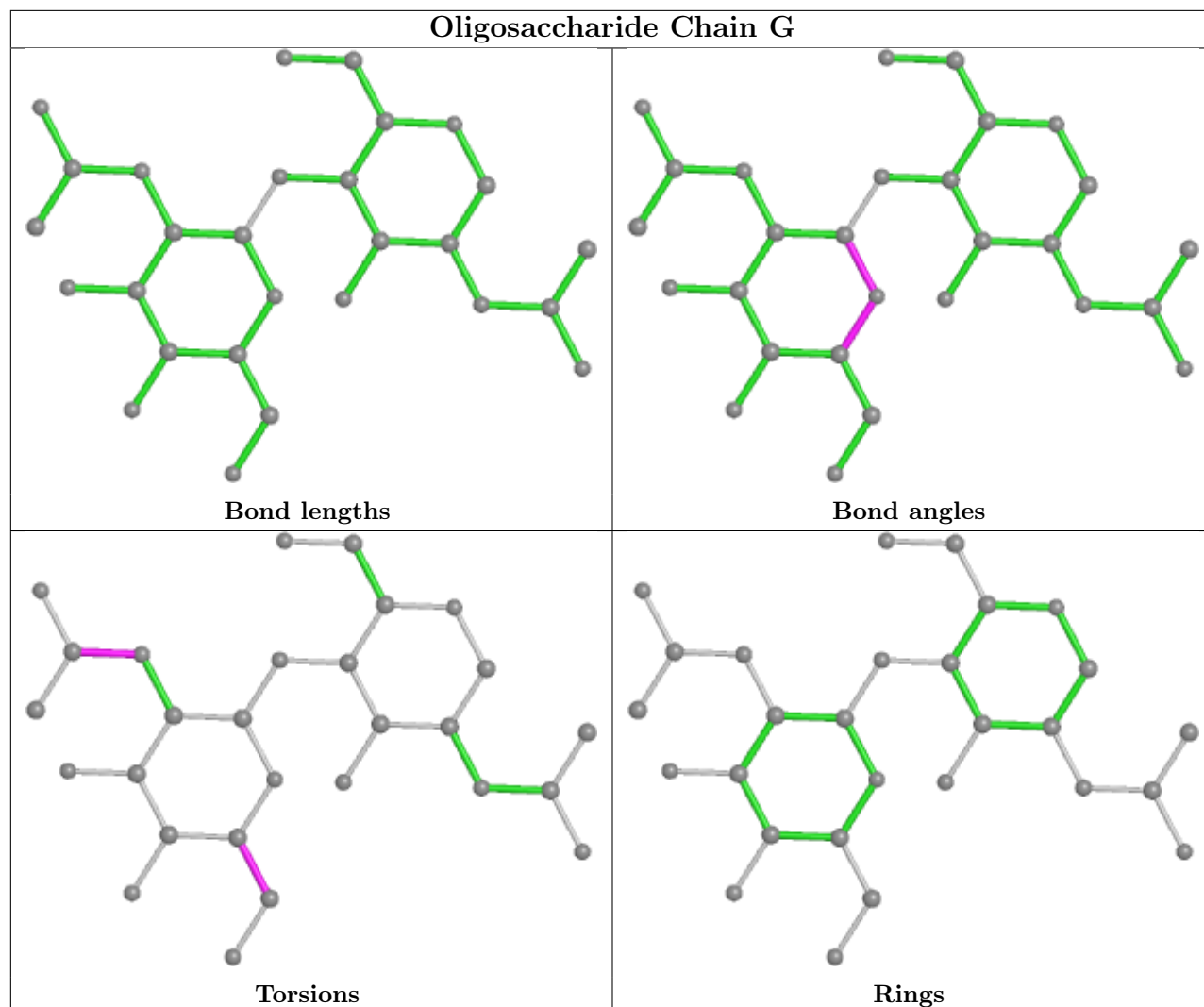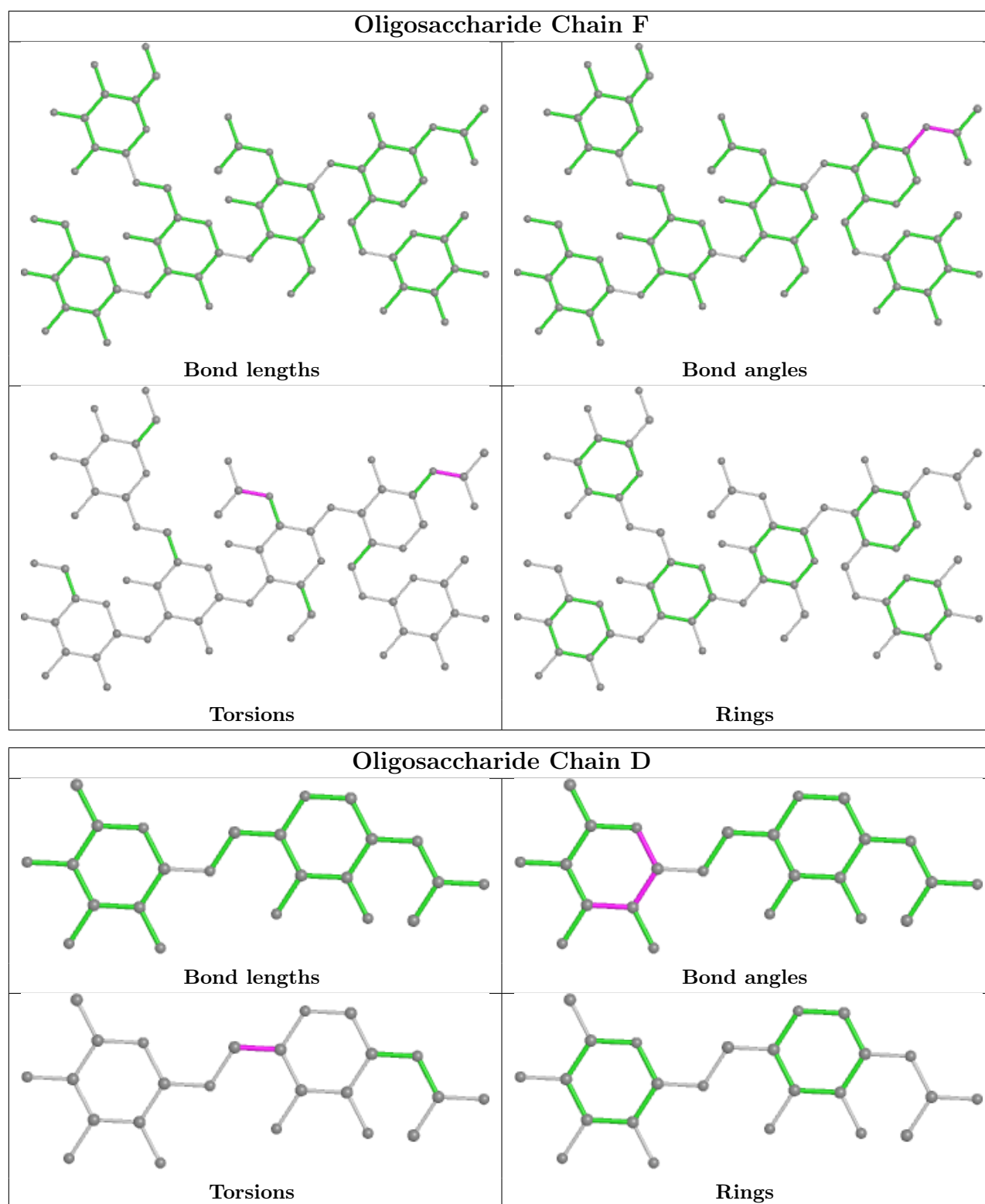
5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\#|Z| > 2$
6	UDP	B	402	5	24,26,26	0.53	0	37,40,40	0.51	0
9	PEG	A	405	-	6,6,6	0.09	0	5,5,5	0.13	0
7	GAL	A	403	-	11,11,12	0.61	0	15,15,17	2.28	4 (26%)
6	UDP	A	402	5	24,26,26	0.53	0	37,40,40	0.48	0
8	B3P	B	404	-	18,18,18	0.63	0	21,23,23	1.53	2 (9%)
8	B3P	A	404	-	18,18,18	0.60	0	21,23,23	1.66	4 (19%)
9	PEG	A	406	-	6,6,6	0.22	0	5,5,5	0.19	0
9	PEG	A	407	-	6,6,6	0.11	0	5,5,5	0.07	0
7	GAL	B	403	-	11,11,12	0.61	0	15,15,17	2.27	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
6	UDP	B	402	5	-	7/16/32/32	0/2/2/2
9	PEG	A	405	-	-	3/4/4/4	-
7	GAL	A	403	-	-	2/2/19/22	0/1/1/1
6	UDP	A	402	5	-	3/16/32/32	0/2/2/2
8	B3P	B	404	-	-	4/28/28/28	-
8	B3P	A	404	-	-	6/28/28/28	-
9	PEG	A	406	-	-	3/4/4/4	-
9	PEG	A	407	-	-	2/4/4/4	-
7	GAL	B	403	-	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	403	GAL	O5-C1-C2	6.13	120.24	110.77
7	B	403	GAL	O5-C1-C2	6.11	120.20	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	403	GAL	C1-O5-C5	4.82	118.72	112.19
7	A	403	GAL	C1-O5-C5	4.81	118.70	112.19
8	B	404	B3P	C3-N1-C4	-4.59	109.57	116.08
8	A	404	B3P	C3-N1-C4	-4.51	109.68	116.08
8	A	404	B3P	C2-N2-C8	-3.80	110.69	116.08
8	B	404	B3P	C2-N2-C8	-3.47	111.15	116.08
8	A	404	B3P	O2-C10-C8	-2.50	106.58	111.63
7	A	403	GAL	C2-C3-C4	-2.14	107.20	110.89
7	A	403	GAL	C1-C2-C3	2.14	112.29	109.67
7	B	403	GAL	C1-C2-C3	2.13	112.29	109.67
7	B	403	GAL	C2-C3-C4	-2.12	107.23	110.89
8	A	404	B3P	O4-C5-C4	-2.09	107.39	111.63

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	402	UDP	PA-O3A-PB-O3B
6	B	402	UDP	C5'-O5'-PA-O1A
6	B	402	UDP	C5'-O5'-PA-O2A
8	A	404	B3P	N1-C4-C5-O4
8	A	404	B3P	C6-C4-C5-O4
8	A	404	B3P	C7-C4-C5-O4
8	A	404	B3P	N1-C4-C6-O5
8	A	404	B3P	C5-C4-C6-O5
8	A	404	B3P	C7-C4-C6-O5
9	A	407	PEG	O1-C1-C2-O2
7	B	403	GAL	O5-C5-C6-O6
7	A	403	GAL	O5-C5-C6-O6
7	A	403	GAL	C4-C5-C6-O6
6	B	402	UDP	O4'-C4'-C5'-O5'
7	B	403	GAL	C4-C5-C6-O6
9	A	406	PEG	O2-C3-C4-O4
9	A	407	PEG	C4-C3-O2-C2
9	A	406	PEG	O1-C1-C2-O2
9	A	406	PEG	C4-C3-O2-C2
9	A	405	PEG	O2-C3-C4-O4
8	B	404	B3P	C7-C4-C6-O5
8	B	404	B3P	C5-C4-C6-O5
6	B	402	UDP	C2'-C1'-N1-C6
9	A	405	PEG	C1-C2-O2-C3
6	B	402	UDP	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
6	B	402	UDP	O4'-C1'-N1-C6
8	B	404	B3P	C3-C1-C2-N2
6	A	402	UDP	PA-O3A-PB-O1B
8	B	404	B3P	N1-C4-C6-O5
6	B	402	UDP	C5'-O5'-PA-O3A
6	A	402	UDP	PB-O3A-PA-O2A
9	A	405	PEG	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	405	PEG	1	0
8	B	404	B3P	1	0
8	A	404	B3P	1	0
9	A	406	PEG	1	0
9	A	407	PEG	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 UDP B 402

Bond lengths

Bond angles

Torsions

Rings

Ligand GAL A 403

Bond lengths

Bond angles

Torsions

Rings

Ligand UDP A 402

Bond lengths

Bond angles

Torsions

Rings

Ligand B3P B 404

Bond lengths

Bond angles

Torsions

Rings

Ligand B3P A 404

Bond lengths

Bond angles

Torsions

Rings

Ligand GAL B 403

Bond lengths

Bond angles

Torsions

Rings
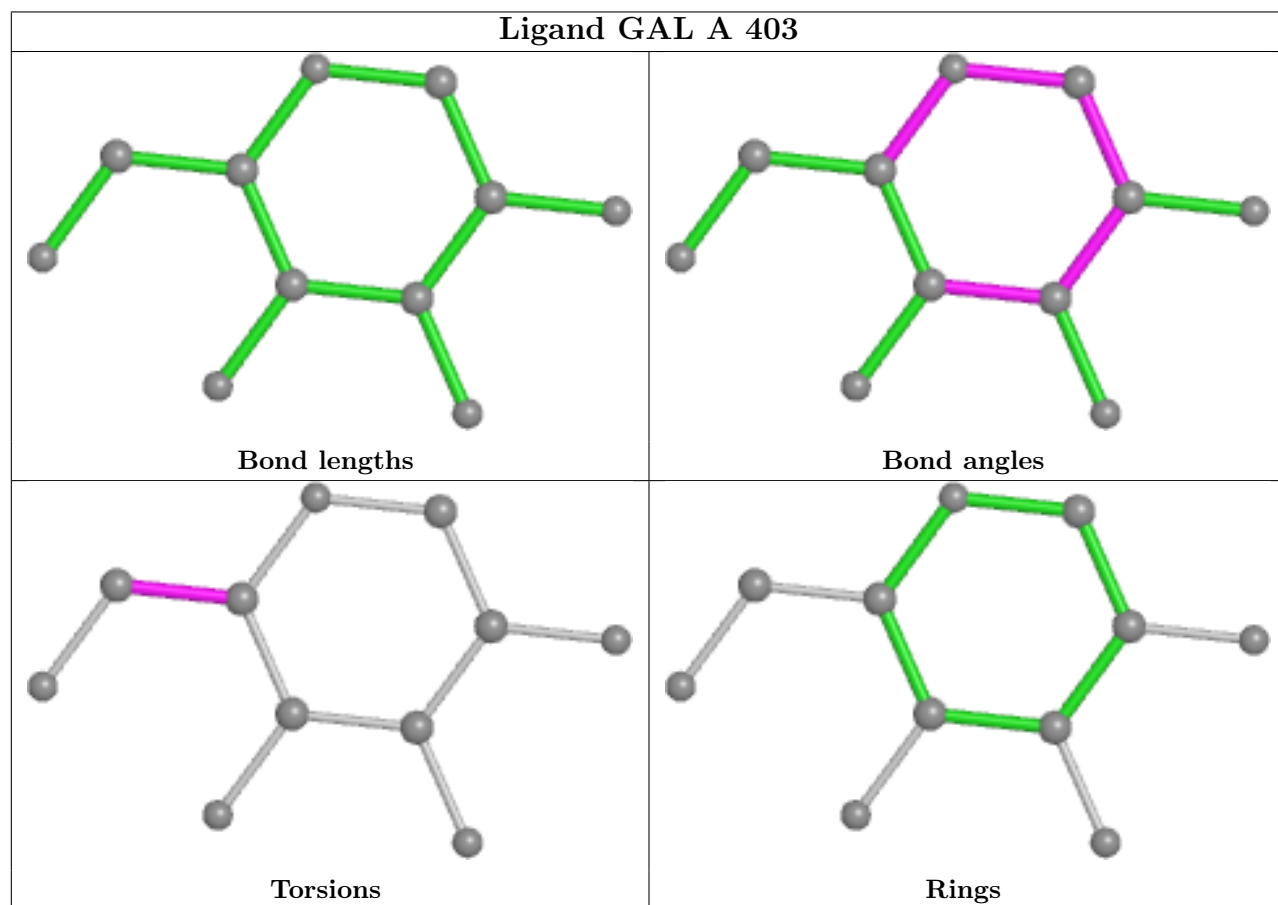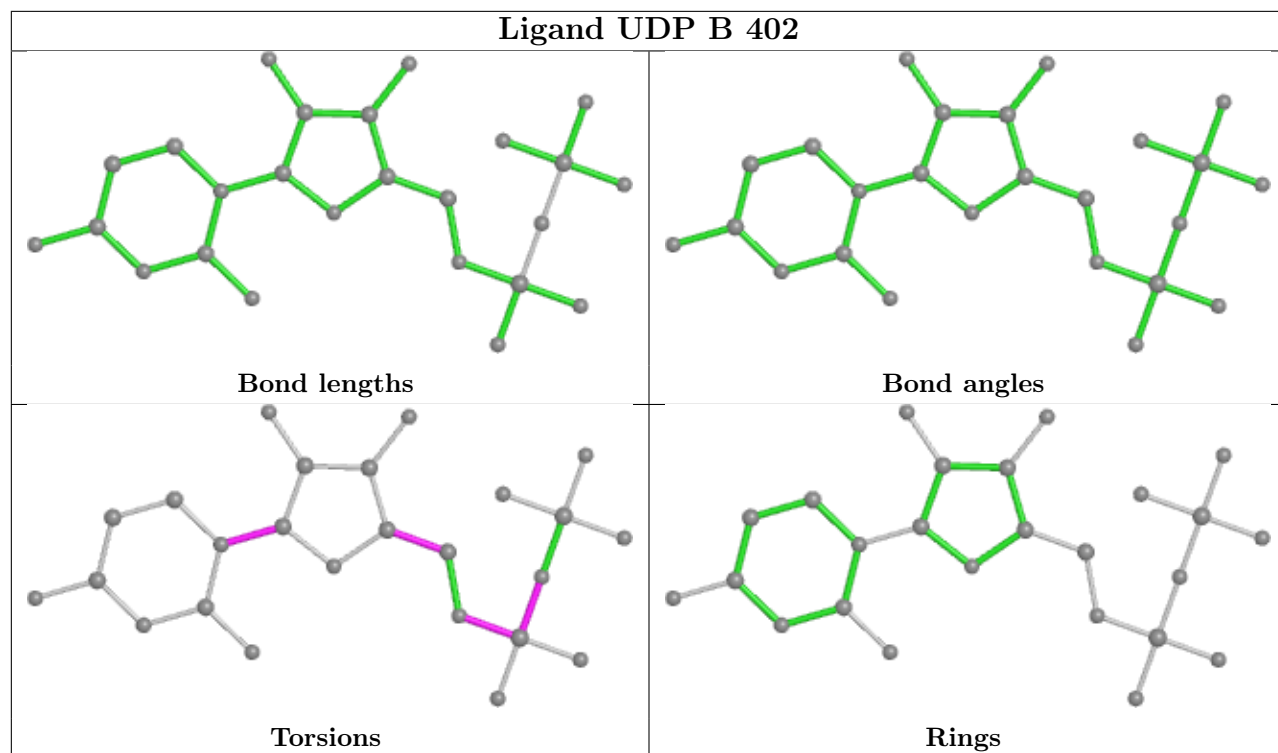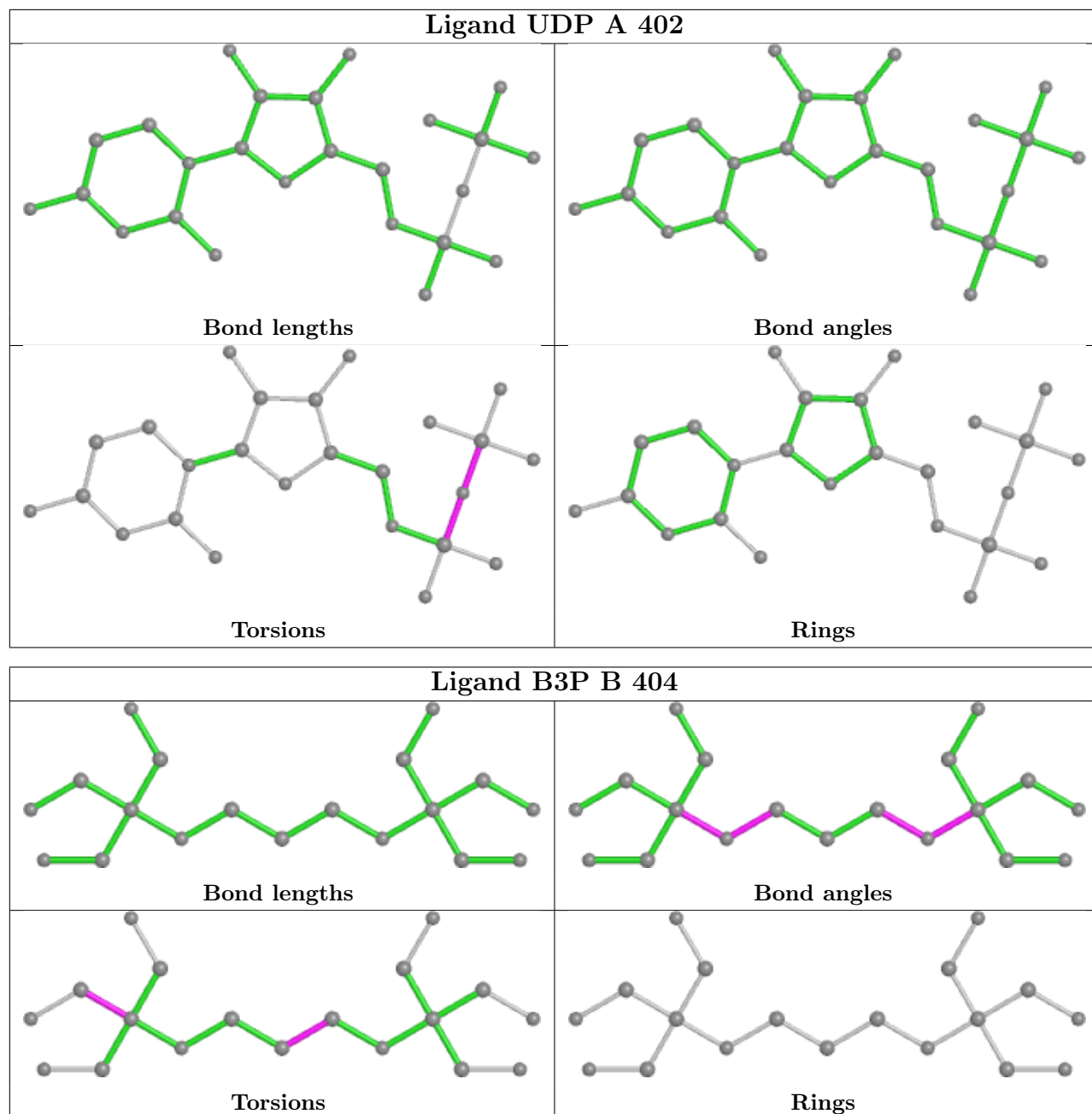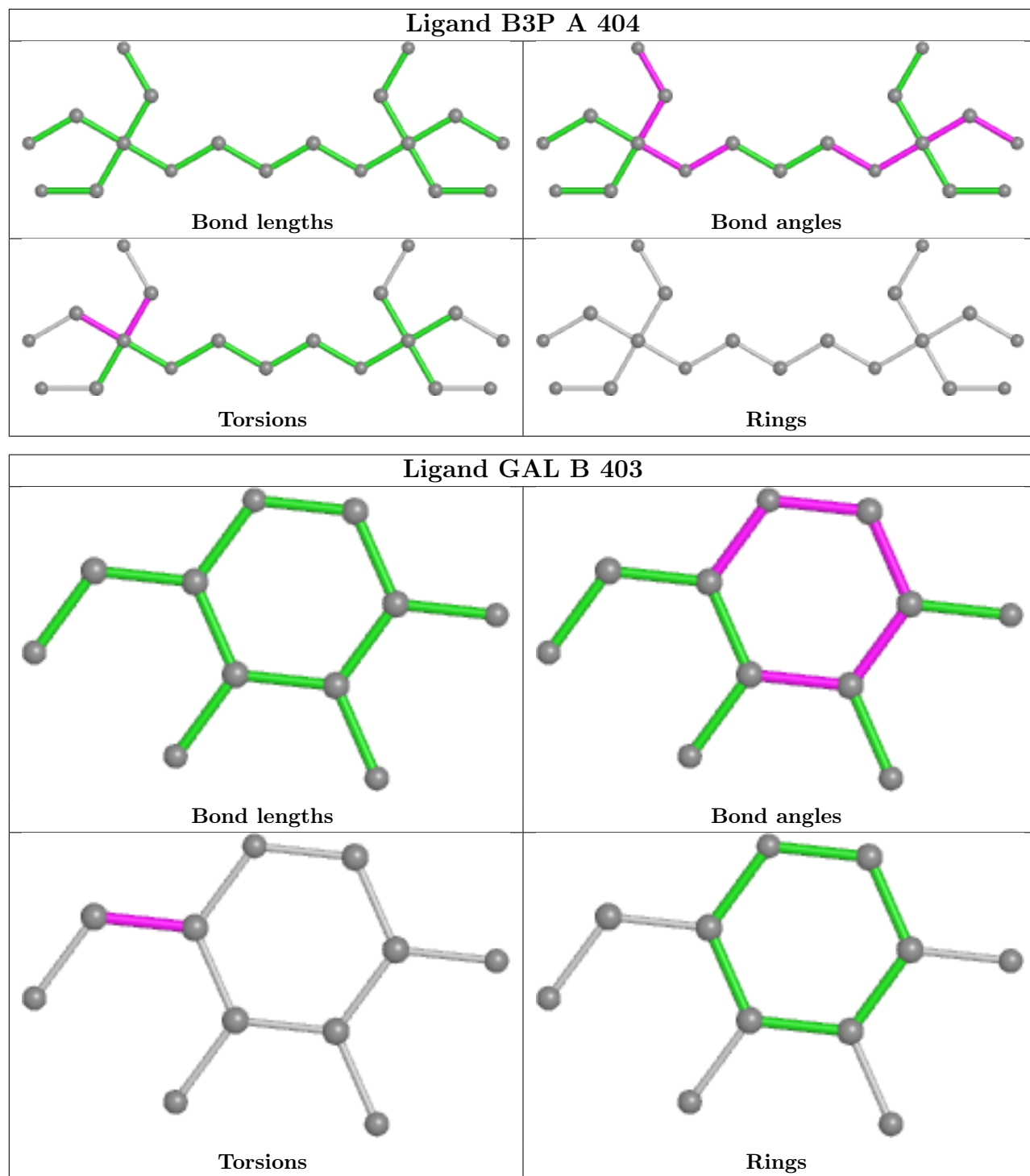
5.7 Other polymers ⓘ

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 ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3　Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

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 E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
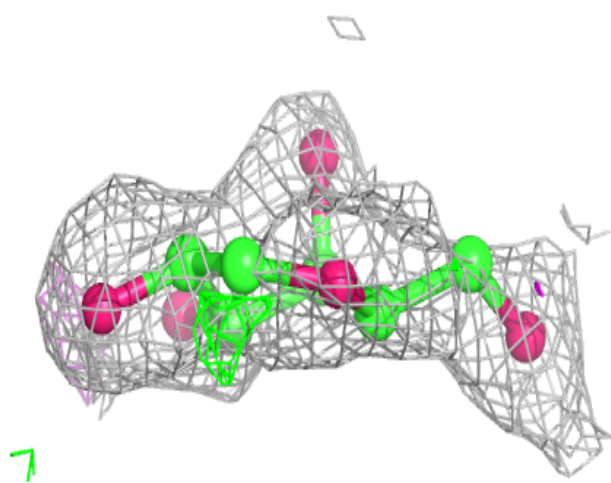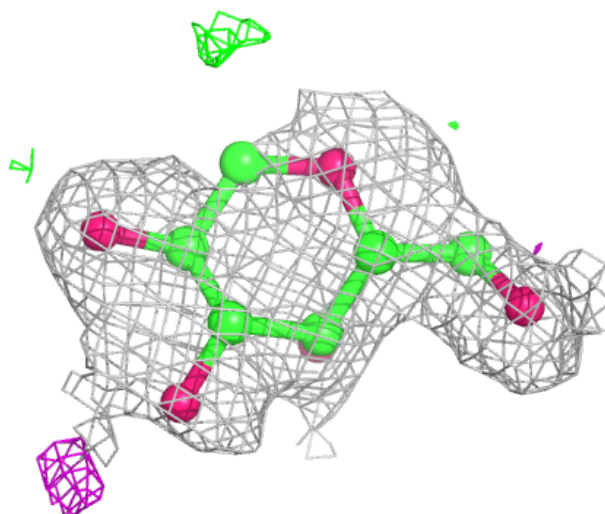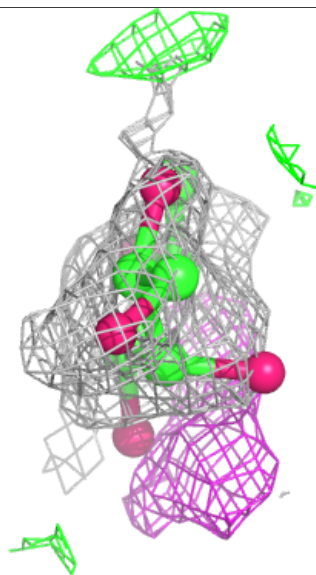and green (positive)
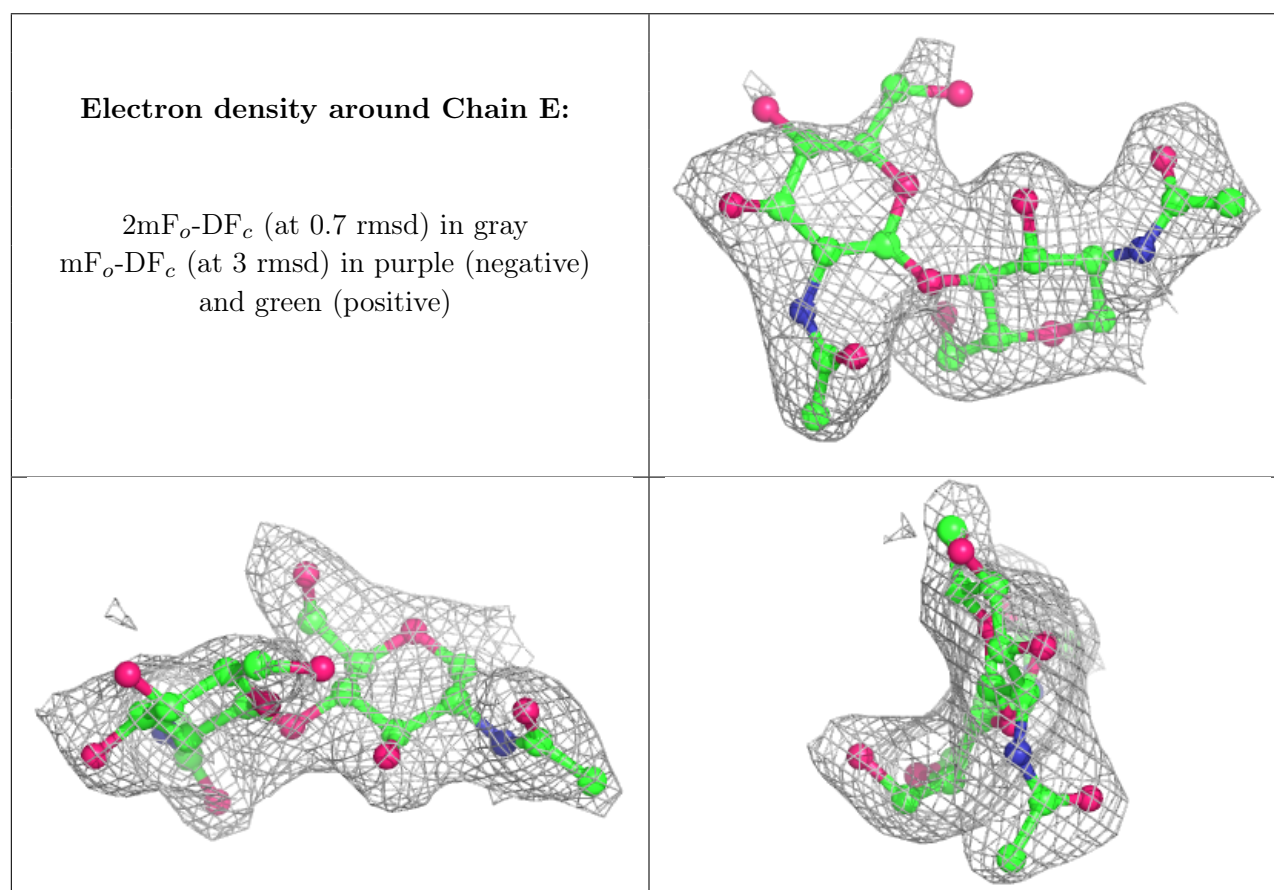
Electron density around Chain G:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
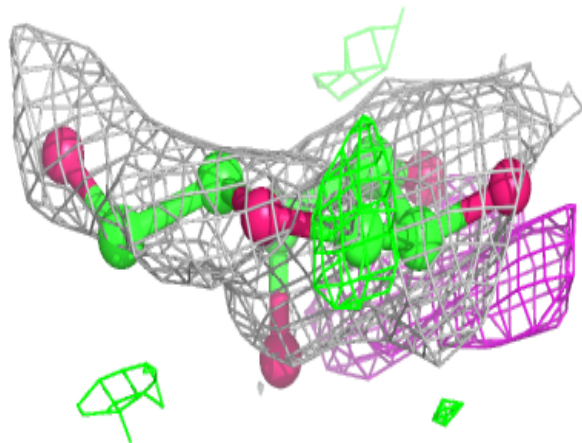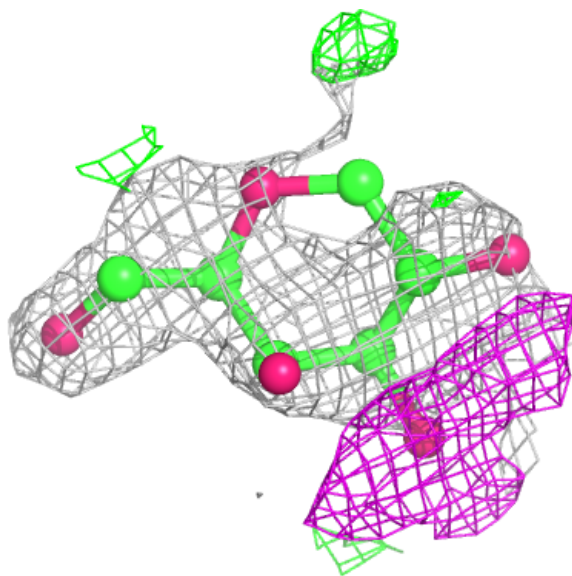and green (positive)
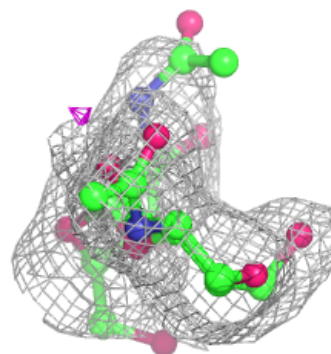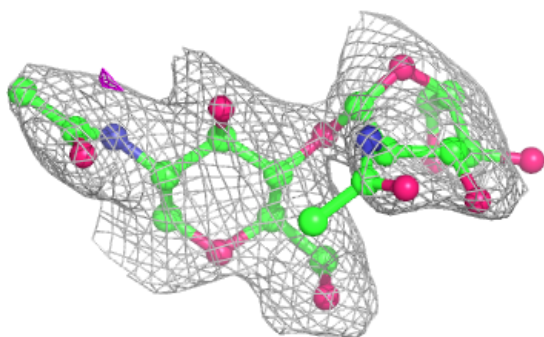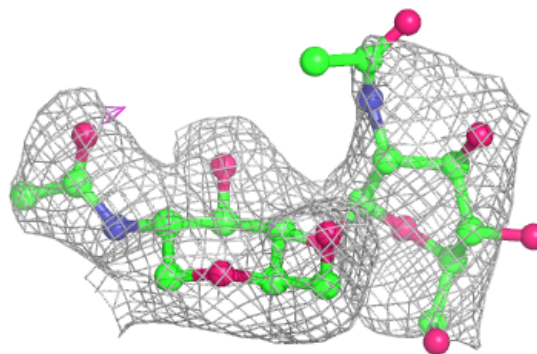
Electron density around Chain F:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
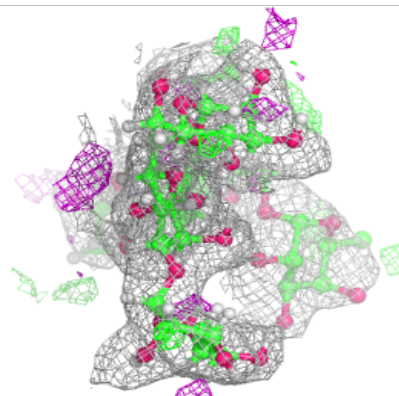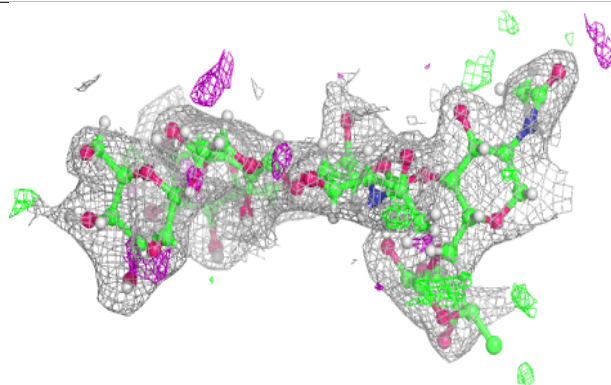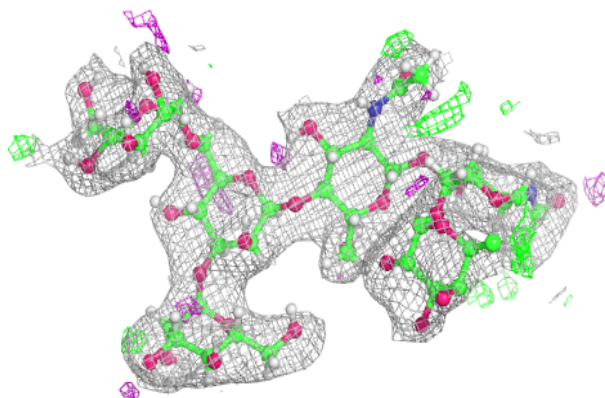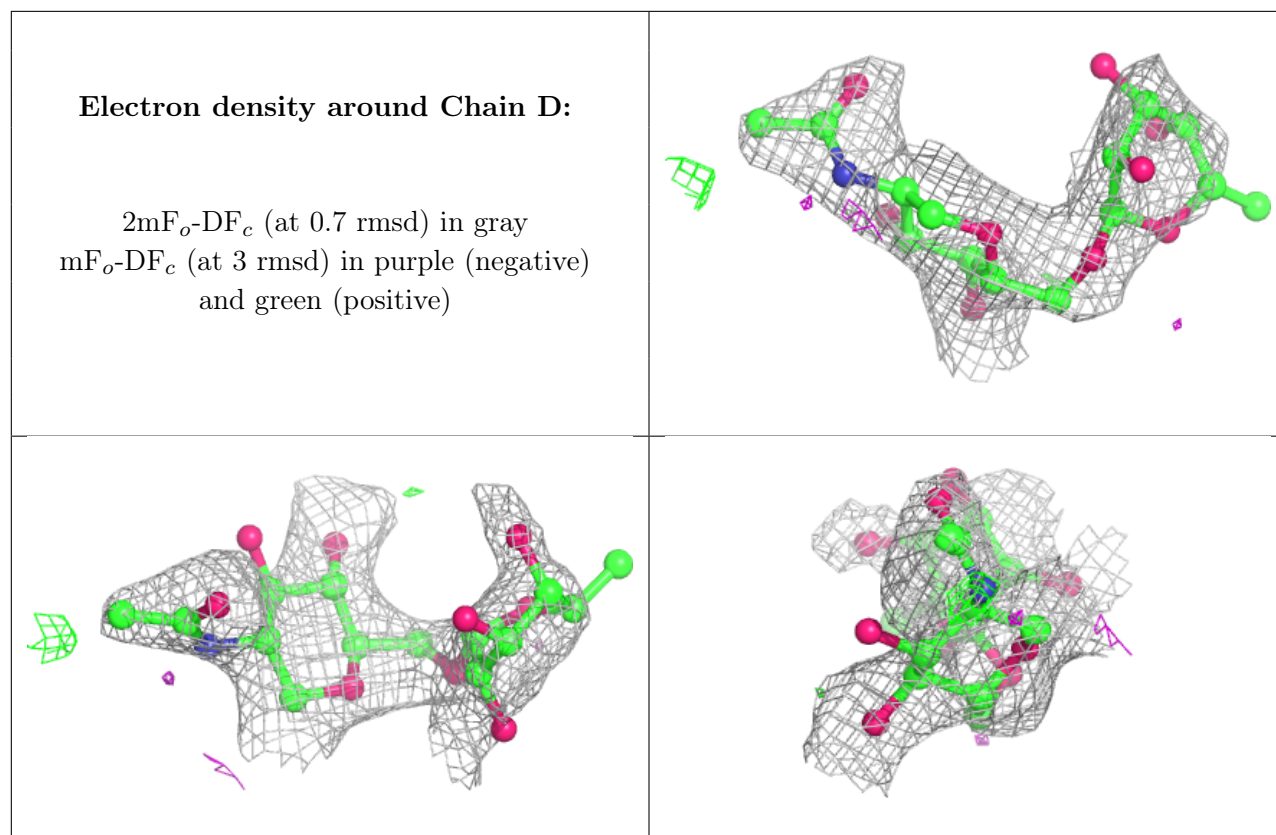
Electron density around Chain D:

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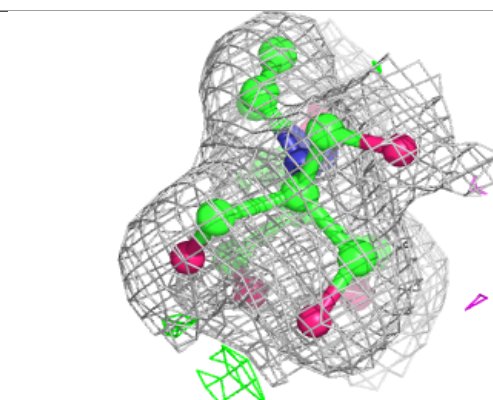mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

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 MN A 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
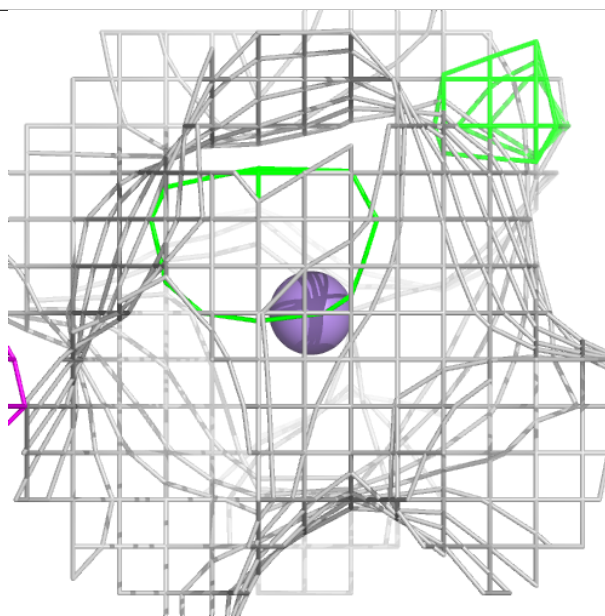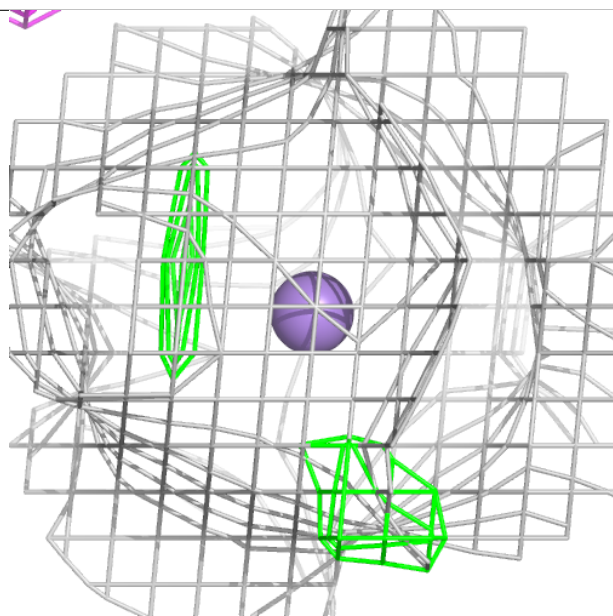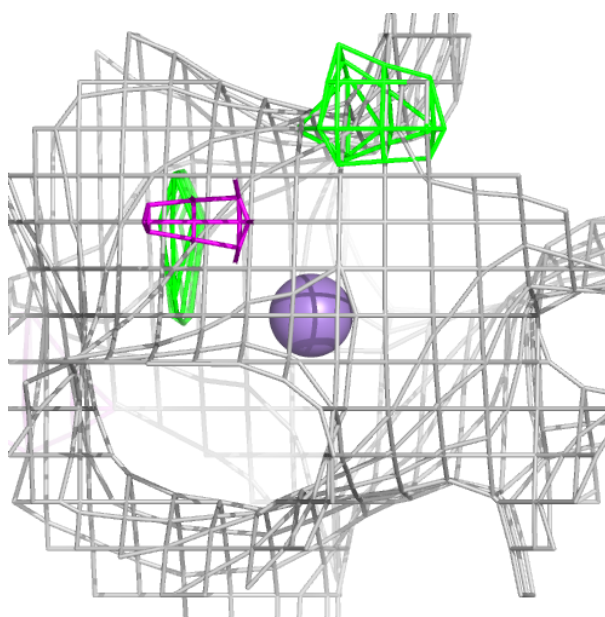
Electron density around MN B 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
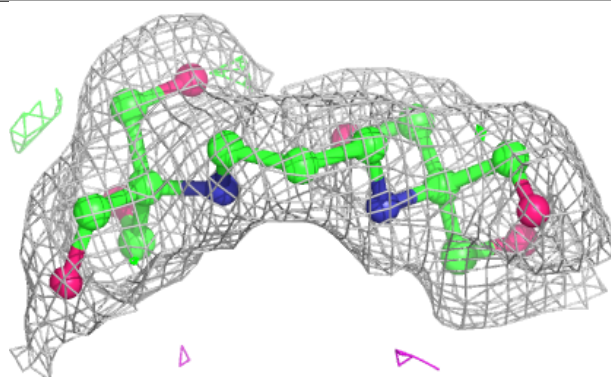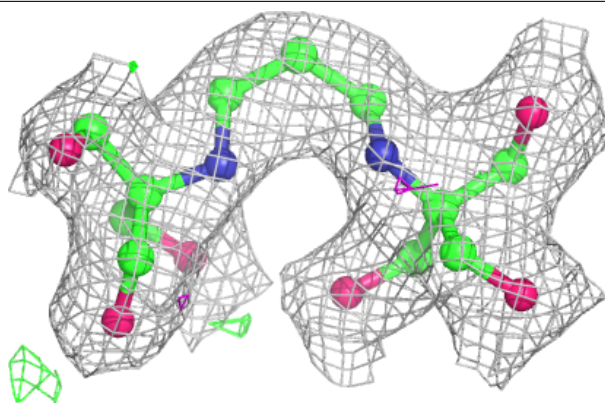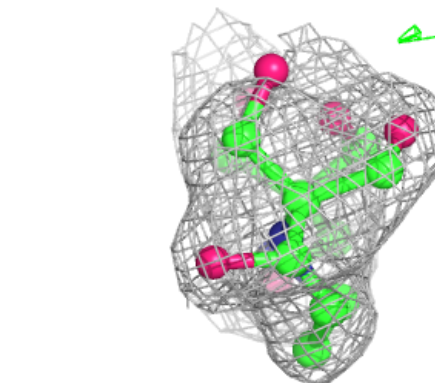mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
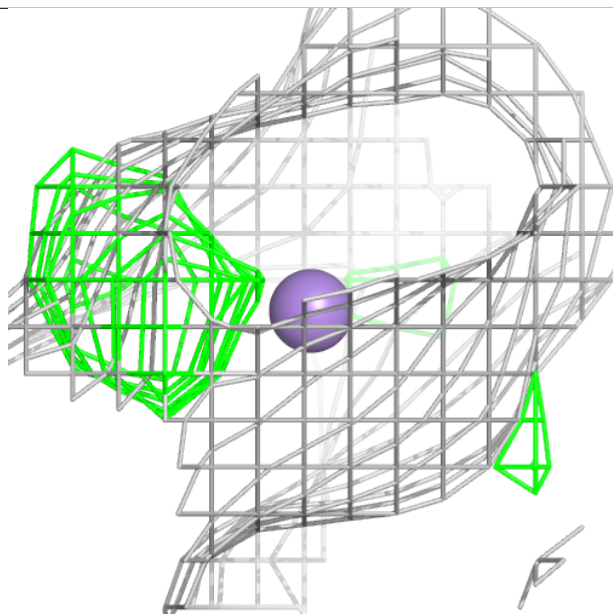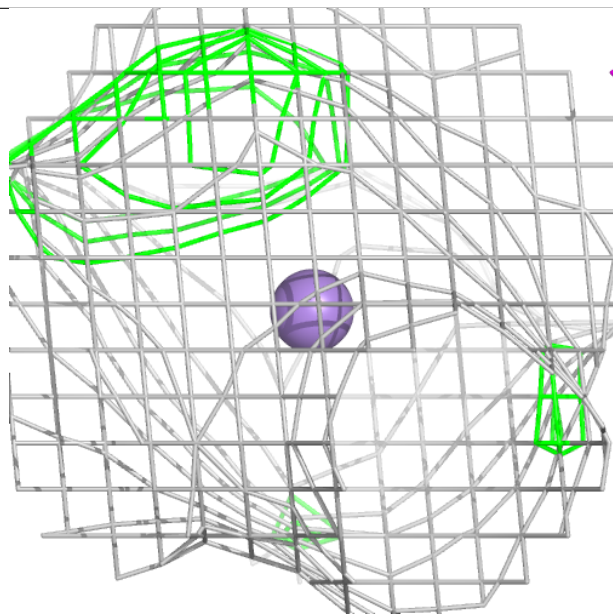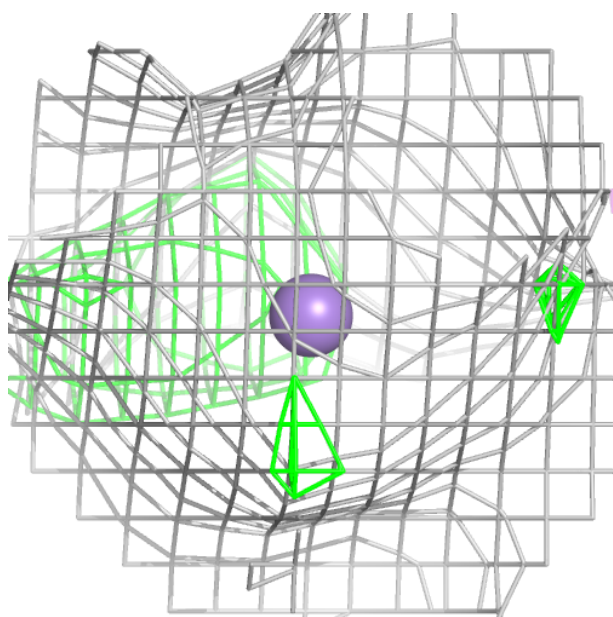
Electron density around UDP A 402:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
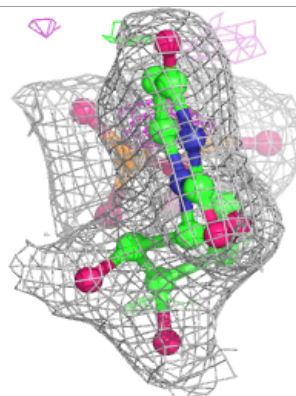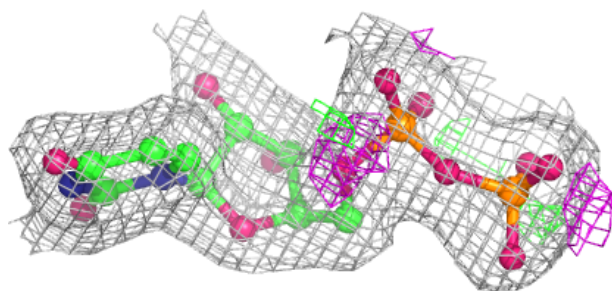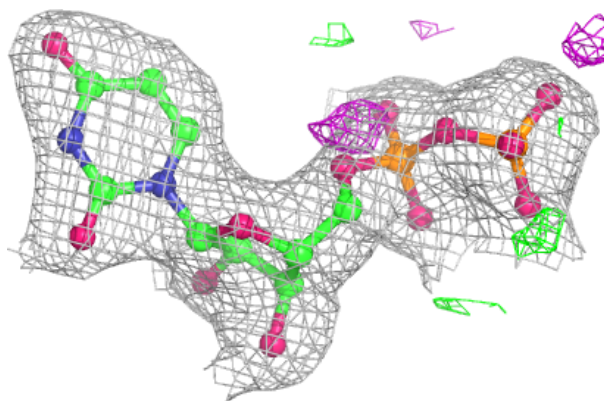
Electron density around UDP B 402:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
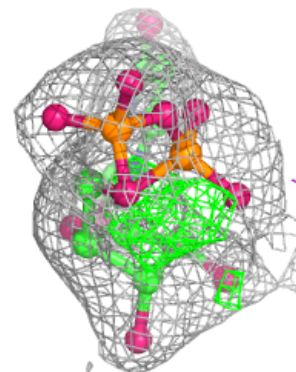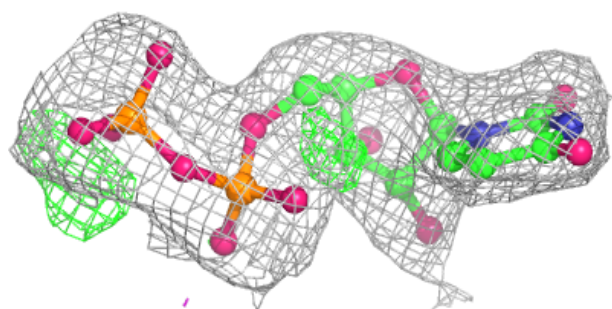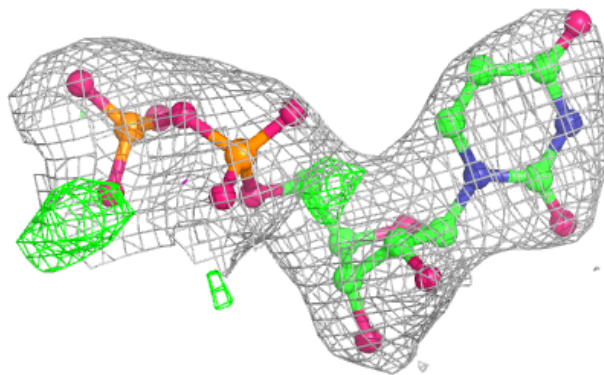
Electron density around GAL A 403:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
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and green (positive)
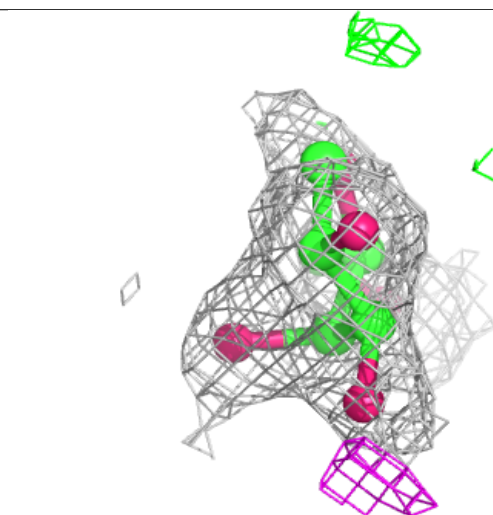
Electron density around GAL B 403:

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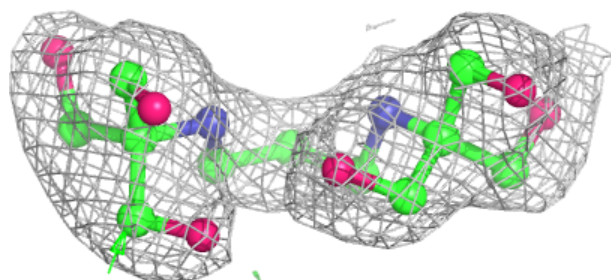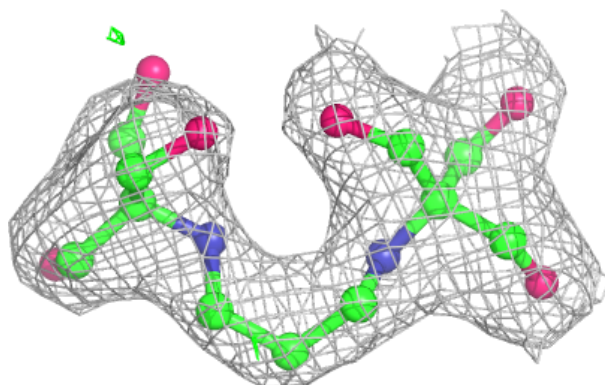$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around B3P A 404:

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

Electron density around B3P B 404:

$2mF_o$-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 ⓘ

EDS failed to run properly - this section is therefore empty.