

wwPDB X-ray Structure Validation Summary Report (i)

Sep 17, 2023 – 09:24 PM EDT

PDB ID : 4XX6

Title : Crystal structure of a glycosylated endo-beta-1,4-xylanase (glycoside hydrolase

family 10/GH10) enzyme from Gloeophyllum trabeum

Authors: Stogios, P.J.; Nocek, B.; Xu, X.; Cui, H.; Lowden, M.; Savchenko, A.

Deposited on : 2015-01-29

Resolution : 1.95 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 (i) 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 (1)) 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 : 2.35.1 buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

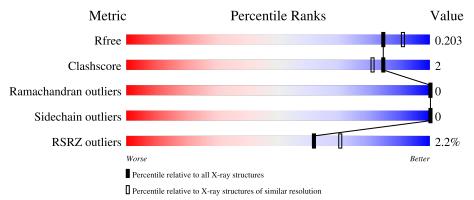
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of c	hain	
1	A	321	96%		
1	В	321	95%		5%
2	С	8	62%	38%	
3	D	9	56%	33%	11%
4	E	4	50%	50%	



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Mol	Chain	Length	(Quality of chain	
5	F	6	33%	50%	17%
6	G	8	759	%	25%
7	Н	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
5	MAN	F	6	-	-	-	X



2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 6233 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 Beta-xylanase.

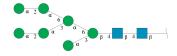
Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	Δ	318	Total	С	N	О	S	0	2	0
1	Λ	310	2515	1618	413	476	8	U	2	
1	В	321	Total	С	N	О	S	0	9	0
1	Ъ	921	2533	1627	416	482	8		<u> </u>	

• Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf	Trace
2	С	8	Total C 94 5	N 2 2	O 40	0	0	0

• Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf	Trace
3	D	9	Total 105	C 58	N 2	O 45	0	0	0

• Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos

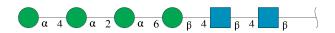


e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf	Trace
4	E	4	Total 50	C 28	N 2	O 20	0	0	0

• Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	A	Atoms		ZeroOcc	AltConf	Trace	
5	F	6	Total 72	C 40	N 2	O 30	0	0	0

• Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	A	A ton	ns		ZeroOcc	AltConf	Trace
6	G	8	Total 94	C 52	N 2	O 40	0	0	0

• Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



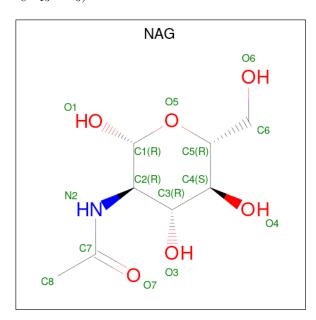


\mathbf{Mol}	Chain	Residues	A	tom	$1\mathbf{S}$		$\mathbf{ZeroOcc}$	AltConf	Trace	
7	Н	2	Total 28	C 16	N 2	O 10	0	0	0	

• Molecule 8 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total X 1 1	0	0
8	В	1	Total X 1 1	0	0

 \bullet Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\rm C_8H_{15}NO_6).$



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

• Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

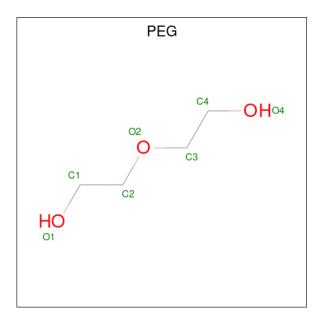
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Mg 1 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	В	1	Total Mg 1 1	0	0

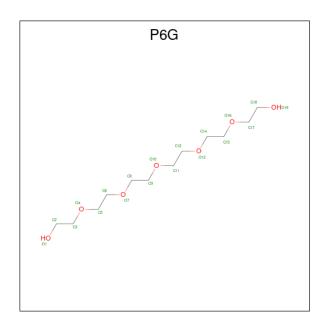
 \bullet Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 7 4 3	0	0
11	В	1	Total C O 7 4 3	0	0
11	В	1	Total C O 7 4 3	0	0

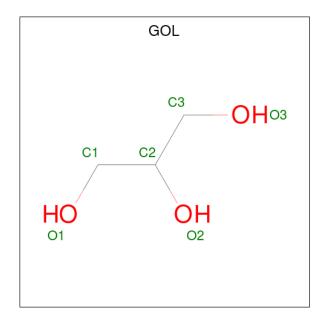
• Molecule 12 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 18 12 6	0	0
12	A	1	Total C O 13 8 5	0	0

 \bullet Molecule 13 is GLYCEROL (three-letter code: GOL) (formula: $\mathrm{C_3H_8O_3}).$



ľ	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	13	A	1	Total C O 6 3 3	0	0
	13	A	1	Total C O 6 3 3	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C O 6 3 3	0	0
13	A	1	Total C O 6 3 3	0	0
13	В	1	Total C O 6 3 3	0	0
13	В	1	Total C O 6 3 3	0	0
13	В	1	Total C O 6 3 3	0	0

• Molecule 14 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	В	1	Total Cl 1 1	0	0

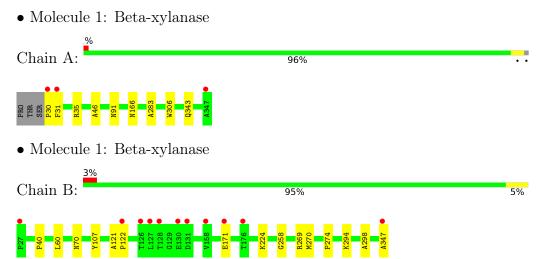
• Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	293	Total O 306 306	0	13
15	В	288	Total O 295 295	0	7



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.



Chain C: 62% 38%

 $\bullet \ \, Molecule \ 3: \ alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranos$

Chain D: 56% 33% 11%

• Molecule 4: 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

Chain E: 50% 50%



NAG1	NAG2	BMA3	MAN4

 $\bullet \ \, Molecule 5: \ alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-acetamido-2-deoxy-beta-D-glucopyranose-(1-4$

Chain F: 33% 50% 17%

NAG2 NAG2 BMA3 MAN4 MAN5 MAN6

 $\bullet \ \, \text{Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-b$

Chain G: 75% 25%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7 MAN7

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	52.41Å 99.34Å 147.27Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.20 - 1.95	Depositor
Resolution (A)	30.20 - 1.95	EDS
% Data completeness	91.7 (30.20-1.95)	Depositor
(in resolution range)	86.6 (30.20-1.95)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) > 1$	4.57 (at 1.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
D.D.	0.154 , 0.204	Depositor
R, R_{free}	0.153 , 0.203	DCC
R_{free} test set	2000 reflections (3.92%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.40, 66.9	EDS
L-test for twinning ²	$< L > = 0.48, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6233	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: BMA, GOL, UNX, NAG, MAN, PEG, P6G, CL, MG

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	
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.40	0/2596	0.53	0/3563
1	В	0.39	0/2615	0.53	0/3589
All	All	0.40	0/5211	0.53	0/7152

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	2515	0	2370	8	0
1	В	2533	0	2382	11	0
2	С	94	0	79	0	0
3	D	105	0	88	2	0
4	Е	50	0	43	3	0
5	F	72	0	61	1	0
6	G	94	0	79	0	0
7	Н	28	0	25	0	0
8	A	1	0	0	0	0
8	В	1	0	0	0	0
9	A	14	0	13	0	0



Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	В	28	0	26	0	0
10	A	1	0	0	0	0
10	В	1	0	0	0	0
11	A	7	0	10	0	0
11	В	14	0	20	3	0
12	A	31	0	39	2	0
13	A	24	0	32	1	0
13	В	18	0	24	2	0
14	В	1	0	0	0	0
15	A	306	0	0	1	0
15	В	295	0	0	0	1
All	All	6233	0	5291	25	1

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.

The worst 5 of 25 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:B:269:ARG:HH22	13:B:424:GOL:H32	1.46	0.80
1:B:298:ALA:HA	11:B:422:PEG:H22	1.69	0.75
1:A:35:ARG:HE	12:A:426:P6G:H171	1.63	0.64
1:B:171:GLU:O	1:B:171:GLU:HG3	1.98	0.61
1:B:294:LYS:NZ	1:B:347:ALA:O	2.40	0.54

All (1) 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
15:B:611:HOH:O	15:B:680:HOH:O[1_655]	2.19	0.01

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	$318/321 \ (99\%)$	313 (98%)	5 (2%)	0	100	100
1	В	321/321 (100%)	315 (98%)	6 (2%)	0	100	100
All	All	639/642 (100%)	628 (98%)	11 (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	$262/263 \; (100\%)$	262 (100%)	0	100 100
1	В	265/263 (101%)	265 (100%)	0	100 100
All	All	527/526 (100%)	527 (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)

37 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).

N (T 1	TD.	GI :	Ъ	т. 1	Во	ond leng	ths	В	ond ang	les
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	С	1	2,1	14,14,15	0.30	0	17,19,21	0.60	0
2	NAG	С	2	2	14,14,15	0.53	0	17,19,21	0.51	0
2	BMA	С	3	2	11,11,12	0.60	0	15,15,17	0.89	0
2	MAN	С	4	2	11,11,12	0.76	0	15,15,17	0.86	0
2	MAN	С	5	2	11,11,12	0.87	1 (9%)	15,15,17	0.97	1 (6%)
2	MAN	С	6	2	11,11,12	1.05	0	15,15,17	1.83	2 (13%)
2	MAN	С	7	2	11,11,12	0.68	0	15,15,17	1.13	1 (6%)
2	MAN	С	8	2	11,11,12	0.61	0	15,15,17	0.84	0
3	NAG	D	1	3,1	14,14,15	0.43	0	17,19,21	0.65	0
3	NAG	D	2	3	14,14,15	0.38	0	17,19,21	0.63	0
3	BMA	D	3	3	11,11,12	0.97	1 (9%)	15,15,17	0.99	1 (6%)
3	MAN	D	4	3	11,11,12	0.89	0	15,15,17	0.94	0
3	MAN	D	5	3	11,11,12	0.83	0	15,15,17	0.94	0
3	MAN	D	6	3	11,11,12	0.85	0	15,15,17	0.88	0
3	MAN	D	7	3	11,11,12	0.79	0	15,15,17	1.02	1 (6%)
3	MAN	D	8	3	11,11,12	0.65	0	15,15,17	0.82	0
3	MAN	D	9	3	11,11,12	1.00	0	15,15,17	0.92	0
4	NAG	Е	1	4,1	14,14,15	0.56	0	17,19,21	0.76	0
4	NAG	Е	2	4	14,14,15	0.39	0	17,19,21	0.60	0
4	BMA	Е	3	4	11,11,12	1.09	1 (9%)	15,15,17	1.46	2 (13%)
4	MAN	E	4	4	11,11,12	0.82	1 (9%)	15,15,17	0.88	0
5	NAG	F	1	5,1	14,14,15	0.29	0	17,19,21	0.47	0
5	NAG	F	2	5	14,14,15	0.62	1 (7%)	17,19,21	0.71	0
5	BMA	F	3	5	11,11,12	1.02	1 (9%)	15,15,17	1.80	3 (20%)
5	MAN	F	4	5	11,11,12	0.72	0	15,15,17	0.83	0
5	MAN	F	5	5	11,11,12	1.25	2 (18%)	15,15,17	1.17	1 (6%)
5	MAN	F	6	5	11,11,12	0.85	0	15,15,17	0.85	0
6	NAG	G	1	1,6	14,14,15	0.52	0	17,19,21	0.44	0
6	NAG	G	2	6	14,14,15	0.18	0	17,19,21	0.62	0
6	BMA	G	3	6	11,11,12	0.63	0	15,15,17	0.75	0
6	MAN	G	4	6	11,11,12	0.88	0	15,15,17	1.00	0
6	MAN	G	5	6	11,11,12	0.78	1 (9%)	15,15,17	0.85	0
6	MAN	G	6	6	11,11,12	0.74	0	15,15,17	0.84	0
6	MAN	G	7	6	11,11,12	0.82	0	15,15,17	1.05	2 (13%)
6	MAN	G	8	6	11,11,12	0.66	0	15,15,17	0.87	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
MIOI	туре		nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
7	NAG	Н	1	7,1	14,14,15	0.33	0	17,19,21	0.39	0
7	NAG	Н	2	7	14,14,15	0.22	0	17,19,21	0.38	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
2	NAG	С	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	С	2	2	-	0/6/23/26	0/1/1/1
2	BMA	С	3	2	-	0/2/19/22	0/1/1/1
2	MAN	С	4	2	-	0/2/19/22	0/1/1/1
2	MAN	С	5	2	-	2/2/19/22	0/1/1/1
2	MAN	С	6	2	-	0/2/19/22	0/1/1/1
2	MAN	С	7	2	-	0/2/19/22	1/1/1/1
2	MAN	С	8	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	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
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
3	MAN	D	6	3	-	0/2/19/22	0/1/1/1
3	MAN	D	7	3	-	2/2/19/22	0/1/1/1
3	MAN	D	8	3	-	0/2/19/22	0/1/1/1
3	MAN	D	9	3	-	2/2/19/22	0/1/1/1
4	NAG	Е	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Е	2	4	-	1/6/23/26	0/1/1/1
4	BMA	Е	3	4	-	1/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	MAN	F	5	5	-	1/2/19/22	0/1/1/1
5	MAN	F	6	5	-	1/2/19/22	1/1/1/1
6	NAG	G	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	1/6/23/26	0/1/1/1
6	BMA	G	3	6	-	0/2/19/22	0/1/1/1
6	MAN	G	4	6	-	0/2/19/22	0/1/1/1



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	G	5	6	-	0/2/19/22	0/1/1/1
6	MAN	G	6	6	-	0/2/19/22	0/1/1/1
6	MAN	G	7	6	-	1/2/19/22	0/1/1/1
6	MAN	G	8	6	-	2/2/19/22	0/1/1/1
7	NAG	Н	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	Н	2	7	-	2/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(ext{\AA})$
5	F	5	MAN	O4-C4	2.58	1.49	1.43
4	Е	3	BMA	O5-C5	2.44	1.48	1.43
3	D	3	BMA	C2-C3	2.33	1.55	1.52
5	F	5	MAN	C4-C5	2.18	1.57	1.53
5	F	2	NAG	O5-C1	-2.16	1.40	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
2	С	6	MAN	O3-C3-C2	5.36	120.25	109.99
5	F	3	BMA	C1-O5-C5	5.10	119.10	112.19
4	E	3	BMA	C1-C2-C3	-4.24	104.46	109.67
2	С	6	MAN	C1-C2-C3	-3.21	105.72	109.67
6	G	7	MAN	O2-C2-C3	-2.93	104.27	110.14

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	3	BMA	O5-C5-C6-O6
2	С	5	MAN	O5-C5-C6-O6
7	Н	2	NAG	O5-C5-C6-O6
3	D	9	MAN	C4-C5-C6-O6
3	D	9	MAN	O5-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	С	7	MAN	C1-C2-C3-C4-C5-O5
5	F	6	MAN	C1-C2-C3-C4-C5-O5

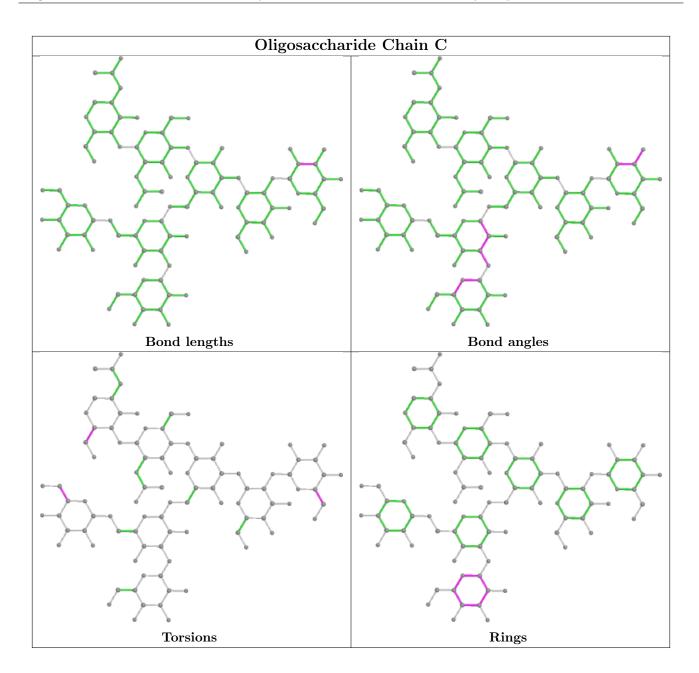


9 monomers are involved in 6 short contacts:

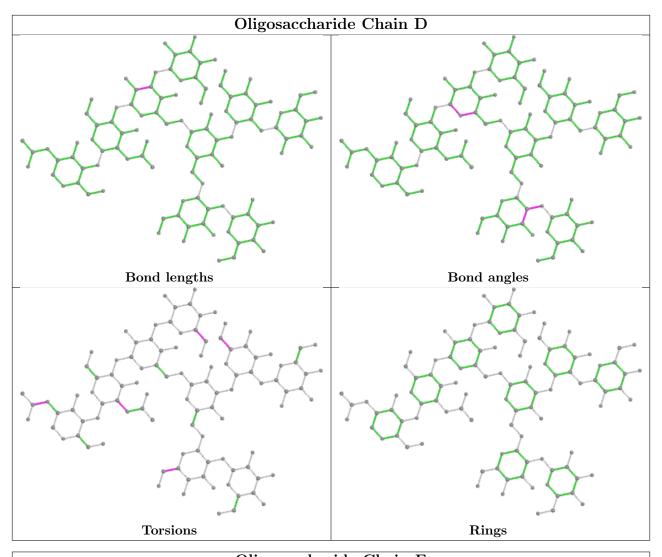
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	5	MAN	1	0
4	Е	4	MAN	1	0
3	D	9	MAN	1	0
3	D	1	NAG	1	0
4	Е	3	BMA	2	0
5	F	6	MAN	1	0
4	Е	1	NAG	1	0
4	Е	2	NAG	1	0
3	D	3	BMA	1	0

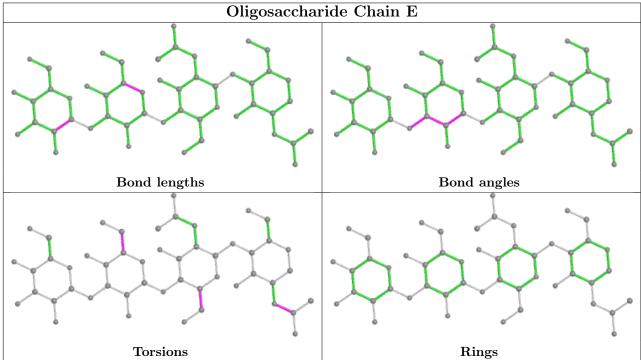
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



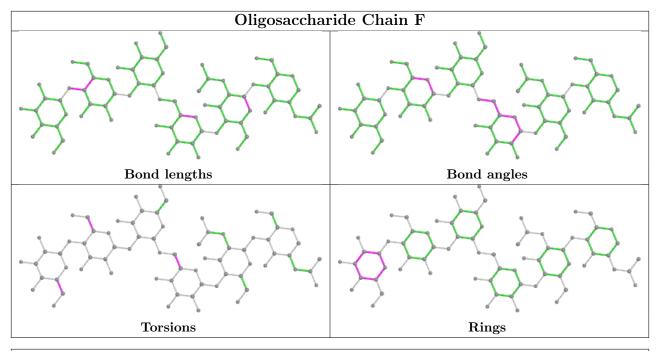


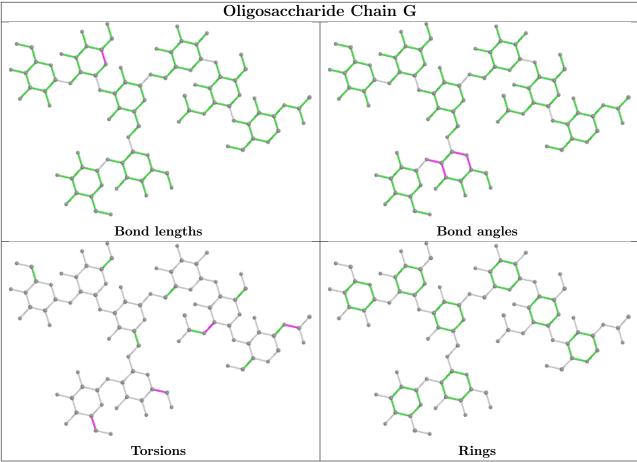




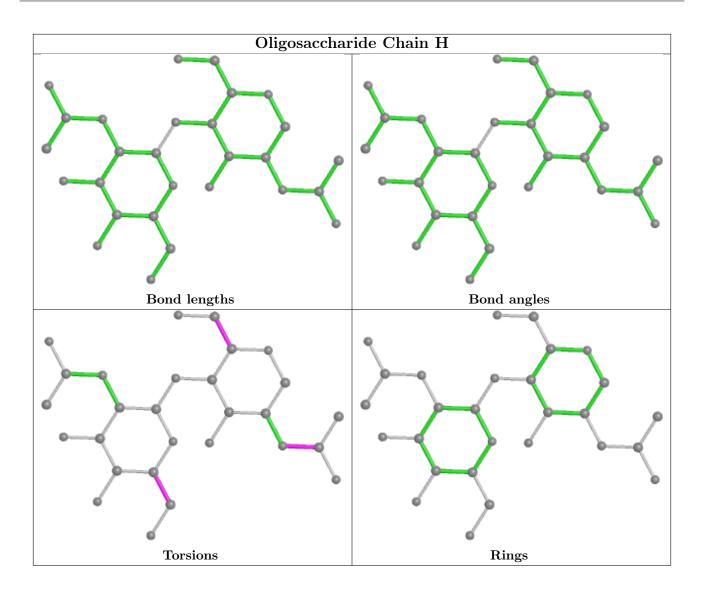












5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 2 are unknown and 3 are monoatomic - leaving 15 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).

Mal	Tuna	Chain	Res	Link	Bond length			hs Bond angles		
Mol Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
13	GOL	A	429	-	5,5,5	0.34	0	5,5,5	0.32	0
13	GOL	В	424	-	5,5,5	0.37	0	5,5,5	0.19	0
13	GOL	В	425	-	5,5,5	0.37	0	5,5,5	0.23	0



Mol	Trino	Chain	Res	Link	Во	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	Ites Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	GOL	A	430	-	5,5,5	0.36	0	5,5,5	0.28	0
9	NAG	В	419	1	14,14,15	0.30	0	17,19,21	0.55	0
11	PEG	В	422	-	6,6,6	0.65	0	5,5,5	0.24	0
11	PEG	A	425	-	6,6,6	0.65	0	5,5,5	0.20	0
9	NAG	В	416	1	14,14,15	0.19	0	17,19,21	0.66	1 (5%)
9	NAG	A	423	1	14,14,15	0.33	0	17,19,21	0.41	0
12	P6G	A	427	-	12,12,18	0.66	0	11,11,17	0.98	1 (9%)
13	GOL	В	426	-	5,5,5	0.35	0	5,5,5	0.32	0
13	GOL	A	428	-	5,5,5	0.35	0	5,5,5	0.32	0
11	PEG	В	423	-	6,6,6	0.65	0	5,5,5	0.33	0
13	GOL	A	431	-	5,5,5	0.35	0	5,5,5	0.21	0
12	P6G	A	426	-	17,17,18	0.58	0	16,16,17	1.84	4 (25%)

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
13	GOL	A	429	-	-	2/4/4/4	-
13	GOL	В	424	-	-	4/4/4/4	-
13	GOL	В	425	-	-	2/4/4/4	-
13	GOL	A	430	-	-	2/4/4/4	-
9	NAG	В	419	1	-	2/6/23/26	0/1/1/1
11	PEG	В	422	-	-	0/4/4/4	-
11	PEG	A	425	-	-	0/4/4/4	-
9	NAG	В	416	1	-	4/6/23/26	0/1/1/1
9	NAG	A	423	1	-	2/6/23/26	0/1/1/1
12	P6G	A	427	-	-	1/10/10/16	-
13	GOL	В	426	-	-	2/4/4/4	-
13	GOL	A	428	-	-	0/4/4/4	-
11	PEG	В	423	-	-	2/4/4/4	_
13	GOL	A	431	-	-	2/4/4/4	-
12	P6G	A	426	-	-	6/15/15/16	-

There are no bond length outliers.

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



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
12	A	426	P6G	O7-C8-C9	4.30	129.76	110.39
12	A	426	P6G	O10-C9-C8	-3.57	94.32	110.39
12	A	426	P6G	C8-O7-C6	-3.08	99.95	113.29
9	В	416	NAG	C1-O5-C5	2.26	115.26	112.19
12	A	427	P6G	O13-C12-C11	2.20	120.30	110.39

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	429	GOL	O1-C1-C2-C3
13	A	430	GOL	O1-C1-C2-C3
13	В	424	GOL	O1-C1-C2-O2
13	В	424	GOL	O1-C1-C2-C3
13	В	424	GOL	C1-C2-C3-O3

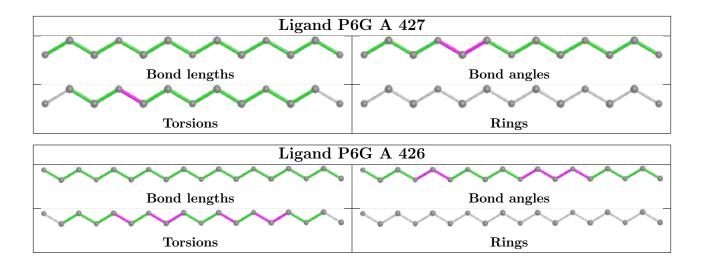
There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	В	424	GOL	2	0
11	В	422	PEG	2	0
13	A	428	GOL	1	0
11	В	423	PEG	1	0
12	A	426	P6G	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 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.





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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	318/321 (99%)	-0.13	3 (0%) 84 89	10, 19, 37, 99	0
1	В	321/321 (100%)	-0.02	11 (3%) 45 55	10, 21, 41, 64	0
All	All	639/642 (99%)	-0.08	14 (2%) 62 70	10, 20, 40, 99	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	PHE	10.5
1	A	30	PRO	9.6
1	В	127	LEU	5.1
1	A	347	ALA	3.4
1	В	347	ALA	2.8

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
5	MAN	F	6	11/12	0.44	0.69	96,100,105,106	0
4	MAN	Е	4	11/12	0.56	0.30	79,88,100,101	0
4	BMA	Е	3	11/12	0.62	0.30	62,78,84,88	0
3	MAN	D	9	11/12	0.70	0.39	68,83,90,92	0
3	MAN	D	6	11/12	0.73	0.32	48,65,74,77	0

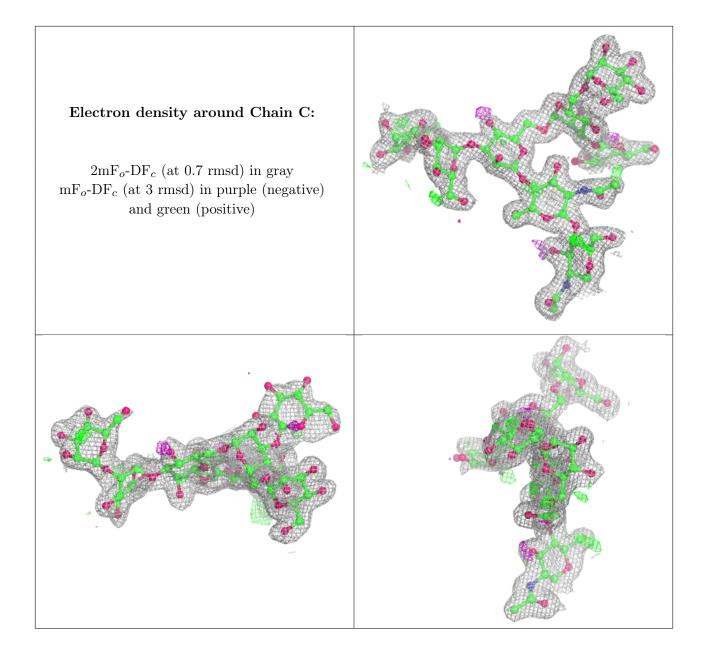


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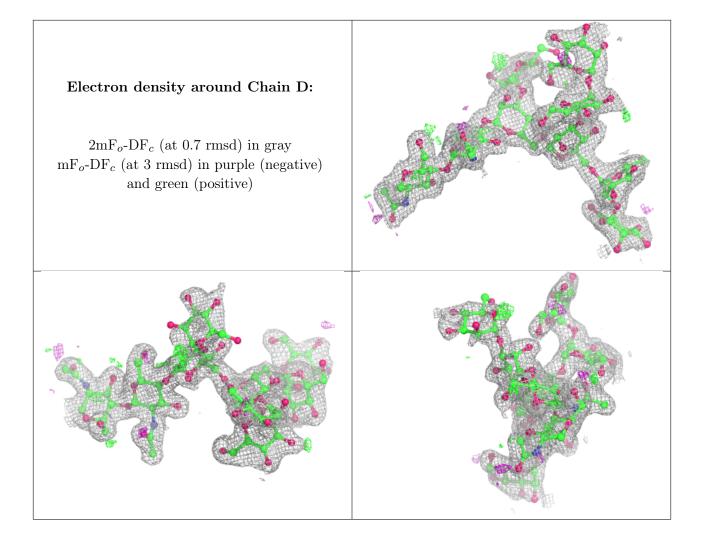
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	MAN	С	7	11/12	0.77	0.32	62,70,79,86	0
5	BMA	F	3	11/12	0.80	0.28	27,61,96,103	0
7	NAG	Н	2	14/15	0.81	0.41	76,82,86,92	0
4	NAG	Е	2	14/15	0.85	0.28	27,58,68,71	0
6	MAN	G	6	11/12	0.86	0.39	50,58,70,71	0
7	NAG	Н	1	14/15	0.87	0.32	41,59,65,68	0
5	MAN	F	5	11/12	0.88	0.18	41,50,83,88	0
2	MAN	С	5	11/12	0.89	0.20	41,46,58,64	0
3	MAN	D	8	11/12	0.89	0.30	55,58,62,67	0
3	MAN	D	5	11/12	0.90	0.13	27,30,36,38	0
4	NAG	Е	1	14/15	0.91	0.14	24,36,52,52	0
6	MAN	G	8	11/12	0.91	0.21	43,45,55,56	0
5	MAN	F	4	11/12	0.92	0.13	26,32,38,41	0
6	MAN	G	5	11/12	0.92	0.16	22,24,30,35	0
2	MAN	С	4	11/12	0.93	0.15	25,31,38,38	0
3	MAN	D	7	11/12	0.93	0.22	36,42,55,64	0
5	NAG	F	2	14/15	0.93	0.19	20,25,38,39	0
2	BMA	С	3	11/12	0.93	0.15	18,27,30,31	0
6	MAN	G	7	11/12	0.94	0.19	28,34,46,50	0
6	MAN	G	4	11/12	0.94	0.15	20,26,34,34	0
3	BMA	D	3	11/12	0.94	0.17	23,28,41,52	0
6	BMA	G	3	11/12	0.94	0.13	23,28,40,43	0
2	MAN	С	6	11/12	0.95	0.17	24,30,37,45	0
2	NAG	С	1	14/15	0.95	0.09	12,17,29,33	0
2	MAN	С	8	11/12	0.95	0.11	23,31,35,39	0
6	NAG	G	2	14/15	0.95	0.09	14,17,30,32	0
6	NAG	G	1	14/15	0.96	0.08	16,18,38,53	0
3	NAG	D	1	14/15	0.96	0.08	10,17,30,40	0
3	MAN	D	4	11/12	0.96	0.16	20,24,31,34	0
5	NAG	F	1	14/15	0.96	0.12	13,21,27,42	0
3	NAG	D	2	14/15	0.96	0.08	11,15,25,26	0
2	NAG	С	2	14/15	0.97	0.09	12,21,27,28	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.





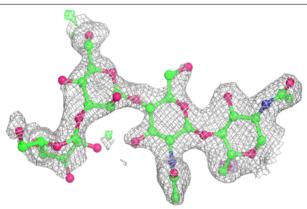


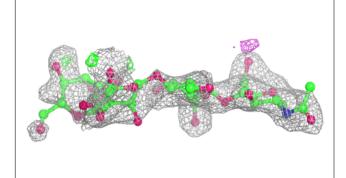


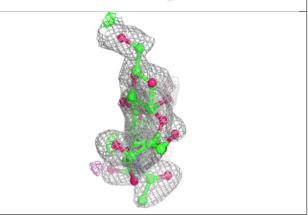


Electron density around Chain E:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

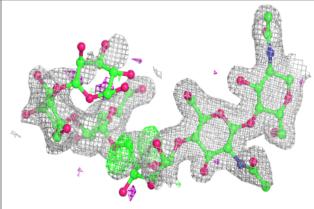


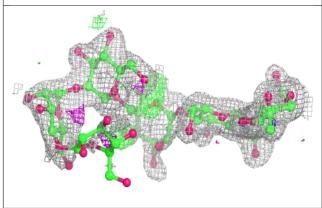


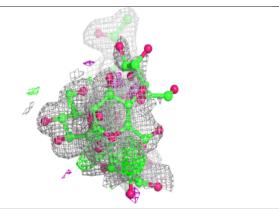


Electron density around Chain F:

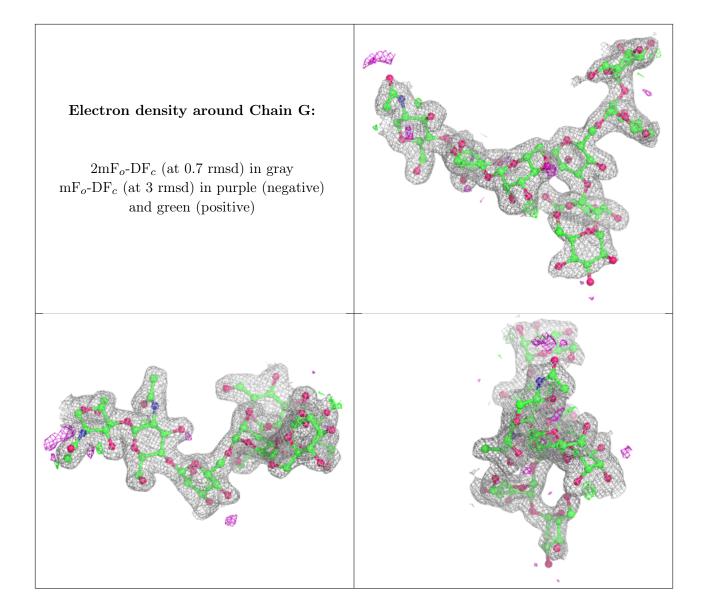
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



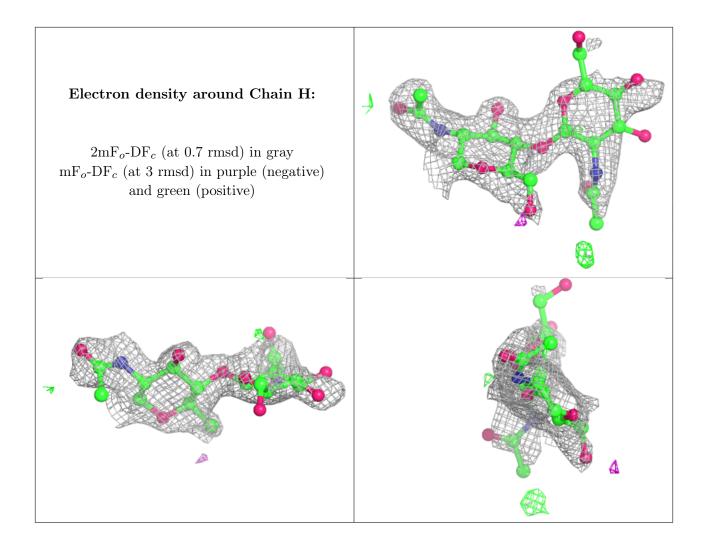












6.4 Ligands (i)

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

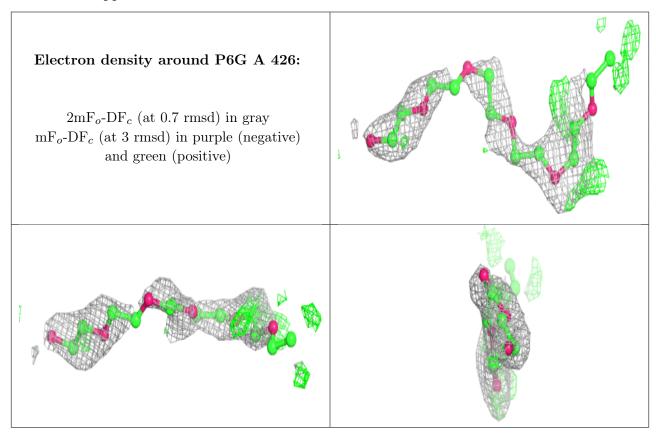
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
13	GOL	A	431	6/6	0.53	0.28	57,69,71,74	0
13	GOL	В	425	6/6	0.58	0.30	61,78,79,85	0
13	GOL	A	430	6/6	0.67	0.34	83,85,89,90	0
13	GOL	В	426	6/6	0.67	0.30	75,76,81,84	0
12	P6G	A	426	18/19	0.68	0.27	50,66,80,81	0
13	GOL	A	428	6/6	0.73	0.24	62,63,65,68	0
9	NAG	A	423	14/15	0.74	0.30	47,57,73,73	0
13	GOL	A	429	6/6	0.78	0.32	58,62,62,62	0
11	PEG	В	423	7/7	0.81	0.28	44,58,62,66	0
8	UNX	A	401	1/1	0.84	0.72	30,30,30,30	0



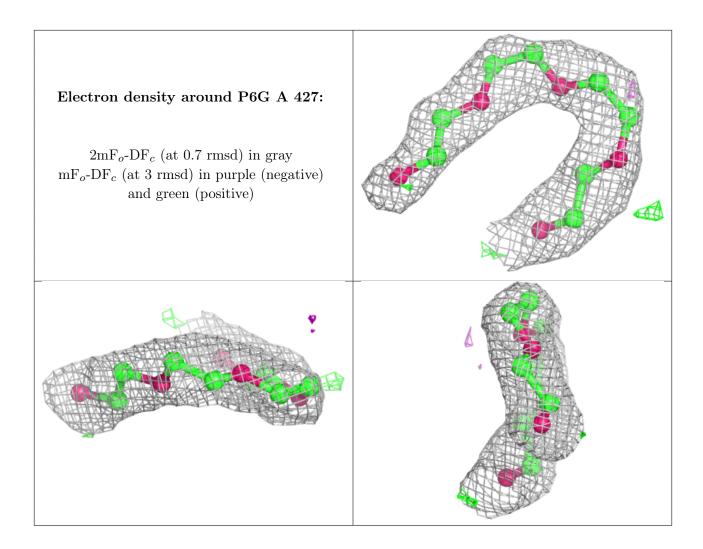
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
9	NAG	В	419	14/15	0.86	0.26	39,54,71,77	0
13	GOL	В	424	6/6	0.87	0.12	58,59,59,60	0
8	UNX	В	401	1/1	0.89	0.62	30,30,30,30	0
9	NAG	В	416	14/15	0.90	0.40	40,62,68,72	0
12	P6G	A	427	13/19	0.91	0.18	36,44,54,56	0
11	PEG	A	425	7/7	0.91	0.25	40,47,50,53	0
11	PEG	В	422	7/7	0.92	0.24	42,50,63,67	0
10	MG	В	420	1/1	0.95	0.04	23,23,23,23	0
10	MG	A	424	1/1	0.97	0.09	21,21,21,21	0
14	CL	В	421	1/1	0.98	0.08	21,21,21,21	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.







6.5 Other polymers (i)

There are no such residues in this entry.

