

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID : 6QWN	
Title : Protein peptide complex	
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Deposited on : 2019-03-05	
Resolution : $3.89 \text{ Å}(\text{reported})$	

This is a wwPDB X-ray Structure Validation Summary 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	:	1.8.4, 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 3.89 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.



Motric	Whole archive	Similar resolution		
WIEUTIC	$(\# {\it Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R _{free}	130704	$1002 \ (4.14-3.66)$		
Clashscore	141614	1004 (4.12-3.68)		
Ramachandran outliers	138981	1021 (4.14-3.66)		
Sidechain outliers	138945	1014 (4.14-3.66)		
RSRZ outliers	127900	1275 (4.20-3.60)		

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	of chain	
			2%		
1	А	379	63%	25%	• 12%
	_		5%		
1	В	379	63%	26%	11%
			7%		
1	С	379	62%	27%	11%
			3%		
1	D	379	63%	26%	• 11%
			16%		
1	Ε	379	59%	26%	15%

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Mol	Chain	Length	Quality of ch	ain	
2	F	56	64%	20%	16%
2	G	56	2% 68%	16%	16%
2	Н	56	59%	25%	16%
2	Ι	56	57%	27%	16%
2	J	56	55%	29%	16%
3	K	4	75%		25%
4	L	2	100%		
5	М	3	100%		
6	Ν	2	50%	50%	
7	Ο	3	100%		

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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
3	MAN	Κ	4	-	-	-	Х
4	NAG	L	2	-	-	-	Х



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2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15070 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		Atoms					AltConf	Trace
1	Δ	225	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	A	ეეე	2585	1649	429	493	14	0	0	0
1	В	338	Total	С	Ν	Ο	S	0	0	0
1	D	000	2601	1659	432	496	14	0	0	0
1	С	338	Total	С	Ν	Ο	S	0	0	0
1		000	2612	1667	432	500	13	0	0	0
1	Л	336	Total	С	Ν	Ο	S	0	0	0
1	D	550	2589	1653	430	493	13	0	0	0
1	F	300	Total	С	Ν	Ο	S	0	0	0
		522	2489	1590	414	472	13	0	U	

• Molecule 1 is a protein called Pollen-specific leucine-rich repeat extensin-like protein 1.

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	29	MET	-	initiating methionine	UNP Q9LJ64
А	30	GLU	-	expression tag	UNP Q9LJ64
А	401	LEU	-	expression tag	UNP Q9LJ64
А	402	GLU	-	expression tag	UNP Q9LJ64
А	403	GLY	-	expression tag	UNP Q9LJ64
А	404	SER	-	expression tag	UNP Q9LJ64
А	405	GLU	-	expression tag	UNP Q9LJ64
А	406	ASN	-	expression tag	UNP Q9LJ64
А	407	LEU	-	expression tag	UNP Q9LJ64
В	29	MET	-	initiating methionine	UNP Q9LJ64
В	30	GLU	-	expression tag	UNP Q9LJ64
В	401	LEU	-	expression tag	UNP Q9LJ64
В	402	GLU	-	expression tag	UNP Q9LJ64
В	403	GLY	-	expression tag	UNP Q9LJ64
В	404	SER	-	expression tag	UNP Q9LJ64
В	405	GLU	-	expression tag	UNP Q9LJ64
В	406	ASN	-	expression tag	UNP Q9LJ64
В	407	LEU	-	expression tag	UNP Q9LJ64
С	29	MET	-	initiating methionine	UNP Q9LJ64

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Chain	Residue	Modelled	Actual Comment		Reference
С	30	GLU	-	expression tag	UNP Q9LJ64
С	401	LEU	-	expression tag	UNP Q9LJ64
С	402	GLU	-	expression tag	UNP Q9LJ64
С	403	GLY	-	expression tag	UNP Q9LJ64
С	404	SER	-	expression tag	UNP Q9LJ64
С	405	GLU	-	expression tag	UNP Q9LJ64
С	406	ASN	-	expression tag	UNP Q9LJ64
С	407	LEU	-	expression tag	UNP Q9LJ64
D	29	MET	-	initiating methionine	UNP Q9LJ64
D	30	GLU	-	expression tag	UNP Q9LJ64
D	401	LEU	-	expression tag	UNP Q9LJ64
D	402	GLU	-	expression tag	UNP Q9LJ64
D	403	GLY	-	expression tag	UNP Q9LJ64
D	404	SER	-	expression tag	UNP Q9LJ64
D	405	GLU	-	expression tag	UNP Q9LJ64
D	406	ASN	-	expression tag	UNP Q9LJ64
D	407	LEU	-	expression tag	UNP Q9LJ64
Е	29	MET	-	initiating methionine	UNP Q9LJ64
E	30	GLU	-	expression tag	UNP Q9LJ64
Е	401	LEU	-	expression tag	UNP Q9LJ64
Е	402	GLU	-	expression tag	UNP Q9LJ64
E	403	GLY	-	expression tag	UNP Q9LJ64
Е	404	SER	-	expression tag	UNP Q9LJ64
Е	405	GLU	-	expression tag	UNP Q9LJ64
Е	406	ASN	-	expression tag	UNP Q9LJ64
E	407	LEU	-	expression tag	UNP Q9LJ64

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• Molecule 2 is a protein called Protein RALF-like 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	47	Total	С	Ν	0	S	0	0	0
	T,	41	403	244	90	65	4	0	0	0
2	C	47	Total	С	Ν	Ο	S	0	0	0
2	G	41	403	244	90	65	4	0	0	0
2	п	47	Total	С	Ν	Ο	\mathbf{S}	0	0	0
2	11	41	403	244	90	65	4			0
0	т	47	Total	С	Ν	0	S	0	0	0
	41	403	244	90	65	4	0	0	0	
0	9 I	J 47	Total	С	Ν	Ο	S	0	0	0
	J		356	219	70	63	4	U	U	U

There are 10 discrepancies between the modelled and reference sequences:



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U V	

Chain	Residue	Modelled	Actual	Comment	Reference
F	1052	MET	-	initiating methionine	UNP Q9FZA0
F	1053	GLY	-	expression tag	UNP Q9FZA0
G	1052	MET	-	initiating methionine	UNP Q9FZA0
G	1053	GLY	-	expression tag	UNP Q9FZA0
Н	1052	MET	-	initiating methionine	UNP Q9FZA0
Н	1053	GLY	-	expression tag	UNP Q9FZA0
Ι	1052	MET	-	initiating methionine	UNP Q9FZA0
Ι	1053	GLY	-	expression tag	UNP Q9FZA0
J	1052	MET	-	initiating methionine	UNP Q9FZA0
J	1053	GLY	-	expression tag	UNP Q9FZA0

• Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	4	Total 50	C 28	N 2	O 20	0	0	0

• Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	L	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-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
5	М	3	Total 39	C 22	N 2	O 15	0	0	0

• Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
6	Ν	2	Total 28	C 16	N 2	0 10	0	0	0

• Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	О	3	Total 39	C 22	N 2	O 15	39	0	0

• Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	1	Total C N O 14 8 1 5	0	0
8	D	1	Total C N O 14 8 1 5	0	0
8	D	1	Total C N O 14 8 1 5	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: Pollen-specific leucine-rich repeat extensin-like protein 1

 \bullet Molecule 1: Pollen-specific leucine-rich repeat extensin-like protein 1









 $\bullet \ Molecule \ 3: \ alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose \\ eta-D-glucopyranose \ (1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose \ (1-4)-2-acetamido-2-deoxy-beta-D-glucopyra$

Chain K·	750/	25%
	1370	2570

NAG1 NAG2 BMA3 MAN4

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

100%

100%

NAG1 NAG2

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

VAG1 VAG2 BMA3

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:	50%	50%
MAG1 MAG2		

• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:	100%
Unann U.	100%

NAG1 NAG2 BMA3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	205.84Å 114.09Å 146.98Å	Deperitor
a, b, c, α , β , γ	90.00° 116.25° 90.00°	Depositor
$\mathbf{B}_{\mathrm{ascolution}}\left(\overset{\mathrm{A}}{\mathbf{\lambda}}\right)$	49.44 - 3.89	Depositor
Resolution (A)	49.46 - 3.89	EDS
% Data completeness	99.7(49.44-3.89)	Depositor
(in resolution range)	99.9 (49.46 - 3.89)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	0.46	Depositor
$< I/\sigma(I) > 1$	$1.06 (at 3.88 \text{\AA})$	Xtriage
Refinement program	PHENIX	Depositor
P. P.	0.282 , 0.329	Depositor
Π, Π_{free}	0.285 , 0.333	DCC
R_{free} test set	1409 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	126.7	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 70.7	EDS
L-test for twinning ²	$< L >=0.41, < L^2>=0.24$	Xtriage
	0.038 for $1/2$ *h- $3/2$ *k,- $1/2$ *h- $1/2$ *k,- $1/2$ *h	
Estimated twinning fraction	$+1/2^{*}k$ -l	Xtriage
	$0.048 \text{ for } 1/2^{h}+3/2^{k},1/2^{h}-1/2^{k},-1/2^{h}-1/2^{h}$	0-
E.E. completion	$\frac{1/2^{k-1}}{0.87}$	EDC
$\mathbf{F}_{o}, \mathbf{F}_{c}$ correlation	0.87	
Total number of atoms	15070	wwPDB-VP
Average B, all atoms (A^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.75% 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: BMA, NAG, 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	Bo	ond angles
MIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.26	0/2647	0.49	0/3588
1	В	0.26	0/2665	0.48	1/3614~(0.0%)
1	С	0.26	0/2675	0.49	0/3626
1	D	0.26	0/2652	0.49	0/3595
1	Е	0.26	0/2546	0.50	0/3447
2	F	0.25	0/411	0.46	0/546
2	G	0.25	0/411	0.47	0/546
2	Н	0.32	0/411	0.55	0/546
2	Ι	0.25	0/411	0.46	0/546
2	J	0.26	0/364	0.61	0/492
All	All	0.26	0/15193	0.49	1/20546~(0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	383	LEU	CA-CB-CG	5.77	128.57	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	А	128	ASN	Peptide

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	2585	0	2489	66	0
1	В	2601	0	2503	76	0
1	С	2612	0	2510	78	0
1	D	2589	0	2492	76	0
1	Е	2489	0	2409	69	0
2	F	403	0	400	12	0
2	G	403	0	400	8	0
2	Н	403	0	400	14	0
2	Ι	403	0	400	13	0
2	J	356	0	312	14	0
3	K	50	0	43	0	0
4	L	28	0	25	0	0
5	М	39	0	34	0	0
6	N	28	0	25	0	0
7	0	39	0	34	0	0
8	А	14	0	13	0	0
8	D	28	0	26	1	0
All	All	15070	0	14515	372	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.

The worst 5 of 372 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:ARG:HD3	1:D:374:PRO:HD2	1.59	0.84
1:B:130:ALA:O	1:B:154:ASN:ND2	2.12	0.81
1:C:306:LEU:HD11	1:C:330:ILE:HG12	1.64	0.80
1:E:250:PHE:HB2	1:E:272:ASN:HD21	1.46	0.80
1:D:365:ASP:OD1	1:D:368:ASN:ND2	2.15	0.79



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	\mathbf{ntiles}
1	А	331/379~(87%)	289 (87%)	41 (12%)	1 (0%)	41	75
1	В	336/379~(89%)	301 (90%)	35 (10%)	0	100	100
1	С	334/379~(88%)	299 (90%)	34 (10%)	1 (0%)	41	75
1	D	332/379~(88%)	297 (90%)	33 (10%)	2 (1%)	25	63
1	Е	312/379~(82%)	274 (88%)	37~(12%)	1 (0%)	41	75
2	F	45/56~(80%)	36~(80%)	9 (20%)	0	100	100
2	G	45/56~(80%)	38~(84%)	6~(13%)	1 (2%)	6	38
2	Η	45/56~(80%)	32 (71%)	13 (29%)	0	100	100
2	Ι	45/56~(80%)	35~(78%)	10 (22%)	0	100	100
2	J	45/56~(80%)	36~(80%)	9 (20%)	0	100	100
All	All	1870/2175 (86%)	1637 (88%)	227 (12%)	6 (0%)	41	75

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	247	HIS
1	С	131	ASP
2	G	1092	ASN
1	D	345	PHE
1	Е	188	ALA

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.



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	292/331~(88%)	291 (100%)	1 (0%)	92	95
1	В	294/331~(89%)	293 (100%)	1 (0%)	92	95
1	С	294/331~(89%)	294 (100%)	0	100	100
1	D	292/331~(88%)	289~(99%)	3 (1%)	76	86
1	Е	282/331~(85%)	282 (100%)	0	100	100
2	F	42/48~(88%)	42 (100%)	0	100	100
2	G	42/48~(88%)	42 (100%)	0	100	100
2	Н	42/48~(88%)	41 (98%)	1 (2%)	49	69
2	Ι	42/48~(88%)	41 (98%)	1 (2%)	49	69
2	J	33/48~(69%)	33 (100%)	0	100	100
All	All	1655/1895~(87%)	1648 (100%)	7 (0%)	91	94

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

5 of 7 residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	D	96	ASN
1	D	200	ARG
2	Ι	1089	ARG
1	D	325	PHE
2	Н	1078	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	128	ASN
1	А	263	ASN
1	В	247	HIS
1	Е	70	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)

14 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	$_{\rm ths}$	B	ond ang	les
	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	K	1	1,3	14,14,15	0.30	0	17,19,21	0.57	0
3	NAG	K	2	3	14,14,15	0.28	0	17,19,21	0.67	0
3	BMA	K	3	3	11,11,12	0.62	0	$15,\!15,\!17$	0.87	0
3	MAN	К	4	3	11,11,12	0.65	0	$15,\!15,\!17$	0.99	2 (13%)
4	NAG	L	1	1,4	14,14,15	0.36	0	17,19,21	0.94	1 (5%)
4	NAG	L	2	4	14,14,15	0.34	0	17,19,21	1.18	2 (11%)
5	NAG	М	1	1,5	14,14,15	0.31	0	17,19,21	0.86	1 (5%)
5	NAG	М	2	5	14,14,15	0.33	0	17,19,21	0.85	2 (11%)
5	BMA	М	3	5	11,11,12	0.89	1 (9%)	15,15,17	0.91	1 (6%)
6	NAG	Ν	1	1,6	14,14,15	0.30	0	17,19,21	0.87	1 (5%)
6	NAG	N	2	6	14,14,15	0.27	0	17,19,21	0.62	0
7	NAG	0	1	1,7	14,14,15	0.30	0	17,19,21	0.57	0
7	NAG	0	2	7	14,14,15	0.28	0	17,19,21	0.75	0
7	BMA	0	3	7	11,11,12	0.59	0	15,15,17	0.80	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
3	NAG	К	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
3	MAN	K	4	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	L	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
5	NAG	М	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	М	2	5	-	0/6/23/26	0/1/1/1
5	BMA	М	3	5	-	2/2/19/22	0/1/1/1
6	NAG	Ν	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Ν	2	6	-	2/6/23/26	0/1/1/1
7	NAG	0	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	0	2	7	-	0/6/23/26	0/1/1/1
7	BMA	0	3	7	-	0/2/19/22	0/1/1/1

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All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
5	М	3	BMA	C1-C2	2.33	1.57	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	L	2	NAG	C1-O5-C5	3.05	116.33	112.19
4	L	1	NAG	O3-C3-C2	2.66	114.96	109.47
6	Ν	1	NAG	C1-O5-C5	2.42	115.47	112.19
3	Κ	4	MAN	C1-O5-C5	2.35	115.38	112.19
5	М	2	NAG	O4-C4-C3	-2.28	105.08	110.35

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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























5.6 Ligand geometry (i)

3 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	Turne	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Dec		Bond lengths			Bond angles		
MOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2								
8	NAG	А	501	1	14,14,15	0.28	0	17,19,21	0.64	0								
8	NAG	D	501	1	14,14,15	0.30	0	17,19,21	0.77	0								
8	NAG	D	502	1	14,14,15	0.30	0	17,19,21	0.71	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	NAG	А	501	1	-	4/6/23/26	0/1/1/1
8	NAG	D	501	1	-	2/6/23/26	0/1/1/1
8	NAG	D	502	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	А	501	NAG	C8-C7-N2-C2
8	А	501	NAG	O7-C7-N2-C2
8	D	501	NAG	O7-C7-N2-C2
8	D	501	NAG	C8-C7-N2-C2
8	А	501	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	NAG	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, 95th 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	$OWAB(Å^2)$	Q<0.9
1	А	335/379~(88%)	0.34	8 (2%) 59 48	64, 105, 151, 181	0
1	В	338/379~(89%)	0.42	20 (5%) 22 17	68, 112, 159, 199	0
1	C	338/379~(89%)	0.61	27 (7%) 12 10	63, 122, 179, 200	0
1	D	336/379~(88%)	0.33	11 (3%) 46 36	81, 114, 155, 171	0
1	E	322/379~(84%)	0.97	61 (18%) 1 1	112, 162, 202, 241	0
2	F	47/56~(83%)	0.56	6(12%) 3 4	89, 118, 143, 152	0
2	G	47/56~(83%)	0.37	1 (2%) 63 53	90, 121, 151, 160	0
2	Н	47/56~(83%)	0.22	0 100 100	92, 124, 150, 168	0
2	Ι	47/56~(83%)	0.60	3 (6%) 19 14	98, 136, 163, 181	0
2	J	47/56~(83%)	0.53	3 (6%) 19 14	134, 169, 186, 190	0
All	All	1904/2175~(87%)	0.52	140 (7%) 14 11	63, 122, 183, 241	0

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	348	GLY	6.2
1	С	314	GLN	6.1
1	Е	262	LYS	5.9
1	Е	269	PHE	5.9
2	Ι	1107	ARG	5.4

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)

SUGAR-RSR INFOmissingINFO

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	$B-factors(A^2)$	Q<0.9
8	NAG	D	502	14/15	0.63	0.37	109,138,153,155	0
8	NAG	А	501	14/15	0.70	0.36	133,148,158,162	0
8	NAG	D	501	14/15	0.81	0.32	92,122,128,131	0

6.5 Other polymers (i)

There are no such residues in this entry.

