

Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2020 – 04:58 AM BST

PDB ID	:	4JZJ
Title	:	Crystal Structure of Receptor-Fab Complex
Authors	:	Broughton, S.E.; Parker, M.W.
Deposited on	:	2013-04-03
Resolution	:	2.80 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 as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.80 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	3140(2.80-2.80)			
Clashscore	141614	3569(2.80-2.80)			
Ramachandran outliers	138981	3498 (2.80-2.80)			
Sidechain outliers	138945	3500 (2.80-2.80)			
RSRZ outliers	127900	3078 (2.80-2.80)			

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	С	287	9% 70% 15%	• 13%
1	D	287	9% 65% 21%	• 13%
2	А	221	^{2%} 78%	17% ••
2	Н	221	84%	13% •
3	В	220	90%	8% •
3	L	220	85%	12% •



Mol	Chain	Length	Quality of chain						
4	Е	7	43%	57%					
5	F	5	40%	60%					
6	G	3	67%	33%					

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density	
5	NAG	F	1	-	-	Х	-	
5	NAG	F	2	-	-	Х	-	
5	FUL	F	4	-	-	Х	-	
6	NAG	G	1	-	-	Х	-	
8	GOL	Н	301	-	-	-	Х	



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 10972 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 Interleukin-3 receptor subunit alpha.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	С	250	Total 2024	C 1283	N 359	O 369	S 13	0	0	0
1	D	251	Total 2035	C 1293	N 359	O 370	S 13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	144	LYS	ASN	SEE REMARK 999	UNP P26951
С	?	-	ARG	deletion	UNP P26951
С	298	VAL	ALA	engineered mutation	UNP P26951
D	144	LYS	ASN	SEE REMARK 999	UNP P26951
D	?	-	ARG	deletion	UNP P26951
D	298	VAL	ALA	engineered mutation	UNP P26951

• Molecule 2 is a protein called Fab Heavy Chain.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	Δ 214	Total	С	Ν	Ο	S	0	0	0	
	214	1628	1041	267	311	9	0	0		
0	ц	215	Total	С	Ν	Ο	S	0	0	0
	2 П	210	1634	1044	268	313	9		0	0

• Molecule 3 is a protein called Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3 B	219	Total	С	Ν	Ο	S	0	0	0
JU	D		1699	1062	282	350	5	0		
2	т	210	Total	С	Ν	Ο	S	0	0	0
3		219	1699	1062	282	350	5	0	0	

• Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran



ose-(1-6)] beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)] 2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Е	7	Total 81	С 46	N 2	O 33	0	0	0

• Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-3)][beta-L-fucopyranose-(1-6)]2-acetami do-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf	Trace
5	F	5	Total 59	$\begin{array}{c} \mathrm{C} \\ \mathrm{34} \end{array}$	N 2	O 23	0	0	0

• Molecule 6 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	3	Total 34	C 20	N 1	O 13	0	0	0

• Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	C	1	Total	С	Ν	Ο	0	0	
1	U	T	14	8	1	5	0	0	
7	л	1	Total	С	Ν	Ο	0	0	
1	D	T	14	8	1	5	0	0	

• Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	Н	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0



• Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	С	9	Total O 9 9	0	0
9	D	7	Total O 7 7	0	0
9	А	2	Total O 2 2	0	0
9	В	6	Total O 6 6	0	0
9	Н	12	Total O 12 12	0	0
9	L	3	Total O 3 3	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: Interleukin-3 receptor subunit alpha



SER THR SER SER SER G114 0151 1148 0151 7153 7153 7155 7155 7155 7155 7156 7156 7156 7156	S186 1196 1198 1198 1198 1200 1200 1200 1200 1200 1200 1221		
• Molecule 2: Fab Heav	y Chain		
Chain H:	84%	13% •	
87 87 821 821 823 835 835 8436 8436 8436 8436 8436 8436 8440 8440 8440 8440 8440 8440 8440 844	D50 854 457 759 77 778 178 178 178 178 178 178 812 8122 812	8134 SER SER THR SER THR SER GLY GLY 0151 T152 T155	116 C
1185 1190 1196 1231			
• Molecule 3: Fab Ligh	t Chain		
Chain B:	90%	8% •	
D1 S14 S14 121 121 121 128 149 126 126 126	869 1108 1108 1138 1142 1142 1142 1142 1142 1142 1142 114	1184 1188 1188 1188 1187 1187 1187 1187	SXD
• Molecule 3: Fab Ligh	t Chain		
Chain L:	85%	12% ·	
명 전 전 전 전 전 전 전 전 전 전 전 전 전 전 전 전 전 전 전	139 140 171 178 178 170 1702 1702 1702 1702 1702 1702 1702	0130 1138 1138 1138 1138 1138 1138 1138	7203 7210
CKS CKS			
• Molecule 4: alpha-D-: se-(1-4)-2-acetamido-2- pyranose-(1-6)]2-acetam	mannopyranose-(1-3)-[alpha-1 deoxy-beta-D-glucopyranose- nido-2-deoxy-beta-D-glucopyr	D-mannopyranose-(1-6) -(1-4)-[beta-L-fucopyrar ranose]beta-D-mannopyrano 10se-(1-3)][beta-L-fuco

Chain E:	43%	57%
NAG 1 NAG 2 BNA3 BNA3 MAN4 FUL6 FUL6 FUL6		

 • Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-3)][beta-L-fucopyranose-(1-6)] 2-acetamido-2-deoxy-beta-D-glucopyranose e

Chain F:	40%	60%
NAG1 NAG2 BMA3 FUL4 FUL4		



67%

Chain G:

33%

NAG1 FUC2 FUL3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	88.30Å 120.65Å 92.97Å	Deperitor
a, b, c, α , β , γ	90.00° 97.45° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	49.67 - 2.80	Depositor
Resolution (A)	49.67 - 2.80	EDS
% Data completeness	99.1 (49.67-2.80)	Depositor
(in resolution range)	$99.1 \ (49.67 - 2.80)$	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	$3.22 (at 2.81 \text{\AA})$	Xtriage
Refinement program	PHENIX dev_1218	Depositor
B B.	0.185 , 0.244	Depositor
II, II, <i>free</i>	0.191 , 0.244	DCC
R_{free} test set	2381 reflections $(5.05%)$	wwPDB-VP
Wilson B-factor ($Å^2$)	72.1	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.31 , 37.7	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10972	wwPDB-VP
Average B, all atoms $(Å^2)$	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.51% 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: GOL, BMA, NAG, FUC, FUL, 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	Bo	nd lengths	Bo	ond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	С	0.60	1/2074~(0.0%)	0.72	1/2814~(0.0%)
1	D	0.51	0/2087	0.70	1/2830~(0.0%)
2	А	0.48	0/1671	0.63	0/2270
2	Н	0.56	0/1677	0.68	1/2278~(0.0%)
3	В	0.52	0/1737	0.65	0/2362
3	L	0.58	0/1737	0.65	0/2362
All	All	0.54	1/10983~(0.0%)	0.68	$3/14916 \ (0.0\%)$

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	С	79	THR	C-N	5.69	1.47	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	281	LEU	CA-CB-CG	7.03	131.47	115.30
1	С	151	LEU	CA-CB-CG	5.75	128.52	115.30
2	Н	185	LEU	CA-CB-CG	5.04	126.90	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	С	2024	0	1958	28	0
1	D	2035	0	1968	39	0
2	А	1628	0	1608	19	0
2	Н	1634	0	1613	12	0
3	В	1699	0	1630	10	0
3	L	1699	0	1630	18	0
4	Ε	81	0	70	9	0
5	F	59	0	51	33	0
6	G	34	0	31	10	0
7	С	14	0	13	2	0
7	D	14	0	13	2	0
8	D	6	0	8	1	0
8	Н	6	0	8	1	0
9	А	2	0	0	1	0
9	В	6	0	0	0	0
9	С	9	0	0	0	0
9	D	7	0	0	0	0
9	H	12	0	0	3	0
9	L	3	0	0	0	0
All	All	10972	0	10601	159	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (159) 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:C:46:ASN:HD22	7:C:408:NAG:C1	0.99	1.57
5:F:1:NAG:H62	5:F:2:NAG:C7	1.36	1.51
1:D:109:ASN:HD21	6:G:1:NAG:C1	1.22	1.48
5:F:1:NAG:C6	5:F:2:NAG:C7	2.27	1.11
1:C:80:ASN:CG	4:E:1:NAG:C1	2.23	1.06
5:F:1:NAG:H62	5:F:2:NAG:O7	1.57	1.01
5:F:1:NAG:C6	5:F:2:NAG:O7	2.09	1.01
5:F:1:NAG:C5	5:F:2:NAG:O7	2.09	1.01
5:F:1:NAG:H62	5:F:2:NAG:C8	1.99	0.91
1:C:80:ASN:OD1	4:E:1:NAG:C1	2.20	0.88
5:F:1:NAG:H5	5:F:2:NAG:O7	1.73	0.87
5:F:1:NAG:O7	5:F:4:FUL:C1	2.22	0.87
5:F:1:NAG:C7	5:F:4:FUL:C1	2.57	0.83
1:C:56:ALA:HB2	4:E:7:FUL:O3	1.79	0.82
5:F:1:NAG:C6	5:F:2:NAG:C1	2.59	0.80



A 4 1	A 4 5 77 0	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
5:F:1:NAG:O3	5:F:1:NAG:C7	2.28	0.80
3:B:151:LYS:HB3	3:B:203:THR:HG23	1.65	0.78
4:E:3:BMA:H62	4:E:5:MAN:O2	1.84	0.77
1:C:80:ASN:ND2	4:E:1:NAG:C2	2.48	0.77
1:C:37:GLN:HE21	1:C:73:ILE:HG12	1.51	0.76
1:C:238:GLU:OE2	1:C:274:ARG:NH1	2.20	0.73
1:C:262:LEU:HG	1:C:263:ASN:HB3	1.72	0.72
1:D:125:ALA:CB	6:G:1:NAG:H82	2.19	0.72
1:D:109:ASN:CG	6:G:1:NAG:C1	2.59	0.71
1:C:80:ASN:ND2	4:E:1:NAG:O5	2.25	0.70
1:D:109:ASN:HD21	6:G:1:NAG:C2	2.04	0.70
5:F:1:NAG:O4	5:F:4:FUL:C2	2.41	0.69
1:D:30:LEU:HD13	1:D:94:ILE:HG23	1.76	0.68
1:C:51:GLU:OE2	3:L:102:TYR:OH	2.05	0.67
1:D:153:TYR:CD1	1:D:161:ARG:HG2	2.30	0.66
3:L:17:GLU:HG3	3:L:18:ARG:H	1.63	0.64
5:F:2:NAG:O7	5:F:2:NAG:C1	2.41	0.64
1:C:46:ASN:HD21	7:C:408:NAG:C1	2.02	0.64
5:F:2:NAG:C1	5:F:5:FUL:H61	2.29	0.63
5:F:2:NAG:H5	5:F:5:FUL:H61	1.82	0.62
2:H:36:TRP:CE3	2:H:81:LEU:HD22	2.34	0.62
3:B:14:SER:HB2	3:B:17:GLU:HG3	1.82	0.62
5:F:1:NAG:O4	5:F:4:FUL:O2	2.16	0.62
2:H:151:ASP:OD1	2:H:178:GLN:NE2	2.33	0.61
5:F:1:NAG:H81	5:F:4:FUL:O5	2.00	0.61
5:F:1:NAG:C8	5:F:4:FUL:O5	2.48	0.61
1:C:24:ASN:HB3	1:C:25:PRO:HD3	1.85	0.59
5:F:1:NAG:O4	5:F:4:FUL:H2	2.02	0.58
1:D:125:ALA:HB1	6:G:1:NAG:H82	1.85	0.58
8:H:301:GOL:H2	9:H:409:HOH:O	2.04	0.57
1:D:93:TRP:CE2	5:F:1:NAG:H3	2.39	0.57
1:C:37:GLN:NE2	1:C:73:ILE:HG12	2.20	0.56
1:D:50:ILE:HG12	1:D:85:VAL:HG12	1.87	0.56
1:D:109:ASN:OD1	6:G:1:NAG:C1	2.54	0.56
1:D:53:VAL:HA	1:D:59:SER:HB2	1.88	0.55
5:F:1:NAG:H4	5:F:1:NAG:O7	2.07	0.55
5:F:1:NAG:C7	5:F:4:FUL:O5	2.54	0.55
5:F:1:NAG:O7	5:F:4:FUL:O5	2.23	0.55
5:F:1:NAG:C4	5:F:2:NAG:O7	2.54	0.55
1:C:30:LEU:HD23	1:C:94:ILE:HG23	1.88	0.54
3:L:102:TYR:CD1	3:L:102:TYR:N	2.76	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
7:D:409:NAG:C1	6:G:1:NAG:O4	2.55	0.54
1:D:144:LYS:N	1:D:145:ARG:HA	2.22	0.54
3:B:38:TYR:CE1	3:B:56:TRP:HZ3	2.26	0.53
5:F:1:NAG:O4	5:F:2:NAG:O7	2.25	0.53
2:A:36:TRP:CD2	2:A:81:LEU:HD13	2.43	0.53
1:D:26:PRO:HB3	1:D:45:ARG:HD3	1.91	0.53
3:L:11:LEU:HD23	3:L:110:LEU:HD13	1.91	0.53
3:B:55:TYR:HE2	3:B:61:GLU:OE1	1.92	0.52
5:F:1:NAG:C4	5:F:1:NAG:O7	2.58	0.51
4:E:3:BMA:C6	4:E:5:MAN:O2	2.57	0.51
5:F:2:NAG:H82	5:F:5:FUL:C1	2.40	0.51
3:L:169:VAL:HG22	3:L:181:LEU:HD12	1.92	0.51
1:C:63:VAL:HG13	3:L:33:GLY:HA3	1.93	0.51
1:C:182:LEU:HD12	1:C:196:ASP:HB3	1.94	0.50
2:A:32:TYR:CG	2:A:98:ARG:HD3	2.46	0.50
1:D:156:ASP:HB3	1:D:162:ILE:HD13	1.94	0.50
3:L:39:LEU:HG	3:L:40:THR:N	2.26	0.50
2:A:33:TYR:HB2	2:A:99:SER:HB3	1.93	0.49
1:C:234:LYS:HD2	1:C:276:ARG:NH2	2.27	0.49
1:C:263:ASN:HB2	1:C:264:PRO:HA	1.93	0.49
1:D:144:LYS:HB2	1:D:146:GLN:N	2.27	0.49
1:D:182:LEU:HD12	1:D:196:ASP:HB3	1.93	0.49
1:D:272:ARG:HH21	1:D:274:ARG:NH1	2.10	0.48
2:H:168:SER:HB2	9:H:411:HOH:O	2.12	0.48
3:B:184:THR:HG22	3:B:186:THR:HG23	1.95	0.48
2:H:152:TYR:CE1	2:H:157:VAL:HG13	2.49	0.48
3:L:21:ILE:HD12	3:L:79:LEU:HD23	1.95	0.48
1:C:138:LEU:HD22	1:C:164:CYS:HB3	1.96	0.48
1:D:32:MET:HE2	1:D:39:LEU:HD13	1.96	0.47
2:A:43:LYS:HD3	2:A:43:LYS:HA	1.52	0.47
5:F:2:NAG:H3	5:F:5:FUL:H61	1.95	0.47
1:C:56:ALA:HB2	4:E:7:FUL:HO3	1.77	0.47
2:H:76:ILE:O	2:H:78:THR:HG23	2.13	0.47
1:D:75:LEU:HB3	8:D:410:GOL:H32	1.97	0.47
2:A:196:LEU:HA	2:A:196:LEU:HD12	1.71	0.46
3:L:71:SER:OG	3:L:78:THR:HG22	2.16	0.46
2:A:38:ARG:HB3	2:A:94:TYR:CE1	2.51	0.46
1:D:35:LYS:HG3	1:D:36:ALA:H	1.79	0.46
1:D:85:VAL:HG22	1:D:90:PHE:O	2.16	0.46
2:A:95:TYR:CE1	3:B:49:PRO:HB3	2.51	0.46
2:H:7:SER:HB3	2:H:21:SER:H	1.81	0.46



	t a c	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:54:LYS:O	1:C:57:ASP:HB2	2.16	0.46
1:D:143:ALA:HA	1:D:145:ARG:NE	2.31	0.45
1:D:173:SER:HB2	1:D:176:SER:HB2	1.99	0.45
1:D:150:CYS:HB3	1:D:153:TYR:CZ	2.52	0.45
2:A:69:THR:HG23	2:A:82:GLN:HB3	1.99	0.45
2:H:168:SER:CB	9:H:411:HOH:O	2.64	0.45
1:D:242:GLN:HB3	1:D:248:VAL:HA	1.99	0.45
2:A:47:TRP:CZ2	2:A:49:GLY:HA2	2.52	0.45
7:D:409:NAG:C1	6:G:1:NAG:HO4	2.28	0.45
3:L:3:VAL:H	3:L:26:SER:HB2	1.82	0.45
1:D:135:GLN:CD	1:D:161:ARG:HD3	2.37	0.45
1:D:114:ILE:HD12	1:D:169:ILE:HD13	1.99	0.44
1:D:141:ASN:OD1	1:D:147:GLN:HG2	2.17	0.44
1:D:54:LYS:HD2	1:D:58:TYR:CE2	2.52	0.44
3:L:153:GLN:HG2	3:L:160:LEU:HD22	2.00	0.44
2:A:11:VAL:HG21	2:A:154:PRO:HG3	2.00	0.44
1:D:125:ALA:HB1	6:G:1:NAG:C8	2.48	0.44
1:C:274:ARG:CZ	1:C:281:LEU:HD21	2.48	0.44
1:D:30:LEU:HD22	1:D:94:ILE:HD13	2.00	0.44
3:L:126:PRO:HB3	3:L:137:SER:H	1.83	0.44
3:L:17:GLU:CG	3:L:18:ARG:H	2.30	0.44
1:D:40:THR:HG22	1:D:41:TRP:H	1.82	0.44
1:C:268:THR:HA	1:C:288:GLN:O	2.18	0.43
1:D:93:TRP:NE1	5:F:1:NAG:H3	2.34	0.43
2:A:148:LEU:HA	2:A:148:LEU:HD12	1.88	0.43
2:A:148:LEU:HD12	2:A:186:SER:HB3	1.99	0.43
2:A:100:HIS:CE1	2:A:102:LEU:HD12	2.53	0.43
1:C:210:PRO:HG2	1:C:271:ILE:HG23	1.99	0.43
1:D:153:TYR:CG	1:D:161:ARG:HG2	2.54	0.43
1:D:125:ALA:HB3	6:G:1:NAG:H82	1.98	0.43
2:A:19:LYS:HG3	2:A:82:GLN:HG3	1.99	0.43
5:F:1:NAG:O3	5:F:1:NAG:O7	2.30	0.43
5:F:1:NAG:O7	5:F:1:NAG:C3	2.56	0.43
1:C:254:ARG:HA	1:C:254:ARG:HD2	1.97	0.42
2:H:35:LYS:HG2	2:H:50:ASP:OD1	2.19	0.42
3:B:136:ALA:N	3:B:187:LEU:O	2.41	0.42
2:H:144:ALA:HB2	2:H:190:THR:HG22	2.01	0.42
3:B:149:GLU:HG3	3:B:149:GLU:O	2.19	0.42
3:B:21:ILE:HG12	3:B:108:THR:HG21	2.02	0.42
1:D:108:GLU:OE2	1:D:128:PRO:HD2	2.19	0.42
5:F:2:NAG:O5	5:F:4:FUL:H2	2.19	0.42



		Interatomic	Clash
Atom-1	Atom-2	$distance (m \AA)$	overlap (Å)
3:B:100:TYR:CD2	3:B:100:TYR:C	2.92	0.42
3:L:203:THR:HG22	3:L:210:PRO:HB3	2.02	0.42
2:H:57:ALA:HB2	4:E:5:MAN:H61	2.01	0.41
3:L:39:LEU:HD11	3:L:94:CYS:HB2	2.02	0.41
3:L:130:GLN:HG2	3:L:135:THR:O	2.20	0.41
1:D:169:ILE:HG13	1:D:169:ILE:H	1.59	0.41
3:L:3:VAL:H	3:L:26:SER:CB	2.34	0.41
2:H:23:LYS:CB	2:H:78:THR:HG22	2.50	0.41
1:D:54:LYS:O	1:D:54:LYS:HD3	2.20	0.41
2:H:196:LEU:HA	2:H:196:LEU:HD23	1.84	0.41
1:C:113:TRP:HD1	1:C:115:HIS:HB3	1.85	0.41
1:C:52:CYS:O	1:C:59:SER:HB2	2.21	0.41
2:A:153:PHE:HA	2:A:154:PRO:HA	1.71	0.41
2:A:168:SER:HB2	9:A:401:HOH:O	2.20	0.41
2:A:206:ASN:OD1	2:A:213:LYS:HE2	2.20	0.41
1:D:33:LYS:HE2	1:D:40:THR:OG1	2.21	0.41
3:L:101:PRO:O	3:L:103:THR:N	2.53	0.41
5:F:2:NAG:C5	5:F:5:FUL:H61	2.49	0.40
2:A:54:SER:O	2:A:74:LYS:HE3	2.21	0.40
2:A:6:GLN:HG2	2:A:22:CYS:HB2	2.02	0.40
1:C:116:ASP:HB2	1:C:119:PHE:HD2	1.86	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	Percen	\mathbf{tiles}
1	С	240/287~(84%)	222~(92%)	15 (6%)	3 (1%)	12	36
1	D	243/287~(85%)	220 (90%)	20 (8%)	3 (1%)	13	39
2	А	210/221~(95%)	197 (94%)	12 (6%)	1 (0%)	29	61
2	Н	$211/221 \ (96\%)$	201 (95%)	9 (4%)	1 (0%)	29	61



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
3	В	217/220~(99%)	205~(94%)	12~(6%)	0	100	100
3	L	217/220~(99%)	212~(98%)	5 (2%)	0	100	100
All	All	1338/1456~(92%)	1257 (94%)	73 (6%)	8 (1%)	25	56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	254	ARG
1	D	35	LYS
1	D	48	THR
1	D	287	PRO
2	Н	220	PRO
1	С	73	ILE
1	С	287	PRO
2	А	44	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	С	223/256~(87%)	210~(94%)	13~(6%)	20 50
1	D	223/256~(87%)	203~(91%)	20 (9%)	9 28
2	А	181/187~(97%)	166~(92%)	15 (8%)	11 32
2	Н	182/187~(97%)	171 (94%)	11 (6%)	19 48
3	В	194/195~(100%)	185~(95%)	9~(5%)	27 60
3	L	194/195~(100%)	183 (94%)	11 (6%)	20 50
All	All	1197/1276~(94%)	1118 (93%)	79 (7%)	16 44

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	35	LYS
1	С	46	ASN



Mol	Chain	Res	Type
1	С	47	VAL
1	С	55	ASP
1	С	57	ASP
1	С	74	SER
1	С	170	SER
1	С	174	SER
1	С	179	SER
1	С	262	LEU
1	С	263	ASN
1	С	275	GLU
1	С	277	VAL
1	D	27	ILE
1	D	40	THR
1	D	55	ASP
1	D	68	CYS
1	D	87	ASN
1	D	91	SER
1	D	169	ILE
1	D	176	SER
1	D	179	SER
1	D	195	THR
1	D	197	LYS
1	D	199	VAL
1	D	213	THR
1	D	233	ARG
1	D	250	THR
1	D	255	ASP
1	D	257	THR
1	D	269	VAL
1	D	276	ARG
1	D	281	LEU
2	A	43	LYS
2	A	54	SER
2	A	65	LYS
2	A	79	THR
2	A	82	GLN
2	A	85	SER
2	A	119	SER
2	A	127	SER
2	A	151	ASP
2	A	156	PRO
2	A	157	VAL



Mol	Chain	Res	Type
2	А	168	SER
2	А	198	THR
2	А	200	THR
2	А	203	CYS
3	В	1	ASP
3	В	69	SER
3	В	100	TYR
3	В	128	ASP
3	В	142	LEU
3	В	149	GLU
3	В	156	VAL
3	В	186	THR
3	В	203	THR
2	Н	7	SER
2	Н	40	MET
2	Н	45	LEU
2	Н	54	SER
2	Н	59	PHE
2	Н	69	THR
2	Н	82	GLN
2	Н	98	ARG
2	Н	122	SER
2	Н	158	THR
2	Н	167	THR
3	L	5	THR
3	L	18	ARG
3	L	26	SER
3	L	53	LEU
3	L	78	THR
3	L	80	THR
3	L	103	THR
3	L	133	SER
3	L	135	THR
3	L	143	ASN
3	L	203	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type	
1	С	37	GLN	
1	С	44	ASN	
1	С	46	ASN	



Mol	Chain	Res	Type
1	С	224	HIS
1	D	99	ASN
1	D	109	ASN
2	A	67	GLN
2	А	178	GLN
3	L	27	GLN
3	L	31	ASN
3	L	35	GLN
3	Ĺ	143	ASN
3	L	144	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)

15 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	Tune	Chain	Dec	Tink	Bo	Bond lengths		Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	1	1,4	14,14,15	1.15	1 (7%)	17,19,21	2.17	7 (41%)
4	NAG	Е	2	4	14,14,15	0.80	0	17,19,21	1.25	2 (11%)
4	BMA	E	3	4	11,11,12	0.69	0	15,15,17	1.17	1(6%)
4	MAN	E	4	4	11,11,12	0.68	0	15,15,17	1.39	3 (20%)
4	MAN	E	5	4	11,11,12	0.61	0	15,15,17	1.46	3 (20%)
4	FUL	E	6	4	10, 10, 11	0.81	0	14,14,16	<mark>3.01</mark>	6 (42%)
4	FUL	Е	7	4	10,10,11	0.60	0	14,14,16	1.96	4 (28%)



Mal	Tune	Chain	Dec	Tink	Bo	ond leng	$_{\rm sths}$	E	Sond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
5	NAG	F	1	1,5	14, 14, 15	0.94	0	17,19,21	<mark>5.85</mark>	11 (64%)
5	NAG	F	2	5	14, 14, 15	1.85	6 (42%)	17,19,21	<mark>3.25</mark>	8 (47%)
5	BMA	F	3	5	11,11,12	0.76	0	15,15,17	1.65	4 (26%)
5	FUL	F	4	5	10, 10, 11	0.48	0	14,14,16	0.97	1 (7%)
5	FUL	F	5	5	10, 10, 11	0.30	0	14,14,16	0.62	0
6	NAG	G	1	$1,\!6$	14, 14, 15	0.47	0	17,19,21	1.71	4 (23%)
6	FUC	G	2	6	10, 10, 11	0.77	0	14,14,16	1.26	2 (14%)
6	FUL	G	3	6	10, 10, 11	0.83	0	14,14,16	2.17	3 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	Е	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Е	2	4	-	2/6/23/26	0/1/1/1
4	BMA	Е	3	4	-	2/2/19/22	0/1/1/1
4	MAN	Е	4	4	-	0/2/19/22	0/1/1/1
4	MAN	Е	5	4	-	0/2/19/22	0/1/1/1
4	FUL	Е	6	4	-	-	0/1/1/1
4	FUL	Е	7	4	-	-	0/1/1/1
5	NAG	F	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	F	2	5	-	3/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
5	FUL	F	4	5	-	-	0/1/1/1
5	FUL	F	5	5	-	-	0/1/1/1
6	NAG	G	1	1,6	-	2/6/23/26	0/1/1/1
6	FUC	G	2	6	-	-	0/1/1/1
6	FUL	G	3	6	-	_	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
5	F	2	NAG	C2-N2	-3.30	1.40	1.46
5	F	2	NAG	C3-C2	-2.87	1.46	1.52
5	F	2	NAG	O5-C1	-2.44	1.39	1.43
5	F	2	NAG	C1-C2	-2.28	1.48	1.52
5	F	2	NAG	07-C7	-2.16	1.18	1.23



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
5	F	2	NAG	C7-N2	-2.09	1.27	1.34
4	Е	1	NAG	C1-C2	-2.06	1.49	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	F	1	NAG	C4-C3-C2	-15.03	88.99	111.02
5	F	1	NAG	C3-C4-C5	-10.22	92.01	110.24
4	Е	6	FUL	C1-C2-C3	-9.33	98.20	109.67
5	F	2	NAG	O4-C4-C3	-8.89	89.80	110.35
5	F	1	NAG	C1-C2-N2	7.35	123.05	110.49
5	F	1	NAG	C2-N2-C7	-7.31	112.49	122.90
5	F	1	NAG	O5-C1-C2	-7.09	100.10	111.29
6	G	3	FUL	C1-C2-C3	6.57	117.74	109.67
5	F	2	NAG	C2-N2-C7	-5.86	114.56	122.90
5	F	1	NAG	C1-O5-C5	5.77	120.01	112.19
5	F	1	NAG	O4-C4-C3	4.94	121.76	110.35
5	F	2	NAG	C3-C4-C5	-4.79	101.70	110.24
4	Е	1	NAG	C1-O5-C5	4.13	117.79	112.19
6	G	1	NAG	O5-C5-C6	4.12	113.66	107.20
4	Е	7	FUL	C1-O5-C5	3.86	121.53	112.78
5	F	1	NAG	O3-C3-C4	3.77	119.06	110.35
6	G	1	NAG	C3-C4-C5	-3.74	103.57	110.24
4	Е	5	MAN	C1-O5-C5	3.49	116.92	112.19
4	Е	6	FUL	C3-C4-C5	3.43	115.11	109.77
4	Е	1	NAG	O5-C5-C4	-3.35	102.67	110.83
4	Е	1	NAG	C6-C5-C4	3.35	120.85	113.00
4	Е	1	NAG	O4-C4-C5	3.29	117.47	109.30
5	F	3	BMA	C2-C3-C4	3.29	116.58	110.89
5	F	2	NAG	O5-C1-C2	-3.26	106.14	111.29
5	F	2	NAG	O7-C7-C8	2.97	127.58	122.06
6	G	3	FUL	O5-C1-C2	2.90	115.24	110.77
4	Е	2	NAG	O5-C1-C2	-2.87	106.76	111.29
5	F	3	BMA	C1-O5-C5	-2.86	108.32	112.19
4	Е	1	NAG	O6-C6-C5	2.84	121.05	111.29
4	Е	4	MAN	C1-O5-C5	2.81	116.00	112.19
6	G	3	FUL	C2-C3-C4	2.79	115.72	110.89
4	Е	7	FUL	C2-C3-C4	2.77	115.69	110.89
4	Е	3	BMA	C1-C2-C3	2.76	113.05	109.67
4	Е	4	MAN	C3-C4-C5	2.75	115.14	110.24
4	Е	4	MAN	O5-C5-C6	2.69	111.43	107.20
4	Е	6	FUL	O5-C5-C4	2.65	114.27	109.52



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	F	3	BMA	O5-C5-C6	2.64	111.34	107.20
6	G	2	FUC	O5-C1-C2	-2.64	106.70	110.77
4	Ε	7	FUL	C3-C4-C5	2.50	113.67	109.77
5	F	2	NAG	O7-C7-N2	-2.40	117.54	121.95
4	Ε	2	NAG	O4-C4-C3	-2.35	104.91	110.35
4	Е	6	FUL	O5-C1-C2	-2.32	107.19	110.77
4	Е	7	FUL	O5-C5-C6	2.28	112.23	107.33
5	F	1	NAG	O7-C7-N2	-2.27	117.77	121.95
5	F	4	FUL	C1-O5-C5	-2.26	107.65	112.78
6	G	2	FUC	C3-C4-C5	2.23	113.25	109.77
5	F	2	NAG	O5-C5-C6	-2.22	103.72	107.20
5	F	1	NAG	O5-C5-C4	2.22	116.23	110.83
4	Ε	6	FUL	C1-O5-C5	-2.20	107.78	112.78
6	G	1	NAG	C1-O5-C5	-2.19	109.22	112.19
6	G	1	NAG	O3-C3-C4	2.18	115.39	110.35
4	Ε	1	NAG	O5-C1-C2	-2.18	107.85	111.29
5	F	2	NAG	C1-O5-C5	2.18	115.14	112.19
4	Ε	5	MAN	O2-C2-C1	2.15	113.56	109.15
4	Е	5	MAN	C3-C4-C5	2.15	114.07	110.24
4	Ε	1	NAG	O4-C4-C3	2.13	115.28	110.35
5	F	3	BMA	C1-C2-C3	2.11	112.26	109.67
4	Ε	6	FUL	O2-C2-C3	2.08	114.31	110.14
5	F	1	NAG	O6-C6-C5	-2.01	104.41	111.29

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Ε	1	NAG	C8-C7-N2-C2
4	Е	1	NAG	O7-C7-N2-C2
4	Е	3	BMA	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
4	Ε	3	BMA	C4-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
6	G	1	NAG	C4-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	F	1	NAG	C1-C2-N2-C7
4	Е	2	NAG	C4-C5-C6-O6
5	F	3	BMA	C4-C5-C6-O6
4	Е	2	NAG	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6



5

5

Continued from previous page									
\mathbf{Mol}	Mol Chain Res Type Atoms								
5	F	2	NAG	C1-C2-N2-C7					

1

2

There are no ring outliers.

F

F

9 monomers are involved in 52 short contacts:

NAG

NAG

C3-C2-N2-C7

C3-C2-N2-C7

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	4	FUL	10	0
4	Ε	3	BMA	2	0
5	F	1	NAG	26	0
4	Е	1	NAG	4	0
4	Ε	5	MAN	3	0
5	F	5	FUL	5	0
6	G	1	NAG	10	0
4	Е	7	FUL	2	0
5	F	2	NAG	17	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)

4 ligands 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	Tune	Chain	Bos	5 Link	Bond lengths			Bond angles		
	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	D	410	-	$5,\!5,\!5$	0.35	0	5, 5, 5	0.41	0
7	NAG	С	408	1	14, 14, 15	0.72	1 (7%)	$17,\!19,\!21$	1.74	3 (17%)
7	NAG	D	409	-	14,14,15	0.70	0	17,19,21	1.67	2 (11%)
8	GOL	Н	301	-	$5,\!5,\!5$	0.45	0	5, 5, 5	0.61	0



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	D	410	-	-	4/4/4/4	-
7	NAG	С	408	1	-	1/6/23/26	0/1/1/1
7	NAG	D	409	-	-	2/6/23/26	0/1/1/1
8	GOL	Н	301	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
7	С	408	NAG	C1-C2	2.16	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	D	409	NAG	O5-C1-C2	-5.45	102.68	111.29
7	С	408	NAG	O5-C1-C2	-3.58	105.63	111.29
7	С	408	NAG	C1-O5-C5	3.15	116.46	112.19
7	D	409	NAG	C3-C4-C5	2.79	115.22	110.24
7	С	408	NAG	C3-C4-C5	-2.79	105.27	110.24

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	410	GOL	O1-C1-C2-C3
8	Н	301	GOL	O1-C1-C2-C3
8	Н	301	GOL	C1-C2-C3-O3
7	D	409	NAG	C8-C7-N2-C2
7	D	409	NAG	O7-C7-N2-C2
8	Н	301	GOL	O1-C1-C2-O2
8	D	410	GOL	C1-C2-C3-O3
8	D	410	GOL	O1-C1-C2-O2
8	Н	301	GOL	O2-C2-C3-O3
8	D	410	GOL	O2-C2-C3-O3
7	С	408	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 6 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	410	GOL	1	0
7	С	408	NAG	2	0
7	D	409	NAG	2	0
8	Н	301	GOL	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	<RSRZ $>$	#RSRZ $>$ 2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	$Q{<}0.9$
1	С	250/287~(87%)	0.58	27 (10%) 5 3	21, 38, 93, 116	0
1	D	251/287~(87%)	0.58	27 (10%) 5 3	29, 57, 96, 113	0
2	А	214/221~(96%)	0.19	4 (1%) 66 59	32, 50, 78, 94	0
2	Н	215/221~(97%)	-0.11	1 (0%) 91 88	22, 38, 59, 77	0
3	В	219/220~(99%)	0.22	8 (3%) 41 31	23, 45, 90, 102	0
3	L	219/220~(99%)	0.01	1 (0%) 91 88	22, 42, 67, 87	0
All	All	1368/1456~(93%)	0.26	68 (4%) 28 19	21, 45, 87, 116	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	214	ALA	5.8
1	С	251	GLU	5.3
1	D	268	THR	5.1
1	С	250	THR	5.0
1	D	239	LEU	4.9
1	D	290	PHE	4.8
1	С	239	LEU	4.7
3	В	215	PHE	4.7
1	С	214	ALA	4.7
1	D	267	TYR	4.5
1	D	269	VAL	4.3
1	С	222	PHE	4.3
1	С	249	ILE	4.3
1	D	288	GLN	4.2
1	С	269	VAL	4.1
3	В	198	TYR	4.0
1	С	252	GLN	4.0
3	В	160	LEU	3.9
1	D	289	ARG	3.6



Continued from previous page										
Mol	Chain	Res	Type	RSRZ						
1	D	241	ILE	3.6						
1	С	270	GLN	3.5						
1	D	223	MET	3.5						
1	D	261	LEU	3.4						
1	С	212	MET	3.4						
1	D	221	SER	3.3						
1	D	63	VAL	3.3						
3	В	200	CYS	3.2						
1	D	212	MET	3.2						
1	С	254	ARG	3.1						
1	С	215	LYS	3.1						
1	D	43	LEU	3.1						
1	D	64	ASN	3.1						
1	D	27	ILE	3.0						
1	С	248	VAL	3.0						
1	D	255	ASP	3.0						
3	В	197	VAL	3.0						
1	С	223	MET	2.9						
1	С	240	GLN	2.9						
1	С	221	SER	2.9						
1	С	258	SER	2.8						
1	С	225	TRP	2.7						
1	С	260	GLN	2.7						
1	С	253	VAL	2.6						
1	С	271	ILE	2.5						
2	А	72	ALA	2.5						
1	D	41	TRP	2.5						
1	С	48	THR	2.5						
1	С	288	GLN	2.5						
1	D	47	VAL	2.4						
1	С	261	LEU	2.4						
1	С	238	GLU	2.4						
1	D	242	GLN	2.4						
2	Н	27	TYR	2.3						
1	D	48	THR	2.3						
1	С	241	ILE	2.3						
3	В	152	VAL	2.3						
1	D	30	LEU	2.3						
1	D	222	PHE	2.3						
3	L	53	LEU	2.3						
3	В	155	LYS	2.2						
2	А	196	LEU	2.2						



Mol	Chain Res		Type	RSRZ
2	А	27	TYR	2.2
2	А	101	LEU	2.1
1	D	98	GLU	2.1
1	С	259	PHE	2.1
1	D	254	ARG	2.1
3	В	192	TYR	2.1
1	D	104	TRP	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
5	NAG	F	1	14/15	0.58	0.23	70,70,71,71	0
5	FUL	F	5	10/11	0.72	0.30	57, 58, 58, 58	0
5	BMA	F	3	11/12	0.75	0.18	$91,\!103,\!107,\!109$	0
5	FUL	F	4	10/11	0.76	0.30	20,20,20,20	0
4	MAN	Е	4	11/12	0.77	0.20	108,116,121,121	0
5	NAG	F	2	14/15	0.81	0.22	27,29,30,30	0
4	FUL	Е	6	10/11	0.82	0.26	79,95,101,104	0
6	FUC	G	2	10/11	0.84	0.28	112,122,131,133	0
6	NAG	G	1	14/15	0.86	0.18	88,94,103,116	0
4	NAG	Е	1	14/15	0.88	0.17	46,47,48,48	0
4	BMA	Е	3	11/12	0.89	0.14	$85,\!93,\!105,\!108$	0
4	MAN	Е	5	11/12	0.90	0.18	83,94,96,101	0
6	FUL	G	3	10/11	0.92	0.18	104,112,116,119	0
4	FUL	Е	7	10/11	0.92	0.35	62,70,79,84	0
4	NAG	E	2	14/15	0.94	0.20	60,69,74,82	0

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





6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B}$ -factors(${ m \AA}^2$)	Q<0.9
7	NAG	С	408	14/15	0.74	0.22	$105,\!120,\!134,\!135$	0
8	GOL	Н	301	6/6	0.76	0.50	47,47,47,47	0
8	GOL	D	410	6/6	0.79	0.25	83,83,83,83	0
7	NAG	D	409	14/15	0.90	0.20	81,81,81,81	0

6.5 Other polymers (i)

There are no such residues in this entry.

