Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 06:42 PM EDT

PDB ID	:	4XWH
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 (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 (i)) were used in the production of this report:

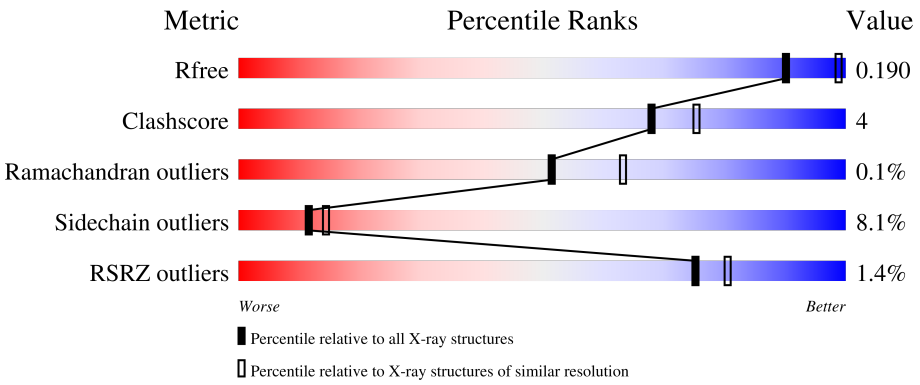
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 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}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (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 <=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	% 86% 12% • •
2	B	3	100%
3	C	2	100%
3	D	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
3	NAG	C	2	-	-	-	X
3	NAG	D	2	-	-	-	X
4	NAG	A	2010	-	-	-	X

2 Entry composition (i)

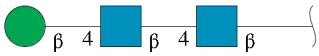
There are 7 unique types of molecules in this entry. The entry contains 6204 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	P	S			
1	A	720	5750	3698	1006	1025	1	20	0	8	0

- 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.

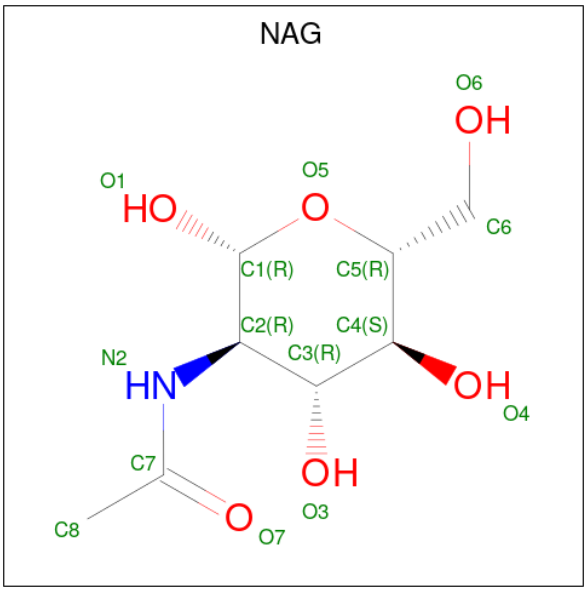


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	39	22	2	15	0	0	0

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

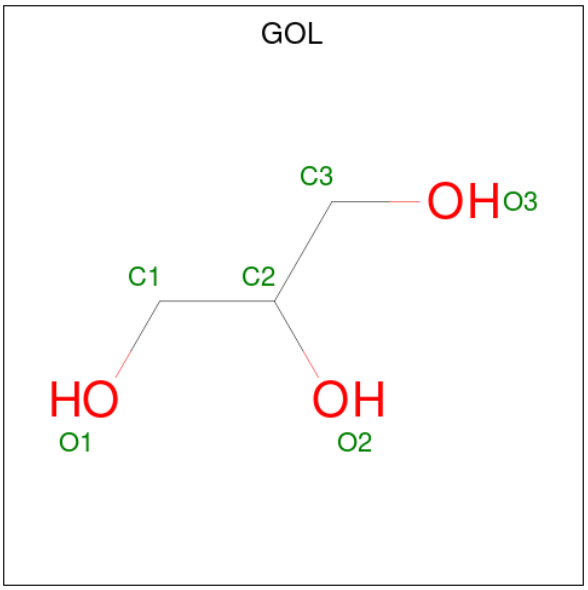
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	2	28	16	2	10	0	0	0
3	D	2	28	16	2	10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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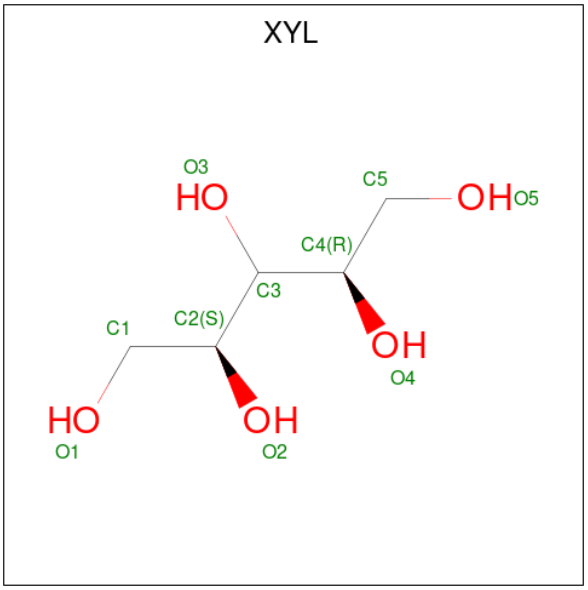
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	3	3	0	0
			Total	C	O		
5	A	1	6	3	3	0	0

- Molecule 6 is Xylitol (three-letter code: XYL) (formula: $C_5H_{12}O_5$).



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

- Molecule 7 is water.

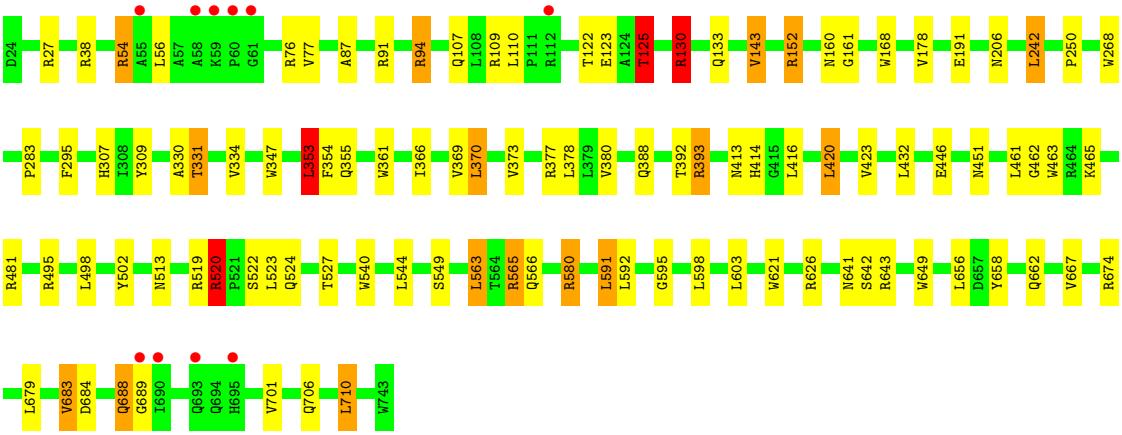
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	279	279	279	0	0

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.

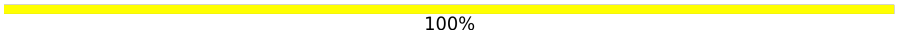
• Molecule 1: Alpha-N-acetylglucosaminidase

Chain A:



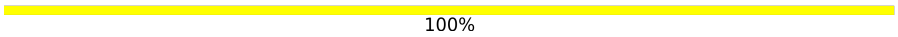
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



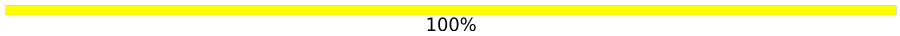
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



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

Chain D:



NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	205.09Å 205.09Å 78.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.32 49.26 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.6 (100.00-2.32) 99.6 (49.26-2.32)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.32Å)	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 (4.90%)	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)	0.35 , 36.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical 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.

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, XYL, NAG, BMA, NEP

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	0.67	0/5929	0.96	35/8085 (0.4%)

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 (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	565	ARG	NE-CZ-NH2	-15.58	112.51	120.30
1	A	38	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	A	38	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	A	130	ARG	NE-CZ-NH1	10.73	125.66	120.30
1	A	643	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	A	54	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	A	565	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	A	643	ARG	NE-CZ-NH2	-9.65	115.47	120.30
1	A	377	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	A	54	ARG	NE-CZ-NH2	-8.75	115.93	120.30
1	A	130	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	A	377	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	A	520	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	A	94	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	565	ARG	CG-CD-NE	-6.96	97.17	111.80
1	A	674	ARG	NE-CZ-NH2	-6.82	116.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	143	VAL	CB-CA-C	-6.66	98.75	111.40
1	A	125	THR	CB-CA-C	-5.86	95.79	111.60
1	A	481	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	580	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	626	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	481	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	495	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	76	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	152[A]	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	152[B]	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	38	ARG	CG-CD-NE	-5.39	100.48	111.80
1	A	520	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	565	ARG	CD-NE-CZ	5.34	131.08	123.60
1	A	495	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	27	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	38	ARG	CD-NE-CZ	5.07	130.70	123.60
1	A	353	LEU	CA-CB-CG	5.06	126.94	115.30
1	A	143	VAL	CG1-CB-CG2	5.04	118.97	110.90

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 (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	5750	0	5593	41	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	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	279	0	0	2	0
All	All	6204	0	5764	44	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 (44) 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
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:91:ARG:HH12	1:A:123:GLU:CD	2.24	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

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	725/720 (101%)	706 (97%)	18 (2%)	1 (0%)	51 63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	GLN

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	586/578 (101%)	538 (92%)	48 (8%)	11 14

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	56	LEU
1	A	77	VAL
1	A	107	GLN
1	A	109	ARG
1	A	110	LEU
1	A	122	THR
1	A	125	THR
1	A	130	ARG
1	A	143	VAL
1	A	168	TRP
1	A	191	GLU
1	A	242	LEU
1	A	250	PRO
1	A	331	THR
1	A	353	LEU
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	498	LEU
1	A	520	ARG
1	A	522	SER
1	A	523	LEU
1	A	524	GLN
1	A	527	THR
1	A	544	LEU
1	A	549	SER

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Mol	Chain	Res	Type
1	A	563	LEU
1	A	591	LEU
1	A	592	LEU
1	A	598	LEU
1	A	603	LEU
1	A	641	ASN
1	A	649	TRP
1	A	656	LEU
1	A	667	VAL
1	A	683	VAL
1	A	688	GLN
1	A	710	LEU

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	127	ASN
1	A	160	ASN
1	A	176	GLN
1	A	186	GLN
1	A	315	ASN
1	A	350	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	645	GLN
1	A	654	ASN
1	A	669	ASN
1	A	694	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	10,14,15	5.64	3 (30%)	5,20,22	1.62	1 (20%)

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	16.69	1.61	1.47
1	A	307	NEP	CD2-CG	4.09	1.42	1.36
1	A	307	NEP	P-O2P	-3.61	1.47	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	307	NEP	O2P-P-O3P	-3.36	106.18	113.44

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	1,2	14,14,15	0.47	0	17,19,21	1.41	2 (11%)
2	NAG	B	2	2	14,14,15	0.86	0	17,19,21	1.65	2 (11%)
2	BMA	B	3	2	11,11,12	0.80	0	15,15,17	1.66	3 (20%)
3	NAG	C	1	3,1	14,14,15	0.44	0	17,19,21	2.05	6 (35%)
3	NAG	C	2	3	14,14,15	0.85	0	17,19,21	1.85	3 (17%)
3	NAG	D	1	3,1	14,14,15	0.78	0	17,19,21	1.74	5 (29%)
3	NAG	D	2	3	14,14,15	0.88	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	1,2	-	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	3,1	-	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	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	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	2.39	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	NAG	C1-O5-C5	6.41	120.88	112.19
3	C	2	NAG	C1-O5-C5	5.03	119.01	112.19
2	B	2	NAG	C4-C3-C2	4.64	117.82	111.02
2	B	3	BMA	C1-O5-C5	4.34	118.07	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	C1-O5-C5	3.60	117.07	112.19
2	B	1	NAG	C1-C2-N2	-3.51	104.49	110.49
2	B	3	BMA	O2-C2-C1	3.02	115.32	109.15
3	D	1	NAG	C2-N2-C7	3.00	127.17	122.90
3	D	1	NAG	O5-C5-C6	-2.72	102.93	107.20
3	D	1	NAG	O7-C7-N2	2.63	126.79	121.95
3	C	2	NAG	O5-C5-C6	2.55	111.20	107.20
2	B	3	BMA	O2-C2-C3	-2.54	105.06	110.14
2	B	2	NAG	C2-N2-C7	2.45	126.39	122.90
3	D	2	NAG	C2-N2-C7	2.44	126.38	122.90
3	C	1	NAG	O5-C1-C2	-2.26	107.71	111.29
3	C	1	NAG	O6-C6-C5	-2.20	103.74	111.29
2	B	1	NAG	C2-N2-C7	2.18	126.01	122.90
3	C	1	NAG	C1-C2-N2	2.09	114.05	110.49
3	D	1	NAG	C4-C3-C2	2.05	114.02	111.02
3	C	1	NAG	O5-C5-C6	-2.03	104.02	107.20
3	C	1	NAG	O5-C5-C4	2.01	115.72	110.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

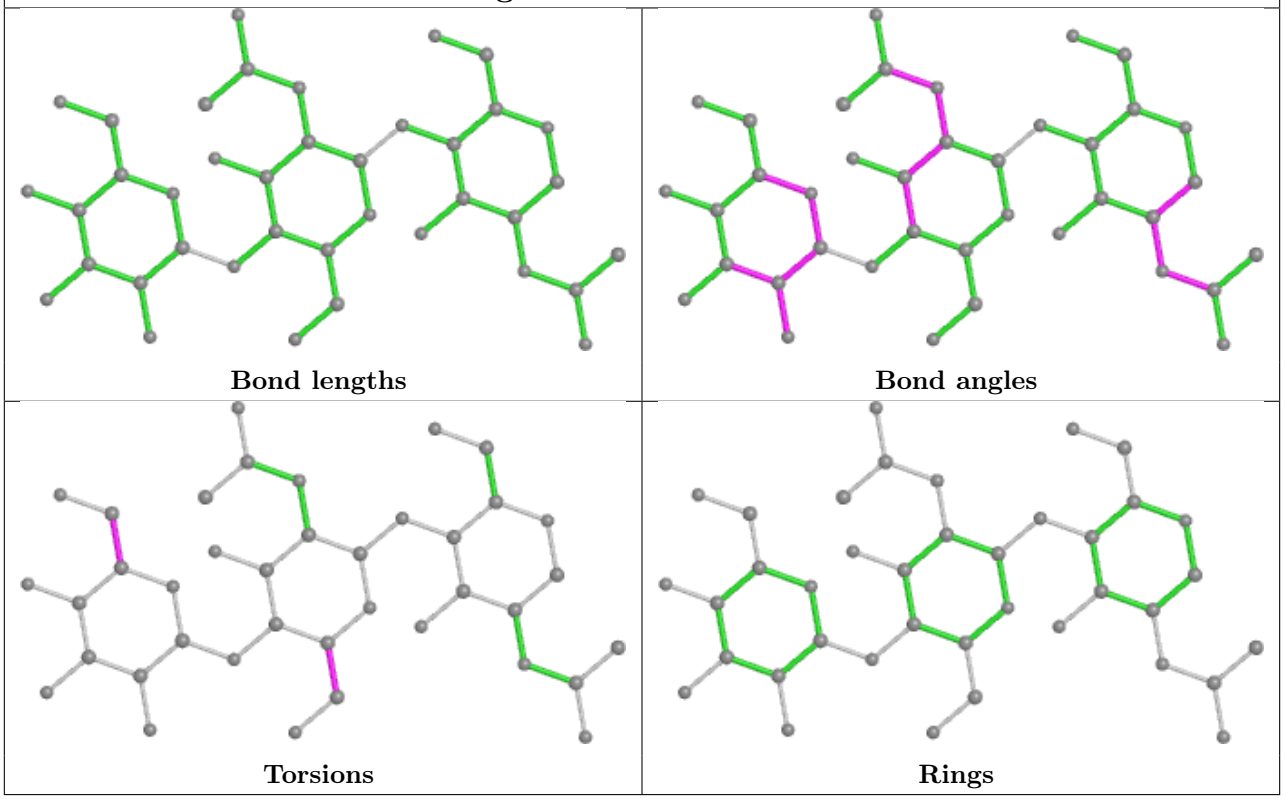
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

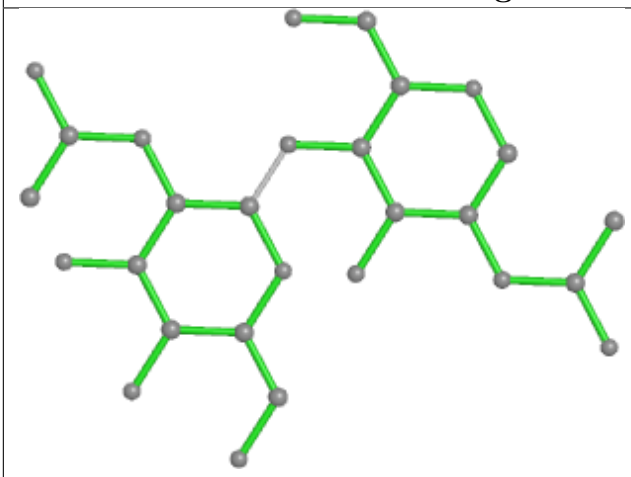
No monomer is involved in short contacts.

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

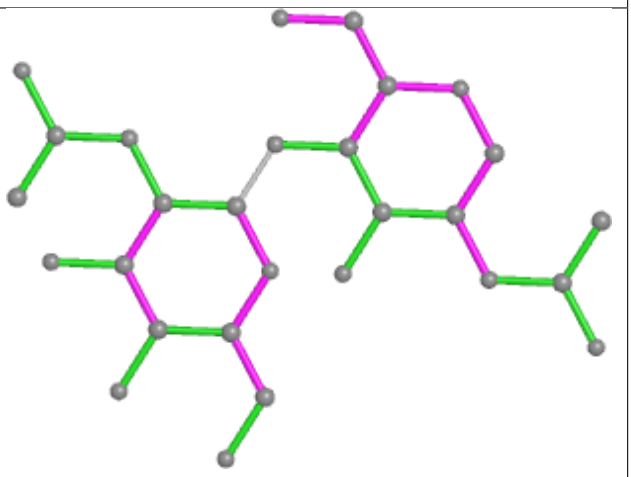
Oligosaccharide Chain B



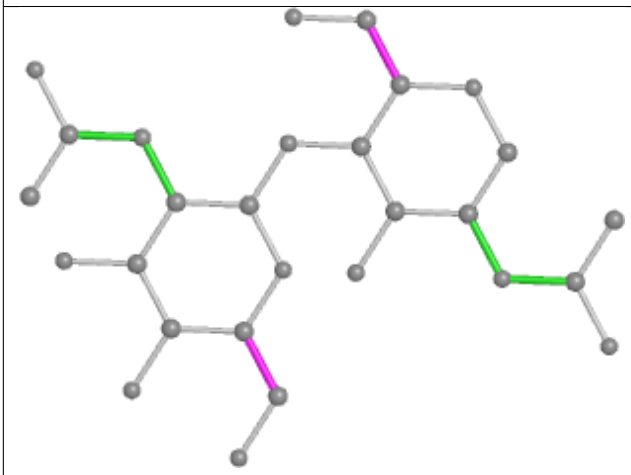
Oligosaccharide Chain C



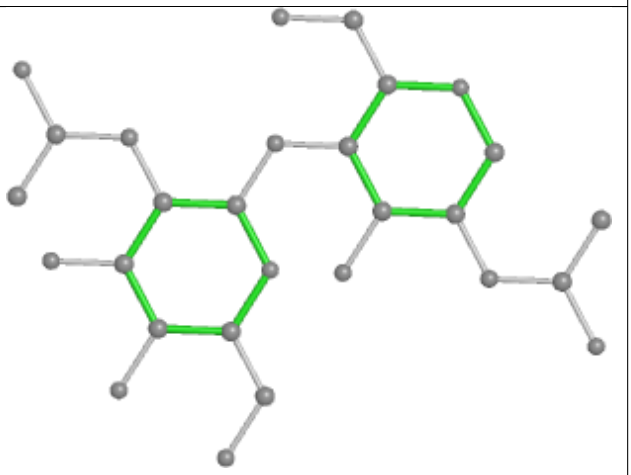
Bond lengths



Bond angles

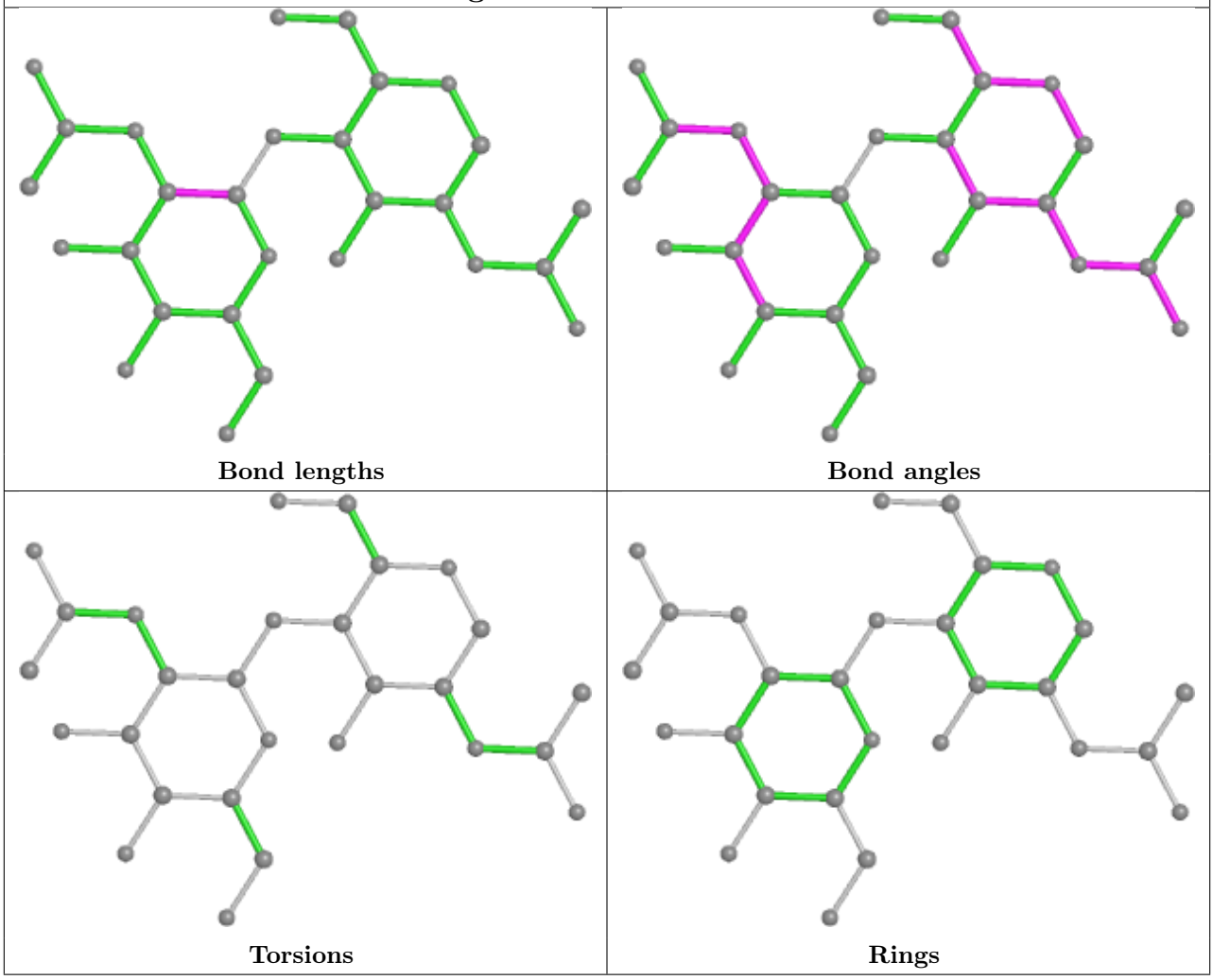


Torsions



Rings

Oligosaccharide Chain D



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	2014	-	9,9,9	0.66	0	11,11,11	2.21	4 (36%)
5	GOL	A	2013	-	5,5,5	0.51	0	5,5,5	0.35	0
4	NAG	A	2010	1	14,14,15	1.05	0	17,19,21	1.61	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	XYL	A	2015	-	9,9,9	0.71	0	11,11,11	2.10	4 (36%)
4	NAG	A	2009	1	14,14,15	0.91	0	17,19,21	1.75	4 (23%)
5	GOL	A	2012	-	5,5,5	0.53	0	5,5,5	0.51	0
5	GOL	A	2011	-	5,5,5	0.25	0	5,5,5	0.51	0
4	NAG	A	2004	1	14,14,15	0.67	0	17,19,21	1.78	6 (35%)

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	2014	-	-	7/12/12/12	-
5	GOL	A	2013	-	-	4/4/4/4	-
4	NAG	A	2010	1	-	1/6/23/26	0/1/1/1
6	XYL	A	2015	-	-	7/12/12/12	-
4	NAG	A	2009	1	-	1/6/23/26	0/1/1/1
5	GOL	A	2012	-	-	0/4/4/4	-
5	GOL	A	2011	-	-	2/4/4/4	-
4	NAG	A	2004	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	2014	XYL	C1-C2-C3	5.01	123.27	112.41
4	A	2004	NAG	C1-O5-C5	4.69	118.54	112.19
4	A	2009	NAG	C1-O5-C5	4.06	117.69	112.19
4	A	2009	NAG	O5-C5-C6	4.00	113.48	107.20
6	A	2015	XYL	O1-C1-C2	-3.73	102.95	111.07
6	A	2015	XYL	C1-C2-C3	3.40	119.78	112.41
6	A	2015	XYL	O4-C4-C5	3.21	116.68	109.14
4	A	2010	NAG	O5-C5-C6	3.18	112.20	107.20
4	A	2010	NAG	C2-N2-C7	3.08	127.28	122.90
6	A	2014	XYL	O2-C2-C3	-2.96	101.89	109.10
4	A	2010	NAG	O5-C1-C2	-2.93	106.67	111.29
4	A	2009	NAG	C6-C5-C4	-2.46	107.25	113.00
6	A	2015	XYL	C4-C3-C2	2.44	118.43	113.36
4	A	2010	NAG	O3-C3-C2	2.39	114.40	109.47
6	A	2014	XYL	O1-C1-C2	2.36	116.22	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2009	NAG	C2-N2-C7	2.29	126.16	122.90
4	A	2004	NAG	C6-C5-C4	-2.28	107.67	113.00
4	A	2004	NAG	C4-C3-C2	2.26	114.33	111.02
4	A	2004	NAG	O5-C1-C2	-2.18	107.84	111.29
4	A	2004	NAG	O3-C3-C4	-2.15	105.38	110.35
4	A	2010	NAG	C4-C3-C2	-2.09	107.95	111.02
6	A	2014	XYL	C4-C3-C2	-2.08	109.03	113.36
4	A	2004	NAG	O5-C5-C6	2.06	110.44	107.20

There are no chirality outliers.

All (22) 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	O2-C2-C3-O3
6	A	2014	XYL	C1-C2-C3-C4
6	A	2015	XYL	C1-C2-C3-O3
6	A	2015	XYL	O2-C2-C3-O3
6	A	2015	XYL	O2-C2-C3-C4
5	A	2011	GOL	C1-C2-C3-O3
5	A	2013	GOL	O2-C2-C3-O3
6	A	2014	XYL	O2-C2-C3-C4
6	A	2015	XYL	O1-C1-C2-O2
4	A	2010	NAG	C3-C2-N2-C7
6	A	2015	XYL	O1-C1-C2-C3
6	A	2015	XYL	C2-C3-C4-C5
5	A	2011	GOL	O2-C2-C3-O3
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

There are no ring outliers.

2 monomers are involved in 8 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2015	XYL	4	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%)	-0.37	10 (1%) 75 80	36, 50, 76, 102	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	695	HIS	3.5
1	A	60	PRO	3.5
1	A	55	ALA	2.5
1	A	58	ALA	2.5
1	A	690	ILE	2.4
1	A	693	GLN	2.4
1	A	61	GLY	2.4
1	A	59	LYS	2.2
1	A	689	GLY	2.1
1	A	112	ARG	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	0.09	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

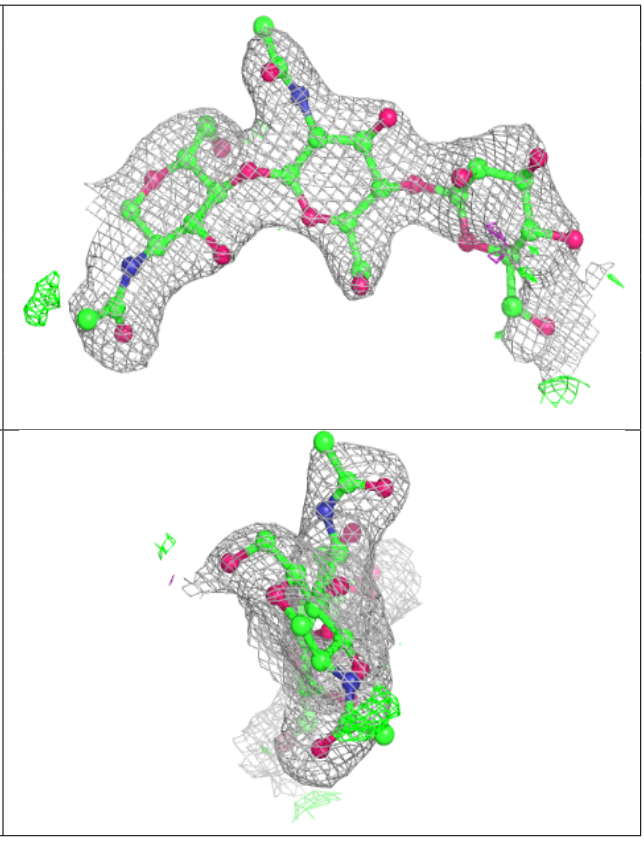
labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	B	3	11/12	0.68	0.34	101,113,120,121	0
3	NAG	C	2	14/15	0.79	0.51	111,119,127,128	0
3	NAG	D	2	14/15	0.80	0.48	115,122,127,128	0
3	NAG	D	1	14/15	0.90	0.18	76,89,98,108	0
2	NAG	B	2	14/15	0.92	0.33	74,87,97,109	0
3	NAG	C	1	14/15	0.95	0.26	78,86,96,109	0
2	NAG	B	1	14/15	0.95	0.16	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.

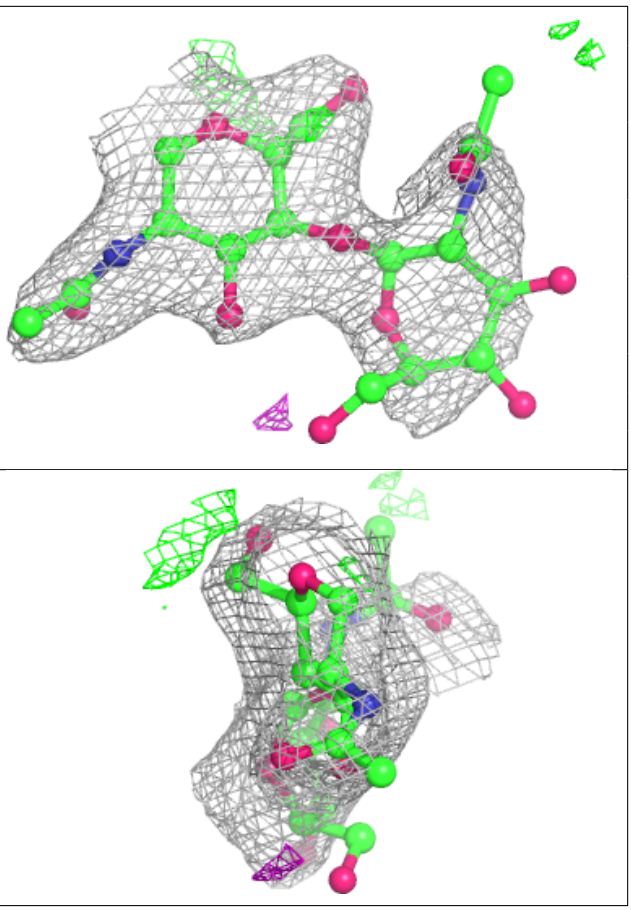
Electron density around Chain B:

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



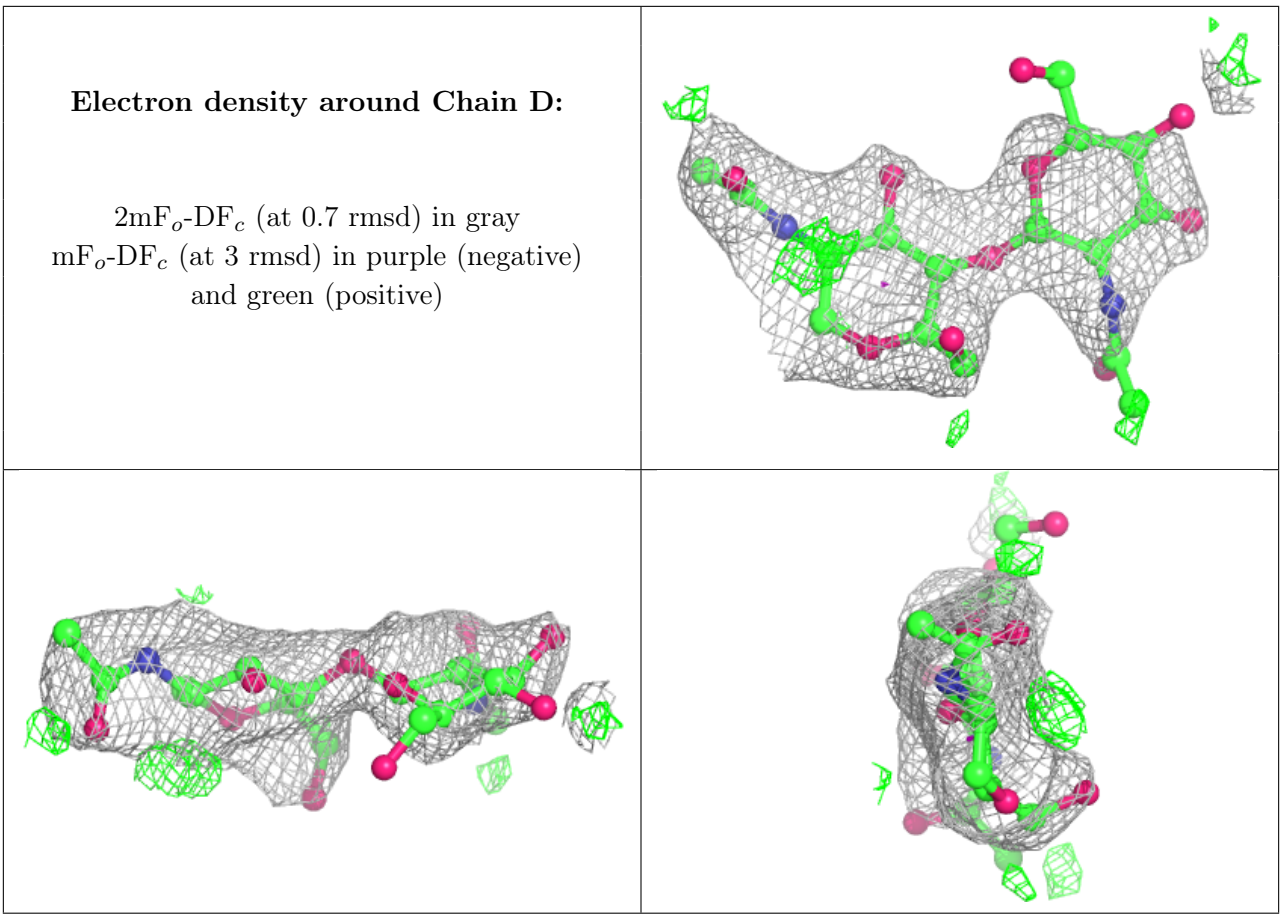
Electron density around Chain C:

$2mF_o$-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 D:

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



6.4 Ligands (i)

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
4	NAG	A	2010	14/15	0.63	0.48	116,127,133,133	0
5	GOL	A	2012	6/6	0.75	0.20	74,78,85,89	0
5	GOL	A	2013	6/6	0.79	0.20	70,72,76,79	0
4	NAG	A	2009	14/15	0.80	0.39	106,111,114,114	0
6	XYL	A	2014	10/10	0.86	0.38	75,82,89,94	0
4	NAG	A	2004	14/15	0.91	0.28	84,94,98,104	0
6	XYL	A	2015	10/10	0.91	0.20	48,52,57,62	0
5	GOL	A	2011	6/6	0.92	0.28	51,61,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.