

Full wwPDB X-ray Structure Validation Report (i)

Aug 18, 2021 – 06:03 am BST

PDB ID	:	7BG0
Title	:	Fusion of MBP and the backbone of the long-acting amylin analog AM833.
Authors	:	Johansson, E.
Deposited on	:	2021-01-05
$\operatorname{Resolution}$:	2.89 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 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	:	2.23.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution $(\#Entries, resolution range(Å))$
P	130704	(7, 2000, 200, 100, 100, 100, 100, 100, 10
Itfree	100704	1907 (2.90-2.90)
Clashscore	141614	2172(2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	408	^{2%} 79%	19% ••
1	В	408	% 75%	14% • 9%
1	D	408	68%	20% • 10%
1	Е	408	8%	20% ••
2	С	2	50%	50%



Mol	Chain	Length	Quality	of chain
2	F	2	50%	50%



$7 \mathrm{BG0}$

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11933 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 Maltose/maltodextrin-binding periplasmic protein,Islet amyloid polypeptide.

Mol	Chain	Residues		At	\mathbf{oms}			ZeroOcc	AltConf	Trace
1 A		402	Total	С	Ν	Ο	S	0	0	0
	A	403	3102	1991	512	591	8	0	0	0
1	D	971	Total	С	Ν	Ο	S	0	0	0
	D	571	2863	1844	467	546	6	0	0	0
1	р	266	Total	С	Ν	Ο	S	0	0	0
	D	300	2831	1825	460	540	6	0	0	0
1 F		40.1	Total	С	Ν	Ο	S	0	0	0
		401	3091	1984	510	589	8	0	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	26	MET	-	initiating methionine	UNP POAEX9
А	385	ALA	GLU	engineered mutation	UNP P0AEX9
А	388	ALA	-	linker	UNP P0AEX9
A	389	ALA	-	linker	UNP P0AEX9
A	390	ALA	-	linker	UNP P0AEX9
A	391	GLN	-	linker	UNP P0AEX9
A	392	THR	-	linker	UNP P0AEX9
А	393	ASN	-	linker	UNP P0AEX9
A	394	ALA	-	linker	UNP P0AEX9
A	395	ALA	-	linker	UNP P0AEX9
A	396	ALA	-	linker	UNP POAEX9
A	410	GLU	ASN	engineered mutation	UNP P10997
А	413	ARG	VAL	engineered mutation	UNP P10997
A	421	PRO	ALA	engineered mutation	UNP P10997
A	424	PRO	SER	engineered mutation	UNP P10997
A	425	PRO	SER	engineered mutation	UNP P10997
A	433	PRO	TYR	engineered mutation	UNP P10997
В	26	MET	-	initiating methionine	UNP POAEX9
В	385	ALA	GLU	engineered mutation	UNP POAEX9
В	388	ALA	-	linker	UNP POAEX9



	Bosiduo	Modelled	Actual	Commont	Boforonco
			Actual		
	389	ALA	-		UNP PUAEA9
B	390	ALA	-		UNP PUAEX9
B	391	GLN	-	linker	UNP PUAEX9
B	392	THR	-	linker	UNP POAEX9
B	393	ASN	-	linker	UNP POAEX9
B	394	ALA	-	linker	UNP POAEX9
B	395	ALA	-	linker	UNP POAEX9
B	396	ALA	-	linker	UNP POAEX9
B	410	GLU	ASN	engineered mutation	UNP P10997
B	413	ARG	VAL	engineered mutation	UNP P10997
<u> </u>	421	PRO	ALA	engineered mutation	UNP P10997
B	424	PRO	SER	engineered mutation	UNP P10997
B	425	PRO	SER	engineered mutation	UNP P10997
B	433	PRO	TYR	engineered mutation	UNP P10997
D	26	MET	-	initiating methionine	UNP POAEX9
D	385	ALA	GLU	engineered mutation	UNP POAEX9
D	388	ALA	_	linker	UNP P0AEX9
D	389	ALA	-	linker	UNP P0AEX9
D	390	ALA	-	linker	UNP POAEX9
D	391	GLN	-	linker	UNP POAEX9
D	392	THR	-	linker	UNP POAEX9
D	393	ASN	-	linker	UNP POAEX9
D	394	ALA	-	linker	UNP POAEX9
D	395	ALA	-	linker	UNP POAEX9
D	396	ALA	_	linker	UNP POAEX9
D	410	GLU	ASN	engineered mutation	UNP P10997
D	413	ARG	VAL	engineered mutation	UNP P10997
D	421	PRO	ALA	engineered mutation	UNP P10997
D	424	PRO	SER	engineered mutation	UNP P10997
D	425	PRO	SER	engineered mutation	UNP P10997
D	433	PRO	TYR	engineered mutation	UNP P10997
Е	26	MET	_	initiating methionine	UNP POAEX9
Е	385	ALA	GLU	engineered mutation	UNP POAEX9
Е	388	ALA	_	linker	UNP POAEX9
E	389	ALA	_	linker	UNP POAEX9
Е	390	ALA	_	linker	UNP POAEX9
E	391	GLN	-	linker	UNP POAEX9
E	392	THR	_	linker	UNP POAEX9
Ē	393	ASN	_	linker	UNP POAEX9
Ē	394	ALA	_	linker	UNP POAEX9
E	395	ALA	_	linker	UNP POAEX9
E	396	ALA	_	linker	UNP POAEX9

Contin $d f_{a}$



Chain	Residue	Modelled	Actual	Comment	Reference
Е	410	GLU	ASN	engineered mutation	UNP P10997
Е	413	ARG	VAL	engineered mutation	UNP P10997
Е	421	PRO	ALA	engineered mutation	UNP P10997
Е	424	PRO	SER	engineered mutation	UNP P10997
Е	425	PRO	SER	engineered mutation	UNP P10997
Е	433	PRO	TYR	engineered mutation	UNP P10997

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	С	2	Total C O 23 12 11	0	0	0
2	F	2	Total C O 23 12 11	0	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: Maltose/maltodextrin-binding periplasmic protein,Islet amyloid polypeptide



• Molecule 1: Maltose/maltodextrin-binding periplasmic protein,Islet amyloid polypeptide





N308 N308 V1309 1.131 L311 1.310 L316 1.316 L316 1.316 L316 1.316 L316 1.316 L316 1.330 L316 1.330 L330 1.332 L330 1.332 L330 1.332 L330 1.332 L330 1.333 L330 1.334 M345 M345 M365 1.335 M365 1.335 M365 1.335 M365 1.335 M365 1.335 M365 1.337 M365 1.337 M365 1.337 M365 1.337 M365 1.337 M37 1.337 M37 1.337 M37 1.337 M37 1.338 M37 1.338 M37 1.338

• Molecule 1: Maltose/maltodextrin-binding periplasmic protein,Islet amyloid polypeptide



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

Chain C:	50%	50%
<mark>6101</mark>		

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

Chain F:

50%

50%

GLC1 GLC2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	Н 3	Depositor
Cell constants	179.13Å 179.13Å 150.21Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	37.55 - 2.89	Depositor
Resolution (A)	41.36 - 2.89	EDS
% Data completeness	99.4 (37.55-2.89)	Depositor
(in resolution range $)$	87.3(41.36-2.89)	EDS
R _{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.54 (at 2.90 \text{\AA})$	Xtriage
Refinement program	PHENIX dev_3965	Depositor
D D .	0.220 , 0.279	Depositor
Π, Π_{free}	0.220 , 0.281	DCC
R_{free} test set	1986 reflections (4.98%)	wwPDB-VP
Wilson B-factor $(Å^2)$	56.1	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 34.9	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11933	wwPDB-VP
Average B, all atoms $(Å^2)$	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.82% 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: GLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	Bond lengths		Bond angles	
10101	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.28	0/3177	0.47	0/4318
1	В	0.28	0/2932	0.46	0/3982
1	D	0.27	0/2900	0.48	1/3939~(0.0%)
1	Е	0.28	0/3166	0.51	2/4303~(0.0%)
All	All	0.28	0/12175	0.48	3/16542~(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	Е	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	Е	413	ARG	CB-CG-CD	-7.14	93.02	111.60
1	Е	413	ARG	CG-CD-NE	6.04	124.48	111.80
1	D	273	LEU	CA-CB-CG	5.84	128.73	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Е	413	ARG	Sidechain



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	3102	0	3068	61	0
1	В	2863	0	2838	46	0
1	D	2831	0	2804	68	0
1	Е	3091	0	3056	75	0
2	С	23	0	21	0	0
2	F	23	0	21	2	0
All	All	11933	0	11808	194	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 (194) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1		Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:A:105:ILE:HG22	1:A:107:PRO:HD3	1.56	0.87
1:E:183:THR:HG22	1:E:187:ILE:HD11	1.59	0.84
1:D:105:ILE:HG22	1:D:107:PRO:HD3	1.60	0.82
1:B:105:ILE:HG22	1:B:107:PRO:HD3	1.63	0.79
1:A:59:ILE:HG12	1:B:301:LEU:HD21	1.65	0.78
1:E:64:GLU:HG2	1:E:66:PRO:HD3	1.65	0.78
1:D:299:LYS:O	1:D:301:LEU:N	2.16	0.77
1:D:66:PRO:HD2	1:D:69:LEU:HD12	1.67	0.77
1:D:287:VAL:HB	1:E:90:HIS:HD2	1.50	0.75
1:D:36:TRP:HB3	1:D:69:LEU:HD11	1.70	0.72
1:D:356:MET:HB2	1:E:90:HIS:CE1	2.25	0.71
1:E:179:GLU:HB2	1:E:182:PHE:HE2	1.56	0.70
1:E:105:ILE:HG22	1:E:107:PRO:HD3	1.74	0.70
1:D:258:TRP:HB2	1:D:324:PRO:HG2	1.74	0.70
1:D:284:PHE:HD1	1:D:356:MET:HG2	1.56	0.69
1:A:417:ASN:N	1:A:417:ASN:OD1	2.25	0.68
1:E:179:GLU:HB2	1:E:182:PHE:CE2	2.28	0.67
1:B:207:VAL:O	1:B:391:GLN:NE2	2.27	0.67
1:A:38:ASN:ND2	1:A:40:ASP:OD1	2.29	0.65
1:E:154:THR:OG1	1:E:157:GLU:HG2	1.96	0.65
1:B:298:ASN:N	1:B:298:ASN:OD1	2.29	0.65



Interatomic Clash					
Atom-1	Atom-2	distance $(Å)$	overlap(Å)		
1:E:66:PBO:HG2	1:E:69:LEU:HD13	1.80	0.64		
1:E:338:ALA:HA	1:E:340:ASP:N	2.12	0.64		
1:E:338:ALA:HB2	1:E:343:ILE:HB	1.80	0.64		
1:A:338:ALA:HB2	1:A:343:ILE:HB	1.81	0.63		
1:B:258:TRP:HB2	1:B:324:PRO:HG2	1.79	0.63		
1:A:338:ALA:HA	1:A:340:ASP:N	2.14	0.62		
1:A:32:LYS:O	1:B:298:ASN:ND2	2.22	0.61		
1:A:90:HIS:HD2	1:B:287:VAL:HB	1.64	0.61		
1:D:284:PHE:CD1	1:D:356:MET:HG2	2.35	0.60		
1:E:153:LYS:N	1:E:157:GLU:OE2	2.29	0.60		
1:D:298:ASN:ND2	1:E:29:GLU:O	2.35	0.59		
1:A:59:ILE:HG12	1:B:301:LEU:CD2	2.32	0.59		
1:D:306:LEU:HD21	1:E:85:ILE:HD13	1.86	0.58		
1:B:268:TYR:OH	1:B:342:ARG:NH1	2.36	0.58		
1:A:207:VAL:CG1	1:A:395:ALA:HB2	2.33	0.58		
1:D:255:PRO:HB2	1:D:324:PRO:HB2	1.86	0.58		
1:A:115:LEU:HD23	1:A:133:PRO:HG2	1.86	0.57		
1:D:356:MET:HB2	1:E:90:HIS:HE1	1.69	0.57		
1:E:36:TRP:CG	1:E:83:PRO:HG3	2.38	0.57		
1:D:298:ASN:OD1	1:E:31:GLY:N	2.38	0.57		
1:E:88:TRP:HB3	1:E:93:PHE:HE1	1.69	0.56		
1:D:270:VAL:HG22	1:E:142:ILE:HG22	1.86	0.56		
1:E:32:LYS:HD3	1:E:60:LYS:HB3	1.88	0.56		
1:B:235:ASP:OD2	1:B:238:ILE:HG12	2.06	0.55		
1:A:90:HIS:CE1	1:B:356:MET:HB2	2.42	0.55		
1:A:207:VAL:HG11	1:A:395:ALA:HB2	1.89	0.54		
1:D:359:ILE:HD12	1:D:361:GLN:HB2	1.88	0.54		
1:A:109:LYS:NZ	1:A:113:ASP:OD2	2.32	0.54		
1:D:49:VAL:HA	1:D:52:LYS:HE3	1.90	0.54		
1:E:90:HIS:CD2	1:E:122:ALA:HB1	2.43	0.53		
1:B:123:VAL:HG21	1:B:133:PRO:HD3	1.91	0.53		
1:B:284:PHE:CD1	1:B:356:MET:HG2	2.43	0.53		
1:A:54:GLU:O	1:A:58:GLY:HA2	2.09	0.53		
1:D:275:THR:O	1:E:155:TRP:N	2.35	0.53		
1:E:36:TRP:CD2	1:E:83:PRO:HG3	2.43	0.53		
1:A:57:THR:O	1:A:59:ILE:HD12	2.08	0.53		
1:E:105:ILE:HD12	1:E:132:TYR:CE1	2.43	0.53		
1:D:323:LYS:HD3	1:E:42:GLY:HA2	1.91	0.53		
1:B:215:LYS:HD3	1:B:387:LEU:HD12	1.90	0.52		
1:E:70:GLU:H	1:E:70:GLU:CD	2.12	0.52		
1:D:287:VAL:HB	1:E:90:HIS:CD2	2.40	0.52		



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:106:THR:O	1:E:106:THR:OG1	2.27	0.52	
1:E:116:TYR:O	1:E:119:THR:OG1	2.25	0.52	
1:A:32:LYS:HA	1:A:59:ILE:CG2	2.39	0.52	
1:B:36:TRP:HB3	1:B:69:LEU:HD13	1.92	0.51	
1:E:37:ILE:HA	1:E:87:PHE:HB2	1.93	0.51	
1:B:73:PHE:CG	1:B:86:ILE:HD12	2.45	0.51	
1:D:255:PRO:O	1:D:258:TRP:N	2.35	0.51	
1:D:270:VAL:HG12	1:D:345:ALA:HB3	1.91	0.51	
1:A:148:LEU:HD21	1:A:152:PRO:HD3	1.92	0.51	
1:A:183:THR:HG23	1:B:221:LEU:HD13	1.91	0.51	
1:D:258:TRP:CH2	1:D:342:ARG:HG3	2.46	0.51	
1:A:328:VAL:HA	1:B:135:ALA:HA	1.93	0.51	
1:D:298:ASN:HD21	1:E:30:GLU:HA	1.76	0.51	
1:D:283:PRO:HB3	1:E:185:PRO:HG3	1.92	0.50	
1:A:31:GLY:O	1:A:59:ILE:HG23	2.11	0.50	
1:B:317:GLU:HG2	1:B:321:LYS:HE2	1.93	0.50	
1:B:317:GLU:O	1:B:321:LYS:HG3	2.11	0.50	
1:E:148:LEU:HD11	1:E:151:PRO:HA	1.94	0.50	
1:A:90:HIS:CD2	1:B:287:VAL:H	2.29	0.50	
1:D:247:GLU:HA	1:E:170:LYS:HD2	1.94	0.50	
1:D:284:PHE:HD2	1:E:184:TRP:CD1	2.30	0.50	
1:D:287:VAL:H	1:E:90:HIS:CD2	2.30	0.50	
1:A:305:PHE:HE1	1:B:50:GLY:HA2	1.77	0.49	
1:D:185:PRO:HG3	1:E:283:PRO:HA	1.94	0.49	
1:D:123:VAL:HG21	1:D:133:PRO:HD3	1.92	0.49	
1:B:148:LEU:HD21	1:B:152:PRO:HD3	1.94	0.49	
1:A:418:ASN:CG	1:A:419:PHE:H	2.16	0.49	
1:B:161:LEU:HG	1:B:165:LEU:HD12	1.95	0.49	
1:A:223:ASP:O	1:A:227:ASN:ND2	2.46	0.49	
1:D:303:LYS:HG3	1:D:307:GLU:OE1	2.13	0.49	
1:A:144:ASN:HB3	1:A:147:LEU:HB2	1.93	0.48	
1:D:256:TRP:HA	1:D:324:PRO:HD2	1.96	0.48	
1:D:322:ASP:OD2	1:E:44:ASN:HB2	2.13	0.48	
1:D:328:VAL:HA	1:E:135:ALA:HA	1.95	0.48	
1:E:27:LYS:N	1:E:81:ASP:OD1	2.47	0.48	
1:A:159:PRO:HA	1:B:229:HIS:CD2	2.49	0.48	
1:D:349:ASN:ND2	1:E:140:SER:HA	2.29	0.48	
1:A:305:PHE:CE1	1:B:50:GLY:HA2	2.49	0.47	
1:D:142:ILE:HG12	1:E:270:VAL:HG22	1.95	0.47	
1:D:247:GLU:O	1:E:170:LYS:HB3	2.14	0.47	
1:D:277:LYS:NZ	1:E:190:ASP:OD1	2.30	0.47	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:36:TRP:HB3	1:E:69:LEU:HD11	1.96	0.46
1:E:187:ILE:HD12	1:E:187:ILE:H	1.80	0.46
1:D:215:LYS:O	1:D:219:THR:HB	2.15	0.46
1:A:270:VAL:HG22	1:B:142:ILE:HG12	1.98	0.46
1:A:283:PRO:HA	1:B:185:PRO:HG3	1.98	0.46
1:B:242:ALA:O	1:B:247:GLU:HB3	2.16	0.46
1:D:309:TYR:O	1:D:315:GLY:HA3	2.16	0.46
1:D:309:TYR:CE2	1:E:53:PHE:HD1	2.34	0.46
1:E:155:TRP:O	1:E:158:ILE:HD12	2.16	0.46
1:E:158:ILE:N	1:E:159:PRO:HD2	2.31	0.45
1:A:116:TYR:HE2	1:B:334:GLU:HG2	1.81	0.45
1:B:48:GLU:O	1:B:51:LYS:HB2	2.16	0.45
1:E:418:ASN:C	1:E:420:GLY:H	2.19	0.45
1:A:70:GLU:OE1	1:A:70:GLU:N	2.36	0.45
1:A:135:ALA:HA	1:B:328:VAL:HA	1.99	0.45
1:E:73:PHE:CE1	1:E:86:ILE:HB	2.52	0.45
1:E:271:THR:OG1	1:E:272:VAL:N	2.50	0.45
1:A:76:VAL:O	1:A:79:THR:OG1	2.34	0.45
1:A:56:ASP:N	1:A:56:ASP:OD1	2.50	0.45
1:D:115:LEU:HB2	1:D:120:TRP:NE1	2.32	0.45
1:D:292:ILE:HG21	1:D:299:LYS:HE3	1.99	0.45
1:E:336:GLU:O	1:E:339:LYS:HG3	2.17	0.45
1:D:202:TYR:CZ	1:D:357:PRO:HG3	2.52	0.44
1:A:54:GLU:OE1	1:A:60:LYS:NZ	2.40	0.44
1:A:152:PRO:CD	1:B:250:MET:HE1	2.47	0.44
1:B:258:TRP:CH2	1:B:342:ARG:HG3	2.52	0.44
1:A:148:LEU:HD12	1:A:149:PRO:HD2	1.99	0.44
1:D:273:LEU:HD22	1:D:349:ASN:ND2	2.32	0.44
1:D:207:VAL:O	1:D:391:GLN:NE2	2.51	0.44
1:D:214:ALA:HA	1:E:187:ILE:HG22	1.99	0.44
1:A:257:ALA:O	1:A:261:ILE:HG13	2.18	0.44
1:A:255:PRO:HA	1:A:258:TRP:CE2	2.52	0.44
1:D:270:VAL:HB	1:D:342:ARG:HB2	2.00	0.44
1:D:255:PRO:O	1:D:257:ALA:N	2.51	0.44
1:A:35:ILE:HG12	1:A:85:ILE:HB	1.98	0.44
1:D:70:GLU:HB3	1:D:88:TRP:CZ2	2.53	0.44
1:A:428:VAL:HG21	1:E:237:SER:HB3	1.99	0.43
1:A:53:PHE:O	1:A:57:THR:N	2.45	0.43
1:B:52:LYS:HE3	1:B:52:LYS:HB2	1.55	0.43
1:E:311:LEU:HD23	1:E:311:LEU:HA	1.89	0.43
1:D:252:ILE:HD12	1:E:175:PHE:CD2	2.53	0.43



	, a c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:105:ILE:CG2	1:E:107:PRO:HD3	2.46	0.43
1:E:92:ARG:NH1	2:F:2:GLC:O4	2.52	0.43
1:E:31:GLY:O	1:E:59:ILE:HG23	2.19	0.43
1:D:186:LEU:HD23	1:E:221:LEU:HB2	2.01	0.43
1:E:184:TRP:HA	1:E:187:ILE:CD1	2.49	0.43
1:A:418:ASN:C	1:A:420:GLY:H	2.23	0.42
1:D:261:ILE:H	1:D:261:ILE:HG13	1.71	0.42
1:E:162:ASP:O	1:E:166:LYS:HG3	2.19	0.42
1:A:368:ALA:HB1	1:A:390:ALA:HA	2.01	0.42
1:A:37:ILE:HA	1:A:87:PHE:HB2	2.01	0.42
1:D:217:GLY:HA3	1:E:187:ILE:HA	2.00	0.42
1:E:148:LEU:HD22	1:E:149:PRO:HD2	2.00	0.42
1:A:153:LYS:HA	1:A:153:LYS:HD2	1.78	0.42
1:A:292:ILE:HD12	1:B:105:ILE:HD11	2.02	0.42
1:B:67:ASP:OD1	1:E:237:SER:OG	2.30	0.42
1:B:255:PRO:HA	1:B:258:TRP:CD2	2.54	0.42
1:A:270:VAL:HB	1:A:342:ARG:HG2	2.02	0.42
1:A:94:GLY:HA3	1:B:358:ASN:O	2.20	0.42
1:A:347:MET:O	1:A:347:MET:HE3	2.20	0.42
1:D:215:LYS:HD3	1:D:387:LEU:HD12	2.00	0.42
1:A:221:LEU:HB2	1:B:186:LEU:HD23	2.01	0.42
1:A:218:LEU:HD23	1:A:383:VAL:HG13	2.02	0.41
1:B:47:ALA:O	1:B:51:LYS:HG3	2.20	0.41
1:A:141:LEU:HD22	1:B:274:PRO:HG3	2.02	0.41
1:E:41:LYS:HD3	1:E:41:LYS:HA	1.88	0.41
1:A:271:THR:OG1	1:A:272:VAL:N	2.53	0.41
1:D:27:LYS:HD2	1:D:27:LYS:HA	1.80	0.41
1:D:169:GLY:O	1:D:170:LYS:HD3	2.20	0.41
1:D:209:VAL:O	1:D:387:LEU:HD22	2.20	0.41
1:E:38:ASN:ND2	1:E:88:TRP:HZ3	2.18	0.41
1:E:68:LYS:HA	1:E:68:LYS:HD2	1.66	0.41
1:A:54:GLU:OE2	1:A:60:LYS:HD2	2.20	0.41
1:D:235:ASP:OD1	1:D:237:SER:N	2.53	0.41
1:D:298:ASN:ND2	1:E:30:GLU:HA	2.34	0.41
1:D:375:ASN:HB3	1:D:381:GLN:HB2	2.02	0.41
1:E:119:THR:HB	1:E:133:PRO:HB2	2.02	0.41
1:D:275:THR:OG1	1:E:154:THR:HG22	2.20	0.41
1:B:207:VAL:HG11	1:B:395:ALA:HB2	2.03	0.41
1:D:48:GLU:OE1	1:D:51:LYS:HE3	2.21	0.41
1:D:366:TRP:CD1	2:F:2:GLC:H4	2.56	0.41
1:E:70:GLU:HB2	1:E:92:ARG:HD3	2.02	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:A:185:PRO:HG3	1:B:283:PRO:HA	2.03	0.41	
1:D:133:PRO:O	1:D:134:ILE:HD13	2.21	0.41	
1:D:314:GLU:H	1:D:314:GLU:CD	2.24	0.41	
1:D:259:SER:HA	1:D:262:ASP:OD2	2.21	0.40	
1:D:32:LYS:O	1:E:298:ASN:ND2	2.54	0.40	
1:A:59:ILE:HG21	1:B:301:LEU:HD23	2.03	0.40	
1:A:105:ILE:HD12	1:A:132:TYR:CE1	2.56	0.40	
1:A:207:VAL:HG23	1:B:194:ALA:O	2.21	0.40	
1:A:428:VAL:HG11	1:E:237:SER:OG	2.21	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	Perce	\mathbf{ntiles}
1	А	401/408~(98%)	380~(95%)	17~(4%)	4 (1%)	15	45
1	В	369/408~(90%)	350~(95%)	18 (5%)	1 (0%)	41	71
1	D	364/408~(89%)	345~(95%)	14 (4%)	5(1%)	11	36
1	E	399/408~(98%)	380~(95%)	16 (4%)	3 (1%)	19	51
All	All	1533/1632~(94%)	1455(95%)	65(4%)	13 (1%)	19	51

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	428	VAL
1	D	256	TRP
1	D	300	GLU
1	Е	149	PRO
1	D	234	THR
1	А	149	PRO



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Mol	Chain	Res	Type
1	В	194	ALA
1	D	194	ALA
1	Е	191	GLY
1	Е	397	LYS
1	А	397	LYS
1	D	299	LYS
1	А	191	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric Outlier		Percentiles	
1	А	319/324~(98%)	310~(97%)	9~(3%)	43 76	
1	В	292/324~(90%)	275~(94%)	17~(6%)	20 50	
1	D	290/324~(90%)	278~(96%)	12~(4%)	30 64	
1	Ε	318/324~(98%)	307~(96%)	11 (4%)	36 70	
All	All	1219/1296~(94%)	1170~(96%)	49~(4%)	31 65	

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	55	LYS
1	А	81	ASP
1	А	140	SER
1	А	174	MET
1	А	201	LYS
1	А	209	VAL
1	А	323	LYS
1	А	408	LEU
1	А	417	ASN
1	В	48	GLU
1	В	51	LYS
1	В	69	LEU
1	В	75	GLN
1	В	92	ARG



Mol	Chain Res		Type
1	В	168	LYS
1	В	201	LYS
1	В	210	ASP
1	В	221	LEU
1	В	284	PHE
1	В	298	ASN
1	В	303	LYS
1	В	304	GLU
1	В	313	ASP
1	В	354	GLU
1	В	367	TYR
1	В	371	THR
1	D	86	ILE
1	D	164	GLU
1	D	201	LYS
1	D	210	ASP
1	D	219	THR
1	D	226	LYS
1	D	235	ASP
1	D	296	SER
1	D	321	LYS
1	D	362	MET
1	D	371	THR
1	D	382	THR
1	Е	56	ASP
1	Е	68	LYS
1	Е	140	SER
1	Е	143	TYR
1	Е	145	LYS
1	Е	171	SER
1	E	199	ASN
1	Е	201	LYS
1	Е	304	GLU
1	Е	408	LEU
1	Е	426	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type	
1	А	90	HIS	
1	В	231	ASN	
1	Ε	90	HIS	



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Mol	Chain	\mathbf{Res}	Type	
1	Ε	227	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)

4 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	al Turna Chain Dag Lind		Tink	Bo	ond leng	$_{\rm sths}$	Bond angles			
	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	С	1	2	12,12,12	0.53	0	17,17,17	0.56	0
2	GLC	C	2	2	11,11,12	0.57	0	15,15,17	0.89	1 (6%)
2	GLC	F	1	2	12,12,12	0.55	0	17,17,17	0.98	0
2	GLC	F	2	2	11,11,12	0.54	0	15,15,17	1.02	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	С	1	2	-	2/2/22/22	0/1/1/1
2	GLC	С	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	2/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1



There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	F	2	GLC	C1-O5-C5	2.76	115.93	112.19
2	С	2	GLC	C1-O5-C5	2.21	115.19	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
2	F	1	GLC	C4-C5-C6-O6
2	F	1	GLC	O5-C5-C6-O6
2	С	1	GLC	C4-C5-C6-O6
2	С	1	GLC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	GLC	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)

There are no ligands in this entry.

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	403/408~(98%)	-0.07	7 (1%) 70 69	32, 53, 92, 114	0
1	В	371/408~(90%)	-0.17	4 (1%) 80 80	35, 57, 83, 98	0
1	D	366/408~(89%)	0.38	31 (8%) 10 8	35, 82, 119, 128	0
1	Е	401/408~(98%)	0.36	34 (8%) 10 8	34, 66, 122, 134	0
All	All	1541/1632~(94%)	0.12	76 (4%) 29 26	32, 60, 117, 134	0

All (76) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	А	427	ASN	6.6
1	Е	49	VAL	5.4
1	Е	147	LEU	5.4
1	D	311	LEU	5.3
1	Е	53	PHE	4.5
1	Е	172	ALA	4.4
1	Е	173	LEU	4.3
1	D	222	VAL	4.1
1	D	295	ALA	3.9
1	Е	63	VAL	3.6
1	Е	161	LEU	3.5
1	D	326	GLY	3.4
1	Е	158	ILE	3.4
1	Е	427	ASN	3.2
1	Е	32	LYS	3.2
1	Е	168	LYS	3.2
1	Е	33	LEU	3.1
1	D	367	TYR	3.0
1	D	316	LEU	3.0
1	А	57	THR	2.9
1	А	428	VAL	2.9



Mol	Chain	Res	Type	RSRZ
1	Е	167	ALA	2.9
1	D	372	ALA	2.9
1	Е	70	GLU	2.9
1	D	373	VAL	2.8
1	Е	35	ILE	2.8
1	D	309	TYR	2.8
1	D	290	ALA	2.8
1	D	308	ASN	2.8
1	D	336	GLU	2.7
1	D	369	VAL	2.7
1	D	230	MET	2.7
1	D	381	GLN	2.7
1	Е	164	GLU	2.6
1	Е	146	ASP	2.6
1	Е	416	SER	2.6
1	Е	67	ASP	2.6
1	В	396	ALA	2.6
1	Е	72	LYS	2.5
1	D	209	VAL	2.5
1	Е	98	GLN	2.5
1	D	232	ALA	2.5
1	Е	175	PHE	2.4
1	D	335	GLU	2.4
1	D	333	TYR	2.4
1	Е	165	LEU	2.4
1	Е	163	LYS	2.3
1	D	252	ILE	2.3
1	Е	87	PHE	2.3
1	D	387	LEU	2.3
1	D	218	LEU	2.3
1	Е	62	THR	2.3
1	D	231	ASN	2.2
1	E	55	LYS	2.2
1	А	417	ASN	2.2
1	В	395	ALA	2.2
1	E	$13\overline{2}$	TYR	2.2
1	E	178	GLN	2.2
1	E	114	LYS	2.2
1	E	144	ASN	2.2
1	Е	153	LYS	2.2
1	D	224	LEU	2.2
1	D	246	GLY	2.2



Mol	Chain	\mathbf{Res}	Type	RSRZ
1	D	256	TRP	2.1
1	D	390	ALA	2.1
1	В	397	LYS	2.1
1	А	429	GLY	2.1
1	А	163	LYS	2.1
1	D	325	LEU	2.1
1	D	310	LEU	2.1
1	D	321	LYS	2.1
1	В	224	LEU	2.0
1	Е	156	GLU	2.0
1	А	160	ALA	2.0
1	D	330	LEU	2.0
1	Е	46	LEU	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	F	1	12/12	0.92	0.14	$91,\!96,\!101,\!101$	0
2	GLC	С	1	12/12	0.95	0.17	$42,\!51,\!56,\!57$	0
2	GLC	F	2	11/12	0.95	0.18	79,83,87,89	0
2	GLC	С	2	11/12	0.97	0.18	41,43,48,49	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

