

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	5EJZ
Title	:	Bacterial Cellulose Synthase Product-Bound State
Authors	:	Morgan, J.L.W.; Zimmer, J.
Deposited on	:	2015-11-02
Resolution	:	2.94 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (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	:	2.35.1
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

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 2.94 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{Entries,\ resolution\ range}({ m \AA}))$			
R _{free}	130704	2969 (2.98-2.90)			
Clashscore	141614	3218 (2.98-2.90)			
Ramachandran outliers	138981	3122 (2.98-2.90)			
Sidechain outliers	138945	3124 (2.98-2.90)			
RSRZ outliers	127900	2902 (2.98-2.90)			

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	803	5% 76%	14%	9%
2	В	724	2% 77%	14%	10%
3	D	9	100%		
4	С	18	50% 50	%	

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
4	SHG	С	18	-	-	-	Х
7	MG	А	922	-	-	-	Х



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 11078 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Putative cellulose synthase.

Mol	Chain	Residues		A	toms		ZeroOcc	AltConf	Trace	
1	А	728	Total 5739	C 3725	N 1000	O 982	S 32	0	1	0

Chain Residue Modelled Actual Comment Reference UNP Q3J125 А 0 MET _ initiating methionine GLY $\overline{\text{UNP}}$ Q3J125 А 1 expression tag _ Α 789 HIS expression tag UNP Q3J125 _ Α 790 HIS expression tag UNP Q3J125 _ А 791HIS **UNP Q3J125** _ expression tag А 792 HIS expression tag UNP Q3J125 _ HIS А 793 expression tag UNP Q3J125 _ А 794 HIS _ expression tag UNP Q3J125 795 LYS А expression tag UNP Q3J125 _ А 796 LEU UNP Q3J125 expression tag -А 797 HIS expression tag **UNP Q3J125** _ HIS А 798 **UNP Q3J125** expression tag _ А 799 HIS expression tag UNP Q3J125 -Α HIS UNP Q3J125 800 expression tag _ HIS UNP Q3J125 А 801 expression tag UNP Q3J125 А HIS 802 expression tag _

There are 16 discrepancies between the modelled and reference sequences:

• Molecule 2 is a protein called Putative cellulose synthase.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
2	В	655	Total 4887	C 3100	N 864	O 907	S 16	0	0	0

• Molecule 3 is a protein called poly(unk).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	9	Total 45	С 27	N 9	O 9	0	0	0

• Molecule 4 is an oligosaccharide called 2-deoxy-2-fluoro-beta-D-glucopyranose-(1-4)-beta-D-glucopy

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	С	18	Total 199	C 108	F 1	O 90	0	0	0

• Molecule 5 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidooctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclodode cine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula: $C_{20}H_{24}N_{10}O_{14}P_2$).



Mol	Chain	Residues		At	oms		ZeroOcc	AltConf		
5	Λ	1	Total	С	Ν	Ο	Р	0	0	
J A	1	46	20	10	14	2	0	0		
5	Λ	1	Total	С	Ν	Ο	Р	0	0	
5	5 A	L	46	20	10	14	2	0	0	

• Molecule 6 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	А	1	Total 25	С 9	N 2	O 12	Р 2	0	0

• Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	Total Mg 1 1	0	0
7	В	1	Total Mg 1 1	0	0

• Molecule 8 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	1	Total C N O P 38 28 1 8 1	0	0
8	В	1	Total C 9 9	0	0
8	В	1	Total C 11 11	0	0

• Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
9	А	1	Total 20	C 10	N 1	0 8	Р 1	0	0

• Molecule 10 is UNDECANE (three-letter code: UND) (formula: $C_{11}H_{24}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	В	1	Total C 11 11	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: Putative cellulose synthase

100%



• Molecule 3: poly(unk)

Chain D:

There are no outlier residues recorded for this chain.

 $\label{eq:2-decoy-2-fluoro-beta-D-glucopyranose-(1-4)-beta-D-glucopyranos$

Chair	ı C										50%		50%	
BGC1 BGC2 BGC3 BGC4	BGC5 BGC6 BCC6	BGC8	BGC9	BGC11	BGC12	BGC13	BGC14	BGC15	oTODd	SHG18				



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	67.27Å 216.84Å 221.12Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	34.35 - 2.94	Depositor
Resolution (A)	38.70 - 2.94	EDS
% Data completeness	98.5 (34.35-2.94)	Depositor
(in resolution range)	98.5 (38.70-2.94)	EDS
R_{merge}	0.12	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.87 (at 2.95 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
D D.	0.206 , 0.233	Depositor
Π, Π_{free}	0.210 , 0.235	DCC
R_{free} test set	3431 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	73.0	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31 , 45.8	EDS
L-test for twinning ²	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11078	wwPDB-VP
Average B, all atoms $(Å^2)$	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.

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: UND, MG, PLC, UDP, BGC, 3PE, C2E, SHG

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	0.23	0/5888	0.40	0/8007	
2	В	0.24	0/5006	0.43	0/6865	
All	All	0.23	0/10894	0.41	0/14872	

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	5739	0	5855	89	0
2	В	4887	0	4966	85	0
3	D	45	0	13	0	0
4	С	199	0	163	14	0
5	А	92	0	44	1	0
6	А	25	0	11	4	0
7	А	1	0	0	0	0
7	В	1	0	0	0	0
8	А	38	0	53	2	0
8	В	20	0	38	1	0
9	A	20	0	14	0	0



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	В	11	0	24	2	0
All	All	11078	0	11181	174	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 8.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:77:GLN:NE2	2:B:168:GLU:CB	2.16	1.09
1:A:173:ARG:HD2	1:A:173:ARG:O	1.57	1.05
2:B:77:GLN:HG3	2:B:168:GLU:OE1	1.58	1.03
2:B:77:GLN:NE2	2:B:168:GLU:HB3	1.71	1.02
2:B:77:GLN:CD	2:B:168:GLU:HB3	1.82	1.00
1:A:340:ILE:CD1	1:A:501:ALA:HB3	1.92	0.99
1:A:340:ILE:HD13	1:A:501:ALA:HB1	1.46	0.97
1:A:340:ILE:CD1	1:A:501:ALA:CB	2.45	0.94
1:A:480:GLU:OE2	4:C:14:BGC:O6	1.86	0.92
2:B:352:ALA:HB3	2:B:354:GLN:HE22	1.36	0.90
2:B:77:GLN:NE2	2:B:168:GLU:HB2	1.85	0.89
1:A:340:ILE:HD13	1:A:501:ALA:CB	2.04	0.87
2:B:352:ALA:HB3	2:B:354:GLN:NE2	1.90	0.86
2:B:77:GLN:HE22	2:B:335:TYR:HB3	1.41	0.85
1:A:340:ILE:HD11	1:A:501:ALA:HB3	1.59	0.82
2:B:78:GLN:HG3	2:B:336:PHE:CD1	2.15	0.80
2:B:516:GLU:OE2	2:B:598:GLY:HA3	1.81	0.80
1:A:616:ARG:NH2	5:A:919:C2E:O61	2.15	0.80
2:B:516:GLU:CG	2:B:600:LEU:HB3	2.12	0.80
2:B:77:GLN:NE2	2:B:335:TYR:HB3	1.98	0.79
1:A:548:ASP:OD1	4:C:7:BGC:O6	2.01	0.79
2:B:77:GLN:NE2	2:B:168:GLU:OE1	2.18	0.76
2:B:77:GLN:CG	2:B:168:GLU:OE1	2.33	0.76
2:B:354:GLN:OE1	2:B:354:GLN:N	2.18	0.75
1:A:371:GLU:OE2	1:A:578:GLN:NE2	2.20	0.74
1:A:243:VAL:HG22	1:A:323:VAL:HG22	1.70	0.73
1:A:66:ARG:NH1	1:A:123:ALA:O	2.25	0.70
2:B:336:PHE:HB3	2:B:419:SER:OG	1.92	0.70
1:A:340:ILE:HG22	1:A:340:ILE:O	1.90	0.69
1:A:382:ARG:NH1	1:A:504:ALA:O	2.24	0.69
2:B:516:GLU:HG3	2:B:600:LEU:HB3	1.74	0.69
1:A:508:LYS:NZ	6:A:921:UDP:O2A	2.26	0.68



	,	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:77:GLN:O	2:B:78:GLN:HB3	1.95	0.67
2:B:516:GLU:HG2	2:B:600:LEU:CB	2.25	0.67
1:A:399:ARG:O	1:A:407:ARG:NH1	2.27	0.67
2:B:352:ALA:HB3	2:B:354:GLN:OE1	1.95	0.67
2:B:77:GLN:HE22	2:B:168:GLU:HB2	1.56	0.67
2:B:251:THR:HG22	2:B:252:GLY:N	2.11	0.66
1:A:343:ASP:OD1	1:A:344:ALA:N	2.28	0.66
1:A:173:ARG:HD2	1:A:173:ARG:C	2.15	0.65
2:B:583:GLN:HA	2:B:586:ILE:HG12	1.79	0.65
2:B:482:THR:HG22	2:B:502:VAL:HB	1.78	0.65
1:A:108:GLU:OE2	4:C:12:BGC:O2	2.12	0.64
2:B:352:ALA:HB3	2:B:354:GLN:CD	2.16	0.64
1:A:186:ARG:HG2	1:A:194:LEU:HD21	1.79	0.64
2:B:387:PRO:HG3	4:C:5:BGC:O6	1.98	0.64
2:B:516:GLU:HG3	2:B:516:GLU:O	1.98	0.64
1:A:382:ARG:NH2	6:A:921:UDP:O2B	2.31	0.63
2:B:516:GLU:HG2	2:B:600:LEU:HB3	1.78	0.63
1:A:372:THR:HG22	1:A:512:LEU:HD21	1.79	0.63
1:A:369:GLN:HG3	1:A:370:PRO:HD2	1.81	0.62
2:B:245:LYS:HB3	2:B:246:PRO:HD2	1.82	0.62
1:A:340:ILE:HD11	1:A:501:ALA:CB	2.20	0.62
2:B:390:ARG:HH22	4:C:5:BGC:C6	2.13	0.62
2:B:390:ARG:HH22	4:C:5:BGC:H6C1	1.64	0.62
1:A:345:GLU:HA	1:A:390:MET:HE2	1.83	0.60
2:B:235:PRO:O	2:B:236:ASP:HB2	2.00	0.60
1:A:351:HIS:HD1	1:A:410:TYR:HH	1.48	0.60
1:A:382:ARG:HH22	1:A:506:THR:HG1	1.48	0.59
1:A:259:THR:HG21	1:A:323:VAL:HG21	1.84	0.59
2:B:78:GLN:HG3	2:B:336:PHE:HD1	1.63	0.59
2:B:100:GLN:HE21	2:B:136:VAL:HG23	1.68	0.59
2:B:148:ASP:HB3	2:B:305:LEU:HG	1.85	0.58
2:B:244:SER:OG	2:B:248:SER:HB3	2.03	0.58
1:A:340:ILE:O	1:A:340:ILE:CG2	2.52	0.58
1:A:343:ASP:OD2	4:C:17:BGC:H4	2.03	0.58
2:B:185:PRO:HG2	2:B:188:ALA:HB2	1.84	0.58
2:B:360:ILE:HA	2:B:444:THR:HG23	1.86	0.57
1:A:439:GLU:HB2	4:C:8:BGC:H6C2	1.87	0.56
1:A:394:LYS:O	1:A:399:ARG:NH1	2.38	0.56
2:B:244:SER:OG	2:B:248:SER:CB	2.53	0.56
1:A:512:LEU:HD12	1:A:578:GLN:HB3	1.87	0.56
2:B:106:ILE:HG22	2:B:171:LEU:HD22	1.88	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:368:LEU:HD22	1:A:583:PRO:HG2	1.88	0.55
1:A:35:ALA:O	1:A:79:ARG:NH2	2.40	0.55
1:A:179:ASP:OD1	1:A:201:ARG:NH1	2.40	0.55
1:A:184:ASP:HB3	1:A:202:ARG:HH12	1.72	0.55
1:A:132:ARG:HG3	1:A:265:GLU:CD	2.27	0.55
1:A:311:ARG:HH22	2:B:719:THR:HG23	1.71	0.54
2:B:77:GLN:HG3	2:B:333:ASN:HB3	1.90	0.54
1:A:482:ALA:HB2	1:A:569:ALA:HB1	1.90	0.53
1:A:135:GLN:HG3	1:A:136:PRO:HD2	1.90	0.53
1:A:340:ILE:HG23	1:A:503:PHE:HD1	1.74	0.53
1:A:218:THR:OG1	1:A:219:ARG:N	2.42	0.53
2:B:352:ALA:CB	2:B:354:GLN:HE22	2.16	0.51
1:A:419:PHE:HA	1:A:422:VAL:HG22	1.92	0.51
2:B:245:LYS:HB3	2:B:246:PRO:CD	2.39	0.51
1:A:497:ARG:HD2	1:A:500:SER:HB3	1.91	0.51
1:A:154:ASP:OD1	1:A:154:ASP:N	2.43	0.51
1:A:300:MET:HA	1:A:470:GLN:HB3	1.92	0.51
1:A:345:GLU:HA	1:A:390:MET:CE	2.40	0.51
2:B:587:GLN:O	2:B:591:ARG:HB2	2.10	0.51
1:A:362:ARG:HH12	1:A:697:ARG:HD2	1.75	0.50
1:A:176:VAL:HG22	1:A:215:VAL:HB	1.93	0.50
2:B:320:THR:HA	2:B:445:ASP:HA	1.94	0.50
2:B:264:ASP:OD1	2:B:267:ARG:NH2	2.45	0.50
2:B:302:THR:O	2:B:304:THR:HG23	2.12	0.49
2:B:678:SER:O	2:B:682:VAL:HG23	2.12	0.49
2:B:77:GLN:OE1	2:B:168:GLU:O	2.30	0.49
2:B:77:GLN:OE1	2:B:77:GLN:N	2.45	0.49
1:A:436:PHE:HA	8:A:923:PLC:H1'2	1.95	0.49
1:A:161:ALA:HB1	1:A:683:GLU:HG2	1.93	0.49
2:B:189:ILE:O	2:B:272:ARG:NH1	2.45	0.49
1:A:173:ARG:C	1:A:173:ARG:CD	2.80	0.48
2:B:224:ARG:HD3	2:B:469:ALA:HA	1.95	0.48
2:B:575:GLN:HE21	10:B:802:UND:H21	1.78	0.48
2:B:514:ASN:O	2:B:515:GLU:HG3	2.14	0.48
2:B:238:ALA:HB2	2:B:488:ALA:HB2	1.94	0.48
2:B:516:GLU:HG2	2:B:600:LEU:HB2	1.94	0.48
1:A:512:LEU:O	1:A:578:GLN:O	2.31	0.48
2:B:140:LEU:HB3	2:B:144:VAL:HB	1.96	0.47
10:B:802:UND:H42	8:B:803:PLC:H4'2	1.95	0.47
1:A:362:ARG:NH1	1:A:697:ARG:HD2	2.29	0.47
1:A:419:PHE:CD2	1:A:420:PRO:HD3	2.49	0.47



	lo do pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:220:GLU:OE2	2:B:224:ARG:NH2	2.48	0.47
2:B:251:THR:CG2	2:B:252:GLY:N	2.78	0.47
2:B:353:SER:O	2:B:355:LYS:HD2	2.13	0.47
1:A:270:PHE:HB3	1:A:355:TRP:HB3	1.96	0.47
1:A:274:THR:OG1	1:A:321:ALA:O	2.23	0.46
1:A:37:VAL:HG13	1:A:41:ALA:HB3	1.98	0.46
1:A:389:GLN:NE2	1:A:498:PRO:O	2.49	0.46
1:A:387:MET:HG3	1:A:417:TRP:CD1	2.50	0.46
1:A:464:ASN:O	1:A:468:ALA:HB2	2.16	0.46
2:B:377:LYS:HB2	2:B:416:SER:HB2	1.98	0.46
1:A:18:LEU:HD22	2:B:711:ILE:HG23	1.97	0.46
1:A:397:LEU:HD21	1:A:411:LEU:HD13	1.96	0.46
2:B:358:ILE:HG13	2:B:403:PHE:HE2	1.80	0.46
1:A:147:PRO:HA	1:A:178:CYS:HB2	1.98	0.46
1:A:452:MET:HE2	4:C:11:BGC:O6	2.15	0.45
2:B:466:VAL:HG13	2:B:470:SER:OG	2.17	0.45
2:B:617:GLU:HG3	2:B:620:LYS:HB2	1.98	0.45
1:A:390:MET:HE3	1:A:390:MET:HB2	1.61	0.45
2:B:105:ASP:HA	2:B:160:ARG:HE	1.81	0.45
4:C:10:BGC:O3	4:C:11:BGC:O5	2.25	0.45
2:B:251:THR:HG22	2:B:252:GLY:H	1.82	0.45
2:B:456:MET:O	2:B:458:ASP:N	2.49	0.45
1:A:42:GLN:OE1	1:A:79:ARG:NH1	2.51	0.44
2:B:76:GLY:N	2:B:171:LEU:O	2.40	0.44
2:B:505:LEU:HD21	2:B:527:LEU:HD12	2.00	0.44
1:A:452:MET:HE2	1:A:558:TRP:HE1	1.83	0.43
1:A:452:MET:CE	4:C:11:BGC:O6	2.67	0.43
2:B:612:MET:HG2	2:B:654:VAL:HG22	2.01	0.43
1:A:274:THR:HG22	1:A:360:ILE:HG23	1.99	0.43
1:A:345:GLU:HB2	1:A:390:MET:CE	2.49	0.43
2:B:55:TRP:CE3	2:B:189:ILE:HG13	2.54	0.43
2:B:334:ARG:HA	2:B:334:ARG:HD3	1.84	0.43
1:A:276:HIS:HE1	1:A:318:CYS:HB3	1.84	0.42
1:A:513:SER:O	1:A:577:GLN:HG3	2.18	0.42
2:B:387:PRO:HB3	4:C:5:BGC:H6	1.85	0.42
2:B:307:PRO:HA	2:B:308:PRO:HD3	1.85	0.42
1:A:189:SER:HA	1:A:190:PRO:HD3	1.92	0.42
2:B:266:ASP:OD1	2:B:285:PRO:HD3	2.20	0.42
1:A:91:PRO:HA	1:A:92:PRO:HD3	1.90	0.41
1:A:312:TRP:HB3	1:A:405:ALA:HB1	2.02	0.41
2:B:77:GLN:CD	2:B:168:GLU:OE1	2.58	0.41



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:B:556:ALA:HB2	2:B:576:THR:HG23	2.01	0.41	
2:B:234:LEU:HB3	2:B:237:GLU:HB2	2.01	0.41	
1:A:144:ILE:HG21	1:A:163:ALA:HB1	2.03	0.41	
1:A:148:SER:HA	6:A:921:UDP:O2'	2.20	0.41	
1:A:248:ASP:HB2	1:A:368:LEU:HG	2.02	0.41	
1:A:447:GLU:OE2	2:B:355:LYS:NZ	2.53	0.41	
2:B:368:LEU:HA	2:B:369:PRO:HD3	1.84	0.41	
2:B:448:VAL:HA	2:B:449:PRO:HD3	1.89	0.41	
1:A:186:ARG:HG2	1:A:194:LEU:CD2	2.50	0.41	
1:A:547:GLY:O	4:C:7:BGC:O6	2.38	0.41	
2:B:466:VAL:HG22	2:B:498:VAL:CG1	2.50	0.41	
1:A:366:ALA:HB3	1:A:690:PHE:HD1	1.85	0.41	
1:A:151:GLU:OE2	6:A:921:UDP:O2'	2.32	0.41	
1:A:420:PRO:O	1:A:424:MET:HG2	2.21	0.41	
1:A:497:ARG:HD2	1:A:500:SER:CB	2.50	0.41	
8:A:923:PLC:H71	4:C:6:BGC:O3	2.21	0.41	
1:A:17:LEU:HD23	1:A:20:LEU:HD12	2.02	0.40	
1:A:89:LEU:HA	1:A:90:PRO:HD2	1.91	0.40	
2:B:78:GLN:O	2:B:78:GLN:CG	2.70	0.40	

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
1	А	727/803~(90%)	701 (96%)	24 (3%)	2(0%)	41	69	
2	В	651/724~(90%)	624 (96%)	25~(4%)	2(0%)	41	69	
All	All	1378/1527~(90%)	1325 (96%)	49 (4%)	4 (0%)	41	69	

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	А	498	PRO
2	В	457	ALA
1	А	401	GLY
2	В	493	PRO

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	599/661~(91%)	594 (99%)	5 (1%)	81 93		
2	В	520/572~(91%)	517~(99%)	3 (1%)	86 95		
All	All	1119/1233 (91%)	1111 (99%)	8 (1%)	84 94		

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	37	VAL
1	А	77	VAL
1	А	325	ARG
1	А	512	LEU
1	А	578	GLN
2	В	326	VAL
2	В	669	LEU
2	В	693	ARG

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

Mol	Chain	Res	Type
1	А	222	ASN
2	В	77	GLN
2	В	100	GLN
2	В	514	ASN
2	В	575	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)

18 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	Turne	Chain	Dec	Tink	Bo	ond leng	ths	Bond angles		
	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BGC	С	1	4	12,12,12	1.22	1 (8%)	17,17,17	1.49	4 (23%)
4	BGC	С	10	4	11,11,12	1.65	3 (27%)	15,15,17	1.65	1 (6%)
4	BGC	С	11	4	11,11,12	1.64	2 (18%)	15,15,17	1.10	1 (6%)
4	BGC	С	12	4	11,11,12	1.71	3 (27%)	15,15,17	0.78	0
4	BGC	С	13	4	11,11,12	1.57	2 (18%)	15,15,17	1.09	1 (6%)
4	BGC	С	14	4	11,11,12	1.67	2 (18%)	15,15,17	1.69	3 (20%)
4	BGC	С	15	4	11,11,12	1.61	2 (18%)	15,15,17	1.54	4 (26%)
4	BGC	С	16	4	11,11,12	1.54	1 (9%)	15,15,17	2.20	4 (26%)
4	BGC	С	17	4	11,11,12	1.76	3 (27%)	15,15,17	0.88	0
4	SHG	С	18	4	11,11,12	1.67	1 (9%)	10,15,17	0.63	0
4	BGC	С	2	4	11,11,12	1.77	3 (27%)	15,15,17	1.56	4 (26%)
4	BGC	С	3	4	11,11,12	1.69	2 (18%)	15,15,17	2.02	3 (20%)
4	BGC	С	4	4	11,11,12	1.70	3 (27%)	15,15,17	2.15	5 (33%)
4	BGC	С	5	4	11,11,12	1.60	2 (18%)	15,15,17	1.91	4 (26%)
4	BGC	С	6	4	11,11,12	2.12	3 (27%)	15,15,17	1.00	1 (6%)
4	BGC	С	7	4	11,11,12	1.73	3 (27%)	15,15,17	0.97	0
4	BGC	С	8	4	11,11,12	1.68	3 (27%)	15,15,17	1.70	4 (26%)
4	BGC	С	9	4	11,11,12	1.71	3 (27%)	15,15,17	1.28	1 (6%)



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGC	С	1	4	-	2/2/22/22	0/1/1/1
4	BGC	С	10	4	-	1/2/19/22	0/1/1/1
4	BGC	С	11	4	-	2/2/19/22	0/1/1/1
4	BGC	С	12	4	-	0/2/19/22	0/1/1/1
4	BGC	С	13	4	-	2/2/19/22	0/1/1/1
4	BGC	С	14	4	-	2/2/19/22	0/1/1/1
4	BGC	С	15	4	-	2/2/19/22	0/1/1/1
4	BGC	С	16	4	-	2/2/19/22	0/1/1/1
4	BGC	С	17	4	-	2/2/19/22	0/1/1/1
4	SHG	С	18	4	-	2/2/19/22	0/1/1/1
4	BGC	С	2	4	-	2/2/19/22	0/1/1/1
4	BGC	С	3	4	-	1/2/19/22	0/1/1/1
4	BGC	С	4	4	-	2/2/19/22	0/1/1/1
4	BGC	С	5	4	-	0/2/19/22	0/1/1/1
4	BGC	С	6	4	-	1/2/19/22	0/1/1/1
4	BGC	С	7	4	-	2/2/19/22	0/1/1/1
4	BGC	С	8	4	-	2/2/19/22	0/1/1/1
4	BGC	С	9	4	-	1/2/19/22	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	С	6	BGC	O5-C1	5.54	1.52	1.43
4	С	14	BGC	O5-C1	4.40	1.50	1.43
4	С	9	BGC	O5-C1	4.40	1.50	1.43
4	С	4	BGC	O5-C1	4.39	1.50	1.43
4	С	18	SHG	O5-C1	4.37	1.50	1.43
4	С	12	BGC	O5-C1	4.35	1.50	1.43
4	С	3	BGC	O5-C1	4.34	1.50	1.43
4	С	7	BGC	O5-C1	4.29	1.50	1.43
4	С	17	BGC	O5-C1	4.28	1.50	1.43
4	С	2	BGC	O5-C1	4.27	1.50	1.43
4	С	8	BGC	O5-C1	4.23	1.50	1.43
4	С	11	BGC	O5-C1	4.11	1.50	1.43
4	С	10	BGC	O5-C1	4.06	1.50	1.43
4	С	16	BGC	O5-C1	4.02	1.50	1.43



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	С	15	BGC	O5-C1	3.99	1.50	1.43
4	С	5	BGC	O5-C1	3.93	1.50	1.43
4	С	13	BGC	O5-C1	3.76	1.49	1.43
4	С	1	BGC	O5-C1	3.10	1.50	1.42
4	С	6	BGC	C2-C3	-2.88	1.48	1.52
4	С	17	BGC	C2-C3	-2.87	1.48	1.52
4	С	2	BGC	C2-C3	-2.71	1.48	1.52
4	С	6	BGC	O5-C5	2.59	1.48	1.43
4	С	13	BGC	C2-C3	-2.53	1.48	1.52
4	С	10	BGC	C2-C3	-2.49	1.48	1.52
4	С	15	BGC	C2-C3	-2.47	1.48	1.52
4	С	7	BGC	C2-C3	-2.45	1.48	1.52
4	С	12	BGC	C2-C3	-2.40	1.49	1.52
4	С	11	BGC	C2-C3	-2.40	1.49	1.52
4	С	9	BGC	C2-C3	-2.38	1.49	1.52
4	С	3	BGC	C2-C3	-2.36	1.49	1.52
4	С	5	BGC	O2-C2	2.29	1.48	1.43
4	С	7	BGC	O5-C5	2.27	1.48	1.43
4	С	8	BGC	C2-C3	-2.26	1.49	1.52
4	С	2	BGC	O5-C5	2.24	1.48	1.43
4	С	14	BGC	C2-C3	-2.22	1.49	1.52
4	С	4	BGC	C2-C3	-2.14	1.49	1.52
4	С	8	BGC	O5-C5	2.13	1.47	1.43
4	С	17	BGC	O5-C5	2.12	1.47	1.43
4	С	12	BGC	O5-C5	2.08	1.47	1.43
4	С	4	BGC	O5-C5	2.02	1.47	1.43
4	С	9	BGC	O5-C5	2.01	1.47	1.43
4	С	10	BGC	O5-C5	2.01	1.47	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
4	С	16	BGC	C1-C2-C3	5.96	116.99	109.67
4	С	4	BGC	C1-C2-C3	5.55	116.49	109.67
4	С	3	BGC	C1-C2-C3	4.85	115.63	109.67
4	С	10	BGC	C1-C2-C3	4.84	115.62	109.67
4	С	14	BGC	C1-C2-C3	4.63	115.35	109.67
4	С	5	BGC	C1-C2-C3	4.21	114.84	109.67
4	С	5	BGC	C2-C3-C4	4.15	118.07	110.89
4	С	4	BGC	C2-C3-C4	3.90	117.65	110.89
4	C	3	BGC	C2-C3-C4	3.71	117.31	110.89
4	С	16	BGC	C2-C3-C4	3.41	116.80	110.89



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	С	1	BGC	C3-C4-C5	3.29	116.11	110.24
4	С	1	BGC	O5-C5-C4	3.19	115.49	109.69
4	С	2	BGC	C3-C4-C5	3.03	115.64	110.24
4	С	8	BGC	C1-C2-C3	2.98	113.33	109.67
4	С	3	BGC	C3-C4-C5	2.93	115.47	110.24
4	С	8	BGC	C3-C4-C5	2.88	115.37	110.24
4	С	8	BGC	C2-C3-C4	2.86	115.84	110.89
4	С	9	BGC	C1-C2-C3	2.78	113.08	109.67
4	С	15	BGC	C3-C4-C5	2.64	114.95	110.24
4	С	5	BGC	C1-O5-C5	-2.57	108.71	112.19
4	С	5	BGC	O4-C4-C5	-2.53	103.01	109.30
4	С	2	BGC	C2-C3-C4	2.53	115.27	110.89
4	С	15	BGC	C2-C3-C4	2.42	115.09	110.89
4	С	4	BGC	C6-C5-C4	-2.42	107.33	113.00
4	С	14	BGC	O5-C1-C2	2.40	114.47	110.77
4	С	6	BGC	C1-C2-C3	2.38	112.60	109.67
4	С	15	BGC	C1-C2-C3	2.34	112.54	109.67
4	С	1	BGC	C4-C3-C2	2.28	114.80	110.82
4	С	15	BGC	C1-O5-C5	-2.27	109.12	112.19
4	С	4	BGC	C3-C4-C5	2.22	114.21	110.24
4	С	16	BGC	C1-O5-C5	-2.13	109.30	112.19
4	С	11	BGC	C3-C4-C5	2.12	114.02	110.24
4	С	1	BGC	C6-C5-C4	-2.11	108.07	113.00
4	С	2	BGC	C6-C5-C4	-2.10	108.08	113.00
4	С	16	BGC	C3-C4-C5	2.08	113.96	110.24
4	С	8	BGC	C1-O5-C5	-2.03	109.44	112.19
4	С	14	BGC	C2-C3-C4	2.03	114.41	110.89
4	С	2	BGC	C1-C2-C3	2.02	112.15	109.67
4	С	4	BGC	O3-C3-C4	-2.01	105.69	110.35
4	С	13	BGC	C6-C5-C4	-2.00	108.31	113.00

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	С	7	BGC	O5-C5-C6-O6
4	С	18	SHG	C4-C5-C6-O6
4	С	2	BGC	O5-C5-C6-O6
4	С	16	BGC	O5-C5-C6-O6
4	С	17	BGC	O5-C5-C6-O6
4	С	14	BGC	O5-C5-C6-O6
4	С	1	BGC	O5-C5-C6-O6



Mol	Chain	Res	Type	Atoms
4	С	7	BGC	C4-C5-C6-O6
4	С	4	BGC	O5-C5-C6-O6
4	С	16	BGC	C4-C5-C6-O6
4	С	8	BGC	O5-C5-C6-O6
4	С	18	SHG	O5-C5-C6-O6
4	С	14	BGC	C4-C5-C6-O6
4	С	11	BGC	O5-C5-C6-O6
4	С	17	BGC	C4-C5-C6-O6
4	С	8	BGC	C4-C5-C6-O6
4	С	11	BGC	C4-C5-C6-O6
4	С	4	BGC	C4-C5-C6-O6
4	С	2	BGC	C4-C5-C6-O6
4	С	13	BGC	C4-C5-C6-O6
4	С	9	BGC	O5-C5-C6-O6
4	С	13	BGC	O5-C5-C6-O6
4	С	10	BGC	O5-C5-C6-O6
4	С	6	BGC	O5-C5-C6-O6
4	С	3	BGC	O5-C5-C6-O6
4	С	15	BGC	C4-C5-C6-O6
4	С	1	BGC	C4-C5-C6-O6
4	С	15	BGC	O5-C5-C6-O6

Continued from previous page...

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	С	14	BGC	1	0
4	С	11	BGC	3	0
4	С	17	BGC	1	0
4	С	5	BGC	4	0
4	С	12	BGC	1	0
4	С	8	BGC	1	0
4	С	6	BGC	1	0
4	С	7	BGC	2	0
4	С	10	BGC	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)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	Tinle	Bo	ond leng	$_{\rm sths}$	Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PLC	В	803	-	8,8,41	0.30	0	7,7,49	0.77	0
8	PLC	А	923	-	37,37,41	1.11	4 (10%)	43,45,49	1.08	2(4%)
5	C2E	А	920	-	44,52,52	0.99	2 (4%)	52,82,82	1.03	5 (9%)
8	PLC	В	804	-	10,10,41	0.30	0	9,9,49	0.80	0
6	UDP	А	921	7	24,26,26	1.00	1 (4%)	37,40,40	1.75	5 (13%)
9	3PE	А	924	-	19,19,50	1.36	4 (21%)	22,24,55	1.49	2 (9%)
5	C2E	А	919	-	44,52,52	0.96	2 (4%)	52,82,82	1.07	5 (9%)
10	UND	В	802	-	10,10,10	0.26	0	9,9,9	0.54	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
8	PLC	В	803	-	-	0/6/6/45	-
8	PLC	А	923	-	-	25/41/41/45	-
5	C2E	А	920	-	-	0/22/62/62	0/6/7/7
8	PLC	В	804	-	-	6/8/8/45	-
6	UDP	А	921	7	-	3/16/32/32	0/2/2/2
9	3PE	А	924	-	-	5/22/22/54	-
5	C2E	А	919	-	-	2/22/62/62	0/6/7/7



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	UND	В	802	-	-	1/8/8/8	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
9	А	924	3PE	O21-C2	-2.52	1.40	1.46
9	А	924	3PE	O31-C31	2.45	1.40	1.33
8	А	923	PLC	O2-C2	-2.44	1.40	1.46
8	А	923	PLC	O3-CB	2.43	1.40	1.33
9	А	924	3 PE	O21-C21	2.34	1.40	1.35
5	А	920	C2E	C6-N1	-2.34	1.34	1.37
5	А	919	C2E	C6-N1	-2.33	1.34	1.37
5	А	920	C2E	C61-N11	-2.30	1.34	1.37
5	А	919	C2E	C61-N11	-2.28	1.34	1.37
8	А	923	PLC	O2-C'	2.15	1.40	1.34
9	А	924	3 PE	O31-C3	-2.11	1.40	1.45
8	А	923	PLC	O3-C3	-2.08	1.40	1.45
6	А	921	UDP	C5-C4	-2.01	1.39	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	А	921	UDP	C4-N3-C2	-5.60	119.20	126.58
9	А	924	3PE	O21-C21-C22	4.83	119.98	111.09
8	А	923	PLC	O2-C'-C1'	3.92	119.96	111.50
6	А	921	UDP	C5-C4-N3	3.79	120.50	114.84
6	А	921	UDP	N3-C2-N1	3.54	119.59	114.89
9	А	924	3PE	O31-C31-C32	3.36	120.19	111.38
6	А	921	UDP	O4-C4-C5	-3.27	119.42	125.16
6	А	921	UDP	PA-O3A-PB	-2.86	123.00	132.83
8	А	923	PLC	O3-CB-C1B	2.59	120.05	111.91
5	А	919	C2E	C81-N71-C51	2.58	107.91	102.99
5	А	920	C2E	C81-N71-C51	2.54	107.84	102.99
5	А	919	C2E	C8-N7-C5	2.54	107.82	102.99
5	А	920	C2E	C8-N7-C5	2.52	107.80	102.99
5	А	919	C2E	C3'-C2'-C1'	2.47	105.37	99.89
5	А	919	C2E	C51-C61-N11	2.41	118.21	113.95
5	A	919	C2E	C5-C6-N1	2.37	118.14	113.95
5	А	920	C2E	C51-C61-N11	2.33	118.07	113.95
5	A	920	C2E	C5-C6-N1	2.29	117.99	113.95
5	А	920	C2E	C3'-C2'-C1'	2.19	104.73	99.89



There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
6	А	921	UDP	C5'-O5'-PA-O2A
6	А	921	UDP	C5'-O5'-PA-O3A
8	А	923	PLC	O3P-C1-C2-O2
8	А	923	PLC	O4P-C4-C5-N
8	А	923	PLC	C5-C4-O4P-P
8	А	923	PLC	C1-O3P-P-O1P
8	А	923	PLC	C4-O4P-P-O1P
9	А	924	3PE	C1-O11-P-O14
9	А	924	3PE	O13-C11-C12-N
9	А	924	3PE	O32-C31-O31-C3
9	А	924	3PE	C32-C31-O31-C3
8	А	923	PLC	O2-C2-C3-O3
8	А	923	PLC	C1-O3P-P-O4P
8	А	923	PLC	C4-O4P-P-O3P
8	А	923	PLC	C6B-C7B-C8B-C9B
8	А	923	PLC	C1'-C2'-C3'-C4'
8	А	923	PLC	CB-C1B-C2B-C3B
8	А	923	PLC	C5B-C6B-C7B-C8B
8	А	923	PLC	C7B-C8B-C9B-CAA
8	В	804	PLC	C5'-C6'-C7'-C8'
8	В	804	PLC	C7'-C8'-C9'-CA'
8	А	923	PLC	C4B-C5B-C6B-C7B
8	А	923	PLC	C1-C2-C3-O3
8	В	804	PLC	C8'-C9'-CA'-CB'
8	А	923	PLC	C8B-C9B-CAA-CBA
10	В	802	UND	C7-C8-C9-C10
8	А	923	PLC	C1'-C'-O2-C2
8	А	923	PLC	C3B-C4B-C5B-C6B
8	А	923	PLC	O'-C'-O2-C2
9	А	924	3PE	C1-O11-P-O13
6	А	921	UDP	C5'-O5'-PA-O1A
8	А	923	PLC	O3P-C1-C2-C3
8	В	804	PLC	C3'-C4'-C5'-C6'
8	А	923	PLC	C'-C1'-C2'-C3'
8	В	804	PLC	C2'-C3'-C4'-C5'
8	А	923	PLC	C2B-C1B-CB-O3
8	В	804	PLC	C1'-C2'-C3'-C4'
8	А	923	PLC	C1B-CB-O3-C3
8	А	923	PLC	OB-CB-O3-C3
5	А	919	C2E	O4A-C4A-C5A-O5A



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Mol	Chain	Res	Type	Atoms
8	А	923	PLC	C2B-C1B-CB-OB
5	А	919	C2E	C2'-C3'-O3'-P11

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	В	803	PLC	1	0
8	А	923	PLC	2	0
6	А	921	UDP	4	0
5	А	919	C2E	1	0
10	В	802	UND	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 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	$OWAB(Å^2)$	Q < 0.9
1	А	728/803~(90%)	0.20	42 (5%) 23 21	55, 79, 133, 176	0
2	В	655/724~(90%)	-0.13	16 (2%) 59 59	49, 72, 116, 161	0
3	D	0/9	-	-	-	-
All	All	1383/1536~(90%)	0.05	58 (4%) 36 35	49, 75, 126, 176	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res Type		RSRZ	
1	А	16	VAL	5.3	
1	А	13	VAL	5.2	
1	А	15	PRO	4.3	
2	В	77	GLN	4.2	
1	А	318	CYS	4.1	
1	А	499	ARG	3.7	
1	А	188	MET	3.7	
2	В	593	LEU	3.6	
2	В	78	GLN	3.5	
2	В	595	PRO	3.5	
2	В	594	ARG	3.5	
1	А	398	PHE	3.4	
1	А	192	PRO	3.4	
1	А	739	ARG	3.3	
1	А	496	LEU	3.3	
1	А	221	ARG	3.2	
1	А	393	LEU	3.1	
1	А	502	ARG	3.1	
1	А	17	LEU	3.1	
1	А	134	LEU	3.0	
1	A	740	ARG	2.9	
1	А	94	LEU	2.9	
2	В	590	ARG	2.9	



Mol	Chain	Res	Type	RSRZ	
1	А	187	CYS	2.8	
2	В	169	PHE	2.8	
1	А	514	GLU	2.7	
1	А	497	ARG	2.7	
2	В	531	THR	2.7	
1	А	543	VAL	2.7	
1	А	14	VAL	2.7	
1	А	264	VAL	2.6	
1	А	735	PRO	2.6	
2	В	130	PHE	2.6	
1	А	620	ARG	2.6	
2	В	544	GLY	2.6	
1	А	498	PRO	2.6	
1	А	335	PHE	2.6	
2	В	589	VAL	2.6	
1	А	19	PHE	2.5	
1	А	194	LEU	2.5	
1	А	501	ALA	2.5	
1	А	737	ARG	2.4	
1	А	137	GLU	2.4	
1	А	738	ARG	2.4	
1	А	706	PRO	2.4	
2	В	592	MET	2.3	
1	А	120	PHE	2.3	
1	А	705	ARG	2.3	
1	А	319	GLY	2.3	
2	В	494	ASP	2.3	
1	А	297	GLU	2.2	
1	А	235	GLU	2.2	
1	А	20	LEU	2.1	
2	В	131	GLY	2.1	
2	В	596	GLY	2.1	
2	В	247	TRP	2.1	
1	А	400	ARG	2.0	
1	A	240	GLU	2.0	

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

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



6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
4	SHG	С	18	11/12	0.78	0.41	100,108,125,138	0
4	BGC	С	1	12/12	0.82	0.31	120,132,137,143	0
4	BGC	С	2	11/12	0.88	0.18	100,107,112,112	0
4	BGC	С	8	11/12	0.90	0.25	$67,\!85,\!116,\!135$	0
4	BGC	С	17	11/12	0.91	0.40	77,82,98,99	0
4	BGC	С	3	11/12	0.91	0.14	$81,\!91,\!107,\!109$	0
4	BGC	С	16	11/12	0.92	0.38	69,75,90,100	0
4	BGC	С	6	11/12	0.92	0.22	$50,\!58,\!80,\!103$	0
4	BGC	С	5	11/12	0.92	0.21	49,52,86,113	0
4	BGC	С	15	11/12	0.93	0.32	62, 76, 87, 89	0
4	BGC	С	10	11/12	0.93	0.26	65, 96, 113, 131	0
4	BGC	С	13	11/12	0.94	0.29	66,71,88,92	0
4	BGC	С	14	11/12	0.94	0.28	57,74,80,87	0
4	BGC	С	9	11/12	0.94	0.23	84,91,101,106	0
4	BGC	С	7	11/12	0.95	0.14	$49,\!57,\!76,\!89$	0
4	BGC	С	4	11/12	0.95	0.18	$56,\!67,\!86,\!93$	0
4	BGC	С	12	11/12	0.96	0.26	64,80,89,94	0
4	BGC	С	11	11/12	0.97	0.20	77,86,100,103	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
7	MG	А	922	1/1	0.73	0.93	$98,\!98,\!98,\!98$	0
7	MG	В	801	1/1	0.81	0.13	$61,\!61,\!61,\!61$	0
8	PLC	А	923	38/42	0.83	0.46	87,124,155,157	0
8	PLC	В	804	11/42	0.85	0.42	72,83,94,97	0
10	UND	В	802	11/11	0.87	0.37	63,68,80,82	0
9	3PE	А	924	20/51	0.91	0.26	87,105,115,120	0
8	PLC	В	803	9/42	0.91	0.26	49,77,87,92	0
6	UDP	А	921	25/25	0.94	0.18	77,102,116,116	0
5	C2E	А	920	46/46	0.95	0.13	49,74,90,101	0
5	C2E	А	919	46/46	0.96	0.14	49,68,83,95	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.

