

Full wwPDB X-ray Structure Validation Report (i)

Apr 22, 2024 – 01:34 PM EDT

:	8TZU
:	OC43 S1b domain in complex with WNb 293 and WNb 317
:	Pymm, P.; Feng, J.; Tham, W.H.
:	2023-08-27
:	2.90 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	:	2.36.2
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)	:	2.36.2

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 2.90 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.



Motria	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	А	275	86%	8% 6%
1	В	275	91%	7% •
1	F	275	89%	7% •
2	С	121	98%	
2	G	121	% 	11% •



Mol	Chain	Length	Quality of chain		
2	Н	121	2% 	11%	
3	D	128	5% 	11%	·
3	Е	128	97%		•
4	Κ	2	50% 50%		
4	L	2	100%		
4	Ν	2	100%		
5	Ι	4	75%	25%	
6	J	3	67% 33	3%	_

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
6	NAG	J	2	-	-	-	Х
7	GOL	А	702	-	-	-	Х



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10985 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1 A	258	Total	С	Ν	0	S	0	0	0	
		1974	1241	339	375	19	0	0		
1	1 B	269	Total	С	Ν	0	S	0	0	0
1			2059	1295	351	390	23			
1	1 F	962	Total	С	Ν	0	S	0	0	0
	205	2012	1266	342	381	23	0	0	U	

• Molecule 1 is a protein called Spike protein S1.

• Molecule 2 is a protein called WNb 317.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2 C	120	Total	С	Ν	0	S	0	0	0	
		913	571	159	179	4	0	0	0	
0	<u>р</u> С	190	Total	С	Ν	0	\mathbf{S}	0	0	0
	G	120	913	571	159	179	4			0
0	9 II	190	Total	С	Ν	0	S	0	0	0
	120	913	571	159	179	4	0		0	

• Molecule 3 is a protein called WNb 293.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	2 D	197	Total	С	Ν	0	S	0	0	0
3 D	121	965	605	167	190	3	0	0	0	
9	Б	199	Total	С	Ν	0	S	0	0	0
o E	128	974	611	169	191	3	0	0	0	

• Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf	Trace
4	L	2	Total 28	C 16	N 2	O 10	0	0	0
4	Ν	2	Total 28	C 16	N 2	0 10	0	0	0
4	К	2	Total 28	C 16	N 2	O 10	0	0	0

• Molecule 5 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	I	Aton	ns		ZeroOcc	AltConf	Trace
5	Ι	4	Total 49	C 28	N 2	O 19	0	0	0

• Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[al pha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf	Trace
6	J	3	Total 38	C 22	N 2	O 14	0	0	0

• Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	17	Total O 17 17	0	0
8	В	18	Total O 18 18	0	0
8	С	5	Total O 5 5	0	0
8	D	7	Total O 7 7	0	0
8	Е	5	$\begin{array}{cc} \text{Total} & \text{O} \\ 5 & 5 \end{array}$	0	0
8	F	10	Total O 10 10	0	0
8	Н	5	$\begin{array}{cc} \text{Total} & \text{O} \\ 5 & 5 \end{array}$	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: Spike protein S1





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

α	•	т
(Ch	am	1.
011	am	ш.

100%

NAG 1 NAG 2

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain N:

100%

NAG1 NAG2

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



50%

Chain K:

NAG 1 NAG 2

 $\bullet \ {\rm Molecule \ 5: \ beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alp ha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose}$

Chain I:	75%	25%
NAG1 NAG2 BMA3 FUC4		

50%

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

Chain J:	67%	33%
NAG2 FUC3		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	98.91Å 150.61Å 155.11Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	49.46 - 2.90	Depositor
Resolution (A)	49.46 - 2.90	EDS
% Data completeness	$100.0 \ (49.46-2.90)$	Depositor
(in resolution range)	$100.0 \ (49.46-2.90)$	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.45 (at 2.91 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
D D.	0.227 , 0.266	Depositor
Π, Π_{free}	0.224 , 0.262	DCC
R_{free} test set	2621 reflections (5.04%)	wwPDB-VP
Wilson B-factor $(Å^2)$	78.8	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 50.5	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10985	wwPDB-VP
Average B, all atoms $(Å^2)$	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.12% 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, NAG, BMA, FUC

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	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.26	0/2022	0.47	0/2746
1	В	0.26	0/2110	0.46	0/2867
1	F	0.26	0/2060	0.48	0/2797
2	С	0.26	0/932	0.51	0/1262
2	G	0.25	0/932	0.51	0/1262
2	Н	0.25	0/932	0.52	0/1262
3	D	0.26	0/990	0.51	0/1344
3	Е	0.25	0/999	0.51	0/1355
All	All	0.26	0/10977	0.49	0/14895

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	1974	0	1860	10	0
1	В	2059	0	1952	10	0
1	F	2012	0	1904	9	0
2	С	913	0	873	2	0
2	G	913	0	873	7	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Н	913	0	870	8	0
3	D	965	0	894	8	0
3	Е	974	0	907	2	0
4	K	28	0	25	1	0
4	L	28	0	25	0	0
4	Ν	28	0	25	0	0
5	Ι	49	0	43	0	0
6	J	38	0	34	1	0
7	А	12	0	16	0	0
7	С	12	0	16	0	0
8	А	17	0	0	0	0
8	В	18	0	0	0	0
8	С	5	0	0	0	0
8	D	7	0	0	0	0
8	Е	5	0	0	0	0
8	F	10	0	0	1	0
8	Н	5	0	0	0	0
All	All	10985	0	10317	55	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 3.

All (55) 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)
3:D:91:THR:HG23	3:D:123:THR:HA	1.74	0.69
2:G:67:ARG:NH2	2:G:90:ASP:OD2	2.29	0.66
1:F:526:ASN:ND2	8:F:701:HOH:O	2.31	0.62
2:G:91:THR:HG23	2:G:117:THR:HA	1.80	0.62
1:B:580:GLN:HB3	2:C:106:PRO:HG3	1.81	0.62
3:E:91:THR:HG23	3:E:123:THR:HA	1.81	0.61
4:K:1:NAG:H83	4:K:1:NAG:H3	1.86	0.57
1:F:475:ARG:NH2	2:H:60:TYR:O	2.37	0.57
6:J:1:NAG:H3	6:J:1:NAG:H83	1.88	0.54
1:F:393:LYS:NZ	1:F:395:TYR:OH	2.37	0.53
1:B:400:SER:HA	1:B:610:GLY:HA3	1.91	0.52
3:D:52:SER:O	3:D:72:ARG:NH1	2.41	0.52
2:G:39:GLN:HB2	2:G:45:ARG:HG2	1.92	0.52
2:H:93:VAL:HG22	2:H:115:GLN:HG2	1.92	0.52
2:G:89:GLU:OE1	2:G:89:GLU:N	2.41	0.51
2:G:40:ALA:HB3	2:G:43:LYS:HE3	1.93	0.51



	lo de pagem	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:500:PRO:HA	1:B:528:LEU:HD12	1.92	0.50	
1:A:403:THR:OG1	1:A:603:ILE:HB	2.13	0.48	
1:B:400:SER:HB3	1:B:606:ASP:HB2	1.96	0.48	
3:E:22:CYS:HB3	3:E:79:VAL:HG13	1.96	0.48	
1:A:365:PHE:HB2	1:A:402:ILE:HB	1.96	0.47	
3:D:6:GLU:OE1	3:D:6:GLU:N	2.45	0.47	
3:D:22:CYS:HB3	3:D:79:VAL:HG13	1.96	0.47	
1:A:409:ILE:HD11	1:A:599:PHE:HB2	1.97	0.47	
1:B:607:VAL:HG22	1:B:608:ASN:HD22	1.80	0.47	
1:A:504:ASN:HD22	1:A:518:ILE:HG21	1.80	0.47	
3:D:40:ALA:HB1	3:D:41:PRO:HD2	1.96	0.46	
1:B:399:PHE:HE1	1:B:607:VAL:HG23	1.81	0.46	
1:A:503:LEU:HB3	1:A:506:SER:HB3	1.96	0.46	
2:G:12:VAL:HG11	2:G:86:LEU:HD13	1.97	0.46	
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.48	0.46	
1:B:409:ILE:HD11	1:B:599:PHE:HB2	1.99	0.45	
1:B:465:GLY:HA3	1:B:576:THR:HG23	1.98	0.45	
3:D:12:VAL:HG12	1:F:383:SER:HB2	1.98	0.45	
2:H:18:LEU:HD12	2:H:19:ARG:H	1.81	0.45	
2:H:12:VAL:HG11	2:H:86:LEU:HD13	1.99	0.44	
3:D:97:ALA:HB2	3:D:116:TRP:CZ3	2.53	0.44	
1:A:350:ASN:HA	1:A:445:LEU:HD11	2.00	0.44	
2:H:18:LEU:HD12	2:H:19:ARG:N	2.31	0.44	
2:G:27:ARG:HG2	2:G:28:THR:HG23	2.00	0.44	
1:B:365:PHE:CE1	1:B:404:ILE:HD12	2.53	0.43	
2:C:65:LYS:HB2	2:C:65:LYS:HE3	1.75	0.43	
1:F:452:VAL:HG11	1:F:485:VAL:HG22	1.99	0.43	
3:D:126:SER:O	3:D:127:HIS:ND1	2.52	0.43	
1:A:346:GLU:OE1	1:A:346:GLU:N	2.44	0.42	
1:A:573:ASN:HA	1:A:574:SER:HA	1.75	0.42	
1:F:563:LEU:HD21	1:F:585:TRP:HB3	2.02	0.42	
2:H:33:ALA:HB2	2:H:53:TRP:HE3	1.84	0.42	
1:B:455:PHE:HA	1:B:468:GLU:HG2	2.01	0.42	
1:F:416:ASP:O	1:F:426:GLN:HG3	2.20	0.42	
1:A:421:ASN:OD1	1:A:422:LEU:N	2.53	0.41	
1:F:393:LYS:HD3	1:F:393:LYS:HA	1.90	0.41	
1:A:389:ILE:HB	1:A:437:THR:HG23	2.03	0.41	
1:F:428:PHE:HB3	1:F:491:CYS:SG	2.60	0.41	
2:H:94:TYR:O	2:H:113:GLY:HA2	2.20	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	Percentiles
1	А	252/275~(92%)	244 (97%)	8 (3%)	0	100 100
1	В	265/275~(96%)	255~(96%)	9~(3%)	1 (0%)	34 66
1	F	255/275~(93%)	240 (94%)	15 (6%)	0	100 100
2	С	118/121~(98%)	114 (97%)	4(3%)	0	100 100
2	G	118/121~(98%)	113 (96%)	5 (4%)	0	100 100
2	Н	118/121~(98%)	115~(98%)	3~(2%)	0	100 100
3	D	125/128~(98%)	123 (98%)	2(2%)	0	100 100
3	E	126/128~(98%)	122 (97%)	4 (3%)	0	100 100
All	All	1377/1444~(95%)	1326 (96%)	50 (4%)	1 (0%)	51 82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	606	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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	222/237~(94%)	219~(99%)	3~(1%)	67	89	
1	В	233/237~(98%)	230~(99%)	3 (1%)	69	90	
1	F	228/237~(96%)	223~(98%)	5 (2%)	52	81	
2	С	95/97~(98%)	95 (100%)	0	100	100	



Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
2	G	95/97~(98%)	95~(100%)	0	100	100	
2	Н	95/97~(98%)	95 (100%)	0	100	100	
3	D	98/101~(97%)	98 (100%)	0	100	100	
3	Ε	99/101~(98%)	99 (100%)	0	100	100	
All	All	1165/1204~(97%)	1154 (99%)	11 (1%)	78	93	

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	454	ARG
1	А	535	THR
1	А	604	LEU
1	В	485	VAL
1	В	508	VAL
1	В	602	PHE
1	F	380	GLN
1	F	410	PRO
1	F	453	SER
1	F	575	CYS
1	F	588	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	608	ASN
3	D	82	GLN
1	F	418	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)

13 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	Tuno	Chain	Dog	Link	Bo	ond leng	\mathbf{ths}	Bond angles		
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
5	NAG	Ι	1	1,5	14,14,15	0.24	0	17,19,21	0.55	0
5	NAG	Ι	2	5	14,14,15	0.26	0	17,19,21	0.49	0
5	BMA	I	3	5	11,11,12	0.61	0	$15,\!15,\!17$	0.92	1 (6%)
5	FUC	Ι	4	5	10,10,11	0.74	0	14,14,16	0.92	0
6	NAG	J	1	1,6	14,14,15	0.45	0	17,19,21	1.28	2 (11%)
6	NAG	J	2	6	14,14,15	0.29	0	17,19,21	0.45	0
6	FUC	J	3	6	10,10,11	0.75	0	14,14,16	0.73	0
4	NAG	K	1	1,4	14,14,15	0.42	0	17,19,21	1.22	1 (5%)
4	NAG	K	2	4	14,14,15	0.27	0	17,19,21	0.50	0
4	NAG	L	1	1,4	14,14,15	0.24	0	17,19,21	0.46	0
4	NAG	L	2	4	14,14,15	0.25	0	17,19,21	0.42	0
4	NAG	N	1	1,4	14,14,15	0.23	0	17,19,21	0.51	0
4	NAG	N	2	4	14,14,15	0.23	0	17,19,21	0.44	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
5	NAG	Ι	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Ι	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Ι	3	5	-	0/2/19/22	0/1/1/1
5	FUC	Ι	4	5	-	-	0/1/1/1
6	NAG	J	1	1,6	-	5/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	FUC	J	3	6	-	-	0/1/1/1
4	NAG	К	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	K	2	4	-	1/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1



001000	e entrada ji ente precesa e pagem											
Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings					
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1					
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1					
4	NAG	Ν	2	4	-	2/6/23/26	0/1/1/1					

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	J	1	NAG	C2-N2-C7	4.29	129.01	122.90
4	Κ	1	NAG	C2-N2-C7	4.18	128.85	122.90
6	J	1	NAG	C1-C2-N2	2.15	114.17	110.49
5	Ι	3	BMA	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	1	NAG	C8-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
4	Ν	2	NAG	C8-C7-N2-C2
4	Ν	2	NAG	O7-C7-N2-C2
4	Κ	1	NAG	C8-C7-N2-C2
4	Κ	1	NAG	O7-C7-N2-C2
6	J	1	NAG	C8-C7-N2-C2
6	J	1	NAG	O7-C7-N2-C2
6	J	1	NAG	C4-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
4	Κ	2	NAG	O5-C5-C6-O6
4	Κ	1	NAG	C3-C2-N2-C7
6	J	1	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	NAG	1	0
6	J	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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).

Mol Typ	Turne	Chain	Ros	Dog Link	Bond lengths			Bond angles		
	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	А	702	-	$5,\!5,\!5$	0.91	0	$5,\!5,\!5$	1.12	0
7	GOL	С	202	-	$5,\!5,\!5$	0.92	0	$5,\!5,\!5$	0.97	0
7	GOL	А	701	-	$5,\!5,\!5$	0.71	0	$5,\!5,\!5$	1.07	0



Mol	Tuno	Chain	Dog	Link	B	Bond lengths		E	Bond angles		
	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts RM	RMSZ	# Z > 2	
7	GOL	С	201	-	$5,\!5,\!5$	0.92	0	$5,\!5,\!5$	0.98	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
7	GOL	А	702	-	-	0/4/4/4	-
7	GOL	С	202	-	-	0/4/4/4	-
7	GOL	А	701	-	-	0/4/4/4	-
7	GOL	С	201	-	-	0/4/4/4	-

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></rsrz>	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	258/275~(93%)	0.38	16 (6%) 20 16	51, 72, 137, 184	0
1	В	269/275~(97%)	0.27	18 (6%) 17 13	49, 70, 140, 174	0
1	F	263/275~(95%)	0.88	47 (17%) 1 1	69, 100, 164, 195	0
2	С	120/121~(99%)	0.09	0 100 100	47, 73, 99, 144	0
2	G	120/121 (99%)	0.29	1 (0%) 86 86	56, 87, 112, 138	0
2	Н	120/121 (99%)	0.18	2 (1%) 70 69	58, 70, 94, 134	0
3	D	127/128~(99%)	0.35	6 (4%) 31 28	61, 87, 130, 153	0
3	Е	128/128~(100%)	0.32	7 (5%) 25 21	50, 75, 111, 150	0
All	All	1405/1444 (97%)	0.39	97 (6%) 16 13	47, 79, 140, 195	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	611	LEU	8.6
1	F	340	LEU	6.7
1	В	398	CYS	6.4
1	А	373	SER	6.1
1	F	497	ASN	6.0
1	F	341	PRO	5.5
1	А	370	PHE	5.4
1	В	611	LEU	5.4
1	А	378	PHE	5.2
1	А	377	SER	5.1
1	F	401	SER	5.0
1	А	374	SER	4.8
1	F	518	ILE	4.7
1	F	502	LYS	4.6
1	F	342	ASN	4.4
1	F	369	ASN	4.3



Mol	Chain	Res	Type	RSRZ
1	F	527	TYR	4.2
1	А	381	ALA	4.1
1	F	505	GLY	4.0
1	F	613	CYS	3.9
1	F	528	LEU	3.9
1	В	342	ASN	3.9
1	F	365	PHE	3.8
1	F	574	SER	3.7
1	F	605	HIS	3.7
1	F	498	PHE	3.6
1	F	519	GLY	3.6
3	Е	68	PHE	3.5
1	A	371	ASN	3.5
1	F	370	PHE	3.5
1	В	369	ASN	3.5
1	А	382	ASP	3.5
1	F	571	GLY	3.4
1	F	503	LEU	3.3
1	F	507	CYS	3.3
1	А	402	ILE	3.2
1	F	520	THR	3.2
3	D	117	GLY	3.1
1	А	379	ILE	3.1
1	В	341	PRO	3.1
1	В	367	ASN	3.1
3	Е	84	ASN	3.0
3	D	118	GLN	3.0
1	В	613	CYS	3.0
3	Е	13	GLN	2.9
1	F	516	ASN	2.9
3	Е	86	LEU	2.9
3	Е	20	LEU	2.8
1	F	402	ILE	2.8
1	В	610	GLY	2.8
1	В	609	SER	2.8
1	F	344	ASN	2.7
1	A	372	MET	2.7
2	G	10	GLY	2.7
1	F	399	PHE	2.7
1	F	367	ASN	2.6
1	F	407	PHE	2.6
1	F	533	LEU	2.6



Mol	Chain	Res	Type	RSRZ
1	F	554	VAL	2.6
1	А	375	LEU	2.5
1	F	501	CYS	2.5
1	В	380	GLN	2.5
1	F	504	ASN	2.5
3	D	1	GLN	2.5
1	F	360	TRP	2.5
2	Н	2	VAL	2.4
1	F	366	SER	2.4
1	F	345	ILE	2.4
1	В	377	SER	2.3
1	В	543	GLY	2.3
1	F	396	GLY	2.3
1	А	401	SER	2.2
1	F	362	ARG	2.2
3	Е	14	ALA	2.2
1	F	464	PHE	2.2
1	В	370	PHE	2.2
1	А	383	SER	2.2
1	F	368	CYS	2.2
1	F	517	GLY	2.2
1	А	515	ASN	2.2
1	В	368	CYS	2.2
3	D	4	LEU	2.2
1	F	614	SER	2.2
1	В	399	PHE	2.1
3	D	29	PHE	2.1
1	А	608	ASN	2.1
3	D	74	ASN	2.1
1	В	402	ILE	2.1
1	F	343	CYS	2.1
1	F	398	CYS	2.1
1	F	525	THR	2.1
1	F	500	PRO	2.1
1	В	515	ASN	2.0
3	Е	18	LEU	2.0
1	F	599	PHE	2.0
1	В	612	THR	2.0
2	Н	28	THR	2.0

Continued from previous page...



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	$B-factors(A^2)$	Q<0.9
4	NAG	K	2	14/15	0.68	0.23	162,173,179,183	0
4	NAG	N	2	14/15	0.69	0.30	132,158,169,172	0
5	BMA	Ι	3	11/12	0.69	0.38	135,159,169,174	0
6	NAG	J	2	14/15	0.69	0.47	151,177,182,182	0
6	NAG	J	1	14/15	0.70	0.27	140,166,177,180	0
4	NAG	N	1	14/15	0.74	0.18	91,126,144,161	0
4	NAG	K	1	14/15	0.78	0.18	136,149,159,162	0
4	NAG	L	1	14/15	0.79	0.18	129,144,157,171	0
4	NAG	L	2	14/15	0.82	0.23	139,168,174,175	0
6	FUC	J	3	10/11	0.85	0.48	171,182,190,191	0
5	NAG	Ι	2	14/15	0.86	0.33	114,130,144,147	0
5	FUC	Ι	4	10/11	0.87	0.49	114,136,143,145	0
5	NAG	Ι	1	14/15	0.89	0.23	68,98,122,123	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
7	GOL	А	702	6/6	0.49	0.69	73,99,116,119	0
7	GOL	А	701	6/6	0.70	0.22	98,102,122,122	0
7	GOL	С	202	6/6	0.84	0.21	79,96,100,103	0
7	GOL	С	201	6/6	0.89	0.20	60,74,92,99	0

6.5 Other polymers (i)

There are no such residues in this entry.

