

wwPDB X-ray Structure Validation Summary Report (i)

Aug 29, 2023 – 01:56 pm BST

PDB ID	:	8BXL
Title	:	Patulin Synthase from Penicillium expansum
Authors	:	Tjallinks, G.; Boverio, A.; Rozeboom, H.J.; Fraaije, M.W.
Deposited on	:	2022-12-09
Resolution	:	2.40 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	:	2.35
buster-report	:	1.1.7(2018)
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 2.40 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.



Motric	Whole archive	Similar resolution				
IVIEUTIC	$(\# { m Entries})$	(#Entries, resolution range(Å))				
R _{free}	130704	3907 (2.40-2.40)				
Clashscore	141614	4398 (2.40-2.40)				
Ramachandran outliers	138981	4318 (2.40-2.40)				
Sidechain outliers	138945	4319 (2.40-2.40)				
RSRZ outliers	127900	3811 (2.40-2.40)				

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	٨	600	% •		
	А	628	87%	6%	• 6%
	P				
1	В	628	87%	6%	• 6%
			2%		
1	\mathbf{C}	628	87%	6%	• 6%
			10%		
1	D	628	87%	6%	6%
			2%		
1	Ε	628	87%	6%	6%



Conti	nuea jron	i previous	page	
Mol	Chain	Length	Quality of chain	
1	F	628	% 89% 5	% 6%
2	G	3	100%	
2	Н	3	100%	
2	Ι	3	100%	
2	J	3	100%	
2	K	3	100%	
3	L	2	100%	

 α tia d fa

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
6	PEG	F	610	-	-	Х	-
7	GOL	Е	607	-	-	Х	Х



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 29074 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	В	500	Total	С	Ν	0	\mathbf{S}	0	0	0
1	D	090	4526	2865	785	862	14	0	0	0
1	С	500	Total	С	Ν	0	S	0	0	0
1		0.50	4490	2846	778	852	14	0	0	0
1	П	500	Total	С	Ν	0	S	0	0	0
1	D	590	4446	2822	764	846	14		0	
1	Λ	500	Total	С	Ν	0	S	0	0	0
1	Л	090	4530	2867	785	864	14	0	0	0
1	F	500	Total	С	Ν	0	S	0	0	0
1	Г	590	4506	2852	781	859	14	0	0	0
1	1 E	500	Total	С	Ν	0	S	0	0	0
		590	4530	2867	785	864	14	0	U	U

• Molecule 1 is a protein called Patulin synthase.

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



Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf	Trace	
2	G	3	Total	С	Ν	Ο	0	0	0	
	ŭ	0	39	22	2	15	0	0	0	
0	Ц	2	Total	С	Ν	0	0	0	0	
	11	5	39	22	2	15	0	0	U	
0	0 I	3	Total	С	Ν	0	0	0	0	
	1		39	22	2	15	0	0	0	
0	т	2	Total	С	Ν	0	0	0	0	
	1	0	39	22	2	15	0	0	U	
2	V	2	Total	С	Ν	0	0	0	0	
	n	3	39	22	2	15	0	0	U	



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- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf	Trace
3	L	2	Total 28	C 16	N 2	O 10	0	0	0

• Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	
4		1	Total	С	Ν	Ο	Р	0	0	
4	D	I	53	27	9	15	2	0	0	
4	C	1	Total	С	Ν	0	Р	0	0	
4		1	53	27	9	15	2	0	0	
4	Л	1	Total	С	Ν	0	Р	0	0	
4	4 D	T	53	27	9	15	2	0	0	
4	Δ	1	Total	С	Ν	0	Р	0	0	
4	Л	I	53	27	9	15	2	0	0	
4	Б	1	Total	С	Ν	0	Р	0	0	
4 Г	Г	L	53	27	9	15	2	0	U	
	1	Total	С	Ν	Ο	Р	0	0		
4			53	27	9	15	2	0		

• Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:



 $C_8H_{15}NO_6$).



Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
5	D	1	Total	С	Ν	0	0	0
G	В	1	14	8	1	5	0	0
5	D	1	Total	С	Ν	0	0	0
5	D	L	14	8	1	5	0	0
5	Р	1	Total	С	Ν	0	0	0
5	D	L	14	8	1	5	0	0
5	В	1	Total	С	Ν	0	0	0
0	D	T	14	8	1	5	0	0
5	С	1	Total	С	Ν	0	0	0
0	U	T	14	8	1	5	0	0
5	С	1	Total	С	Ν	Ο	0	0
0	0	T	14	8	1	5	0	0
5	С	1	Total	С	Ν	Ο	0	0
		1	14	8	1	5	Ŭ	
5	С	1	Total	С	Ν	Ο	0	0
		-	14	8	1	5		
5	D	1	Total	С	Ν	Ο	0	0
	_	_	14	8	1	5	Ŭ,	
5	D	1	Total	С	Ν	O	0	0
			14	8	1	5	_	-
5	D	1	Total	C	N	Õ	0	0
			14	8	1	5		-
5	D	1	Total	C	N	Õ	0	0
			14	8	1	5		-
5	А	1	Total	C	N	Õ	0	0
-		_	14	8	1	5	Ŭ	÷



Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
F	٨	1	Total	С	Ν	0	0	0
5	A	1	14	8	1	5	0	0
5	Λ	1	Total	С	Ν	0	0	0
0	A	1	14	8	1	5	0	0
5	Δ	1	Total	С	Ν	0	0	0
5	A	1	14	8	1	5	0	0
5	Б	1	Total	С	Ν	0	0	0
5	Г	1	14	8	1	5	0	0
5	F	1	Total	С	Ν	0	0	0
5	Ľ	1	14	8	1	5		0
5	F	1	Total	С	Ν	0	0	0
5	Ľ	I	14	8	1	5	0	0
5	F	1	Total	С	Ν	0	0	0
5	Ľ	T	14	8	1	5	0	0
5	F	1	Total	С	Ν	0	0	0
5	Ľ	T	14	8	1	5	0	0
5	F	1	Total	С	Ν	0	0	0
5	Ľ	1	14	8	1	5	0	0
5	F	1	Total	С	Ν	0	0	0
5		L	14	8	1	5	0	U
5	F	1	Total	С	Ν	0	0	0
0			14	8	1	5	0	

• Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0

• Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





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

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	В	199	Total O 200 200	0	1
8	С	170	Total O 170 170	0	0
8	D	63	$\begin{array}{cc} \text{Total} & \text{O} \\ 63 & 63 \end{array}$	0	0
8	А	154	Total O 158 158	0	4
8	F	187	Total O 187 187	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	Е	206	Total O 209 209	0	3



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: Patulin synthase



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

Chain G:

100%

NAG1 NAG2 MAN3



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

Chain H:

100%

NAG1 NAG2 MAN3

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

Chain I:

100%

NAG1 NAG2 MAN3

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

Chain J:	100%	

NAG1 NAG2 MANG

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

Chain K:

100%

NAG1 NAG2 MAN3

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

100%

NAG1 NAG2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	104.84Å 144.16 Å 155.24 Å	Deperitor
a, b, c, α , β , γ	90.00° 91.53° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	48.74 - 2.40	Depositor
Resolution (A)	48.69 - 2.40	EDS
% Data completeness	100.0 (48.74-2.40)	Depositor
(in resolution range)	$100.0 \ (48.69-2.40)$	EDS
R _{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.97 (at 2.39 \text{\AA})$	Xtriage
Refinement program	REFMAC v7.1.018	Depositor
D D.	0.182 , 0.222	Depositor
n, n_{free}	0.188 , 0.226	DCC
R_{free} test set	9411 reflections (5.23%)	wwPDB-VP
Wilson B-factor $(Å^2)$	36.0	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, 49.6	EDS
L-test for twinning ²	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	29074	wwPDB-VP
Average B, all atoms $(Å^2)$	40.0	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 22.65 % 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 5.4539e-03. 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, PEG, GOL, MAN, FAD

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	
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.65	0/4646	0.80	3/6332~(0.0%)
1	В	0.66	0/4642	0.79	2/6327~(0.0%)
1	С	0.65	0/4606	0.79	3/6284~(0.0%)
1	D	0.65	0/4562	0.77	1/6233~(0.0%)
1	Е	0.66	0/4646	0.81	5/6332~(0.1%)
1	F	0.65	0/4622	0.78	1/6305~(0.0%)
All	All	0.65	0/27724	0.79	15/37813~(0.0%)

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	А	0	1
1	В	0	1
1	С	0	2
1	D	0	1
1	Ε	0	1
1	F	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	Е	157	ARG	NE-CZ-NH2	8.75	124.67	120.30
1	А	157	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	F	157	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	Е	172	ASN	CB-CA-C	7.53	125.45	110.40



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	160	ASN	CB-CA-C	-7.09	96.22	110.40

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	378	GLU	Peptide
1	В	378	GLU	Peptide
1	С	378	GLU	Peptide
1	С	381	PRO	Peptide
1	D	378	GLU	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	4530	0	4370	30	0
1	В	4526	0	4366	31	0
1	С	4490	0	4310	36	0
1	D	4446	0	4227	34	0
1	Ε	4530	0	4370	28	0
1	F	4506	0	4324	25	0
2	G	39	0	34	0	0
2	Н	39	0	34	0	0
2	Ι	39	0	34	2	0
2	J	39	0	34	0	0
2	Κ	39	0	34	2	0
3	L	28	0	25	0	0
4	А	53	0	31	5	0
4	В	53	0	31	5	0
4	С	53	0	31	6	0
4	D	53	0	31	6	0
4	Ε	53	0	31	5	0
4	F	53	0	31	5	0
5	A	56	0	52	3	0
5	В	56	0	52	1	0
5	С	56	0	52	5	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	56	0	52	2	0
5	Е	56	0	52	3	0
5	F	56	0	52	1	0
6	А	21	0	30	2	0
6	В	28	0	40	1	0
6	С	14	0	20	2	0
6	D	14	0	20	2	0
6	Ε	28	0	40	3	0
6	F	35	0	50	12	0
7	А	6	0	8	2	0
7	В	6	0	8	3	0
7	С	6	0	8	3	0
7	D	6	0	8	1	0
7	Ε	6	0	8	4	0
7	F	12	0	16	4	0
8	А	158	0	0	4	0
8	В	200	0	0	5	0
8	С	170	0	0	3	0
8	D	63	0	0	3	0
8	Е	209	0	0	1	0
8	F	187	0	0	1	0
All	All	29074	0	26916	180	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 3.

The worst 5 of 180 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:438:VAL:HG21	1:A:479:ALA:HB1	1.47	0.96
1:D:438:VAL:HG21	1:D:479:ALA:HB1	1.48	0.94
1:B:438:VAL:HG21	1:B:479:ALA:HB1	1.48	0.93
1:A:157:ARG:NH1	8:A:744[B]:HOH:O	1.91	0.91
1:A:371:THR:HG21	7:A:606:GOL:H2	1.52	0.91

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	entiles
1	А	588/628~(94%)	570~(97%)	16 (3%)	2(0%)	41	55
1	В	588/628~(94%)	569~(97%)	16 (3%)	3~(0%)	29	41
1	С	588/628~(94%)	568~(97%)	17 (3%)	3~(0%)	29	41
1	D	588/628~(94%)	570~(97%)	16 (3%)	2(0%)	41	55
1	Е	588/628~(94%)	570~(97%)	16 (3%)	2(0%)	41	55
1	F	588/628~(94%)	569~(97%)	17 (3%)	2(0%)	41	55
All	All	3528/3768~(94%)	3416 (97%)	98 (3%)	14 (0%)	34	48

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	371	THR
1	С	371	THR
1	D	371	THR
1	А	371	THR
1	F	371	THR

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	n Analysed Rotameric Outliers		Percentiles		
1	А	472/500~(94%)	461 (98%)	11 (2%)	50 70	
1	В	471/500~(94%)	463 (98%)	8 (2%)	60 78	
1	С	462/500~(92%)	453~(98%)	9~(2%)	57 75	



Mol	Chain	Analysed Rotameric Outliers		Percentiles		
1	D	452/500~(90%)	442 (98%)	10 (2%)	52	71
1	Ε	472/500~(94%)	462~(98%)	10 (2%)	53	72
1	F	466/500~(93%)	457~(98%)	9~(2%)	57	75
All	All	2795/3000~(93%)	2738~(98%)	57 (2%)	55	74

Continued from previous page...

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	115	GLN
1	Е	490	THR
1	А	384	LYS
1	Е	466	TRP
1	Е	216	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	Е	343	GLN
1	Е	516	HIS
1	А	115	GLN
1	А	343	GLN
1	А	488	ASN

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)

17 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



Mol	Tuno	Chain	Dog	Link	Bo	ond leng	ths	В	ond ang	les
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	NAG	G	1	1,2	14,14,15	0.73	0	$17,\!19,\!21$	2.13	3 (17%)
2	NAG	G	2	2	14,14,15	0.80	0	17,19,21	1.79	3 (17%)
2	MAN	G	3	2	11,11,12	0.80	0	$15,\!15,\!17$	2.14	4 (26%)
2	NAG	Н	1	1,2	14,14,15	0.45	0	17,19,21	2.95	3 (17%)
2	NAG	Н	2	2	14,14,15	0.61	0	17,19,21	1.73	4 (23%)
2	MAN	Н	3	2	11,11,12	0.87	0	$15,\!15,\!17$	1.61	3 (20%)
2	NAG	Ι	1	1,2	14,14,15	0.55	0	17,19,21	2.28	4 (23%)
2	NAG	Ι	2	2	14,14,15	0.53	0	17,19,21	1.77	3 (17%)
2	MAN	Ι	3	2	11,11,12	0.67	0	$15,\!15,\!17$	1.76	3 (20%)
2	NAG	J	1	1,2	14,14,15	0.78	1 (7%)	17,19,21	2.01	4 (23%)
2	NAG	J	2	2	14,14,15	0.61	0	17,19,21	1.17	1 (5%)
2	MAN	J	3	2	11,11,12	0.69	0	$15,\!15,\!17$	1.59	2 (13%)
2	NAG	K	1	1,2	14,14,15	0.74	0	17,19,21	2.67	5 (29%)
2	NAG	K	2	2	14,14,15	0.75	0	17,19,21	2.04	7 (41%)
2	MAN	K	3	2	11,11,12	0.85	0	$15,\!15,\!17$	1.82	3 (20%)
3	NAG	L	1	1,3	14,14,15	0.55	0	17,19,21	2.20	4 (23%)
3	NAG	L	2	3	14,14,15	0.98	1 (7%)	17,19,21	2.04	7 (41%)

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).

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	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	MAN	G	3	2	-	2/2/19/22	1/1/1/1
2	NAG	Н	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Н	2	2	-	2/6/23/26	0/1/1/1
2	MAN	Н	3	2	-	2/2/19/22	1/1/1/1
2	NAG	Ι	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Ι	2	2	-	2/6/23/26	0/1/1/1
2	MAN	Ι	3	2	-	1/2/19/22	1/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	4/6/23/26	0/1/1/1
2	MAN	J	3	2	-	2/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	1/6/23/26	0/1/1/1
2	MAN	K	3	2	-	1/2/19/22	1/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
3	L	2	NAG	C4-C5	2.35	1.58	1.53
2	J	1	NAG	O7-C7	-2.15	1.18	1.23

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Н	1	NAG	C1-O5-C5	10.11	125.89	112.19
2	Κ	1	NAG	C1-O5-C5	9.13	124.56	112.19
3	L	1	NAG	C1-O5-C5	7.40	122.22	112.19
2	Ι	1	NAG	C1-O5-C5	7.21	121.96	112.19
2	G	3	MAN	C1-O5-C5	5.91	120.19	112.19

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	3	MAN	O5-C5-C6-O6
2	Ι	1	NAG	C4-C5-C6-O6
2	G	3	MAN	C4-C5-C6-O6
2	J	3	MAN	C4-C5-C6-O6
2	J	3	MAN	O5-C5-C6-O6

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	3	MAN	C1-C2-C3-C4-C5-O5
2	Ι	3	MAN	C1-C2-C3-C4-C5-O5
2	Н	3	MAN	C1-C2-C3-C4-C5-O5



Mol	Chain	Res	Type	Atoms
2	Κ	3	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Ι	3	MAN	1	0
2	Ι	2	NAG	1	0
2	Ι	1	NAG	1	0
2	K	1	NAG	1	0
2	K	3	MAN	1	0
2	K	2	NAG	2	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)

57 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	Type	Chain	Dec	Tink	Bond lengths			Bond angles			
	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2		
6	PEG	А	608	-	6,6,6	0.33	0	$5,\!5,\!5$	0.35	0	
7	GOL	А	606	-	$5,\!5,\!5$	0.39	0	$5,\!5,\!5$	0.56	0	
6	PEG	Е	605	-	$6,\!6,\!6$	0.28	0	$5,\!5,\!5$	0.14	0	
6	PEG	В	610	-	6,6,6	0.38	0	$5,\!5,\!5$	0.29	0	



Mal	T a	Chain	Dag	T : 1-	Bond lengths		Bond angles			
NIOI	Type	Chain	Res	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	FAD	В	601	-	53,58,58	0.88	1 (1%)	68,89,89	0.90	2 (2%)
6	PEG	D	603	-	6,6,6	0.37	0	$5,\!5,\!5$	0.24	0
5	NAG	А	607	1	14,14,15	0.61	0	17,19,21	2.06	7 (41%)
4	FAD	D	601	-	53,58,58	0.65	0	68,89,89	0.86	3 (4%)
6	PEG	А	603	-	6,6,6	0.22	0	$5,\!5,\!5$	0.14	0
5	NAG	С	602	1	14,14,15	0.91	1 (7%)	17,19,21	1.99	6 (35%)
6	PEG	F	603	-	6,6,6	0.30	0	$5,\!5,\!5$	0.21	0
5	NAG	D	602	1	14,14,15	0.77	0	17,19,21	1.63	<mark>5 (29%)</mark>
6	PEG	F	608	-	6,6,6	0.33	0	$5,\!5,\!5$	0.35	0
5	NAG	С	604	1	14,14,15	0.42	0	17,19,21	1.34	2 (11%)
5	NAG	В	604	1	14,14,15	0.87	1 (7%)	17,19,21	1.71	3 (17%)
6	PEG	С	605	_	6,6,6	0.22	0	5,5,5	0.26	0
5	NAG	D	604	1	14,14,15	0.56	0	17,19,21	2.41	3 (17%)
4	FAD	F	601	-	53,58,58	0.65	0	68,89,89	0.81	3 (4%)
5	NAG	Е	609	1	14,14,15	0.53	0	17,19,21	1.58	4 (23%)
6	PEG	В	608	_	6,6,6	0.38	0	5,5,5	0.23	0
5	NAG	F	612	1	14,14,15	0.66	0	17,19,21	1.51	3 (17%)
7	GOL	F	606	-	5,5,5	0.25	0	5,5,5	0.52	0
5	NAG	F	607	1	14,14,15	0.46	0	17,19,21	2.23	5 (29%)
5	NAG	Е	604	1	14,14,15	0.75	0	17,19,21	2.71	7 (41%)
6	PEG	В	605	-	6,6,6	0.52	0	5,5,5	0.38	0
6	PEG	D	605	-	6,6,6	0.18	0	5,5,5	0.18	0
6	PEG	А	605	-	6,6,6	0.31	0	$5,\!5,\!5$	0.31	0
6	PEG	С	603	-	6,6,6	0.29	0	$5,\!5,\!5$	0.32	0
7	GOL	С	606	-	5,5,5	0.17	0	5,5,5	0.42	0
7	GOL	E	607	-	5,5,5	0.32	0	$5,\!5,\!5$	0.55	0
7	GOL	F	609	-	5,5,5	0.21	0	5,5,5	0.59	0
5	NAG	F	604	1	14,14,15	0.43	0	17,19,21	1.83	1 (5%)
5	NAG	С	607	1	14,14,15	0.29	0	17,19,21	1.31	2 (11%)
5	NAG	F	602	1	14,14,15	0.74	0	17,19,21	2.04	<mark>6 (35%)</mark>
6	PEG	F	611	-	6,6,6	0.19	0	$5,\!5,\!5$	0.12	0
6	PEG	Е	602	-	6,6,6	0.44	0	$5,\!5,\!5$	0.32	0
4	FAD	A	601	-	53,58,58	0.75	0	68,89,89	0.84	1 (1%)
5	NAG	D	607	1	14,14,15	0.25	0	17,19,21	1.40	3 (17%)
5	NAG	С	608	1	14,14,15	0.50	0	17,19,21	0.86	0
5	NAG	D	608	1	14,14,15	0.62	0	17,19,21	1.55	4 (23%)
5	NAG	А	609	1	14,14,15	0.42	0	17,19,21	1.17	1 (5%)
4	FAD	Е	603	-	53,58,58	0.64	0	68,89,89	0.91	4 (5%)



Mol Type		Chain	Bos	Link	Bo	ond leng	$_{\rm ths}$	Bond angles		
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
5	NAG	В	607	1	14,14,15	0.46	0	17,19,21	1.50	4 (23%)
6	PEG	В	603	-	6,6,6	0.32	0	$5,\!5,\!5$	0.25	0
6	PEG	F	610	-	6,6,6	0.32	0	$5,\!5,\!5$	0.50	0
6	PEG	F	605	-	6,6,6	0.41	0	$5,\!5,\!5$	0.33	0
7	GOL	В	606	-	5,5,5	0.18	0	$5,\!5,\!5$	0.38	0
7	GOL	D	606	-	$5,\!5,\!5$	0.13	0	$5,\!5,\!5$	0.35	0
5	NAG	А	604	1	14,14,15	0.77	1 (7%)	17,19,21	1.56	2 (11%)
5	NAG	В	609	1	14,14,15	0.60	0	17,19,21	1.82	4 (23%)
5	NAG	А	602	1	14,14,15	0.84	0	17,19,21	1.61	4 (23%)
5	NAG	Е	608	1	14,14,15	0.30	0	17,19,21	1.30	2 (11%)
5	NAG	В	602	1	14,14,15	0.65	0	17,19,21	1.71	4 (23%)
4	FAD	С	601	-	53,58,58	0.66	1 (1%)	68,89,89	0.85	1 (1%)
5	NAG	Е	610	1	14,14,15	0.47	0	17,19,21	1.85	5 (29%)
6	PEG	Е	601	-	6,6,6	0.18	0	5, 5, 5	0.13	0
6	PEG	Е	606	-	6,6,6	0.38	0	5,5,5	0.33	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
6	PEG	А	608	-	-	2/4/4/4	-
7	GOL	А	606	-	-	4/4/4/4	-
6	PEG	Е	605	-	-	2/4/4/4	-
6	PEG	В	610	-	-	4/4/4/4	-
4	FAD	В	601	-	-	2/30/50/50	0/6/6/6
6	PEG	D	603	-	-	2/4/4/4	-
5	NAG	А	607	1	-	2/6/23/26	0/1/1/1
4	FAD	D	601	-	-	2/30/50/50	0/6/6/6
6	PEG	А	603	-	-	1/4/4/4	-
5	NAG	С	602	1	-	2/6/23/26	0/1/1/1
6	PEG	F	603	-	-	3/4/4/4	-
5	NAG	D	602	1	-	1/6/23/26	0/1/1/1
6	PEG	F	608	-	-	2/4/4/4	-
5	NAG	С	604	1	-	5/6/23/26	0/1/1/1
5	NAG	В	604	1	-	2/6/23/26	0/1/1/1
6	PEG	С	605	-	-	3/4/4/4	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	D	604	1	-	2/6/23/26	0/1/1/1
4	FAD	F	601	-	-	5/30/50/50	0/6/6/6
5	NAG	Е	609	1	-	2/6/23/26	0/1/1/1
6	PEG	В	608	-	-	2/4/4/4	-
5	NAG	F	612	1	-	0/6/23/26	0/1/1/1
7	GOL	F	606	-	-	0/4/4/4	-
5	NAG	F	607	1	-	0/6/23/26	0/1/1/1
5	NAG	Ε	604	1	-	2/6/23/26	0/1/1/1
6	PEG	В	605	-	-	1/4/4/4	-
6	PEG	D	605	-	-	2/4/4/4	-
6	PEG	А	605	-	-	3/4/4/4	-
6	PEG	С	603	-	-	1/4/4/4	-
7	GOL	С	606	-	-	2/4/4/4	-
7	GOL	Е	607	-	-	4/4/4/4	-
7	GOL	F	609	-	-	2/4/4/4	-
5	NAG	F	604	1	-	2/6/23/26	0/1/1/1
5	NAG	С	607	1	-	2/6/23/26	0/1/1/1
5	NAG	F	602	1	-	2/6/23/26	0/1/1/1
6	PEG	F	611	-	-	1/4/4/4	-
6	PEG	Е	602	-	-	4/4/4/4	-
4	FAD	А	601	-	-	3/30/50/50	0/6/6/6
5	NAG	D	607	1	-	2/6/23/26	0/1/1/1
5	NAG	С	608	1	-	4/6/23/26	0/1/1/1
5	NAG	D	608	1	-	2/6/23/26	0/1/1/1
5	NAG	А	609	1	-	1/6/23/26	0/1/1/1
4	FAD	Е	603	-	-	2/30/50/50	0/6/6/6
5	NAG	В	607	1	-	2/6/23/26	0/1/1/1
6	PEG	В	603	-	-	2/4/4/4	-
6	PEG	F	610	-	_	2/4/4/4	-
6	PEG	F	605	-	-	3/4/4/4	-
7	GOL	В	606	-	-	0/4/4/4	-
7	GOL	D	606	-	-	2/4/4/4	-
5	NAG	А	604	1	-	2/6/23/26	0/1/1/1
5	NAG	В	609	1	-	0/6/23/26	0/1/1/1
5	NAG	А	602	1	-	2/6/23/26	0/1/1/1
5	NAG	Е	608	1	-	2/6/23/26	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	В	602	1	-	0/6/23/26	0/1/1/1
4	FAD	С	601	-	-	2/30/50/50	0/6/6/6
5	NAG	Е	610	1	-	2/6/23/26	0/1/1/1
6	PEG	Е	601	-	-	4/4/4/4	-
6	PEG	Е	606	-	-	3/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
4	В	601	FAD	C1'-C2'	-3.43	1.47	1.52
5	В	604	NAG	C1-C2	2.72	1.56	1.52
4	С	601	FAD	C1'-C2'	-2.26	1.49	1.52
5	А	604	NAG	C1-C2	2.08	1.55	1.52
5	С	602	NAG	O4-C4	2.04	1.47	1.43

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	D	604	NAG	C1-O5-C5	8.23	123.35	112.19
5	F	607	NAG	C1-O5-C5	7.20	121.94	112.19
5	F	604	NAG	C1-O5-C5	5.98	120.30	112.19
5	Е	604	NAG	C2-N2-C7	5.46	130.68	122.90
5	В	604	NAG	C2-N2-C7	4.93	129.92	122.90

There are no chirality outliers.

5 of 120 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	С	601	FAD	PA-O3P-P-O5'
4	D	601	FAD	PA-O3P-P-O5'
4	Е	603	FAD	PA-O3P-P-O5'
5	С	604	NAG	C3-C2-N2-C7
5	С	604	NAG	C8-C7-N2-C2

There are no ring outliers.

34 monomers are involved in 83 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	А	606	GOL	2	0
6	Е	605	PEG	1	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	601	FAD	5	0
6	D	603	PEG	1	0
4	D	601	FAD	6	0
6	А	603	PEG	1	0
6	F	603	PEG	1	0
6	F	608	PEG	1	0
5	С	604	NAG	3	0
5	В	604	NAG	1	0
6	С	605	PEG	1	0
5	D	604	NAG	2	0
4	F	601	FAD	5	0
5	Е	609	NAG	3	0
7	F	606	GOL	1	0
6	D	605	PEG	1	0
6	А	605	PEG	1	0
6	С	603	PEG	1	0
7	С	606	GOL	3	0
7	Е	607	GOL	4	0
7	F	609	GOL	3	0
5	F	604	NAG	1	0
5	С	607	NAG	1	0
6	Е	602	PEG	1	0
4	А	601	FAD	5	0
5	С	608	NAG	1	0
4	Е	603	FAD	5	0
6	В	603	PEG	1	0
6	F	610	PEG	10	0
7	В	606	GOL	3	0
7	D	606	GOL	1	0
5	А	604	NAG	3	0
4	С	601	FAD	6	0
6	Е	606	PEG	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.



The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.































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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	590/628~(93%)	-0.17	9 (1%) 73 72	19, 32, 52, 86	0
1	В	590/628~(93%)	-0.24	2 (0%) 94 93	19, 31, 50, 71	0
1	С	590/628~(93%)	-0.07	13 (2%) 62 60	26, 39, 61, 87	0
1	D	590/628~(93%)	0.48	63 (10%) 6 5	28, 53, 80, 104	0
1	Ε	590/628~(93%)	-0.15	11 (1%) 66 64	20, 32, 54, 80	0
1	F	590/628~(93%)	-0.13	6 (1%) 82 80	23, 38, 58, 87	0
All	All	3540/3768~(93%)	-0.05	104 (2%) 51 50	19, 37, 66, 104	0

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	387	ALA	5.1
1	D	491	ALA	4.7
1	D	386	SER	4.7
1	D	306	ALA	4.3
1	D	431	TYR	4.2

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.



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
2	MAN	J	3	11/12	0.67	0.28	55,74,92,95	0
2	MAN	Ι	3	11/12	0.71	0.31	70,89,104,105	0
2	MAN	G	3	11/12	0.76	0.27	$57,\!84,\!93,\!95$	0
2	MAN	K	3	11/12	0.76	0.26	54,76,91,99	0
2	MAN	Н	3	11/12	0.80	0.37	$53,\!76,\!105,\!108$	0
3	NAG	L	2	14/15	0.90	0.20	41,52,59,61	0
2	NAG	Н	2	14/15	0.92	0.26	50,62,74,74	0
2	NAG	Ι	2	14/15	0.92	0.25	53,66,82,99	0
2	NAG	Н	1	14/15	0.93	0.19	$26,\!37,\!45,\!46$	0
2	NAG	J	2	14/15	0.95	0.20	44,54,74,85	0
3	NAG	L	1	14/15	0.95	0.13	23,33,42,54	0
2	NAG	Ι	1	14/15	0.95	0.11	$37,\!42,\!53,\!55$	0
2	NAG	K	2	14/15	0.96	0.17	38,45,55,73	0
2	NAG	G	1	14/15	0.96	0.13	22,28,36,46	0
2	NAG	J	1	14/15	0.96	0.12	24,28,34,52	0
2	NAG	K	1	14/15	0.96	0.11	22,29,34,47	0
2	NAG	G	2	14/15	0.97	0.22	36,49,64,67	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	$B-factors(A^2)$	Q<0.9
7	GOL	F	606	6/6	0.53	0.39	$56,\!68,\!78,\!80$	0
6	PEG	F	610	7/7	0.55	0.29	67,86,106,122	0
7	GOL	Е	607	6/6	0.60	0.40	41,64,88,88	0
6	PEG	F	611	7/7	0.61	0.15	$62,\!85,\!98,\!100$	0
5	NAG	С	604	14/15	0.62	0.35	51,69,112,130	0
7	GOL	D	606	6/6	0.69	0.38	78,89,97,98	0
7	GOL	А	606	6/6	0.71	0.31	43,52,53,56	0
7	GOL	F	609	6/6	0.73	0.26	$61,\!73,\!86,\!89$	0
7	GOL	В	606	6/6	0.74	0.26	40,52,76,79	0
6	PEG	В	608	7/7	0.74	0.12	56,68,83,100	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
7	GOL	С	606	6/6	0.79	0.36	66,73,84,94	0
6	PEG	Е	606	7/7	0.81	0.14	46,50,56,66	0
6	PEG	С	603	7/7	0.81	0.21	42,58,63,76	0
6	PEG	Е	602	7/7	0.82	0.17	49,52,64,71	0
6	PEG	В	605	7/7	0.84	0.16	43,43,50,51	0
5	NAG	А	607	14/15	0.84	0.26	51,73,106,159	0
6	PEG	С	605	7/7	0.85	0.15	45,51,58,65	0
5	NAG	С	607	14/15	0.85	0.38	59,78,85,86	0
5	NAG	D	608	14/15	0.85	0.24	55,73,100,113	0
5	NAG	С	602	14/15	0.85	0.16	$36,\!56,\!68,\!79$	0
6	PEG	F	605	7/7	0.87	0.15	47,49,54,67	0
5	NAG	В	604	14/15	0.87	0.27	47,58,73,76	0
5	NAG	С	608	14/15	0.87	0.23	58,79,89,94	0
5	NAG	D	607	14/15	0.88	0.21	62,77,88,94	0
5	NAG	D	602	14/15	0.88	0.15	$38,\!53,\!62,\!71$	0
5	NAG	D	604	14/15	0.88	0.41	61,93,104,110	0
6	PEG	В	603	7/7	0.88	0.19	$26,\!43,\!53,\!53$	0
6	PEG	D	603	7/7	0.88	0.21	$51,\!54,\!70,\!72$	0
6	PEG	F	603	7/7	0.88	0.20	$39,\!45,\!62,\!65$	0
6	PEG	А	608	7/7	0.89	0.29	40,50,58,70	0
6	PEG	В	610	7/7	0.89	0.14	$45,\!48,\!54,\!55$	0
6	PEG	E	601	7/7	0.90	0.32	47,53,58,60	0
5	NAG	F	602	14/15	0.90	0.14	$37,\!54,\!63,\!75$	0
5	NAG	А	602	14/15	0.91	0.12	$34,\!41,\!53,\!74$	0
5	NAG	F	604	14/15	0.91	0.29	45,62,73,92	0
6	PEG	А	603	7/7	0.91	0.17	37,45,60,61	0
5	NAG	F	612	14/15	0.91	0.12	$38,\!50,\!64,\!65$	0
5	NAG	E	609	14/15	0.91	0.24	$31,\!44,\!58,\!61$	0
5	NAG	E	610	14/15	0.91	0.14	$38,\!51,\!62,\!62$	0
6	PEG	E	605	7/7	0.92	0.14	$35,\!40,\!55,\!56$	0
5	NAG	A	604	14/15	0.92	0.23	33,42,53,59	0
6	PEG	D	605	7/7	0.92	0.28	$55,\!62,\!66,\!68$	0
5	NAG	В	607	14/15	0.93	0.29	45,57,71,81	0
6	PEG	F	608	7/7	0.93	0.14	$38,\!42,\!55,\!59$	0
5	NAG	A	609	14/15	0.93	0.19	44,63,75,84	0
6	PEG	A	605	7/7	0.94	0.13	37,45,51,54	0
5	NAG	E	604	14/15	0.94	0.12	35,42,55,60	0
5	NAG	В	602	14/15	0.94	0.13	31,43,60,65	0
5	NAG	E	608	14/15	0.95	0.19	45,64,74,74	0
5	NAG	F	607	14/15	0.95	0.20	44,55,67,71	0
5	NAG	В	609	14/15	0.96	0.11	33,46,56,58	0
4	FAD	D	601	$53/\overline{53}$	0.96	0.18	24,37,46,54	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FAD	С	601	53/53	0.96	0.17	$25,\!36,\!44,\!49$	0
4	FAD	А	601	53/53	0.97	0.16	18,24,32,39	0
4	FAD	В	601	53/53	0.98	0.17	17,25,32,35	0
4	FAD	F	601	53/53	0.98	0.16	18,27,40,42	0
4	FAD	Е	603	53/53	0.98	0.16	18,26,35,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.















6.5 Other polymers (i)

There are no such residues in this entry.

