



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:35 PM UTC

PDB ID : 5W0A / pdb_00005w0a
Title : Crystal structure of Trichoderma harzianum endoglucanase I
Authors : Godoy, A.S.; Pellegrini, V.O.A.; Sonoda, M.T.; Kadowaki, M.A.; Nascimento, A.S.; Polikarpov, I.
Deposited on : 2017-05-30
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

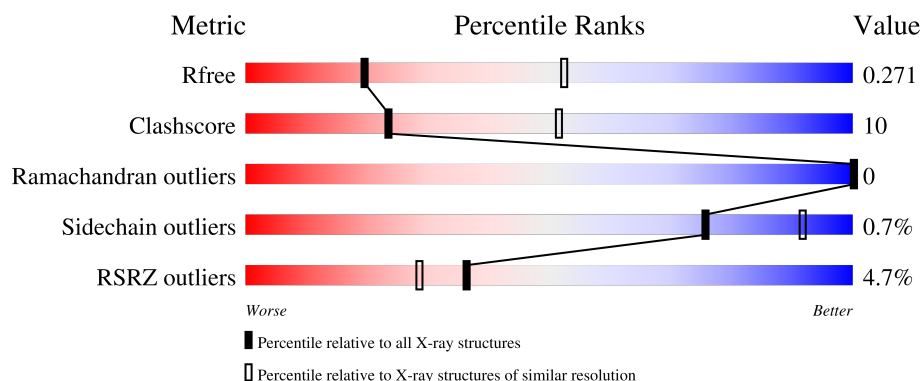
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	373	5% 77% 21% .
1	B	373	5% 75% 23% .
2	C	3	33% 67%
2	D	3	100%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	404	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5583 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 Glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2734	1676	466	568	24			
1	B	373	Total	C	N	O	S	0	0	0
			2730	1674	465	567	24			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	VAL	ALA	conflict	UNP A0A0F9XHQ5
A	87	SER	ASN	conflict	UNP A0A0F9XHQ5
A	91	MET	LEU	conflict	UNP A0A0F9XHQ5
A	99	SER	THR	conflict	UNP A0A0F9XHQ5
A	189	HIS	ASN	conflict	UNP A0A0F9XHQ5
A	231	ASN	SER	conflict	UNP A0A0F9XHQ5
A	294	PRO	SER	conflict	UNP A0A0F9XHQ5
A	296	ALA	GLY	conflict	UNP A0A0F9XHQ5
A	373	GLY	-	expression tag	UNP A0A0F9XHQ5
B	75	VAL	ALA	conflict	UNP A0A0F9XHQ5
B	87	SER	ASN	conflict	UNP A0A0F9XHQ5
B	91	MET	LEU	conflict	UNP A0A0F9XHQ5
B	99	SER	THR	conflict	UNP A0A0F9XHQ5
B	189	HIS	ASN	conflict	UNP A0A0F9XHQ5
B	231	ASN	SER	conflict	UNP A0A0F9XHQ5
B	294	PRO	SER	conflict	UNP A0A0F9XHQ5
B	296	ALA	GLY	conflict	UNP A0A0F9XHQ5
B	373	GLY	-	expression tag	UNP A0A0F9XHQ5

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



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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

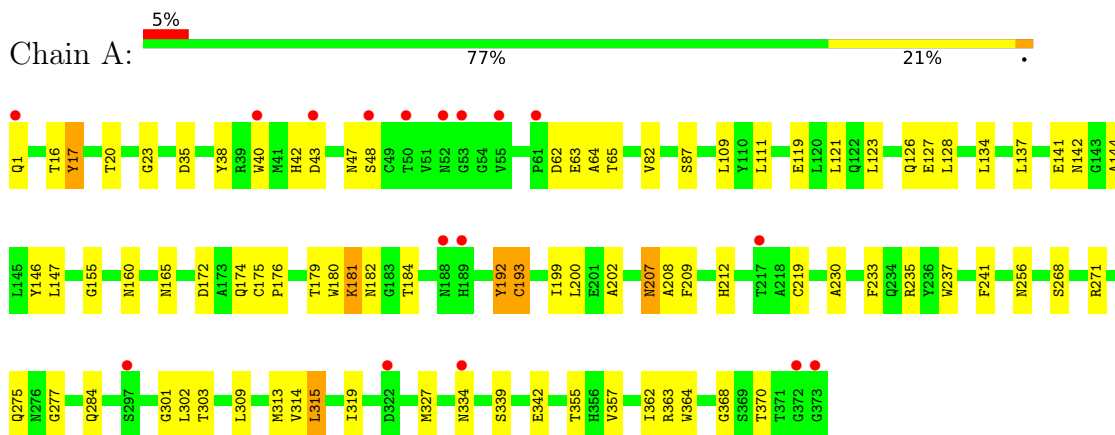
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	6	Total	O	0	0
			6	6		

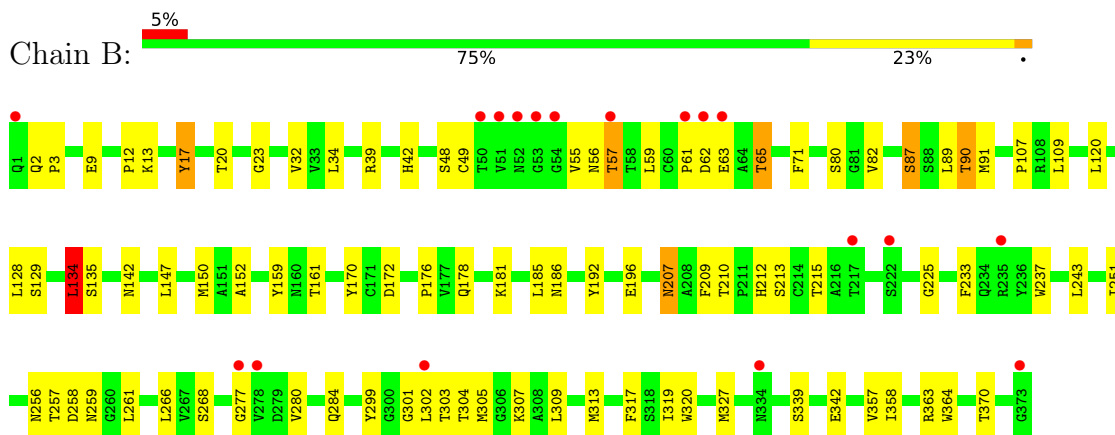
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glucanase



- Molecule 1: Glucanase



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



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

Chain D:  100%

MAG1
MAG2
BGLA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.58Å 99.33Å 114.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 2.90 29.82 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.82-2.90) 99.6 (29.82-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.11rc2_2531: ???)	Depositor
R, R_{free}	0.234 , 0.274 0.232 , 0.271	Depositor DCC
R_{free} test set	1938 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5583	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	1.13	28/2796 (1.0%)	0.80	5/3815 (0.1%)
1	B	0.77	9/2792 (0.3%)	0.75	2/3810 (0.1%)
All	All	0.97	37/5588 (0.7%)	0.78	7/7625 (0.1%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	CYS	C-O	-13.60	1.17	1.23
1	A	207	ASN	C-O	-10.19	1.11	1.23
1	A	17	TYR	C-O	-8.34	1.14	1.23
1	A	119	GLU	C-O	-8.09	1.14	1.24
1	A	315	LEU	C-O	-8.03	1.14	1.24
1	B	90	THR	C-O	-7.59	1.14	1.24
1	A	314	VAL	C-O	-7.56	1.15	1.24
1	A	192	TYR	C-O	-7.50	1.15	1.24
1	A	111	LEU	C-O	-7.47	1.14	1.24
1	A	165	ASN	CA-C	-7.43	1.42	1.52
1	A	155	GLY	C-O	-7.42	1.14	1.24
1	A	271	ARG	C-O	-7.42	1.15	1.24
1	A	208	ALA	C-O	-7.21	1.15	1.23
1	B	209	PHE	C-O	-7.07	1.15	1.24
1	A	175	CYS	CA-C	-6.96	1.47	1.53
1	A	175	CYS	N-CA	-6.95	1.41	1.46
1	A	209	PHE	C-O	-6.92	1.15	1.24
1	A	165	ASN	C-O	-6.78	1.15	1.24
1	A	181	LYS	C-O	-6.54	1.15	1.23
1	A	193	CYS	CA-C	-6.49	1.44	1.52
1	B	134	LEU	C-O	-6.49	1.14	1.24
1	B	17	TYR	C-O	-6.37	1.16	1.23
1	B	13	LYS	C-O	-6.37	1.16	1.24
1	A	277	GLY	C-O	-6.26	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	CYS	C-O	-6.25	1.16	1.23
1	A	172	ASP	C-O	-6.08	1.17	1.23
1	A	199	ILE	C-O	-6.04	1.16	1.24
1	B	207	ASN	C-O	-5.97	1.16	1.23
1	A	212	HIS	C-O	-5.93	1.17	1.24
1	B	49	CYS	C-O	-5.77	1.16	1.24
1	A	176	PRO	C-O	-5.63	1.17	1.23
1	B	277	GLY	C-O	-5.54	1.15	1.23
1	A	179	THR	C-O	-5.46	1.17	1.24
1	B	57	THR	C-O	-5.45	1.17	1.24
1	A	174	GLN	C-O	-5.23	1.17	1.24
1	A	275	GLN	CA-C	-5.23	1.45	1.52
1	A	119	GLU	N-CA	-5.01	1.40	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	GLU	N-CA-C	-6.37	105.55	113.38
1	A	175	CYS	CA-C-N	6.08	125.84	119.76
1	A	175	CYS	C-N-CA	6.08	125.84	119.76
1	A	64	ALA	N-CA-C	-6.05	103.33	112.04
1	B	65	THR	OG1-CB-CG2	5.94	121.18	109.30
1	B	87	SER	CB-CA-C	-5.84	99.50	110.01
1	A	207	ASN	N-CA-C	5.36	117.00	108.79

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	2734	0	2506	46	0
1	B	2730	0	2500	63	0
2	C	39	0	34	0	0
2	D	39	0	34	0	0
3	A	14	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	13	0	0
4	A	7	0	0	0	0
4	B	6	0	0	0	0
All	All	5583	0	5099	109	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 10.

All (109) 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:178:GLN:O	1:B:186:ASN:ND2	2.09	0.84
1:B:150:MET:HE3	1:B:170:TYR:HA	1.60	0.83
1:A:1:GLN:HE21	1:A:180:TRP:HE1	1.28	0.81
3:A:404:NAG:O7	3:A:404:NAG:O3	2.03	0.76
1:A:1:GLN:HB3	1:A:160:ASN:HA	1.67	0.76
1:B:17:TYR:HB2	1:B:363:ARG:HG2	1.71	0.73
1:B:9:GLU:OE1	1:B:39:ARG:NH2	2.22	0.71
1:A:1:GLN:OE1	1:A:1:GLN:N	2.19	0.71
1:B:56:ASN:HB3	1:B:59:LEU:HB2	1.72	0.70
1:A:1:GLN:NE2	1:A:180:TRP:HE1	1.90	0.69
1:A:17:TYR:HB2	1:A:363:ARG:HG2	1.74	0.69
1:A:207:ASN:ND2	1:A:237:TRP:CE3	2.62	0.67
1:B:34:LEU:O	1:B:39:ARG:NH1	2.28	0.67
1:B:9:GLU:CD	1:B:39:ARG:NH2	2.54	0.65
1:B:20:THR:OG1	1:B:23:GLY:N	2.28	0.65
1:B:305:MET:HE2	1:B:313:MET:HE1	1.79	0.65
1:A:137:LEU:HD11	1:A:357:VAL:HB	1.79	0.64
1:A:363:ARG:NH1	1:A:370:THR:O	2.29	0.64
1:A:1:GLN:NE2	1:A:180:TRP:NE1	2.45	0.64
1:A:1:GLN:HE21	1:A:180:TRP:NE1	1.96	0.64
1:A:128:LEU:HD12	1:A:364:TRP:HB3	1.81	0.62
1:A:233:PHE:CE1	1:A:284:GLN:HG2	2.34	0.61
1:B:304:THR:O	1:B:307:LYS:HG3	2.01	0.61
1:B:210:THR:HG1	1:B:212:HIS:HE2	1.49	0.60
1:A:137:LEU:HD23	1:A:355:THR:OG1	2.01	0.59
1:A:42:HIS:ND1	1:A:43:ASP:O	2.34	0.59
1:B:181:LYS:HB3	1:B:186:ASN:HB3	1.86	0.58
1:B:233:PHE:CE1	1:B:284:GLN:HG2	2.39	0.57
1:B:9:GLU:CD	1:B:39:ARG:HH21	2.12	0.56
1:B:90:THR:HG23	1:B:358:ILE:HG12	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:ARG:NH1	1:B:370:THR:O	2.35	0.56
1:A:142:ASN:O	1:A:319:ILE:HA	2.06	0.56
1:A:202:ALA:HB2	1:A:207:ASN:HB2	1.88	0.56
1:B:91:MET:HE1	1:B:317:PHE:HB3	1.89	0.55
1:B:62:ASP:OD1	1:B:65:THR:OG1	2.20	0.54
1:B:181:LYS:HG3	1:B:192:TYR:HB2	1.89	0.54
1:B:57:THR:HG22	1:B:57:THR:O	2.07	0.53
1:B:63:GLU:HG2	1:B:185:LEU:HB2	1.90	0.53
1:B:55:VAL:HG11	1:B:185:LEU:HD11	1.89	0.53
1:B:63:GLU:HG3	1:B:185:LEU:H	1.73	0.52
1:B:142:ASN:O	1:B:319:ILE:HA	2.10	0.52
1:B:258:ASP:OD1	1:B:259:ASN:N	2.41	0.51
1:B:339:SER:OG	1:B:342:GLU:HB2	2.09	0.51
1:A:42:HIS:HA	1:A:48:SER:HA	1.91	0.51
1:B:2:GLN:O	1:B:71:PHE:HA	2.11	0.51
1:B:305:MET:CE	1:B:313:MET:HE1	2.42	0.50
1:B:63:GLU:OE1	1:B:159:TYR:HB2	2.11	0.50
1:B:172:ASP:OD1	1:B:176:PRO:HD3	2.12	0.50
1:B:256:ASN:HB2	1:B:268:SER:OG	2.12	0.49
1:A:87:SER:H	1:B:87:SER:HB2	1.78	0.49
1:B:215:THR:HG23	1:B:299:TYR:HD1	1.77	0.49
1:A:20:THR:OG1	1:A:23:GLY:N	2.46	0.49
1:B:82:VAL:HG13	1:B:89:LEU:HD11	1.95	0.49
1:A:256:ASN:HB2	1:A:268:SER:OG	2.12	0.49
1:A:235:ARG:HA	1:A:241:PHE:CE2	2.49	0.48
1:A:35:ASP:HB3	1:A:38:TYR:CD1	2.48	0.48
1:A:182:ASN:HB2	1:A:192:TYR:CE2	2.49	0.47
1:B:2:GLN:HG3	1:B:3:PRO:HD2	1.95	0.47
1:A:16:THR:HG22	1:A:362:ILE:HB	1.96	0.47
1:B:80:SER:O	1:B:107:PRO:HG3	2.14	0.47
1:A:137:LEU:HD22	1:A:141:GLU:HG2	1.97	0.47
1:B:266:LEU:O	1:B:302:LEU:HD23	2.14	0.46
1:B:299:TYR:O	1:B:304:THR:HG21	2.16	0.46
1:A:147:LEU:HB2	1:A:313:MET:HE3	1.98	0.46
1:A:235:ARG:NH1	1:A:235:ARG:HB3	2.30	0.46
1:A:62:ASP:HB2	1:A:65:THR:OG1	2.15	0.45
1:A:144:ALA:HA	1:A:200:LEU:O	2.16	0.45
1:B:61:PRO:HD2	1:B:65:THR:HG21	1.97	0.45
1:B:210:THR:HG22	1:B:225:GLY:HA2	1.97	0.45
1:B:305:MET:HE3	1:B:305:MET:HA	1.97	0.45
1:B:134:LEU:O	1:B:135:SER:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:PHE:CZ	1:B:284:GLN:HG2	2.51	0.45
1:B:309:LEU:HG	1:B:313:MET:HE3	1.97	0.45
1:B:320:TRP:CZ3	1:B:327:MET:HE1	2.52	0.45
1:A:123:LEU:HA	1:A:126:GLN:HB2	1.99	0.45
1:B:128:LEU:HD12	1:B:364:TRP:HB3	1.99	0.44
1:B:120:LEU:HD11	1:B:152:ALA:HB2	1.98	0.44
1:A:127:GLU:CD	1:A:368:GLY:H	2.26	0.44
1:B:129:SER:HA	1:B:251:ILE:O	2.17	0.44
1:A:147:LEU:CB	1:A:313:MET:HE3	2.48	0.44
1:B:172:ASP:HB2	1:B:196:GLU:OE2	2.18	0.43
1:A:40:TRP:CZ2	1:A:42:HIS:HB3	2.52	0.43
1:A:142:ASN:HB2	1:A:327:MET:HE3	2.00	0.43
1:B:237:TRP:CD1	1:B:237:TRP:C	2.97	0.43
1:A:43:ASP:HB2	1:A:47:ASN:O	2.19	0.43
1:A:301:GLY:C	1:A:303:THR:H	2.27	0.42
1:B:213:SER:HB3	1:B:304:THR:OG1	2.19	0.42
1:A:309:LEU:HD23	1:A:313:MET:HE2	2.02	0.42
1:B:147:LEU:HB3	1:B:313:MET:HB2	2.01	0.42
1:A:193:CYS:HB3	1:A:219:CYS:SG	2.59	0.42
1:A:339:SER:HB2	1:A:342:GLU:H	1.84	0.42
1:B:61:PRO:HD2	1:B:65:THR:CG2	2.49	0.42
1:B:243:LEU:HD12	1:B:280:VAL:HG21	2.02	0.41
1:A:146:TYR:O	1:A:315:LEU:HD12	2.20	0.41
1:A:230:ALA:HA	1:A:334:ASN:O	2.21	0.41
1:A:82:VAL:HG21	1:A:109:LEU:HD21	2.01	0.41
1:B:12:PRO:HG2	1:B:32:VAL:CG2	2.51	0.41
1:B:61:PRO:HG2	1:B:65:THR:HG21	2.03	0.41
1:B:257:THR:HG21	1:B:261:LEU:O	2.21	0.41
1:B:301:GLY:C	1:B:303:THR:H	2.28	0.41
1:B:59:LEU:HA	1:B:59:LEU:HD23	1.76	0.41
1:B:91:MET:HB2	1:B:357:VAL:HG12	2.01	0.41
1:B:42:HIS:HA	1:B:48:SER:HA	2.03	0.41
1:B:82:VAL:HG21	1:B:109:LEU:HD21	2.03	0.41
1:A:121:LEU:HD22	1:A:364:TRP:CZ2	2.55	0.41
1:B:2:GLN:HG3	1:B:161:THR:OG1	2.21	0.41
1:A:123:LEU:HB2	1:A:309:LEU:HD22	2.02	0.40
1:A:302:LEU:HD12	1:A:302:LEU:HA	1.90	0.40
1:A:181:LYS:HG3	1:A:192:TYR:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	371/373 (100%)	364 (98%)	7 (2%)	0	100	100
1	B	371/373 (100%)	359 (97%)	12 (3%)	0	100	100
All	All	742/746 (100%)	723 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/300 (100%)	297 (99%)	2 (1%)	76	92
1	B	298/300 (99%)	296 (99%)	2 (1%)	76	92
All	All	597/600 (100%)	593 (99%)	4 (1%)	76	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	LEU
1	A	184	THR
1	B	134	LEU
1	B	207	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	188	ASN
1	A	189	HIS
1	A	231	ASN
1	A	234	GLN
1	A	284	GLN
1	A	352	ASN
1	B	28	GLN
1	B	231	ASN
1	B	284	GLN
1	B	351	ASN

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 ⓘ

6 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	2,1	14,14,15	2.55	3 (21%)	17,19,21	1.54	3 (17%)
2	NAG	C	2	2	14,14,15	0.49	0	17,19,21	0.60	0
2	BMA	C	3	2	11,11,12	0.95	0	15,15,17	1.35	2 (13%)
2	NAG	D	1	2,1	14,14,15	2.15	6 (42%)	17,19,21	2.11	2 (11%)
2	NAG	D	2	2	14,14,15	1.93	3 (21%)	17,19,21	3.41	9 (52%)
2	BMA	D	3	2	11,11,12	0.88	0	15,15,17	1.67	1 (6%)

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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
2	BMA	D	3	2	-	1/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	C1-C2	6.80	1.61	1.52
2	C	1	NAG	O5-C1	-5.84	1.33	1.43
2	D	2	NAG	O5-C1	-4.58	1.36	1.43
2	D	1	NAG	O5-C1	-3.50	1.37	1.43
2	D	1	NAG	O7-C7	-3.44	1.15	1.23
2	D	1	NAG	C8-C7	-3.38	1.43	1.50
2	C	1	NAG	C3-C2	3.03	1.58	1.52
2	D	2	NAG	O7-C7	-2.95	1.16	1.23
2	D	2	NAG	C1-C2	-2.78	1.48	1.52
2	D	1	NAG	O5-C5	-2.74	1.38	1.43
2	D	1	NAG	C7-N2	-2.62	1.25	1.34
2	D	1	NAG	C2-N2	-2.50	1.42	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	O5-C1-C2	-7.71	99.36	111.29
2	D	1	NAG	O5-C1-C2	-7.38	99.87	111.29
2	D	2	NAG	C2-N2-C7	6.43	131.51	122.90
2	D	2	NAG	C1-C2-N2	-6.09	100.83	110.43
2	D	3	BMA	C1-O5-C5	5.17	119.11	112.19
2	C	1	NAG	C4-C3-C2	4.74	117.97	111.02
2	D	2	NAG	C1-O5-C5	4.50	118.22	112.19
2	D	2	NAG	C3-C4-C5	-3.47	103.94	110.23
2	C	3	BMA	C1-O5-C5	3.00	116.20	112.19
2	D	2	NAG	C8-C7-N2	2.67	120.55	116.12
2	D	2	NAG	O3-C3-C4	-2.55	104.38	110.38
2	D	2	NAG	O3-C3-C2	2.50	114.59	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C5-C4	-2.46	104.83	110.83
2	D	2	NAG	O7-C7-N2	-2.44	117.66	121.98
2	C	3	BMA	O5-C5-C6	-2.21	103.36	107.66
2	C	1	NAG	C1-O5-C5	-2.17	109.28	112.19
2	D	1	NAG	O3-C3-C4	-2.09	105.45	110.38

There are no chirality outliers.

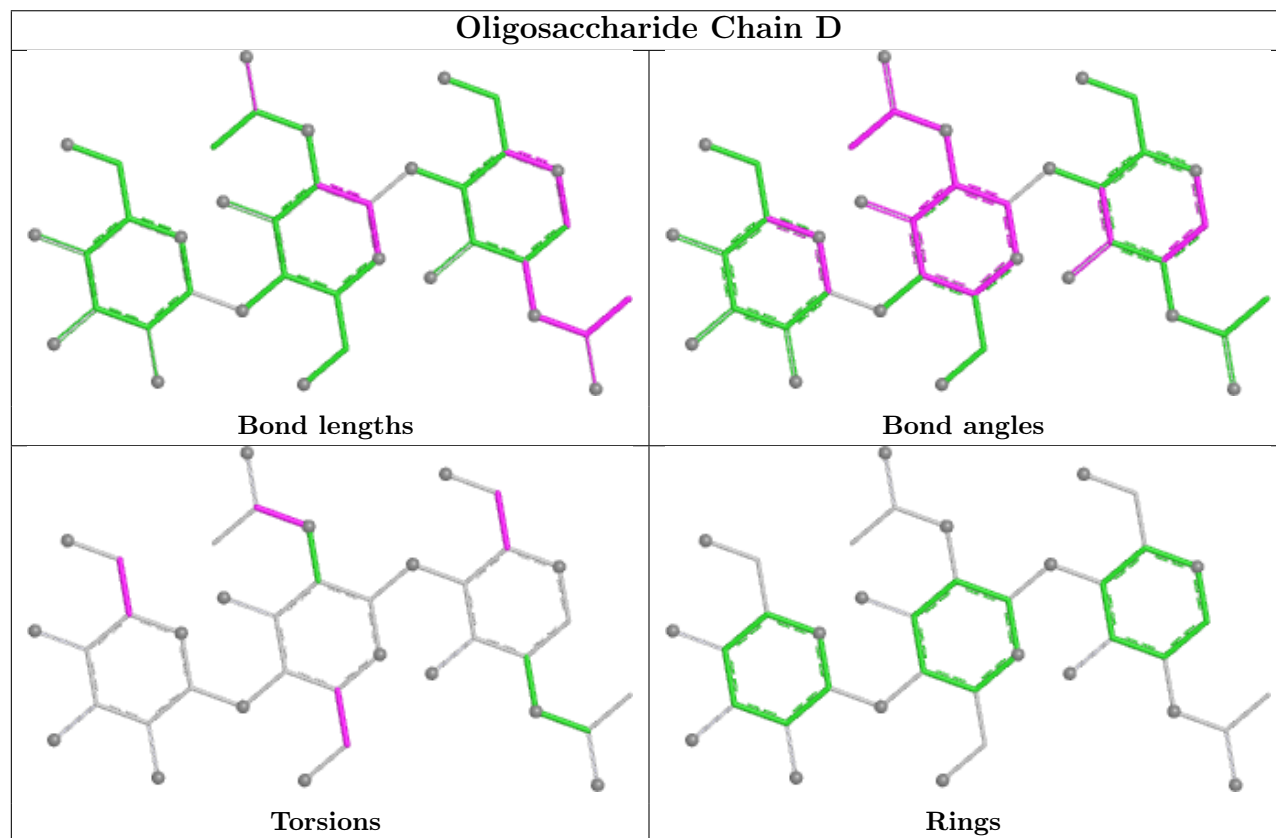
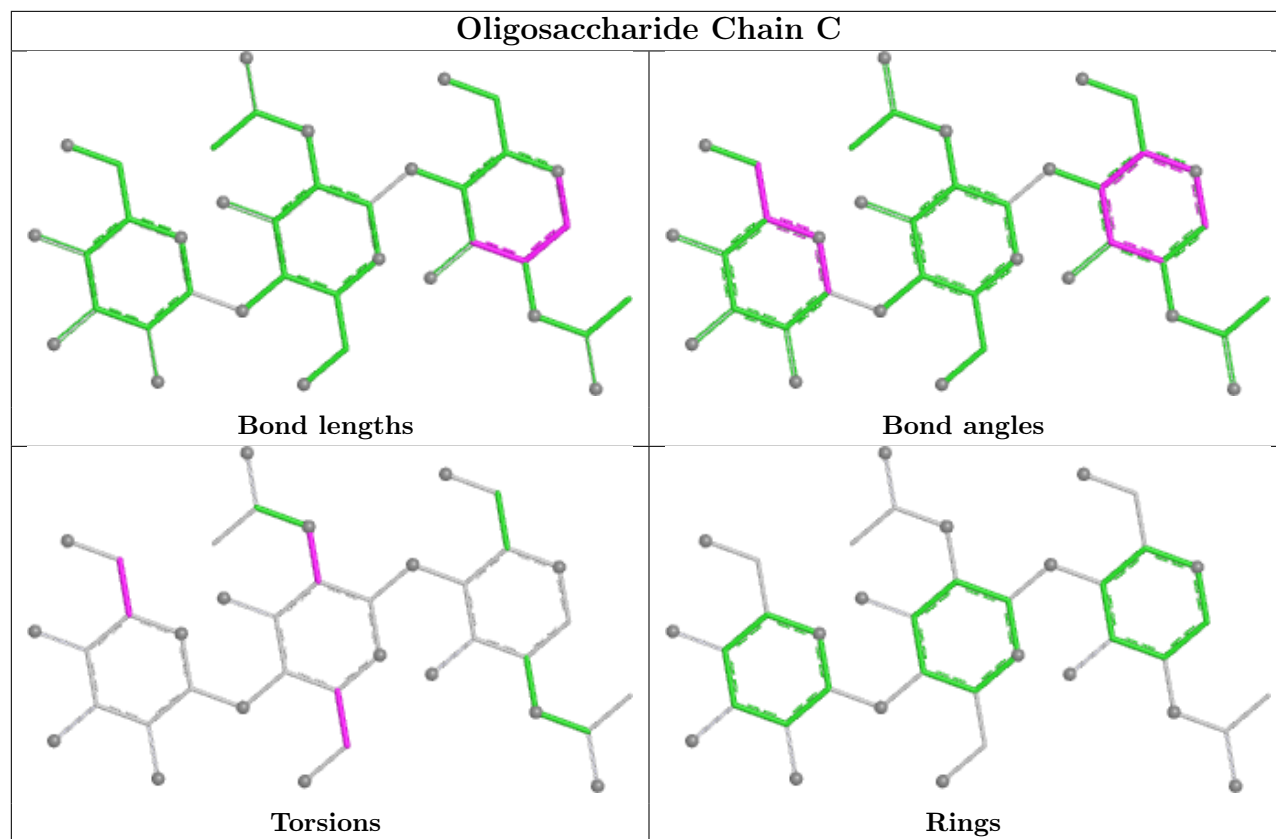
All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	C	3	BMA	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry

2 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	$\# Z > 2$
3	NAG	B	401	1	14,14,15	1.05	2 (14%)	17,19,21	2.88	8 (47%)
3	NAG	A	404	1	14,14,15	2.41	10 (71%)	17,19,21	2.63	10 (58%)

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
3	NAG	B	401	1	-	1/6/23/26	0/1/1/1
3	NAG	A	404	1	-	5/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	404	NAG	O7-C7	-3.46	1.15	1.23
3	A	404	NAG	C4-C5	-3.38	1.45	1.53
3	A	404	NAG	C7-N2	-2.81	1.25	1.34
3	A	404	NAG	C1-C2	-2.75	1.48	1.52
3	A	404	NAG	C2-N2	-2.61	1.41	1.46
3	A	404	NAG	C3-C2	-2.57	1.47	1.52
3	A	404	NAG	O5-C1	-2.49	1.39	1.43
3	A	404	NAG	O5-C5	-2.34	1.38	1.43
3	A	404	NAG	C8-C7	-2.24	1.45	1.50
3	A	404	NAG	O3-C3	-2.23	1.37	1.43
3	B	401	NAG	O7-C7	-2.18	1.18	1.23
3	B	401	NAG	C1-C2	-2.09	1.49	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	NAG	O5-C1-C2	6.77	121.76	111.29
3	B	401	NAG	C1-O5-C5	6.64	121.08	112.19
3	A	404	NAG	C2-N2-C7	4.88	129.44	122.90
3	A	404	NAG	O5-C1-C2	-4.42	104.45	111.29
3	A	404	NAG	C1-O5-C5	4.40	118.08	112.19
3	B	401	NAG	O3-C3-C4	-2.89	103.57	110.38
3	A	404	NAG	C3-C4-C5	-2.88	105.00	110.23
3	A	404	NAG	C4-C3-C2	-2.87	106.81	111.02
3	B	401	NAG	C1-C2-N2	-2.85	105.93	110.43
3	B	401	NAG	C4-C3-C2	2.81	115.13	111.02
3	B	401	NAG	O3-C3-C2	-2.80	103.58	109.40
3	A	404	NAG	O4-C4-C5	-2.69	102.70	109.32
3	B	401	NAG	C2-N2-C7	2.48	126.22	122.90
3	A	404	NAG	O5-C5-C6	2.47	112.48	107.66
3	A	404	NAG	O7-C7-N2	-2.35	117.82	121.98
3	A	404	NAG	C1-C2-N2	-2.18	106.99	110.43
3	B	401	NAG	O4-C4-C5	2.08	114.44	109.32
3	A	404	NAG	C6-C5-C4	-2.02	108.05	113.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	NAG	C3-C2-N2-C7
3	B	401	NAG	C1-C2-N2-C7
3	A	404	NAG	O5-C5-C6-O6
3	A	404	NAG	C8-C7-N2-C2
3	A	404	NAG	C4-C5-C6-O6
3	A	404	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	373/373 (100%)	0.29	17 (4%) 37 29	6, 16, 41, 62	0
1	B	373/373 (100%)	0.43	18 (4%) 35 28	7, 20, 40, 61	0
All	All	746/746 (100%)	0.36	35 (4%) 36 28	6, 18, 40, 62	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	GLY	4.4
1	B	51	VAL	3.6
1	A	1	GLN	3.4
1	B	373	GLY	3.1
1	B	277	GLY	3.1
1	A	48	SER	2.9
1	B	222	SER	2.9
1	B	334	ASN	2.8
1	B	217	THR	2.8
1	A	188	ASN	2.7
1	B	52	ASN	2.7
1	A	334	ASN	2.7
1	B	57	THR	2.6
1	A	43	ASP	2.6
1	A	297	SER	2.6
1	A	372	GLY	2.6
1	B	53	GLY	2.6
1	B	61	PRO	2.6
1	A	40	TRP	2.5
1	A	217	THR	2.5
1	B	62	ASP	2.4
1	A	373	GLY	2.4
1	A	53	GLY	2.3
1	B	1	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	63	GLU	2.2
1	A	52	ASN	2.2
1	B	278	VAL	2.2
1	A	50	THR	2.2
1	A	61	PRO	2.1
1	B	50	THR	2.1
1	B	235	ARG	2.1
1	A	55	VAL	2.1
1	A	189	HIS	2.1
1	B	302	LEU	2.1
1	A	322	ASP	2.1

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

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

6.3 Carbohydrates ⓘ

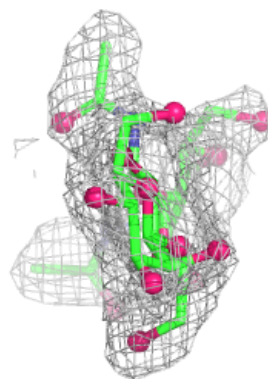
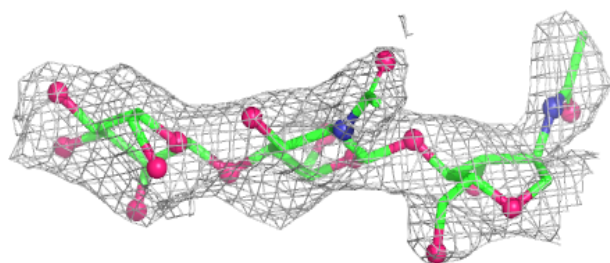
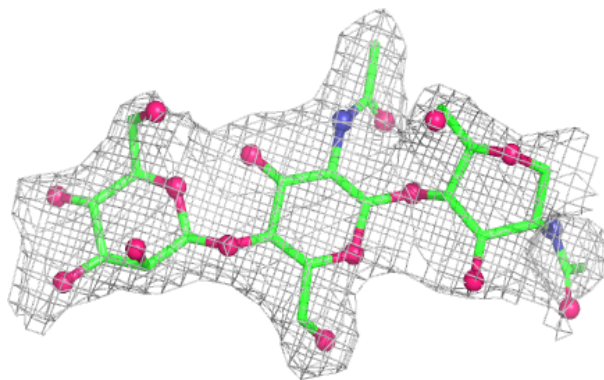
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	1	14/15	0.79	0.16	33,40,49,53	0
2	NAG	C	2	14/15	0.81	0.13	29,32,38,41	0
2	BMA	C	3	11/12	0.86	0.13	22,26,32,37	0
2	NAG	D	2	14/15	0.89	0.11	11,16,19,20	0
2	BMA	D	3	11/12	0.89	0.12	17,18,22,25	0
2	NAG	D	1	14/15	0.95	0.07	10,13,16,17	0

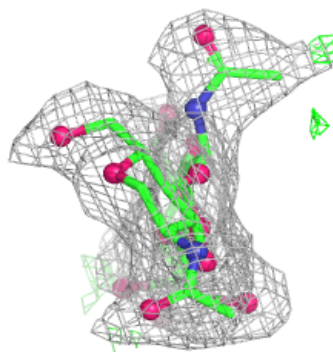
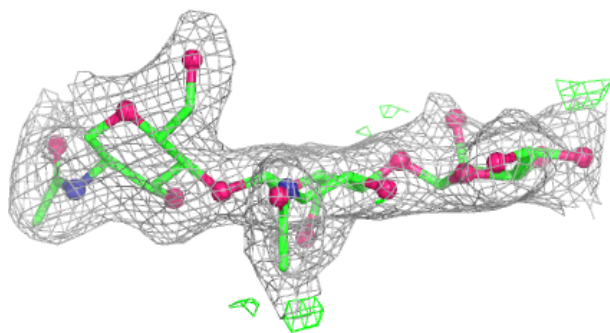
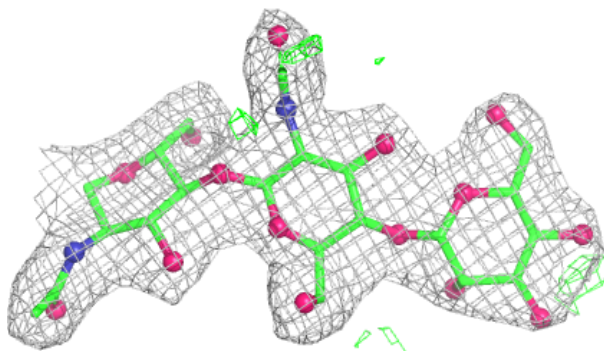
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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($\text{\AA}^2$)	Q<0.9
3	NAG	B	401	14/15	0.58	0.19	39,52,60,61	0
3	NAG	A	404	14/15	0.84	0.14	12,20,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.