



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 03:15 PM UTC

PDB ID : 3OG2 / pdb_00003og2
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

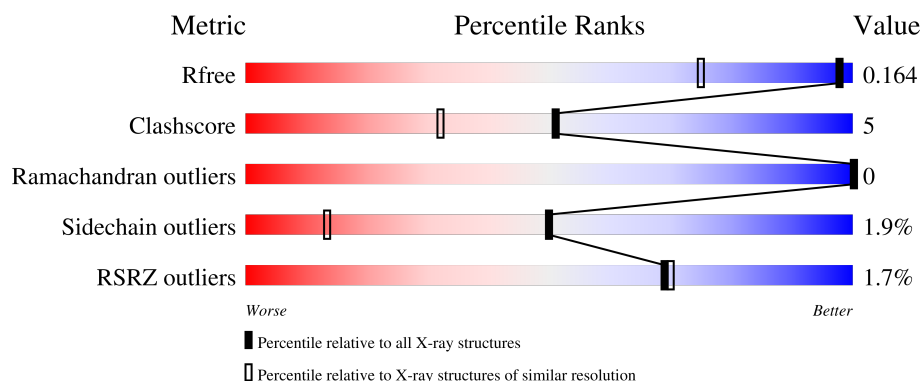
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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

Mol	Chain	Length	Quality of chain
1	A	1003	2% 88% 9% ..
2	B	7	14% 71% 14%
3	C	12	67% 33%
4	D	2	50% 50%

2 Entry composition [i](#)

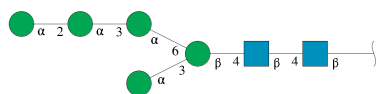
There are 7 unique types of molecules in this entry. The entry contains 9055 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

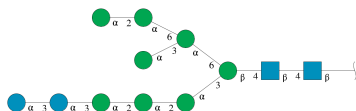
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	986	7773	5016	1298	1450	9	0	27	0

- 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
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

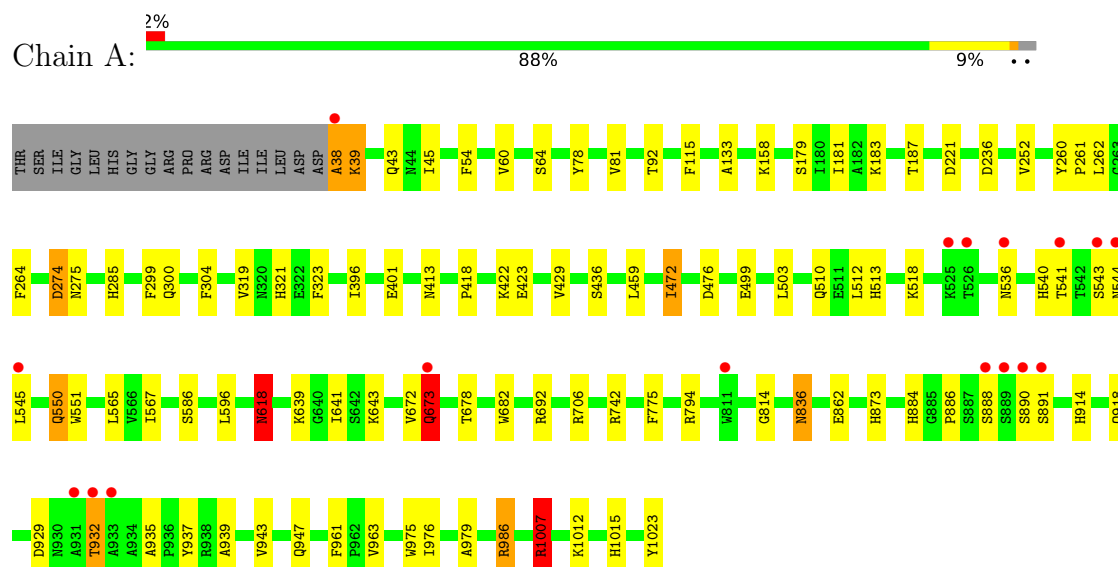
- Molecule 7 is water.

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

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.

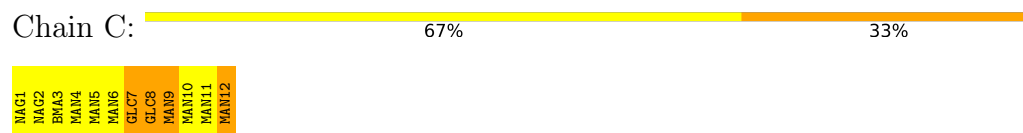
• Molecule 1: Beta-galactosidase



• 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



• 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



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

Chain D:



MAG1
MAG2

4 Data and refinement statistics

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 20.00 – 1.20	Depositor EDS
% Data completeness (in resolution range)	86.2 (20.00-1.20) 83.2 (20.00-1.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.20Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.139 , 0.171 0.134 , 0.164	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)	0.44 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.86	2/8059 (0.0%)	1.32	43/10981 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	551	TRP	NE1-CE2	-5.70	1.31	1.37
1	A	1023	TYR	C-OXT	5.52	1.34	1.23

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1007	ARG	CD-NE-CZ	10.65	139.31	124.40
1	A	932	THR	CA-C-N	-10.54	107.18	122.77
1	A	932	THR	C-N-CA	-10.54	107.18	122.77
1	A	929	ASP	CA-CB-CG	8.09	120.69	112.60
1	A	794	ARG	NE-CZ-NH2	7.46	125.91	119.20
1	A	285	HIS	CA-CB-CG	-7.28	106.52	113.80
1	A	862	GLU	CB-CA-C	-7.23	97.33	109.48
1	A	536	ASN	OD1-CG-ND2	7.05	129.65	122.60
1	A	518	LYS	CA-C-O	-6.59	114.56	121.55
1	A	963	VAL	CA-C-O	-6.57	116.53	119.94
1	A	541	THR	O-C-N	-6.51	114.94	123.21
1	A	274	ASP	CA-C-O	6.30	128.09	121.15
1	A	536	ASN	CA-CB-CG	-6.30	106.30	112.60
1	A	396	ILE	CA-C-N	-6.25	112.81	122.49
1	A	396	ILE	C-N-CA	-6.25	112.81	122.49
1	A	476	ASP	CA-CB-CG	-6.19	106.41	112.60
1	A	986	ARG	NE-CZ-NH2	6.18	124.76	119.20
1	A	413	ASN	OD1-CG-ND2	6.02	128.62	122.60
1	A	513	HIS	CA-CB-CG	-6.01	107.79	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1015	HIS	CB-CG-ND1	6.00	131.71	122.70
1	A	299	PHE	CA-CB-CG	-5.92	107.89	113.80
1	A	236	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	836	ASN	CA-CB-CG	-5.77	106.83	112.60
1	A	1015	HIS	CB-CG-CD2	-5.70	123.79	131.20
1	A	274	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	54	PHE	CA-CB-CG	5.42	119.22	113.80
1	A	937	TYR	O-C-N	5.35	129.35	123.25
1	A	618	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	A	261	PRO	O-C-N	-5.25	114.99	122.35
1	A	551	TRP	CB-CG-CD1	5.25	134.77	126.90
1	A	775	PHE	CA-CB-CG	5.25	119.05	113.80
1	A	43	GLN	CA-C-N	-5.23	114.28	122.49
1	A	43	GLN	C-N-CA	-5.23	114.28	122.49
1	A	115	PHE	CA-CB-CG	-5.21	108.59	113.80
1	A	221	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	975	TRP	CA-CB-CG	-5.21	103.70	113.60
1	A	914	HIS	CA-CB-CG	-5.17	108.63	113.80
1	A	706	ARG	CG-CD-NE	-5.05	100.89	112.00
1	A	550	GLN	OE1-CD-NE2	5.03	127.63	122.60
1	A	38	ALA	CA-C-N	5.02	131.56	121.81
1	A	38	ALA	C-N-CA	5.02	131.56	121.81
1	A	673	GLN	CA-C-O	5.01	125.84	120.38
1	A	961	PHE	CA-CB-CG	-5.01	108.79	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7773	0	7625	77	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	12	0	16	0	0
7	A	993	0	0	13	0
All	All	9055	0	7877	83	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 (83) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:133:ALA:HB1	1:A:181[A]:ILE:HD13	1.88	0.54
1:A:673:GLN:HA	1:A:673:GLN:NE2	2.22	0.52
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:886:PRO:HD2	1:A:891:SER:HG	1.74	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	816 (98%)	16 (2%)	50 13

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
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	672	VAL
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	1007	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	140	ASN
1	A	225	ASN
1	A	283	GLN
1	A	458	GLN
1	A	540	HIS
1	A	573	ASN
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
1	A	1015	HIS
1	A	1020	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	1.01	1 (7%)	17,19,21	1.56	2 (11%)
2	NAG	B	2	2	14,14,15	0.66	0	17,19,21	0.98	1 (5%)
2	BMA	B	3	2	11,11,12	0.82	0	15,15,17	0.79	0
2	MAN	B	4	2	11,11,12	0.88	0	15,15,17	1.16	1 (6%)
2	MAN	B	5	2	11,11,12	0.80	0	15,15,17	1.62	1 (6%)
2	MAN	B	6	2	11,11,12	1.00	1 (9%)	15,15,17	1.67	5 (33%)
2	MAN	B	7	2	11,11,12	1.24	1 (9%)	15,15,17	2.40	4 (26%)
3	NAG	C	1	3,1	14,14,15	0.78	0	17,19,21	1.05	1 (5%)
3	MAN	C	10	3	11,11,12	0.79	1 (9%)	15,15,17	1.39	3 (20%)
3	MAN	C	11	3	11,11,12	0.95	1 (9%)	15,15,17	2.35	6 (40%)
3	MAN	C	12	3	11,11,12	0.76	0	15,15,17	1.73	2 (13%)
3	NAG	C	2	3	14,14,15	0.60	0	17,19,21	1.52	3 (17%)
3	BMA	C	3	3	11,11,12	0.79	0	15,15,17	1.46	3 (20%)
3	MAN	C	4	3	11,11,12	0.86	0	15,15,17	2.33	4 (26%)
3	MAN	C	5	3	11,11,12	0.74	0	15,15,17	0.94	1 (6%)
3	MAN	C	6	3	11,11,12	0.85	1 (9%)	15,15,17	1.62	3 (20%)
3	GLC	C	7	3	11,11,12	1.00	1 (9%)	15,15,17	2.37	3 (20%)
3	GLC	C	8	3	11,11,12	0.70	0	15,15,17	2.61	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	C	9	3	11,11,12	0.53	0	15,15,17	1.71	4 (26%)
4	NAG	D	1	4,1	14,14,15	0.63	0	17,19,21	2.33	5 (29%)
4	NAG	D	2	4	14,14,15	0.59	0	17,19,21	1.02	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	-	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
3	NAG	C	2	3	-	1/6/23/26	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	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	2.80	1.56	1.52
3	C	11	MAN	C2-C3	2.33	1.56	1.52
3	C	7	GLC	O5-C1	-2.29	1.39	1.43
2	B	6	MAN	C2-C3	2.26	1.55	1.52
3	C	6	MAN	C2-C3	2.16	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	MAN	C2-C3	2.14	1.55	1.52
3	C	10	MAN	C2-C3	2.07	1.55	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	MAN	C1-O5-C5	7.09	121.68	112.19
3	C	4	MAN	C1-O5-C5	6.92	121.46	112.19
3	C	11	MAN	C1-O5-C5	6.87	121.39	112.19
3	C	7	GLC	C1-O5-C5	6.59	121.02	112.19
3	C	8	GLC	O5-C5-C6	6.07	119.49	107.66
4	D	1	NAG	C1-O5-C5	5.82	119.99	112.19
3	C	8	GLC	C1-C2-C3	5.59	117.79	109.64
3	C	12	MAN	C1-O5-C5	5.47	119.52	112.19
2	B	5	MAN	C1-O5-C5	4.88	118.73	112.19
2	B	1	NAG	O5-C1-C2	-4.39	104.49	111.29
4	D	1	NAG	C4-C3-C2	4.32	117.34	111.02
3	C	9	MAN	C1-O5-C5	4.13	117.72	112.19
3	C	7	GLC	C1-C2-C3	4.00	115.46	109.64
3	C	2	NAG	C2-N2-C7	-3.88	117.70	122.90
3	C	6	MAN	O3-C3-C2	-3.83	102.23	110.05
3	C	8	GLC	O6-C6-C5	3.74	124.07	111.33
2	B	6	MAN	O5-C5-C4	-3.69	101.86	110.83
3	C	4	MAN	C6-C5-C4	-3.28	104.98	113.02
3	C	6	MAN	O4-C4-C3	3.22	117.97	110.38
2	B	7	MAN	O3-C3-C4	-3.19	102.86	110.38
4	D	1	NAG	O7-C7-C8	-3.06	116.61	122.05
3	C	8	GLC	C1-O5-C5	3.00	116.21	112.19
2	B	7	MAN	C6-C5-C4	-2.95	105.78	113.02
4	D	1	NAG	C2-N2-C7	2.92	126.81	122.90
3	C	11	MAN	C2-C3-C4	-2.88	105.80	110.86
3	C	7	GLC	O2-C2-C3	2.84	116.04	110.15
3	C	5	MAN	C1-O5-C5	2.79	115.93	112.19
3	C	11	MAN	C1-C2-C3	-2.73	105.68	109.64
2	B	6	MAN	O3-C3-C2	-2.71	104.53	110.05
3	C	10	MAN	C1-O5-C5	2.67	115.77	112.19
2	B	4	MAN	C1-O5-C5	2.62	115.70	112.19
3	C	6	MAN	O6-C6-C5	-2.61	102.45	111.33
3	C	9	MAN	O5-C5-C6	2.51	112.55	107.66
3	C	1	NAG	O5-C1-C2	-2.49	107.45	111.29
4	D	2	NAG	O7-C7-C8	-2.48	117.63	122.05
2	B	7	MAN	O6-C6-C5	-2.47	102.91	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	BMA	C1-C2-C3	-2.47	106.04	109.64
3	C	3	BMA	O3-C3-C2	2.47	115.08	110.05
3	C	2	NAG	O7-C7-N2	-2.41	117.71	121.98
3	C	11	MAN	O2-C2-C3	-2.38	105.22	110.15
3	C	9	MAN	C1-C2-C3	2.30	112.99	109.64
3	C	9	MAN	O3-C3-C4	-2.29	104.98	110.38
2	B	6	MAN	O3-C3-C4	-2.27	105.03	110.38
3	C	4	MAN	O5-C5-C6	-2.25	103.28	107.66
3	C	3	BMA	C1-O5-C5	-2.24	109.19	112.19
2	B	2	NAG	O5-C1-C2	-2.21	107.88	111.29
3	C	10	MAN	O6-C6-C5	-2.20	103.83	111.33
2	B	6	MAN	O6-C6-C5	-2.17	103.93	111.33
3	C	2	NAG	O5-C1-C2	-2.17	107.94	111.29
3	C	12	MAN	C1-C2-C3	-2.17	106.49	109.64
3	C	10	MAN	O3-C3-C2	-2.14	105.68	110.05
3	C	11	MAN	O5-C5-C4	2.13	116.00	110.83
3	C	4	MAN	C3-C4-C5	2.06	113.97	110.23
3	C	11	MAN	O3-C3-C4	-2.06	105.53	110.38
4	D	2	NAG	C8-C7-N2	2.06	119.53	116.12
2	B	1	NAG	C4-C3-C2	-2.05	108.02	111.02
2	B	6	MAN	C3-C4-C5	-2.02	106.57	110.23
4	D	1	NAG	O5-C1-C2	-2.01	108.19	111.29

There are no chirality outliers.

All (11) torsion outliers are listed below:

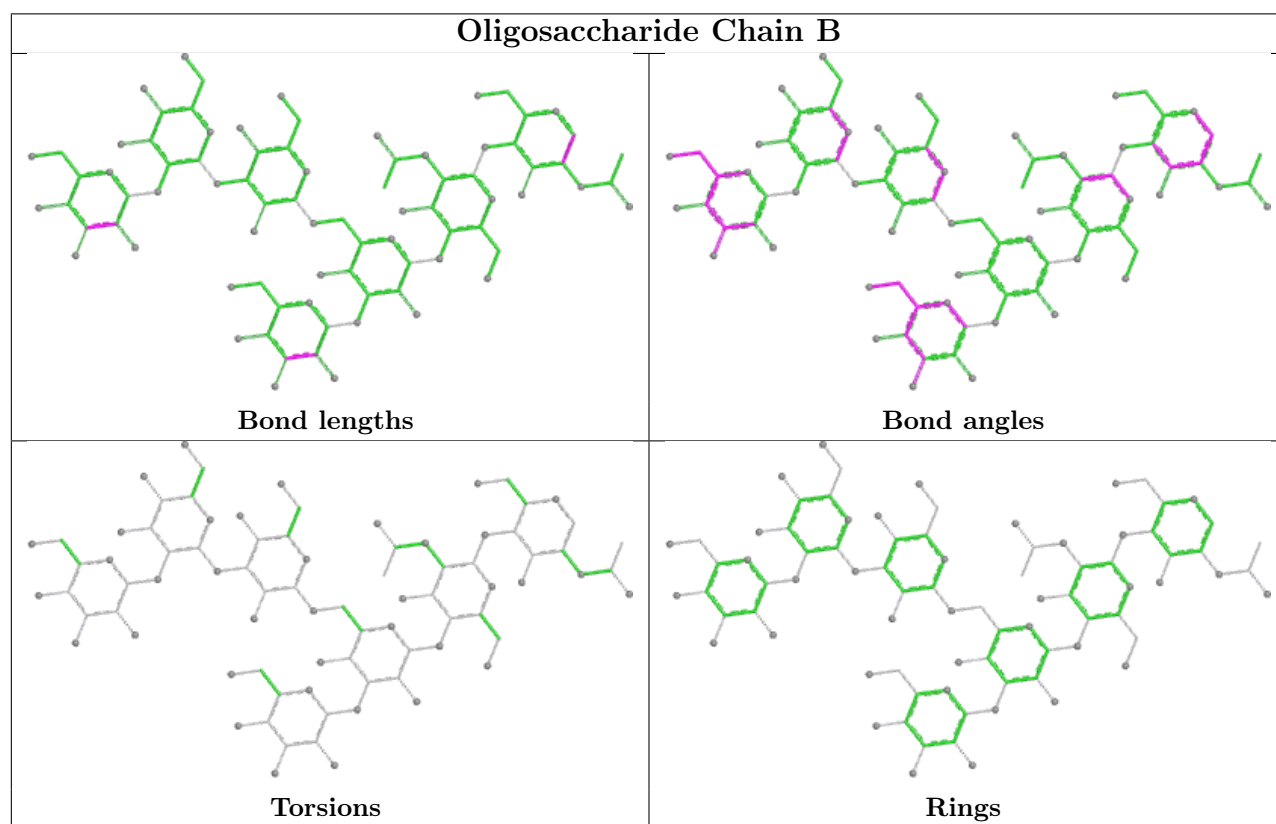
Mol	Chain	Res	Type	Atoms
3	C	10	MAN	O5-C5-C6-O6
4	D	1	NAG	O7-C7-N2-C2
3	C	8	GLC	O5-C5-C6-O6
3	C	10	MAN	C4-C5-C6-O6
3	C	12	MAN	C4-C5-C6-O6
3	C	12	MAN	O5-C5-C6-O6
3	C	7	GLC	C4-C5-C6-O6
3	C	8	GLC	C4-C5-C6-O6
3	C	7	GLC	O5-C5-C6-O6
4	D	1	NAG	C1-C2-N2-C7
3	C	2	NAG	O7-C7-N2-C2

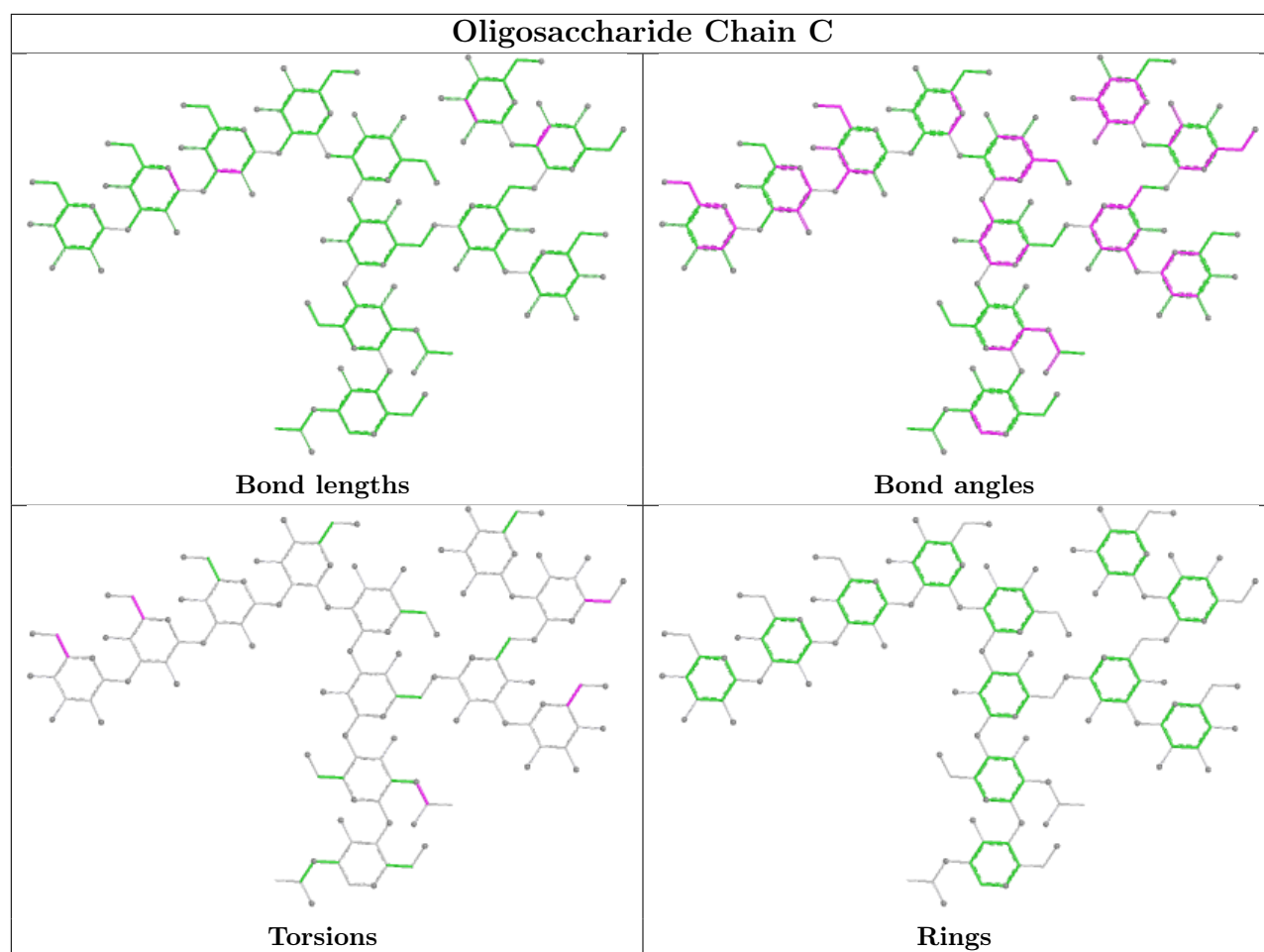
There are no ring outliers.

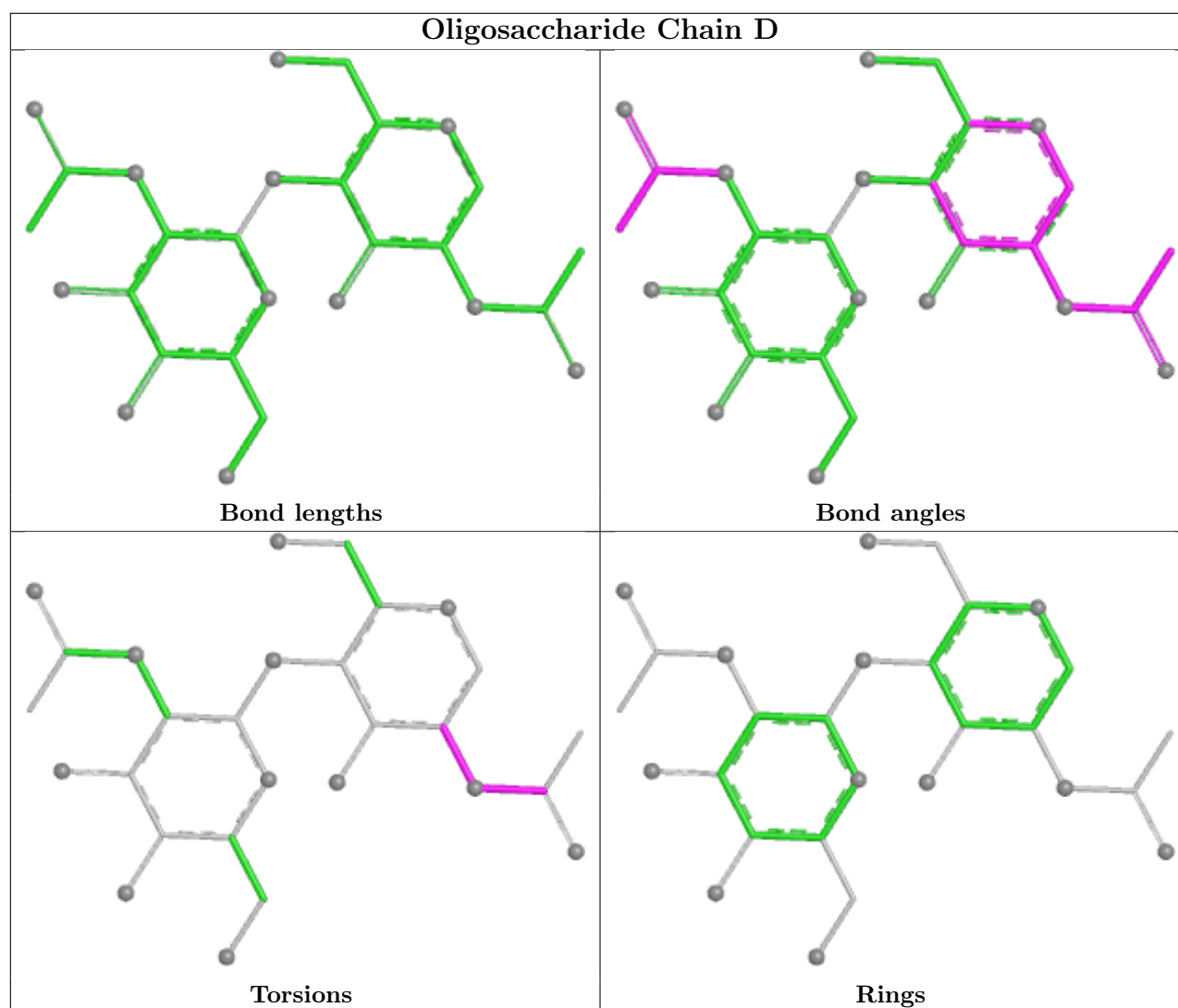
6 monomers are involved in 10 short contacts:

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







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	$\# Z > 2$
6	GOL	A	1048	-	5,5,5	0.77	0	5,5,5	0.48	0
5	NAG	A	1044	1	14,14,15	0.75	0	17,19,21	1.90	5 (29%)
5	NAG	A	1045	1	14,14,15	0.48	0	17,19,21	1.63	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	A	1049	-	5,5,5	0.19	0	5,5,5	1.44	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
6	GOL	A	1048	-	-	0/4/4/4	-
5	NAG	A	1044	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1045	1	-	2/6/23/26	0/1/1/1
6	GOL	A	1049	-	-	3/4/4/4	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1044	NAG	O5-C1-C2	-4.45	104.41	111.29
5	A	1045	NAG	O7-C7-C8	-3.44	115.93	122.05
5	A	1044	NAG	O7-C7-C8	-2.80	117.07	122.05
5	A	1044	NAG	C1-C2-N2	2.66	114.62	110.43
6	A	1049	GOL	O2-C2-C3	2.64	120.13	109.18
5	A	1045	NAG	C8-C7-N2	2.62	120.46	116.12
5	A	1044	NAG	O7-C7-N2	2.59	126.56	121.98
5	A	1045	NAG	O5-C1-C2	-2.53	107.37	111.29
5	A	1045	NAG	O3-C3-C2	-2.34	104.53	109.40
5	A	1044	NAG	O5-C5-C6	2.26	112.06	107.66
5	A	1045	NAG	C1-C2-N2	2.03	113.64	110.43

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%)	-0.44	17 (1%) 69 70	5, 11, 33, 69	27 (2%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	931	ALA	4.6
1	A	933	ALA	4.6
1	A	932	THR	4.4
1	A	38	ALA	3.9
1	A	891	SER	3.5
1	A	543	SER	3.2
1	A	888	SER	2.6
1	A	673	GLN	2.4
1	A	890	SER	2.4
1	A	889	SER	2.4
1	A	526	THR	2.3
1	A	544	ASN	2.3
1	A	545	LEU	2.3
1	A	536	ASN	2.2
1	A	541	THR	2.1
1	A	525	LYS	2.1
1	A	811	TRP	2.1

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,

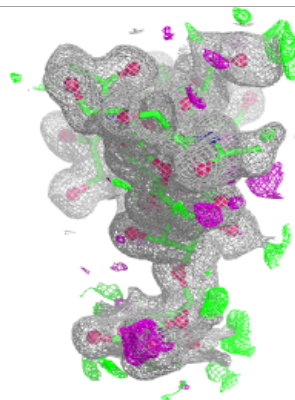
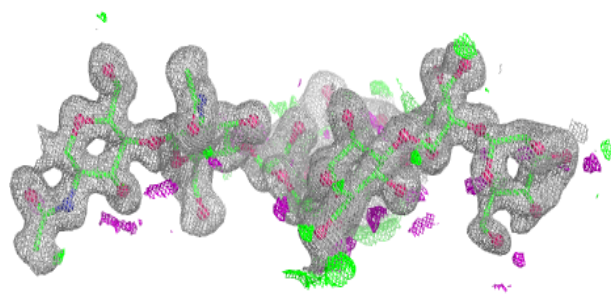
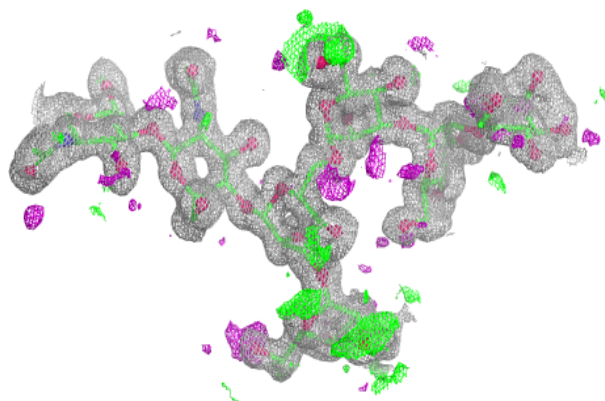
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	C	12	11/12	0.69	0.21	41,55,72,74	0
3	GLC	C	8	11/12	0.76	0.18	66,75,88,91	0
4	NAG	D	2	14/15	0.77	0.19	55,86,102,108	0
3	MAN	C	10	11/12	0.83	0.14	34,40,66,76	0
3	GLC	C	7	11/12	0.86	0.13	35,50,55,66	0
3	MAN	C	11	11/12	0.89	0.11	32,37,51,59	0
4	NAG	D	1	14/15	0.90	0.13	29,43,58,68	0
2	MAN	B	7	11/12	0.93	0.09	18,20,26,27	0
3	MAN	C	9	11/12	0.94	0.08	21,26,34,39	0
2	MAN	B	6	11/12	0.94	0.10	20,26,47,52	0
3	MAN	C	4	11/12	0.95	0.09	18,25,38,45	0
3	MAN	C	6	11/12	0.95	0.07	19,25,36,36	0
3	NAG	C	1	14/15	0.97	0.06	11,14,28,37	0
3	NAG	C	2	14/15	0.97	0.07	12,19,45,46	0
3	MAN	C	5	11/12	0.98	0.05	17,20,25,30	0
2	MAN	B	5	11/12	0.98	0.05	11,11,17,28	0
2	BMA	B	3	11/12	0.99	0.04	10,12,15,17	0
2	MAN	B	4	11/12	0.99	0.04	9,10,14,22	0
2	NAG	B	1	14/15	0.99	0.04	9,11,22,24	0
3	BMA	C	3	11/12	0.99	0.06	14,15,17,18	0
2	NAG	B	2	14/15	0.99	0.03	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.

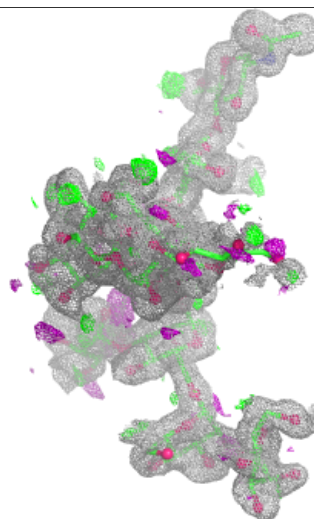
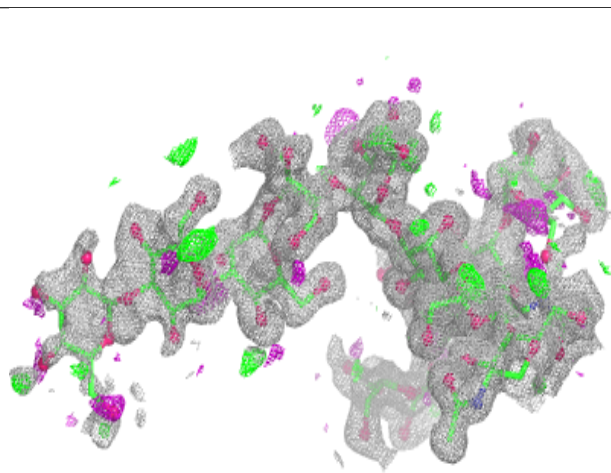
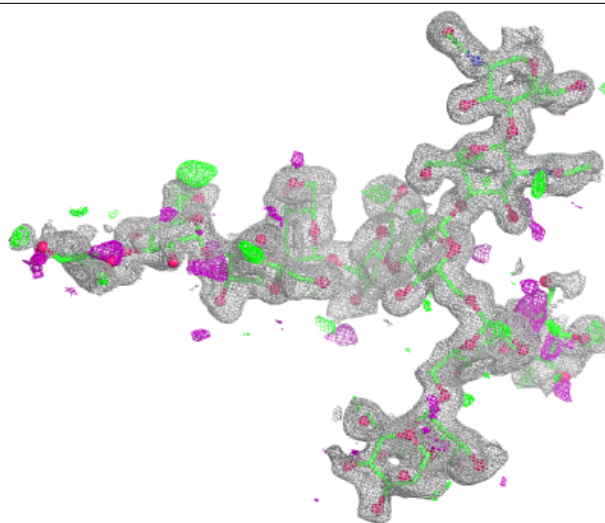
Electron density around Chain B:

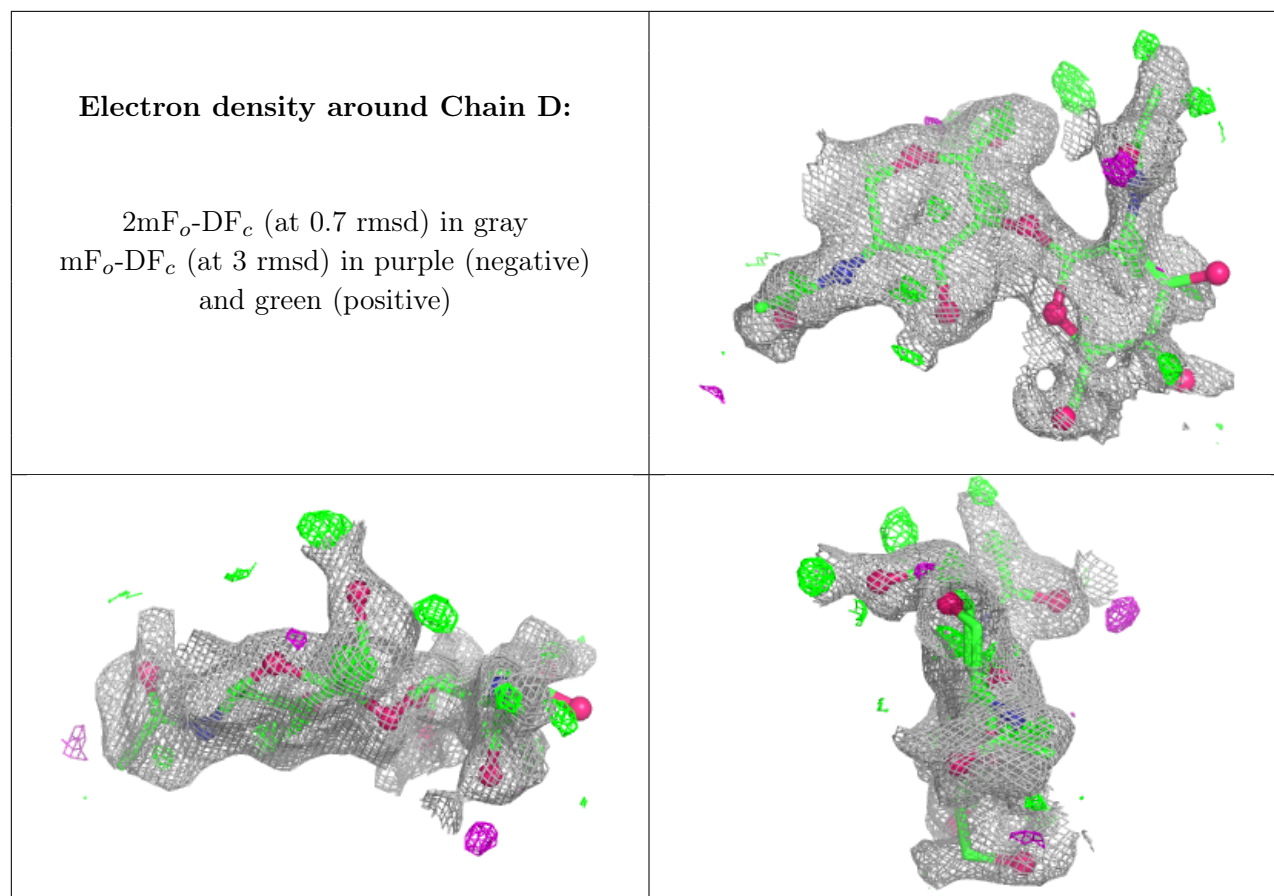
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	A	1049	6/6	0.86	0.15	23,48,51,59	0
5	NAG	A	1045	14/15	0.89	0.12	27,42,59,65	0
5	NAG	A	1044	14/15	0.91	0.10	23,35,50,55	0
6	GOL	A	1048	6/6	0.99	0.03	11,12,12,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.