Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 09:46 AM EDT

PDB ID	:	3OG2
Title	:	Native crystal structure of Trichoderma reesei beta-galactosidase
Authors	:	Maksimainen, M.; Rouvinen, J.
Deposited on	:	2010-08-16
Resolution	:	1.20 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:

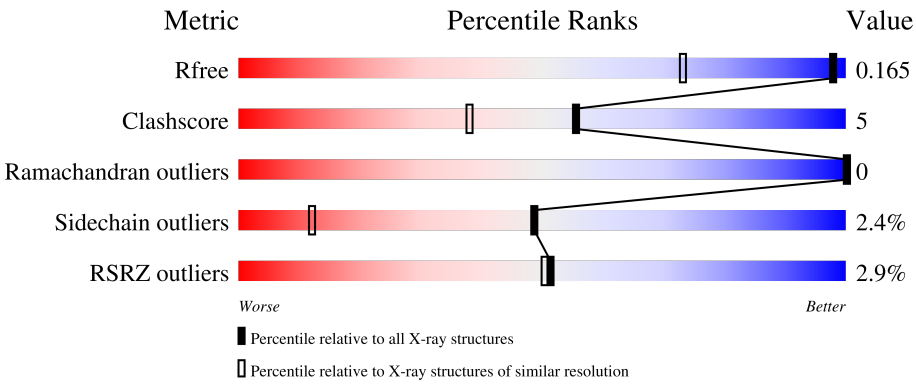
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.20 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	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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	1003	3%, 87%, 11%, • •
2	B	7	14%, 71%, 14%
3	C	12	67%, 33%
4	D	2	50%, 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	C	12	-	-	-	X

2 Entry composition (i)

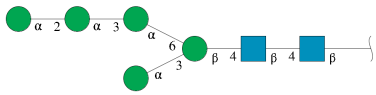
There are 7 unique types of molecules in this entry. The entry contains 9055 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-galactosidase.

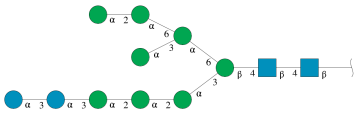
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	986	7773	5016	1298	1450	9	0	27	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	7	83	46	2	35	0	0	0

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

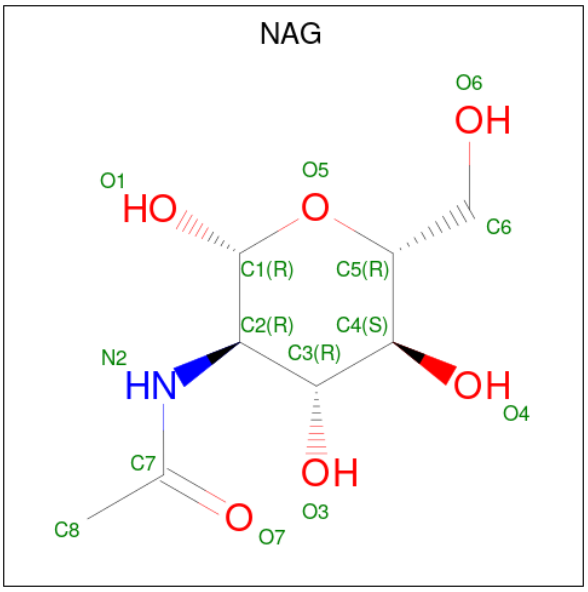


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	12	138	76	2	60	0	0	0

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

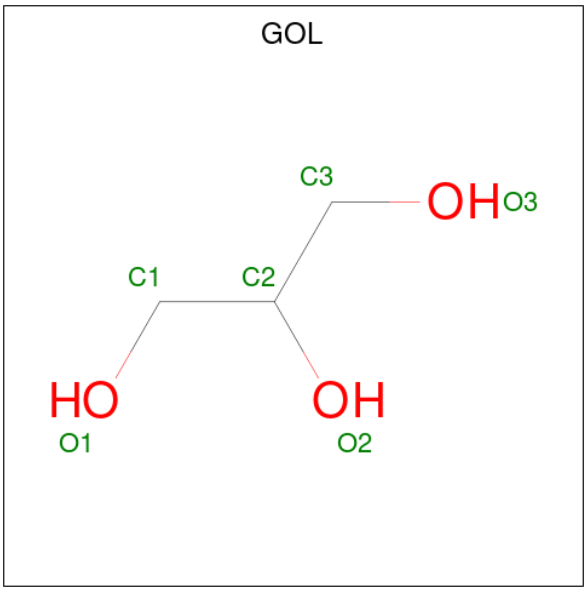
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	2	28	16	2	10	0	0	0

- Molecule 5 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		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

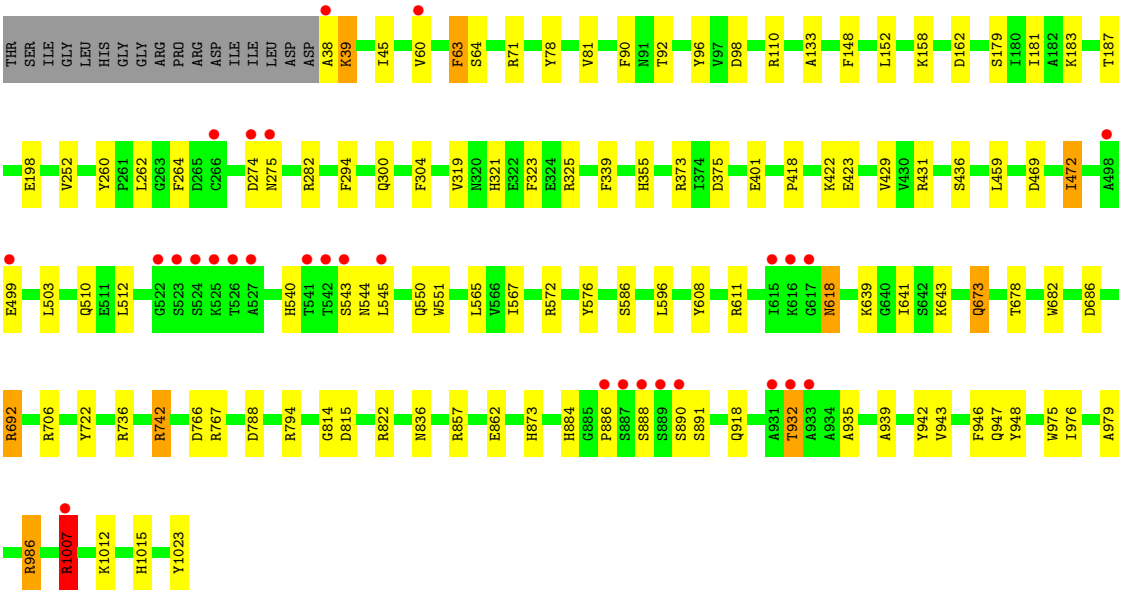
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	993	993	993	0	0

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.

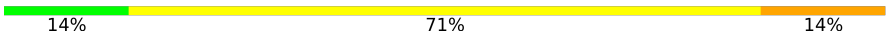
• Molecule 1: Beta-galactosidase

Chain A:



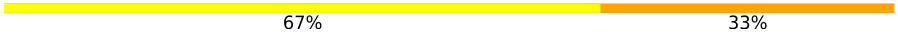
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

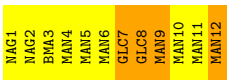
Chain B:



• Molecule 3: alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:





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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.30Å 69.10Å 81.50Å 109.10° 97.30° 114.50°	Depositor
Resolution (Å)	20.00 – 1.20 47.87 – 1.20	Depositor EDS
% Data completeness (in resolution range)	86.2 (20.00-1.20) 88.4 (47.87-1.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 1.20Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.139 , 0.171 0.136 , 0.165	Depositor DCC
R_{free} test set	35989 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	8.6	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 63.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.014 for k,h,-h-k-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	9055	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: MAN, NAG, GOL, GLC, BMA

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	0.71	1/8059 (0.0%)	1.25	66/10981 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1023	TYR	C-OXT	5.92	1.34	1.23

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	942	TYR	CB-CG-CD2	11.84	128.10	121.00
1	A	794	ARG	NE-CZ-NH2	11.22	125.91	120.30
1	A	1007	ARG	CD-NE-CZ	11.22	139.31	123.60
1	A	71	ARG	NE-CZ-NH2	-10.91	114.84	120.30
1	A	1007	ARG	NE-CZ-NH1	10.07	125.34	120.30
1	A	942	TYR	CB-CG-CD1	-9.81	115.11	121.00
1	A	373	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	A	986	ARG	NE-CZ-NH2	8.93	124.76	120.30
1	A	857	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	A	110	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	A	71	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	572	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	A	722	TYR	CB-CG-CD2	-7.65	116.41	121.00
1	A	576	TYR	CB-CG-CD2	-7.57	116.46	121.00
1	A	942	TYR	CG-CD1-CE1	7.54	127.33	121.30
1	A	572	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	692	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	A	1007	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	339	PHE	CB-CG-CD2	-7.16	115.79	120.80
1	A	767	ARG	NE-CZ-NH1	-7.14	116.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	282	ARG	NE-CZ-NH1	-7.07	116.77	120.30
1	A	742	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	A	766	ASP	CB-CG-OD1	6.93	124.54	118.30
1	A	431	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	A	862	GLU	CB-CA-C	-6.54	97.33	110.40
1	A	706	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	110	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	551	TRP	CD1-CG-CD2	-6.39	101.19	106.30
1	A	576	TYR	CB-CG-CD1	6.35	124.81	121.00
1	A	942	TYR	CG-CD2-CE2	-6.31	116.25	121.30
1	A	96	TYR	CB-CG-CD2	-6.26	117.24	121.00
1	A	815	ASP	CB-CG-OD1	-6.26	112.67	118.30
1	A	686	ASP	CB-CG-OD1	6.23	123.90	118.30
1	A	822	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	325	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	325	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	A	608	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	A	551	TRP	CB-CG-CD1	5.98	134.77	127.00
1	A	63	PHE	CB-CG-CD1	5.96	124.97	120.80
1	A	788	ASP	CB-CG-OD1	5.86	123.58	118.30
1	A	162	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	A	294	PHE	CB-CG-CD2	-5.82	116.73	120.80
1	A	932	THR	C-N-CA	-5.81	107.18	121.70
1	A	736	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	A	767	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	A	611	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	862	GLU	CG-CD-OE1	5.63	129.55	118.30
1	A	572	ARG	CD-NE-CZ	5.56	131.38	123.60
1	A	152	LEU	CB-CG-CD2	5.55	120.44	111.00
1	A	862	GLU	CG-CD-OE2	-5.51	107.28	118.30
1	A	469	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	611	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	339	PHE	CB-CG-CD1	5.41	124.59	120.80
1	A	722	TYR	CB-CG-CD1	5.38	124.23	121.00
1	A	90	PHE	CB-CG-CD2	-5.37	117.04	120.80
1	A	608	TYR	CB-CG-CD1	5.29	124.18	121.00
1	A	975	TRP	CA-CB-CG	-5.26	103.70	113.70
1	A	551	TRP	CE2-CD2-CG	5.26	111.51	107.30
1	A	98	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	946	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	A	706	ARG	CG-CD-NE	-5.19	100.89	111.80
1	A	282	ARG	NH1-CZ-NH2	5.19	125.11	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	148	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	A	63	PHE	CB-CG-CD2	-5.13	117.21	120.80
1	A	375	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	431	ARG	NE-CZ-NH1	5.09	122.84	120.30

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	7773	0	7625	76	0
2	B	83	0	70	1	0
3	C	138	0	115	8	0
4	D	28	0	25	1	0
5	A	28	0	26	0	0
6	A	12	0	16	0	0
7	A	993	0	0	13	0
All	All	9055	0	7877	82	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 5.

All (82) 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:264[B]:PHE:CG	1:A:304[B]:PHE:CE2	2.03	1.44
1:A:264[B]:PHE:CB	1:A:304[B]:PHE:CE2	2.28	1.15
1:A:264[B]:PHE:CD1	1:A:304[B]:PHE:HE2	1.67	1.13
1:A:264[B]:PHE:CG	1:A:304[B]:PHE:HE2	1.55	1.09
1:A:264[B]:PHE:CB	1:A:304[B]:PHE:CZ	2.42	1.02
1:A:264[B]:PHE:HB3	1:A:304[B]:PHE:CE2	2.05	0.90
1:A:264[B]:PHE:HB2	1:A:304[B]:PHE:CZ	2.08	0.89
1:A:264[B]:PHE:CD2	1:A:304[B]:PHE:CE2	2.62	0.87
1:A:422:LYS:HG2	1:A:423:GLU:HG3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264[B]:PHE:CD1	1:A:304[B]:PHE:CE2	2.52	0.86
1:A:264[B]:PHE:HB3	1:A:304[B]:PHE:CZ	2.12	0.84
1:A:264[B]:PHE:CD2	1:A:304[B]:PHE:CD2	2.66	0.84
1:A:1007:ARG:HH11	1:A:1007:ARG:HG3	1.47	0.78
7:A:1818:HOH:O	3:C:8:GLC:H61	1.83	0.78
1:A:512:LEU:HD11	1:A:550:GLN:HG2	1.67	0.75
3:C:9:MAN:C2	3:C:12:MAN:H5	2.22	0.70
1:A:158[B]:LYS:HE2	7:A:1567:HOH:O	1.92	0.67
1:A:60[B]:VAL:HG21	1:A:596:LEU:CD1	2.25	0.66
1:A:673:GLN:HE21	1:A:673:GLN:HA	1.60	0.66
1:A:429:VAL:HG22	1:A:472[A]:ILE:HD13	1.79	0.65
3:C:9:MAN:H2	3:C:12:MAN:H5	1.77	0.65
1:A:264[B]:PHE:CG	1:A:304[B]:PHE:CD2	2.77	0.63
1:A:1012:LYS:HE3	7:A:1704:HOH:O	1.99	0.61
1:A:262[B]:LEU:HD22	1:A:323[B]:PHE:CE1	2.37	0.60
1:A:304[B]:PHE:CZ	3:C:7:GLC:H4	2.37	0.59
1:A:60[B]:VAL:HG21	1:A:596:LEU:HD12	1.83	0.59
1:A:943:VAL:HG22	1:A:976[A]:ILE:CD1	2.34	0.58
7:A:1278:HOH:O	3:C:8:GLC:H62	2.03	0.58
1:A:886:PRO:HD2	1:A:891:SER:OG	2.05	0.57
1:A:935:ALA:HB2	1:A:986:ARG:HD2	1.86	0.57
1:A:510:GLN:HA	1:A:510:GLN:OE1	2.02	0.56
1:A:262[B]:LEU:HD22	1:A:323[B]:PHE:HE1	1.70	0.56
1:A:873:HIS:H	1:A:873:HIS:CD2	2.24	0.55
1:A:673:GLN:HA	1:A:673:GLN:NE2	2.22	0.54
1:A:133:ALA:HB1	1:A:181[A]:ILE:HD13	1.88	0.54
1:A:510:GLN:HG2	7:A:2036:HOH:O	2.10	0.51
1:A:78:TYR:O	1:A:81[A]:VAL:HG23	2.10	0.51
7:A:1825:HOH:O	2:B:7:MAN:H3	2.09	0.51
1:A:38:ALA:N	1:A:39:LYS:HE2	2.25	0.51
1:A:565:LEU:HG	1:A:567[B]:ILE:HD11	1.92	0.51
1:A:678:THR:HG23	7:A:1647:HOH:O	2.10	0.50
1:A:401:GLU:HB2	1:A:418:PRO:HG2	1.94	0.49
1:A:304[B]:PHE:CE1	3:C:7:GLC:H4	2.46	0.49
1:A:422:LYS:CG	1:A:423:GLU:HG3	2.36	0.49
1:A:544:ASN:O	1:A:545:LEU:HB2	2.12	0.49
1:A:459:LEU:HD13	1:A:540:HIS:HD2	1.79	0.47
1:A:321:HIS:HE1	7:A:1825:HOH:O	1.98	0.47
1:A:943:VAL:HG22	1:A:976[A]:ILE:HD12	1.96	0.46
1:A:692:ARG:NH1	7:A:1795:HOH:O	2.49	0.46
1:A:459:LEU:HD13	1:A:540:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:LEU:CG	1:A:567[B]:ILE:HD11	2.46	0.46
1:A:503:LEU:HD23	1:A:567[B]:ILE:HD12	1.98	0.46
1:A:45[B]:ILE:HD12	1:A:187:THR:HA	1.98	0.45
1:A:939:ALA:HA	1:A:979:ALA:O	2.17	0.45
1:A:264[B]:PHE:CD2	1:A:304[B]:PHE:HD2	2.33	0.45
1:A:158[B]:LYS:HD2	1:A:814:GLY:HA2	1.98	0.45
1:A:682:TRP:O	1:A:884:HIS:HD2	2.00	0.45
1:A:260:TYR:HA	1:A:300:GLN:HB2	1.99	0.44
1:A:304[B]:PHE:HZ	3:C:7:GLC:H4	1.79	0.44
1:A:436:SER:OG	4:D:1:NAG:H5	2.18	0.44
1:A:1007:ARG:HG3	1:A:1007:ARG:NH1	2.17	0.44
1:A:264[B]:PHE:HB3	1:A:304[B]:PHE:CD2	2.49	0.44
3:C:9:MAN:H2	3:C:12:MAN:C5	2.46	0.44
1:A:836:ASN:ND2	7:A:1996:HOH:O	2.51	0.43
1:A:319:VAL:HG13	1:A:323[A]:PHE:CD2	2.54	0.43
1:A:836:ASN:ND2	7:A:1549:HOH:O	2.49	0.43
1:A:918:GLN:HG3	1:A:1007:ARG:HD3	2.01	0.43
1:A:565:LEU:HD21	1:A:567[B]:ILE:HD11	2.01	0.42
1:A:618:ASN:HD21	1:A:643:LYS:HD2	1.85	0.42
1:A:873:HIS:HE1	7:A:1239:HOH:O	2.02	0.42
1:A:618:ASN:ND2	1:A:643:LYS:HD2	2.35	0.41
1:A:60[B]:VAL:HG21	1:A:596:LEU:HD13	1.99	0.41
1:A:262[B]:LEU:HA	1:A:262[B]:LEU:HD12	1.67	0.41
1:A:64:SER:HA	1:A:92:THR:O	2.20	0.41
1:A:274:ASP:O	1:A:275:ASN:HB2	2.21	0.41
1:A:565:LEU:CD2	1:A:567[B]:ILE:HD11	2.51	0.41
1:A:38:ALA:HB2	1:A:252:VAL:O	2.22	0.40
1:A:429:VAL:HG22	1:A:472[B]:ILE:HG12	2.03	0.40
1:A:422:LYS:HE2	1:A:423:GLU:OE2	2.21	0.40
1:A:499:GLU:OE1	1:A:499:GLU:N	2.49	0.40
1:A:179[B]:SER:OG	1:A:183:LYS:NZ	2.54	0.40
1:A:183:LYS:HG3	7:A:1498:HOH:O	2.22	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	1012/1003 (101%)	983 (97%)	29 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	832/819 (102%)	812 (98%)	20 (2%)	49 12

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	63	PHE
1	A	198	GLU
1	A	355	HIS
1	A	472[A]	ILE
1	A	472[B]	ILE
1	A	543	SER
1	A	586	SER
1	A	618	ASN
1	A	639	LYS
1	A	641	ILE
1	A	673	GLN
1	A	742	ARG
1	A	888	SER
1	A	890	SER
1	A	932	THR
1	A	947	GLN
1	A	948	TYR
1	A	1007	ARG

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Mol	Chain	Res	Type
1	A	1015	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	A	225	ASN
1	A	413	ASN
1	A	540	HIS
1	A	618	ASN
1	A	664	HIS
1	A	673	GLN
1	A	747	GLN
1	A	836	ASN
1	A	870	GLN
1	A	873	HIS
1	A	884	HIS

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)

21 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	0.97	1 (7%)	17,19,21	1.54	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	B	2	2	14,14,15	0.67	0	17,19,21	0.97	1 (5%)
2	BMA	B	3	2	11,11,12	0.82	0	15,15,17	0.86	0
2	MAN	B	4	2	11,11,12	0.90	0	15,15,17	1.20	1 (6%)
2	MAN	B	5	2	11,11,12	0.83	1 (9%)	15,15,17	1.65	2 (13%)
2	MAN	B	6	2	11,11,12	1.03	1 (9%)	15,15,17	1.74	6 (40%)
2	MAN	B	7	2	11,11,12	1.27	1 (9%)	15,15,17	2.44	4 (26%)
3	NAG	C	1	3,1	14,14,15	0.76	0	17,19,21	1.06	1 (5%)
3	MAN	C	10	3	11,11,12	0.81	1 (9%)	15,15,17	1.48	4 (26%)
3	MAN	C	11	3	11,11,12	0.98	1 (9%)	15,15,17	2.41	6 (40%)
3	MAN	C	12	3	11,11,12	0.78	0	15,15,17	1.80	2 (13%)
3	NAG	C	2	3	14,14,15	0.59	0	17,19,21	1.51	3 (17%)
3	BMA	C	3	3	11,11,12	0.80	0	15,15,17	1.55	3 (20%)
3	MAN	C	4	3	11,11,12	0.89	0	15,15,17	2.38	4 (26%)
3	MAN	C	5	3	11,11,12	0.75	0	15,15,17	0.97	1 (6%)
3	MAN	C	6	3	11,11,12	0.87	1 (9%)	15,15,17	1.68	3 (20%)
3	GLC	C	7	3	11,11,12	1.04	1 (9%)	15,15,17	2.49	3 (20%)
3	GLC	C	8	3	11,11,12	0.71	0	15,15,17	3.09	5 (33%)
3	MAN	C	9	3	11,11,12	0.54	0	15,15,17	1.87	4 (26%)
4	NAG	D	1	4,1	14,14,15	0.65	0	17,19,21	2.31	5 (29%)
4	NAG	D	2	4	14,14,15	0.59	0	17,19,21	1.06	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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	0/2/19/22	0/1/1/1
2	MAN	B	6	2	-	0/2/19/22	0/1/1/1
2	MAN	B	7	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	MAN	C	10	3	-	2/2/19/22	0/1/1/1
3	MAN	C	11	3	-	0/2/19/22	0/1/1/1
3	MAN	C	12	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
3	GLC	C	7	3	-	2/2/19/22	0/1/1/1
3	GLC	C	8	3	-	2/2/19/22	0/1/1/1
3	MAN	C	9	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	2.56	1.56	1.52
3	C	7	GLC	O5-C1	-2.43	1.39	1.43
3	C	11	MAN	C2-C3	2.40	1.56	1.52
2	B	6	MAN	C2-C3	2.33	1.55	1.52
3	C	6	MAN	C2-C3	2.23	1.55	1.52
2	B	7	MAN	C2-C3	2.21	1.55	1.52
3	C	10	MAN	C2-C3	2.13	1.55	1.52
2	B	5	MAN	O5-C1	-2.09	1.40	1.43

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	8	GLC	O5-C5-C6	7.83	119.49	107.20
2	B	7	MAN	C1-O5-C5	7.01	121.68	112.19
3	C	4	MAN	C1-O5-C5	6.84	121.46	112.19
3	C	11	MAN	C1-O5-C5	6.79	121.39	112.19
3	C	8	GLC	C1-C2-C3	6.61	117.79	109.67
3	C	7	GLC	C1-O5-C5	6.52	121.02	112.19
4	D	1	NAG	C1-O5-C5	5.76	119.99	112.19
3	C	12	MAN	C1-O5-C5	5.41	119.52	112.19
2	B	5	MAN	C1-O5-C5	4.82	118.73	112.19
3	C	7	GLC	C1-C2-C3	4.72	115.46	109.67
4	D	1	NAG	C4-C3-C2	4.32	117.34	111.02
2	B	1	NAG	O5-C1-C2	-4.30	104.49	111.29
3	C	9	MAN	C1-O5-C5	4.08	117.72	112.19
3	C	6	MAN	O3-C3-C2	-4.05	102.23	109.99
3	C	8	GLC	O6-C6-C5	3.73	124.07	111.29
2	B	6	MAN	O5-C5-C4	-3.69	101.86	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2	NAG	C2-N2-C7	-3.66	117.70	122.90
3	C	4	MAN	C6-C5-C4	-3.43	104.98	113.00
3	C	9	MAN	O5-C5-C6	3.41	112.55	107.20
3	C	6	MAN	O4-C4-C3	3.30	117.97	110.35
3	C	11	MAN	C1-C2-C3	-3.25	105.68	109.67
2	B	7	MAN	O3-C3-C4	-3.24	102.86	110.35
2	B	7	MAN	C6-C5-C4	-3.09	105.78	113.00
3	C	8	GLC	C1-O5-C5	2.96	116.21	112.19
3	C	3	BMA	C1-C2-C3	-2.95	106.04	109.67
3	C	7	GLC	O2-C2-C3	2.95	116.04	110.14
3	C	11	MAN	C2-C3-C4	-2.94	105.80	110.89
4	D	1	NAG	O7-C7-C8	-2.93	116.61	122.06
2	B	6	MAN	O3-C3-C2	-2.85	104.53	109.99
3	C	5	MAN	C1-O5-C5	2.76	115.93	112.19
4	D	1	NAG	C2-N2-C7	2.75	126.81	122.90
3	C	8	GLC	O5-C1-C2	2.74	115.00	110.77
3	C	9	MAN	C1-C2-C3	2.70	112.99	109.67
3	C	3	BMA	O3-C3-C2	2.66	115.08	109.99
3	C	10	MAN	C1-O5-C5	2.64	115.77	112.19
2	B	4	MAN	C1-O5-C5	2.59	115.70	112.19
3	C	12	MAN	C1-C2-C3	-2.58	106.49	109.67
3	C	6	MAN	O6-C6-C5	-2.58	102.45	111.29
3	C	4	MAN	O5-C5-C6	-2.50	103.28	107.20
3	C	11	MAN	O2-C2-C3	-2.46	105.22	110.14
2	B	7	MAN	O6-C6-C5	-2.44	102.91	111.29
3	C	1	NAG	O5-C1-C2	-2.43	107.45	111.29
4	D	2	NAG	O7-C7-C8	-2.38	117.63	122.06
3	C	9	MAN	O3-C3-C4	-2.32	104.98	110.35
3	C	2	NAG	O7-C7-N2	-2.31	117.71	121.95
2	B	6	MAN	O3-C3-C4	-2.30	105.03	110.35
3	C	10	MAN	O3-C3-C2	-2.25	105.68	109.99
3	C	10	MAN	O5-C1-C2	-2.23	107.34	110.77
3	C	3	BMA	C1-O5-C5	-2.22	109.19	112.19
4	D	2	NAG	O5-C5-C6	2.19	110.63	107.20
3	C	10	MAN	O6-C6-C5	-2.17	103.83	111.29
2	B	5	MAN	C1-C2-C3	2.16	112.33	109.67
2	B	2	NAG	O5-C1-C2	-2.16	107.88	111.29
2	B	6	MAN	O6-C6-C5	-2.14	103.93	111.29
3	C	11	MAN	O5-C5-C4	2.13	116.00	110.83
3	C	2	NAG	O5-C1-C2	-2.12	107.94	111.29
2	B	6	MAN	C1-C2-C3	-2.10	107.09	109.67
3	C	4	MAN	C3-C4-C5	2.09	113.97	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	11	MAN	O3-C3-C4	-2.08	105.53	110.35
2	B	6	MAN	C3-C4-C5	-2.06	106.57	110.24
2	B	1	NAG	C4-C3-C2	-2.05	108.02	111.02
4	D	2	NAG	C8-C7-N2	2.02	119.53	116.10
4	D	1	NAG	O3-C3-C4	2.02	115.02	110.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	10	MAN	O5-C5-C6-O6
4	D	1	NAG	O7-C7-N2-C2
3	C	8	GLC	O5-C5-C6-O6
3	C	12	MAN	C4-C5-C6-O6
3	C	10	MAN	C4-C5-C6-O6
3	C	12	MAN	O5-C5-C6-O6
3	C	7	GLC	C4-C5-C6-O6
3	C	8	GLC	C4-C5-C6-O6
3	C	7	GLC	O5-C5-C6-O6

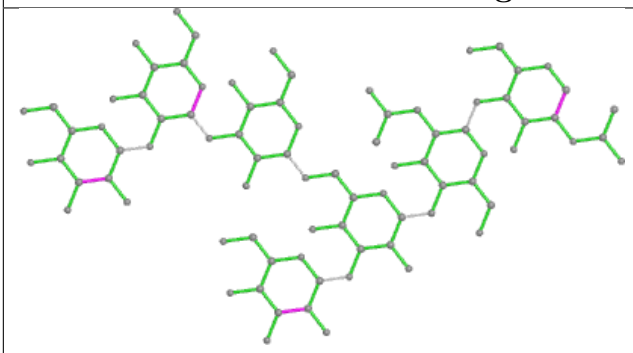
There are no ring outliers.

6 monomers are involved in 10 short contacts:

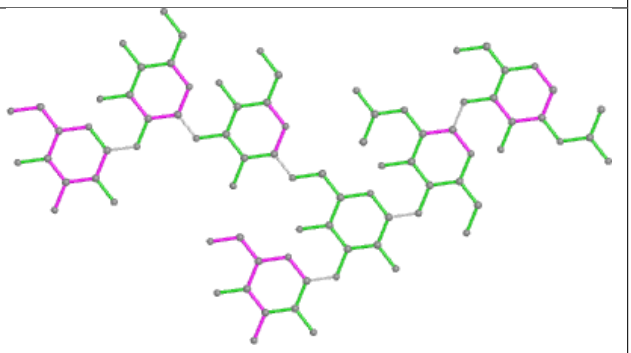
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	12	MAN	3	0
3	C	8	GLC	2	0
4	D	1	NAG	1	0
2	B	7	MAN	1	0
3	C	9	MAN	3	0
3	C	7	GLC	3	0

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

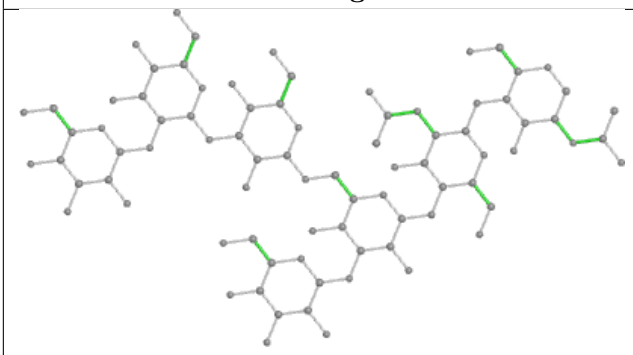
Oligosaccharide Chain B



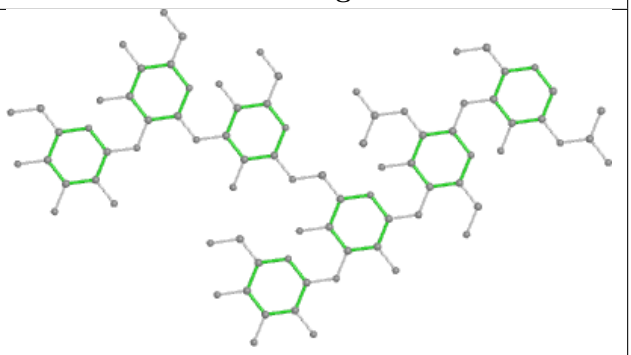
Bond lengths



Bond angles

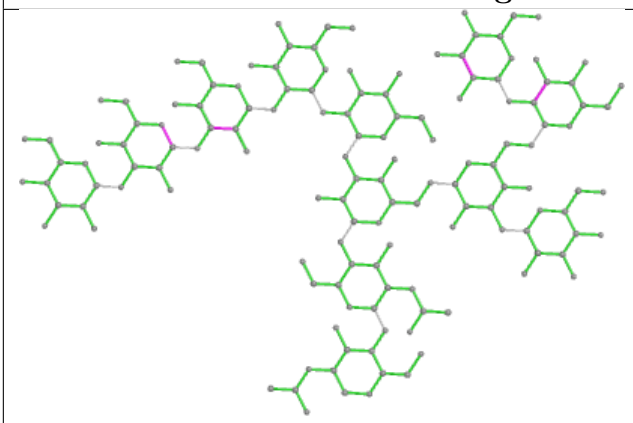


Torsions

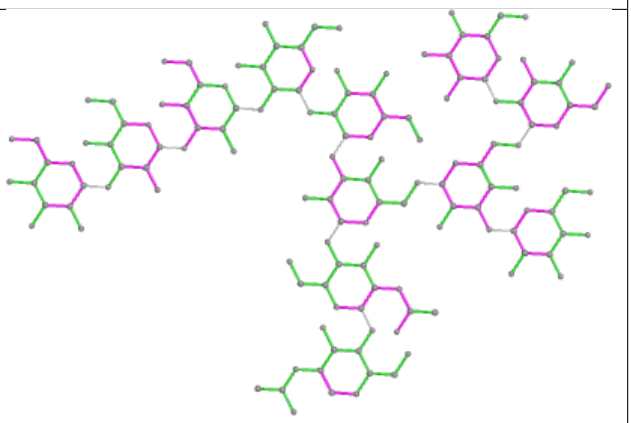


Rings

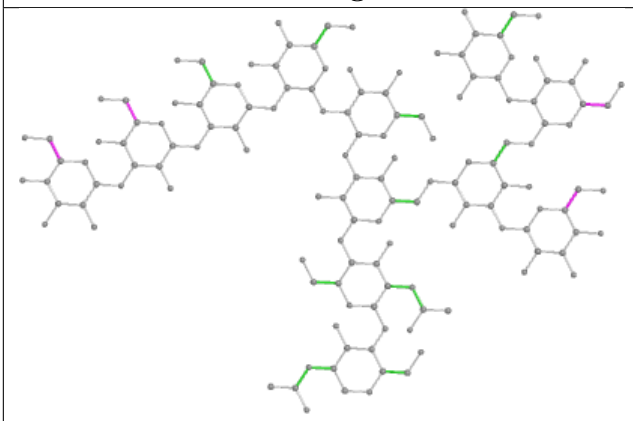
Oligosaccharide Chain C



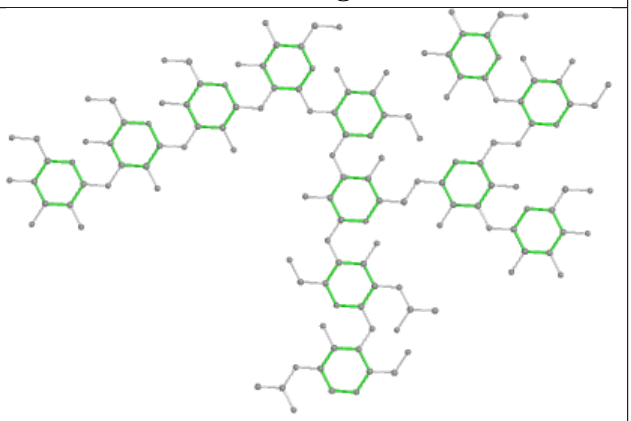
Bond lengths



Bond angles

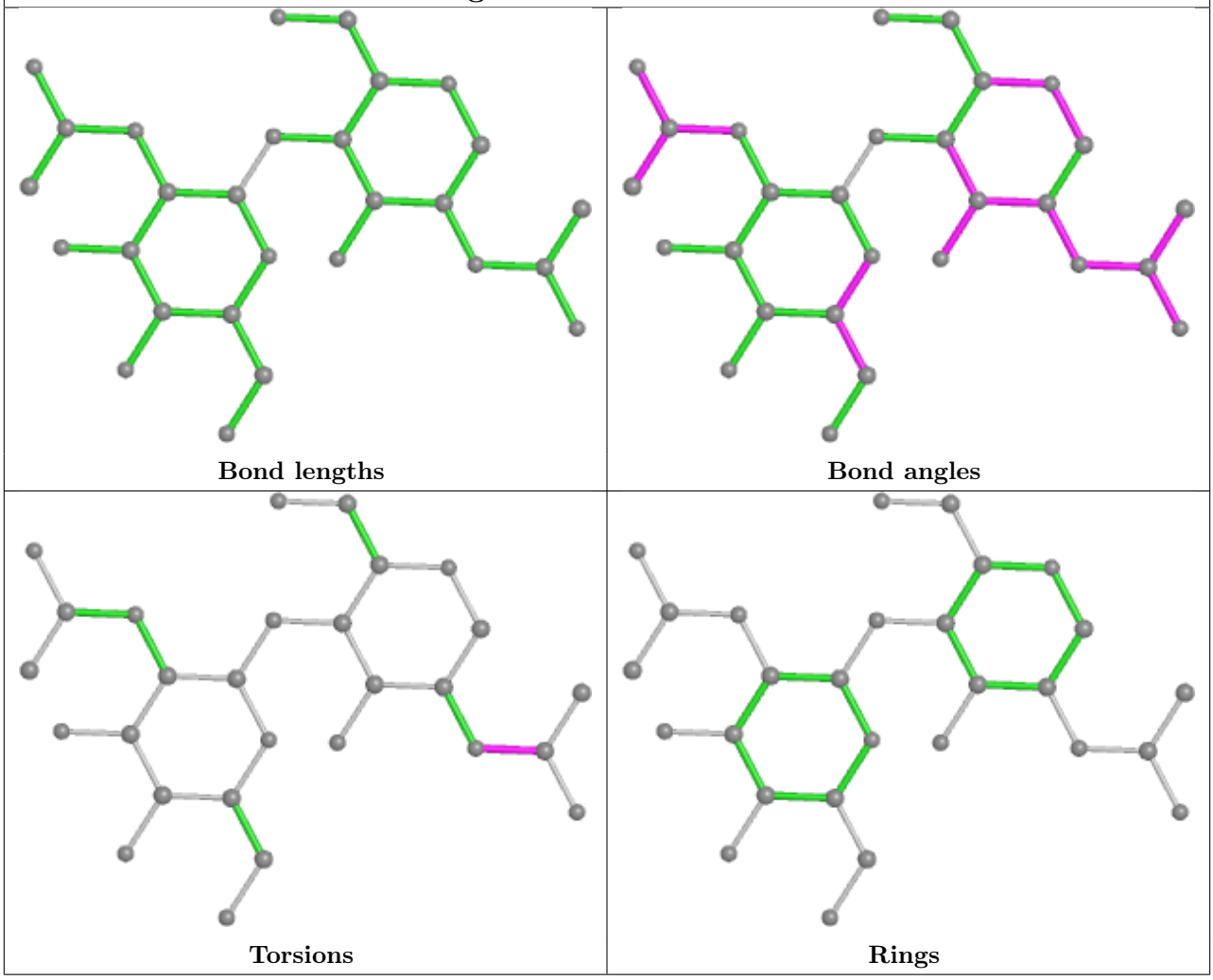


Torsions



Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
5	NAG	A	1044	1	14,14,15	0.73	0	17,19,21	1.92	5 (29%)
6	GOL	A	1049	-	5,5,5	0.19	0	5,5,5	1.37	1 (20%)
5	NAG	A	1045	1	14,14,15	0.48	0	17,19,21	1.61	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GOL	A	1048	-	5,5,5	0.76	0	5,5,5	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1044	1	-	0/6/23/26	0/1/1/1
6	GOL	A	1049	-	-	3/4/4/4	-
5	NAG	A	1045	1	-	2/6/23/26	0/1/1/1
6	GOL	A	1048	-	-	0/4/4/4	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1044	NAG	O5-C1-C2	-4.36	104.41	111.29
5	A	1045	NAG	O7-C7-C8	-3.30	115.93	122.06
5	A	1044	NAG	O5-C5-C6	3.09	112.06	107.20
5	A	1044	NAG	O7-C7-C8	-2.69	117.07	122.06
5	A	1045	NAG	C8-C7-N2	2.57	120.46	116.10
5	A	1044	NAG	O7-C7-N2	2.51	126.56	121.95
6	A	1049	GOL	O2-C2-C3	2.50	120.13	109.12
5	A	1045	NAG	O5-C1-C2	-2.48	107.37	111.29
5	A	1044	NAG	C1-C2-N2	2.42	114.62	110.49
5	A	1045	NAG	O3-C3-C2	-2.38	104.53	109.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1049	GOL	O2-C2-C3-O3
6	A	1049	GOL	C1-C2-C3-O3
5	A	1045	NAG	C4-C5-C6-O6
5	A	1045	NAG	O5-C5-C6-O6
6	A	1049	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	986/1003 (98%)	-0.27	29 (2%) 51 50	7, 12, 33, 69	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	525	LYS	5.7
1	A	526	THR	5.4
1	A	933	ALA	5.1
1	A	888	SER	4.9
1	A	886	PRO	4.4
1	A	932	THR	4.2
1	A	543	SER	4.2
1	A	931	ALA	4.0
1	A	545	LEU	3.9
1	A	889	SER	3.8
1	A	498	ALA	3.7
1	A	523	SER	3.3
1	A	38	ALA	3.1
1	A	887	SER	2.7
1	A	890	SER	2.7
1	A	274	ASP	2.7
1	A	524	SER	2.6
1	A	60[A]	VAL	2.6
1	A	541	THR	2.5
1	A	499	GLU	2.4
1	A	275	ASN	2.3
1	A	616	LYS	2.3
1	A	527	ALA	2.3
1	A	522	GLY	2.2
1	A	617	GLY	2.2
1	A	1007	ARG	2.2
1	A	266[A]	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	615[A]	ILE	2.1
1	A	542	THR	2.0

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

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

6.3 Carbohydrates (i)

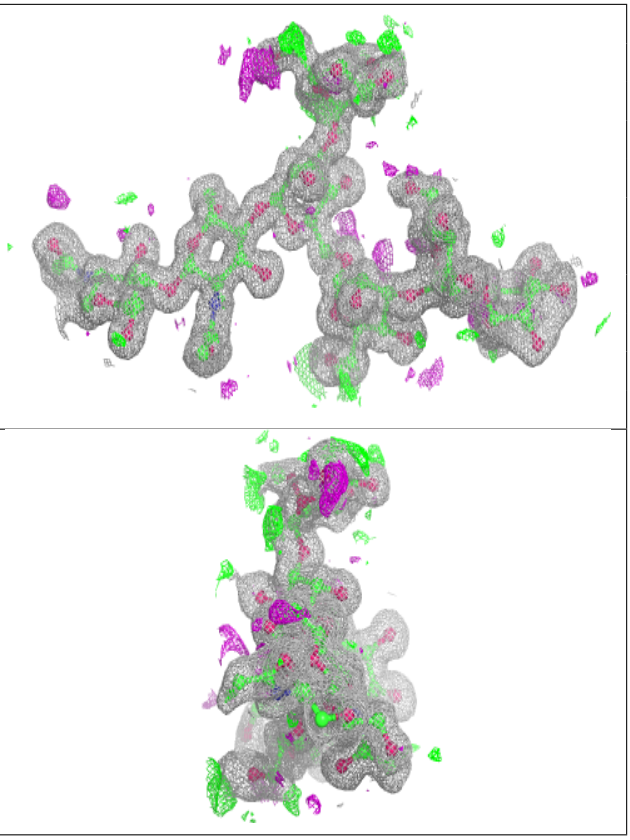
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

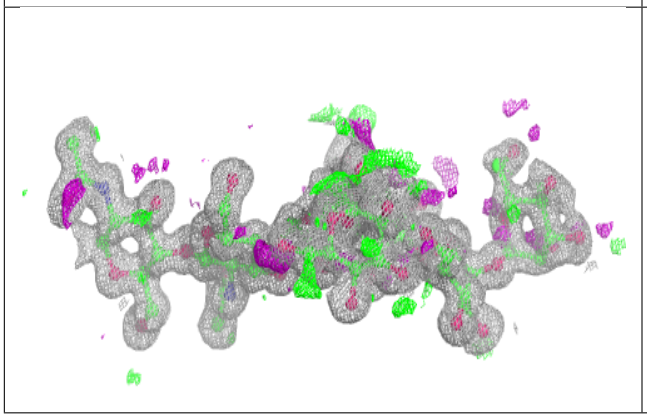
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	C	12	11/12	0.57	0.41	41,55,72,74	0
3	MAN	C	11	11/12	0.79	0.32	32,37,51,59	0
3	GLC	C	8	11/12	0.79	0.35	66,75,88,91	0
4	NAG	D	2	14/15	0.80	0.25	55,86,102,108	0
3	GLC	C	7	11/12	0.81	0.18	35,50,55,66	0
3	MAN	C	10	11/12	0.83	0.33	34,40,66,76	0
4	NAG	D	1	14/15	0.89	0.15	29,43,58,68	0
2	MAN	B	7	11/12	0.93	0.14	18,20,26,27	0
2	MAN	B	6	11/12	0.93	0.25	20,26,47,52	0
3	MAN	C	6	11/12	0.94	0.16	19,25,36,36	0
3	MAN	C	9	11/12	0.95	0.17	21,26,34,39	0
3	MAN	C	4	11/12	0.96	0.13	18,25,38,45	0
3	MAN	C	5	11/12	0.97	0.12	17,20,25,30	0
3	NAG	C	1	14/15	0.97	0.07	11,14,28,37	0
3	NAG	C	2	14/15	0.98	0.09	12,19,45,46	0
2	BMA	B	3	11/12	0.98	0.07	10,12,15,17	0
2	NAG	B	1	14/15	0.99	0.04	9,11,22,24	0
2	MAN	B	4	11/12	0.99	0.04	9,10,14,22	0
2	MAN	B	5	11/12	0.99	0.06	11,11,17,28	0
3	BMA	C	3	11/12	0.99	0.07	14,15,17,18	0
2	NAG	B	2	14/15	0.99	0.04	8,10,13,15	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:

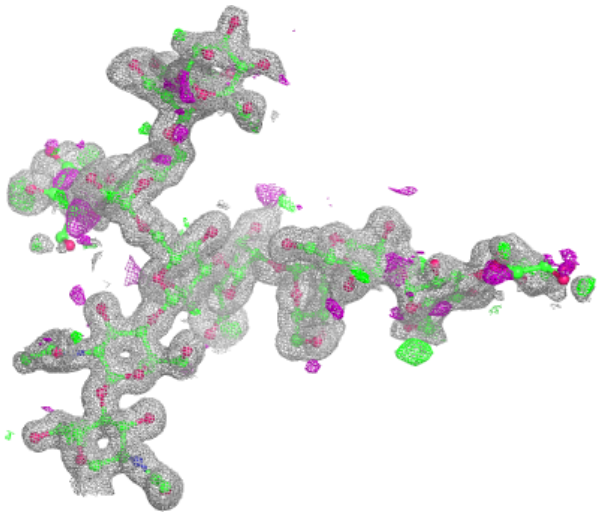
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

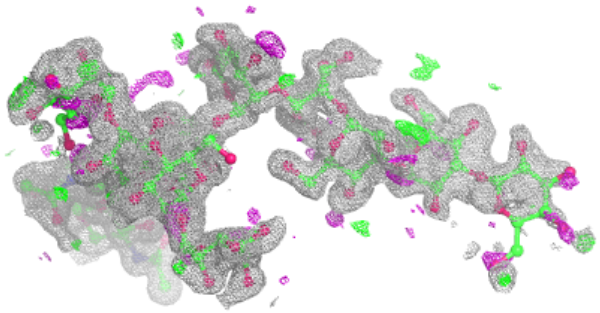


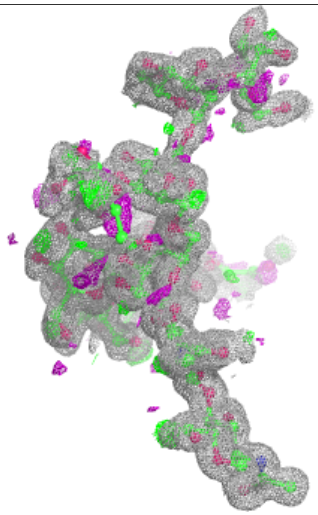


Electron density around Chain C:

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

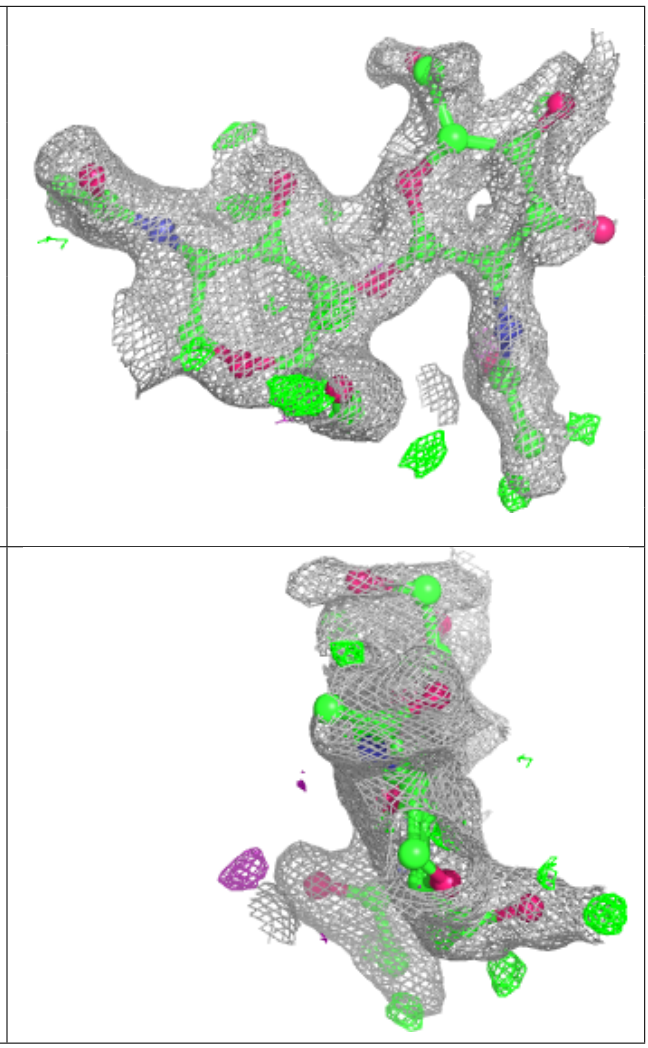






Electron density around Chain D:

$2mF_o$-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
6	GOL	A	1049	6/6	0.81	0.17	23,48,51,59	0
5	NAG	A	1045	14/15	0.90	0.22	27,42,59,65	0
5	NAG	A	1044	14/15	0.91	0.13	23,35,50,55	0
6	GOL	A	1048	6/6	0.99	0.04	11,12,12,14	0

6.5 Other polymers (i)

There are no such residues in this entry.