



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:15 PM UTC

PDB ID : 4XWH / pdb_00004xwh
Title : Crystal structure of the human N-acetyl-alpha-glucosaminidase
Authors : Birrane, G.; Meiyappan, M.; Dassier, A.
Deposited on : 2015-01-28
Resolution : 2.32 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

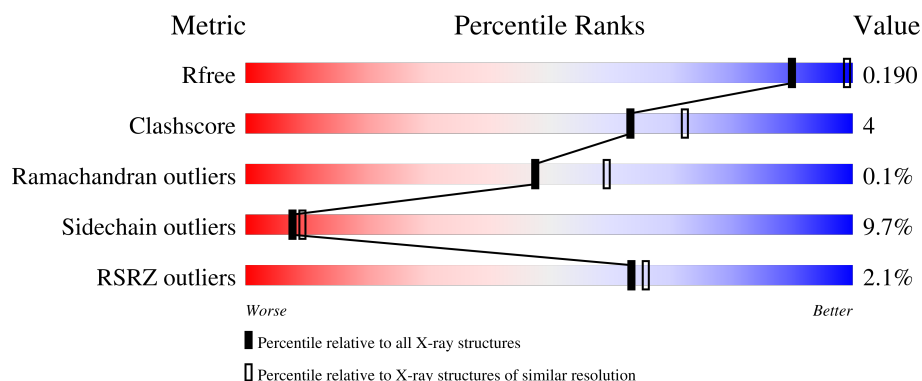
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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 $\leq 5\%$. 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	720	2% 85% 11% .
2	B	3	100%
3	C	2	100%
3	D	2	100%

2 Entry composition [i](#)

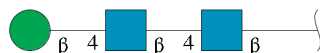
There are 7 unique types of molecules in this entry. The entry contains 6204 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-N-acetylglucosaminidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	720	Total	C	N	O	P	S	0	8	0
			5750	3698	1006	1025	1	20			

- Molecule 2 is an oligosaccharide called 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
2	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 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
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



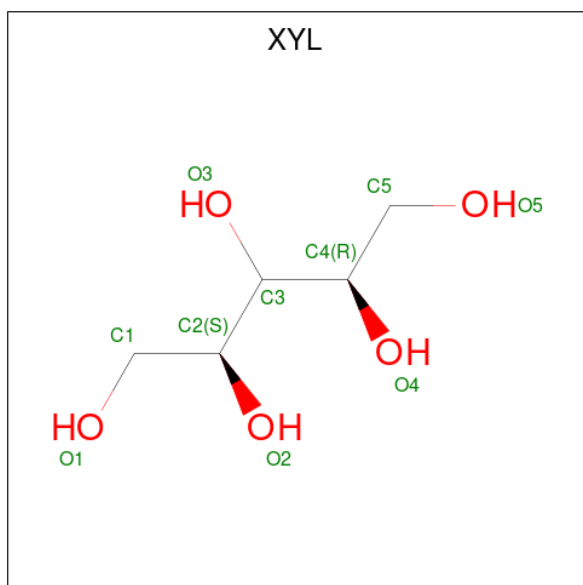
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 6 is Xylitol (CCD ID: XYL) (formula: $C_5H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	5	5		
6	A	1	Total	C	O	0	0
			10	5	5		

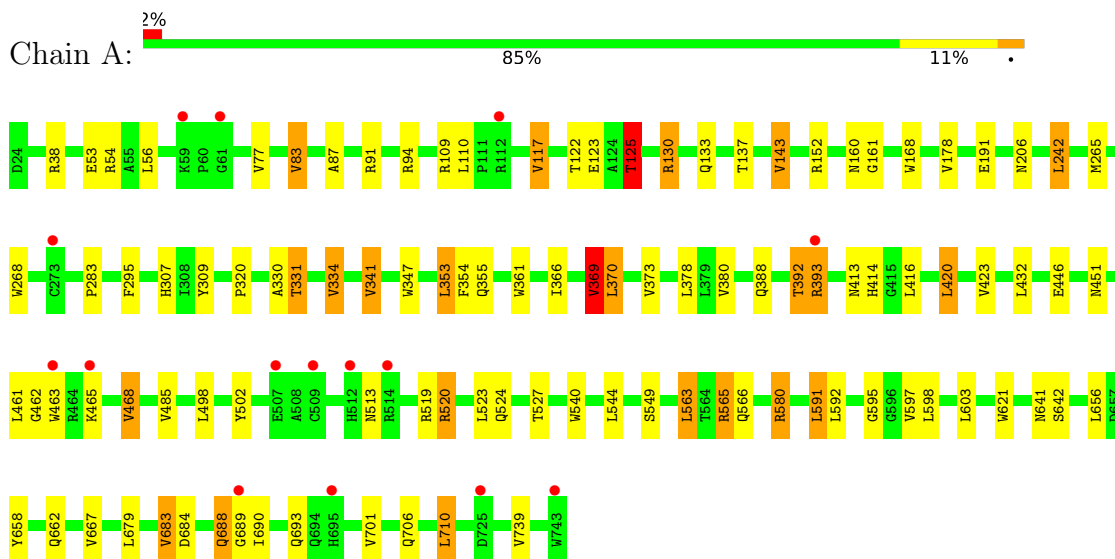
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	279	Total	O	0	0
			279	279		

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 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.

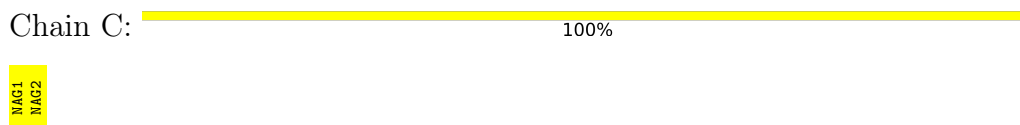
- Molecule 1: Alpha-N-acetylglucosaminidase



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



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



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



MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	205.09 Å 205.09 Å 78.40 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.32 100.00 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.6 (100.00-2.32) 99.6 (100.00-2.32)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.32 Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.166 , 0.186 0.172 , 0.190	Depositor DCC
R_{free} test set	3993 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.016 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6204	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NEP, BMA, GOL, XYL

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	0.86	0/5929	1.00	13/8085 (0.2%)

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	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	VAL	CB-CA-C	-10.26	98.75	111.88
1	A	125	THR	CB-CA-C	-8.37	95.79	109.27
1	A	565	ARG	NE-CZ-NH2	-7.43	112.51	119.20
1	A	468	VAL	N-CA-CB	6.83	116.43	110.08
1	A	565	ARG	CG-CD-NE	-6.74	97.17	112.00
1	A	143	VAL	N-CA-CB	6.22	117.42	110.51
1	A	392	THR	N-CA-C	5.70	118.23	111.33
1	A	341	VAL	N-CA-C	5.55	116.39	111.90
1	A	690	ILE	N-CA-C	5.44	114.47	108.05
1	A	369	VAL	N-CA-CB	5.35	117.42	110.57
1	A	38	ARG	CG-CD-NE	-5.24	100.48	112.00
1	A	117	VAL	CB-CA-C	5.17	116.01	110.53
1	A	83	VAL	N-CA-CB	5.04	118.15	110.58

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	689	GLY	Peptide

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	5750	0	5593	44	0
2	B	39	0	34	0	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
4	A	42	0	39	0	0
5	A	18	0	24	0	0
6	A	20	0	24	9	0
7	A	279	0	0	2	0
All	All	6204	0	5764	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 4.

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)
1:A:331:THR:HG21	1:A:369:VAL:HB	1.55	0.89
1:A:413:ASN:HD22	1:A:513:ASN:H	1.35	0.73
1:A:125:THR:HG23	1:A:463:TRP:HA	1.71	0.72
1:A:520:ARG:HD3	1:A:701:VAL:HG11	1.78	0.65
1:A:679[B]:LEU:O	1:A:683:VAL:HG13	2.00	0.62
1:A:463:TRP:CD1	6:A:2014:XYL:HO3	2.18	0.62
6:A:2015:XYL:H11	6:A:2015:XYL:O4	2.01	0.61
1:A:152[A]:ARG:NH1	7:A:2260:HOH:O	2.27	0.60
1:A:160:ASN:ND2	6:A:2014:XYL:O5	2.36	0.58
1:A:591:LEU:HD13	1:A:683:VAL:HG12	1.87	0.57
1:A:420:LEU:HD22	1:A:502:TYR:HB3	1.87	0.56
1:A:684:ASP:O	1:A:688:GLN:HG2	2.07	0.55
1:A:540:TRP:HA	1:A:563:LEU:HD13	1.91	0.53
1:A:393[B]:ARG:HG3	1:A:393[B]:ARG:HH11	1.74	0.53
1:A:414:HIS:CD2	1:A:662:GLN:H	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:LEU:HA	1:A:451:ASN:HD21	1.75	0.52
6:A:2015:XYL:O4	6:A:2015:XYL:C1	2.57	0.52
1:A:414:HIS:HD2	1:A:662:GLN:H	1.58	0.51
1:A:125:THR:CG2	1:A:462:GLY:O	2.58	0.51
1:A:595:GLY:HA3	1:A:679[A]:LEU:HD13	1.93	0.50
1:A:353:LEU:HD13	1:A:354:PHE:CD1	2.47	0.50
1:A:366:ILE:HG22	1:A:370:LEU:HD22	1.94	0.49
1:A:265:MET:HE1	1:A:320:PRO:HD3	1.96	0.47
1:A:658:TYR:CE2	6:A:2015:XYL:H2	2.48	0.47
1:A:580:ARG:HD2	7:A:2206:HOH:O	2.13	0.47
1:A:206:ASN:HB3	1:A:268:TRP:CD2	2.50	0.47
1:A:130:ARG:HD2	1:A:161:GLY:O	2.15	0.46
6:A:2014:XYL:O1	6:A:2014:XYL:O4	2.32	0.46
1:A:446:GLU:OE2	6:A:2015:XYL:O3	2.34	0.46
1:A:87:ALA:HB1	6:A:2014:XYL:H2	1.98	0.46
1:A:91:ARG:HH12	1:A:123:GLU:CD	2.24	0.45
1:A:621:TRP:CZ3	1:A:642:SER:HB3	2.52	0.45
1:A:355:GLN:HE21	1:A:388:GLN:HG3	1.82	0.44
1:A:565:ARG:HH22	1:A:566:GLN:NE2	2.16	0.44
1:A:242:LEU:O	1:A:309:TYR:HA	2.17	0.44
1:A:331:THR:HG21	1:A:369:VAL:HA	2.00	0.43
1:A:334:VAL:HG22	1:A:347:TRP:CH2	2.53	0.43
1:A:331:THR:HG21	1:A:369:VAL:CB	2.39	0.43
1:A:393[B]:ARG:HG3	1:A:393[B]:ARG:NH1	2.34	0.42
1:A:706:GLN:HG2	1:A:710:LEU:HD22	2.00	0.42
1:A:353:LEU:HD22	1:A:361:TRP:CE2	2.54	0.42
1:A:283:PRO:HB3	1:A:330:ALA:HA	2.01	0.41
1:A:178:VAL:HG21	1:A:295:PHE:HA	2.02	0.41
1:A:679[A]:LEU:O	1:A:683:VAL:HG13	2.20	0.41
1:A:519:ARG:HA	1:A:519:ARG:HD3	1.87	0.40
1:A:94:ARG:NH2	6:A:2014:XYL:H4	2.37	0.40
1:A:265:MET:HA	1:A:265:MET:HE2	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	725/720 (101%)	706 (97%)	18 (2%)	1 (0%)	48 59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	GLN

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	586/578 (101%)	529 (90%)	57 (10%)	8 9

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	54	ARG
1	A	56	LEU
1	A	77	VAL
1	A	83	VAL
1	A	109	ARG
1	A	110	LEU
1	A	117	VAL
1	A	122	THR
1	A	125	THR
1	A	130	ARG
1	A	137	THR
1	A	143	VAL
1	A	168	TRP
1	A	191	GLU
1	A	242	LEU

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Mol	Chain	Res	Type
1	A	331	THR
1	A	334	VAL
1	A	341	VAL
1	A	353	LEU
1	A	369	VAL
1	A	370	LEU
1	A	373	VAL
1	A	378	LEU
1	A	380	VAL
1	A	392	THR
1	A	393[A]	ARG
1	A	393[B]	ARG
1	A	420	LEU
1	A	423	VAL
1	A	432	LEU
1	A	461	LEU
1	A	465	LYS
1	A	468	VAL
1	A	485	VAL
1	A	498	LEU
1	A	520	ARG
1	A	523	LEU
1	A	524	GLN
1	A	527	THR
1	A	544	LEU
1	A	549	SER
1	A	563	LEU
1	A	580	ARG
1	A	591	LEU
1	A	592	LEU
1	A	597	VAL
1	A	598	LEU
1	A	603	LEU
1	A	641	ASN
1	A	656	LEU
1	A	667	VAL
1	A	683	VAL
1	A	688	GLN
1	A	693	GLN
1	A	710	LEU
1	A	739	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	176	GLN
1	A	186	GLN
1	A	318	GLN
1	A	355	GLN
1	A	357	GLN
1	A	413	ASN
1	A	414	HIS
1	A	451	ASN
1	A	524	GLN
1	A	566	GLN
1	A	624	GLN
1	A	654	ASN
1	A	660	ASN
1	A	669	ASN
1	A	694	GLN
1	A	695	HIS
1	A	700	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	NEP	A	307	1	11,14,15	3.57	3 (27%)	8,20,22	1.31	1 (12%)

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
1	NEP	A	307	1	-	1/5/12/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	NEP	P-O3P	10.37	1.61	1.46
1	A	307	NEP	P-O2P	-3.55	1.47	1.56
1	A	307	NEP	CD2-CG	3.50	1.42	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	NEP	O2P-P-O3P	-2.75	106.18	112.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	307	NEP	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

7 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	NAG	B	1	2,1	14,14,15	0.47	0	17,19,21	1.47	3 (17%)
2	NAG	B	2	2	14,14,15	0.85	0	17,19,21	1.67	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	B	3	2	11,11,12	0.79	0	15,15,17	1.59	3 (20%)
3	NAG	C	1	1,3	14,14,15	0.46	0	17,19,21	2.08	5 (29%)
3	NAG	C	2	3	14,14,15	0.88	0	17,19,21	1.82	2 (11%)
3	NAG	D	1	1,3	14,14,15	0.79	0	17,19,21	1.76	5 (29%)
3	NAG	D	2	3	14,14,15	0.93	1 (7%)	17,19,21	1.31	2 (11%)

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	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	C1-C2	2.62	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	6.49	120.88	112.19
3	C	2	NAG	C1-O5-C5	5.09	119.01	112.19
2	B	2	NAG	C4-C3-C2	4.64	117.82	111.02
2	B	3	BMA	C1-O5-C5	4.39	118.07	112.19
2	B	1	NAG	C1-C2-N2	-3.77	104.49	110.43
3	D	1	NAG	C1-O5-C5	3.64	117.07	112.19
3	D	2	NAG	C4-C3-C2	3.63	116.34	111.02
3	C	2	NAG	C4-C3-C2	-3.61	105.72	111.02
3	D	1	NAG	C2-N2-C7	3.18	127.17	122.90
3	D	1	NAG	O7-C7-N2	2.72	126.79	121.98
2	B	3	BMA	O2-C2-C1	2.66	115.32	109.22
2	B	2	NAG	C2-N2-C7	2.60	126.39	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C2-N2-C7	2.59	126.38	122.90
2	B	3	BMA	O2-C2-C3	-2.46	105.06	110.15
3	D	1	NAG	O5-C5-C6	-2.43	102.93	107.66
2	B	1	NAG	C2-N2-C7	2.32	126.01	122.90
3	C	1	NAG	O5-C1-C2	-2.31	107.71	111.29
3	C	1	NAG	C1-C2-N2	2.30	114.05	110.43
3	C	1	NAG	O6-C6-C5	-2.23	103.74	111.33
2	B	2	NAG	C1-C2-N2	-2.08	107.15	110.43
3	D	1	NAG	C4-C3-C2	2.05	114.02	111.02
3	C	1	NAG	O5-C5-C4	2.01	115.72	110.83
2	B	1	NAG	C8-C7-N2	-2.01	112.78	116.12

There are no chirality outliers.

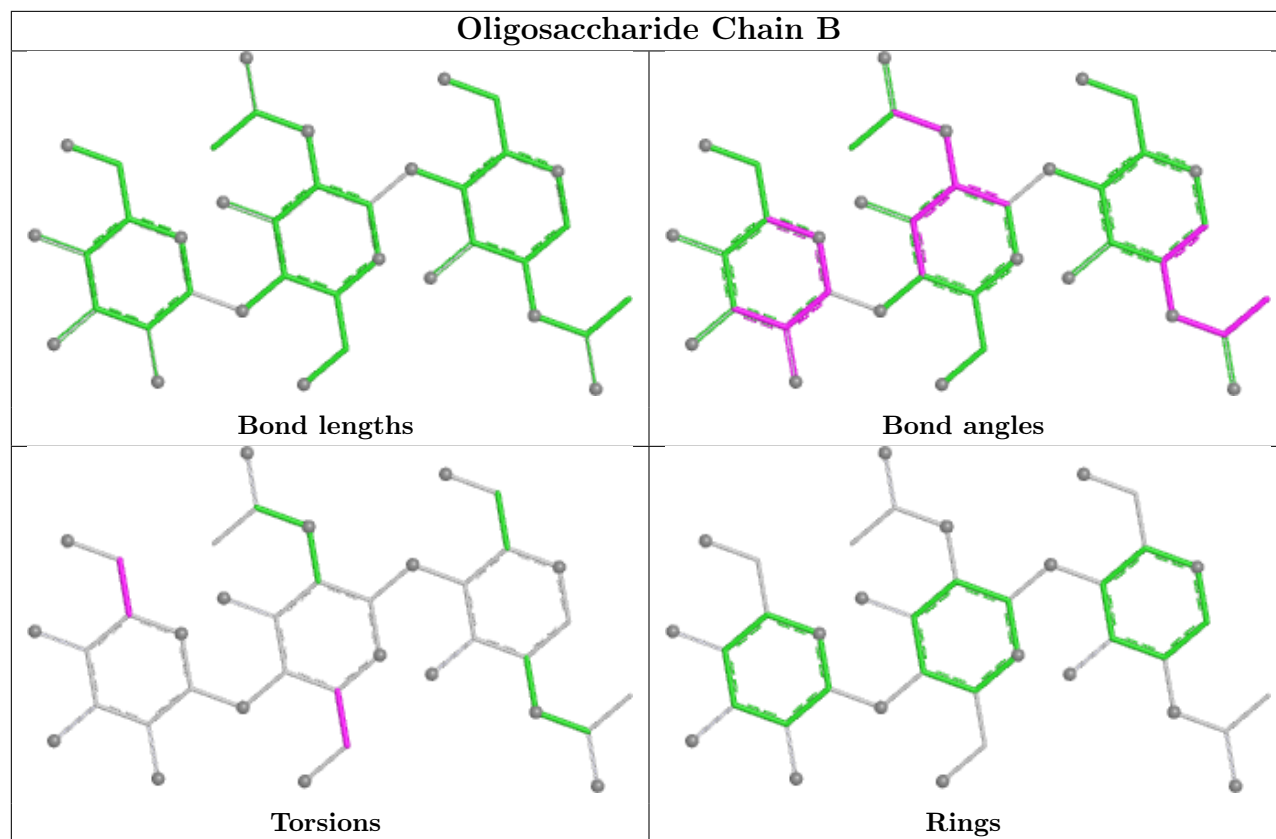
All (7) torsion outliers are listed below:

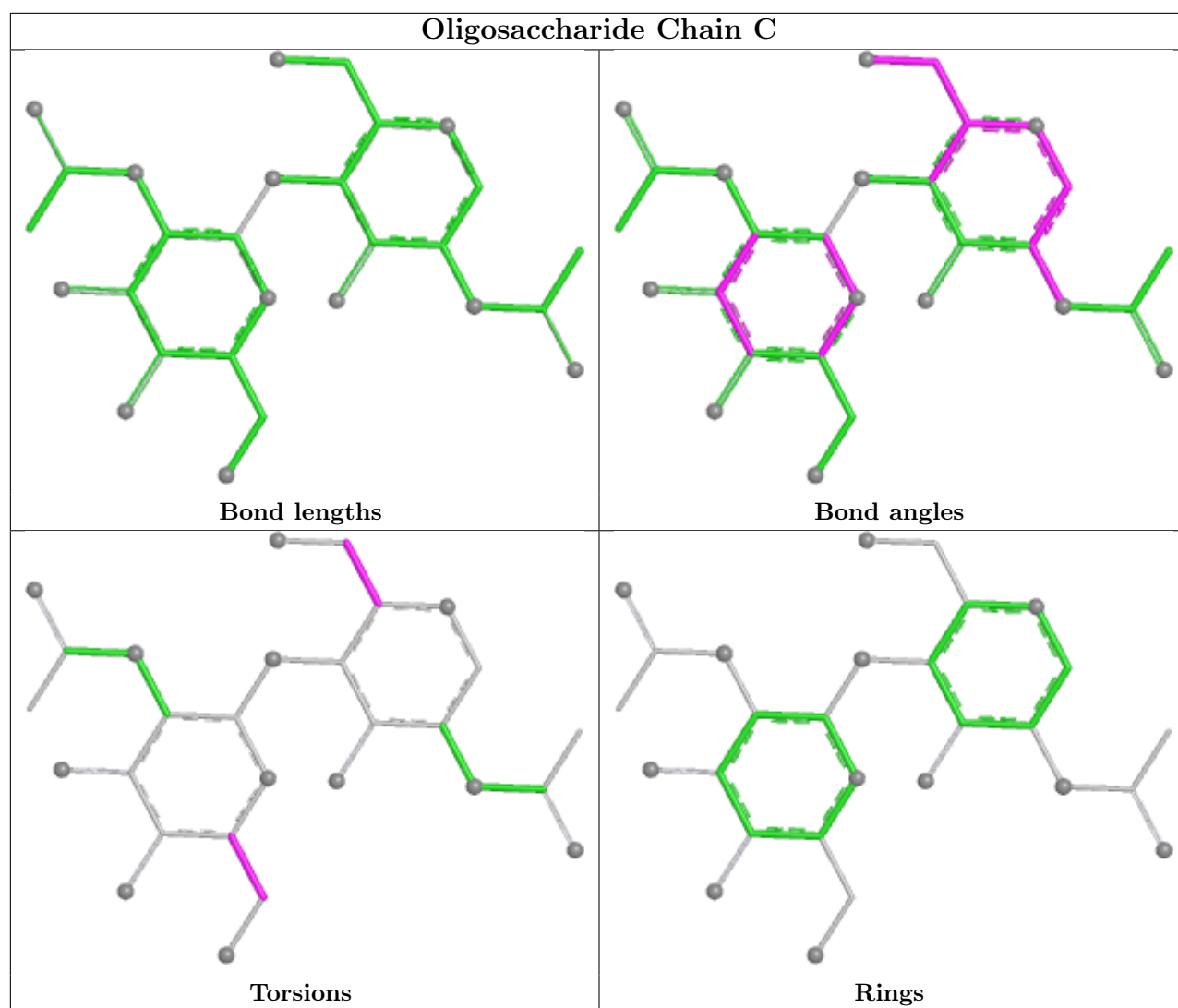
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

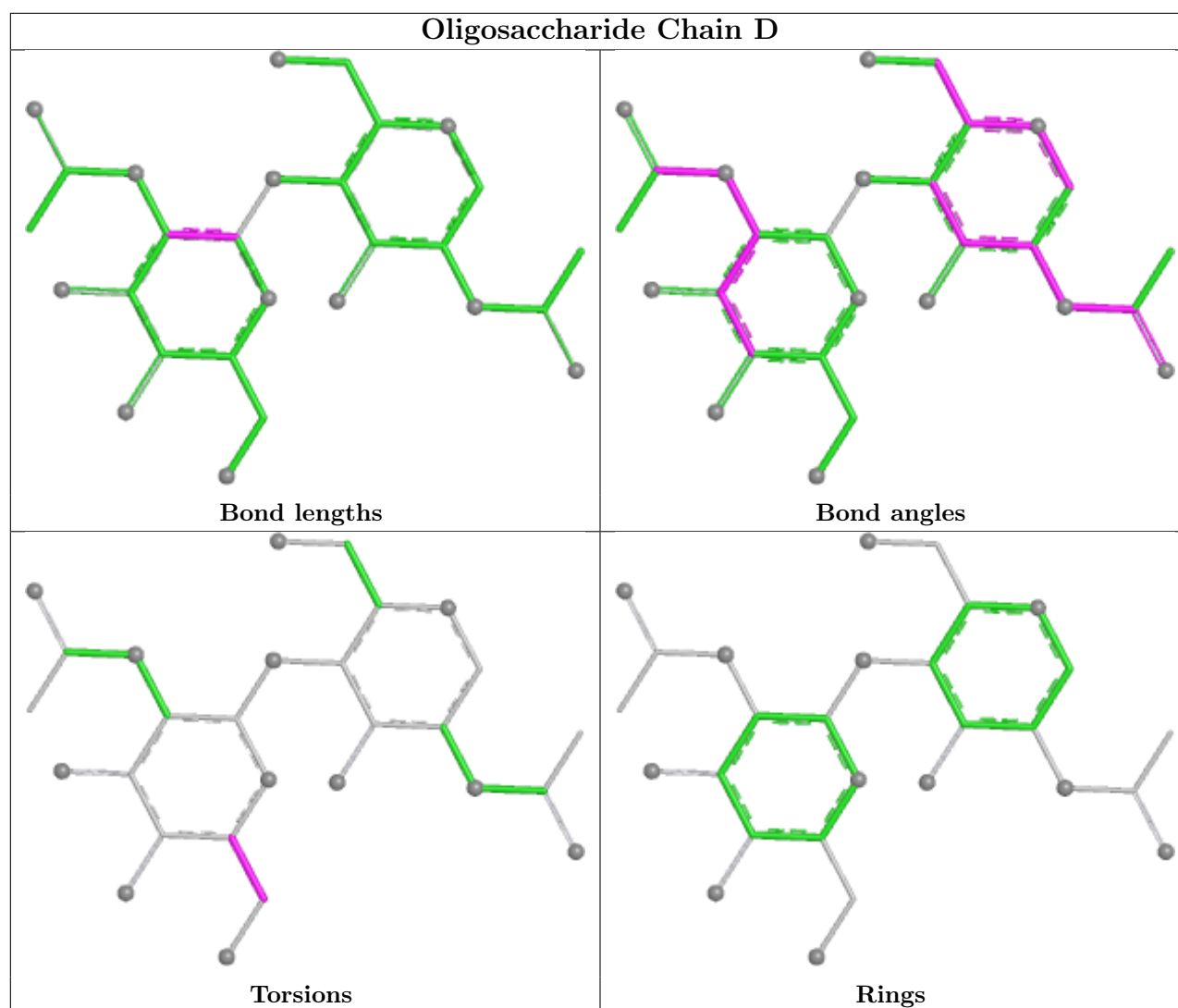
There are no ring outliers.

No monomer is involved in short contacts.

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](#)

8 ligands 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	$\# Z > 2$
6	XYL	A	2015	-	9,9,9	0.73	0	11,11,11	2.26	4 (36%)
5	GOL	A	2012	-	5,5,5	0.55	0	5,5,5	0.53	0
4	NAG	A	2004	1	14,14,15	0.67	0	17,19,21	1.75	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	2009	1	14,14,15	0.93	0	17,19,21	1.65	4 (23%)
5	GOL	A	2011	-	5,5,5	0.25	0	5,5,5	0.56	0
6	XYL	A	2014	-	9,9,9	0.70	0	11,11,11	2.40	4 (36%)
5	GOL	A	2013	-	5,5,5	0.53	0	5,5,5	0.36	0
4	NAG	A	2010	1	14,14,15	1.07	0	17,19,21	1.55	5 (29%)

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	XYL	A	2015	-	-	8/12/12/12	-
5	GOL	A	2012	-	-	0/4/4/4	-
4	NAG	A	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2009	1	-	1/6/23/26	0/1/1/1
5	GOL	A	2011	-	-	2/4/4/4	-
6	XYL	A	2014	-	-	8/12/12/12	-
5	GOL	A	2013	-	-	4/4/4/4	-
4	NAG	A	2010	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2014	XYL	C1-C2-C3	5.45	123.27	112.17
4	A	2004	NAG	C1-O5-C5	4.74	118.54	112.19
4	A	2009	NAG	C1-O5-C5	4.11	117.69	112.19
6	A	2015	XYL	O1-C1-C2	-3.91	102.95	111.16
6	A	2015	XYL	C1-C2-C3	3.73	119.78	112.17
6	A	2015	XYL	O4-C4-C5	3.37	116.68	109.03
4	A	2010	NAG	C2-N2-C7	3.27	127.28	122.90
6	A	2014	XYL	O2-C2-C3	-3.14	101.89	109.25
4	A	2009	NAG	O5-C5-C6	2.99	113.48	107.66
4	A	2010	NAG	O5-C1-C2	-2.99	106.67	111.29
6	A	2015	XYL	C4-C3-C2	2.92	118.43	113.57
6	A	2014	XYL	C4-C3-C2	-2.73	109.03	113.57
4	A	2009	NAG	C2-N2-C7	2.43	126.16	122.90
6	A	2014	XYL	O1-C1-C2	2.41	116.22	111.16
4	A	2010	NAG	O3-C3-C2	2.41	114.40	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2009	NAG	C6-C5-C4	-2.35	107.25	113.02
4	A	2010	NAG	O5-C5-C6	2.33	112.20	107.66
4	A	2004	NAG	C4-C3-C2	2.26	114.33	111.02
4	A	2004	NAG	O5-C1-C2	-2.23	107.84	111.29
4	A	2004	NAG	C6-C5-C4	-2.18	107.67	113.02
4	A	2004	NAG	O3-C3-C4	-2.12	105.38	110.38
4	A	2010	NAG	C4-C3-C2	-2.09	107.95	111.02

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2013	GOL	O1-C1-C2-O2
5	A	2013	GOL	O1-C1-C2-C3
5	A	2013	GOL	C1-C2-C3-O3
6	A	2014	XYL	C1-C2-C3-O3
6	A	2015	XYL	C1-C2-C3-C4
6	A	2014	XYL	C1-C2-C3-C4
6	A	2014	XYL	O2-C2-C3-O3
6	A	2015	XYL	C1-C2-C3-O3
6	A	2015	XYL	O2-C2-C3-O3
5	A	2011	GOL	C1-C2-C3-O3
5	A	2013	GOL	O2-C2-C3-O3
6	A	2015	XYL	O1-C1-C2-O2
6	A	2015	XYL	O2-C2-C3-C4
6	A	2014	XYL	O2-C2-C3-C4
4	A	2010	NAG	C3-C2-N2-C7
6	A	2015	XYL	C2-C3-C4-C5
5	A	2011	GOL	O2-C2-C3-O3
6	A	2015	XYL	O1-C1-C2-C3
6	A	2014	XYL	O4-C4-C5-O5
4	A	2009	NAG	O5-C5-C6-O6
6	A	2014	XYL	O1-C1-C2-O2
6	A	2014	XYL	C3-C4-C5-O5
6	A	2014	XYL	O1-C1-C2-C3
6	A	2015	XYL	O3-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2015	XYL	4	0
6	A	2014	XYL	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	719/720 (99%)	-0.12	15 (2%) 63 66	27, 50, 76, 102	8 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	LYS	4.9
1	A	695	HIS	4.0
1	A	393[A]	ARG	3.8
1	A	743	TRP	3.5
1	A	512[A]	HIS	3.3
1	A	273	CYS	3.3
1	A	463	TRP	3.0
1	A	465	LYS	2.9
1	A	112	ARG	2.8
1	A	689	GLY	2.6
1	A	61	GLY	2.5
1	A	514	ARG	2.5
1	A	507	GLU	2.2
1	A	509	CYS	2.1
1	A	725	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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.

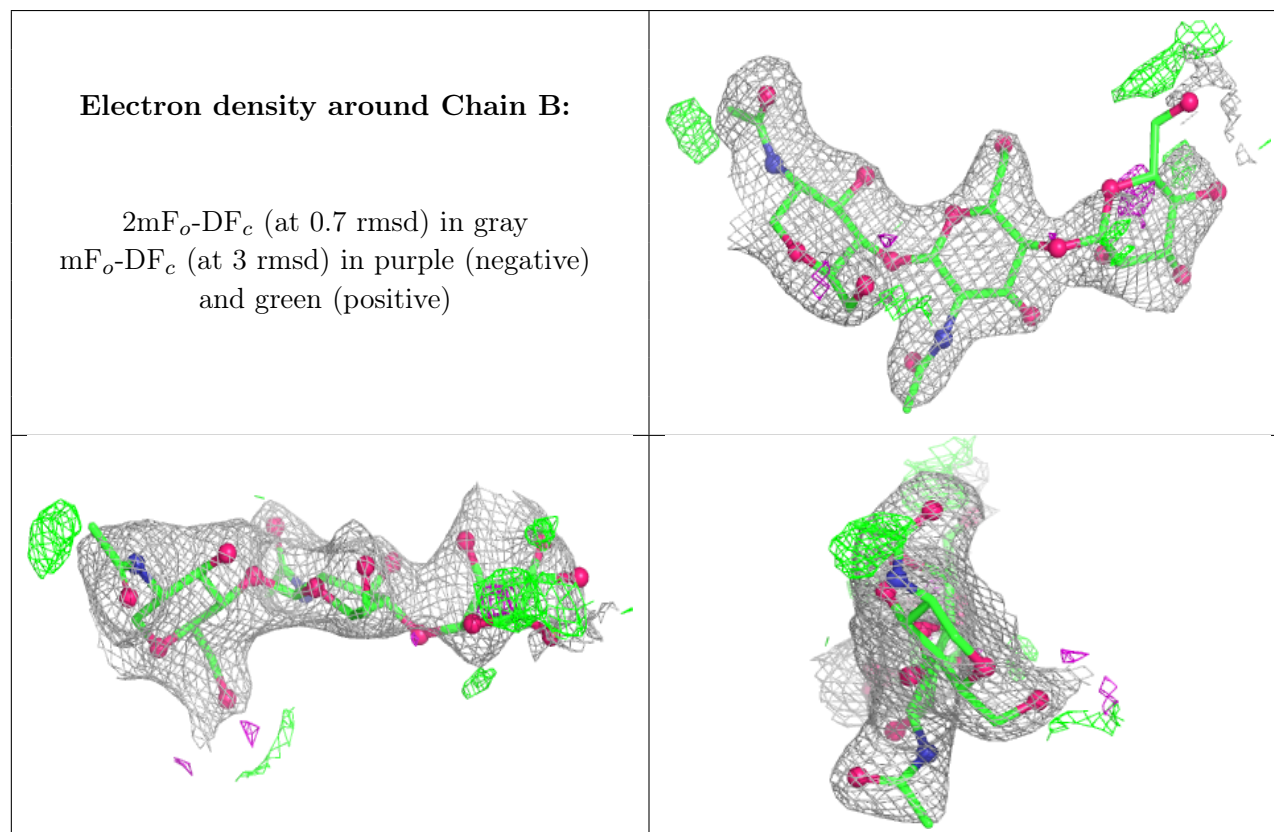
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	NEP	A	307	14/15	0.97	0.07	42,45,60,61	0

6.3 Carbohydrates [i](#)

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

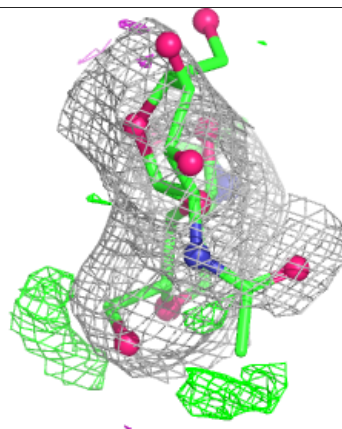
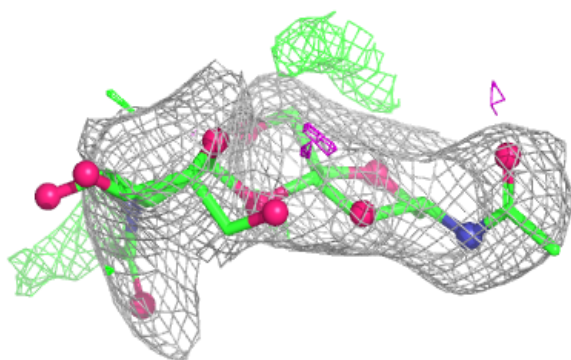
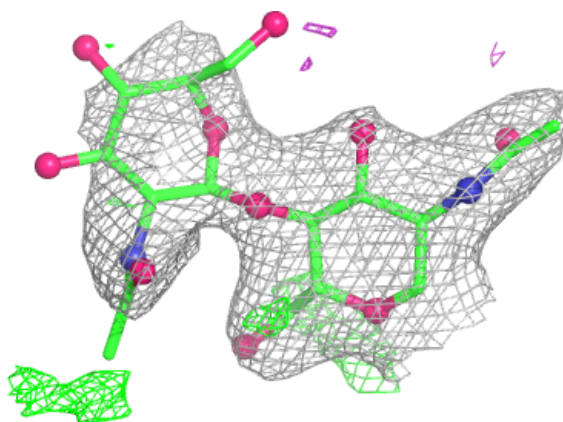
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	B	3	11/12	0.47	0.25	101,113,120,121	0
3	NAG	C	2	14/15	0.64	0.24	111,119,127,128	0
3	NAG	D	2	14/15	0.67	0.21	115,122,127,128	0
3	NAG	C	1	14/15	0.85	0.14	78,86,96,109	0
3	NAG	D	1	14/15	0.90	0.14	76,89,98,108	0
2	NAG	B	2	14/15	0.90	0.16	74,87,97,109	0
2	NAG	B	1	14/15	0.92	0.11	61,69,76,78	0

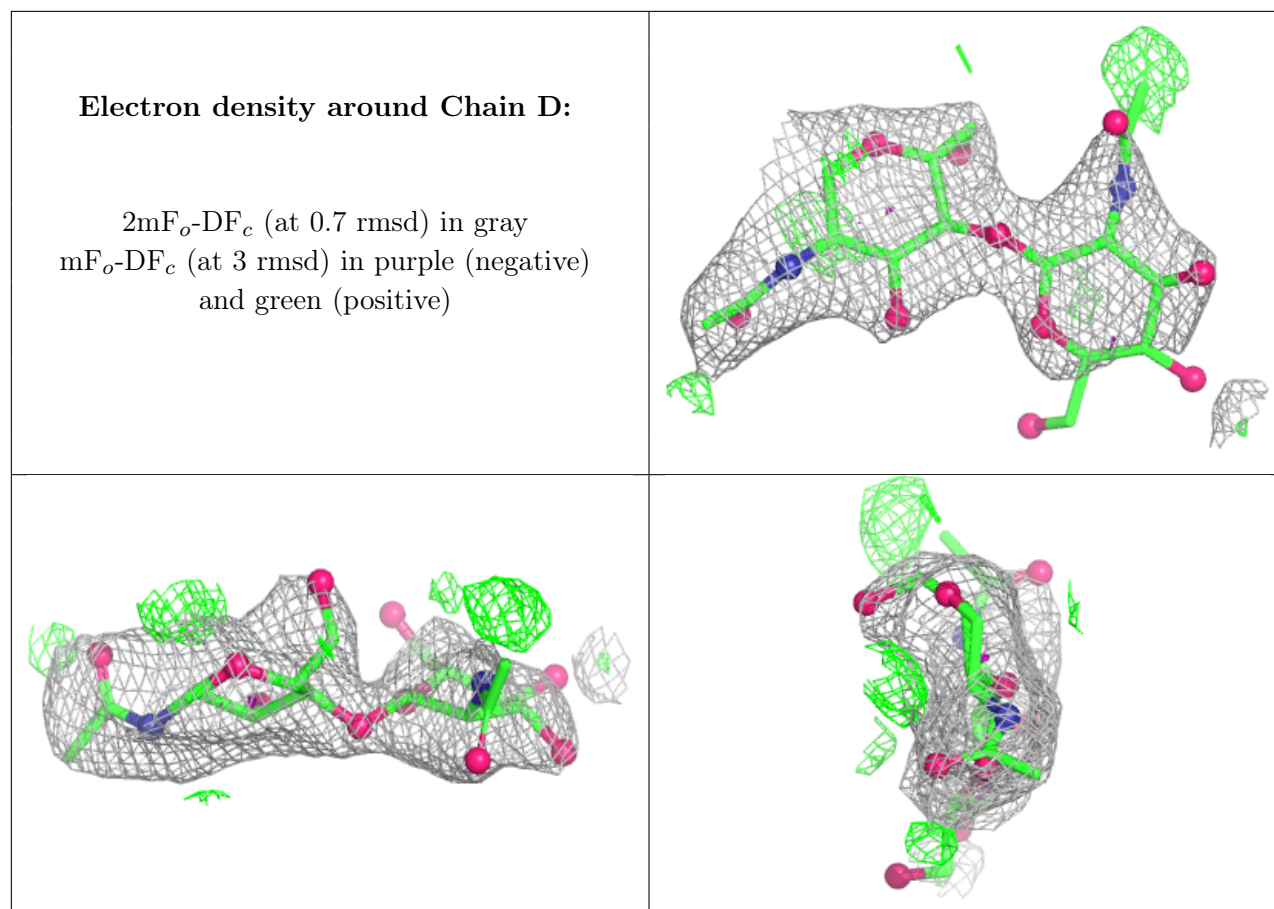
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	A	2010	14/15	0.40	0.30	116,127,133,133	0
4	NAG	A	2009	14/15	0.65	0.22	106,111,114,114	0
4	NAG	A	2004	14/15	0.81	0.20	84,94,98,104	0
5	GOL	A	2012	6/6	0.81	0.27	74,78,85,89	0
6	XYL	A	2014	10/10	0.86	0.22	75,82,89,94	0
5	GOL	A	2013	6/6	0.89	0.20	70,72,76,79	0
6	XYL	A	2015	10/10	0.90	0.17	48,52,57,62	0
5	GOL	A	2011	6/6	0.93	0.17	51,61,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.