

wwPDB X-ray Structure Validation Summary Report (i)

Aug 17, 2023 – 10:23 AM JST

PDB ID	:	8IDP
Title	:	Crystal structure of reducing-end xylose-releasing exoxylanase in GH30 from
		Talaromyces cellulolyticus
Authors	:	Nakamichi, Y.; Watanabe, M.; Fujii, T.; Inoue, H.; Morita, T.
Deposited on	:	2023-02-14
Resolution	:	1.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.80 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	5950(1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	Quali	ty of chain	
1	А	462	% • •	% •	•
1	В	462	% 	% 59	% •
1	С	462	2% 	% •	•
1	D	462	% 92	•	·
2	Е	11	45%	45% 9%	%
2	K	11	36%	64%	



Mol	Chain	Length	Qua	lity of chain	
3	F	6	50%	50%	
3	L	6	50%	50%	
4	G	2	50%	50%	
4	Ι	2	50%	50%	
4	М	2		100%	
4	0	2	50%	50%	
5	Н	9	22%	67%	11%
6	J	5	60%	40%	
6	Р	5	60%	40%	
7	Ν	9	33%	56%	11%

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
9	GOL	С	1908	-	-	Х	-



2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 16663 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	1 1 446	446	Total	С	Ν	0	\mathbf{S}	0	6	0
	440	3531	2234	591	690	16	0	0	0	
1	1 C	446	Total	С	Ν	0	S	0	1	0
	440	3512	2222	587	687	16	0	4	0	
1	р	446	Total	С	Ν	0	S	0	2	0
	440	3507	2221	586	684	16	0	3	0	
1 D	445	Total	С	Ν	0	S	0	3	0	
		3498	2214	586	682	16			0	

• Molecule 1 is a protein called Reducing-end xylose-releasing exoxylanase Xyn30A.

• Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran ose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra nose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyr anose-(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
2	Е	11	Total 127	С 70	N 2	O 55	0	0	0
2	K	11	Total 127	С 70	N 2	O 55	0	0	0

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





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	F	6	Total C N O 72 40 2 30	0	0	0
3	L	6	Total C N O 72 40 2 30	0	0	0

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	C	9	Total C N	0	0	0	0
4	4 G	2	28 16 2	10	0	0	0
4 I	0	Total C N	0	0	0	0	
4	4 1	2	28 16 2	10	0	0	0
4	М	0	Total C N	0	0	0	0
4 M	2	28 16 2	10	0	0	0	
4 O	0	0	Total C N	0	0	0	0
	0	Δ	28 16 2	10			U

• Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran ose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deox y-beta-D-glucopyranose.



Mol	Chain	Residues	ŀ	Aton	ns		ZeroOcc	AltConf	Trace
5	Н	9	Total 105	C 58	N 2	0 45	0	0	0

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





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	J	5	Total C N O 61 34 2 25	0	0	0
6	Р	5	O1 O4 2 26 Total C N O 61 34 2 25	0	0	0

• Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran ose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deox y-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
7	Ν	9	Total 105	C 58	N 2	0 45	0	0	0

• Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	A	tor	ns		ZeroOcc	AltConf
8	А	1	Total 14	C 8	N 1	O 5	0	0
8	С	1	Total 14	C 8	N 1	O 5	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	С	1	Total C N O	0	0
			14 8 1 5		
8	В	1	Total C N O	0	0
0	D	1	14 8 1 5	0	0
8	В	B 1	Total C N O	0	Ο
0	D		14 8 1 5	0	0
0	Л	1	Total C N O	0	0
0	D		14 8 1 5	0	0
0	р	1	Total C N O	0	Ο
0	D	1	14 8 1 5	0	0

• Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	1	Total C O 12 6 6	0	1
9	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
9	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
9	С	1	Total C O 12 6 6	0	1
9	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
9	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
9	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
9	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
9	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
9	В	1	Total C O 12 6 6	0	1
9	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
9	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
9	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
9	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	1	Total C O 13 8 5	0	0
10	С	1	Total C O 13 8 5	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	1	Total C O 13 8 5	0	0

• Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Ato	ms	ZeroOcc	AltConf
11	В	1	Total 7	C O 4 3	0	0

• Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	А	366	Total O 366 366	0	0
12	С	363	Total O 363 363	0	0
12	В	412	Total O 412 412	0	0
12	D	380	Total O 380 380	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: Reducing-end xylose-releasing exoxylanase Xyn30A





A419 R420 R421 P423 L442 L442 L442 L442 E462

 $\label{eq:2} \bullet \mbox{Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)-2] - acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-acetamido-2-acetamido-2-acetamido-2-acetamido-2-acetamido-2-acetamido-2-acetamido-2-acetamido-2-acetamido-2-acetamido-2-acetamido-2-acetamido-2-acetamido-2-acetamido-2-acetamido-2-acetamido-2-acetamido-2-acetamido-2-$

Chain E:	45%	45%	9%
NAG1 NAG2 BMA3 BMA3 MAN4 MAN5 MAN5 MAN5 MAN5 MAN10 MAN10 MAN10			

 $\label{eq:mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-[alpha-D-mannopyranose-(1-4)-2]-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy$

Chain K:	36%	64%
NAG1 NAG2 BMA3 BMA4 MAN5 MAN5 MAN5 MAN5 MAN10 MAN11		

 $\label{eq:mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]} beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2$

Chain F:	50%	50%
<u>م م 4 م م</u>		

• Molecule 3: 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

MACI BANG2 MAN9 MAN5 MAN5 MAN5

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

Chain G:

50%

50%



NAC NAC BMA BMA MAN MAN MAN



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

50%

Chain I:

NAG1 NAG2

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

Chain M:	100%
NAG1 NAG2	
• Molecule 4	2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-acet
opyranose	

Chain O:	50%	50%
MGC2 MGC2		

50%

• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranoy-2-deoxy-beta-D-glucopyranoy-2-deoxy-beta-D-glucopyranoy-

Chain H:	22%	67%	11%
NAG1 NAG2 BMA3 MAN4 MAN5 MAN5 MAN5	MAN9 MAN9		

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

Chain J:	60%	40%
NAG1 NAG2 NAA3 NAN4 MAN5 MAN5		

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

Chain P:	60%	40%
NAG1 BMAG2 MAN4 MAN4 MAN5		



NAG BMA BMA MAN MAN MAN MAN

• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-4)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranoy-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-b

Chain N:	33%	56%	11%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	138.46Å 120.07Å 122.83Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	40.94 - 1.80	Depositor
Resolution (A)	40.94 - 1.80	EDS
% Data completeness	99.5 (40.94-1.80)	Depositor
(in resolution range)	99.5(40.94-1.80)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.54 (at 1.79 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.12	Depositor
D D.	0.165 , 0.195	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.165 , 0.195	DCC
R_{free} test set	9420 reflections (5.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	20.9	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.36 , 44.4	EDS
L-test for twinning ²	$< L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	0.054 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16663	wwPDB-VP
Average B, all atoms $(Å^2)$	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 46.53 % 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 1.1297e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

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: PEG, BMA, PG4, GOL, NAG, MAN

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).

Mal	Chain	Bond lengths		Bond angles	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.40	0/3631	0.60	0/4957
1	В	0.41	0/3607	0.60	0/4925
1	С	0.41	0/3612	0.59	0/4931
1	D	0.42	0/3597	0.61	0/4909
All	All	0.41	0/14447	0.60	0/19722

There are no bond length outliers.

There are no bond angle outliers.

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	А	3531	0	3283	9	0
1	В	3507	0	3264	13	0
1	С	3512	0	3264	14	0
1	D	3498	0	3252	11	0
2	Е	127	0	106	1	0
2	Κ	127	0	106	0	0
3	F	72	0	61	0	0
3	L	72	0	61	0	0
4	G	28	0	25	0	0



8I]	DP

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Ι	28	0	25	0	0
4	М	28	0	25	0	0
4	0	28	0	25	0	0
5	Н	105	0	88	1	0
6	J	61	0	52	0	0
6	Р	61	0	52	0	0
7	Ν	105	0	88	1	0
8	А	14	0	13	0	0
8	В	28	0	26	0	0
8	С	28	0	26	0	0
8	D	28	0	26	0	0
9	А	24	0	32	2	0
9	В	18	0	24	2	0
9	С	42	0	56	8	0
9	D	24	0	31	3	0
10	А	13	0	18	2	0
10	С	13	0	18	2	0
10	D	13	0	18	1	0
11	В	7	0	10	0	0
12	А	366	0	0	1	0
12	В	412	0	0	0	0
12	С	363	0	0	3	0
12	D	380	0	0	2	0
All	All	16663	0	14075	55	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 2.

The worst 5 of 55 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:C:163:ASN:HA	9:C:1904:GOL:H31	1.73	0.71	
1:A:417:LEU:HA	1:A:420:ARG:HH21	1.61	0.65	
9:C:1908:GOL:H12	10:C:1909:PG4:H42	1.82	0.62	
9:C:1908:GOL:C1	10:C:1909:PG4:H42	2.29	0.62	
1:D:28:GLN:NE2	12:D:1201:HOH:O	2.33	0.62	

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	Perce	ntiles
1	А	450/462~(97%)	432 (96%)	15 (3%)	3 (1%)	22	10
1	В	447/462~(97%)	430 (96%)	15 (3%)	2~(0%)	34	21
1	С	448/462~(97%)	429 (96%)	16 (4%)	3 (1%)	22	10
1	D	444/462~(96%)	429 (97%)	12 (3%)	3 (1%)	22	10
All	All	1789/1848~(97%)	1720 (96%)	58 (3%)	11 (1%)	25	12

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	273	SER
1	А	273	SER
1	С	273	SER
1	С	333	TRP
1	В	333	TRP

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	А	377/383~(98%)	373~(99%)	4 (1%)	73 68		
1	В	374/383~(98%)	372 (100%)	2 (0%)	88 87		
1	С	375/383~(98%)	372~(99%)	3 (1%)	81 78		
1	D	373/383~(97%)	370~(99%)	3 (1%)	81 78		
All	All	1499/1532~(98%)	1487 (99%)	12 (1%)	81 78		



5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	В	136	ASN
1	В	333	TRP
1	D	333	TRP
1	D	136	ASN
1	А	420	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	С	33	GLN
1	С	109	GLN
1	В	26	ASN
1	В	415	GLN
1	D	255	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)

70 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 Tw	Turne	Chain	Dog	Tink	Bond lengths			Bond angles		
	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	NAG	Е	1	2,1	14,14,15	0.58	0	17,19,21	0.60	0
2	MAN	Е	10	2	11,11,12	0.69	0	$15,\!15,\!17$	1.10	2 (13%)



	T		D	т 1.	Bo	Bond lengths		Bond angles			
NIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	MAN	Е	11	2	$11,\!11,\!12$	0.85	1 (9%)	$15,\!15,\!17$	0.98	2 (13%)	
2	NAG	Е	2	2	14,14,15	0.22	0	17,19,21	0.55	0	
2	BMA	Е	3	2	11,11,12	0.78	0	15,15,17	0.89	0	
2	MAN	Е	4	2	$11,\!11,\!12$	0.84	0	$15,\!15,\!17$	1.12	2 (13%)	
2	MAN	Е	5	2	11,11,12	0.85	0	15,15,17	0.98	1 (6%)	
2	MAN	Е	6	2	11,11,12	0.95	0	15,15,17	0.87	0	
2	MAN	Е	7	2	11,11,12	0.68	0	15,15,17	1.12	2 (13%)	
2	MAN	Е	8	2	11,11,12	1.06	0	15,15,17	0.92	0	
2	MAN	Е	9	2	11,11,12	1.07	0	15,15,17	1.16	1 (6%)	
3	NAG	F	1	1,3	14,14,15	0.15	0	17,19,21	0.65	0	
3	NAG	F	2	3	14,14,15	0.44	0	17,19,21	0.45	0	
3	BMA	F	3	3	11,11,12	0.77	0	15,15,17	0.86	0	
3	MAN	F	4	3	11,11,12	0.86	0	15,15,17	1.03	2 (13%)	
3	MAN	F	5	3	11,11,12	1.09	1 (9%)	15,15,17	1.03	1 (6%)	
3	MAN	F	6	3	11,11,12	0.88	0	15,15,17	1.09	1 (6%)	
4	NAG	G	1	4,1	14,14,15	0.31	0	17,19,21	0.75	1 (5%)	
4	NAG	G	2	4	14,14,15	0.33	0	17,19,21	0.50	0	
5	NAG	Н	1	5,1	14,14,15	0.42	0	17,19,21	0.61	0	
5	NAG	Н	2	5	14,14,15	0.37	0	17,19,21	0.54	0	
5	BMA	Н	3	5	11,11,12	0.74	0	$15,\!15,\!17$	0.91	1 (6%)	
5	MAN	Н	4	5	11,11,12	0.81	0	15,15,17	1.41	2 (13%)	
5	MAN	Н	5	5	11,11,12	0.60	0	15,15,17	1.24	2 (13%)	
5	MAN	Н	6	5	11,11,12	0.72	0	15,15,17	1.13	2 (13%)	
5	MAN	Н	7	5	11,11,12	1.07	2 (18%)	15,15,17	1.49	3 (20%)	
5	MAN	Н	8	5	11,11,12	0.63	0	15,15,17	1.05	2 (13%)	
5	MAN	Н	9	5	11,11,12	0.92	0	15,15,17	0.96	2 (13%)	
4	NAG	Ι	1	4,1	14,14,15	0.28	0	17,19,21	0.56	0	
4	NAG	Ι	2	4	14,14,15	0.24	0	17,19,21	0.64	1 (5%)	
6	NAG	J	1	1,6	14,14,15	0.21	0	17,19,21	0.62	0	
6	NAG	J	2	6	14,14,15	0.42	0	17,19,21	0.60	0	
6	BMA	J	3	6	11,11,12	0.79	0	15,15,17	0.85	0	
6	MAN	J	4	6	11,11,12	0.87	0	$15,\!15,\!17$	1.05	2 (13%)	
6	MAN	J	5	6	11,11,12	0.87	0	15,15,17	1.01	1 (6%)	
2	NAG	K	1	2,1	14,14,15	0.56	0	17,19,21	0.56	0	
2	MAN	K	10	2	11,11,12	0.77	0	15,15,17	1.20	2 (13%)	
2	MAN	K	11	2	11,11,12	0.92	0	15,15,17	1.17	2 (13%)	
2	NAG	K	2	2	14,14,15	0.37	0	17,19,21	0.57	0	
2	BMA	K	3	2	11,11,12	0.67	0	15,15,17	$0.8\overline{6}$	0	



Mal	Tuno	Chain	Dog	Link	Bo	Bond lengths		Bond angles		
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	K	4	2	11,11,12	0.79	0	$15,\!15,\!17$	0.95	0
2	MAN	К	5	2	11,11,12	0.77	0	$15,\!15,\!17$	1.51	3 (20%)
2	MAN	К	6	2	11,11,12	0.86	0	$15,\!15,\!17$	1.08	1 (6%)
2	MAN	K	7	2	11,11,12	0.72	0	$15,\!15,\!17$	1.13	2 (13%)
2	MAN	K	8	2	11,11,12	0.84	0	$15,\!15,\!17$	0.88	1 (6%)
2	MAN	K	9	2	11,11,12	0.79	1 (9%)	$15,\!15,\!17$	1.07	1 (6%)
3	NAG	L	1	1,3	14,14,15	0.19	0	17,19,21	0.59	0
3	NAG	L	2	3	14,14,15	0.58	0	17,19,21	0.56	0
3	BMA	L	3	3	11,11,12	0.70	0	$15,\!15,\!17$	0.83	0
3	MAN	L	4	3	11,11,12	0.81	0	$15,\!15,\!17$	1.10	2 (13%)
3	MAN	L	5	3	11,11,12	0.96	0	$15,\!15,\!17$	1.19	1 (6%)
3	MAN	L	6	3	11,11,12	1.01	1 (9%)	$15,\!15,\!17$	0.98	1 (6%)
4	NAG	М	1	4,1	14,14,15	0.27	0	17,19,21	0.63	0
4	NAG	М	2	4	14,14,15	0.53	0	17,19,21	0.56	0
7	NAG	N	1	7,1	14,14,15	0.50	0	17,19,21	0.68	0
7	NAG	N	2	7	14,14,15	0.29	0	17,19,21	0.55	0
7	BMA	Ν	3	7	$11,\!11,\!12$	0.71	0	$15,\!15,\!17$	0.79	0
7	MAN	Ν	4	7	11,11,12	0.94	1 (9%)	$15,\!15,\!17$	1.16	1 (6%)
7	MAN	Ν	5	7	11,11,12	1.15	1 (9%)	$15,\!15,\!17$	1.18	2 (13%)
7	MAN	Ν	6	7	11,11,12	0.85	0	$15,\!15,\!17$	0.91	1 (6%)
7	MAN	Ν	7	7	11,11,12	0.90	0	$15,\!15,\!17$	1.23	2 (13%)
7	MAN	Ν	8	7	11,11,12	0.54	0	$15,\!15,\!17$	0.97	2 (13%)
7	MAN	Ν	9	7	11,11,12	0.78	0	$15,\!15,\!17$	1.00	1 (6%)
4	NAG	0	1	4,1	$14,\!14,\!15$	0.31	0	17,19,21	0.63	0
4	NAG	Ο	2	4	14,14,15	0.42	0	$17,\!19,\!21$	0.61	1 (5%)
6	NAG	Р	1	1,6	14,14,15	0.20	0	17,19,21	0.57	0
6	NAG	Р	2	6	14,14,15	0.34	0	17,19,21	0.45	0
6	BMA	Р	3	6	11,11,12	0.70	0	$15,\!15,\!17$	0.73	0
6	MAN	Р	4	6	11,11,12	1.25	2 (18%)	15, 15, 17	0.91	0
6	MAN	Р	5	6	11,11,12	0.76	0	$15,\!15,\!17$	1.22	2 (13%)

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	Е	1	2,1	-	0/6/23/26	0/1/1/1
2	MAN	Е	10	2	-	0/2/19/22	0/1/1/1



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings		
2	MAN	Е	11	2	-	0/2/19/22	0/1/1/1		
2	NAG	Е	2	2	-	0/6/23/26	0/1/1/1		
2	BMA	Е	3	2	-	0/2/19/22	0/1/1/1		
2	MAN	Е	4	2	-	0/2/19/22	0/1/1/1		
2	MAN	Е	5	2	-	2/2/19/22	0/1/1/1		
2	MAN	Е	6	2	-	0/2/19/22	0/1/1/1		
2	MAN	Е	7	2	-	0/2/19/22	0/1/1/1		
2	MAN	Е	8	2	-	1/2/19/22	0/1/1/1		
2	MAN	Е	9	2	-	0/2/19/22	0/1/1/1		
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1		
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1		
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1		
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1		
3	MAN	F	5	3	-	1/2/19/22	0/1/1/1		
3	MAN	F	6	3	-	1/2/19/22	0/1/1/1		
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1		
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1		
5	NAG	Н	1	5,1	-	0/6/23/26	0/1/1/1		
5	NAG	Н	2	5	-	0/6/23/26	0/1/1/1		
5	BMA	Н	3	5	-	0/2/19/22	0/1/1/1		
5	MAN	Н	4	5	-	0/2/19/22	0/1/1/1		
5	MAN	Н	5	5	-	0/2/19/22	0/1/1/1		
5	MAN	Н	6	5	-	0/2/19/22	0/1/1/1		
5	MAN	Н	7	5	-	2/2/19/22	0/1/1/1		
5	MAN	Н	8	5	-	0/2/19/22	0/1/1/1		
5	MAN	Н	9	5	-	0/2/19/22	0/1/1/1		
4	NAG	Ι	1	4,1	-	0/6/23/26	0/1/1/1		
4	NAG	Ι	2	4	-	0/6/23/26	0/1/1/1		
6	NAG	J	1	1,6	-	0/6/23/26	0/1/1/1		
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1		
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1		
6	MAN	J	4	6	-	1/2/19/22	0/1/1/1		
6	MAN	J	5	6	-	2/2/19/22	0/1/1/1		
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1		
2	MAN	K	10	2	-	0/2/19/22	0/1/1/1		
2	MAN	K	11	2	-	0/2/19/22	0/1/1/1		
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1		
2	BMA	K	3	2	-	0/2/19/22	0/1/1/1		
2	MAN	K	4	2	-	0/2/19/22	0/1/1/1		
2	MAN	K	5	2	-	2/2/19/22	0/1/1/1		
2	MAN	K	6	2	-	0/2/19/22	0/1/1/1		



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	K	7	2	-	0/2/19/22	0/1/1/1
2	MAN	K	8	2	-	0/2/19/22	0/1/1/1
2	MAN	K	9	2	-	0/2/19/22	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
3	MAN	L	4	3	-	2/2/19/22	0/1/1/1
3	MAN	L	5	3	-	1/2/19/22	0/1/1/1
3	MAN	L	6	3	-	0/2/19/22	0/1/1/1
4	NAG	М	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	М	2	4	-	0/6/23/26	0/1/1/1
7	NAG	N	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	0/6/23/26	0/1/1/1
7	BMA	N	3	7	-	0/2/19/22	0/1/1/1
7	MAN	N	4	7	-	0/2/19/22	0/1/1/1
7	MAN	N	5	7	-	0/2/19/22	0/1/1/1
7	MAN	N	6	7	-	0/2/19/22	0/1/1/1
7	MAN	N	7	7	-	0/2/19/22	0/1/1/1
7	MAN	N	8	7	-	0/2/19/22	0/1/1/1
7	MAN	N	9	7	-	0/2/19/22	0/1/1/1
4	NAG	0	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	0	2	4	-	0/6/23/26	0/1/1/1
6	NAG	Р	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	Р	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Р	3	6	-	0/2/19/22	0/1/1/1
6	MAN	Р	4	6	-	0/2/19/22	0/1/1/1
6	MAN	Р	5	6	-	0/2/19/22	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	F	5	MAN	C2-C3	2.43	1.56	1.52
6	Р	4	MAN	O5-C1	-2.42	1.39	1.43
7	Ν	5	MAN	O5-C5	2.33	1.48	1.43
6	Р	4	MAN	C2-C3	2.24	1.55	1.52
2	Е	11	MAN	O5-C5	2.19	1.47	1.43

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	L	5	MAN	C1-O5-C5	3.81	117.35	112.19
5	Н	5	MAN	C1-O5-C5	3.71	117.21	112.19



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Κ	5	MAN	C1-O5-C5	3.67	117.16	112.19
6	Р	5	MAN	C1-O5-C5	3.62	117.09	112.19
7	Ν	7	MAN	C1-O5-C5	3.58	117.04	112.19

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	5	MAN	C4-C5-C6-O6
6	J	5	MAN	O5-C5-C6-O6
3	L	4	MAN	C4-C5-C6-O6
3	L	4	MAN	O5-C5-C6-O6
2	Е	5	MAN	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Е	9	MAN	1	0
5	Н	7	MAN	1	0
7	N	5	MAN	1	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)

29 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).

Mal	Tuno	Chain	Dec	Link	Bo	ond leng	$_{\rm ths}$	Bond angles		
MOI	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
10	PG4	D	1107	-	12,12,12	0.17	0	11,11,11	0.57	0
8	NAG	D	1101	1	14,14,15	0.60	0	17,19,21	0.55	0
9	GOL	D	1102	-	$5,\!5,\!5$	1.07	0	$5,\!5,\!5$	0.95	0
9	GOL	С	1905	-	$5,\!5,\!5$	0.81	0	$5,\!5,\!5$	1.20	0





Mal	Type	Chain	Dog	Link	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
8	NAG	А	501	1	14,14,15	0.42	0	17,19,21	0.91	1 (5%)
9	GOL	С	1908	-	$5,\!5,\!5$	0.97	0	$5,\!5,\!5$	0.95	0
10	PG4	С	1909	-	12,12,12	0.15	0	11,11,11	0.80	1 (9%)
9	GOL	С	1901[B]	-	$5,\!5,\!5$	0.78	0	$5,\!5,\!5$	0.99	0
9	GOL	С	1901[A]	-	$5,\!5,\!5$	0.64	0	5,5,5	1.19	1 (20%)
9	GOL	В	2102	-	$5,\!5,\!5$	0.98	0	$5,\!5,\!5$	0.84	0
10	PG4	А	505	-	12,12,12	0.17	0	11,11,11	0.59	0
8	NAG	В	2101	1	14,14,15	0.34	0	17,19,21	0.65	0
9	GOL	D	1106	-	$5,\!5,\!5$	0.97	0	$5,\!5,\!5$	0.76	0
8	NAG	В	2104	1	14,14,15	0.20	0	17,19,21	0.50	0
9	GOL	В	2103[A]	-	$5,\!5,\!5$	0.81	0	$5,\!5,\!5$	1.06	0
8	NAG	С	1903	1	14,14,15	0.39	0	17,19,21	0.48	0
9	GOL	В	2103[B]	-	$5,\!5,\!5$	0.67	0	5, 5, 5	1.10	0
9	GOL	С	1904	-	$5,\!5,\!5$	0.93	0	$5,\!5,\!5$	1.20	1 (20%)
8	NAG	D	1103	1	14,14,15	0.27	0	17,19,21	0.65	1 (5%)
9	GOL	А	502[A]	-	$5,\!5,\!5$	0.70	0	$5,\!5,\!5$	1.15	1 (20%)
9	GOL	D	1105	-	$5,\!5,\!5$	0.63	0	5,5,5	1.01	0
9	GOL	А	502[B]	-	$5,\!5,\!5$	0.90	0	$5,\!5,\!5$	0.98	0
9	GOL	С	1907	-	$5,\!5,\!5$	1.12	0	$5,\!5,\!5$	0.85	0
9	GOL	А	504	-	$5,\!5,\!5$	0.68	0	$5,\!5,\!5$	1.19	0
9	GOL	А	503	-	$5,\!5,\!5$	0.79	0	$5,\!5,\!5$	0.93	0
9	GOL	D	1104	-	5,5,5	0.81	0	5,5,5	1.23	1 (20%)
11	PEG	В	2105	-	6,6,6	0.15	0	$5,\!5,\!5$	0.07	0
9	GOL	С	1906	-	$5,\!5,\!5$	0.93	0	$5,\!5,\!5$	1.02	0
8	NAG	С	1902	1	14,14,15	0.29	0	17,19,21	0.48	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
10	PG4	D	1107	-	-	2/10/10/10	-
8	NAG	D	1101	1	-	0/6/23/26	0/1/1/1
9	GOL	D	1102	-	-	0/4/4/4	-
9	GOL	С	1905	-	-	4/4/4/4	-
8	NAG	А	501	1	-	2/6/23/26	0/1/1/1
9	GOL	С	1908	-	-	0/4/4/4	-
10	PG4	С	1909	-	-	8/10/10/10	-
9	GOL	С	1901[B]	-	-	2/4/4/4	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	С	1901[A]	-	-	0/4/4/4	-
9	GOL	В	2102	-	-	2/4/4/4	-
10	PG4	А	505	-	-	7/10/10/10	-
8	NAG	В	2101	1	-	0/6/23/26	0/1/1/1
9	GOL	D	1106	-	-	2/4/4/4	-
8	NAG	В	2104	1	-	2/6/23/26	0/1/1/1
9	GOL	В	2103[A]	-	-	1/4/4/4	-
8	NAG	С	1903	1	-	0/6/23/26	0/1/1/1
9	GOL	В	2103[B]	-	-	2/4/4/4	-
9	GOL	С	1904	-	-	4/4/4/4	-
8	NAG	D	1103	1	-	1/6/23/26	0/1/1/1
9	GOL	А	502[A]	-	-	2/4/4/4	-
9	GOL	D	1105	-	-	2/4/4/4	-
9	GOL	А	502[B]	-	-	2/4/4/4	-
9	GOL	С	1907	-	-	2/4/4/4	-
9	GOL	А	504	-	-	2/4/4/4	-
9	GOL	А	503	-	-	4/4/4/4	-
9	GOL	D	1104	-	-	2/4/4/4	-
11	PEG	В	2105	-	-	3/4/4/4	-
9	GOL	С	1906	-	-	1/4/4/4	-
8	NAG	С	1902	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
8	А	501	NAG	C1-O5-C5	3.19	116.51	112.19
9	D	1104	GOL	C3-C2-C1	-2.36	102.55	111.70
8	D	1103	NAG	C1-O5-C5	2.26	115.25	112.19
9	С	1904	GOL	C3-C2-C1	-2.23	103.04	111.70
9	А	502[A]	GOL	C3-C2-C1	-2.22	103.07	111.70

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	А	502[A]	GOL	C1-C2-C3-O3
9	А	502[A]	GOL	O2-C2-C3-O3



Mol	Chain	Res	Type	Atoms
9	А	503	GOL	O1-C1-C2-C3
9	С	1901[B]	GOL	C1-C2-C3-O3
9	С	1904	GOL	O1-C1-C2-C3

Continued from previous page...

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes
10	D	1107	PG4	1	0
9	D	1102	GOL	1	0
9	С	1908	GOL	4	0
10	С	1909	PG4	2	0
9	В	2102	GOL	2	0
10	А	505	PG4	2	0
9	D	1106	GOL	1	0
9	С	1904	GOL	3	0
9	А	504	GOL	1	0
9	А	503	GOL	1	0
9	D	1104	GOL	1	0
9	С	1906	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 (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, 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	А	446/462~(96%)	-0.12	6 (1%) 77 74	14, 20, 34, 62	0
1	В	446/462~(96%)	-0.21	5 (1%) 80 78	14, 19, 33, 60	0
1	С	446/462~(96%)	-0.18	9 (2%) 65 61	14, 20, 37, 57	0
1	D	445/462~(96%)	-0.22	6 (1%) 77 74	15, 19, 34, 58	0
All	All	1783/1848~(96%)	-0.18	26 (1%) 73 70	14, 20, 35, 62	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	56	THR	6.5
1	А	417	LEU	4.8
1	В	443	HIS	4.7
1	А	418	LYS	4.6
1	D	443	HIS	4.6

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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
6	MAN	Р	4	11/12	0.63	0.31	37,44,48,51	0
6	MAN	J	5	11/12	0.70	0.29	44,50,57,59	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(A ²)	Q<0.9
2	MAN	E	9	11/12	0.71	0.24	33,36,39,39	0
3	MAN	F'	5	11/12	0.74	0.34	42,47,55,56	0
3	MAN	F	6	11/12	0.75	0.24	36,42,47,49	0
4	NAG	0	2	14/15	0.75	0.28	34,39,43,43	0
6	MAN	P	5	11/12	0.76	0.29	44,47,53,59	0
3	MAN	L	5	11/12	0.77	0.34	38,47,54,55	0
5	MAN	Н	7	11/12	0.79	0.18	34,36,39,45	0
6	MAN	J	4	11/12	0.81	0.25	47,55,59,63	0
2	MAN	K	5	11/12	0.81	0.21	38,43,51,53	0
3	MAN	F	4	11/12	0.82	0.35	41,45,53,55	0
2	MAN	E	6	11/12	0.83	0.37	$43,\!51,\!57,\!59$	0
3	BMA	F	3	11/12	0.84	0.15	27,33,35,36	0
4	NAG	G	2	14/15	0.84	0.20	32,36,44,49	0
4	NAG	Ι	2	14/15	0.84	0.26	$31,\!39,\!48,\!52$	0
7	MAN	Ν	9	11/12	0.85	0.14	$34,\!38,\!40,\!42$	0
3	MAN	L	4	11/12	0.86	0.37	$42,\!46,\!52,\!54$	0
2	MAN	Е	7	11/12	0.86	0.13	$25,\!30,\!31,\!32$	0
3	MAN	L	6	11/12	0.86	0.19	38,40,46,46	0
4	NAG	М	2	14/15	0.87	0.16	$29,\!35,\!45,\!48$	0
2	MAN	Е	5	11/12	0.87	0.13	34,41,44,44	0
2	MAN	Е	10	11/12	0.88	0.13	28,29,35,37	0
2	MAN	K	6	11/12	0.89	0.23	40,44,49,49	0
2	MAN	K	10	11/12	0.89	0.14	24,26,28,29	0
6	BMA	J	3	11/12	0.89	0.18	29,34,41,42	0
2	MAN	Е	8	11/12	0.89	0.15	26,31,33,34	0
5	MAN	Н	6	11/12	0.91	0.11	$26,\!31,\!37,\!38$	0
2	MAN	K	7	11/12	0.91	0.10	23,27,29,29	0
2	MAN	K	8	11/12	0.91	0.15	30,33,37,38	0
2	NAG	K	1	14/15	0.91	0.12	20,24,29,29	0
3	NAG	F	2	14/15	0.91	0.17	24,26,30,37	0
2	MAN	K	4	11/12	0.91	0.12	31,35,36,40	0
5	BMA	Н	3	11/12	0.91	0.09	23,27,30,31	0
5	MAN	Н	4	11/12	0.91	0.11	29,32,41,41	0
6	NAG	Р	1	14/15	0.92	0.10	19,26,29,30	0
6	BMA	Р	3	11/12	0.92	0.17	27,33,38,39	0
5	MAN	Н	5	11/12	0.92	0.12	27,33,37,39	0
4	NAG	0	1	14/15	0.92	0.11	16,20,23,26	0
2	BMA	K	3	11/12	0.92	0.10	24,26,30,31	0
4	NAG	Ι	1	14/15	0.93	0.09	17,18,24,25	0
2	NAG	Е	1	14/15	0.93	0.10	22,26,29,30	0
6	NAG	Р	2	14/15	0.93	0.13	23,27,31,37	0
5	MAN	Н	9	11/12	0.93	0.13	37,42,49,50	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	J	2	14/15	0.93	0.11	24,30,33,39	0
3	BMA	L	3	11/12	0.93	0.19	25,31,37,40	0
7	NAG	N	1	14/15	0.93	0.10	20,25,32,34	0
7	MAN	N	8	11/12	0.93	0.11	23,28,32,33	0
2	MAN	Е	4	11/12	0.93	0.10	28,29,32,32	0
5	NAG	Н	1	14/15	0.94	0.09	25,27,29,29	0
2	NAG	K	2	14/15	0.94	0.10	22,25,28,28	0
2	MAN	Κ	9	11/12	0.94	0.14	29,34,38,41	0
2	MAN	Е	11	11/12	0.94	0.08	$26,\!31,\!35,\!39$	0
2	MAN	K	11	11/12	0.94	0.09	25,27,32,33	0
3	NAG	L	1	14/15	0.94	0.09	20,25,31,34	0
3	NAG	L	2	14/15	0.94	0.16	23,26,31,37	0
6	NAG	J	1	14/15	0.94	0.09	22,27,32,33	0
7	MAN	N	6	11/12	0.94	0.13	29,32,36,37	0
3	NAG	F	1	14/15	0.94	0.08	20,24,33,36	0
2	NAG	Е	2	14/15	0.94	0.09	22,25,29,31	0
7	MAN	N	4	11/12	0.95	0.08	23,24,25,26	0
2	BMA	Е	3	11/12	0.95	0.09	23,26,27,28	0
7	MAN	N	7	11/12	0.95	0.08	24,26,28,28	0
4	NAG	G	1	14/15	0.95	0.07	16,18,23,24	0
5	MAN	Н	8	11/12	0.95	0.07	29,31,34,34	0
7	NAG	N	2	14/15	0.96	0.08	22,25,27,28	0
4	NAG	М	1	14/15	0.96	0.07	15,19,21,23	0
5	NAG	Н	2	14/15	0.96	0.09	23,27,29,30	0
7	BMA	Ν	3	11/12	0.97	0.06	23,25,29,30	0
7	MAN	N	5	11/12	0.97	0.10	23,26,27,29	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.









































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, 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	${f B} ext{-factors}({ m \AA}^2)$	Q < 0.9
8	NAG	А	501	14/15	0.78	0.28	$44,\!51,\!57,\!59$	0
8	NAG	С	1902	14/15	0.80	0.30	$41,\!47,\!50,\!52$	0
9	GOL	С	1904	6/6	0.80	0.14	24,32,34,38	0
10	PG4	С	1909	13/13	0.80	0.36	32,37,43,49	0
9	GOL	А	504	6/6	0.81	0.21	$26,\!34,\!36,\!39$	0
10	PG4	D	1107	13/13	0.82	0.25	$29,\!35,\!46,\!47$	0
9	GOL	А	502[A]	6/6	0.83	0.18	24,25,28,28	6
9	GOL	A	502[B]	6/6	0.83	0.18	24,27,29,29	6
8	NAG	В	2104	14/15	0.84	0.19	40,44,51,52	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q<0.9
9	GOL	С	1905	6/6	0.84	0.24	$31,\!32,\!36,\!42$	0
9	GOL	С	1908	6/6	0.85	0.37	$30,\!35,\!38,\!39$	0
11	PEG	В	2105	7/7	0.85	0.20	$29,\!35,\!37,\!44$	0
8	NAG	D	1103	14/15	0.86	0.20	39,46,50,54	0
9	GOL	В	2103[A]	6/6	0.86	0.16	20,26,27,30	6
9	GOL	В	2103[B]	6/6	0.86	0.16	23,25,27,30	6
9	GOL	С	1907	6/6	0.87	0.26	$19,\!30,\!37,\!39$	0
9	GOL	С	1906	6/6	0.87	0.20	39,39,42,43	0
9	GOL	D	1106	6/6	0.87	0.22	$32,\!33,\!35,\!37$	0
10	PG4	А	505	13/13	0.88	0.22	31,36,40,46	0
9	GOL	D	1104	6/6	0.88	0.17	$26,\!28,\!33,\!35$	0
9	GOL	А	503	6/6	0.89	0.28	$28,\!31,\!38,\!44$	0
9	GOL	С	1901[A]	6/6	0.89	0.17	$22,\!26,\!27,\!28$	6
9	GOL	D	1105	6/6	0.89	0.14	$25,\!30,\!33,\!42$	0
9	GOL	С	1901[B]	6/6	0.89	0.17	$21,\!25,\!28,\!28$	6
8	NAG	С	1903	14/15	0.91	0.10	$21,\!25,\!29,\!32$	0
8	NAG	D	1101	14/15	0.93	0.09	$19,\!23,\!30,\!31$	0
9	GOL	D	1102	6/6	0.94	0.13	20,28,29,29	0
8	NAG	В	2101	14/15	0.94	0.14	20,22,27,34	0
9	GOL	B	2102	6/6	0.95	0.14	18,27,28,31	0

6.5 Other polymers (i)

There are no such residues in this entry.

