



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:37 PM UTC

PDB ID : 2Z8G / pdb_00002z8g
Title : Aspergillus niger ATCC9642 isopullulanase complexed with isopanose
Authors : Mizuno, M.; Koide, A.; Yamamura, A.; Akeboshi, H.; Yoshida, H.; Kamitori, S.; Sakano, Y.; Nishikawa, A.; Tonozuka, T.
Deposited on : 2007-09-05
Resolution : 1.70 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

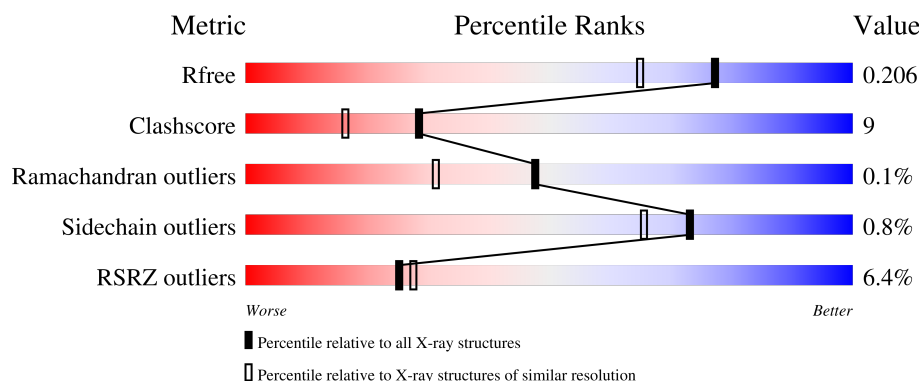
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	549	5% 83% 16% .
1	B	549	7% 81% 18% .
2	C	3	67% 33%
2	D	3	67% 33%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10037 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 Isopullulanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4242	2676	710	845	11			
1	B	549	Total	C	N	O	S	0	0	0
			4242	2676	710	845	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ARG	-	expression tag	UNP O00105
A	17	GLU	-	expression tag	UNP O00105
A	18	PHE	-	expression tag	UNP O00105
A	19	MET	-	expression tag	UNP O00105
B	16	ARG	-	expression tag	UNP O00105
B	17	GLU	-	expression tag	UNP O00105
B	18	PHE	-	expression tag	UNP O00105
B	19	MET	-	expression tag	UNP O00105

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-6)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			34	18	16			
2	D	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

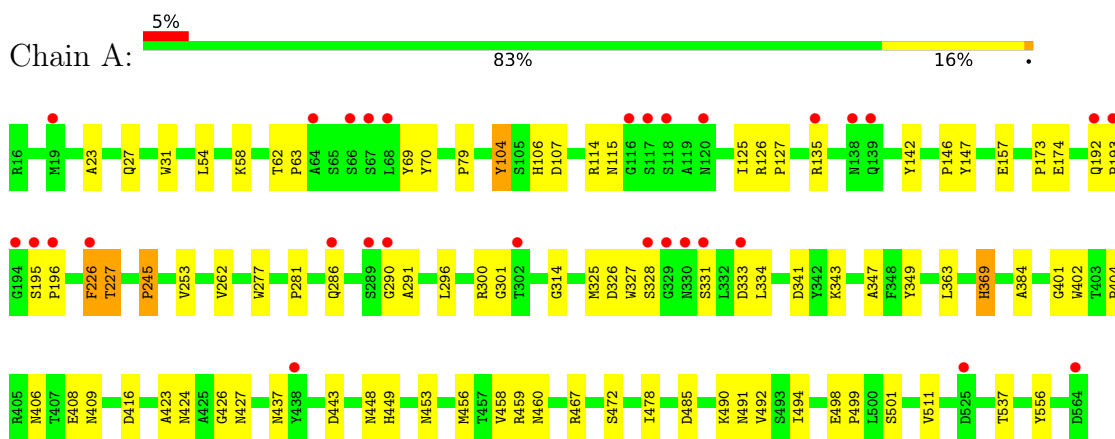
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	645	Total	O	0	0
			645	645		
4	B	518	Total	O	0	0
			518	518		

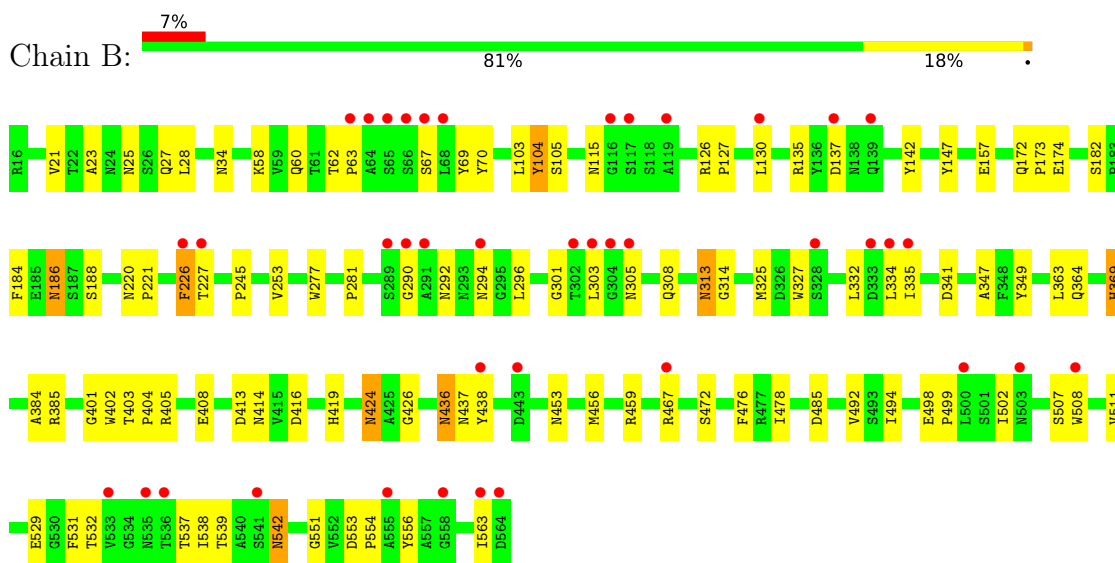
3 Residue-property plots [i](#)

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: Isopullulanase



- Molecule 1: Isopullulanase



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-6)-beta-D-glucopyranos e





- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-6)-beta-D-glucopyranose

Chain D:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.67Å 99.39Å 134.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.69 – 1.70 49.69 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.69-1.70) 99.2 (49.69-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 1.70Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.187 , 0.211 0.182 , 0.206	Depositor DCC
R_{free} test set	12328 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtrriage
Anisotropy	0.213	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10037	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.0029e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NAG, GLC, BGC

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	0.35	0/4357	0.92	14/5962 (0.2%)
1	B	0.34	0/4357	0.90	7/5962 (0.1%)
All	All	0.34	0/8714	0.91	21/11924 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	PHE	N-CA-C	-7.42	94.99	110.80
1	A	369	HIS	N-CA-C	-7.29	96.64	108.52
1	B	369	HIS	N-CA-C	-6.88	97.30	108.52
1	B	226	PHE	N-CA-C	-6.82	96.27	110.80
1	A	253	VAL	N-CA-C	6.31	117.38	108.36
1	B	478	ILE	N-CA-C	6.25	116.87	107.80
1	A	245	PRO	N-CA-C	-6.04	101.72	111.03
1	A	478	ILE	N-CA-C	6.02	116.53	107.80
1	B	245	PRO	N-CA-C	-6.02	101.76	111.03
1	B	174	GLU	N-CA-C	-5.99	104.68	112.23
1	A	174	GLU	N-CA-C	-5.96	104.72	112.23
1	A	325	MET	N-CA-C	5.87	118.07	108.55
1	B	253	VAL	N-CA-C	5.79	116.64	108.36
1	B	325	MET	N-CA-C	5.75	117.87	108.55
1	A	227	THR	N-CA-C	-5.63	98.80	110.80
1	A	458	VAL	N-CA-C	-5.39	100.12	107.99
1	A	286	GLN	N-CA-C	-5.33	103.66	110.53
1	A	262	VAL	N-CA-C	-5.29	100.58	108.46
1	A	406	ASN	N-CA-C	-5.09	99.49	108.20
1	A	501	SER	N-CA-C	5.03	117.42	111.33
1	A	114	ARG	N-CA-C	-5.01	101.93	109.85

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	4242	0	3978	59	0
1	B	4242	0	3979	91	0
2	C	34	0	30	0	0
2	D	34	0	30	0	0
3	A	168	0	156	7	0
3	B	154	0	143	6	0
4	A	645	0	0	6	0
4	B	518	0	0	5	0
All	All	10037	0	8316	152	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 9.

All (152) 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:25:ASN:HD22	1:B:27:GLN:H	1.08	0.96
1:B:539:THR:H	1:B:542:ASN:HD21	1.27	0.80
1:A:226:PHE:O	1:A:227:THR:HG23	1.82	0.79
1:B:226:PHE:O	1:B:227:THR:HG23	1.84	0.76
1:B:539:THR:H	1:B:542:ASN:ND2	1.83	0.75
1:B:436:ASN:HD22	1:B:437:ASN:H	1.33	0.75
1:A:347:ALA:H	1:A:369:HIS:HD2	1.34	0.75
1:A:192:GLN:HB3	1:A:193:PRO:HD2	1.69	0.74
1:B:25:ASN:ND2	1:B:27:GLN:H	1.85	0.74
1:B:347:ALA:H	1:B:369:HIS:HD2	1.34	0.72
1:B:303:LEU:HD21	1:B:334:LEU:HB2	1.71	0.71
1:B:186:ASN:C	1:B:186:ASN:HD22	1.99	0.71
1:B:303:LEU:HD22	1:B:335:ILE:HG13	1.72	0.69
1:B:157:GLU:OE2	1:B:419:HIS:HE1	1.75	0.69
1:A:404:PRO:HB2	1:A:456:MET:HE3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ASN:ND2	1:B:437:ASN:H	1.91	0.68
1:B:135:ARG:HG2	1:B:142:TYR:HB2	1.76	0.67
1:B:308:GLN:NE2	1:B:327:TRP:HE1	1.92	0.67
1:A:146:PRO:HG3	4:A:1290:HOH:O	1.95	0.66
1:A:135:ARG:HG2	1:A:142:TYR:HB2	1.76	0.66
1:A:331:SER:HB3	1:A:333:ASP:OD1	1.97	0.65
1:B:404:PRO:HB2	1:B:456:MET:HE3	1.78	0.64
1:A:423:ALA:H	1:A:427:ASN:ND2	1.96	0.63
1:B:308:GLN:HE21	1:B:327:TRP:HE1	1.45	0.63
1:B:414:ASN:ND2	1:B:467:ARG:HH12	1.96	0.63
1:B:25:ASN:ND2	1:B:28:LEU:H	1.97	0.62
1:B:127:PRO:HG2	1:B:130:LEU:HD13	1.82	0.62
1:B:127:PRO:HG2	1:B:130:LEU:CD1	2.30	0.61
1:B:34:ASN:HB2	4:B:1355:HOH:O	2.01	0.59
1:A:226:PHE:O	1:A:227:THR:CG2	2.49	0.59
1:A:460:ASN:ND2	3:A:1007:NAG:H83	2.18	0.59
1:B:226:PHE:O	1:B:227:THR:CG2	2.51	0.59
1:B:23:ALA:HB2	1:B:70:TYR:CG	2.39	0.58
1:B:542:ASN:C	1:B:542:ASN:HD22	2.12	0.58
1:B:498:GLU:HB3	1:B:499:PRO:HD2	1.85	0.57
1:A:424:ASN:H	1:A:427:ASN:ND2	2.02	0.56
1:B:538:ILE:HA	1:B:542:ASN:HD21	1.70	0.56
1:A:192:GLN:HG2	4:A:1366:HOH:O	2.06	0.56
1:A:453:ASN:ND2	1:A:456:MET:HE2	2.21	0.56
1:A:23:ALA:HB2	1:A:70:TYR:CG	2.42	0.55
1:B:437:ASN:HD22	1:B:437:ASN:C	2.14	0.55
1:B:115:ASN:ND2	3:B:1002:NAG:H82	2.22	0.55
1:B:539:THR:N	1:B:542:ASN:HD21	2.01	0.55
1:A:62:THR:HB	1:A:63:PRO:HA	1.90	0.54
1:B:529:GLU:HB2	1:B:563:ILE:HB	1.90	0.54
1:A:424:ASN:HD22	1:A:426:GLY:H	1.56	0.54
1:A:126:ARG:HA	1:A:127:PRO:C	2.33	0.54
1:A:453:ASN:ND2	3:A:1011:NAG:H83	2.23	0.54
1:B:332:LEU:HD12	1:B:332:LEU:N	2.22	0.53
1:B:332:LEU:HD13	4:B:1204:HOH:O	2.07	0.53
1:A:347:ALA:H	1:A:369:HIS:CD2	2.23	0.53
1:A:300:ARG:HD2	1:A:326:ASP:O	2.08	0.53
1:A:437:ASN:HD22	1:A:437:ASN:C	2.16	0.53
1:B:127:PRO:HB3	1:B:416:ASP:OD2	2.08	0.53
1:A:423:ALA:H	1:A:427:ASN:HD22	1.57	0.53
1:A:424:ASN:HD22	1:A:426:GLY:N	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ASN:HD22	1:B:437:ASN:N	2.04	0.53
1:B:424:ASN:HD22	1:B:426:GLY:N	2.06	0.52
1:A:79:PRO:HG2	4:A:1543:HOH:O	2.08	0.52
1:B:104:TYR:CE2	1:B:147:TYR:HA	2.46	0.51
1:B:453:ASN:HA	3:B:1008:NAG:H82	1.92	0.51
1:B:327:TRP:CD1	1:B:335:ILE:HD13	2.46	0.51
3:B:1003:NAG:O3	3:B:1003:NAG:H83	2.11	0.50
1:A:460:ASN:CG	3:A:1007:NAG:H83	2.36	0.50
1:A:498:GLU:HB3	1:A:499:PRO:HD2	1.94	0.50
1:A:125:ILE:N	1:A:125:ILE:HD12	2.27	0.50
1:B:62:THR:HB	1:B:63:PRO:HA	1.93	0.49
1:A:157:GLU:HB3	1:A:173:PRO:HG3	1.94	0.49
1:A:363:LEU:O	1:A:384:ALA:HA	2.12	0.49
1:B:424:ASN:HD22	1:B:426:GLY:H	1.60	0.49
1:B:172:GLN:HG2	1:B:419:HIS:CD2	2.47	0.49
1:B:437:ASN:HD22	1:B:438:TYR:N	2.09	0.49
1:B:553:ASP:CG	1:B:554:PRO:HD2	2.38	0.49
1:B:58:LYS:HB3	1:B:69:TYR:HB3	1.95	0.49
1:B:126:ARG:HA	1:B:127:PRO:C	2.39	0.48
1:A:281:PRO:HG3	1:A:296:LEU:HD13	1.96	0.48
1:B:157:GLU:HB3	1:B:173:PRO:HG3	1.96	0.48
1:B:459:ARG:HA	1:B:485:ASP:O	2.13	0.48
1:B:499:PRO:O	1:B:502:ILE:HG12	2.14	0.47
1:A:467:ARG:HD2	4:A:1343:HOH:O	2.13	0.47
1:B:103:LEU:HA	1:B:182:SER:O	2.14	0.47
1:B:414:ASN:HD22	1:B:467:ARG:HH12	1.61	0.47
1:B:508:TRP:HB3	1:B:551:GLY:HA3	1.96	0.47
1:A:127:PRO:HB3	1:A:416:ASP:OD2	2.14	0.47
1:A:314:GLY:HA2	1:A:341:ASP:O	2.14	0.47
1:A:449:HIS:HD2	4:A:1078:HOH:O	1.98	0.47
3:A:1005:NAG:H62	1:B:184:PHE:CD1	2.49	0.47
1:B:301:GLY:HA3	1:B:327:TRP:CE2	2.49	0.47
1:B:419:HIS:HD2	4:B:1322:HOH:O	1.98	0.47
1:A:58:LYS:HB3	1:A:69:TYR:HB3	1.97	0.47
1:A:104:TYR:CE2	1:A:147:TYR:HA	2.50	0.46
1:A:54:LEU:HD11	3:A:1002:NAG:H61	1.97	0.46
1:A:277:TRP:CD1	1:A:349:TYR:HB3	2.51	0.46
1:B:472:SER:HB3	1:B:494:ILE:HG23	1.96	0.46
1:B:186:ASN:ND2	1:B:188:SER:H	2.14	0.46
1:B:511:VAL:HA	1:B:556:TYR:CE1	2.50	0.46
1:B:21:VAL:O	1:B:21:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ALA:N	1:A:369:HIS:HD2	2.09	0.45
1:B:281:PRO:HG3	1:B:296:LEU:HD13	1.97	0.45
1:B:459:ARG:NH1	1:B:485:ASP:OD2	2.41	0.45
1:B:532:THR:HG22	1:B:537:THR:HA	1.99	0.45
1:A:448:ASN:CG	3:A:1006:NAG:H82	2.42	0.45
1:B:363:LEU:O	1:B:384:ALA:HA	2.17	0.45
1:A:27:GLN:NE2	3:B:1005:NAG:O3	2.49	0.45
1:A:290:GLY:O	1:A:291:ALA:C	2.59	0.45
1:B:303:LEU:HD22	1:B:335:ILE:CG1	2.43	0.45
1:A:472:SER:HB3	1:A:494:ILE:HG23	1.99	0.44
1:A:106:HIS:HD2	1:A:107:ASP:O	1.99	0.44
1:A:31:TRP:CZ3	1:A:245:PRO:HB3	2.53	0.44
1:A:300:ARG:NE	1:A:328:SER:OG	2.48	0.44
1:A:490:LYS:O	1:A:491:ASN:HB2	2.16	0.44
1:A:492:VAL:HG13	1:A:492:VAL:O	2.18	0.44
1:B:115:ASN:CG	3:B:1002:NAG:H82	2.43	0.44
1:B:277:TRP:CD1	1:B:349:TYR:HB3	2.52	0.44
1:B:290:GLY:O	1:B:292:ASN:N	2.42	0.44
1:B:369:HIS:HE1	4:B:1321:HOH:O	2.00	0.44
1:A:195:SER:OG	1:A:196:PRO:HD2	2.18	0.43
1:A:343:LYS:HD2	1:A:343:LYS:N	2.33	0.43
1:B:314:GLY:HA2	1:B:341:ASP:O	2.17	0.43
1:B:453:ASN:ND2	1:B:456:MET:HE2	2.33	0.43
1:A:511:VAL:HA	1:A:556:TYR:CE1	2.54	0.43
1:B:60:GLN:NE2	1:B:67:SER:OG	2.52	0.43
1:B:313:ASN:C	1:B:313:ASN:HD22	2.26	0.43
1:B:305:ASN:ND2	3:B:1005:NAG:H82	2.33	0.43
1:A:401:GLY:O	1:A:402:TRP:HB2	2.18	0.43
1:B:220:ASN:HB3	1:B:221:PRO:HD2	2.01	0.42
1:B:294:ASN:HB2	4:B:1337:HOH:O	2.18	0.42
1:B:385:ARG:HA	1:B:413:ASP:O	2.18	0.42
1:B:137:ASP:HB3	1:B:142:TYR:HE2	1.85	0.42
1:B:403:THR:O	1:B:405:ARG:HG3	2.20	0.42
1:B:542:ASN:ND2	1:B:542:ASN:C	2.75	0.42
1:B:186:ASN:C	1:B:186:ASN:ND2	2.70	0.42
1:A:537:THR:HG23	4:A:1576:HOH:O	2.19	0.42
1:B:105:SER:HA	1:B:147:TYR:CE1	2.55	0.42
1:B:347:ALA:N	1:B:369:HIS:HD2	2.09	0.41
1:B:492:VAL:HG13	1:B:531:PHE:CD1	2.55	0.41
1:B:364:GLN:HA	1:B:385:ARG:O	2.20	0.41
1:B:408:GLU:HA	1:B:459:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:LEU:HD12	1:A:334:LEU:N	2.36	0.41
1:A:408:GLU:HG3	1:A:409:ASN:ND2	2.36	0.41
1:B:25:ASN:ND2	1:B:28:LEU:N	2.68	0.41
1:B:476:PHE:O	1:B:507:SER:HA	2.21	0.41
1:A:459:ARG:HA	1:A:485:ASP:O	2.21	0.41
3:A:1002:NAG:O3	3:A:1002:NAG:H83	2.21	0.41
1:B:220:ASN:HB3	1:B:221:PRO:CD	2.51	0.40
1:B:401:GLY:O	1:B:402:TRP:HB2	2.20	0.40
1:B:499:PRO:HG2	1:B:502:ILE:HG12	2.03	0.40
1:B:332:LEU:N	1:B:332:LEU:CD1	2.84	0.40
1:A:301:GLY:HA3	1:A:327:TRP:CE2	2.56	0.40
1:A:408:GLU:HA	1:A:459:ARG:O	2.21	0.40
1:A:443:ASP:OD2	1:A:443:ASP:C	2.64	0.40
1:B:127:PRO:HG2	1:B:130:LEU:HD11	2.04	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	547/549 (100%)	517 (94%)	29 (5%)	1 (0%)	43	28
1	B	547/549 (100%)	513 (94%)	34 (6%)	0	100	100
All	All	1094/1098 (100%)	1030 (94%)	63 (6%)	1 (0%)	48	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	ASN

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	466/466 (100%)	465 (100%)	1 (0%)	87	84
1	B	466/466 (100%)	460 (99%)	6 (1%)	61	48
All	All	932/932 (100%)	925 (99%)	7 (1%)	73	65

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	TYR
1	B	104	TYR
1	B	186	ASN
1	B	313	ASN
1	B	424	ASN
1	B	436	ASN
1	B	542	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	41	GLN
1	A	51	GLN
1	A	106	HIS
1	A	122	ASN
1	A	131	ASN
1	A	138	ASN
1	A	274	GLN
1	A	323	ASN
1	A	330	ASN
1	A	369	HIS
1	A	386	ASN
1	A	414	ASN
1	A	424	ASN
1	A	427	ASN

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Mol	Chain	Res	Type
1	A	437	ASN
1	A	449	HIS
1	A	486	ASN
1	A	516	ASN
1	B	25	ASN
1	B	27	GLN
1	B	41	GLN
1	B	60	GLN
1	B	81	ASN
1	B	91	GLN
1	B	139	GLN
1	B	186	ASN
1	B	220	ASN
1	B	274	GLN
1	B	286	GLN
1	B	308	GLN
1	B	313	ASN
1	B	323	ASN
1	B	330	ASN
1	B	364	GLN
1	B	369	HIS
1	B	386	ASN
1	B	414	ASN
1	B	419	HIS
1	B	424	ASN
1	B	436	ASN
1	B	437	ASN
1	B	486	ASN
1	B	516	ASN
1	B	520	GLN
1	B	542	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	BGC	C	1	2	12,12,12	0.36	0	17,17,17	0.44	0
2	GLC	C	2	2	11,11,12	0.45	0	15,15,17	0.65	1 (6%)
2	GLC	C	3	2	11,11,12	0.51	0	15,15,17	0.46	0
2	BGC	D	1	2	12,12,12	0.37	0	17,17,17	0.48	0
2	GLC	D	2	2	11,11,12	0.49	0	15,15,17	0.64	1 (6%)
2	GLC	D	3	2	11,11,12	0.52	0	15,15,17	0.47	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
2	BGC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	1/2/19/22	0/1/1/1
2	GLC	D	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	C1-O5-C5	2.19	115.13	112.19
2	C	2	GLC	C1-O5-C5	2.10	115.00	112.19

There are no chirality outliers.

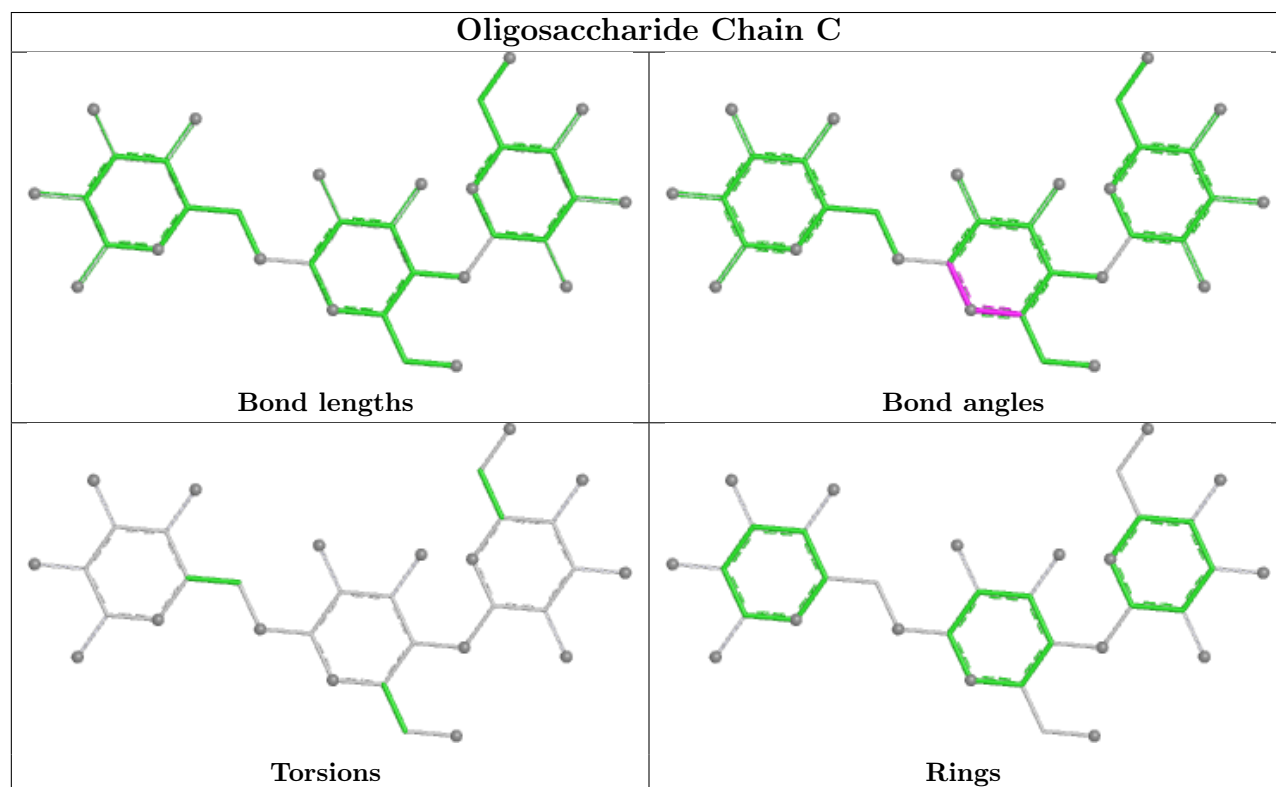
All (1) torsion outliers are listed below:

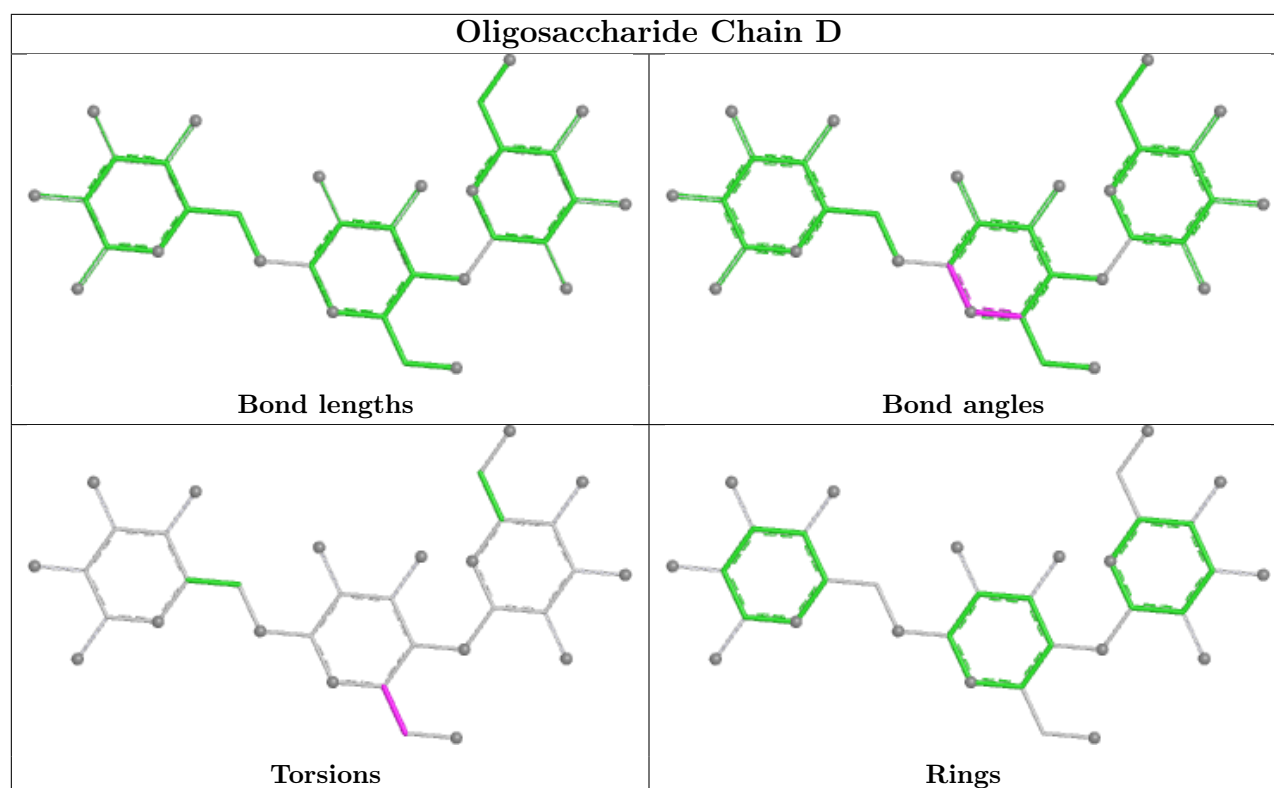
Mol	Chain	Res	Type	Atoms
2	D	2	GLC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

23 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	A	1009	1	14,14,15	0.59	0	17,19,21	0.86	1 (5%)
3	NAG	A	1006	1	14,14,15	0.52	0	17,19,21	0.70	1 (5%)
3	NAG	B	1008	1	14,14,15	0.48	0	17,19,21	0.71	1 (5%)
3	NAG	A	1004	1	14,14,15	0.48	0	17,19,21	0.65	0
3	NAG	A	1000	1	14,14,15	0.54	0	17,19,21	0.68	1 (5%)
3	NAG	A	1010	1	14,14,15	0.54	0	17,19,21	0.66	0
3	NAG	B	1007	1	14,14,15	0.56	0	17,19,21	0.63	0
3	NAG	A	1011	1	14,14,15	0.47	0	17,19,21	0.67	0
3	NAG	B	1002	1	14,14,15	0.51	0	17,19,21	0.68	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	1002	1	14,14,15	0.49	0	17,19,21	0.70	1 (5%)
3	NAG	A	1003	1	14,14,15	0.55	0	17,19,21	0.70	0
3	NAG	B	1003	1	14,14,15	0.58	0	17,19,21	0.65	0
3	NAG	B	1000	1	14,14,15	0.54	0	17,19,21	0.68	1 (5%)
3	NAG	B	1001	1	14,14,15	0.52	0	17,19,21	0.72	1 (5%)
3	NAG	A	1005	1	14,14,15	0.50	0	17,19,21	0.70	1 (5%)
3	NAG	B	1009	1	14,14,15	0.51	0	17,19,21	0.71	1 (5%)
3	NAG	B	1005	1	14,14,15	0.49	0	17,19,21	0.71	1 (5%)
3	NAG	B	1010	1	14,14,15	0.51	0	17,19,21	0.65	0
3	NAG	A	1008	1	14,14,15	0.49	0	17,19,21	0.76	1 (5%)
3	NAG	B	1004	1	14,14,15	0.47	0	17,19,21	0.79	1 (5%)
3	NAG	A	1007	1	14,14,15	0.54	0	17,19,21	0.71	0
3	NAG	A	1001	1	14,14,15	0.52	0	17,19,21	0.76	1 (5%)
3	NAG	B	1006	1	14,14,15	0.53	0	17,19,21	0.64	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
3	NAG	A	1009	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1006	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1008	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1004	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1000	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1010	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1007	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1011	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1002	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1002	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1003	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1000	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1005	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1009	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1005	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1010	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1008	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1004	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1007	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1006	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1004	NAG	C2-N2-C7	-2.45	119.62	122.90
3	A	1009	NAG	C2-N2-C7	-2.38	119.71	122.90
3	B	1001	NAG	C2-N2-C7	-2.29	119.83	122.90
3	B	1009	NAG	C2-N2-C7	-2.27	119.86	122.90
3	A	1001	NAG	C2-N2-C7	-2.27	119.86	122.90
3	A	1002	NAG	C2-N2-C7	-2.26	119.87	122.90
3	B	1008	NAG	C2-N2-C7	-2.21	119.93	122.90
3	A	1008	NAG	C2-N2-C7	-2.21	119.94	122.90
3	B	1005	NAG	C2-N2-C7	-2.18	119.98	122.90
3	A	1006	NAG	C2-N2-C7	-2.14	120.03	122.90
3	A	1000	NAG	C2-N2-C7	-2.10	120.08	122.90
3	A	1005	NAG	C2-N2-C7	-2.07	120.13	122.90
3	B	1000	NAG	C2-N2-C7	-2.06	120.15	122.90
3	B	1002	NAG	C2-N2-C7	-2.04	120.17	122.90

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	NAG	C8-C7-N2-C2
3	A	1002	NAG	O7-C7-N2-C2
3	A	1006	NAG	C8-C7-N2-C2
3	A	1006	NAG	O7-C7-N2-C2
3	A	1007	NAG	C1-C2-N2-C7
3	A	1007	NAG	C8-C7-N2-C2
3	A	1007	NAG	O7-C7-N2-C2
3	A	1009	NAG	C8-C7-N2-C2
3	A	1009	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	A	1011	NAG	C8-C7-N2-C2
3	A	1011	NAG	O7-C7-N2-C2
3	B	1000	NAG	C8-C7-N2-C2
3	B	1000	NAG	O7-C7-N2-C2
3	B	1001	NAG	C8-C7-N2-C2
3	B	1001	NAG	O7-C7-N2-C2
3	B	1002	NAG	C8-C7-N2-C2
3	B	1002	NAG	O7-C7-N2-C2
3	B	1003	NAG	C8-C7-N2-C2
3	B	1003	NAG	O7-C7-N2-C2
3	B	1004	NAG	C8-C7-N2-C2
3	B	1004	NAG	O7-C7-N2-C2
3	B	1005	NAG	C8-C7-N2-C2
3	B	1005	NAG	O7-C7-N2-C2
3	B	1007	NAG	C8-C7-N2-C2
3	B	1007	NAG	O7-C7-N2-C2
3	B	1009	NAG	C8-C7-N2-C2
3	B	1009	NAG	O7-C7-N2-C2
3	B	1006	NAG	C8-C7-N2-C2
3	A	1000	NAG	C8-C7-N2-C2
3	A	1005	NAG	C8-C7-N2-C2
3	A	1004	NAG	C4-C5-C6-O6
3	A	1008	NAG	C4-C5-C6-O6
3	B	1006	NAG	O7-C7-N2-C2
3	A	1004	NAG	O5-C5-C6-O6
3	B	1002	NAG	O5-C5-C6-O6
3	A	1000	NAG	O7-C7-N2-C2
3	A	1005	NAG	O7-C7-N2-C2
3	A	1010	NAG	C8-C7-N2-C2
3	A	1008	NAG	O5-C5-C6-O6
3	A	1010	NAG	O7-C7-N2-C2
3	B	1006	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1006	NAG	1	0
3	B	1008	NAG	1	0
3	A	1011	NAG	1	0
3	B	1002	NAG	2	0
3	A	1002	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1003	NAG	1	0
3	A	1005	NAG	1	0
3	B	1005	NAG	2	0
3	A	1007	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	549/549 (100%)	0.02	30 (5%)	30 34	10, 16, 29, 46	0
1	B	549/549 (100%)	0.41	40 (7%)	21 23	11, 20, 35, 49	0
All	All	1098/1098 (100%)	0.22	70 (6%)	25 27	10, 18, 33, 49	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	290	GLY	6.2
1	A	330	ASN	6.0
1	A	193	PRO	5.0
1	B	303	LEU	4.7
1	B	68	LEU	4.7
1	B	289	SER	4.7
1	A	226	PHE	4.3
1	A	329	GLY	4.2
1	A	116	GLY	4.1
1	A	68	LEU	4.1
1	B	64	ALA	4.1
1	A	194	GLY	4.1
1	B	226	PHE	4.1
1	B	302	THR	3.9
1	B	500	LEU	3.9
1	B	564	ASP	3.9
1	B	535	ASN	3.8
1	A	331	SER	3.7
1	A	302	THR	3.7
1	A	120	ASN	3.7
1	A	118	SER	3.6
1	A	117	SER	3.5
1	A	192	GLN	3.5
1	B	503	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	438	TYR	3.3
1	A	67	SER	3.2
1	B	294	ASN	3.2
1	A	564	ASP	3.2
1	B	541	SER	3.2
1	B	117	SER	3.1
1	B	438	TYR	3.1
1	A	195	SER	3.0
1	A	289	SER	2.9
1	A	138	ASN	2.9
1	A	333	ASP	2.8
1	A	196	PRO	2.8
1	B	536	THR	2.8
1	B	66	SER	2.8
1	B	119	ALA	2.8
1	B	116	GLY	2.7
1	A	139	GLN	2.7
1	B	67	SER	2.7
1	A	19	MET	2.7
1	A	66	SER	2.6
1	B	291	ALA	2.6
1	B	443	ASP	2.6
1	B	334	LEU	2.5
1	A	135	ARG	2.5
1	B	335	ILE	2.5
1	B	555	ALA	2.5
1	B	139	GLN	2.4
1	B	328	SER	2.3
1	B	558	GLY	2.3
1	A	64	ALA	2.3
1	B	333	ASP	2.3
1	B	137	ASP	2.3
1	B	304	GLY	2.3
1	B	533	VAL	2.3
1	A	525	ASP	2.2
1	B	130	LEU	2.2
1	A	328	SER	2.2
1	B	467	ARG	2.2
1	B	63	PRO	2.2
1	B	65	SER	2.2
1	B	227	THR	2.1
1	B	305	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	563	ILE	2.1
1	A	290	GLY	2.0
1	A	286	GLN	2.0
1	B	508	TRP	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](#)

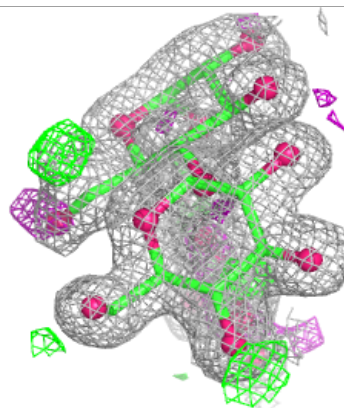
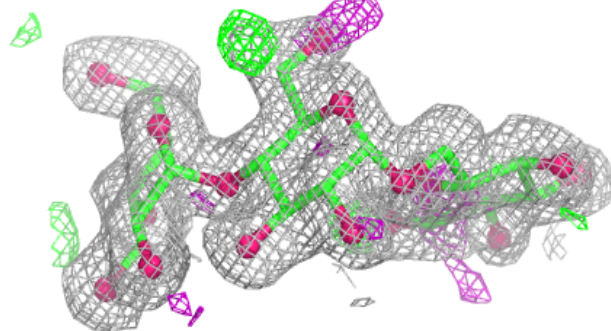
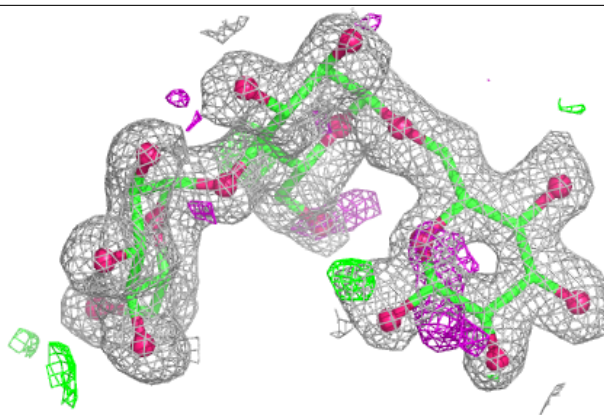
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	D	1	12/12	0.83	0.12	28,33,34,34	0
2	GLC	C	2	11/12	0.87	0.10	19,21,26,27	0
2	BGC	C	1	12/12	0.87	0.12	22,27,27,27	0
2	GLC	D	2	11/12	0.88	0.10	23,24,29,33	0
2	GLC	D	3	11/12	0.92	0.08	19,20,22,24	0
2	GLC	C	3	11/12	0.97	0.06	16,16,19,20	0

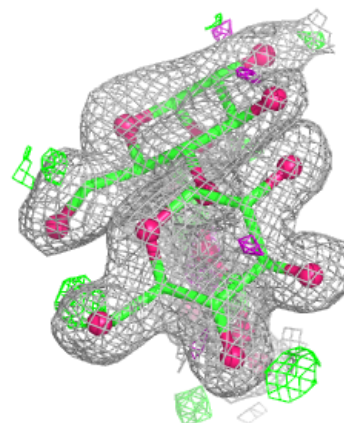
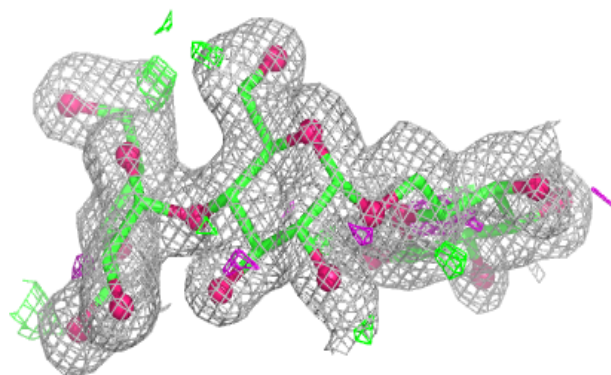
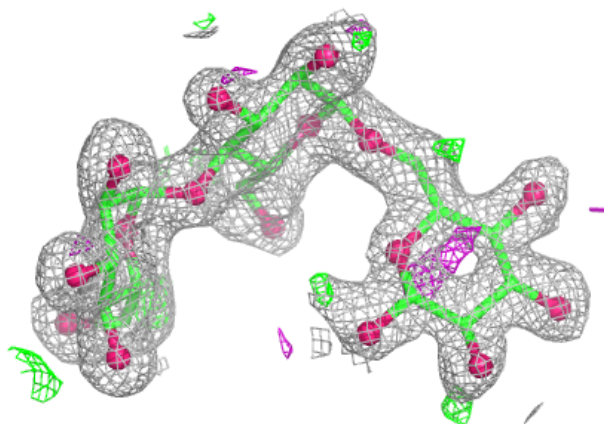
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	1002	14/15	0.48	0.18	51,53,55,56	0
3	NAG	B	1000	14/15	0.57	0.18	43,45,49,50	0
3	NAG	B	1003	14/15	0.64	0.18	54,55,56,57	0
3	NAG	B	1005	14/15	0.67	0.17	48,50,51,52	0
3	NAG	A	1007	14/15	0.71	0.16	29,36,39,40	0
3	NAG	A	1011	14/15	0.75	0.14	36,39,43,45	0
3	NAG	B	1009	14/15	0.75	0.14	29,34,37,37	0
3	NAG	A	1009	14/15	0.78	0.15	32,36,41,41	0
3	NAG	A	1002	14/15	0.80	0.13	36,39,43,43	0
3	NAG	B	1008	14/15	0.81	0.12	34,36,39,40	0
3	NAG	B	1001	14/15	0.81	0.12	30,32,37,38	0
3	NAG	A	1005	14/15	0.82	0.12	28,33,37,38	0
3	NAG	B	1006	14/15	0.83	0.11	28,31,35,35	0
3	NAG	A	1010	14/15	0.84	0.11	35,37,40,40	0
3	NAG	A	1004	14/15	0.84	0.10	32,35,38,42	0
3	NAG	B	1007	14/15	0.86	0.11	32,34,39,39	0
3	NAG	A	1006	14/15	0.88	0.11	26,30,36,36	0
3	NAG	A	1000	14/15	0.88	0.09	24,26,29,31	0
3	NAG	A	1008	14/15	0.88	0.09	18,23,28,34	0
3	NAG	B	1004	14/15	0.89	0.10	22,24,33,34	0
3	NAG	B	1010	14/15	0.90	0.08	24,28,32,35	0
3	NAG	A	1001	14/15	0.91	0.09	19,21,23,26	0
3	NAG	A	1003	14/15	0.94	0.07	19,21,25,27	0

6.5 Other polymers

There are no such residues in this entry.