



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2020 – 12:33 PM EST

PDB ID : 6WMO
Title : Human poly-N-acetyl-lactosamine synthase structure demonstrates a modular assembly of catalytic subsites for GT-A glycosyltransferases
Authors : Kadirvelraj, R.; Wood, Z.A.
Deposited on : 2020-04-21
Resolution : 1.85 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 : 2.14.6
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) : 2.14.6

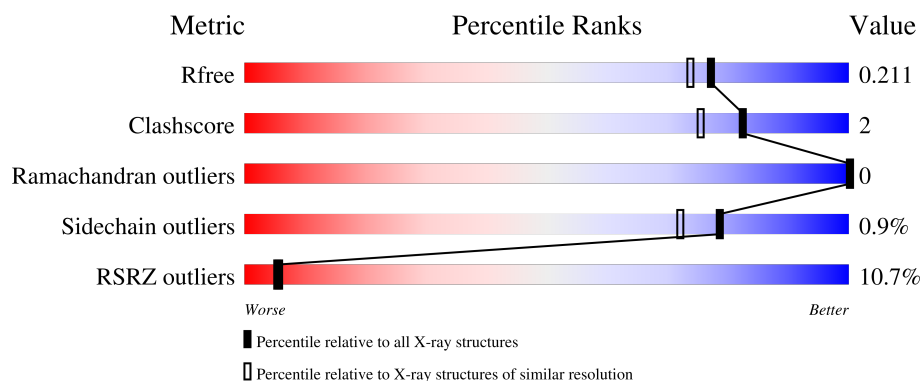
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	364	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>5%</div> <div>11%</div> </div> </div>
1	B	364	<div> <div>12%</div> <div> <div></div> <div>79%</div> <div>7%</div> <div>14%</div> </div> </div>
2	C	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>
2	E	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>
3	D	4	<div> <div></div> <div> <div>25%</div> <div>75%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	4	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	F	4	-	-	-	X
7	EDO	A	412	-	-	X	-
7	EDO	B	415	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5826 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.

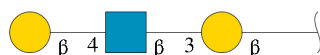
- Molecule 1 is a protein called N-acetylglucosaminide beta-1,3-N-acetylglucosaminyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	8	0
			2714	1743	466	493	12			
1	B	313	Total	C	N	O	S	0	1	0
			2588	1665	443	469	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	expression tag	UNP Q9NY97
B	34	GLY	-	expression tag	UNP Q9NY97

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			37	20	1	16			
2	E	3	Total	C	N	O	0	0	0
			37	20	1	16			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

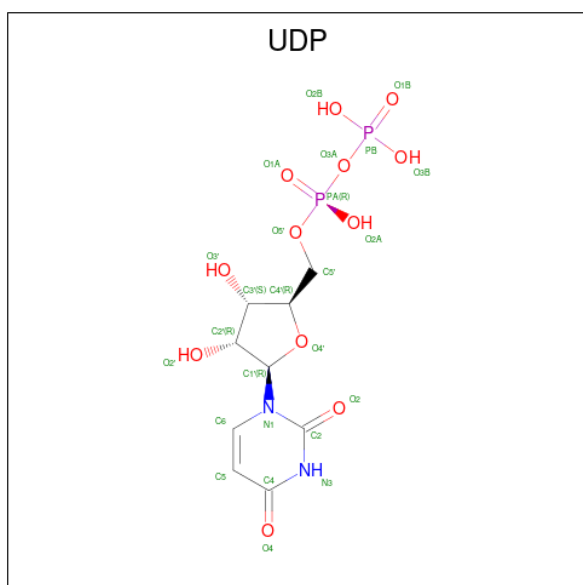


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

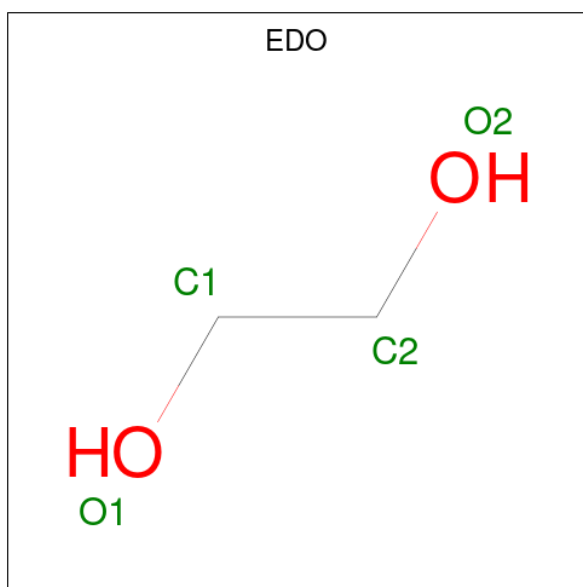
- Molecule 5 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).





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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



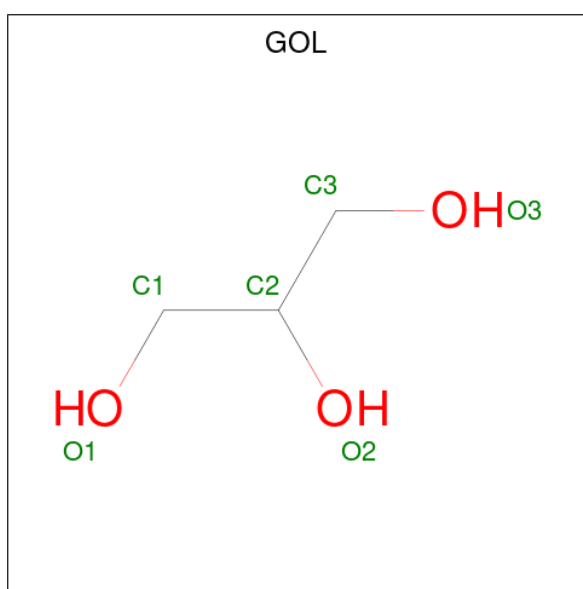
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		

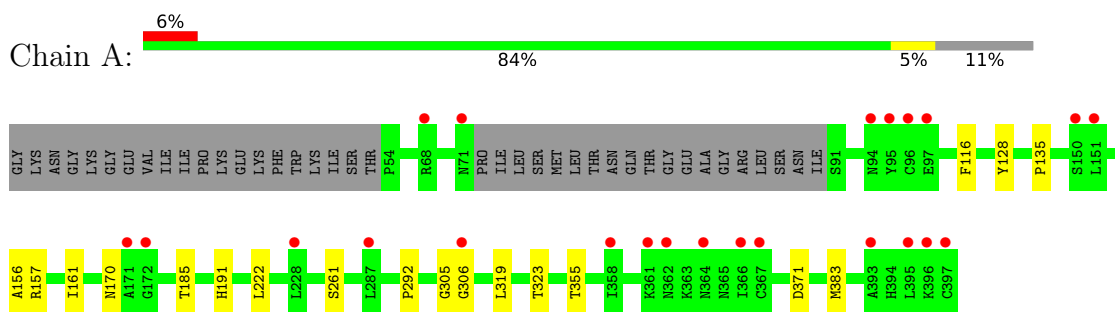
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	121	Total	O	0	0
			121	121		
9	B	109	Total	O	0	0
			109	109		

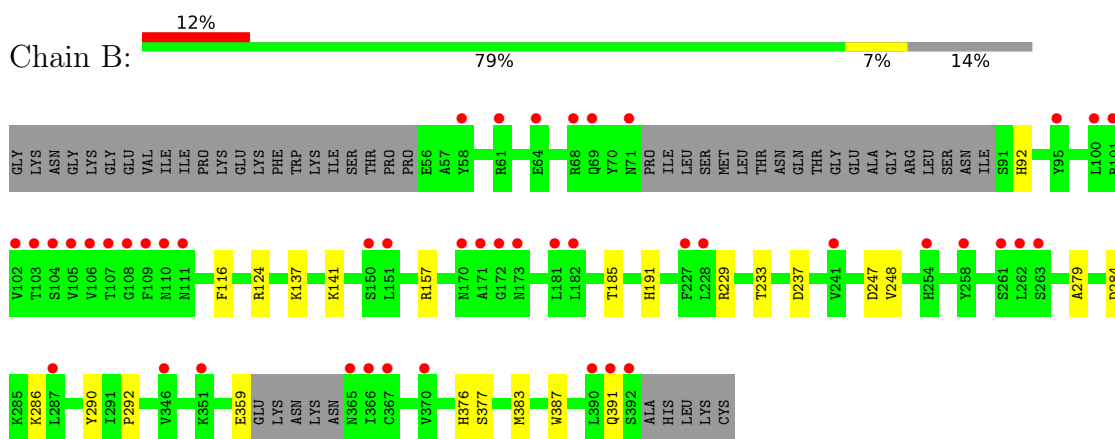
3 Residue-property plots [i](#)

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

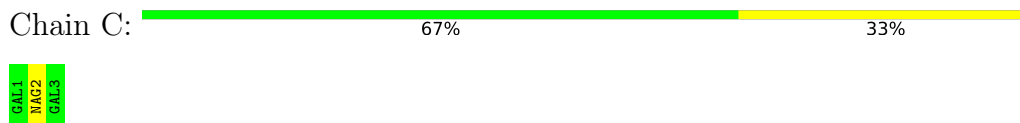
- Molecule 1: N-acetylactosaminide beta-1,3-N-acetylglucosaminyltransferase 2



- Molecule 1: N-acetylactosaminide beta-1,3-N-acetylglucosaminyltransferase 2



- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose





- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.19Å 109.28Å 147.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.85 – 1.85 37.85 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.85-1.85) 99.8 (37.85-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.183 , 0.211 0.183 , 0.211	Depositor DCC
R_{free} test set	3367 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5826	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: GOL, MG, BMA, NAG, EDO, UDP, GAL, MAN

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	0.38	0/2800	0.56	0/3792
1	B	0.38	0/2661	0.55	0/3605
All	All	0.38	0/5461	0.55	0/7397

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	2714	0	2655	10	0
1	B	2588	0	2525	15	0
2	C	37	0	33	0	0
2	E	37	0	33	1	0
3	D	50	0	43	0	0
3	F	50	0	43	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	25	0	11	0	0
5	B	25	0	11	1	0
6	A	28	0	26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	14	0	13	0	0
7	A	4	0	6	4	0
7	B	16	0	23	3	0
8	B	6	0	8	1	0
9	A	121	0	0	1	0
9	B	109	0	0	0	0
All	All	5826	0	5430	27	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 2.

All (27) 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:156:ALA:HB3	7:A:412:EDO:H11	1.73	0.69
1:A:161:ILE:HG13	1:A:383:MET:HE1	1.82	0.61
1:A:305[B]:GLY:O	1:A:355:THR:HG21	2.07	0.54
1:A:306[B]:GLY:HA3	1:A:355:THR:HB	1.92	0.51
1:B:284:ASP:OD1	1:B:286:LYS:HG2	2.11	0.51
1:A:116:PHE:CZ	1:A:292:PRO:HD3	2.48	0.49
7:A:412:EDO:H22	9:A:602:HOH:O	2.13	0.49
1:B:141:LYS:HE3	1:B:237:ASP:OD2	2.14	0.48
1:B:248:VAL:O	1:B:383:MET:HE3	2.13	0.48
5:B:402:UDP:O3B	8:B:413:GOL:H31	2.14	0.47
1:B:137:LYS:NZ	7:B:415:EDO:H12	2.28	0.47
1:A:156:ALA:HB3	7:A:412:EDO:C1	2.41	0.46
1:B:157:ARG:HG3	7:B:411:EDO:H11	1.97	0.45
1:B:279:ALA:HA	2:E:2:NAG:H82	1.98	0.45
1:B:247:ASP:OD2	7:B:412:EDO:O1	2.35	0.45
1:B:247:ASP:C	1:B:383:MET:HE1	2.37	0.45
1:A:128:TYR:CE2	1:A:222:LEU:HD21	2.51	0.45
1:B:290:TYR:CE2	1:B:292:PRO:HG3	2.53	0.43
1:A:319:LEU:O	1:A:323:THR:HG23	2.19	0.43
1:B:185:THR:HB	1:B:191:HIS:CG	2.54	0.43
1:B:116:PHE:CZ	1:B:292:PRO:HD3	2.54	0.42
1:B:92:HIS:HA	1:B:124:ARG:HB3	2.01	0.42
1:B:376:HIS:HA	1:B:377:SER:HA	1.75	0.42
1:B:387:TRP:O	1:B:391:GLN:HG2	2.20	0.42
1:B:229:ARG:O	1:B:233:THR:HG23	2.21	0.41
1:A:185:THR:HB	1:A:191:HIS:CG	2.56	0.41
1:A:157:ARG:HG3	7:A:412:EDO:H12	2.02	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/364 (90%)	318 (97%)	11 (3%)	0	100	100
1	B	308/364 (85%)	301 (98%)	7 (2%)	0	100	100
All	All	637/728 (88%)	619 (97%)	18 (3%)	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	303/331 (92%)	298 (98%)	5 (2%)	60	47
1	B	288/331 (87%)	287 (100%)	1 (0%)	92	91
All	All	591/662 (89%)	585 (99%)	6 (1%)	78	69

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	PRO
1	A	170	ASN
1	A	261[A]	SER
1	A	261[B]	SER
1	A	371	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	359	GLU

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

Mol	Chain	Res	Type
1	B	174	GLN
1	B	260	ASN
1	B	327	HIS

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 ⓘ

14 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	GAL	C	1	2	12,12,12	0.70	0	17,17,17	0.76	0
2	NAG	C	2	2	14,14,15	0.32	0	17,19,21	0.94	1 (5%)
2	GAL	C	3	2	11,11,12	0.81	0	15,15,17	0.70	0
3	NAG	D	1	1,3	14,14,15	0.45	0	17,19,21	1.03	1 (5%)
3	NAG	D	2	3	14,14,15	0.34	0	17,19,21	0.95	1 (5%)
3	BMA	D	3	3	11,11,12	0.23	0	15,15,17	0.63	0
3	MAN	D	4	3	11,11,12	0.67	0	15,15,17	0.91	1 (6%)
2	GAL	E	1	2	12,12,12	0.75	0	17,17,17	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	2	2	14,14,15	0.36	0	17,19,21	0.97	1 (5%)
2	GAL	E	3	2	11,11,12	0.89	0	15,15,17	0.79	0
3	NAG	F	1	1,3	14,14,15	0.57	0	17,19,21	1.02	0
3	NAG	F	2	3	14,14,15	0.40	0	17,19,21	0.95	1 (5%)
3	BMA	F	3	3	11,11,12	0.26	0	15,15,17	0.78	0
3	MAN	F	4	3	11,11,12	0.72	0	15,15,17	1.03	1 (6%)

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	GAL	C	1	2	-	2/2/22/22	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	GAL	C	3	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
2	GAL	E	1	2	-	2/2/22/22	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	GAL	E	3	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	MAN	C1-O5-C5	-2.90	108.27	112.19
3	D	1	NAG	O4-C4-C5	-2.49	103.12	109.30
2	E	2	NAG	C2-N2-C7	2.40	126.31	122.90
3	D	4	MAN	C1-O5-C5	-2.37	108.98	112.19
3	D	2	NAG	C6-C5-C4	-2.21	107.84	113.00
3	F	2	NAG	C6-C5-C4	-2.19	107.88	113.00
2	C	2	NAG	C2-N2-C7	2.16	125.97	122.90

There are no chirality outliers.

All (10) torsion outliers are listed below:

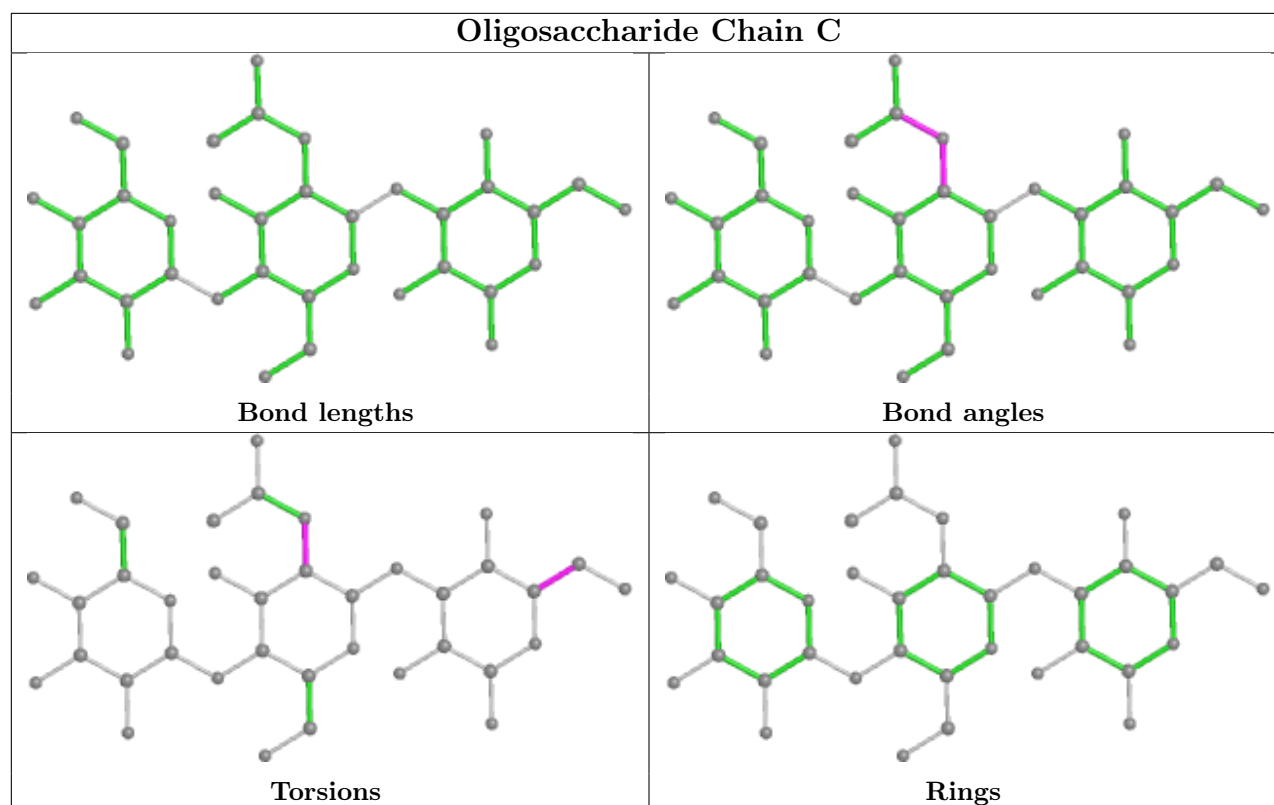
Mol	Chain	Res	Type	Atoms
2	E	1	GAL	C4-C5-C6-O6
2	E	1	GAL	O5-C5-C6-O6
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	F	3	BMA	O5-C5-C6-O6
2	E	2	NAG	C1-C2-N2-C7
2	C	2	NAG	C3-C2-N2-C7
2	C	1	GAL	C4-C5-C6-O6
2	E	2	NAG	C3-C2-N2-C7
2	C	1	GAL	O5-C5-C6-O6

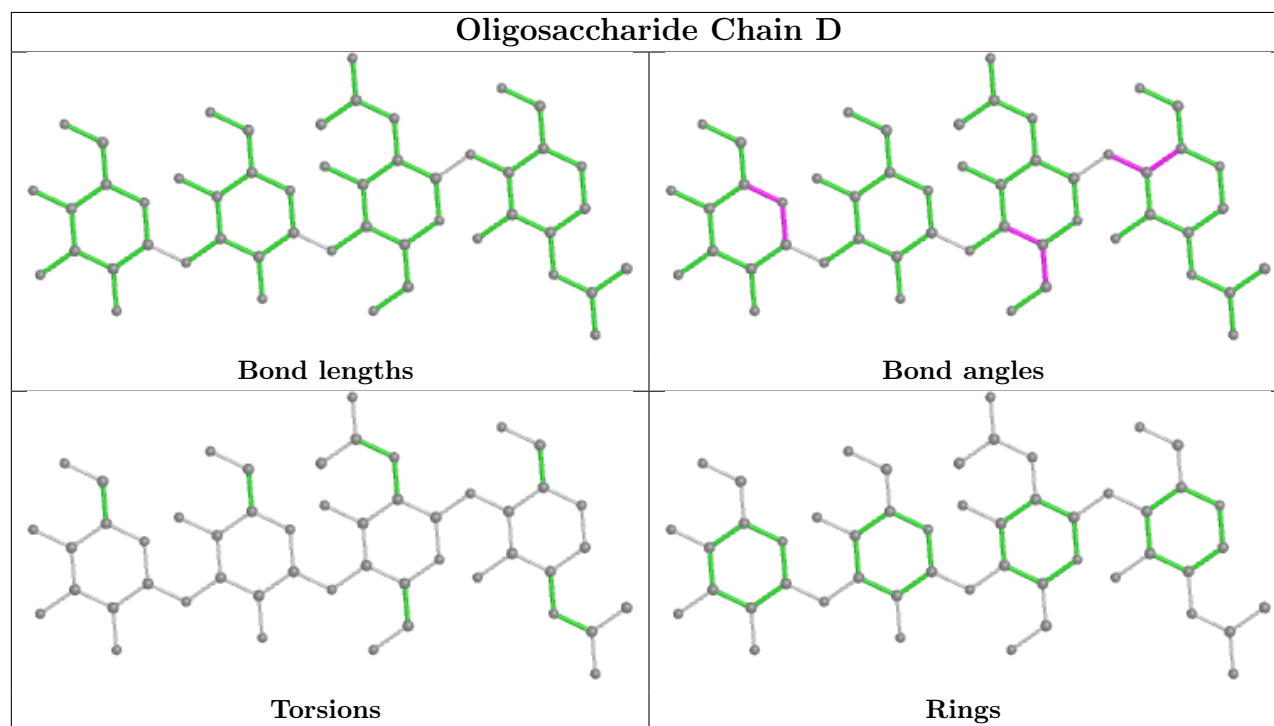
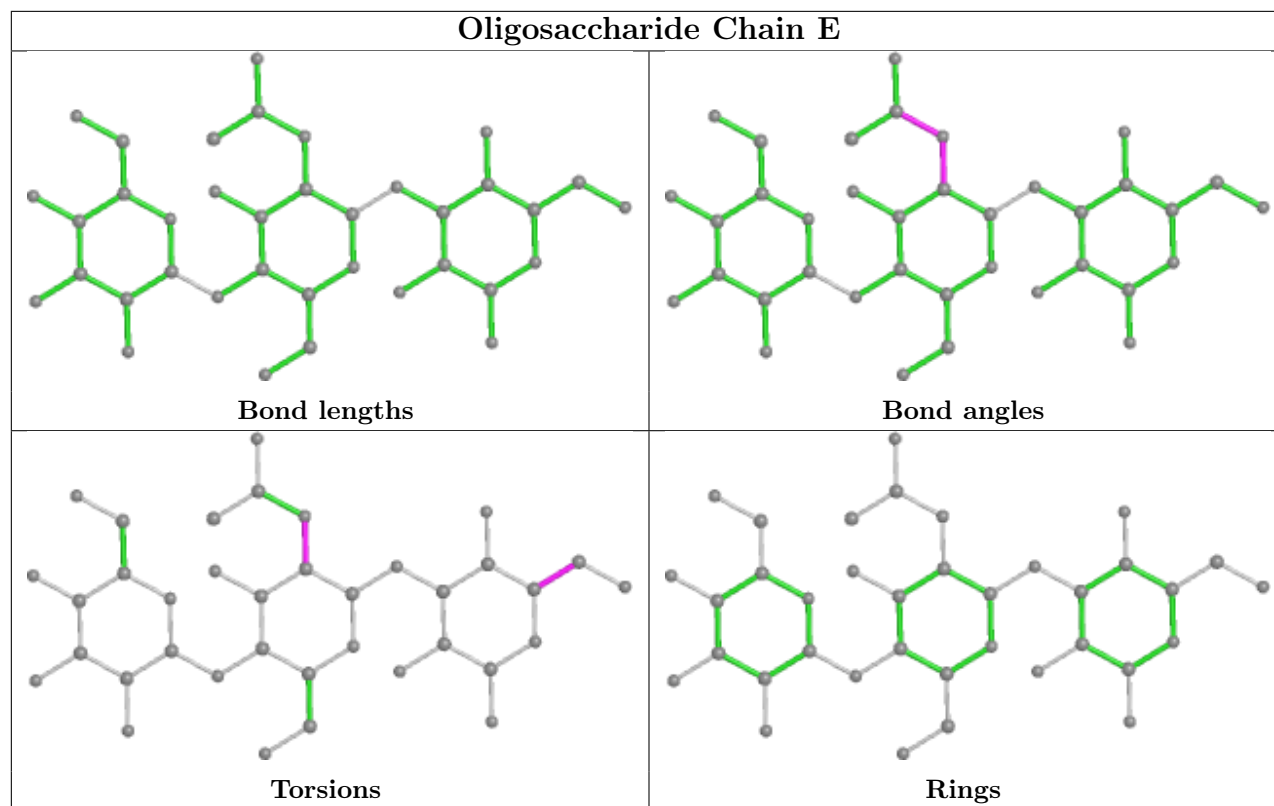
There are no ring outliers.

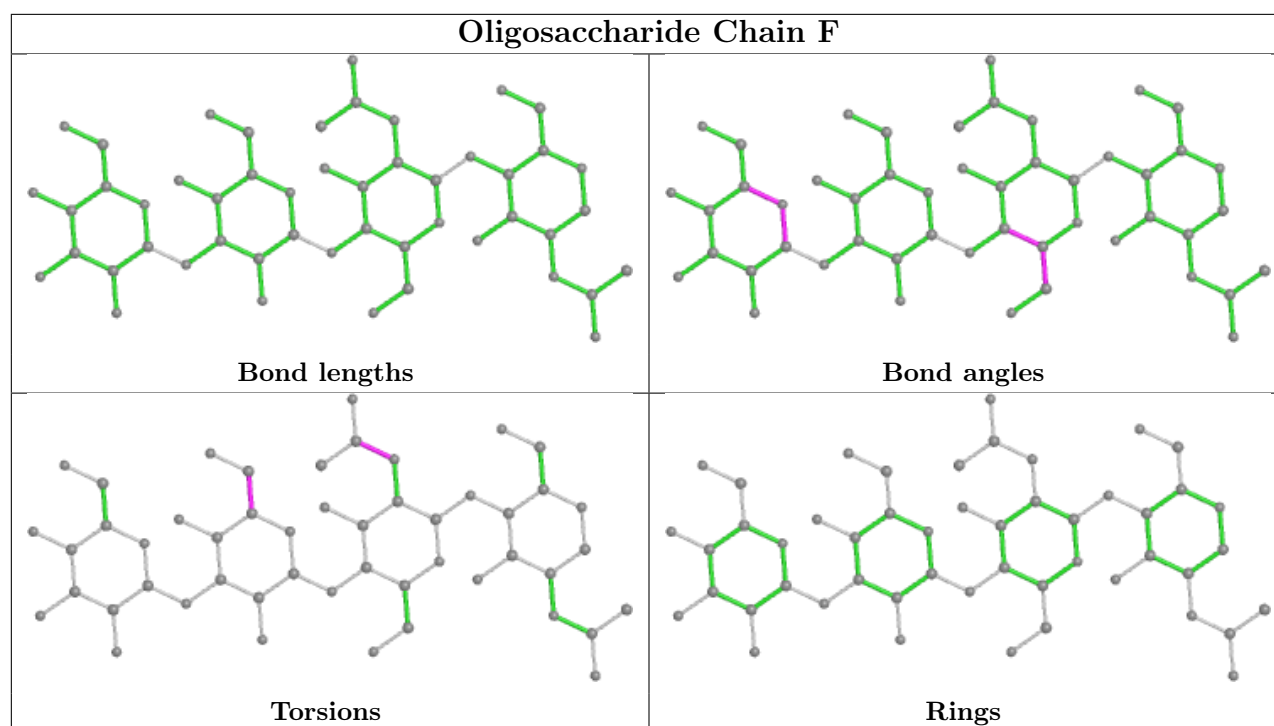
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	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 oligosaccharide.







5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	EDO	B	412	4	3,3,3	0.47	0	2,2,2	0.41	0
6	NAG	A	411	1	14,14,15	0.30	0	17,19,21	1.01	1 (5%)
8	GOL	B	413	-	5,5,5	0.69	0	5,5,5	1.22	0
6	NAG	B	410	1	14,14,15	0.25	0	17,19,21	1.25	2 (11%)
7	EDO	B	411	-	3,3,3	0.10	0	2,2,2	1.10	0
5	UDP	A	402	4	20,26,26	1.10	2 (10%)	25,40,40	0.85	0
5	UDP	B	402	4	20,26,26	1.06	1 (5%)	25,40,40	0.80	0
7	EDO	B	415	-	3,3,3	0.48	0	2,2,2	0.36	0
7	EDO	B	414	-	3,3,3	0.49	0	2,2,2	0.29	0
7	EDO	A	412	-	3,3,3	0.27	0	2,2,2	0.59	0
6	NAG	A	410	1	14,14,15	0.33	0	17,19,21	1.07	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
7	EDO	B	412	4	-	0/1/1/1	-
6	NAG	A	411	1	-	2/6/23/26	0/1/1/1
8	GOL	B	413	-	-	4/4/4/4	-
6	NAG	B	410	1	-	1/6/23/26	0/1/1/1
7	EDO	B	411	-	-	1/1/1/1	-
5	UDP	A	402	4	-	3/14/32/32	0/2/2/2
5	UDP	B	402	4	-	4/14/32/32	0/2/2/2
7	EDO	B	415	-	-	1/1/1/1	-
7	EDO	B	414	-	-	1/1/1/1	-
7	EDO	A	412	-	-	0/1/1/1	-
6	NAG	A	410	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	402	UDP	PB-O1B	2.62	1.59	1.50
5	B	402	UDP	C4-N3	2.42	1.37	1.33
5	A	402	UDP	O4'-C1'	2.28	1.44	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	410	NAG	C1-O5-C5	3.85	117.41	112.19
6	A	410	NAG	C1-O5-C5	3.21	116.55	112.19
6	A	411	NAG	C1-O5-C5	2.99	116.25	112.19
6	B	410	NAG	C6-C5-C4	-2.45	107.27	113.00

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	413	GOL	C1-C2-C3-O3
5	A	402	UDP	C2'-C1'-N1-C6
5	A	402	UDP	O4'-C1'-N1-C6
5	B	402	UDP	C2'-C1'-N1-C6
5	B	402	UDP	O4'-C1'-N1-C6

Continued on next page...

Continued from previous page...

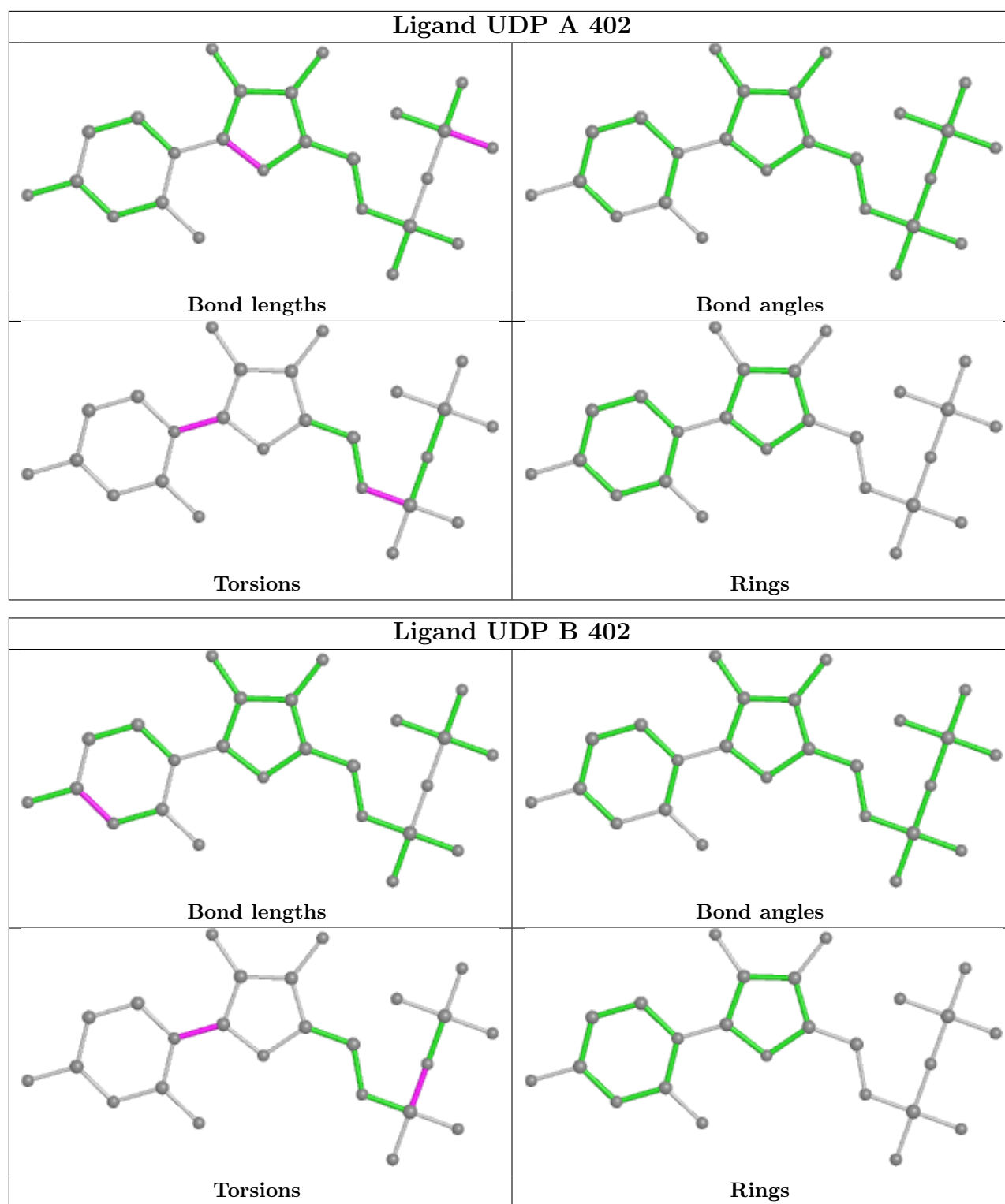
Mol	Chain	Res	Type	Atoms
6	A	410	NAG	O5-C5-C6-O6
6	A	410	NAG	C4-C5-C6-O6
8	B	413	GOL	O2-C2-C3-O3
8	B	413	GOL	O1-C1-C2-C3
6	A	411	NAG	C8-C7-N2-C2
8	B	413	GOL	O1-C1-C2-O2
7	B	414	EDO	O1-C1-C2-O2
6	A	411	NAG	O7-C7-N2-C2
7	B	415	EDO	O1-C1-C2-O2
6	B	410	NAG	O5-C5-C6-O6
7	B	411	EDO	O1-C1-C2-O2
5	B	402	UDP	PB-O3A-PA-O1A
5	B	402	UDP	PB-O3A-PA-O2A
5	A	402	UDP	C5'-O5'-PA-O1A

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	412	EDO	1	0
8	B	413	GOL	1	0
7	B	411	EDO	1	0
5	B	402	UDP	1	0
7	B	415	EDO	1	0
7	A	412	EDO	4	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 ⓘ

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	325/364 (89%)	0.37	23 (7%) 16 15	28, 46, 75, 94	0
1	B	313/364 (85%)	0.71	45 (14%) 2 2	25, 49, 82, 105	0
All	All	638/728 (87%)	0.54	68 (10%) 6 5	25, 47, 81, 105	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	366	ILE	5.4
1	B	101	ARG	4.8
1	B	102	VAL	4.7
1	B	171	ALA	4.7
1	B	365	ASN	4.4
1	A	306[A]	GLY	4.3
1	B	105	VAL	4.3
1	B	100	LEU	4.2
1	A	171	ALA	4.0
1	B	104	SER	3.9
1	B	108	GLY	3.9
1	A	95	TYR	3.8
1	B	228	LEU	3.8
1	B	263	SER	3.8
1	A	397	CYS	3.8
1	B	103	THR	3.7
1	B	107	THR	3.7
1	B	172	GLY	3.6
1	B	109	PHE	3.5
1	B	151	LEU	3.5
1	B	367	CYS	3.4
1	B	173	ASN	3.4
1	A	364	ASN	3.4
1	B	95	TYR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	390	LEU	3.1
1	B	262	LEU	2.9
1	B	111	ASN	2.9
1	B	106	VAL	2.9
1	B	61	ARG	2.8
1	A	367	CYS	2.8
1	A	362	ASN	2.8
1	B	261	SER	2.7
1	B	170	ASN	2.7
1	B	110	ASN	2.7
1	B	69	GLN	2.6
1	B	391	GLN	2.6
1	A	71	ASN	2.6
1	B	58	TYR	2.6
1	A	151	LEU	2.6
1	A	68	ARG	2.5
1	B	64	GLU	2.5
1	B	392	SER	2.5
1	A	395	LEU	2.4
1	A	96	CYS	2.4
1	B	181	LEU	2.4
1	B	71	ASN	2.4
1	B	370	VAL	2.4
1	B	182	LEU	2.3
1	A	172	GLY	2.3
1	A	228	LEU	2.3
1	B	227	PHE	2.3
1	B	287	LEU	2.3
1	A	396	LYS	2.2
1	B	258	TYR	2.2
1	B	68	ARG	2.2
1	B	346	VAL	2.2
1	A	358	ILE	2.1
1	B	351	LYS	2.1
1	A	287	LEU	2.1
1	A	94	ASN	2.1
1	A	361	LYS	2.1
1	A	150[A]	SER	2.1
1	B	150	SER	2.1
1	A	393	ALA	2.1
1	A	366	ILE	2.1
1	B	241	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	254	HIS	2.0
1	A	97	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

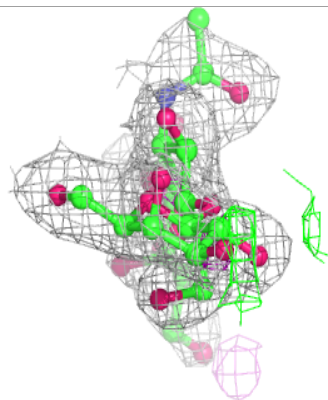
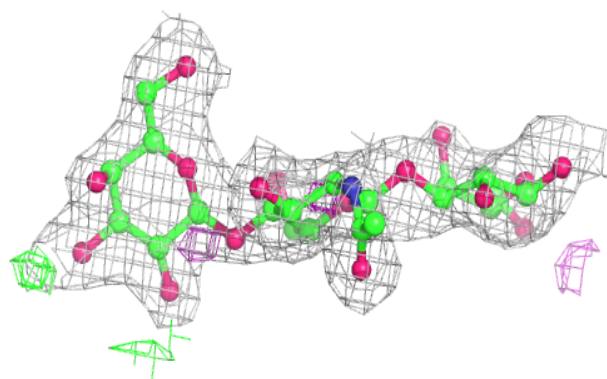
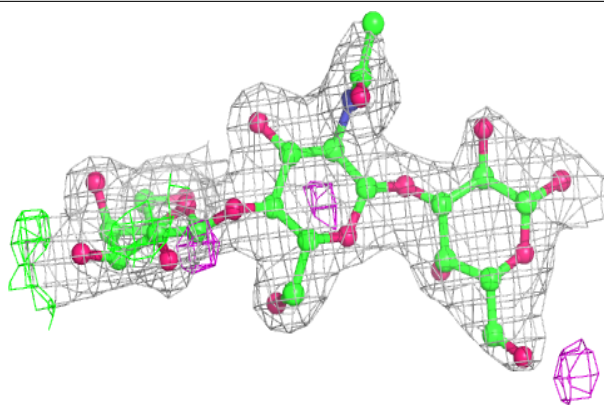
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	F	4	11/12	0.67	0.42	84,94,101,104	11
3	MAN	D	4	11/12	0.73	0.28	89,95,99,102	11
2	GAL	E	1	12/12	0.80	0.20	72,80,84,89	0
3	BMA	F	3	11/12	0.83	0.16	63,70,84,89	0
2	GAL	E	3	11/12	0.83	0.13	31,45,49,54	0
3	BMA	D	3	11/12	0.87	0.19	63,74,85,88	0
2	GAL	C	1	12/12	0.87	0.29	64,76,78,78	0
2	NAG	E	2	14/15	0.88	0.15	48,52,67,68	0
2	NAG	C	2	14/15	0.88	0.27	48,62,68,71	0
2	GAL	C	3	11/12	0.88	0.12	44,52,55,57	0
3	NAG	D	2	14/15	0.93	0.11	41,49,58,59	0
3	NAG	F	2	14/15	0.96	0.10	37,47,57,61	0
3	NAG	F	1	14/15	0.96	0.08	31,35,39,40	0
3	NAG	D	1	14/15	0.96	0.08	28,36,41,43	0

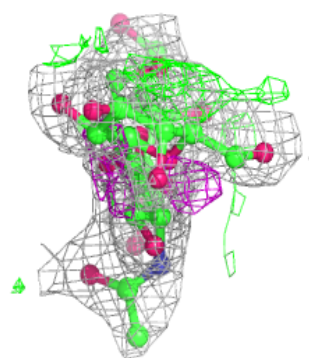
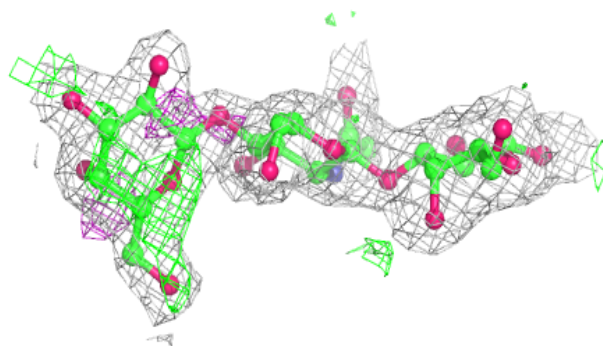
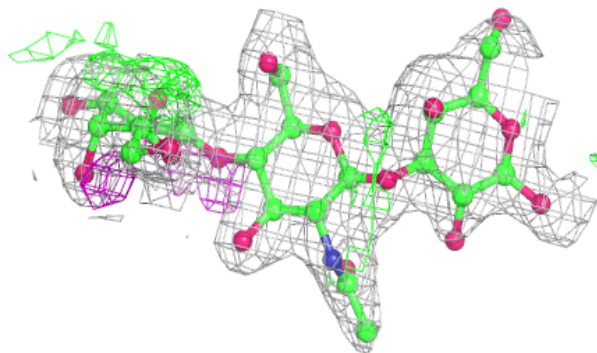
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

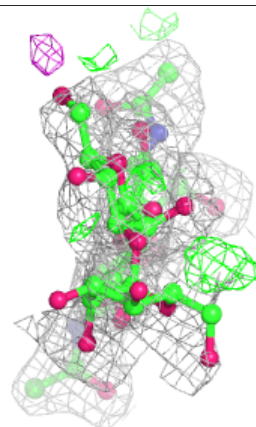
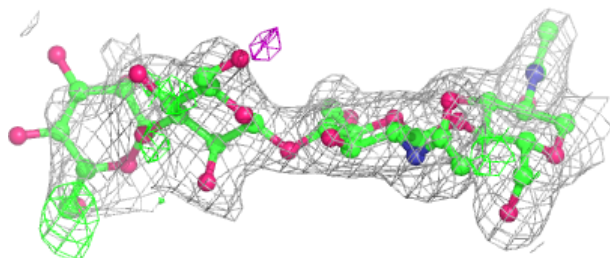
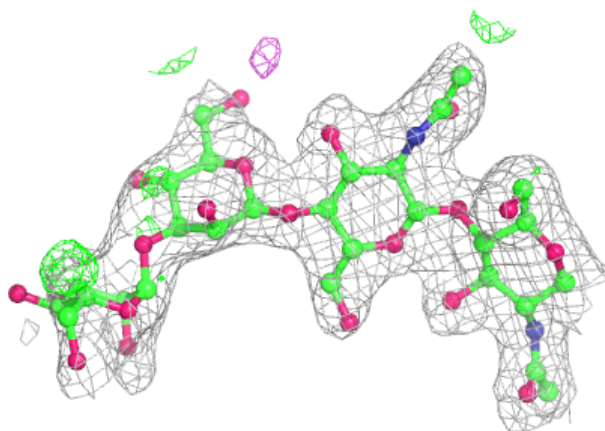
**Electron density around Chain E:**

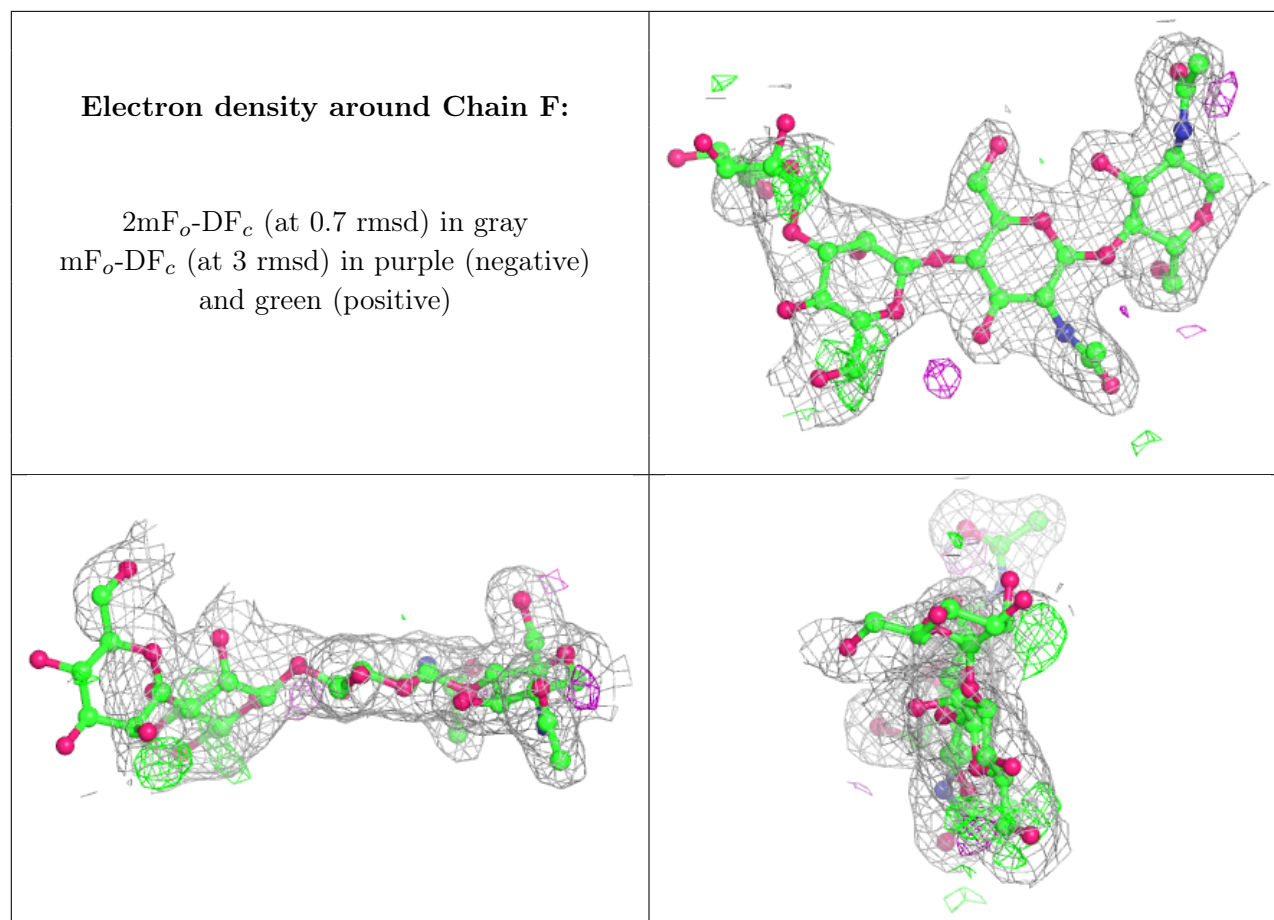
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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 ⓘ

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.

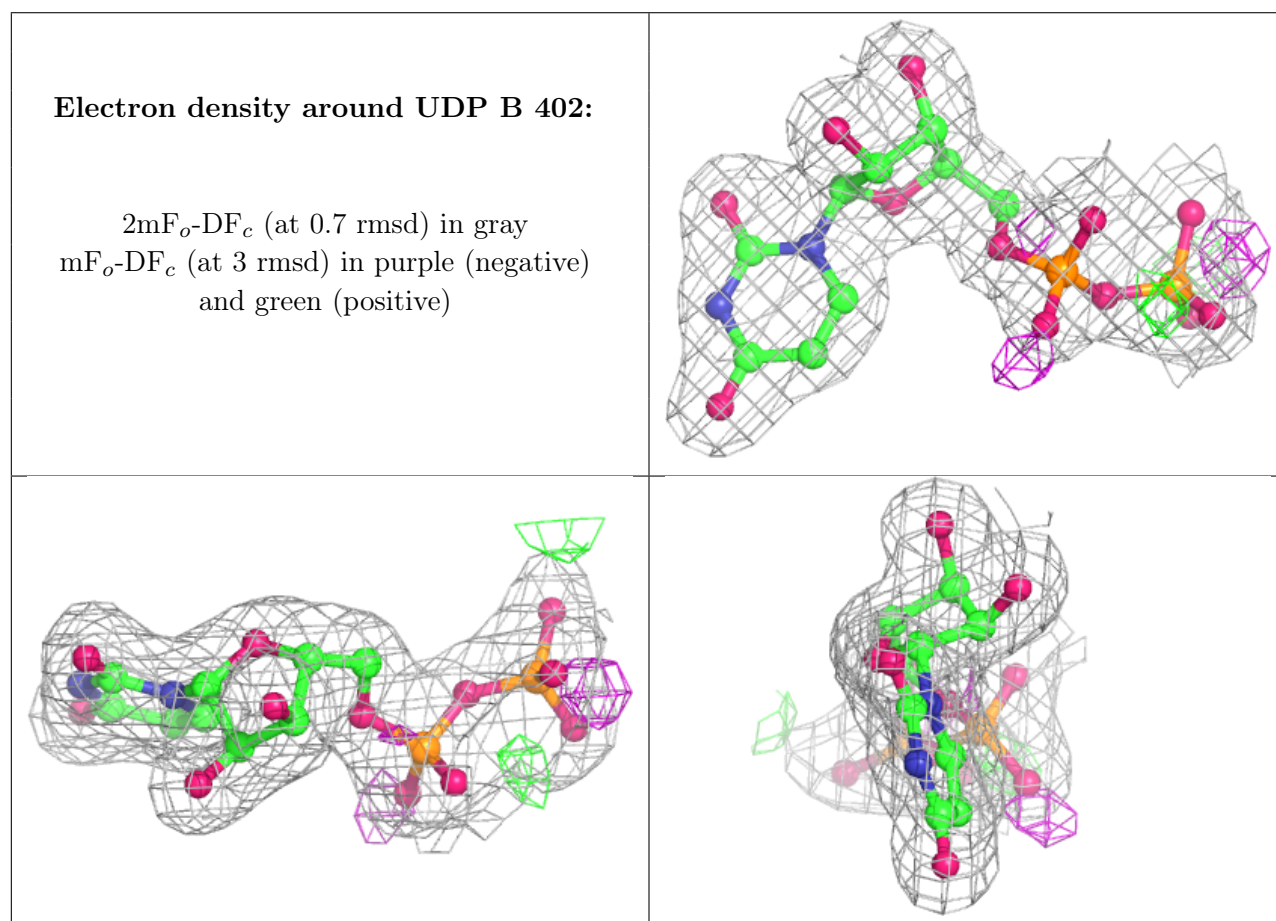
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	EDO	B	415	4/4	0.73	0.60	37,42,46,48	4
6	NAG	B	410	14/15	0.81	0.20	43,50,55,57	14
6	NAG	A	411	14/15	0.83	0.39	57,72,77,80	14
7	EDO	B	412	4/4	0.83	0.17	47,48,49,50	0
6	NAG	A	410	14/15	0.86	0.35	47,67,77,77	14
7	EDO	B	411	4/4	0.87	0.35	29,32,36,43	0
8	GOL	B	413	6/6	0.92	0.30	42,47,57,58	0
4	MG	A	401	1/1	0.94	0.05	38,38,38,38	0
5	UDP	B	402	25/25	0.95	0.14	31,37,42,48	0
7	EDO	B	414	4/4	0.95	0.14	36,45,51,60	0
5	UDP	A	402	25/25	0.96	0.11	28,33,42,50	0
7	EDO	A	412	4/4	0.97	0.32	25,32,38,51	0

Continued on next page...

Continued from previous page...

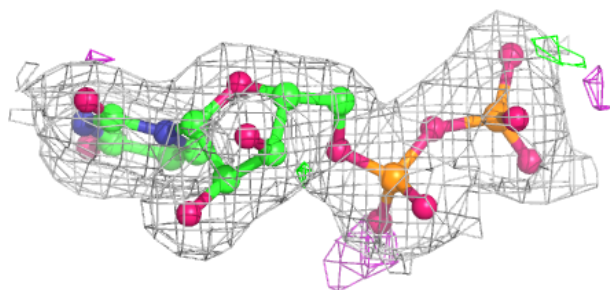
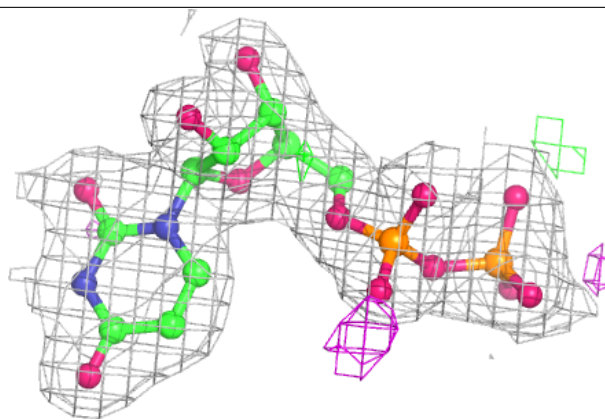
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	B	401	1/1	0.98	0.08	41,41,41,41	0

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



Electron density around UDP A 402:

$2mF_o - DF_c$ (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.