Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2025 – 12:27 AM JST

PDB ID	:	9JLW / pdb_00009jlw
Title	:	Crystal structure of GH57 family amylopullulanase from Aquifex aeolicus mutant D352N in complex with maltoheptaose
Authors	:	Zhu, Z.M.; Wang, W.W.; Li, M.J.; Xu, Q.; Zhou, H.; Huang, L.Q.; Wang, Q.S.; Yu, F.
Deposited on	:	2024-09-19
Resolution	:	1.95 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:

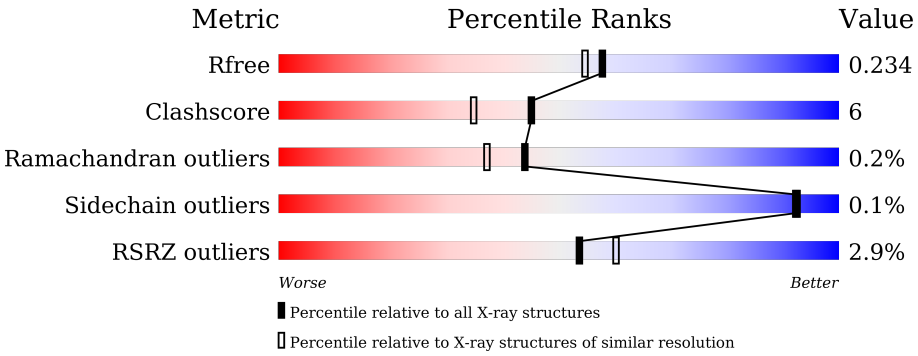
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 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}	164625	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	477	2% 86% 13%
1	B	477	4% 86% 14%
2	C	7	86% 14%
3	D	6	17% 67% 17%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8590 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.

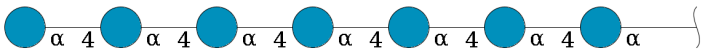
- Molecule 1 is a protein called Glycoside hydrolase family 57 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			4044	2646	648	741	9			
1	B	476	Total	C	N	O	S	0	0	0
			4044	2646	648	741	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	352	ASN	ASP	engineered mutation	UNP O66934
B	352	ASN	ASP	engineered mutation	UNP O66934

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

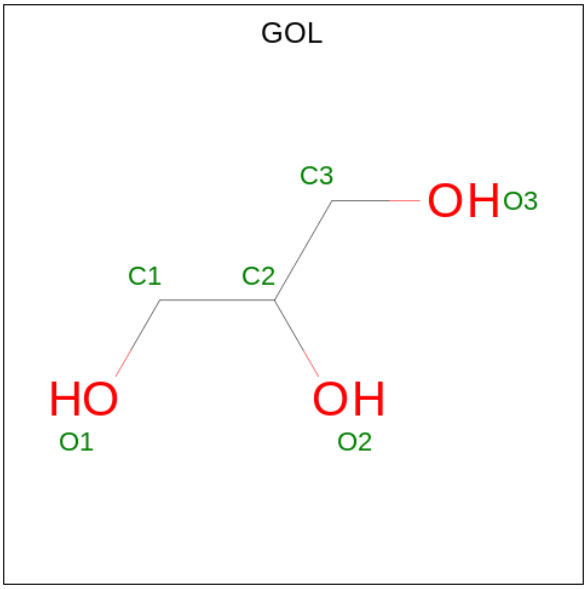


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	O		0	0	0
			78	42	36				

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	6	Total C O 67 36 31	0	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

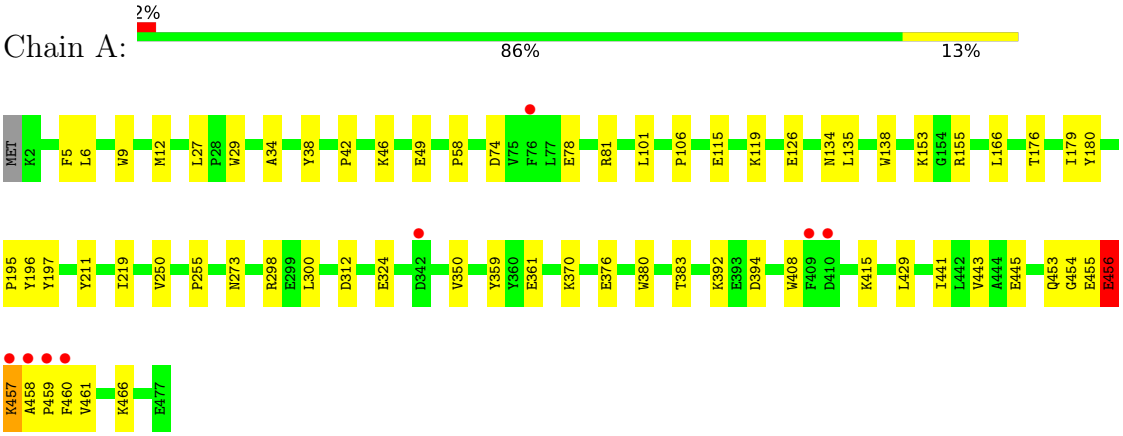
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	190	Total O 190 190	0	0
5	B	155	Total O 155 155	0	0

3 Residue-property plots (i)

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

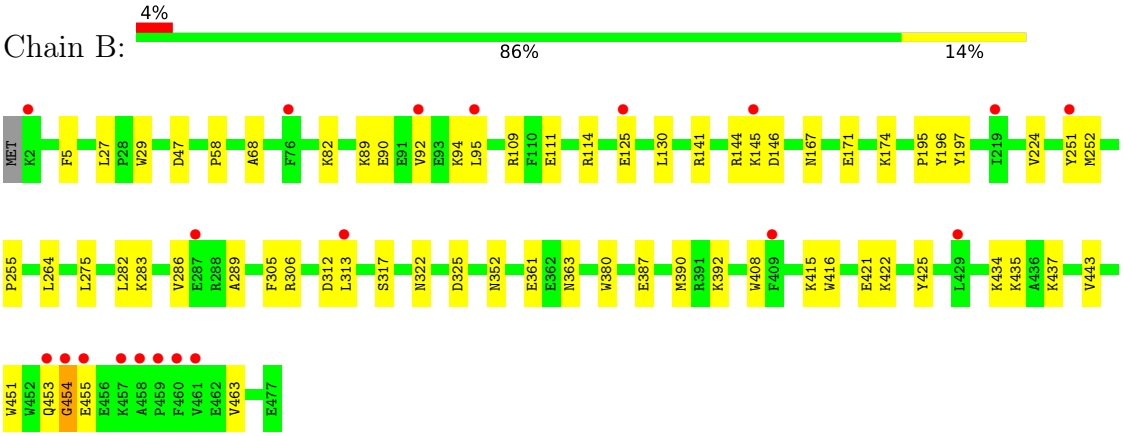
• Molecule 1: Glycoside hydrolase family 57 N-terminal domain-containing protein

Chain A:



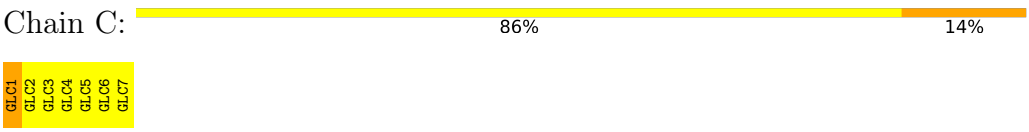
• Molecule 1: Glycoside hydrolase family 57 N-terminal domain-containing protein

Chain B:



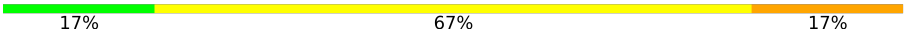
• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

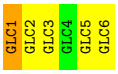
Chain C:



• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	61.42Å 41.15Å 193.21Å 90.00° 94.48° 90.00°	Depositor
Resolution (Å)	59.72 – 1.95 59.72 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.0 (59.72-1.95) 99.0 (59.72-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.195 , 0.233 0.196 , 0.234	Depositor DCC
R_{free} test set	3538 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8590	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.52	7/4157 (0.2%)	0.55	7/5623 (0.1%)
1	B	0.35	1/4157 (0.0%)	0.43	0/5623
All	All	0.44	8/8314 (0.1%)	0.50	7/11246 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	352	ASN	C-O	-13.07	1.08	1.23
1	A	453	GLN	C-O	-12.38	1.09	1.23
1	A	455	GLU	CA-C	-7.30	1.43	1.52
1	A	455	GLU	N-CA	-6.98	1.37	1.46
1	A	454	GLY	CA-C	-6.58	1.44	1.51
1	A	453	GLN	C-N	-6.24	1.27	1.33
1	A	453	GLN	N-CA	-6.16	1.38	1.46
1	A	454	GLY	C-O	-5.71	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	457	LYS	N-CA-C	9.60	124.88	107.99
1	A	458	ALA	CA-C-N	-6.28	113.49	119.90
1	A	458	ALA	C-N-CA	-6.28	113.49	119.90
1	A	455	GLU	CB-CA-C	-6.24	98.73	109.65
1	A	456	GLU	N-CA-CB	-5.63	100.98	110.49
1	A	455	GLU	N-CA-C	-5.55	98.86	108.69
1	A	455	GLU	O-C-N	5.04	129.50	123.36

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	4044	0	3977	43	0
1	B	4044	0	3977	51	0
2	C	78	0	66	4	0
3	D	67	0	57	5	0
4	A	6	0	8	0	0
4	B	6	0	8	1	0
5	A	190	0	0	4	0
5	B	155	0	0	3	0
All	All	8590	0	8093	94	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 6.

All (94) 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:361:GLU:OE1	5:A:601:HOH:O	1.85	0.93
1:A:457:LYS:NZ	1:A:461:VAL:HB	1.94	0.81
1:B:251:TYR:OH	1:B:387:GLU:HA	1.85	0.77
1:B:68:ALA:HB1	1:B:174:LYS:HD2	1.70	0.74
1:B:82:LYS:NZ	5:B:601:HOH:O	2.22	0.73
1:A:5:PHE:CZ	1:A:392:LYS:HE3	2.25	0.72
1:A:457:LYS:HZ1	1:A:461:VAL:HB	1.54	0.70
1:B:145:LYS:HD3	1:B:146:ASP:H	1.55	0.69
1:B:111:GLU:HA	1:B:114:ARG:HG3	1.75	0.68
1:A:81:ARG:NH2	5:A:606:HOH:O	2.30	0.64
1:A:119:LYS:NZ	1:A:126:GLU:OE2	2.29	0.64
1:B:322:ASN:HD22	1:B:325:ASP:H	1.47	0.62
1:B:109:ARG:NH2	1:B:361:GLU:OE1	2.33	0.61
1:A:29:TRP:CD2	2:C:5:GLC:H2	2.37	0.60
1:A:457:LYS:HZ2	1:A:461:VAL:HB	1.66	0.60
1:A:101:LEU:HD13	1:A:459:PRO:HG2	1.84	0.59
1:B:251:TYR:HE1	1:B:390:MET:SD	2.25	0.59
1:B:145:LYS:HD3	1:B:146:ASP:N	2.18	0.58
1:A:46:LYS:NZ	5:A:607:HOH:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:PRO:HB2	1:A:460:PHE:CD2	2.39	0.57
1:A:74:ASP:O	1:A:78:GLU:HG2	2.04	0.57
1:B:195:PRO:HD2	1:B:255:PRO:HD3	1.86	0.57
1:B:282:LEU:HB2	1:B:305:PHE:CD2	2.39	0.57
1:B:29:TRP:CD2	3:D:5:GLC:H2	2.39	0.57
1:B:125:GLU:N	1:B:125:GLU:OE2	2.38	0.56
1:A:466:LYS:NZ	5:A:609:HOH:O	2.39	0.56
1:B:312:ASP:OD1	3:D:1:GLC:H1	2.06	0.55
1:B:435:LYS:O	1:B:437:LYS:NZ	2.38	0.55
1:A:115:GLU:O	1:A:119:LYS:HG3	2.06	0.54
1:B:425:TYR:CE2	1:B:453:GLN:HG3	2.43	0.54
1:B:313:LEU:HA	1:B:317:SER:HB2	1.90	0.54
1:B:141:ARG:HA	1:B:144:ARG:HD3	1.90	0.54
1:B:167:ASN:O	1:B:171:GLU:HG3	2.08	0.54
1:B:114:ARG:NH1	5:B:607:HOH:O	2.41	0.54
1:B:425:TYR:CZ	1:B:453:GLN:HG3	2.42	0.54
1:B:224:VAL:HG11	1:B:434:LYS:HG2	1.90	0.52
1:A:380:TRP:H	1:A:380:TRP:CD1	2.28	0.52
1:B:251:TYR:OH	1:B:387:GLU:OE1	2.28	0.51
1:B:306:ARG:NH2	3:D:1:GLC:O1	2.43	0.51
1:B:415:LYS:HB3	1:B:416:TRP:CZ3	2.45	0.51
1:A:298:ARG:O	1:A:300:LEU:HD13	2.12	0.50
1:B:415:LYS:HE2	1:B:451:TRP:CE2	2.48	0.49
1:A:195:PRO:HD2	1:A:255:PRO:HD3	1.93	0.49
1:A:9:TRP:HB3	1:A:350:VAL:HG22	1.95	0.49
1:B:282:LEU:HG	1:B:289:ALA:HB1	1.94	0.49
1:B:363:ASN:ND2	4:B:501:GOL:H32	2.28	0.49
1:A:12:MET:HB3	1:A:38:TYR:CE1	2.48	0.48
1:B:195:PRO:HD3	1:B:252:MET:HE2	1.94	0.48
1:A:49:GLU:N	1:A:376:GLU:OE2	2.39	0.48
1:B:95:LEU:HD23	1:B:130:LEU:HD23	1.96	0.48
1:A:408:TRP:CZ3	2:C:1:GLC:H62	2.48	0.47
1:B:421:GLU:HB2	1:B:454:GLY:HA2	1.96	0.47
1:A:135:LEU:HD11	1:A:166:LEU:HG	1.97	0.47
1:B:197:TYR:CZ	1:B:443:VAL:HG22	2.50	0.47
1:A:456:GLU:CD	1:A:456:GLU:C	2.82	0.46
1:B:380:TRP:H	1:B:380:TRP:CD1	2.33	0.46
1:A:153:LYS:HE2	1:A:155:ARG:O	2.16	0.46
1:A:176:THR:O	1:A:179:ILE:HG22	2.15	0.46
1:A:312:ASP:OD1	2:C:1:GLC:H1	2.15	0.46
1:A:106:PRO:HD2	1:A:359:TYR:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LYS:HD2	1:A:415:LYS:HA	1.77	0.44
1:B:286:VAL:HB	1:B:289:ALA:HB2	1.99	0.44
1:A:250:VAL:CG2	1:A:273:ASN:HB2	2.48	0.44
1:B:415:LYS:HB3	1:B:416:TRP:CE3	2.52	0.44
1:A:27:LEU:HD21	1:A:460:PHE:HB3	2.00	0.44
1:A:429:LEU:HD21	1:A:445:GLU:HG2	1.99	0.44
1:B:90:GLU:OE2	1:B:94:LYS:NZ	2.42	0.44
1:B:5:PHE:CZ	1:B:392:LYS:HD3	2.53	0.44
1:A:34:ALA:HA	1:A:38:TYR:HB2	2.00	0.43
1:A:211:TYR:OH	1:A:219:ILE:HG12	2.17	0.43
1:B:408:TRP:CZ3	3:D:1:GLC:H62	2.53	0.43
1:A:58:PRO:HG2	1:A:196:TYR:HA	2.00	0.43
1:B:82:LYS:NZ	5:B:608:HOH:O	2.42	0.43
1:A:6:LEU:O	1:A:383:THR:HA	2.19	0.42
1:B:58:PRO:HG2	1:B:196:TYR:HA	2.01	0.42
1:B:283:LYS:HA	1:B:283:LYS:HD2	1.82	0.42
1:B:224:VAL:CG1	1:B:434:LYS:HG2	2.50	0.42
1:B:47:ASP:OD2	1:B:141:ARG:NH2	2.50	0.42
1:B:27:LEU:HG	1:B:463:VAL:HG11	2.02	0.42
1:A:29:TRP:CG	2:C:5:GLC:H2	2.55	0.42
1:B:89:LYS:O	1:B:92:VAL:HG22	2.20	0.42
1:B:174:LYS:HD2	1:B:174:LYS:HA	1.80	0.42
1:A:134:ASN:O	1:A:138:TRP:HD1	2.03	0.41
1:A:197:TYR:CZ	1:A:443:VAL:HG22	2.55	0.41
1:A:394:ASP:OD1	1:A:394:ASP:N	2.54	0.41
1:A:324:GLU:HG3	1:A:370:LYS:HD3	2.02	0.41
1:A:457:LYS:HB3	1:A:457:LYS:HE3	1.90	0.41
1:B:29:TRP:CG	3:D:5:GLC:H2	2.56	0.41
1:B:282:LEU:CG	1:B:289:ALA:HB1	2.51	0.41
1:B:422:LYS:NZ	1:B:455:GLU:OE2	2.51	0.41
1:A:42:PRO:HG3	1:A:180:TYR:CZ	2.55	0.41
1:B:251:TYR:OH	1:B:387:GLU:CA	2.62	0.41
1:B:264:LEU:HD23	1:B:275:LEU:HD21	2.02	0.41
1:A:441:ILE:HD12	1:A:441:ILE:HA	1.97	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	474/477 (99%)	470 (99%)	3 (1%)	1 (0%)	44 37
1	B	474/477 (99%)	468 (99%)	5 (1%)	1 (0%)	44 37
All	All	948/954 (99%)	938 (99%)	8 (1%)	2 (0%)	44 37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	GLU
1	B	454	GLY

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	436/437 (100%)	435 (100%)	1 (0%)	92 92
1	B	436/437 (100%)	436 (100%)	0	100 100
All	All	872/874 (100%)	871 (100%)	1 (0%)	92 92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	456	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	134	ASN
1	A	156	ASN
1	A	273	ASN
1	A	352	ASN
1	B	134	ASN
1	B	322	ASN
1	B	352	ASN
1	B	453	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

13 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	GLC	C	1	2	12,12,12	0.85	0	17,17,17	2.03	4 (23%)
2	GLC	C	2	2	11,11,12	0.70	0	15,15,17	1.42	2 (13%)
2	GLC	C	3	2	11,11,12	0.48	0	15,15,17	1.31	1 (6%)
2	GLC	C	4	2	11,11,12	0.63	0	15,15,17	0.94	1 (6%)
2	GLC	C	5	2	11,11,12	0.55	0	15,15,17	0.79	0
2	GLC	C	6	2	11,11,12	0.64	0	15,15,17	1.15	2 (13%)
2	GLC	C	7	2	11,11,12	0.48	0	15,15,17	1.39	4 (26%)
3	GLC	D	1	3	12,12,12	0.80	0	17,17,17	2.05	4 (23%)
3	GLC	D	2	3	11,11,12	0.65	0	15,15,17	1.59	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GLC	D	3	3	11,11,12	0.47	0	15,15,17	1.19	1 (6%)
3	GLC	D	4	3	11,11,12	0.52	0	15,15,17	0.67	0
3	GLC	D	5	3	11,11,12	0.61	0	15,15,17	0.85	0
3	GLC	D	6	3	11,11,12	0.77	0	15,15,17	0.98	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	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	0/2/19/22	0/1/1/1
2	GLC	C	5	2	-	0/2/19/22	0/1/1/1
2	GLC	C	6	2	-	2/2/19/22	0/1/1/1
2	GLC	C	7	2	-	0/2/19/22	0/1/1/1
3	GLC	D	1	3	-	0/2/22/22	0/1/1/1
3	GLC	D	2	3	-	2/2/19/22	0/1/1/1
3	GLC	D	3	3	-	0/2/19/22	0/1/1/1
3	GLC	D	4	3	-	0/2/19/22	0/1/1/1
3	GLC	D	5	3	-	0/2/19/22	0/1/1/1
3	GLC	D	6	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	GLC	O5-C1-C2	4.91	119.05	110.28
2	C	3	GLC	C1-O5-C5	4.44	118.21	112.19
2	C	1	GLC	C1-O5-C5	4.32	121.81	113.66
2	C	1	GLC	O4-C4-C5	-4.09	99.14	109.30
3	D	1	GLC	C1-O5-C5	3.88	120.99	113.66
2	C	1	GLC	O5-C1-C2	3.82	117.09	110.28
3	D	3	GLC	C1-O5-C5	3.63	117.11	112.19
2	C	2	GLC	O4-C4-C3	3.05	117.40	110.35
3	D	1	GLC	C1-C2-C3	2.96	116.46	110.31
3	D	6	GLC	O5-C1-C2	-2.83	106.40	110.77
3	D	1	GLC	O4-C4-C5	-2.76	102.44	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2	GLC	O4-C4-C3	2.75	116.71	110.35
2	C	2	GLC	O3-C3-C2	-2.64	104.94	109.99
2	C	7	GLC	C1-O5-C5	2.59	115.71	112.19
2	C	7	GLC	C3-C4-C5	2.53	114.74	110.24
2	C	1	GLC	O5-C5-C6	2.50	112.64	106.44
2	C	7	GLC	O5-C1-C2	-2.45	106.98	110.77
3	D	2	GLC	C1-O5-C5	2.43	115.48	112.19
2	C	6	GLC	O5-C1-C2	-2.33	107.17	110.77
2	C	6	GLC	C1-O5-C5	2.28	115.28	112.19
3	D	2	GLC	O4-C4-C5	-2.20	103.83	109.30
2	C	7	GLC	C6-C5-C4	-2.14	107.99	113.00
3	D	2	GLC	C6-C5-C4	-2.07	108.16	113.00
2	C	4	GLC	C1-O5-C5	2.02	114.92	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

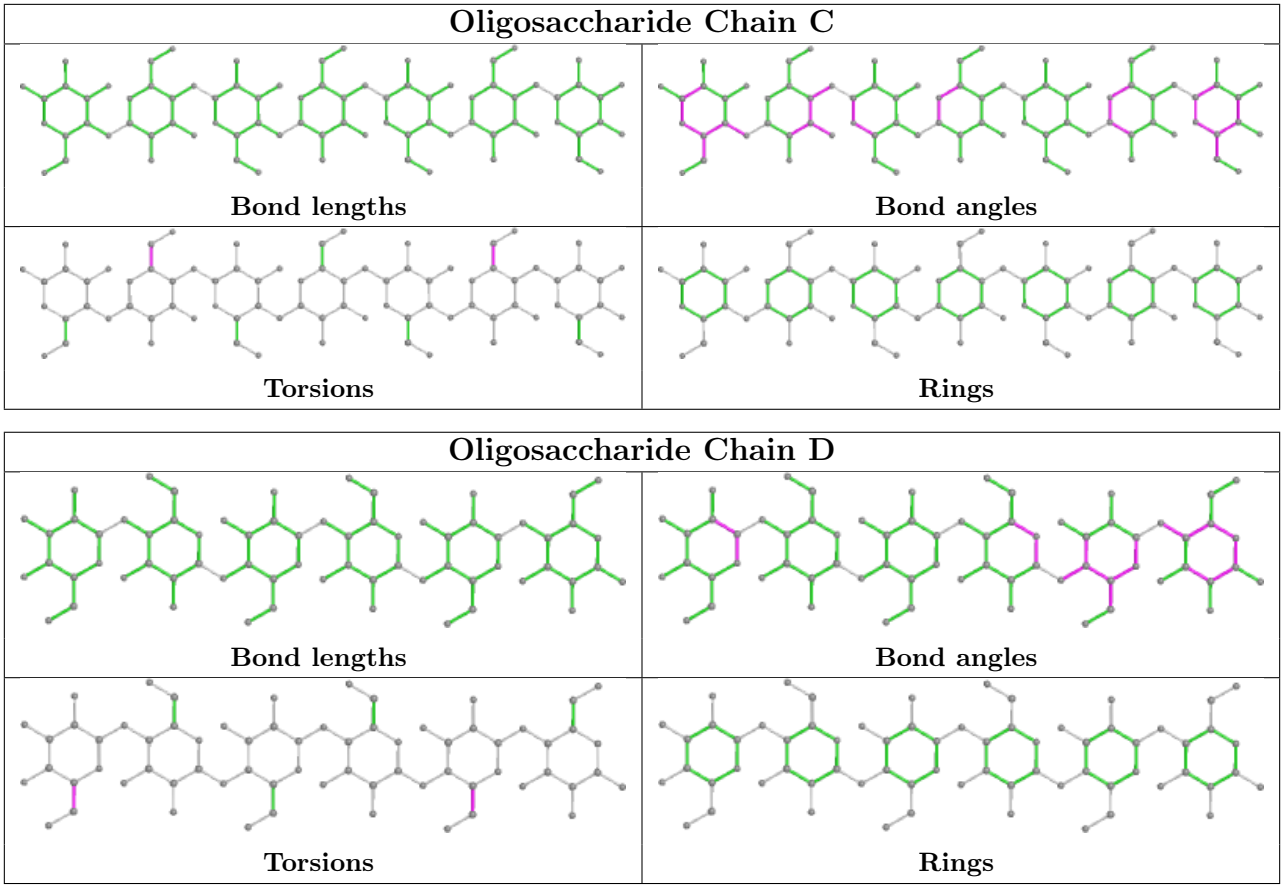
Mol	Chain	Res	Type	Atoms
3	D	2	GLC	O5-C5-C6-O6
3	D	2	GLC	C4-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
3	D	6	GLC	O5-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
3	D	6	GLC	C4-C5-C6-O6
2	C	6	GLC	C4-C5-C6-O6
2	C	6	GLC	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GLC	2	0
3	D	5	GLC	2	0
2	C	5	GLC	2	0
3	D	1	GLC	3	0

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



5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	GOL	A	501	-	5,5,5	0.95	0	5,5,5	0.92	0
4	GOL	B	501	-	5,5,5	0.75	0	5,5,5	0.90	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
4	GOL	A	501	-	-	0/4/4/4	-
4	GOL	B	501	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	476/477 (99%)	0.19	8 (1%) 69 75	15, 25, 44, 99	0
1	B	476/477 (99%)	0.46	20 (4%) 41 48	20, 32, 53, 100	0
All	All	952/954 (99%)	0.32	28 (2%) 54 60	15, 29, 48, 100	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	459	PRO	4.0
1	B	251	TYR	3.9
1	A	76	PHE	3.7
1	B	453	GLN	3.7
1	B	458	ALA	3.5
1	A	342	ASP	3.3
1	A	458	ALA	3.2
1	B	454	GLY	3.2
1	A	457	LYS	2.9
1	B	457	LYS	2.8
1	A	459	PRO	2.7
1	B	460	PHE	2.7
1	B	76	PHE	2.6
1	B	2	LYS	2.5
1	B	92	VAL	2.5
1	A	409	PHE	2.4
1	A	460	PHE	2.3
1	B	455	GLU	2.3
1	B	461	VAL	2.2
1	B	145	LYS	2.2
1	B	125	GLU	2.2
1	B	219	ILE	2.2
1	B	287	GLU	2.1
1	B	409	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	95	LEU	2.1
1	B	313	LEU	2.1
1	A	410	ASP	2.1
1	B	429	LEU	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)

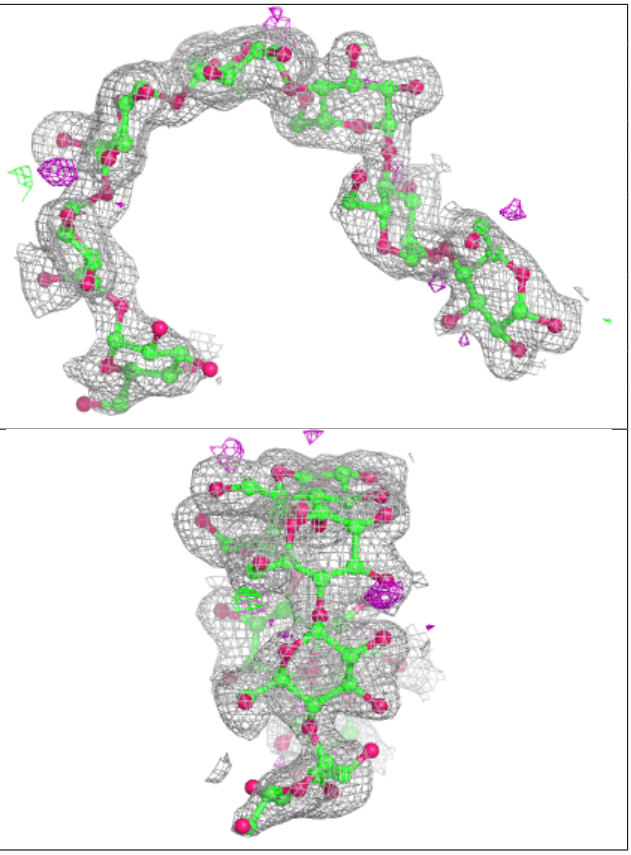
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	GLC	C	7	11/12	0.74	0.12	62,64,69,70	0
3	GLC	D	6	11/12	0.81	0.12	34,41,49,55	0
2	GLC	C	6	11/12	0.85	0.12	30,38,45,55	0
3	GLC	D	2	11/12	0.87	0.12	28,39,47,48	0
2	GLC	C	1	12/12	0.87	0.11	33,41,45,46	0
2	GLC	C	2	11/12	0.89	0.12	24,36,49,57	0
3	GLC	D	1	12/12	0.91	0.09	41,46,51,52	0
2	GLC	C	4	11/12	0.93	0.09	17,22,23,25	0
2	GLC	C	5	11/12	0.94	0.06	18,19,23,24	0
3	GLC	D	3	11/12	0.95	0.07	20,24,27,31	0
3	GLC	D	4	11/12	0.95	0.06	19,24,28,30	0
3	GLC	D	5	11/12	0.95	0.06	25,27,31,34	0
2	GLC	C	3	11/12	0.95	0.07	15,20,23,24	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.

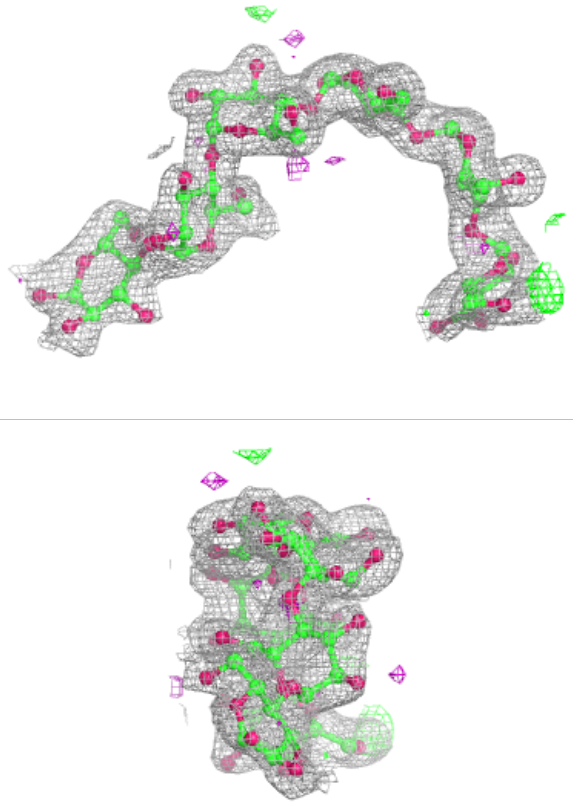
Electron density around Chain C:

$2mF_o$-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, 95^{th} 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
4	GOL	A	501	6/6	0.94	0.09	21,26,28,28	0
4	GOL	B	501	6/6	0.95	0.08	23,28,30,34	0

6.5 Other polymers

There are no such residues in this entry.