Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 06:42 PM EDT

PDB ID	:	1UKC
Title	:	Crystal Structure of Aspergillus niger EstA
Authors	:	Bourne, Y.; Hasper, A.A.; Chahinian, H.; Juin, M.; De Graaff, L.H.; Marchot, P.
Deposited on	:	2003-08-19
Resolution	:	2.10 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:

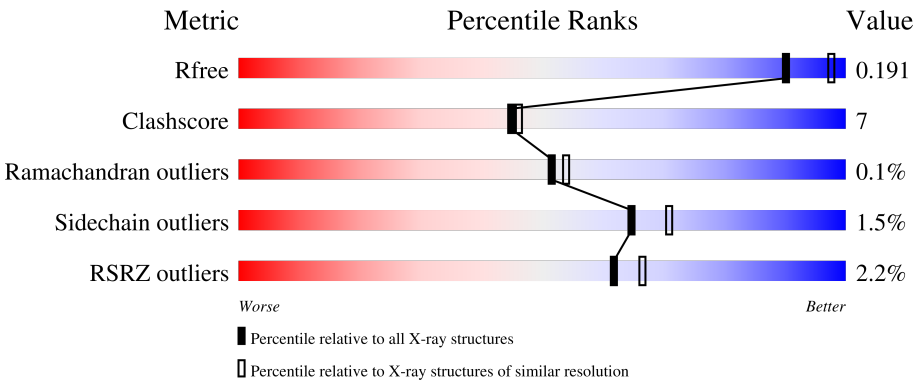
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

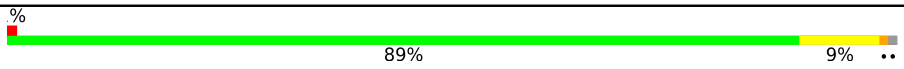
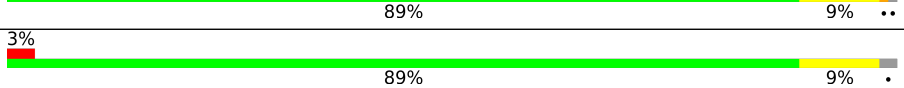
The reported resolution of this entry is 2.10 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	522	
1	B	522	
2	C	3	
3	D	2	

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	D	1	-	-	X	-
4	NAG	A	1502	-	-	-	X
4	NAG	B	1852	-	-	-	X
4	NAG	B	1951	-	-	-	X
7	CL	A	2902	-	-	X	-

2 Entry composition (i)

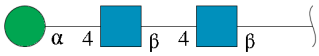
There are 9 unique types of molecules in this entry. The entry contains 9377 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EstA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	517	3986	2520	672	783	11	0	0	0
1	B	513	3953	2502	664	776	11	0	0	0

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

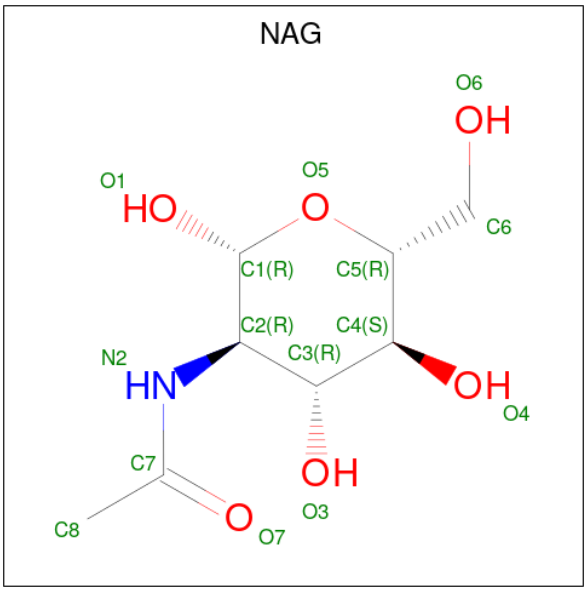


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	39	22	2	15	0	0	0

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

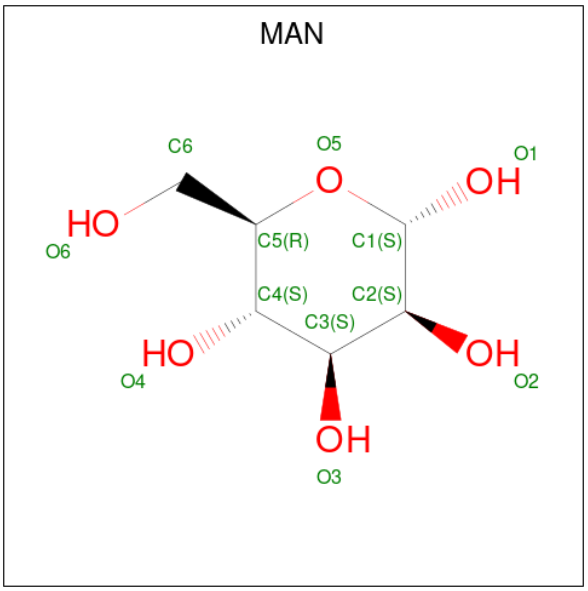
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	2	28	16	2	10	0	0	0

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



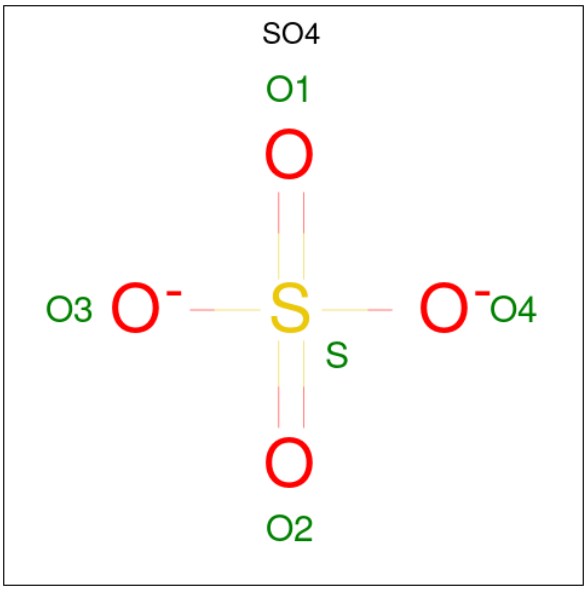
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	B	1	14	8	1	5	0	0
			Total	C	N	O		
4	B	1	14	8	1	5	0	0
			Total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

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

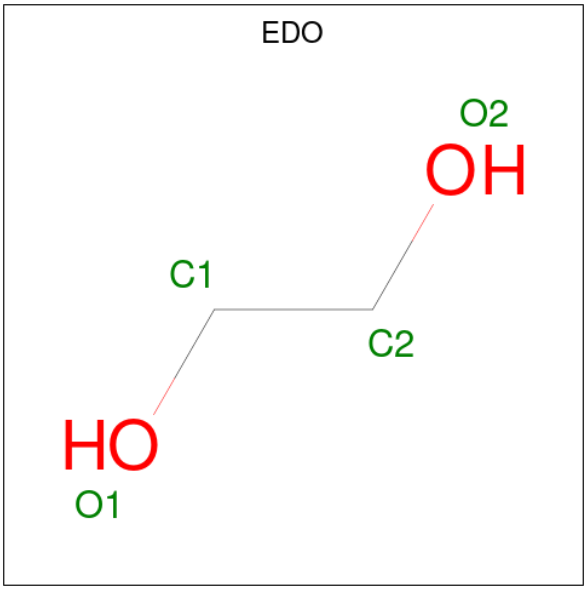


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	B	1	5	4	1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	A	1	1	1	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 9 is water.

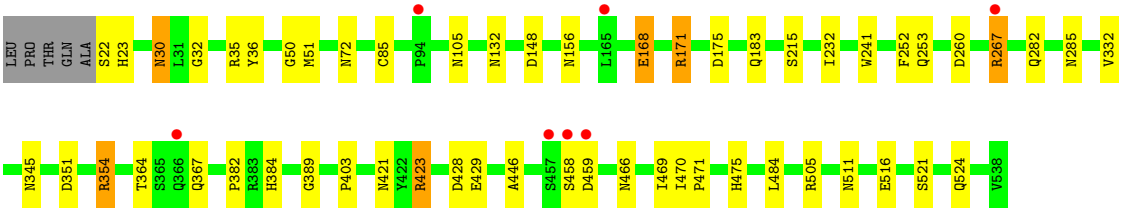
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	643	643	643	0	0
			Total	O		
9	B	506	506	506	0	0

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.

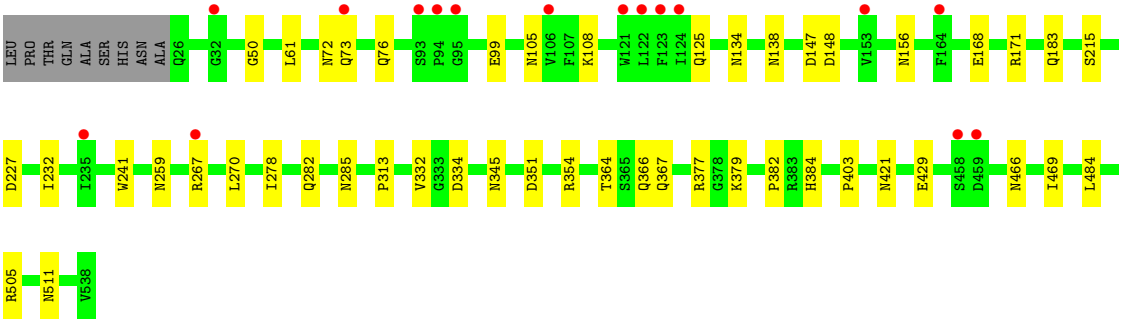
• Molecule 1: EstA

Chain A:



• Molecule 1: EstA

Chain B:



• Molecule 2: alpha-D-mannopyranose-(1-4)-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	167.49Å 167.49Å 112.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.69 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.10) 100.0 (29.69-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.158 , 0.184 0.169 , 0.191	Depositor DCC
R_{free} test set	1006 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9377	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: SO4, CL, NAG, EDO, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.63	0/4092	0.77	9/5581 (0.2%)
1	B	0.59	0/4058	0.70	3/5535 (0.1%)
All	All	0.61	0/8150	0.74	12/11116 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	423	ARG	NE-CZ-NH2	-16.00	112.30	120.30
1	A	423	ARG	NE-CZ-NH1	10.45	125.53	120.30
1	A	171	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	A	459	ASP	CB-CG-OD2	6.17	123.85	118.30
1	B	227	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	428	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	354	ARG	NE-CZ-NH1	-5.37	117.62	120.30
1	A	175	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	260	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	354	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	B	147	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	334	ASP	CB-CG-OD2	5.03	122.83	118.30

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	3986	0	3759	45	1
1	B	3953	0	3731	38	0
2	C	39	0	35	1	0
3	D	28	0	26	11	0
4	A	70	0	65	11	0
4	B	70	0	65	12	0
5	A	22	0	20	0	0
5	B	33	0	30	4	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	1	0	0	3	1
8	A	12	0	18	1	0
8	B	4	0	6	0	0
9	A	643	0	0	7	0
9	B	506	0	0	3	0
All	All	9377	0	7755	96	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 7.

All (96) 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:B:345:ASN:HD21	4:B:1751:NAG:C1	1.08	1.64
1:B:138:ASN:HD21	3:D:1:NAG:C1	1.04	1.59
1:B:511:ASN:HD21	4:B:1851:NAG:C1	1.00	1.55
1:A:72:ASN:HD21	4:A:1501:NAG:C1	1.09	1.54
1:A:345:ASN:HD21	4:A:1701:NAG:C1	1.15	1.51
1:A:511:ASN:HD21	4:A:1801:NAG:C1	0.92	1.51
1:B:259:ASN:HD21	4:B:1951:NAG:C1	1.38	1.37
1:A:35:ARG:NH1	9:A:3524:HOH:O	1.73	1.20
1:A:23:HIS:N	7:A:2902:CL:CL	2.14	1.16
1:B:259:ASN:ND2	4:B:1951:NAG:C1	2.24	0.99
1:A:23:HIS:ND1	7:A:2902:CL:CL	2.41	0.91
1:A:22:SER:N	7:A:2902:CL:CL	2.41	0.90
3:D:1:NAG:HO4	3:D:2:NAG:C1	1.77	0.88
1:A:282:GLN:HE22	1:A:285:ASN:HD22	1.28	0.82
1:B:282:GLN:HE22	1:B:285:ASN:HD22	1.27	0.81
4:A:1801:NAG:O4	4:A:1802:NAG:C1	2.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:ASN:HD21	4:B:1851:NAG:C2	1.96	0.76
1:B:138:ASN:HD21	3:D:1:NAG:C2	1.95	0.76
1:A:351:ASP:OD1	1:A:354:ARG:NH1	2.20	0.75
3:D:1:NAG:C4	3:D:2:NAG:C1	2.67	0.72
1:A:364:THR:H	1:A:367:GLN:NE2	1.89	0.71
1:A:511:ASN:HD21	4:A:1801:NAG:C2	1.98	0.70
1:B:50:GLY:H	1:B:105:ASN:HD22	1.40	0.70
4:B:1851:NAG:O4	4:B:1852:NAG:C1	2.42	0.67
2:C:2:NAG:C4	2:C:3:MAN:C1	2.72	0.67
1:B:364:THR:H	1:B:367:GLN:NE2	1.93	0.66
1:A:50:GLY:H	1:A:105:ASN:HD22	1.44	0.66
1:A:364:THR:H	1:A:367:GLN:HE21	1.44	0.64
1:A:429:GLU:HG2	9:B:3203:HOH:O	1.98	0.63
1:A:511:ASN:CG	4:A:1801:NAG:C1	2.63	0.63
1:B:168:GLU:OE1	1:B:171:ARG:HD2	2.00	0.61
1:B:50:GLY:H	1:B:105:ASN:ND2	1.99	0.60
1:A:423:ARG:HD3	1:A:516:GLU:OE2	2.03	0.59
1:B:345:ASN:HD21	4:B:1751:NAG:C2	2.06	0.59
1:B:332:VAL:O	1:B:421:ASN:HA	2.03	0.58
1:B:72:ASN:HD21	4:B:1551:NAG:C1	2.16	0.58
1:B:421:ASN:HD22	1:B:505:ARG:HB3	1.70	0.56
1:B:232:ILE:HD12	1:B:484:LEU:HD11	1.87	0.56
1:A:30:ASN:ND2	1:A:32:GLY:H	2.03	0.55
1:A:30:ASN:HD22	1:A:32:GLY:H	1.55	0.55
1:A:72:ASN:HD21	4:A:1501:NAG:C2	2.07	0.54
5:B:1652:MAN:C1	3:D:2:NAG:O4	2.56	0.53
1:B:384:HIS:HE1	9:B:3245:HOH:O	1.92	0.53
1:A:332:VAL:O	1:A:421:ASN:HA	2.09	0.53
1:B:511:ASN:CG	4:B:1851:NAG:C1	2.72	0.53
1:A:421:ASN:HD22	1:A:505:ARG:HB3	1.72	0.53
1:B:138:ASN:CG	3:D:1:NAG:C1	2.73	0.53
1:A:521:SER:HA	1:A:524:GLN:HE21	1.75	0.52
1:B:364:THR:H	1:B:367:GLN:HE21	1.57	0.52
1:A:382:PRO:O	1:A:384:HIS:HD2	1.92	0.52
1:B:511:ASN:ND2	4:B:1851:NAG:C2	2.63	0.51
1:A:50:GLY:H	1:A:105:ASN:ND2	2.06	0.51
1:B:241:TRP:CD2	1:B:403:PRO:HB3	2.45	0.51
1:B:511:ASN:ND2	4:B:1851:NAG:O5	2.40	0.51
1:A:511:ASN:ND2	4:A:1801:NAG:C2	2.67	0.50
1:A:423:ARG:NH2	9:A:3183:HOH:O	2.37	0.50
1:A:389:GLY:HA3	9:A:3353:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ARG:HH11	1:A:267:ARG:HB3	1.77	0.50
1:B:345:ASN:ND2	4:B:1751:NAG:C2	2.70	0.50
1:B:138:ASN:ND2	3:D:1:NAG:O5	2.43	0.49
1:B:183:GLN:OE1	1:B:215:SER:HB3	2.12	0.49
3:D:1:NAG:O4	3:D:2:NAG:C2	2.58	0.49
8:A:1932:EDO:H12	9:A:3508:HOH:O	2.12	0.49
5:B:1652:MAN:O3	5:B:1651:MAN:H5	2.13	0.49
1:A:384:HIS:HE1	9:A:3004:HOH:O	1.94	0.49
5:B:1652:MAN:C1	3:D:2:NAG:C4	2.91	0.48
1:A:241:TRP:CD2	1:A:403:PRO:HB3	2.49	0.48
1:B:382:PRO:O	1:B:384:HIS:HD2	1.96	0.48
1:A:470:ILE:HB	1:A:471:PRO:HD3	1.97	0.47
9:A:3396:HOH:O	1:B:379:LYS:HE3	2.14	0.47
1:B:125:GLN:HB2	1:B:134:ASN:HB2	1.97	0.46
4:A:1501:NAG:O4	4:A:1502:NAG:C1	2.64	0.46
1:A:72:ASN:CG	4:A:1501:NAG:C1	2.76	0.46
1:A:168:GLU:OE1	1:A:171:ARG:CD	2.64	0.46
1:A:132:ASN:ND2	1:A:156:ASN:HB3	2.30	0.46
1:A:446:ALA:HA	1:A:470:ILE:HG12	1.98	0.45
1:A:85:CYS:H	1:A:132:ASN:ND2	2.15	0.44
1:B:138:ASN:ND2	3:D:1:NAG:C2	2.66	0.44
1:B:313:PRO:HD2	9:B:3037:HOH:O	2.16	0.44
1:B:125:GLN:NE2	1:B:156:ASN:HD22	2.16	0.44
5:B:1652:MAN:C1	3:D:2:NAG:H4	2.48	0.43
1:B:466:ASN:O	1:B:469:ILE:HG22	2.18	0.43
1:B:351:ASP:OD1	1:B:354:ARG:NH1	2.48	0.43
9:A:3395:HOH:O	1:B:429:GLU:HG2	2.17	0.42
1:A:168:GLU:OE1	1:A:171:ARG:HD2	2.19	0.42
1:A:30:ASN:HD22	1:A:30:ASN:C	2.23	0.42
1:A:132:ASN:HD21	1:A:156:ASN:HB3	1.85	0.42
1:A:232:ILE:HD12	1:A:484:LEU:HD11	2.02	0.42
1:A:252:PHE:CG	1:A:253:GLN:N	2.88	0.42
1:B:125:GLN:HE22	1:B:156:ASN:HD22	1.67	0.42
1:A:183:GLN:OE1	1:A:215:SER:HB3	2.20	0.41
1:B:99:GLU:HG3	1:B:278:ILE:HD13	2.02	0.41
4:A:1801:NAG:C4	4:A:1802:NAG:C1	2.98	0.41
1:A:466:ASN:O	1:A:469:ILE:HG22	2.21	0.40
1:A:36:TYR:CD2	1:A:51:MET:HG2	2.57	0.40
1:A:367:GLN:HE21	1:A:367:GLN:HB2	1.70	0.40

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	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:HIS:NE2	7:A:2902:CL:CL[2_665]	2.12	0.08

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	515/522 (99%)	492 (96%)	23 (4%)	0	100	100
1	B	511/522 (98%)	493 (96%)	17 (3%)	1 (0%)	47	49
All	All	1026/1044 (98%)	985 (96%)	40 (4%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	377	ARG

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	425/429 (99%)	420 (99%)	5 (1%)	71	77
1	B	421/429 (98%)	413 (98%)	8 (2%)	57	63
All	All	846/858 (99%)	833 (98%)	13 (2%)	65	71

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	148	ASP
1	A	168	GLU
1	A	267	ARG
1	A	458	SER
1	B	61	LEU
1	B	73	GLN
1	B	76	GLN
1	B	108	LYS
1	B	148	ASP
1	B	267	ARG
1	B	270	LEU
1	B	366	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	37	GLN
1	A	72	ASN
1	A	105	ASN
1	A	132	ASN
1	A	144	GLN
1	A	156	ASN
1	A	172	GLN
1	A	282	GLN
1	A	341	ASN
1	A	345	ASN
1	A	367	GLN
1	A	384	HIS
1	A	421	ASN
1	A	509	GLN
1	A	511	ASN
1	A	524	GLN
1	B	30	ASN
1	B	72	ASN
1	B	105	ASN
1	B	132	ASN
1	B	138	ASN
1	B	141	GLN
1	B	156	ASN
1	B	259	ASN
1	B	282	GLN

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Mol	Chain	Res	Type
1	B	341	ASN
1	B	345	ASN
1	B	366	GLN
1	B	367	GLN
1	B	384	HIS
1	B	421	ASN
1	B	509	GLN
1	B	511	ASN

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)

5 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	C	1	1,2	14,14,15	0.56	0	17,19,21	1.30	3 (17%)
2	NAG	C	2	2	14,14,15	0.62	0	17,19,21	1.30	3 (17%)
2	MAN	C	3	2	11,11,12	0.82	0	15,15,17	1.67	3 (20%)
3	NAG	D	1	1,3	14,14,15	0.70	0	17,19,21	1.68	2 (11%)
3	NAG	D	2	3	14,14,15	0.64	0	17,19,21	1.58	3 (17%)

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

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	MAN	C1-O5-C5	-4.07	106.68	112.19
3	D	1	NAG	C1-O5-C5	-3.78	107.07	112.19
3	D	2	NAG	C1-O5-C5	-3.75	107.11	112.19
3	D	1	NAG	C3-C4-C5	3.43	116.35	110.24
3	D	2	NAG	O5-C5-C6	3.05	111.98	107.20
2	C	2	NAG	O4-C4-C3	-2.80	103.88	110.35
2	C	2	NAG	C1-O5-C5	-2.56	108.73	112.19
2	C	1	NAG	O5-C1-C2	2.48	115.21	111.29
2	C	2	NAG	C3-C4-C5	2.39	114.49	110.24
2	C	3	MAN	C2-C3-C4	2.38	115.01	110.89
3	D	2	NAG	O4-C4-C3	-2.34	104.94	110.35
2	C	3	MAN	C3-C4-C5	2.32	114.37	110.24
2	C	1	NAG	C3-C4-C5	2.24	114.23	110.24
2	C	1	NAG	C2-N2-C7	-2.10	119.91	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

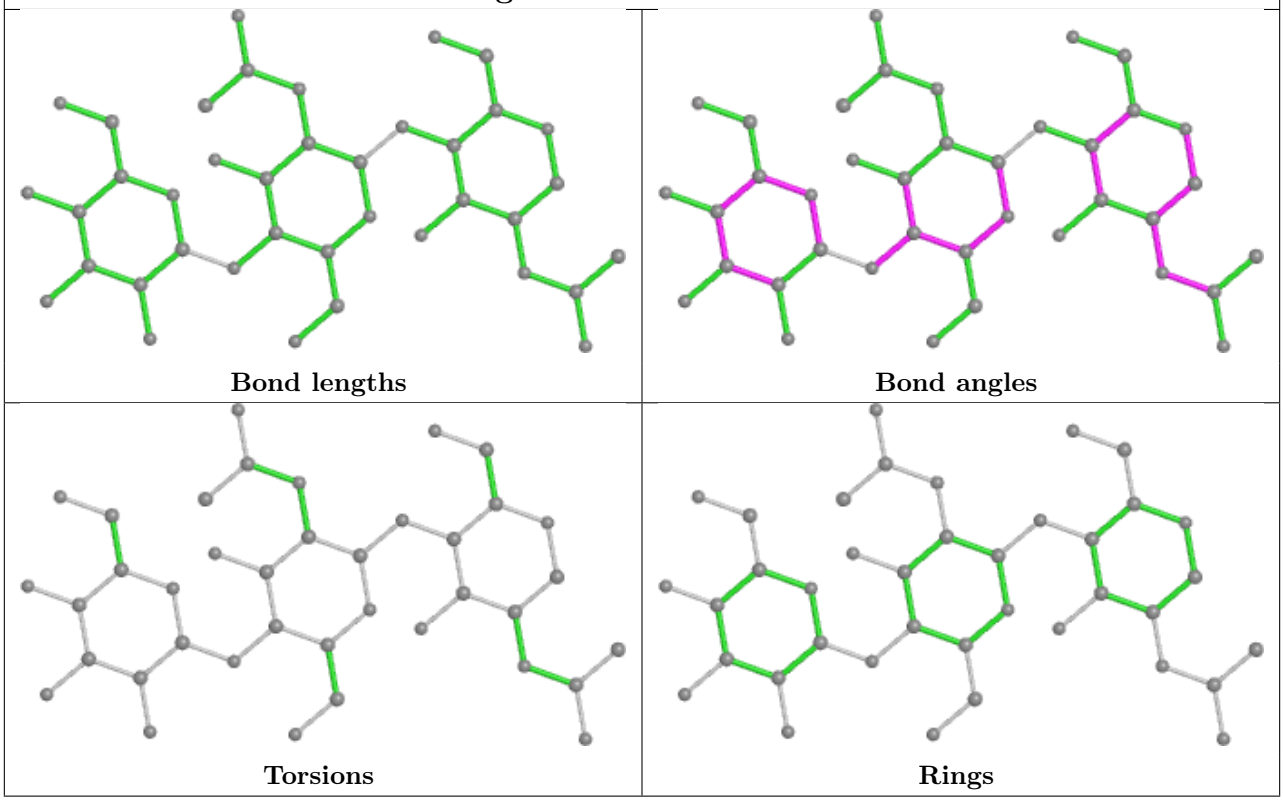
There are no ring outliers.

4 monomers are involved in 12 short contacts:

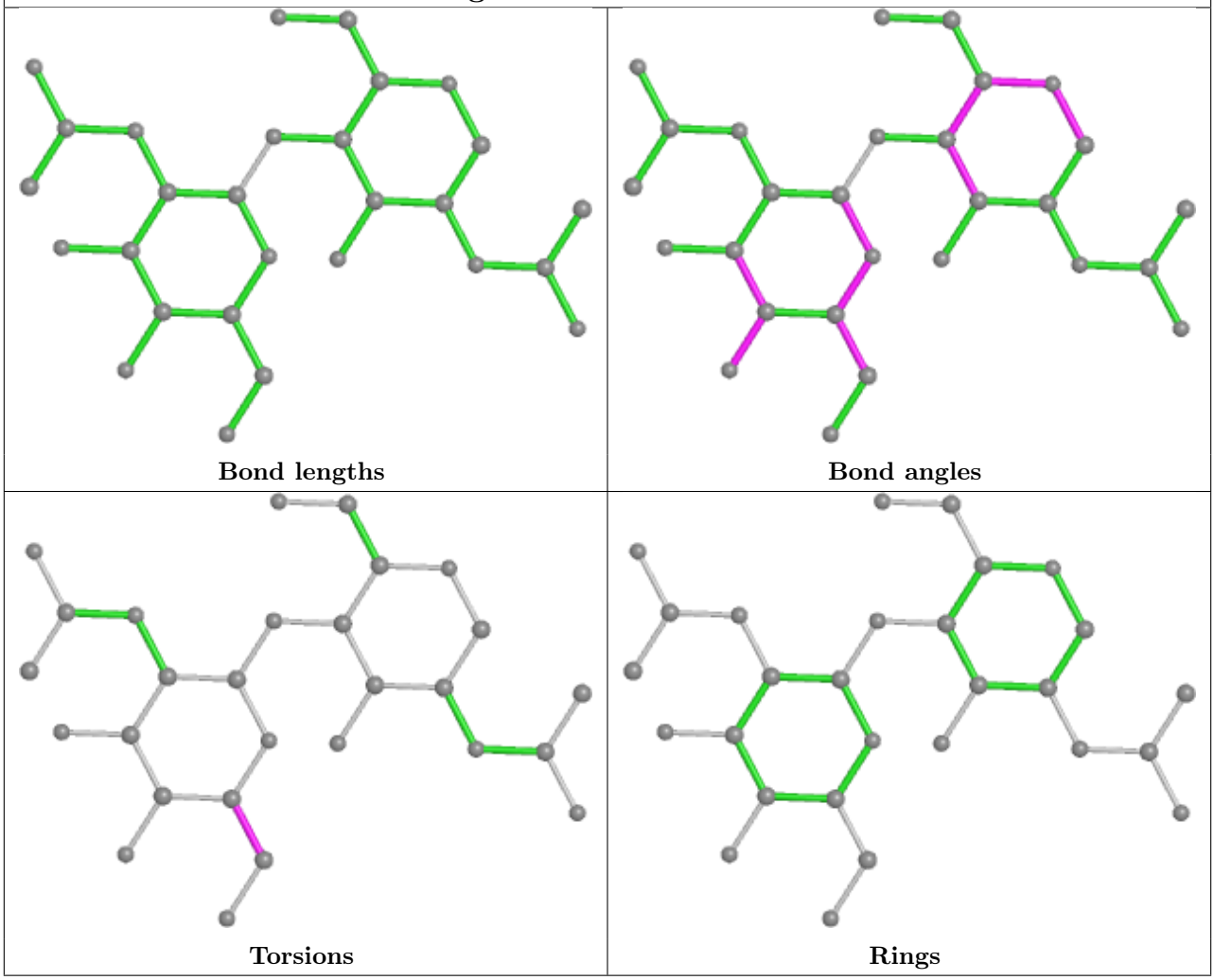
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	8	0
2	C	3	MAN	1	0
3	D	2	NAG	6	0
2	C	2	NAG	1	0

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

Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	1701	1	14,14,15	0.67	0	17,19,21	0.90	0
5	MAN	B	1651	-	11,11,12	0.59	0	15,15,17	1.37	2 (13%)
8	EDO	A	1922	-	3,3,3	0.28	0	2,2,2	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	1751	1	14,14,15	0.66	0	17,19,21	0.81	0
4	NAG	A	1502	-	14,14,15	0.60	0	17,19,21	1.12	2 (11%)
5	MAN	A	1601	-	11,11,12	0.72	0	15,15,17	1.40	3 (20%)
8	EDO	A	1932	-	3,3,3	0.39	0	2,2,2	0.32	0
4	NAG	B	1851	1	14,14,15	0.65	0	17,19,21	1.07	0
4	NAG	A	1801	1	14,14,15	0.56	0	17,19,21	1.16	2 (11%)
5	MAN	B	1652	-	11,11,12	0.75	0	15,15,17	1.49	4 (26%)
4	NAG	A	1501	1	14,14,15	0.63	0	17,19,21	1.17	2 (11%)
5	MAN	B	1653	-	11,11,12	0.89	1 (9%)	15,15,17	2.15	3 (20%)
5	MAN	A	1603	-	11,11,12	0.82	0	15,15,17	2.10	4 (26%)
6	SO4	A	2901	-	4,4,4	0.13	0	6,6,6	0.69	0
8	EDO	A	1902	-	3,3,3	0.37	0	2,2,2	0.10	0
8	EDO	B	1912	-	3,3,3	0.36	0	2,2,2	0.08	0
4	NAG	A	1802	-	14,14,15	0.61	0	17,19,21	0.98	0
6	SO4	B	2951	-	4,4,4	0.21	0	6,6,6	0.50	0
4	NAG	B	1951	-	14,14,15	0.64	0	17,19,21	1.14	2 (11%)
4	NAG	B	1852	-	14,14,15	0.63	0	17,19,21	1.28	3 (17%)
4	NAG	B	1551	-	14,14,15	0.63	0	17,19,21	0.98	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1701	1	-	2/6/23/26	0/1/1/1
5	MAN	B	1651	-	-	2/2/19/22	0/1/1/1
8	EDO	A	1922	-	-	0/1/1/1	-
4	NAG	B	1751	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1502	-	-	4/6/23/26	0/1/1/1
5	MAN	A	1601	-	-	0/2/19/22	0/1/1/1
8	EDO	A	1932	-	-	1/1/1/1	-
4	NAG	B	1851	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1801	1	-	0/6/23/26	0/1/1/1
5	MAN	B	1652	-	-	2/2/19/22	0/1/1/1
4	NAG	A	1501	1	-	0/6/23/26	0/1/1/1
5	MAN	B	1653	-	-	2/2/19/22	0/1/1/1
5	MAN	A	1603	-	-	2/2/19/22	0/1/1/1
8	EDO	A	1902	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	B	1912	-	-	1/1/1/1	-
4	NAG	A	1802	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1951	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1852	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1551	-	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1653	MAN	C2-C3	2.09	1.55	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1653	MAN	C1-C2-C3	6.46	117.61	109.67
5	A	1603	MAN	C1-C2-C3	5.99	117.03	109.67
5	A	1603	MAN	O5-C1-C2	3.50	116.17	110.77
5	A	1601	MAN	C1-C2-C3	3.12	113.50	109.67
5	B	1653	MAN	O5-C1-C2	3.10	115.55	110.77
5	B	1651	MAN	C1-C2-C3	3.02	113.38	109.67
5	A	1603	MAN	C1-O5-C5	3.01	116.27	112.19
5	B	1652	MAN	C3-C4-C5	2.94	115.49	110.24
4	B	1852	NAG	C1-O5-C5	-2.90	108.27	112.19
5	B	1653	MAN	C2-C3-C4	2.84	115.80	110.89
5	B	1652	MAN	C1-O5-C5	-2.78	108.43	112.19
4	B	1951	NAG	C3-C4-C5	2.70	115.06	110.24
5	A	1601	MAN	C2-C3-C4	2.64	115.47	110.89
5	B	1652	MAN	C2-C3-C4	2.53	115.27	110.89
5	B	1651	MAN	C1-O5-C5	2.52	115.61	112.19
4	A	1801	NAG	C3-C4-C5	2.49	114.68	110.24
5	B	1652	MAN	O5-C5-C6	2.38	110.93	107.20
5	A	1603	MAN	C2-C3-C4	2.35	114.95	110.89
4	A	1502	NAG	C3-C4-C5	2.26	114.26	110.24
4	A	1501	NAG	C3-C4-C5	2.22	114.19	110.24
4	B	1551	NAG	C3-C4-C5	2.13	114.04	110.24
4	A	1801	NAG	C1-O5-C5	-2.12	109.32	112.19
4	A	1501	NAG	O4-C4-C3	-2.12	105.46	110.35
4	B	1852	NAG	C4-C3-C2	2.06	114.04	111.02
4	B	1951	NAG	O5-C1-C2	-2.06	108.04	111.29
5	A	1601	MAN	C1-O5-C5	2.02	114.92	112.19
4	A	1502	NAG	O5-C1-C2	-2.01	108.12	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1852	NAG	O5-C1-C2	-2.00	108.13	111.29

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1551	NAG	C8-C7-N2-C2
4	B	1551	NAG	O7-C7-N2-C2
5	A	1603	MAN	O5-C5-C6-O6
5	B	1651	MAN	O5-C5-C6-O6
4	B	1751	NAG	O5-C5-C6-O6
5	B	1652	MAN	O5-C5-C6-O6
5	B	1653	MAN	O5-C5-C6-O6
5	B	1653	MAN	C4-C5-C6-O6
4	A	1802	NAG	C8-C7-N2-C2
5	B	1651	MAN	C4-C5-C6-O6
5	A	1603	MAN	C4-C5-C6-O6
4	A	1802	NAG	O7-C7-N2-C2
4	B	1751	NAG	C4-C5-C6-O6
5	B	1652	MAN	C4-C5-C6-O6
4	A	1502	NAG	C8-C7-N2-C2
4	A	1502	NAG	C4-C5-C6-O6
4	A	1701	NAG	O5-C5-C6-O6
4	A	1701	NAG	C4-C5-C6-O6
4	A	1502	NAG	O7-C7-N2-C2
8	A	1932	EDO	O1-C1-C2-O2
4	B	1852	NAG	C8-C7-N2-C2
4	B	1852	NAG	O7-C7-N2-C2
4	A	1502	NAG	O5-C5-C6-O6
8	A	1902	EDO	O1-C1-C2-O2
8	B	1912	EDO	O1-C1-C2-O2

There are no ring outliers.

13 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1701	NAG	1	0
5	B	1651	MAN	1	0
4	B	1751	NAG	3	0
4	A	1502	NAG	1	0
8	A	1932	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1851	NAG	6	0
4	A	1801	NAG	6	0
5	B	1652	MAN	4	0
4	A	1501	NAG	4	0
4	A	1802	NAG	2	0
4	B	1951	NAG	2	0
4	B	1852	NAG	1	0
4	B	1551	NAG	1	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	517/522 (99%)	-0.35	7 (1%)	75	78	23, 32, 47, 69	0
1	B	513/522 (98%)	-0.26	16 (3%)	49	55	25, 36, 61, 86	0
All	All	1030/1044 (98%)	-0.31	23 (2%)	62	66	23, 34, 55, 86	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	94	PRO	4.3
1	B	458	SER	3.8
1	A	267	ARG	3.6
1	B	267	ARG	3.5
1	A	458	SER	3.5
1	B	121	TRP	2.8
1	A	94	PRO	2.8
1	B	122	LEU	2.7
1	A	165	LEU	2.6
1	B	164	PHE	2.5
1	B	95	GLY	2.4
1	B	235	ILE	2.4
1	A	459	ASP	2.4
1	B	106	VAL	2.3
1	B	93	SER	2.3
1	B	124	ILE	2.3
1	B	153	VAL	2.3
1	A	366	GLN	2.2
1	B	32	GLY	2.2
1	B	123	PHE	2.2
1	A	457	SER	2.1
1	B	459	ASP	2.0
1	B	73	GLN	2.0

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

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

6.3 Carbohydrates (i)

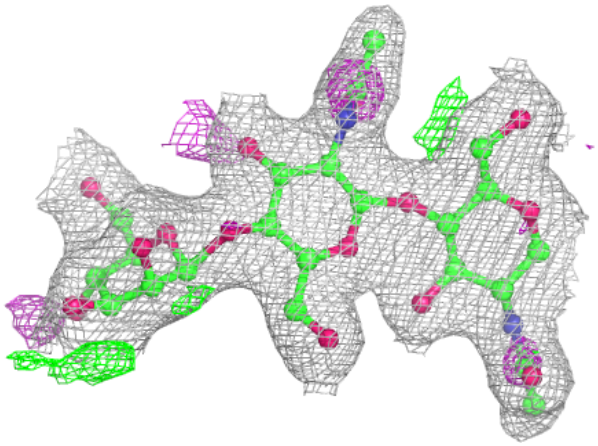
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

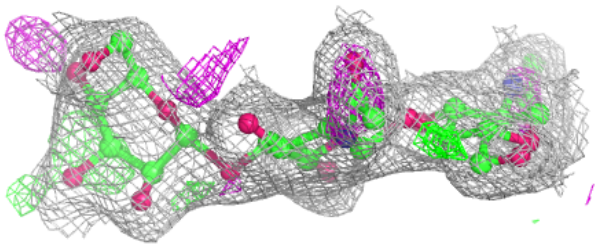
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	D	2	14/15	0.89	0.19	55,63,66,67	0
2	MAN	C	3	11/12	0.92	0.22	63,65,68,68	0
3	NAG	D	1	14/15	0.95	0.11	47,49,51,52	0
2	NAG	C	2	14/15	0.95	0.14	33,35,40,42	0
2	NAG	C	1	14/15	0.98	0.07	28,30,34,35	0

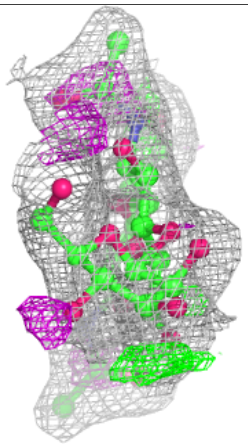
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

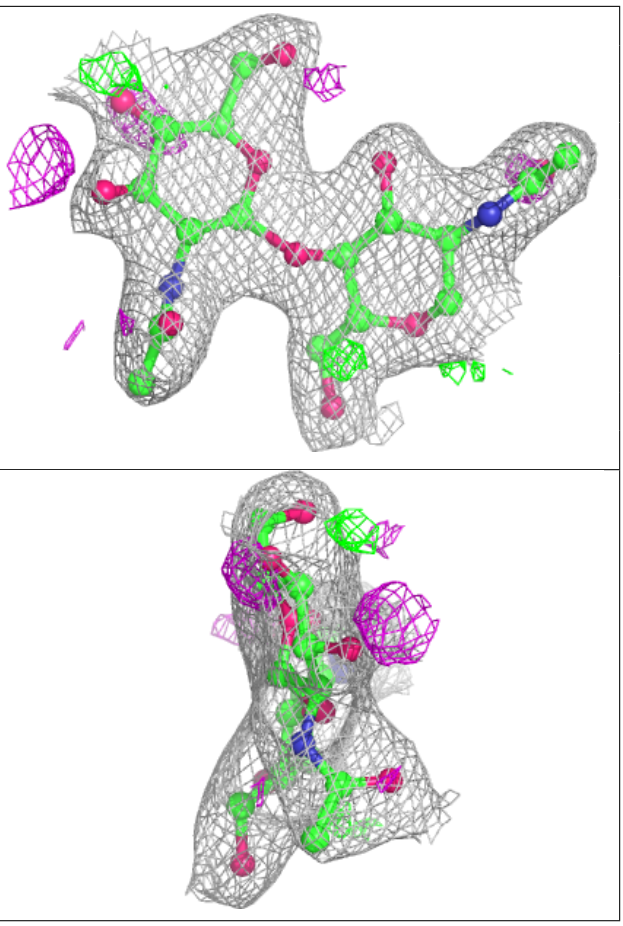






Electron density around Chain D:

$2mF_o$-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
5	MAN	A	1603	11/12	0.73	0.32	85,85,86,86	0
4	NAG	B	1551	14/15	0.74	0.29	83,83,84,84	0
4	NAG	A	1802	14/15	0.74	0.40	79,80,82,83	0
5	MAN	B	1651	11/12	0.74	0.37	89,89,90,90	0
4	NAG	A	1502	14/15	0.75	0.45	91,92,92,93	0
4	NAG	B	1852	14/15	0.75	0.41	82,84,84,85	0
4	NAG	B	1951	14/15	0.79	0.45	80,81,81,81	0
5	MAN	B	1653	11/12	0.82	0.40	85,86,86,86	0
5	MAN	B	1652	11/12	0.83	0.24	89,90,91,91	0
4	NAG	A	1701	14/15	0.85	0.20	56,58,60,62	0
5	MAN	A	1601	11/12	0.85	0.32	88,88,89,89	0
4	NAG	B	1751	14/15	0.85	0.21	56,59,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	1501	14/15	0.90	0.23	56,59,61,62	0
4	NAG	B	1851	14/15	0.91	0.18	36,46,52,54	0
8	EDO	A	1902	4/4	0.91	0.09	47,49,50,52	0
4	NAG	A	1801	14/15	0.94	0.16	34,42,49,51	0
8	EDO	B	1912	4/4	0.94	0.10	48,52,52,55	0
8	EDO	A	1932	4/4	0.97	0.12	31,37,39,44	0
8	EDO	A	1922	4/4	0.97	0.21	34,39,41,44	0
6	SO4	B	2951	5/5	0.99	0.08	35,36,38,41	0
7	CL	A	2902	1/1	0.99	0.14	12,12,12,12	0
6	SO4	A	2901	5/5	0.99	0.08	30,30,32,37	0

6.5 Other polymers (i)

There are no such residues in this entry.