

# Full wwPDB X-ray Structure Validation Report (i)

#### Sep 3, 2023 – 04:16 AM EDT

PDB ID	:	3RLF
Title	:	Crystal structure of the maltose-binding protein/maltose transporter complex
		in an outward-facing conformation bound to MgAMPPNP
Authors	:	Oldham, M.L.; Chen, J.
Deposited on	:	2011-04-19
Resolution	:	2.20 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
$\mathrm{EDS}$	:	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 2.20 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.



Motrie	Whole archive	Similar resolution
WIEUTIC	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
R <sub>free</sub>	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	
			12%	
1	Ε	380	89%	9% •
			14%	
2	F	514	86%	8% • 5%
			6%	
3	G	296	90%	6% • •
			4%	
4	А	381	86%	11% ••
			8%	
4	В	381	85%	11% • •



Mol	Chain	Length	Quality of chain
5	С	2	100%



# 2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 15268 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-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Е	374	Total 2914	C 1875	N 476	O 557	S 6	0	2	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Е	371	ALA	-	expression tag	UNP P0AEX9
Е	372	SER	-	expression tag	UNP P0AEX9
Е	373	ALA	-	expression tag	UNP P0AEX9
Е	374	SER	-	expression tag	UNP P0AEX9
Е	375	HIS	-	expression tag	UNP P0AEX9
E	376	HIS	-	expression tag	UNP P0AEX9
Е	377	HIS	-	expression tag	UNP P0AEX9
E	378	HIS	-	expression tag	UNP P0AEX9
Е	379	HIS	-	expression tag	UNP P0AEX9
Е	380	HIS	-	expression tag	UNP P0AEX9

• Molecule 2 is a protein called Maltose transport system permease protein malF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	490	Total 3832	C 2517	N 612	O 686	S 17	0	1	0

• Molecule 3 is a protein called Maltose transport system permease protein malG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	286	Total 2214	C 1484	N 352	O 370	S 8	0	2	0

• Molecule 4 is a protein called Maltose/maltodextrin import ATP-binding protein MalK.



Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
4	Δ	371	Total	С	Ν	Ο	$\mathbf{S}$	0	Ο	0
4 11	011	2876	1819	515	529	13	0	0	0	
4	Р	271	Total	С	Ν	Ο	$\mathbf{S}$	0	1	0
4 D	511	2881	1822	515	531	13	0	1	0	

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	372	ALA	-	expression tag	UNP P68187
А	373	SER	-	expression tag	UNP P68187
А	374	ALA	-	expression tag	UNP P68187
А	375	SER	-	expression tag	UNP P68187
А	376	HIS	-	expression tag	UNP P68187
А	377	HIS	-	expression tag	UNP P68187
А	378	HIS	-	expression tag	UNP P68187
А	379	HIS	-	expression tag	UNP P68187
А	380	HIS	-	expression tag	UNP P68187
А	381	HIS	-	expression tag	UNP P68187
В	372	ALA	-	expression tag	UNP P68187
В	373	SER	-	expression tag	UNP P68187
В	374	ALA	-	expression tag	UNP P68187
В	375	SER	-	expression tag	UNP P68187
В	376	HIS	-	expression tag	UNP P68187
В	377	HIS	-	expression tag	UNP P68187
В	378	HIS	-	expression tag	UNP P68187
В	379	HIS	-	expression tag	UNP P68187
В	380	HIS	-	expression tag	UNP P68187
В	381	HIS	-	expression tag	UNP P68187

• Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	С	2	Total 23	C 12	0 11	0	0	0





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
6	Е	1	Total 34	C 23	0 11	0	0

• Molecule 7 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHO RYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total C O P 51 40 10 1	0	0
7	F	1	Total C 14 14	0	0



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Continued	from	previous	page

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total C 14 14	0	0
7	G	1	Total C 12 12	0	0

• Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

• Molecule 9 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
0	Δ	1	Total	С	Ν	Ο	Р	0	0	
9	A	L	31	10	6	12	3	0	0	
0	Р	1	Total	С	Ν	Ο	Р	0	0	
9	D	L	31	10	6	12	3	0	0	

• Molecule 10 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	Е	62	Total         O           62         62	0	0
10	F	63	Total         O           63         63	0	0
10	G	59	Total         O           59         59	0	0
10	А	81	Total         O           81         81	0	0
10	В	74	Total O 74 74	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.

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- Molecule 1: Maltose-binding periplasmic protein

• Molecule 2: Maltose transport system permease protein malF



• Molecule 3: Maltose transport system permease protein malG





# MET MET V212 MET V212 MET V213 MET VAL MET VAL MET VAL MET VAL MET P331 LUS VAL LUS VAL LUS P335 LUS P336 LUS P335 LUS P335 LUS P45 L16 P45 K60 P116 K72 P124 L49 P1274 L49 P126 K60 P127 K73 P126 K73 P116 L102 P116 L1126 P116 L1126 P116 L1126 P133 F133 P133 F133 P133 F133 P133 F133 P133 F133 P133 F133

• Molecule 4: Maltose/maltodextrin import ATP-binding protein MalK



• Molecule 5: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:

100%





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	72.10Å 95.81Å 109.98Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$86.70^{\circ}$ $82.68^{\circ}$ $76.40^{\circ}$	Depositor
Bosolution(A)	20.00 - 2.20	Depositor
Resolution (A)	19.97 - 2.20	EDS
% Data completeness	86.3 (20.00-2.20)	Depositor
(in resolution range)	86.3(19.97-2.20)	EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.17 (at 2.19 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
B B.	0.223 , $0.254$	Depositor
II, II, <i>free</i>	0.223 , $0.254$	DCC
$R_{free}$ test set	6209 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	39.2	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.39, 56.1	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15268	wwPDB-VP
Average B, all atoms $(Å^2)$	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: UMQ, ANP, GLC, MG, PGV

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		
INIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	Е	0.34	0/2983	0.46	0/4048	
2	F	0.36	0/3927	0.50	0/5344	
3	G	0.37	0/2278	0.49	0/3115	
4	А	0.34	0/2926	0.53	1/3968~(0.0%)	
4	В	0.35	0/2932	0.53	0/3974	
All	All	0.35	0/15046	0.50	1/20449~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	347	LEU	CA-CB-CG	5.08	126.98	115.30

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	Е	2914	0	2888	19	0
2	F	3832	0	3861	32	0
3	G	2214	0	2302	11	0
4	А	2876	0	2941	26	0
4	В	2881	0	2942	29	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	С	23	0	21	0	0
6	Е	34	0	44	0	0
7	F	65	0	100	2	0
7	G	26	0	44	1	0
8	А	1	0	0	0	0
8	В	1	0	0	0	0
9	А	31	0	13	2	0
9	В	31	0	13	2	0
10	А	81	0	0	1	0
10	В	74	0	0	2	0
10	Ε	62	0	0	0	0
10	F	63	0	0	0	0
10	G	59	0	0	0	0
All	All	15268	0	15169	111	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 4.

All (111) 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 $(\text{\AA})$	overlap (Å)	
2:F:471:THR:HG21	2:F:490:ILE:HG21	1.42	1.01	
4:A:39:GLY:H	9:A:2501:ANP:HNB1	1.16	0.94	
4:B:39:GLY:H	9:B:2502:ANP:HNB1	1.18	0.88	
4:A:223:HIS:CE1	4:A:368:GLU:HG2	2.12	0.85	
4:B:344:ALA:N	4:B:344:ALA:CB	2.45	0.80	
4:B:344:ALA:CB	4:B:344:ALA:C	2.51	0.79	
4:B:141:ARG:NH1	10:B:455:HOH:O	2.05	0.78	
1:E:116:ILE:HD11	1:E:242:TYR:HD2	1.51	0.76	
2:F:196:VAL:HG13	2:F:204:PHE:HB3	1.69	0.75	
2:F:471:THR:CG2	2:F:490:ILE:HG21	2.16	0.75	
4:A:288:GLU:HG2	4:B:312:ASN:HB2	1.70	0.73	
2:F:159:LEU:HD11	2:F:188:ALA:HB1	1.70	0.73	
4:A:39:GLY:N	9:A:2501:ANP:HNB1	1.88	0.70	
1:E:116:ILE:HD11	1:E:242:TYR:CD2	2.27	0.69	
3:G:86:TRP:CE2	3:G:90:LYS:HD2	2.29	0.68	
4:B:344:ALA:N	4:B:344:ALA:C	2.47	0.67	
4:B:39:GLY:N	9:B:2502:ANP:HNB1	1.93	0.66	
2:F:196:VAL:CG1	2:F:204:PHE:HB3	2.27	0.65	
4:A:6:LEU:HD22	4:A:22:ILE:HD11	1.78	0.65	
2:F:471:THR:HG21	2:F:490:ILE:CG2	2.22	0.65	



	<b>A b b c</b>	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
4:B:320:ILE:HD11	4:B:327:LEU:HB2	1.80	0.63	
4:A:208:ASP:O	4:A:211:ARG:HG2	2.02	0.59	
1:E:367:ARG:HD2	2:F:460:PRO:HG3	1.84	0.59	
2:F:280:ILE:O	2:F:284:THR:HG23	2.02	0.59	
4:A:312:ASN:HB2	4:B:288:GLU:HG2	1.85	0.59	
2:F:444:ILE:HG13	2:F:466:LEU:HG	1.85	0.57	
4:B:324:ARG:HD3	4:B:324:ARG:H	1.70	0.57	
2:F:471:THR:HG23	2:F:490:ILE:HD13	1.88	0.56	
2:F:36:ALA:O	2:F:38:GLY:N	2.37	0.56	
2:F:59:ASN:HD22	2:F:59:ASN:H	1.54	0.56	
2:F:360:ALA:HB1	2:F:363:SER:HB2	1.90	0.54	
4:A:223:HIS:ND1	4:A:368:GLU:HG2	2.22	0.54	
2:F:212:THR:HG23	2:F:222:ASN:HD21	1.72	0.54	
3:G:45:ALA:HB2	3:G:260:TRP:CE2	2.43	0.54	
4:B:246:VAL:HG23	4:B:281:MET:HG3	1.91	0.53	
4:B:288:GLU:HG3	4:B:330:ARG:HD3	1.91	0.52	
4:A:97:SER:HB3	4:A:114:VAL:HG21	1.91	0.52	
4:A:270:VAL:HG13	4:A:362:CYS:HB3	1.92	0.51	
4:A:208:ASP:HB2	4:A:229:PHE:CE2	2.46	0.51	
4:A:86:LEU:HA	4:A:146:ARG:NH2	2.25	0.50	
3:G:110:PHE:HB3	3:G:178:LYS:HD2	1.93	0.50	
4:B:26:ILE:HG12	4:B:32:VAL:HG21	1.93	0.50	
4:A:288:GLU:HG3	4:A:330:ARG:HD3	1.94	0.50	
3:G:60:LYS:HE2	7:G:4006:PGV:H201	1.94	0.50	
3:G:224:ILE:HG12	3:G:274[A]:ILE:HD12	1.94	0.50	
4:B:146:ARG:HD2	10:B:393:HOH:O	2.12	0.49	
4:B:208:ASP:O	4:B:211:ARG:HG3	2.13	0.49	
4:B:290:LEU:HD22	4:B:345:ILE:HD13	1.94	0.48	
3:G:230:VAL:HB	3:G:231:PRO:HD3	1.95	0.48	
1:E:116:ILE:HG12	1:E:244:VAL:HG22	1.95	0.48	
2:F:445:GLN:HG2	2:F:469:ASN:HD22	1.79	0.47	
1:E:62:TRP:HB3	1:E:67:PHE:HE1	1.79	0.47	
2:F:403:SER:HB3	2:F:417:ILE:HD11	1.96	0.46	
2:F:86:THR:O	2:F:488:ALA:HB1	2.14	0.46	
4:B:145:GLY:O	4:B:149:VAL:HG23	2.16	0.46	
4:A:62:ILE:HB	4:A:67:MET:HG3	1.97	0.46	
2:F:273:ILE:HA	2:F:470:TYR:OH	2.15	0.46	
2:F:376:ASN:HD21	2:F:437:ASN:ND2	2.14	0.46	
1:E:6:LYS:HA	1:E:33:ILE:HG23	1.98	0.46	
4:A:157:LEU:HB3	4:A:160:PRO:HG3	1.96	0.46	
3:G:245:LEU:HG	3:G:249:MET:HE2	1.96	0.46	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:F:372:LEU:HD21	2:F:444:ILE:HD12	1.98	0.46	
4:B:33:VAL:HG22	4:B:204:ILE:HG12	1.97	0.46	
4:B:236:SER:HA	4:B:237:PRO:C	2.35	0.46	
1:E:110:VAL:HG11	1:E:321:MET:HE3	1.96	0.46	
4:A:260:MET:CE	4:A:300:LEU:HD22	2.46	0.45	
4:B:86:LEU:HA	4:B:146:ARG:NH2	2.31	0.45	
3:G:245:LEU:HG	3:G:249:MET:CE	2.47	0.45	
4:B:77:VAL:HG12	4:B:154:VAL:HB	1.99	0.45	
2:F:284:THR:HG21	2:F:467:LEU:H	1.80	0.45	
4:B:100:LEU:HB3	4:B:110:ILE:HG12	1.98	0.45	
4:B:131:PRO:HA	4:B:134:LEU:HD22	1.99	0.45	
2:F:125:TYR:HA	2:F:126:PRO:HD2	1.89	0.44	
4:A:34:PHE:HB2	4:A:190:VAL:HG22	1.98	0.44	
4:A:86:LEU:HA	4:A:146:ARG:HH22	1.82	0.44	
2:F:429:LEU:HD23	3:G:172:LEU:HD22	2.00	0.44	
1:E:18:ASN:O	1:E:22:GLU:HG2	2.18	0.44	
4:B:321:PRO:O	4:B:322:SER:HB3	2.17	0.44	
1:E:192:LEU:HD23	1:E:357:VAL:HG13	1.98	0.44	
4:B:262:ASN:ND2	4:B:264:GLN:HB2	2.33	0.44	
2:F:305:LEU:O	2:F:311:LEU:HD12	2.18	0.44	
2:F:216:ASP:OD1	2:F:218:THR:HG22	2.18	0.43	
2:F:305:LEU:HD23	7:F:4001:PGV:H011	2.00	0.43	
2:F:410:PRO:HB3	7:F:4001:PGV:H02	1.99	0.43	
4:A:113:ARG:HG3	4:A:149:VAL:HG13	2.01	0.43	
4:B:45:LEU:HD12	4:B:207:LEU:HD11	2.00	0.43	
1:E:92:PHE:HD1	1:E:329:ILE:HD11	1.83	0.43	
2:F:232:ASN:O	2:F:257:VAL:HG21	2.18	0.43	
2:F:284:THR:HG22	2:F:466:LEU:HA	2.01	0.43	
4:A:67:MET:HE1	4:A:75:ARG:HA	2.00	0.43	
1:E:371:ALA:HB1	2:F:478:GLY:O	2.19	0.42	
1:E:77:ALA:HB2	1:E:273:LYS:HE3	2.01	0.42	
1:E:229:PRO:HA	1:E:232:TRP:CE2	2.54	0.42	
1:E:349:ASN:HB3	1:E:355:GLN:HB2	2.02	0.42	
4:A:315:GLN:HG2	4:A:330:ARG:HG2	2.01	0.42	
4:B:33:VAL:HA	4:B:189:TYR:O	2.19	0.42	
4:B:50:ALA:HB2	4:B:79:MET:HE3	2.01	0.42	
4:A:151:GLU:O	4:A:185:ARG:NH2	2.52	0.42	
1:E:90:TYR:HA	1:E:91:PRO:HD3	1.95	0.42	
4:B:100:LEU:HD13	4:B:150:ALA:HA	2.00	0.42	
1:E:158:TRP:N	1:E:159:PRO:CD	2.82	0.41	
4:A:364:ARG:HD2	10:A:423:HOH:O	2.18	0.41	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:E:249:THR:HG22	1:E:254:PRO:HA	2.02	0.41	
1:E:47:PHE:HB3	1:E:48:PRO:HD3	2.02	0.41	
1:E:341:TYR:CE2	2:F:460:PRO:HB2	2.56	0.41	
4:A:148:LEU:HD22	4:A:179:LEU:HD22	2.02	0.41	
4:A:236:SER:HA	4:A:237:PRO:C	2.40	0.41	
2:F:81:PHE:HB3	2:F:82:PRO:HD3	2.02	0.40	
3:G:102:LEU:O	3:G:106:CYS:HB2	2.21	0.40	
4:A:87:TYR:HA	4:A:88:PRO:HD3	1.87	0.40	
3:G:177:ILE:HD11	3:G:218:VAL:HG21	2.02	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	Percentile	es
1	Ε	374/380~(98%)	364 (97%)	9(2%)	1 (0%)	41 46	
2	$\mathbf{F}$	487/514~(95%)	471 (97%)	14 (3%)	2(0%)	34 37	
3	G	286/296~(97%)	283~(99%)	2(1%)	1 (0%)	41 46	
4	А	369/381~(97%)	360~(98%)	9(2%)	0	100 100	)
4	В	369/381~(97%)	360~(98%)	8 (2%)	1 (0%)	41 46	
All	All	1885/1952~(97%)	1838 (98%)	42 (2%)	5 (0%)	41 46	

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	37	GLN
2	F	38	GLY
1	Е	165	GLY
4	В	105	ALA
3	G	230	VAL



#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	hain Analysed Rotameric Outliers		Percentiles		
1	Ε	299/305~(98%)	295~(99%)	4 (1%)	69 81	
2	F	403/424~(95%)	395~(98%)	8 (2%)	55 69	
3	G	230/237~(97%)	226~(98%)	4 (2%)	60 74	
4	А	314/323~(97%)	305~(97%)	9~(3%)	42 54	
4	В	315/323~(98%)	303~(96%)	12 (4%)	33 42	
All	All	1561/1612~(97%)	1524 (98%)	37(2%)	49 62	

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Е	65	ASP
1	Е	116	ILE
1	Е	224	MET
1	Е	365	GLN
2	F	59	ASN
2	F	145	LEU
2	F	196	VAL
2	F	284	THR
2	F	306	VAL
2	F	325	TYR
2	F	440	ASN
2	F	471	THR
3	G	106	CYS
3	G	126	LEU
3	G	212	VAL
3	G	235	LEU
4	А	22	ILE
4	А	127	LEU
4	А	219	LEU
4	А	252	ASP
4	А	270	VAL
4	А	288	GLU
4	А	327	LEU



Mol	Chain	Res	Type
4	А	331	GLN
4	А	350	GLU
4	В	15	GLU
4	В	100	LEU
4	В	123	LEU
4	В	127	LEU
4	В	134	LEU
4	В	185	ARG
4	В	211	ARG
4	В	252	ASP
4	В	258	LEU
4	В	288	GLU
4	В	320	ILE
4	В	324	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	Е	218	ASN
2	F	59	ASN
2	F	98	ASN
2	F	222	ASN
2	F	232	ASN
2	F	437	ASN
2	F	440	ASN
3	G	241	ASN
4	В	180	HIS

#### 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)

2 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	$\mathbf{ths}$	В	ond ang	les
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GLC	С	1	5	12,12,12	0.51	0	$17,\!17,\!17$	1.08	1 (5%)
5	GLC	С	2	5	11,11,12	0.35	0	$15,\!15,\!17$	0.98	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
5	GLC	С	1	5	-	0/2/22/22	0/1/1/1
5	GLC	С	2	5	-	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	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
5	С	1	GLC	C1-O5-C5	3.08	119.48	113.66
5	С	2	GLC	C1-O5-C5	2.97	116.21	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	Mol Type Chain F		Dec	Tink	Bo	ond leng	$_{\rm ths}$	Bond angles		
IVIOI	туре	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	ANP	А	2501	8	29,33,33	1.88	8 (27%)	31,52,52	2.17	7 (22%)
7	PGV	F	4001	-	50,50,50	1.08	3 (6%)	53,56,56	1.02	3 (5%)
7	PGV	F	4002	-	13,13,50	0.28	0	12,12,56	0.52	0
9	ANP	В	2502	8	29,33,33	1.83	9 (31%)	31,52,52	1.89	6 (19%)
7	PGV	G	4006	-	13,13,50	0.27	0	12,12,56	0.54	0



Mal Turna		Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Dec	Tink	Bo	ond leng	$\mathbf{ths}$	В	ond ang	les
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2													
6	UMQ	Е	5004	-	$35,\!35,\!35$	0.44	0	46,46,46	0.84	2 (4%)													
7	PGV	G	4009	-	11,11,50	0.27	0	10,10,56	0.53	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
9	ANP	А	2501	8	-	4/14/38/38	0/3/3/3
7	PGV	F	4001	-	-	27/55/55/55	-
7	PGV	F	4002	-	-	9/11/11/55	-
9	ANP	В	2502	8	-	4/14/38/38	0/3/3/3
7	PGV	G	4006	-	-	3/11/11/55	-
6	UMQ	Е	5004	-	-	10/20/60/60	0/2/2/2
7	PGV	G	4009	-	-	7/9/9/55	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(\text{\AA})$	Ideal(Å)
9	А	2501	ANP	PB-N3B	4.41	1.74	1.63
7	F	4001	PGV	O03-C19	4.39	1.46	1.33
9	А	2501	ANP	PG-N3B	4.36	1.74	1.63
7	F	4001	PGV	O01-C1	4.29	1.46	1.34
9	В	2502	ANP	PB-N3B	4.25	1.74	1.63
9	В	2502	ANP	PG-N3B	4.16	1.74	1.63
7	F	4001	PGV	C12-C11	3.63	1.52	1.31
9	В	2502	ANP	PB-O1B	3.46	1.51	1.46
9	В	2502	ANP	PG-01G	3.37	1.51	1.46
9	А	2501	ANP	PB-O1B	3.36	1.51	1.46
9	А	2501	ANP	PG-01G	3.32	1.51	1.46
9	А	2501	ANP	PB-O3A	2.55	1.62	1.59
9	А	2501	ANP	C5-C4	2.53	1.47	1.40
9	В	2502	ANP	C5-C4	2.43	1.47	1.40
9	В	2502	ANP	PG-O3G	-2.38	1.50	1.56
9	А	2501	ANP	PG-O2G	-2.35	1.50	1.56
9	А	2501	ANP	PB-O2B	-2.22	1.50	1.56
9	В	2502	ANP	C2-N3	2.14	1.35	1.32
9	В	2502	ANP	PG-O2G	-2.11	1.51	1.56
9	В	2502	ANP	PB-O2B	-2.01	1.51	1.56



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
9	А	2501	ANP	O1G-PG-N3B	-7.95	100.06	111.77
9	В	2502	ANP	O1G-PG-N3B	-5.91	103.07	111.77
9	А	2501	ANP	O2B-PB-O1B	4.68	119.74	109.92
7	F	4001	PGV	O01-C1-C2	4.16	120.48	111.50
9	В	2502	ANP	O2B-PB-O1B	4.16	118.64	109.92
9	А	2501	ANP	O1B-PB-N3B	-3.61	106.45	111.77
9	А	2501	ANP	N3-C2-N1	-3.50	123.21	128.68
9	В	2502	ANP	N3-C2-N1	-3.39	123.38	128.68
9	В	2502	ANP	O1B-PB-N3B	-3.10	107.20	111.77
9	В	2502	ANP	O2G-PG-O3G	2.72	114.89	107.64
7	F	4001	PGV	O03-C19-C20	2.51	119.80	111.91
9	В	2502	ANP	C4-C5-N7	-2.39	106.91	109.40
9	А	2501	ANP	C4-C5-N7	-2.34	106.96	109.40
6	Е	5004	UMQ	C3'-C4'-C5'	2.27	116.14	110.93
9	A	2501	ANP	O2G-PG-O3G	2.25	113.64	107.64
6	Е	5004	UMQ	C2'-C3'-C4'	2.23	114.77	109.68
7	F	4001	PGV	O01-C1-O02	-2.15	118.50	123.70
9	А	2501	ANP	PB-O3A-PA	-2.09	125.25	132.62

All (18) bond angle outliers are listed below:

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
7	F	4001	PGV	C03-O11-P-O12
7	F	4001	PGV	C03-O11-P-O13
7	F	4001	PGV	C03-O11-P-O14
7	F	4001	PGV	C04-C05-C06-O06
7	F	4001	PGV	C2-C1-O01-C02
9	А	2501	ANP	PG-N3B-PB-O1B
9	А	2501	ANP	PA-O3A-PB-O1B
9	А	2501	ANP	PA-O3A-PB-O2B
9	В	2502	ANP	PB-N3B-PG-O1G
9	В	2502	ANP	PG-N3B-PB-O1B
9	В	2502	ANP	PA-O3A-PB-O1B
9	В	2502	ANP	PA-O3A-PB-O2B
7	F	4001	PGV	O02-C1-O01-C02
7	F	4001	PGV	C10-C11-C12-C13
6	Е	5004	UMQ	O5'-C1'-O1'-CA
7	F	4001	PGV	C20-C19-O03-C01
7	F	4001	PGV	O04-C19-O03-C01
6	Е	5004	UMQ	C2'-C1'-O1'-CA

All (64) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
7	F	4001	PGV	C1-C2-C3-C4
6	Е	5004	UMQ	O5'-C5'-C6'-O6'
6	Е	5004	UMQ	CC-CD-CF-CG
7	F	4001	PGV	C23-C24-C25-C26
7	F	4001	PGV	C25-C26-C27-C28
7	G	4006	PGV	C22-C23-C24-C25
7	G	4009	PGV	C23-C24-C25-C26
7	F	4001	PGV	C22-C23-C24-C25
7	F	4001	PGV	C6-C7-C8-C9
7	F	4001	PGV	C26-C27-C28-C29
7	F	4001	PGV	C11-C10-C9-C8
6	Е	5004	UMQ	CG-CH-CI-CJ
7	F	4001	PGV	C29-C30-C31-C32
7	F	4001	PGV	C4-C5-C6-C7
7	F	4001	PGV	C20-C21-C22-C23
7	G	4009	PGV	C20-C21-C22-C23
7	F	4001	PGV	C21-C22-C23-C24
7	F	4001	PGV	C19-C20-C21-C22
7	F	4001	PGV	C30-C31-C32-C33
7	F	4001	PGV	C2-C3-C4-C5
7	F	4002	PGV	C20-C21-C22-C23
7	F	4002	PGV	C28-C29-C30-C31
7	F	4001	PGV	O05-C05-C06-O06
7	G	4009	PGV	C26-C27-C28-C29
7	F	4002	PGV	C22-C23-C24-C25
7	G	4009	PGV	C25-C26-C27-C28
7	F	4002	PGV	C27-C28-C29-C30
7	F	4001	PGV	C14-C15-C16-C17
7	G	4009	PGV	C27-C28-C29-C30
7	F	4002	PGV	C21-C22-C23-C24
7	F	4001	PGV	O03-C01-C02-C03
6	Е	5004	UMQ	CI-CJ-CK-CL
7	G	4009	PGV	C21-C22-C23-C24
7	F	4001	PGV	O03-C01-C02-O01
7	G	4009	PGV	C19-C20-C21-C22
6	Е	5004	UMQ	CD-CF-CG-CH
7	F	4002	PGV	C19-C20-C21-C22
7	G	4006	PGV	C23-C24-C25-C26
6	Е	5004	UMQ	CB-CC-CD-CF
7	F	4002	PGV	C25-C26-C27-C28
7	F	4002	PGV	C23-C24-C25-C26
6	Е	5004	UMQ	CH-CI-CJ-CK

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Mol	Chain	Res	Type	Atoms
7	G	4006	PGV	C21-C22-C23-C24
7	F	4002	PGV	C26-C27-C28-C29
6	Ε	5004	UMQ	CA-CB-CC-CD
9	А	2501	ANP	PB-N3B-PG-O1G

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	А	2501	ANP	2	0
7	F	4001	PGV	2	0
9	В	2502	ANP	2	0
7	G	4006	PGV	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	<RSRZ $>$	#RSRZ>2		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	Е	374/380~(98%)	0.55	44 (11%) 4	4	30, 66, 111, 133	1 (0%)
2	F	490/514~(95%)	0.83	74 (15%) 2	2	32, 61, 127, 188	0
3	G	286/296~(96%)	0.26	19 (6%) 18	17	28, 44, 81, 108	0
4	А	371/381~(97%)	0.18	15 (4%) 38	36	27,  44,  69,  94	0
4	В	371/381~(97%)	0.25	30 (8%) 12	10	25,  46,  84,  112	0
All	All	1892/1952~(96%)	0.45	182 (9%) 8	6	25, 51, 104, 188	1 (0%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	10	TRP	19.4
2	F	37	GLN	11.0
2	F	38	GLY	8.9
2	F	14	ALA	7.6
2	F	29	TYR	7.4
3	G	70	ALA	6.9
2	F	355	PHE	6.7
4	В	105	ALA	6.5
3	G	72	GLY	6.4
3	G	71	ASP	6.3
1	Е	172	GLU	6.2
2	F	245	ASN	6.0
2	F	11	GLN	5.9
3	G	74	ILE	5.9
4	В	263	ARG	5.9
4	А	372	ALA	5.8
2	F	269	THR	5.8
2	F	22	LEU	5.7
4	В	324	ARG	5.5
2	F	40	TYR	5.5



3RLF
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Mol	Chain	Res	Type	RSRZ
4	В	251	ILE	5.5
4	В	295	ILE	5.5
1	Е	143 GLY		5.3
2	F	25 LEU		5.3
2	F	352	SER	5.3
4	А	104	GLY	5.3
3	G	73	ARG	5.2
2	F	357	VAL	5.2
4	В	260	MET	5.1
2	F	503	ILE	5.0
2	F	12	SER	5.0
1	Е	173	ASN	4.9
4	А	108	GLU	4.9
1	Е	119	LYS	4.9
3	G	114	ARG	4.8
1	Е	373	ALA	4.8
1	Е	374	SER	4.8
4	В	322	SER	4.7
2	F	248	ASP	4.7
2	F	275	LYS	4.6
4	А	294	ASP	4.5
2	F	246	TRP	4.4
2	F	271	GLU	4.3
2	F	15	LEU	4.2
3	G	69	GLN	4.2
2	F	260	GLY	4.2
4	В	294	ASP	4.2
2	F	354	LEU	4.1
2	F	17	TRP	4.1
2	F	13	ASP	4.0
2	F	214	ASP	4.0
2	F	278	LEU	4.0
2	F	216	ASP	4.0
4	А	295	ILE	3.9
2	F	312	ARG	3.9
4	В	296	ALA	3.9
2	F	411	PHE	3.8
2	F	60	ARG	3.8
4	В	261	PRO	3.8
4	А	324	ARG	3.7
1	Е	224	MET	3.7
2	F	16	LYS	3.7



Mol	Mol Chain Res		Type	RSRZ
1	Е	178 ILE		3.7
2	F	353	ALA	3.7
3	G	68	GLU	3.7
3	G	153	PHE	3.7
2	F	20	LEU	3.6
2	F	268	PHE	3.6
4	В	262	ASN	3.6
2	F	19	VAL	3.6
1	Е	123	PRO	3.6
4	А	261	PRO	3.5
1	Е	237	THR	3.5
1	Е	115	LEU	3.5
2	F	18	SER	3.5
3	G	116	PRO	3.4
2	F	349	MET	3.4
2	F	41	LEU	3.3
1	Е	147	LEU	3.3
1	Е	183	VAL	3.3
4	В	340	GLY	3.2
1	Е	170	LYS	3.2
4	В	323	ILE	3.2
4	В	14	GLY	3.2
4	В	15	GLU	3.2
4	В	372	ALA	3.2
2	F	500	ALA	3.2
2	F	247	GLY	3.2
4	А	181	LYS	3.1
2	F	213	LEU	3.1
1	Е	225	THR	3.1
1	E	1	LYS	3.1
1	E	253	GLN	3.1
1	E	364	ALA	3.0
1	E	359	GLU	3.0
1	E	179	LYS	3.0
4	В	297	ASP	3.0
2	F	134	ALA	3.0
1	Е	370	LYS	2.9
1	Е	192	LEU	2.9
2	F	23	LEU	2.9
2	F	21	GLY	2.9
4	В	16	VAL	2.9
2	F	48	ILE	2.9



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Mol	Chain	Res	Type	RSRZ				
1	Е	354	ARG	2.9				
2	F	44	ILE	2.8				
2	F	227	LYS	2.8				
1	Е	165	GLY	2.8				
3	G	11	ALA	2.8				
2	F	237	TYR	2.8				
4	В	259	PRO	2.8				
4	А	107	LYS	2.8				
2	F	303	ALA	2.7				
4	В	273	ARG	2.7				
3	G	133	ALA	2.7				
1	Е	164	ASP	2.7				
2	F	302	LEU	2.6				
2	F	195	LYS	2.6				
1	Е	160	LEU	2.6				
1	Е	174	GLY	2.6				
4	А	262	ASN	2.6				
2	F	219	LEU	2.6				
4	В	321	PRO	2.5				
2	F	280	ILE	2.5				
4	В	357	GLU	2.5				
3	G	152	PRO	2.5				
2	F	250	LYS	2.4				
1	Е	175	LYS	2.4				
2	F	306	VAL	2.4				
3	G	14	PHE	2.4				
4	В	178	ARG	2.4				
3	G	49	LEU	2.4				
1	Е	117	TYR	2.4				
3	G	146	ARG	2.4				
4	В	267	TRP	2.4				
1	Е	114	SER	2.4				
2	F	129	ASP	2.3				
1	Е	116	ILE	2.3				
4	В	353	HIS	2.3				
1	Е	226	ILE	2.3				
1	Е	368	ILE	2.3				
1	Е	146	ALA	2.3				
2	F	305	LEU	2.3				
4	А	74	GLU	2.3				
1	Е	362	LYS	2.3				
1	Е	124	ASN	2.3				



Mol	Chain	Res	Type	RSRZ	
4	А	49	ILE	2.3	
1	Е	168	ALA	2.3	
3	G	18	LEU	2.3	
2	F	345	GLY	2.3	
2	F	238	GLN	2.3	
2	F	490	ILE	2.3	
2	F	135	LEU	2.2	
4	В	181	LYS	2.2	
2	F	128	GLY	2.2	
2	F	356	GLY	2.2	
2	F	209	PRO	2.2	
1	Е	241	ASN	2.2	
4	А	15	GLU	2.2	
2	F	215	GLY	2.2	
4	В	358	ASP	2.2	
2	F	249	GLU	2.2	
4	В	132	LYS	2.2	
2	F	223	GLN	2.2	
1	Е	302	VAL	2.1	
1	Е	356 THR		2.1	
4	А	119	GLU	2.1	
2	F	466	LEU	2.1	
1	Е	161	ILE	2.1	
1	Е	141	ALA	2.1	
2	F	496	LEU	2.1	
4	В	341	ALA	2.1	
4	А	102	LEU	2.1	
2	F	265	THR	2.1	
3	G	75	THR	2.1	
1	Е	254	PRO	2.1	
1	Е	101	GLY	2.0	
2	F	287	PHE	2.0	
2	F	109	LEU	2.0	
3	G	149	GLU	2.0	
4	В	245	LYS	2.0	
2	F	114	TRP	2.0	

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

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



### 6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
5	GLC	С	1	12/12	0.95	0.08	47,49,52,54	0
5	GLC	С	2	11/12	0.95	0.11	46,48,50,51	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,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
7	PGV	F	4002	14/51	0.72	0.25	58,60,65,66	0
7	PGV	G	4009	12/51	0.73	0.23	70,71,74,74	0
6	UMQ	Е	5004	34/34	0.77	0.28	74,80,82,83	0
7	PGV	F	4001	51/51	0.81	0.23	75,83,86,91	0
7	PGV	G	4006	14/51	0.83	0.19	71,75,82,84	0
8	MG	А	1501	1/1	0.98	0.04	28,28,28,28	0
8	MG	В	1502	1/1	0.98	0.11	30,30,30,30	0
9	ANP	А	2501	31/31	0.98	0.09	25,32,41,41	0
9	ANP	В	2502	31/31	0.98	0.10	28,35,41,42	0

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.

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.

