

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	2YLA
Title	:	INHIBITION OF THE PNEUMOCOCCAL VIRULENCE FACTOR STRH
		AND MOLECULAR INSIGHTS INTO N-GLYCAN RECOGNITION AND
		HYDROLYSIS
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Deposited on	:	2011-06-01
Resolution	:	2.70 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

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 2.70 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	Similar resolution
	(#Entries)	(#Entries, resolution range(A))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069(2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	А	442	% 7 9%	12%	•	6%
1	В	442	77%	16%		• 6%
1	С	442	.% 7 9%	12%	•	8%
1	D	442	% 	11%	•	8%



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Mol	Chain	Length		Quality of chain	
2	Е	5	20%	60%	20%
2	F	5	40%	40%	20%
2	Н	5	20%	80%	
3	G	4		100%	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	Е	1	-	-	-	Х
2	BMA	Е	2	-	-	-	Х
2	NAG	Е	5	-	-	-	Х
2	NAG	F	1	-	-	-	Х
2	NAG	F	5	-	-	-	Х
2	NAG	Н	1	-	-	-	Х
2	BMA	Н	2	-	-	-	Х
2	NAG	Н	5	-	-	-	Х
4	EDO	А	1107	-	-	-	Х
4	EDO	В	1110	-	-	-	Х
4	EDO	В	1113	-	-	-	Х
4	EDO	В	1114	-	-	-	Х



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14253 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 A 416	416	Total	С	Ν	0	\mathbf{S}	-91	9	0
1	Л	410	3321	2128	542	639	12	21	2	0
1	р	417	Total	С	Ν	0	S	12	0	0
	D	417	3317	2126	539	640	12	10	0	0
1	C	408	Total	С	Ν	0	S	16	2	0
		U 408	3267	2097	532	626	12	10		0
1	а	408	Total	С	Ν	0	S	28	1	0
	408	3261	2092	531	626	12	20		0	

• Molecule 1 is a protein called BETA-N-ACETYLHEXOSAMINIDASE.

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	623	GLY	-	expression tag	UNP P49610
А	624	SER	-	expression tag	UNP P49610
А	625	HIS	-	expression tag	UNP P49610
А	626	MET	-	expression tag	UNP P49610
А	805	GLN	GLU	engineered mutation	UNP P49610
В	623	GLY	-	expression tag	UNP P49610
В	624	SER	-	expression tag	UNP P49610
В	625	HIS	-	expression tag	UNP P49610
В	626	MET	-	expression tag	UNP P49610
В	805	GLN	GLU	engineered mutation	UNP P49610
С	623	GLY	-	expression tag	UNP P49610
С	624	SER	-	expression tag	UNP P49610
С	625	HIS	-	expression tag	UNP P49610
С	626	MET	-	expression tag	UNP P49610
С	805	GLN	GLU	engineered mutation	UNP P49610
D	623	GLY	-	expression tag	UNP P49610
D	624	SER	-	expression tag	UNP P49610
D	625	HIS	-	expression tag	UNP P49610
D	626	MET	-	expression tag	UNP P49610
D	805	GLN	GLU	engineered mutation	UNP P49610



• Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alp ha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mann opyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	Е	5	Total C N O 65 36 3 26	0	0	0
2	F	5	Total C N O 65 36 3 26	0	0	0
2	Н	5	Total C N O 65 36 3 26	0	0	0

• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alp ha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
3	G	4	Total 51	C 28	N 2	O 21	0	0	0

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).







Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	O 2	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	172	Total O 174 174	0	2
5	В	197	Total O 200 200	0	3
5	С	235	Total O 237 237	0	2
5	D	168	Total O 170 170	0	2



3 Residue-property plots (i)

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



• Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE



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

Chain E:	20%	60%	20%
NAG1 BMA2 MAN3 NAG4 NAG5			

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

Chain F:	40%	40%	20%
NAG1 BMA2 MAN3 NAA3 NAA3 NAA3			

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

Chain H:	20%	80%
NAG 1 BMA 2 MAN3 NAG 4 NAG 5 NAG 5		

 $\bullet \ Molecule \ 3: \ 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose$

Chain G:

100%







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	67.56Å 115.71Å 132.21Å	Depositor
a, b, c, α , β , γ	90.00° 99.67° 90.00°	Depositor
Bosolution(A)	29.97 - 2.70	Depositor
Resolution (A)	29.98 - 2.70	EDS
% Data completeness	$100.0\ (29.97-2.70)$	Depositor
(in resolution range)	$100.0\ (29.98-2.70)$	EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.62 (at 2.68 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
P. P.	0.223 , 0.273	Depositor
n, n_{free}	0.221 , 0.268	DCC
R_{free} test set	2792 reflections $(5.07%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	16.3	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.31 , 27.4	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14253	wwPDB-VP
Average B, all atoms $(Å^2)$	14.0	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 57.09 % 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 2.4880e-05. 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: NAG, MAN, EDO, BMA

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	Bo	ond lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.64	9/3394~(0.3%)	0.60	7/4583~(0.2%)	
1	В	0.56	4/3392~(0.1%)	0.53	2/4583~(0.0%)	
1	С	1.13	5/3342~(0.1%)	0.63	7/4510~(0.2%)	
1	D	1.32	12/3333~(0.4%)	0.66	7/4499~(0.2%)	
All	All	0.97	30/13461~(0.2%)	0.61	23/18175~(0.1%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	В	0	1

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	С	724	GLU	CG-CD	50.47	2.27	1.51
1	D	756	LYS	CE-NZ	-47.28	0.30	1.49
1	D	1037	ALA	CA-CB	-31.76	0.85	1.52
1	С	908	LYS	CD-CE	-27.67	0.82	1.51
1	D	908	LYS	CD-CE	-22.56	0.94	1.51

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	С	724	GLU	CB-CG-CD	-16.62	69.32	114.20
1	D	764	LYS	CD-CE-NZ	-15.43	76.21	111.70
1	А	995	THR	CA-CB-CG2	-13.57	93.40	112.40
1	D	908	LYS	CG-CD-CE	13.29	151.78	111.90



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Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	\mathbf{C}	908	LYS	CG-CD-CE	10.85	144.45	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	803	THR	Peptide

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	3321	0	3252	40	0
1	В	3317	0	3240	36	0
1	С	3267	0	3207	24	0
1	D	3261	0	3194	25	0
2	Ε	65	0	57	1	0
2	F	65	0	57	2	0
2	Н	65	0	57	0	0
3	G	51	0	45	0	0
4	А	8	0	12	0	0
4	В	40	0	60	2	0
4	С	8	0	12	1	0
4	D	4	0	6	0	0
5	А	174	0	0	0	0
5	В	200	0	0	0	0
5	C	237	0	0	0	0
5	D	170	0	0	0	0
All	All	14253	0	13199	128	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 128 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:982:ASN:HD21	1:B:984:ASN:HD22	1.21	0.87
1:A:907:GLN:NE2	1:A:954:ARG:HH12	1.79	0.80
1:D:907:GLN:NE2	1:D:954:ARG:HH12	1.85	0.75
1:B:678:ASP:H	1:B:716:GLN:HE21	1.34	0.73
1:B:845:GLN:HB2	4:B:1114:EDO:H11	1.70	0.73

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	Per	centil	es
1	А	414/442~(94%)	397~(96%)	16 (4%)	1 (0%)	47	73	
1	В	415/442~(94%)	396 (95%)	17 (4%)	2 (0%)	29	54	
1	С	406/442~(92%)	389~(96%)	16 (4%)	1 (0%)	47	73	
1	D	405/442~(92%)	387~(96%)	17 (4%)	1 (0%)	47	73	
All	All	1640/1768~(93%)	1569 (96%)	66 (4%)	5 (0%)	41	66	Γ

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	804	ASP
1	D	1037	ALA
1	А	671	ASP
1	В	805	GLN
1	С	671	ASP

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.



Mol	Chain	Analysed	Rotameric	Outliers	Pe	erce	ntiles
1	А	344/363~(95%)	320~(93%)	24 (7%)		15	35
1	В	343/363~(94%)	321 (94%)	22~(6%)		17	39
1	С	338/363~(93%)	316 (94%)	22~(6%)		17	38
1	D	337/363~(93%)	309~(92%)	28 (8%)		11	25
All	All	1362/1452~(94%)	1266 (93%)	96 (7%)		14	35

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

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	С	887	LEU
1	D	654	ASP
1	С	910	GLU
1	С	1006	GLU
1	D	744	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	907	GLN
1	С	1033	ASN
1	С	922	ASN
1	С	975	ASN
1	D	716	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)

19 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).

Mal	Tuno	Chain	Dog	Tink	Bo	Bond lengths		Bond angles		
IVIOI	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1	2	$15,\!15,\!15$	0.53	0	21,21,21	1.67	5 (23%)
2	BMA	Е	2	2	11,11,12	0.89	0	15,15,17	0.86	0
2	MAN	Е	3	2	11,11,12	0.54	0	$15,\!15,\!17$	0.94	1 (6%)
2	NAG	Е	4	2	14,14,15	0.68	1 (7%)	17,19,21	2.19	3 (17%)
2	NAG	Е	5	2	14,14,15	0.61	0	17,19,21	2.15	3 (17%)
2	NAG	F	1	2	$15,\!15,\!15$	0.45	0	21,21,21	0.84	0
2	BMA	F	2	2	11,11,12	0.91	0	15,15,17	0.84	0
2	MAN	F	3	2	11,11,12	0.55	0	$15,\!15,\!17$	1.19	1 (6%)
2	NAG	F	4	2	14,14,15	0.63	0	17,19,21	2.15	4 (23%)
2	NAG	F	5	2	14,14,15	0.56	0	17,19,21	2.04	3 (17%)
3	NAG	G	1	3	$15,\!15,\!15$	0.57	0	21,21,21	1.45	4 (19%)
3	BMA	G	2	3	11,11,12	0.81	0	$15,\!15,\!17$	0.91	1 (6%)
3	MAN	G	3	3	11,11,12	0.51	0	15,15,17	0.98	1 (6%)
3	NAG	G	4	3	14,14,15	0.63	0	17,19,21	2.17	3 (17%)
2	NAG	Н	1	2	15,15,15	0.57	0	21,21,21	1.46	4 (19%)
2	BMA	Н	2	2	11,11,12	0.85	0	15,15,17	0.87	0
2	MAN	Н	3	2	11,11,12	0.57	0	15,15,17	0.92	1 (6%)
2	NAG	Н	4	2	14,14,15	0.70	1 (7%)	17,19,21	2.10	4 (23%)
2	NAG	Н	5	2	14,14,15	0.59	0	17,19,21	1.23	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	Е	1	2	-	4/6/26/26	0/1/1/1
2	BMA	Е	2	2	-	2/2/19/22	0/1/1/1
2	MAN	Е	3	2	-	2/2/19/22	0/1/1/1
2	NAG	Е	4	2	-	1/6/23/26	0/1/1/1
2	NAG	E	5	2	-	4/6/23/26	0/1/1/1

2YLA

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	1	2	-	2/6/26/26	0/1/1/1
2	BMA	F	2	2	-	0/2/19/22	0/1/1/1
2	MAN	F	3	2	-	1/2/19/22	0/1/1/1
2	NAG	F	4	2	-	1/6/23/26	0/1/1/1
2	NAG	F	5	2	-	3/6/23/26	0/1/1/1
3	NAG	G	1	3	-	5/6/26/26	0/1/1/1
3	BMA	G	2	3	-	0/2/19/22	0/1/1/1
3	MAN	G	3	3	-	1/2/19/22	0/1/1/1
3	NAG	G	4	3	-	3/6/23/26	0/1/1/1
2	NAG	Н	1	2	-	3/6/26/26	0/1/1/1
2	BMA	Н	2	2	-	0/2/19/22	0/1/1/1
2	MAN	Н	3	2	-	2/2/19/22	0/1/1/1
2	NAG	Н	4	2	-	2/6/23/26	0/1/1/1
2	NAG	Н	5	2	-	3/6/23/26	0/1/1/1

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All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	Н	4	NAG	C1-C2	2.22	1.55	1.52
2	Е	4	NAG	C1-C2	2.15	1.55	1.52

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Е	5	NAG	C2-N2-C7	7.11	133.03	122.90
3	G	4	NAG	C1-O5-C5	7.06	121.76	112.19
2	F	4	NAG	C1-O5-C5	6.84	121.45	112.19
2	F	5	NAG	C2-N2-C7	6.72	132.47	122.90
2	Е	4	NAG	C1-O5-C5	6.56	121.08	112.19

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Е	5	NAG	C3-C2-N2-C7
2	F	5	NAG	C3-C2-N2-C7
2	Е	3	MAN	O5-C5-C6-O6
3	G	4	NAG	O5-C5-C6-O6
2	Е	3	MAN	C4-C5-C6-O6



There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	5	NAG	2	0
2	Е	5	NAG	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)

15 ligands are modelled in this entry.



2YLA

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	Turne	Chain	Dec	Tink	В	ond leng	gths	Bond angles			
	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
4	EDO	В	1107	-	$3,\!3,\!3$	0.50	0	$2,\!2,\!2$	0.27	0	
4	EDO	В	1109	-	3,3,3	0.46	0	2,2,2	0.32	0	
4	EDO	В	1110	-	3,3,3	0.48	0	2,2,2	0.31	0	
4	EDO	В	1115	-	$3,\!3,\!3$	0.47	0	$2,\!2,\!2$	0.30	0	
4	EDO	С	1105	-	3,3,3	0.48	0	2,2,2	0.32	0	
4	EDO	В	1114	-	3,3,3	0.49	0	2,2,2	0.15	0	
4	EDO	В	1108	-	3,3,3	0.50	0	2,2,2	0.28	0	
4	EDO	А	1106	-	3,3,3	0.47	0	2,2,2	0.32	0	
4	EDO	В	1111	-	3,3,3	0.50	0	2,2,2	0.24	0	
4	EDO	В	1112	-	3,3,3	0.46	0	2,2,2	0.30	0	
4	EDO	В	1113	-	3,3,3	0.48	0	2,2,2	0.31	0	
4	EDO	D	1106	-	3,3,3	0.48	0	2,2,2	0.27	0	
4	EDO	В	1106	-	3,3,3	0.46	0	$2,\!2,\!2$	0.30	0	
4	EDO	А	1107	-	3,3,3	0.48	0	2,2,2	0.30	0	
4	EDO	С	1106	-	3,3,3	0.45	0	$2,\!2,\!2$	0.31	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	EDO	В	1107	-	-	1/1/1/1	-
4	EDO	В	1109	-	-	0/1/1/1	-
4	EDO	В	1110	-	-	0/1/1/1	-
4	EDO	В	1115	-	-	0/1/1/1	-
4	EDO	С	1105	-	-	1/1/1/1	-
4	EDO	В	1114	-	-	0/1/1/1	-
4	EDO	В	1108	-	-	1/1/1/1	-
4	EDO	А	1106	-	-	1/1/1/1	-
4	EDO	В	1111	-	-	1/1/1/1	-
4	EDO	В	1112	-	-	1/1/1/1	-
4	EDO	В	1113	-	-	0/1/1/1	-
4	EDO	D	1106	-	-	1/1/1/1	-
4	EDO	В	1106	-	-	1/1/1/1	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	А	1107	-	-	0/1/1/1	-
4	EDO	С	1106	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	1106	EDO	O1-C1-C2-O2
4	В	1106	EDO	O1-C1-C2-O2
4	С	1105	EDO	O1-C1-C2-O2
4	В	1107	EDO	O1-C1-C2-O2
4	В	1111	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	1110	EDO	1	0
4	В	1114	EDO	1	0
4	С	1106	EDO	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	416/442~(94%)	-0.26	6 (1%) 75 77	4, 12, 35, 46	14 (3%)
1	В	417/442~(94%)	-0.19	10 (2%) 59 60	3, 11, 41, 54	17 (4%)
1	С	408/442~(92%)	-0.30	4 (0%) 82 83	4, 11, 34, 52	13 (3%)
1	D	408/442~(92%)	-0.28	4 (0%) 82 83	5, 13, 39, 53	21 (5%)
All	All	1649/1768~(93%)	-0.26	24 (1%) 73 76	3, 12, 37, 54	65 (3%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	1000	TYR	5.7
1	В	1008	LEU	5.4
1	В	996	ASN	5.1
1	В	997	LEU	4.4
1	В	1001	SER	3.9

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	\mathbf{RSR}	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	NAG	Е	5	14/15	0.58	0.51	72,72,72,72	0
2	BMA	Е	2	11/12	0.59	0.41	68,70,70,71	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
2	NAG	Н	1	15/15	0.63	0.43	64,65,66,66	0
2	NAG	F	1	15/15	0.65	0.45	61,62,62,62	0
2	NAG	Е	1	15/15	0.65	0.43	70,71,72,72	0
3	BMA	G	2	11/12	0.65	0.39	57,58,59,59	0
2	BMA	Н	2	11/12	0.69	0.41	62,63,64,64	0
2	NAG	Н	5	14/15	0.70	0.42	64,64,64,64	0
2	NAG	F	5	14/15	0.70	0.44	62,63,63,63	0
2	BMA	F	2	11/12	0.72	0.36	58,61,61,61	0
3	NAG	G	1	15/15	0.76	0.39	60,61,62,62	0
2	MAN	Н	3	11/12	0.78	0.28	59,60,61,61	0
2	MAN	Е	3	11/12	0.78	0.28	$65,\!66,\!67,\!67$	0
3	MAN	G	3	11/12	0.81	0.27	$53,\!55,\!56,\!56$	0
2	MAN	F	3	11/12	0.82	0.30	54,56,57,57	0
2	NAG	Н	4	14/15	0.83	0.33	$56,\!57,\!57,\!58$	0
2	NAG	F	4	14/15	0.87	0.31	$50,\!52,\!53,\!53$	0
2	NAG	Е	4	14/15	0.90	0.27	$\overline{62,\!62,\!63,\!63}$	0
3	NAG	G	4	14/15	0.90	0.27	49,50,51,52	0

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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	$B-factors(Å^2)$	Q<0.9
4	EDO	В	1113	4/4	0.67	0.40	85,85,85,85	0
4	EDO	В	1114	4/4	0.69	0.42	29,30,30,31	0
4	EDO	В	1111	4/4	0.71	0.39	36,36,36,37	0
4	EDO	А	1107	4/4	0.74	0.47	63,63,63,63	0
4	EDO	А	1106	4/4	0.75	0.26	37,37,37,37	0
4	EDO	D	1106	4/4	0.76	0.30	38,38,38,38	0
4	EDO	В	1108	4/4	0.79	0.25	39,39,39,39	0
4	EDO	В	1110	4/4	0.79	0.42	36,37,37,37	0
4	EDO	В	1107	4/4	0.81	0.23	27,28,28,28	0
4	EDO	В	1115	4/4	0.86	0.24	41,42,42,42	0
4	EDO	В	1112	4/4	0.86	0.28	49,49,49,49	0
4	EDO	С	1105	4/4	0.88	0.26	20,20,21,21	0
4	EDO	С	1106	4/4	0.88	0.28	42,42,42,43	0
4	EDO	В	1106	4/4	0.88	0.40	43,43,43,44	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
4	EDO	В	1109	4/4	0.91	0.26	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.

