

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

#### Aug 10, 2020 – 10:29 AM BST

:	6VG1
:	xenopus protocadherin 8.1 EC1-6
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:	2020-01-07
:	2.00  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
$\mathrm{EDS}$	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	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)	:	2.13.1

# 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 2.00 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries}, { m resolution\ range}({ m \AA}))$		
$R_{free}$	130704	$8085\ (2.00-2.00)$		
Clashscore	141614	$9178 \ (2.00-2.00)$		
Ramachandran outliers	138981	9054 (2.00-2.00)		
Sidechain outliers	138945	9053 (2.00-2.00)		
RSRZ outliers	127900	7900 (2.00-2.00)		

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 on 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	A	647	14%	74%		25%			
1	В	647	25%	72%		27%			
2	С	4	25%	25%		50%			
2	D	4		50%	25%	25%			

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 crite-



ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MAN	В	722	-	-	-	Х



# 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 19847 atoms, of which 9678 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 protocadherin protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Δ	642	Total	С	Η	Ν	Ο	S	0	0	0
	1 A 042	042	9697	3078	4771	838	997	13	0		
1	В	641	Total	С	Η	Ν	Ο	S	0	0	0
	D	041	9691	3075	4770	837	996	13			

Chain	Residue	Modelled	Actual	Comment	Reference
A	642	HIS	-	expression tag	UNP Q6GLU2
А	643	HIS	-	expression tag	UNP Q6GLU2
A	644	HIS	-	expression tag	UNP Q6GLU2
A	645	HIS	-	expression tag	UNP Q6GLU2
A	646	HIS	-	expression tag	UNP Q6GLU2
A	647	HIS	-	expression tag	UNP Q6GLU2
В	642	HIS	-	expression tag	UNP Q6GLU2
В	643	HIS	-	expression tag	UNP Q6GLU2
В	644	HIS	-	expression tag	UNP Q6GLU2
В	645	HIS	-	expression tag	UNP Q6GLU2
В	646	HIS	-	expression tag	UNP Q6GLU2
В	647	HIS	-	expression tag	UNP Q6GLU2

There are 12 discrepancies between the modelled and reference sequences:

• Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopy ranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	С	4	Total 92	C 28	Н 43	N 2	O 19	0	0	0



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	4	Total 92	C 28	Н 43	N 2	O 19	0	0	0

• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf	
3	А	1	Total	С	Η	Ο	0	0	
	0 11	±	10	2	6	2	0	Ū	
9	D	1	Total	С	Η	Ο	0	0	
3 B		10	2	6	2		0		

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	15	Total Ca 15 15	0	0
4	А	15	Total Ca 15 15	0	0

• Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total Cl 1 1	0	0
5	А	1	Total Cl 1 1	0	0



• Molecule 6 is alpha-D-mannopyranose (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	Δ	1	Total	С	Η	Ο	0	0	
	Л		21	6	10	5	0		
6	Δ	1	Total	С	Η	Ο	0	0	
0	0 A	T	21	6	10	5	0	0	
6	В	1	Total	С	Η	Ο	0	0	
0	D	L	20	6	9	5	0		
6	В	1	Total	С	Η	Ο	0	0	
6	В	D I	21	6	10	5	0	0	

• Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

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

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	81	Total O 81 81	0	0
8	В	57	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 57 & 57 \end{array}$	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: protocadherin protein





Chain C:	25%	25%	50%
NAG1 NAG2 BMA3 FUC4			

• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alp ha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:	50%	25%	25%
NAG1 NAG2 FUC4			



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	146.65Å $42.39$ Å $167.47$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $110.60^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{Bosolution} \left( \overset{\circ}{\mathbf{A}} \right)$	38.27 - 2.00	Depositor
Resolution (A)	38.27 - 2.00	EDS
% Data completeness	45.0 (38.27-2.00)	Depositor
(in resolution range)	41.9(38.27-2.00)	EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.61 (at 2.00 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
D D.	0.253 , $0.297$	Depositor
$\Pi, \Pi_{free}$	0.255 , $0.262$	DCC
$R_{free}$ test set	1775 reflections $(2.98%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	20.8	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , $47.3$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	19847	wwPDB-VP
Average B, all atoms $(Å^2)$	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 32.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6680e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<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: BMA, NAG, CL, NA, CA, EDO, FUC, MAN

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	
	Cham	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.34	0/5010	0.55	0/6823
1	В	0.32	0/5005	0.53	0/6816
All	All	0.33	0/10015	0.54	0/13639

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	4926	4771	4831	119	0
1	В	4921	4770	4828	141	0
2	С	49	43	43	1	0
2	D	49	43	43	2	0
3	А	4	6	6	1	0
3	В	4	6	6	0	0
4	А	15	0	0	0	0
4	В	15	0	0	0	0
5	А	1	0	0	0	0
5	В	1	0	0	0	0
6	А	22	20	20	1	0



	f = f = f = f = f = f = f = f = f = f =						
Mol	Chain	Non-H	${ m H(model)}$	H(added)	Clashes	Symm-Clashes	
6	В	22	19	19	2	0	
7	А	1	0	0	0	0	
7	В	1	0	0	0	0	
8	А	81	0	0	0	0	
8	В	57	0	0	1	0	
All	All	10169	9678	9796	260	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 13.

All (260) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:572:ASP:OD2	1:B:578:ASN:O	1.73	1.06
1:B:574:ASP:OD2	1:B:578:ASN:OD1	1.84	0.94
1:A:567:HIS:HE1	1:A:599:THR:HG22	1.32	0.92
1:B:220:GLU:HB3	1:B:311:ILE:HD11	1.56	0.86
1:B:557:SER:O	1:B:608:VAL:HG21	1.76	0.84
1:B:618:ALA:O	1:B:635:THR:OG1	1.94	0.83
1:A:567:HIS:CE1	1:A:599:THR:HG22	2.19	0.77
1:B:614:GLN:O	1:B:639:LEU:HD13	1.85	0.76
1:B:557:SER:HB2	1:B:608:VAL:HG11	1.68	0.75
1:A:565:VAL:CG2	1:A:602:VAL:HG13	2.16	0.75
1:B:10:GLU:OE1	1:B:57:ARG:NH2	2.20	0.74
1:A:155:ARG:HB2	1:A:159:VAL:HG22	1.69	0.73
1:A:392:GLU:OE2	1:A:426:ASP:OD1	2.06	0.73
1:A:612:ILE:HA	1:A:640:VAL:HG23	1.69	0.73
1:A:156:ALA:N	1:B:287:GLU:OE1	2.15	0.73
1:A:37:GLN:HE21	1:A:40:ASN:HA	1.54	0.72
1:B:293:GLN:HG3	1:B:301:THR:HG22	1.69	0.72
1:A:515:ASP:O	1:A:520:GLN:NE2	2.22	0.71
1:A:327:SER:HB2	1:A:332:VAL:O	1.91	0.70
2:C:1:NAG:H62	2:C:4:FUC:O2	1.91	0.70
1:B:592:VAL:O	1:B:604:LEU:HD12	1.92	0.70
1:B:369:GLU:O	1:B:386:THR:HG21	1.92	0.69
1:A:220:GLU:HB3	1:A:311:ILE:HD11	1.76	0.67
1:A:617:ARG:HG2	1:A:637:THR:HG22	1.76	0.67
1:A:583:TYR:HD1	1:A:622:VAL:HG12	1.59	0.67
1:B:538:ALA:HB2	1:B:630:LEU:HD23	1.77	0.66
1:A:592:VAL:O	1:A:604:LEU:HD12	1.96	0.66
1:B:148:PHE:CE2	1:B:200:VAL:HG11	2.31	0.66



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:616:PHE:O	1:B:637:THR:HG22	1.96	0.65
1:A:19:THR:HG22	1:A:51:GLN:HG3	1.77	0.65
1:A:117:PRO:O	1:A:120:THR:HG23	1.99	0.63
1:A:565:VAL:HG23	1:A:602:VAL:HG13	1.80	0.63
1:B:574:ASP:CG	1:B:578:ASN:OD1	2.37	0.63
1:A:441:LEU:HD23	1:A:532:VAL:CG2	2.29	0.63
1:A:583:TYR:CD1	1:A:622:VAL:HG12	2.34	0.63
1:B:74:LEU:O	1:B:89:VAL:HG12	1.98	0.63
1:B:455:ALA:N	1:B:468:TYR:OH	2.31	0.63
1:B:585:ILE:HD11	1:B:593:PHE:HB2	1.81	0.62
1:A:555:VAL:N	1:A:639:LEU:O	2.33	0.61
1:B:110:VAL:HG11	1:B:122:ILE:HG21	1.82	0.61
1:B:100:SER:HB3	1:B:192:ARG:HB3	1.83	0.60
1:A:563:PHE:HD2	1:A:565:VAL:HG13	1.67	0.60
1:B:148:PHE:HE2	1:B:200:VAL:HG11	1.66	0.60
1:B:287:GLU:OE2	1:B:305:LYS:HE3	2.02	0.60
1:B:639:LEU:HD12	1:B:640:VAL:H	1.66	0.60
1:B:121:ARG:HG2	1:B:165:VAL:HG22	1.85	0.59
1:A:555:VAL:O	1:A:640:VAL:HA	2.03	0.59
1:B:21:ALA:HA	1:B:26:LEU:HD12	1.85	0.58
1:A:499:PHE:HB3	1:A:531:ILE:HD13	1.85	0.58
1:B:565:VAL:HG23	1:B:566:THR:H	1.68	0.58
1:B:567:HIS:CD2	1:B:569:LYS:HG3	2.39	0.58
1:A:574:ASP:CG	1:A:578:ASN:OD1	2.40	0.58
1:A:293:GLN:HG3	1:A:301:THR:HG22	1.85	0.57
1:A:621:SER:OG	1:A:633:THR:HG22	2.04	0.57
1:A:482:THR:HG21	1:A:497:ARG:HH21	1.70	0.56
1:A:217:VAL:HG11	1:A:232:LEU:CD2	2.35	0.56
1:A:305:LYS:HE2	1:A:307:ILE:HD11	1.87	0.56
1:B:585:ILE:O	1:B:585:ILE:HG23	2.05	0.56
1:A:148:PHE:HB3	1:A:164:LEU:HD11	1.87	0.56
1:A:452:THR:HG22	1:A:492:ALA:HA	1.87	0.56
1:B:586:ALA:HB3	1:B:619:THR:OG1	2.06	0.56
1:B:444:ASN:O	1:B:498:THR:HG22	2.06	0.56
1:A:455:ALA:N	1:A:468:TYR:OH	2.35	0.55
1:B:360:GLN:O	1:B:406:LEU:HD23	2.06	0.55
1:A:217:VAL:HG11	1:A:232:LEU:HD21	1.88	0.55
1:B:447:GLY:N	1:B:495:ALA:O	2.39	0.55
1:B:599:THR:O	1:B:599:THR:HG22	2.07	0.55
1:A:46:ARG:HD2	1:A:49:ASP:OD2	2.06	0.55
1:A:585:ILE:HG23	1:A:585:ILE:O	2.07	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:101:PRO:HD2	1:B:192:ARG:O	2.08	0.54
1:A:567:HIS:HD2	1:A:569:LYS:HE2	1.72	0.54
1:B:593:PHE:CE1	1:B:604:LEU:HD13	2.42	0.54
1:A:369:GLU:O	1:A:386:THR:HG21	2.08	0.54
1:A:568:ILE:HG22	1:A:600:GLY:O	2.08	0.54
1:B:189:SER:HB2	1:B:190:PRO:HD3	1.90	0.53
1:B:376:ALA:HB2	1:B:382:MET:HG3	1.89	0.53
1:A:444:ASN:O	1:A:498:THR:HG22	2.08	0.53
1:A:155:ARG:HG3	1:A:159:VAL:CG2	2.38	0.53
1:B:34:LEU:HD23	1:B:76:VAL:HG12	1.90	0.53
1:A:155:ARG:HD3	1:B:287:GLU:OE2	2.08	0.53
1:B:258:GLU:HG3	1:B:259:VAL:N	2.24	0.53
1:A:583:TYR:HB3	1:A:595:ILE:HD11	1.91	0.53
1:A:535:ASN:ND2	1:A:628:PRO:O	2.33	0.53
1:A:484:VAL:HG21	1:A:509:LEU:CD2	2.39	0.53
1:B:195:THR:HG22	1:B:196:THR:N	2.23	0.52
1:B:19:THR:OG1	1:B:22:GLU:HB2	2.10	0.52
2:D:4:FUC:H2	2:D:4:FUC:H63	1.91	0.52
1:B:148:PHE:CE1	1:B:166:LEU:HD13	2.44	0.52
1:A:565:VAL:HG23	1:A:566:THR:N	2.25	0.52
1:A:565:VAL:HG23	1:A:566:THR:H	1.74	0.52
1:B:46:ARG:NH2	1:B:51:GLN:OE1	2.43	0.52
1:A:478:ALA:HB1	1:A:479:PRO:HD2	1.92	0.52
1:A:287:GLU:HG3	1:A:307:ILE:CD1	2.40	0.52
1:B:555:VAL:HG21	1:B:565:VAL:HG12	1.91	0.52
1:B:117:PRO:O	1:B:120:THR:HG23	2.10	0.51
1:A:124:LEU:HD11	1:A:164:LEU:HB2	1.93	0.51
1:B:100:SER:HB3	1:B:192:ARG:HE	1.74	0.51
1:B:535:ASN:OD1	1:B:578:ASN:ND2	2.43	0.51
1:B:449:TYR:CE1	1:B:452:THR:HG23	2.46	0.51
1:A:444:ASN:HD21	1:A:499:PHE:HD2	1.58	0.51
1:B:210:PRO:O	1:B:302:ALA:HB2	2.10	0.51
1:A:449:TYR:CE1	1:A:452:THR:HG23	2.46	0.51
1:B:287:GLU:OE2	1:B:305:LYS:CE	2.59	0.51
1:B:499:PHE:HD1	1:B:504:LEU:HD23	1.76	0.51
1:B:370:HIS:C	1:B:386:THR:HG22	2.31	0.50
1:A:449:TYR:HE1	1:A:452:THR:HG23	1.75	0.50
1:A:588:GLU:HG3	1:A:590:ARG:O	2.11	0.50
1:B:557:SER:HB2	1:B:608:VAL:CG1	2.39	0.50
1:B:129:ASP:HB2	1:B:137:ILE:HG13	1.92	0.50
1:A:155:ARG:HG2	1:A:161:TYR:CE2	2.47	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:568:ILE:HG23	1:B:568:ILE:O	2.12	0.50
1:B:128:THR:N	1:B:137:ILE:HD11	2.27	0.49
1:B:178:TYR:HB2	1:B:200:VAL:HB	1.93	0.49
1:B:449:TYR:OH	1:B:452:THR:HG23	2.13	0.49
1:A:557:SER:O	1:A:608:VAL:HG11	2.12	0.49
1:B:342:GLU:HG2	1:B:372:ARG:HH12	1.77	0.49
1:B:567:HIS:CD2	1:B:569:LYS:HE2	2.48	0.49
1:A:447:GLY:N	1:A:495:ALA:O	2.45	0.49
1:B:499:PHE:CD1	1:B:504:LEU:HD23	2.48	0.49
1:B:565:VAL:HG23	1:B:566:THR:N	2.27	0.49
1:A:210:PRO:O	1:A:302:ALA:HB2	2.12	0.49
1:A:612:ILE:CA	1:A:640:VAL:HG23	2.39	0.49
1:B:517:GLY:O	1:B:520:GLN:HG2	2.13	0.49
1:A:145:ASN:HD21	1:A:148:PHE:HB2	1.78	0.48
1:A:530:LYS:HE2	1:A:532:VAL:HG12	1.95	0.48
1:A:568:ILE:HG23	1:A:568:ILE:O	2.13	0.48
1:A:567:HIS:CE1	1:A:599:THR:O	2.66	0.48
1:A:635:THR:HG23	1:A:635:THR:O	2.12	0.48
1:B:129:ASP:CB	1:B:137:ILE:HG13	2.42	0.48
1:B:370:HIS:HA	1:B:386:THR:HG22	1.95	0.48
1:B:635:THR:O	1:B:635:THR:HG23	2.13	0.48
1:B:79:VAL:HG23	1:B:79:VAL:O	2.13	0.48
1:B:166:LEU:HD21	1:B:170:LEU:HG	1.96	0.48
1:B:367:GLY:HA3	1:B:399:LEU:HD23	1.94	0.48
1:A:580:GLU:O	1:A:624:ASP:HA	2.14	0.48
1:B:585:ILE:HD11	1:B:593:PHE:CB	2.44	0.48
1:B:195:THR:HG21	6:B:722:MAN:H5	1.95	0.48
1:A:610:GLU:HG3	1:A:614:GLN:HG3	1.96	0.48
1:B:370:HIS:O	1:B:386:THR:HG22	2.13	0.48
1:A:399:LEU:HD11	1:A:419:ILE:HD12	1.95	0.47
1:A:585:ILE:O	1:A:585:ILE:CG2	2.62	0.47
1:B:217:VAL:HG11	1:B:232:LEU:HD21	1.96	0.47
1:A:585:ILE:H	1:A:595:ILE:HG21	1.79	0.47
1:B:444:ASN:HD21	1:B:499:PHE:HD2	1.62	0.47
1:A:617:ARG:HG2	1:A:637:THR:CG2	2.45	0.47
1:A:376:ALA:HB2	1:A:382:MET:HG3	1.97	0.47
1:A:475:VAL:HG13	1:A:475:VAL:O	2.14	0.47
1:A:95:ASP:OD1	1:A:96:ILE:N	2.48	0.47
1:A:557:SER:O	1:A:608:VAL:HG21	2.15	0.47
1:A:501:HIS:CD2	1:A:505:GLN:HG3	2.50	0.47
1:B:323:THR:O	1:B:323:THR:HG23	2.15	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:327:SER:CB	1:A:332:VAL:O	2.63	0.47
1:B:127:ALA:CB	1:B:137:ILE:HD13	2.45	0.47
1:B:335:ILE:HD12	1:B:345:VAL:HG22	1.96	0.47
1:B:127:ALA:HB3	1:B:137:ILE:HD13	1.97	0.46
1:B:181:GLU:OE2	6:B:722:MAN:H5	2.15	0.46
1:B:95:ASP:OD1	1:B:96:ILE:N	2.48	0.46
1:B:110:VAL:CG1	1:B:122:ILE:HG21	2.46	0.46
1:A:335:ILE:HD12	1:A:345:VAL:HG22	1.96	0.46
1:B:217:VAL:HG11	1:B:232:LEU:CD2	2.45	0.46
1:B:438:VAL:HG11	1:B:450:ILE:CG2	2.46	0.46
1:A:483:TYR:CZ	1:A:497:ARG:NH1	2.83	0.46
1:B:181:GLU:HG2	1:B:195:THR:CG2	2.46	0.46
1:A:258:GLU:HG3	1:A:259:VAL:N	2.31	0.46
1:A:140:PHE:HB3	1:A:150:ILE:CD1	2.46	0.46
1:B:220:GLU:CB	1:B:311:ILE:HD11	2.38	0.46
1:A:165:VAL:HG12	1:A:167:MET:HE2	1.98	0.45
1:A:585:ILE:CG2	1:A:595:ILE:HB	2.46	0.45
1:A:34:LEU:HD23	1:A:76:VAL:HG12	1.97	0.45
1:A:254:GLN:HG2	1:B:123:PRO:CB	2.46	0.45
1:B:348:ILE:HD11	1:B:383:ILE:HD11	1.98	0.45
1:A:140:PHE:CE1	1:A:184:ALA:HB2	2.51	0.45
1:B:124:LEU:HD11	1:B:164:LEU:HB2	1.99	0.45
1:B:588:GLU:HB3	1:B:618:ALA:HB2	1.98	0.45
1:B:183:LEU:O	1:B:183:LEU:HD12	2.17	0.45
1:A:3:VAL:HG13	1:A:89:VAL:HG23	1.99	0.45
1:A:318:PRO:HA	1:A:351:THR:O	2.17	0.45
1:A:327:SER:HA	1:A:334:TYR:HD2	1.81	0.45
1:B:514:SER:HB3	1:B:522:THR:HG22	1.99	0.45
1:B:453:VAL:HG11	1:B:527:ILE:HD11	2.00	0.44
1:B:501:HIS:CD2	1:B:505:GLN:HG3	2.51	0.44
1:B:578:ASN:ND2	1:B:578:ASN:O	2.50	0.44
1:A:350:THR:O	1:A:379:ASP:HB3	2.17	0.44
1:A:209:SER:HB3	1:A:300:LEU:HB3	1.99	0.44
1:B:107:GLU:HG2	1:B:197:MET:HB2	1.99	0.44
1:B:180:LEU:O	1:B:198:VAL:HB	2.17	0.44
1:B:526:ILE:HD12	1:B:528:LYS:HE3	2.00	0.44
1:A:35:MET:HE1	1:A:86:LEU:HD11	1.98	0.44
1:B:481:THR:O	1:B:481:THR:HG22	2.17	0.44
1:B:79:VAL:HG12	1:B:84:PHE:CD1	2.53	0.44
1:A:183:LEU:C	1:A:183:LEU:HD12	2.38	0.44
1:A:44:HIS:CD2	1:A:55:GLY:HA2	2.53	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:79:VAL:O	1:A:79:VAL:HG23	2.17	0.44
1:B:99:ASN:ND2	8:B:807:HOH:O	2.50	0.44
1:A:195:THR:HG22	1:A:196:THR:N	2.33	0.43
1:B:30:GLY:HA3	1:B:32:PHE:CE2	2.53	0.43
1:A:178:TYR:HB2	1:A:200:VAL:HB	2.00	0.43
1:B:142:ILE:HD13	1:B:150:ILE:CG2	2.48	0.43
1:B:155:ARG:HD3	1:B:159:VAL:HG23	2.00	0.43
1:B:555:VAL:O	1:B:640:VAL:HA	2.18	0.43
1:B:116:ALA:HB1	1:B:120:THR:HG21	1.99	0.43
2:D:4:FUC:C2	2:D:4:FUC:H63	2.47	0.43
1:B:614:GLN:HB3	1:B:616:PHE:CE2	2.53	0.43
1:B:580:GLU:O	1:B:624:ASP:HA	2.19	0.43
1:A:20:LEU:CD1	1:A:76:VAL:HG21	2.48	0.43
1:A:472:GLU:OE2	1:A:479:PRO:CB	2.66	0.43
1:B:24:LEU:HB2	1:B:26:LEU:HG	2.01	0.43
1:A:360:GLN:O	1:A:405:ASP:HA	2.18	0.43
1:A:585:ILE:HG22	1:A:595:ILE:HB	2.01	0.43
1:A:639:LEU:HD23	1:A:640:VAL:N	2.33	0.43
1:B:475:VAL:HG13	1:B:475:VAL:O	2.19	0.43
1:B:155:ARG:HD3	1:B:159:VAL:CG2	2.48	0.43
1:B:449:TYR:HE1	1:B:452:THR:HG23	1.84	0.42
1:B:468:TYR:HB3	1:B:486:LEU:HD21	2.01	0.42
1:B:563:PHE:O	1:B:603:PHE:CD1	2.72	0.42
1:A:348:ILE:HD11	1:A:383:ILE:HD11	2.02	0.42
1:B:101:PRO:O	1:B:194:GLY:HA3	2.20	0.42
1:A:533:ASP:OD2	1:A:574:ASP:HB3	2.20	0.42
1:B:155:ARG:HG2	1:B:161:TYR:CE2	2.54	0.42
1:B:209:SER:HB3	1:B:300:LEU:HB3	2.01	0.42
1:A:254:GLN:OE1	1:A:254:GLN:N	2.51	0.42
1:B:142:ILE:HD13	1:B:150:ILE:HG23	2.01	0.42
1:B:141:GLN:OE1	1:B:183:LEU:HD11	2.19	0.42
1:A:13:PRO:HB3	1:A:55:GLY:O	2.20	0.42
1:A:453:VAL:CG1	1:A:527:ILE:HD11	2.50	0.42
1:A:140:PHE:HB3	1:A:150:ILE:HD12	2.02	0.42
1:A:504:LEU:HD21	1:A:507:LEU:HD13	2.02	0.42
1:B:183:LEU:HB3	1:B:195:THR:HG23	2.01	0.42
1:B:502:GLU:CD	1:B:502:GLU:H	2.23	0.42
1:B:29:GLU:HG2	1:B:30:GLY:N	2.35	0.42
1:B:5:TYR:HB3	1:B:17:ILE:CG2	2.50	0.42
1:A:195:THR:HB	6:A:723:MAN:C5	2.50	0.41
1:B:318:PRO:HA	1:B:351:THR:O	2.21	0.41



		Interatomic	Clash
Atom-1	Atom-2	$distance ( m \AA)$	overlap (Å)
1:B:66:GLN:O	1:B:66:GLN:HG3	2.21	0.41
1:A:235:ASP:H	3:A:705:EDO:H11	1.86	0.41
1:B:480:ILE:HD11	1:B:509:LEU:CD2	2.51	0.41
1:A:553:VAL:O	1:A:638:PHE:HA	2.20	0.41
1:B:561:HIS:CD2	1:B:605:VAL:HA	2.54	0.41
1:A:155:ARG:HG2	1:A:161:TYR:HE2	1.83	0.41
1:A:217:VAL:HG11	1:A:232:LEU:HD22	2.03	0.41
1:B:138:GLN:HG3	1:B:187:GLY:HA3	2.02	0.41
1:B:147:HIS:HB3	1:B:166:LEU:CD1	2.50	0.41
1:A:438:VAL:HG22	1:A:439:SER:N	2.36	0.41
1:B:148:PHE:CZ	1:B:200:VAL:HG11	2.56	0.41
1:B:258:GLU:HG3	1:B:259:VAL:HG23	2.03	0.41
1:A:541:ILE:HD13	1:A:568:ILE:HD11	2.03	0.41
1:B:16:VAL:HG13	1:B:51:GLN:HE21	1.86	0.41
1:B:336:THR:HA	1:B:422:SER:HB3	2.02	0.41
1:B:478:ALA:HB1	1:B:479:PRO:HD2	2.03	0.41
1:A:367:GLY:HA3	1:A:399:LEU:HD23	2.02	0.41
1:B:367:GLY:HA3	1:B:399:LEU:CD2	2.51	0.41
1:B:148:PHE:HE2	1:B:200:VAL:HG21	1.86	0.40
1:A:183:LEU:O	1:A:183:LEU:HD12	2.21	0.40
1:A:474:GLU:N	1:A:474:GLU:OE1	2.54	0.40
1:B:370:HIS:CA	1:B:386:THR:HG22	2.51	0.40
1:A:435:VAL:HG22	1:A:526:ILE:HD11	2.04	0.40
1:B:352:ASP:HB3	1:B:359:GLY:HA2	2.02	0.40
1:B:150:ILE:HG22	1:B:164:LEU:HD12	2.02	0.40
1:A:231:LEU:HD21	1:A:263:PHE:HE1	1.87	0.40
1:B:43:ILE:HG21	1:B:52:LEU:CD1	2.52	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	ntiles
1	А	640/647~(99%)	612 (96%)	28 (4%)	0	100	100
1	В	639/647~(99%)	615~(96%)	24 (4%)	0	100	100
All	All	1279/1294~(99%)	1227 (96%)	52 (4%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	Rotameric Outliers		Percentiles		
1	А	549/555~(99%)	543~(99%)	6 (1%)	73	78		
1	В	549/555~(99%)	543~(99%)	6 (1%)	73	78		
All	All	1098/1110~(99%)	1086~(99%)	12 (1%)	73	78		

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	151	ASP
1	А	201	ARG
1	А	218	MET
1	А	237	LEU
1	А	262	LEU
1	А	460	PHE
1	В	52	LEU
1	В	155	ARG
1	В	218	MET
1	В	297	LEU
1	В	426	ASP
1	В	521	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	37	GLN
	a	1	



Mol	Chain	Res	Type
1	А	44	HIS
1	А	83	GLN
1	А	147	HIS
1	А	277	GLN
1	В	229	HIS
1	В	277	GLN
1	В	368	HIS
1	В	444	ASN
1	В	506	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)

8 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).

Mol Type Chain		Dog	Tink	Bond lengths			Bond angles			
	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	1	1,2	14,14,15	0.60	0	17,19,21	0.89	1 (5%)
2	NAG	С	2	2	14,14,15	0.41	0	17,19,21	0.51	0
2	BMA	C	3	2	11,11,12	1.00	0	15,15,17	0.84	1 (6%)
2	FUC	С	4	2	10,10,11	2.32	2 (20%)	14,14,16	2.07	2 (14%)
2	NAG	D	1	1,2	14,14,15	0.37	0	17,19,21	0.58	0
2	NAG	D	2	2	14,14,15	0.48	0	17,19,21	0.51	0
2	BMA	D	3	2	11,11,12	0.88	1 (9%)	15,15,17	1.04	1 (6%)
2	FUC	D	4	2	10,10,11	1.36	2 (20%)	14,14,16	2.26	2 (14%)



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	С	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	С	2	2	-	2/6/23/26	0/1/1/1
2	BMA	С	3	2	-	2/2/19/22	0/1/1/1
2	FUC	С	4	2	-	-	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	FUC	D	4	2	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
2	С	4	FUC	C2-C3	5.20	1.60	1.52
2	С	4	FUC	C1-C2	4.10	1.61	1.52
2	D	4	FUC	O3-C3	2.78	1.49	1.43
2	D	4	FUC	O2-C2	2.31	1.48	1.43
2	D	3	BMA	C1-C2	2.15	1.57	1.52

All (7) bond angle outliers are listed below
--

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	D	4	FUC	C1-C2-C3	6.76	117.98	109.67
2	С	4	FUC	O2-C2-C1	6.48	122.41	109.15
2	D	4	FUC	C2-C3-C4	3.48	116.91	110.89
2	С	4	FUC	O2-C2-C3	-2.78	104.58	110.14
2	D	3	BMA	C1-C2-C3	2.15	112.30	109.67
2	С	3	BMA	O2-C2-C3	-2.14	105.84	110.14
2	С	1	NAG	C4-C3-C2	2.14	114.15	111.02

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	С	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6



Mol	Chain	Res	Type	Atoms
2	С	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	С	2	NAG	O5-C5-C6-O6
2	С	2	NAG	C4-C5-C6-O6
2	С	3	BMA	C4-C5-C6-O6
2	С	3	BMA	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	1	NAG	1	0
2	С	4	FUC	1	0
2	D	4	FUC	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)

Of 40 ligands modelled in this entry, 34 are monoatomic - leaving 6 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	Tune	Chain	Dog	Tink	Bo	ond leng	$_{\rm ths}$	Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MAN	В	721	1	11,11,12	1.66	2 (18%)	15,15,17	1.37	4 (26%)
3	EDO	А	705	-	3,3,3	0.49	0	2,2,2	0.57	0
6	MAN	В	722	1	11,11,12	1.30	2 (18%)	15,15,17	1.14	1 (6%)
6	MAN	А	723	1	11,11,12	1.02	0	15,15,17	1.39	3 (20%)
3	EDO	В	724	-	3,3,3	0.49	0	2,2,2	0.46	0
6	MAN	А	722	1	11,11,12	0.93	0	15,15,17	1.19	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
6	MAN	В	721	1	-	2/2/19/22	0/1/1/1
3	EDO	А	705	-	-	0/1/1/1	-
6	MAN	В	722	1	-	0/2/19/22	0/1/1/1
6	MAN	А	723	1	-	2/2/19/22	0/1/1/1
3	EDO	В	724	-	-	1/1/1/1	-
6	MAN	А	722	1	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
6	В	721	MAN	O4-C4	3.28	1.50	1.43
6	В	721	MAN	O5-C1	-3.12	1.38	1.43
6	В	722	MAN	C2-C3	2.25	1.55	1.52
6	В	722	MAN	C1-C2	2.10	1.57	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
6	А	723	MAN	C1-O5-C5	3.44	116.85	112.19
6	А	722	MAN	C1-O5-C5	2.48	115.55	112.19
6	В	721	MAN	O2-C2-C3	-2.26	105.62	110.14
6	А	723	MAN	C2-C3-C4	2.20	114.71	110.89
6	А	723	MAN	O5-C5-C4	-2.14	105.63	110.83
6	В	721	MAN	O5-C5-C6	-2.13	103.86	107.20
6	В	721	MAN	C1-O5-C5	2.10	115.04	112.19
6	В	721	MAN	O4-C4-C3	-2.09	105.51	110.35
6	В	722	MAN	C1-O5-C5	2.06	114.99	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	А	723	MAN	O5-C5-C6-O6
6	А	723	MAN	C4-C5-C6-O6
6	В	721	MAN	O5-C5-C6-O6
6	В	721	MAN	C4-C5-C6-O6
3	В	724	EDO	O1-C1-C2-O2



There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	705	EDO	1	0
6	В	722	MAN	2	0
6	А	723	MAN	1	0

### 5.7 Other polymers (i)

There are no such residues in this entry.

### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

### 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	< <b>RSRZ</b> >	#RSRZ>2		$OWAB(Å^2)$	Q<0.9	
1	А	642/647~(99%)	0.81	88 (13%)	3	2	14, 60, 120, 182	0
1	В	641/647~(99%)	1.59	162 (25%)	0	0	21, 75, 143, 217	0
All	All	1283/1294~(99%)	1.20	250 (19%)	1	0	14, 66, 132, 217	0

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	560	PRO	21.4
1	В	616	PHE	20.8
1	В	555	VAL	14.0
1	В	618	ALA	13.0
1	В	554	VAL	12.7
1	А	616	PHE	11.3
1	В	556	PRO	11.2
1	А	615	VAL	11.1
1	А	618	ALA	11.1
1	В	621	SER	11.0
1	В	613	GLY	10.3
1	В	595	ILE	10.2
1	В	563	PHE	10.1
1	В	564	LEU	9.8
1	В	615	VAL	9.7
1	В	605	VAL	9.7
1	В	559	ALA	9.5
1	А	587	ASP	9.5
1	В	587	ASP	9.5
1	А	563	PHE	9.4
1	В	609	SER	9.1
1	В	607	ASP	9.0
1	В	594	THR	9.0
1	В	612	ILE	8.9



6V(	G1
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Mol	Chain	Res	Type	RSRZ
1	В	606	ALA	8.5
1	В	638	PHE	8.4
1	В	557	SER	8.4
1	В	38	PHE	8.2
1	В	553	VAL	8.0
1	А	38	PHE	7.5
1	В	598	ALA	7.5
1	В	636	ILE	7.3
1	В	632	SER	7.1
1	В	622	VAL	7.1
1	А	602	VAL	7.0
1	В	586	ALA	7.0
1	В	597	LYS	7.0
1	A	605	VAL	7.0
1	В	608	VAL	6.9
1	A	607	ASP	6.7
1	В	602	VAL	6.5
1	В	633	THR	6.4
1	А	627	ARG	6.4
1	В	562	GLY	6.4
1	В	585	ILE	6.4
1	В	561	HIS	6.3
1	А	189	SER	6.3
1	В	592	VAL	6.3
1	В	603	PHE	6.2
1	В	614	GLN	6.1
1	В	546	LEU	6.1
1	В	566	THR	6.1
1	В	630	LEU	6.0
1	В	565	VAL	6.0
1	В	440	VAL	5.9
1	В	540	VAL	5.9
1	В	627	ARG	5.9
1	В	16	VAL	5.9
1	A	609	SER	5.9
1	В	620	VAL	5.8
1	В	583	TYR	5.8
1	В	604	LEU	5.8
1	В	541	ILE	5.7
1	В	641	THR	5.6
1	В	568	ILE	5.6
1	В	118	VAL	5.5



Mol	Chain	Res	Type	RSRZ
1	В	37	GLN	5.3
1	В	639	LEU	5.3
1	В	591	ASN	5.3
1	В	625	SER	5.2
1	В	599	THR	5.2
1	В	593	PHE	5.2
1	В	40	ASN	5.1
1	В	188	GLY	5.0
1	В	96	ILE	5.0
1	В	628	PRO	4.9
1	В	629	PRO	4.9
1	В	168	LYS	4.9
1	В	590	ARG	4.9
1	В	619	THR	4.9
1	А	561	HIS	4.8
1	А	558	ARG	4.8
1	А	1	LYS	4.7
1	В	551	ALA	4.6
1	А	595	ILE	4.6
1	А	555	VAL	4.6
1	В	640	VAL	4.6
1	А	582	THR	4.6
1	А	553	VAL	4.6
1	А	546	LEU	4.5
1	В	142	ILE	4.5
1	В	617	ARG	4.5
1	В	610	GLU	4.5
1	А	495	ALA	4.3
1	В	185	MET	4.3
1	А	599	THR	4.3
1	В	577	VAL	4.3
1	В	582	THR	4.3
1	В	1	LYS	4.2
1	В	600	GLY	4.2
1	В	611	ALA	4.2
1	В	195	THR	4.1
1	A	612	ILE	4.1
1	A	603	PHE	4.1
1	В	588	GLU	4.0
1	В	456	ARG	4.0
1	A	37	GLN	4.0
1	В	148	PHE	4.0



6V(	G1
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Mol	Chain	Res	Type	RSRZ
1	В	190	PRO	3.9
1	В	532	VAL	3.9
1	А	590	ARG	3.9
1	А	560	PRO	3.9
1	А	604	LEU	3.8
1	В	596	ASN	3.8
1	В	567	HIS	3.8
1	В	24	LEU	3.8
1	В	558	ARG	3.8
1	В	545	ALA	3.7
1	В	189	SER	3.7
1	А	446	PRO	3.7
1	В	637	THR	3.7
1	В	449	TYR	3.7
1	В	467	ILE	3.6
1	А	600	GLY	3.6
1	А	591	ASN	3.6
1	А	625	SER	3.6
1	В	635	THR	3.6
1	В	134	VAL	3.6
1	В	548	ASN	3.5
1	В	441	LEU	3.5
1	В	27	GLU	3.5
1	В	634	ALA	3.5
1	А	586	ALA	3.4
1	А	594	THR	3.4
1	В	516	GLY	3.4
1	В	549	GLY	3.4
1	В	147	HIS	3.4
1	A	593	PHE	3.4
1	A	554	VAL	3.4
1	В	448	ALA	3.3
1	В	22	GLU	3.3
1	A	188	GLY	3.3
1	A	636	ILE	3.3
1	A	16	VAL	3.3
1	В	144	GLU	3.3
1	A	606	ALA	3.3
1	В	589	GLY	3.2
1	В	184	ALA	3.2
1	В	160	LYS	3.1
1	А	556	PRO	3.1



6V	G1
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Mol	Chain	Res	Type	RSRZ
1	А	628	PRO	3.1
1	В	436	TYR	3.1
1	В	631	SER	3.1
1	В	447	GLY	3.1
1	А	611	ALA	3.1
1	А	619	THR	3.1
1	В	127	ALA	3.0
1	В	140	PHE	3.0
1	А	567	HIS	2.9
1	А	630	LEU	2.9
1	В	167	MET	2.9
1	А	535	ASN	2.9
1	В	6	ARG	2.9
1	А	39	ASN	2.9
1	В	550	SER	2.9
1	В	474	GLU	2.9
1	А	585	ILE	2.9
1	А	614	GLN	2.9
1	А	559	ALA	2.8
1	В	535	ASN	2.8
1	В	534	GLN	2.8
1	А	577	VAL	2.8
1	А	639	LEU	2.8
1	А	588	GLU	2.8
1	А	613	GLY	2.8
1	А	519	PRO	2.8
1	А	633	THR	2.8
1	А	538	ALA	2.8
1	А	469	ARG	2.8
1	В	578	ASN	2.7
1	А	479	PRO	2.7
1	В	181	GLU	2.7
1	В	25	HIS	2.7
1	A	297	LEU	2.7
1	А	597	LYS	2.7
1	В	575	GLU	2.6
1	А	162	ALA	2.6
1	В	439	SER	2.6
1	В	5	TYR	2.6
1	А	564	LEU	2.6
1	В	529	VAL	2.5
1	В	522	THR	2.5



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Mol	Chain	Res	Type	RSRZ
1	В	18	GLY	2.5
1	В	466	VAL	2.5
1	В	107	GLU	2.5
1	А	638	PHE	2.5
1	В	519	PRO	2.5
1	А	589	GLY	2.4
1	В	146	SER	2.4
1	А	641	THR	2.4
1	А	632	SER	2.4
1	В	552	GLU	2.4
1	В	543	GLN	2.4
1	А	581	LEU	2.3
1	В	542	VAL	2.3
1	В	183	LEU	2.3
1	А	551	ALA	2.3
1	А	608	VAL	2.3
1	В	19	THR	2.3
1	В	26	LEU	2.3
1	В	52	LEU	2.3
1	В	521	LEU	2.3
1	В	478	ALA	2.3
1	В	570	ALA	2.3
1	В	166	LEU	2.3
1	В	180	LEU	2.3
1	А	557	SER	2.3
1	В	544	PRO	2.3
1	В	162	ALA	2.2
1	А	592	VAL	2.2
1	В	493	VAL	2.2
1	А	550	SER	2.2
1	A	584	SER	2.2
1	B	626	GLY	2.2
1	B	154	THR	2.2
1	A	635	THR	2.2
1	В	462	HIS	2.2
1	A	$\overline{304}$	CYS	2.2
1	B	581	LEU	2.2
1	B	44	HIS	2.2
1	A	562	GLY	2.2
1	A	25	HIS	2.2
1	В	177	ALA	2.2
1	A	566	THR	2.1



Mol	Chain	Res	Type	RSRZ
1	А	456	ARG	2.1
1	В	297	LEU	2.1
1	В	471	VAL	2.1
1	А	452	THR	2.1
1	А	474	GLU	2.1
1	А	610	GLU	2.1
1	А	52	LEU	2.1
1	В	193	SER	2.1
1	А	640	VAL	2.1
1	В	445	ALA	2.1
1	В	108	ILE	2.0
1	В	129	ASP	2.0
1	В	499	PHE	2.0
1	В	584	SER	2.0
1	A	447	GLY	2.0
1	А	620	VAL	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	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q<0.9
2	BMA	С	3	11/12	0.59	0.28	$75,\!105,\!115,\!135$	0
2	NAG	D	2	14/15	0.69	0.24	$57,\!83,\!113,\!141$	0
2	BMA	D	3	11/12	0.73	0.27	$58,\!83,\!100,\!104$	0
2	FUC	D	4	10/11	0.78	0.17	43,76,96,115	0
2	FUC	С	4	10/11	0.80	0.22	45,72,105,127	0
2	NAG	D	1	14/15	0.85	0.12	36,72,104,114	0
2	NAG	С	2	14/15	0.86	0.20	42,73,106,128	0
2	NAG	С	1	14/15	0.92	0.13	$31,\!56,\!88,\!95$	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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
4	CA	В	719	1/1	0.54	0.15	$154,\!154,\!154,\!154$	0
4	CA	В	707	1/1	0.55	0.11	122,122,122,122	0
6	MAN	В	722	11/12	0.59	0.54	$64,\!110,\!135,\!158$	0
4	CA	В	706	1/1	0.67	0.07	92,92,92,92	0
6	MAN	А	723	11/12	0.69	0.23	$56,\!81,\!104,\!132$	0
4	CA	В	705	1/1	0.78	0.09	75, 75, 75, 75, 75	0
6	MAN	А	722	11/12	0.85	0.24	$49,\!82,\!99,\!109$	0
4	CA	А	719	1/1	0.85	0.07	$91,\!91,\!91,\!91$	0
6	MAN	В	721	11/12	0.86	0.29	$66,\!94,\!131,\!142$	0
4	CA	B	718	1/1	0.87	0.09	88,88,88,88	0
3	EDO	B	724	4/4	0.90	0.15	42,65,79,88	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B$ -factors( $Å^2$ )	Q<0.9
4	CA	В	708	1/1	0.93	0.12	74,74,74,74	0
5	CL	В	720	1/1	0.94	0.26	$69,\!69,\!69,\!69$	0
4	CA	В	714	1/1	0.94	0.10	62,62,62,62	0
3	EDO	А	705	4/4	0.94	0.17	$25,\!57,\!69,\!72$	0
4	CA	А	718	1/1	0.96	0.12	$69,\!69,\!69,\!69$	0
4	CA	В	712	1/1	0.96	0.31	52, 52, 52, 52	0
4	CA	В	717	1/1	0.97	0.09	83,83,83,83	0
5	CL	А	721	1/1	0.97	0.24	$43,\!43,\!43,\!43$	0
4	CA	В	716	1/1	0.97	0.07	59, 59, 59, 59, 59	0
4	CA	А	716	1/1	0.98	0.10	52,52,52,52	0
4	CA	А	707	1/1	0.98	0.14	58, 58, 58, 58	0
4	CA	А	708	1/1	0.98	0.05	56, 56, 56, 56	0
4	CA	А	717	1/1	0.98	0.12	62,62,62,62	0
4	CA	А	706	1/1	0.98	0.15	56, 56, 56, 56	0
7	NA	В	723	1/1	0.98	0.16	46, 46, 46, 46	0
4	CA	В	709	1/1	0.98	0.13	47,47,47,47	0
4	CA	А	711	1/1	0.99	0.14	$34,\!34,\!34,\!34$	0
4	CA	А	715	1/1	0.99	0.10	44,44,44,44	0
4	CA	А	712	1/1	0.99	0.19	$33,\!33,\!33,\!33$	0
4	CA	В	713	1/1	0.99	0.20	$38,\!38,\!38,\!38$	0
4	CA	В	715	1/1	0.99	0.11	$44,\!44,\!44,\!44$	0
4	CA	В	710	1/1	0.99	0.12	$32,\!32,\!32,\!32$	0
4	CA	А	720	1/1	0.99	0.08	$48,\!48,\!48,\!48$	0
4	CA	А	714	1/1	0.99	0.21	29, 29, 29, 29, 29	0
7	NA	A	724	1/1	0.99	0.15	14, 14, 14, 14	0
4	CA	A	713	1/1	1.00	0.16	$1\overline{8,18,18,18}$	0
4	CA	A	709	1/1	1.00	0.12	21,21,21,21	0
4	CA	В	711	1/1	1.00	0.16	28,28,28,28	0
4	CA	A	710	1/1	1.00	0.13	$2\overline{3,23,23,23}$	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

