

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	5GKQ
Title	:	Structure of PL6 family alginate lyase AlyGC mutant-R241A
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Deposited on	:	2016-07-05
Resolution	:	2.56 Å(reported)

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

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

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

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 2.56 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R_{free}	130704	1279(2.58-2.54)		
Clashscore	141614	1327 (2.58-2.54)		
Ramachandran outliers	138981	1312(2.58-2.54)		
Sidechain outliers	138945	1312 (2.58-2.54)		
RSRZ outliers	127900	1269 (2.58-2.54)		

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	726	80%	18%	·
1	В	726	<mark>6%</mark> 79%	19%	
2	С	4	25% 75%		



$5 \mathrm{GKQ}$

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11676 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 AlyGC mutant - R241A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	726	Total 5661	C 3537	N 1009	O 1106	S 9	0	0	0
1	В	726	Total 5661	$\begin{array}{c} \mathrm{C} \\ 3537 \end{array}$	N 1009	O 1106	S 9	0	0	0

• Molecule 2 is an oligosaccharide called beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
2	С	4	Total 49	С 24	O 25	0	0	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Ca 1 1	0	0
3	В	1	Total Ca 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	159	Total O 159 159	0	0
4	В	144	Total O 144 144	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: AlyGC mutant - R241A

V639 V639 V640 N642 N643 N644 N644 N645 F646 N645 N645 N646 N647 N649 N649 N649 N649 N649 N649 N650 N671 N699 N699 N699 N699 N691 N691 N692 N693 N694 </tr

 \bullet Molecule 2: beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid

α · α		
Chain C:	25%	75%

BEM1 BEM2 BEM3 BEM4



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	82.66Å 122.83Å 195.33Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{Baselution}(\mathbf{\hat{A}})$	47.80 - 2.56	Depositor
Resolution (A)	49.30 - 2.56	EDS
% Data completeness	96.0 (47.80-2.56)	Depositor
(in resolution range)	96.1 (49.30-2.56)	EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.60 (at 2.58 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
P. P.	0.191 , 0.228	Depositor
n, n_{free}	0.192 , 0.227	DCC
R_{free} test set	3013 reflections $(4.86%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	45.1	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 32.0	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	0.94	EDS
Total number of atoms	11676	wwPDB-VP
Average B, all atoms $(Å^2)$	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.76% 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: BEM, CA

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		
1VIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.51	0/5770	0.64	0/7823	
1	В	0.53	0/5770	0.66	4/7823~(0.1%)	
All	All	0.52	0/11540	0.65	4/15646~(0.0%)	

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	300	LYS	N-CA-C	-6.01	94.78	111.00
1	В	299	SER	C-N-CA	5.77	136.13	121.70
1	В	714	LEU	N-CA-C	-5.45	96.28	111.00
1	В	712	PHE	C-N-CD	5.37	139.67	128.40

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	5661	0	5522	100	1
1	В	5661	0	5522	104	1
2	С	49	0	27	6	0
3	А	1	0	0	0	0
3	В	1	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	А	159	0	0	15	1
4	В	144	0	0	15	1
All	All	11676	0	11071	205	2

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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 9.

All (205) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:269:ARG:NH1	4:A:901:HOH:O	1.60	1.22
1:B:378:PRO:HD3	1:B:386:GLN:NE2	1.59	1.18
1:B:299:SER:HB3	1:B:300:LYS:HB2	1.11	1.10
1:A:582:GLN:NE2	4:A:902:HOH:O	1.90	1.03
1:A:300:LYS:CD	1:A:301:ILE:H	1.72	1.01
1:A:242:HIS:NE2	2:C:3:BEM:O3	1.96	0.98
1:B:446:SER:OG	1:B:468:GLN:OE1	1.81	0.97
1:A:300:LYS:HD2	1:A:301:ILE:H	1.31	0.95
1:B:299:SER:HB3	1:B:300:LYS:CB	1.96	0.94
2:C:2:BEM:O6A	2:C:3:BEM:O2	1.85	0.93
1:B:562:TYR:OH	4:B:901:HOH:O	1.86	0.93
1:B:299:SER:CB	1:B:300:LYS:HB2	1.97	0.90
1:B:378:PRO:HD3	1:B:386:GLN:HE22	1.38	0.89
1:A:298:ASN:HA	1:A:299:SER:CB	2.04	0.87
1:A:304:TYR:OH	4:A:903:HOH:O	1.91	0.87
1:A:627:ARG:O	4:A:904:HOH:O	1.91	0.86
1:B:82:LYS:NZ	4:B:906:HOH:O	2.08	0.85
1:A:648:GLU:OE1	1:A:651:LYS:NZ	2.11	0.82
1:A:124:ASP:OD2	4:A:905:HOH:O	1.96	0.82
1:B:378:PRO:HD3	1:B:386:GLN:HE21	1.41	0.82
1:A:450:ASN:HD21	1:A:475:SER:H	1.28	0.81
1:B:475:SER:O	1:B:500:ARG:NH1	2.14	0.81
1:A:90:GLU:OE1	4:A:907:HOH:O	1.99	0.81
1:A:674:ASN:H	1:A:698:ASN:HD22	1.28	0.80
1:A:203:GLU:OE1	4:A:906:HOH:O	1.98	0.80
1:B:378:PRO:CD	1:B:386:GLN:NE2	2.45	0.79
1:A:242:HIS:HE2	2:C:3:BEM:HO3	1.30	0.78
1:B:299:SER:HA	1:B:300:LYS:HD2	1.64	0.78
1:B:119:GLU:OE1	4:B:902:HOH:O	2.04	0.75
1:A:300:LYS:CD	1:A:301:ILE:N	2.49	0.75
1:B:341:ASN:OD1	4:B:903:HOH:O	2.04	0.75



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:300:LYS:HD3	1:A:301:ILE:H	1.52	0.74
1:B:674:ASN:H	1:B:698:ASN:HD22	1.34	0.74
1:A:664:HIS:NE2	4:A:912:HOH:O	2.19	0.74
1:B:525:PRO:O	1:B:527:ALA:N	2.22	0.73
1:B:378:PRO:CD	1:B:386:GLN:HE22	2.00	0.72
1:A:298:ASN:HA	1:A:299:SER:HB2	1.71	0.72
1:A:90:GLU:OE2	4:A:908:HOH:O	2.07	0.72
1:B:509:LYS:O	4:B:905:HOH:O	2.08	0.72
1:A:297:PRO:O	1:A:299:SER:HB2	1.89	0.72
1:A:300:LYS:HD3	1:A:301:ILE:N	2.05	0.70
1:A:434:ASP:OD1	4:A:909:HOH:O	2.09	0.69
1:A:269:ARG:HG3	1:A:308:ASP:HB3	1.75	0.68
1:B:187:ARG:HD3	1:B:189:GLY:O	1.94	0.68
1:B:180:SER:OG	1:B:181:ASN:N	2.27	0.67
1:A:188:ILE:O	1:A:221:SER:OG	2.12	0.67
1:B:320:VAL:O	4:B:907:HOH:O	2.13	0.67
1:A:90:GLU:HG2	1:A:128:MET:HG3	1.78	0.65
1:B:119:GLU:OE2	4:B:908:HOH:O	2.15	0.65
1:B:299:SER:HA	1:B:300:LYS:CD	2.27	0.65
1:A:298:ASN:HA	1:A:299:SER:HB3	1.79	0.63
1:B:274:ARG:NH1	4:B:912:HOH:O	2.22	0.60
1:B:299:SER:CA	1:B:300:LYS:HD2	2.31	0.60
1:B:503:LEU:HG	1:B:504:ILE:HG13	1.83	0.60
1:A:520:ASP:OD1	1:A:522:THR:HG23	2.02	0.59
1:B:403:ALA:HB3	1:B:406:GLN:HG3	1.83	0.59
1:B:674:ASN:H	1:B:698:ASN:ND2	1.98	0.59
1:B:187:ARG:NH1	4:B:913:HOH:O	2.23	0.59
1:A:303:ARG:HA	2:C:4:BEM:O6B	2.02	0.59
1:A:556:LEU:HB2	1:A:586:ILE:HG12	1.84	0.59
1:B:300:LYS:HA	1:B:300:LYS:HE2	1.85	0.59
1:A:673:THR:O	1:A:673:THR:OG1	2.21	0.59
1:B:198:SER:HB3	1:B:224:ASN:OD1	2.03	0.58
1:A:77:SER:HA	1:A:108:THR:O	2.04	0.58
1:A:659:ALA:HB2	1:A:683:ILE:HD12	1.85	0.58
1:B:447:PRO:HG3	1:B:470:GLY:HA3	1.85	0.58
1:B:373:ASN:HB3	1:B:389:ILE:HD12	1.86	0.58
1:B:577:GLU:OE2	1:B:579:GLN:NE2	2.37	0.58
1:A:554:GLU:HG2	1:A:584:LYS:HB2	1.85	0.57
1:B:269:ARG:HB3	1:B:308:ASP:HB3	1.86	0.57
1:B:203:GLU:HA	1:B:227:ARG:O	2.04	0.57
1:B:192:HIS:HA	1:B:301:ILE:HD13	1.87	0.57



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:711:LEU:N	1:B:711:LEU:HD12	2.18	0.57	
1:A:723:GLY:N	4:A:940:HOH:O	2.38	0.56	
1:B:614:ASN:ND2	4:B:916:HOH:O	2.30	0.56	
1:B:690:GLU:HG2	1:B:716:GLY:HA3	1.87	0.56	
1:A:593:LEU:HD13	1:A:605:VAL:HG11	1.87	0.56	
1:A:616:SER:HA	1:A:647:ASN:O	2.05	0.56	
1:A:587:THR:HA	1:A:619:GLN:HG3	1.87	0.56	
1:B:90:GLU:HG3	1:B:93:ALA:HB2	1.88	0.55	
1:B:249:GLU:HA	1:B:274:ARG:O	2.06	0.55	
1:A:431:VAL:O	4:A:911:HOH:O	2.18	0.54	
1:B:582:GLN:HG3	1:B:614:ASN:HB3	1.89	0.54	
1:B:147:LYS:HA	1:B:178:LEU:HD11	1.89	0.54	
1:B:614:ASN:HB2	4:B:916:HOH:O	2.07	0.54	
1:B:127:VAL:HB	1:B:151:MET:HG3	1.88	0.54	
1:B:90:GLU:HA	1:B:125:SER:O	2.07	0.54	
1:B:214:VAL:HG12	1:B:635:PHE:CZ	2.43	0.54	
1:A:298:ASN:CA	1:A:299:SER:CB	2.83	0.54	
1:A:371:LEU:CD2	1:A:406:GLN:HG2	2.38	0.54	
1:A:361:ASP:OD1	1:A:363:SER:OG	2.27	0.52	
1:A:329:SER:OG	1:A:360:ASP:OD2	2.28	0.52	
1:B:157:THR:O	1:B:161:GLN:HG3	2.09	0.52	
1:A:566:ASP:OD1	1:A:595:LYS:NZ	2.38	0.52	
1:B:168:ASP:HA	1:B:203:GLU:O	2.10	0.51	
1:B:714:LEU:HD12	1:B:714:LEU:N	2.25	0.51	
1:A:301:ILE:C	1:A:303:ARG:H	2.12	0.51	
1:A:45:GLU:HA	1:A:73:HIS:CD2	2.45	0.51	
1:B:124:ASP:OD2	4:B:910:HOH:O	2.19	0.51	
1:B:582:GLN:OE1	1:B:584:LYS:NZ	2.41	0.50	
1:A:121:PHE:CD2	1:A:570:ARG:HD2	2.47	0.50	
1:A:690:GLU:OE2	1:A:716:GLY:HA3	2.12	0.50	
1:B:77:SER:HA	1:B:108:THR:O	2.12	0.50	
1:A:144:LYS:NZ	1:A:146:ASN:OD1	2.33	0.49	
1:A:537:ARG:NH1	1:B:119:GLU:OE1	2.46	0.49	
1:A:168:ASP:HA	1:A:203:GLU:O	2.13	0.49	
1:B:669:ASN:HB2	1:B:693:THR:HG23	1.95	0.49	
1:B:447:PRO:HA	1:B:472:TYR:CE2	2.47	0.48	
1:A:320:VAL:O	4:A:913:HOH:O	2.20	0.48	
1:B:520:ASP:OD2	4:B:911:HOH:O	2.20	0.48	
1:A:701:GLU:HB2	1:A:727:LEU:HD12	1.95	0.48	
1:A:120:LYS:NZ	4:A:937:HOH:O	2.37	0.48	
1:B:570:ARG:NH1	1:B:596:GLU:OE1	2.46	0.48	



	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:40:GLU:HA	1:A:70:ALA:O	2.14	0.48	
1:A:203:GLU:HA	1:A:227:ARG:O	2.14	0.48	
1:A:227:ARG:HA	1:A:249:GLU:O	2.13	0.48	
1:B:267:ILE:HG12	1:B:293:MET:HG3	1.96	0.48	
1:A:96:ARG:HD2	1:A:97:ASN:ND2	2.29	0.48	
1:B:227:ARG:HA	1:B:249:GLU:O	2.13	0.48	
1:A:371:LEU:HD21	1:A:406:GLN:HG2	1.97	0.47	
1:A:240:LEU:O	1:A:267:ILE:HB	2.14	0.47	
1:B:313:GLU:HA	1:B:343:ASN:O	2.15	0.47	
1:B:656:LYS:HD3	1:B:656:LYS:HA	1.59	0.47	
1:A:561:SER:OG	4:A:914:HOH:O	2.21	0.47	
1:A:610:ILE:O	1:A:641:MET:HA	2.15	0.47	
1:A:293:MET:CE	1:A:327:ALA:HB3	2.45	0.47	
1:A:662:ILE:O	1:A:662:ILE:HG23	2.15	0.47	
1:B:596:GLU:HG3	1:B:602:ILE:HG22	1.96	0.46	
1:B:714:LEU:HD12	1:B:714:LEU:H	1.79	0.46	
1:A:164:HIS:HA	1:A:199:PHE:O	2.15	0.46	
1:B:108:THR:HA	1:B:137:ASP:O	2.16	0.46	
1:A:331:LYS:HD2	1:A:331:LYS:HA	1.78	0.46	
1:B:118:PRO:HA	1:B:541:GLN:HG2	1.98	0.46	
1:B:288:SER:HB3	1:B:322:HIS:O	2.15	0.46	
1:A:274:ARG:HA	1:A:313:GLU:O	2.14	0.46	
1:A:677:ASN:HA	1:A:701:GLU:O	2.16	0.45	
1:B:615:VAL:HB	1:B:646:PHE:HD1	1.81	0.45	
1:A:220:LYS:NZ	2:C:2:BEM:O6A	2.43	0.45	
1:B:674:ASN:N	1:B:698:ASN:HD22	2.06	0.45	
1:B:299:SER:HB3	1:B:300:LYS:CG	2.45	0.45	
1:A:39:PHE:CE2	1:A:74:LEU:HB3	2.51	0.45	
1:A:681:PRO:HB3	1:A:704:PRO:HB2	1.98	0.45	
1:B:268:ASN:O	1:B:307:VAL:HA	2.17	0.45	
1:A:180:SER:OG	1:A:181:ASN:N	2.50	0.45	
1:A:441:LYS:HE2	1:A:443:ILE:HD11	1.99	0.45	
1:B:274:ARG:HA	1:B:313:GLU:O	2.17	0.45	
1:B:297:PRO:HA	1:B:298:ASN:HA	1.73	0.45	
1:A:619:GLN:HB3	1:A:652:GLY:HA3	1.98	0.44	
1:A:371:LEU:HD12	1:A:385:GLU:O	2.16	0.44	
1:A:713:PRO:HA	1:A:714:LEU:HA	1.78	0.44	
1:A:690:GLU:HG2	1:A:716:GLY:H	1.83	0.44	
1:A:72:GLU:HA	1:A:103:SER:O	2.17	0.44	
1:B:711:LEU:HD12	1:B:711:LEU:H	1.81	0.44	
1:B:719:THR:HG22	1:B:721:ILE:HG13	2.00	0.44	



	lo uo pugom	Interatomic Clash			
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:237:THR:HG22	1:A:262:GLY:HA3	1.99	0.44		
1:B:104:HIS:HA	1:B:133:HIS:O	2.18	0.44		
1:B:295:GLY:O	1:B:333:ARG:HA	2.17	0.44		
2:C:3:BEM:H5	2:C:4:BEM:O2	2.18	0.44		
1:A:157:THR:O	1:A:161:GLN:HG3	2.18	0.43		
1:B:86:THR:HG22	4:B:975:HOH:O	2.17	0.43		
1:A:80:VAL:HG22	1:A:111:VAL:HB	2.00	0.43		
1:B:674:ASN:HB2	1:B:698:ASN:HD22	1.83	0.43		
1:B:263:GLY:HA2	1:B:289:GLY:O	2.18	0.43		
1:B:696:THR:HA	1:B:722:SER:O	2.19	0.43		
1:A:580:ASP:HA	1:A:612:ASN:O	2.19	0.43		
1:B:420:LYS:O	1:B:430:LYS:HE2	2.19	0.43		
1:A:152:ALA:HA	1:A:187:ARG:O	2.19	0.43		
1:B:502:THR:HA	1:B:531:THR:O	2.18	0.43		
1:B:116:SER:HA	4:B:951:HOH:O	2.18	0.43		
1:B:520:ASP:OD1	1:B:522:THR:OG1	2.31	0.43		
1:A:111:VAL:HG22	1:A:140:HIS:HB3	2.00	0.43		
1:A:360:ASP:OD1	1:A:361:ASP:N	2.44	0.43		
1:A:297:PRO:C	1:A:299:SER:HB2	2.39	0.42		
1:B:80:VAL:HG22	1:B:111:VAL:HB	2.00	0.42		
1:B:214:VAL:HG13	1:B:633:SER:O	2.18	0.42		
1:B:557:ASP:OD1	1:B:557:ASP:N	2.52	0.42		
1:B:223:LYS:HA	1:B:245:GLY:O	2.20	0.42		
1:B:344:ASN:HA	1:B:369:ASP:O	2.20	0.42		
1:B:371:LEU:CD1	1:B:389:ILE:HD11	2.49	0.42		
1:B:610:ILE:O	1:B:641:MET:HA	2.19	0.42		
1:B:584:LYS:HA	1:B:616:SER:O	2.20	0.42		
1:A:137:ASP:HA	1:A:168:ASP:O	2.20	0.42		
1:A:249:GLU:HA	1:A:274:ARG:O	2.20	0.42		
1:B:400:TYR:CZ	1:B:413:THR:HA	2.55	0.42		
1:B:639:VAL:HG21	1:B:663:LEU:HD22	2.00	0.42		
1:A:237:THR:HG22	1:A:263:GLY:HA3	2.02	0.42		
1:A:544:TYR:CZ	1:A:573:ALA:HB2	2.55	0.42		
1:A:625:VAL:HG13	1:A:663:LEU:CD2	2.50	0.42		
1:B:550:ASN:HA	1:B:580:ASP:O	2.19	0.42		
1:A:269:ARG:CG	1:A:308:ASP:HB3	2.46	0.41		
1:B:544:TYR:CZ	1:B:573:ALA:HB2	2.55	0.41		
1:B:649:VAL:O	1:B:679:SER:HB3	2.21	0.41		
1:B:556:LEU:HD23	1:B:562:TYR:CE1	2.56	0.41		
1:A:311:LEU:HD22	1:A:313:GLU:HG2	2.02	0.41		
1:A:62:THR:O	1:A:65:SER:OG	2.32	0.41		



Jontinued from previous page						
Atom-2	Interatomic distance (Å)	Clash overlap (Å)				
1:B:261:THR:HG22	2.20	0.41				
1:A:513:THR:N	2.36	0.41				
1:A:570:ARG:HD3	1.82	0.41				
1:B:148:GLY:N	2.32	0.40				
1:B:649:VAL:HG11	2.02	0.40				
1:B:168:ASP:O	2.21	0.40				
1:A:163:ASN:HA	2.03	0.40				
1:A:161:GLN:HG2	2.04	0.40				
1:A:318:VAL:O	2.21	0.40				
1:A:598:ASP:N	2.51	0.40				
	Atom-2 1:B:261:THR:HG22 1:A:513:THR:N 1:A:570:ARG:HD3 1:B:148:GLY:N 1:B:649:VAL:HG11 1:B:168:ASP:O 1:A:163:ASN:HA 1:A:161:GLN:HG2 1:A:318:VAL:O 1:A:598:ASP:N	Atom-2Interatomic distance (Å)1:B:261:THR:HG222.201:A:513:THR:N2.361:A:570:ARG:HD31.821:B:148:GLY:N2.321:B:649:VAL:HG112.021:B:168:ASP:O2.211:A:163:ASN:HA2.031:A:161:GLN:HG22.041:A:318:VAL:O2.211:A:598:ASP:N2.51				

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ALA:O	$1:B:298:ASN:OD1[4_557]$	1.48	0.72
4:A:962:HOH:O	4:B:1010:HOH:O[3_547]	2.12	0.08

Torsion angles (i) 5.3

5.3.1Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	724/726~(100%)	688~(95%)	34~(5%)	2(0%)	41	50
1	В	724/726~(100%)	688~(95%)	33~(5%)	3 (0%)	34	45
All	All	1448/1452~(100%)	1376~(95%)	67~(5%)	5(0%)	41	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	299	SER
1	В	300	LYS



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Mol	Chain	Res	Type
1	В	297	PRO
1	А	120	LYS
1	В	526	ASP

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	Analysed	Rotameric	Outliers	Percentiles	
1	А	620/620~(100%)	598~(96%)	22~(4%)	36 48	
1	В	620/620~(100%)	596~(96%)	24~(4%)	32 43	
All	All	1240/1240~(100%)	1194 (96%)	46 (4%)	34 45	

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	51	LEU
1	А	158	GLU
1	А	178	LEU
1	А	221	SER
1	А	240	LEU
1	А	300	LYS
1	А	301	ILE
1	А	311	LEU
1	А	331	LYS
1	А	343	ASN
1	А	363	SER
1	А	394	HIS
1	А	405	THR
1	А	479	SER
1	А	501	SER
1	А	507	ASN
1	А	518	TYR
1	А	562	TYR
1	A	608	LEU
1	А	625	VAL



Mol	Chain	Res	Type
1	А	673	THR
1	А	714	LEU
1	В	5	LEU
1	В	90	GLU
1	В	154	ARG
1	В	180	SER
1	В	186	LEU
1	В	240	LEU
1	В	265	ARG
1	В	269	ARG
1	В	290	LEU
1	В	300	LYS
1	В	301	ILE
1	В	334	SER
1	В	377	LYS
1	В	394	HIS
1	В	402	GLU
1	В	405	THR
1	В	415	LEU
1	В	458	SER
1	В	480	LEU
1	В	562	TYR
1	В	593	LEU
1	В	671	MET
1	В	692	LYS
1	В	714	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	192	HIS
1	А	450	ASN
1	А	698	ASN
1	В	374	GLN
1	В	386	GLN
1	В	450	ASN
1	В	698	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	ol Type Chain Reg		Tiple	Bo	ond leng	$_{\rm ths}$	Bond angles			
	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BEM	С	1	2	13,13,13	0.80	0	18,19,19	1.66	4 (22%)
2	BEM	С	2	2	12,12,13	1.11	2 (16%)	14,17,19	1.33	2 (14%)
2	BEM	С	3	2,3	12,12,13	0.90	0	14,17,19	2.75	5 (35%)
2	BEM	С	4	2	12,12,13	0.90	0	14,17,19	2.24	5 (35%)

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	BEM	С	1	2	-	0/4/24/24	0/1/1/1
2	BEM	С	2	2	-	1/4/21/24	0/1/1/1
2	BEM	С	3	2,3	-	1/4/21/24	0/1/1/1
2	BEM	С	4	2	-	2/4/21/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	С	2	BEM	O6B-C6	-2.32	1.23	1.30
2	С	2	BEM	C5-C6	-2.25	1.48	1.53

All (16) bond angle outliers are listed below:



\mathbf{rt}		$5 \mathrm{GKQ}$
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	3	BEM	C1-C2-C3	7.54	118.93	109.67
2	С	4	BEM	O5-C1-C2	4.50	117.72	110.77
2	С	1	BEM	O5-C5-C6	4.35	117.56	105.88
2	С	4	BEM	C1-C2-C3	4.23	114.86	109.67
2	С	3	BEM	C3-C4-C5	3.67	115.53	109.25
2	С	3	BEM	O2-C2-C1	-3.50	101.99	109.15
2	С	4	BEM	O5-C5-C6	3.33	117.26	106.31
2	С	3	BEM	C2-C3-C4	3.16	116.37	110.89
2	С	2	BEM	O4-C4-C5	2.86	116.16	109.74
2	С	1	BEM	O4-C4-C3	-2.76	103.96	110.35
2	С	4	BEM	C2-C3-C4	2.66	115.50	110.89
2	С	1	BEM	O3-C3-C4	-2.60	104.35	110.35
2	С	3	BEM	O5-C1-C2	2.58	114.75	110.77
2	С	1	BEM	O6B-C6-C5	2.41	122.47	113.65
2	С	4	BEM	O6B-C6-O6A	-2.35	118.76	124.09
2	С	2	BEM	C3-C4-C5	-2.20	105.48	109.25

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	С	3	BEM	C4-C5-C6-O6B
2	С	2	BEM	O5-C5-C6-O6B
2	С	4	BEM	O5-C5-C6-O6B
2	С	4	BEM	O5-C5-C6-O6A

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	2	BEM	2	0
2	С	3	BEM	4	0
2	С	4	BEM	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 $>$	$\langle \mathbf{RSRZ} \rangle $ #RSRZ>2		$OWAB(A^2)$	Q<0.9	
1	А	726/726~(100%)	-0.07	11 (1%)	73	80	26, 38, 54, 84	0
1	В	726/726~(100%)	0.16	40 (5%)	25	32	26, 41, 62, 81	0
All	All	1452/1452~(100%)	0.04	51 (3%)	44	53	26, 39, 59, 84	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	699	VAL	7.9
1	В	698	ASN	5.1
1	А	707	VAL	4.6
1	В	643	ASN	3.5
1	В	674	ASN	3.5
1	В	695	VAL	3.4
1	В	651	LYS	3.2
1	В	724	ASN	3.1
1	В	375	ASP	3.0
1	В	721	ILE	3.0
1	В	702	GLY	3.0
1	А	716	GLY	2.9
1	В	707	VAL	2.8
1	В	727	LEU	2.8
1	В	383	GLY	2.7
1	В	708	VAL	2.6
1	В	376	ALA	2.6
1	В	725	THR	2.6
1	В	377	LYS	2.5
1	В	680	ALA	2.5
1	A	371	LEU	2.5
1	В	413	THR	2.5
1	В	675	GLU	2.5
1	А	660	SER	2.4



Mol	Chain	Res	Type	RSRZ
1	В	683	ILE	2.4
1	А	443	ILE	2.4
1	А	382	LYS	2.4
1	В	697	GLY	2.3
1	В	380	ILE	2.3
1	А	444	ALA	2.3
1	В	719	THR	2.2
1	В	642	ASN	2.2
1	А	469	ALA	2.2
1	В	701	GLU	2.2
1	В	671	MET	2.2
1	В	509	LYS	2.2
1	В	180	SER	2.2
1	А	470	GLY	2.2
1	В	672	THR	2.1
1	В	368	LYS	2.1
1	В	645	ILE	2.1
1	В	298	ASN	2.1
1	В	518	TYR	2.1
1	А	487	ARG	2.1
1	В	400	TYR	2.1
1	В	633	SER	2.1
1	В	660	SER	2.1
1	В	673	THR	2.1
1	В	714	LEU	2.0
1	В	410	GLY	2.0
1	А	404	LYS	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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	BEM	С	1	13/13	0.79	0.20	71,78,85,85	0



0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	$\mathbf{Q} <$	
2	BEM	С	3	12/13	0.80	0.46	74,83,88,91	(
2	BEM	С	4	12/13	0.84	0.41	65,83,89,91	(
2	BEM	С	2	12/13	0.86	0.17	59,78,83,84	(

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The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
3	CA	В	801	1/1	0.76	0.17	76,76,76,76	0
3	CA	А	801	1/1	0.95	0.07	67,67,67,67	0



6.5 Other polymers (i)

There are no such residues in this entry.

