

wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 10:01 AM EDT

PDB ID	:	7LDJ
Title	:	SARS-CoV-2 receptor binding domain in complex with WNb-2
Authors	:	Pymm, P.; Dietrich, M.H.; Tan, L.L.; Adair, A.; Tham, W.H.
Deposited on	:	2021-01-13
Resolution	:	2.36 Å(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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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)	:	2.35.1

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 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	Δ	100	2%	
	A	199	85%	10% • •
	5	100	3%	
1	В	199	83%	16% ••
			5%	
1	С	199	84%	12% •
			10%	
1	D	199	80%	12% • 8%
			2%	
2	E	131	91%	8% ••

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Contr	nueu fron	i previous	page								
Mol	Chain	Length		Quality of chain							
2	F	131	2%		85%			15%			
			.%								
2	G	131			91%			9%			
0	тт	101	5%								
2	Н	131			86%			13%	•		
3	Ι	4		50%			50%		-		
3	K	4			100%						
	т	0									
4	J	6	17%			83%					

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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	BMA	Ι	3	-	-	-	Х
4	FUL	J	6	-	-	-	Х



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10429 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	В	108	Total	С	Ν	0	S	0	1	0
1	D	198	1567	1004	260	295	8		1	0
1	Δ	102	Total	С	Ν	0	O S O O	0	0	
1	А	195	1520	972	253	287	8	0	0	0
1	С	191	Total	С	Ν	0	S	0	0	0
1			1510	967	252	284	7			0
1	1 D	184	Total	С	Ν	0	S	0	1	0
			1478	948	247	276	$\overline{7}$			

• Molecule 1 is a protein called Spike glycoprotein.

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	528	GLY	-	expression tag	UNP P0DTC2
В	529	SER	-	expression tag	UNP P0DTC2
A	528	GLY	-	expression tag	UNP P0DTC2
А	529	SER	-	expression tag	UNP P0DTC2
С	528	GLY	-	expression tag	UNP P0DTC2
С	529	SER	-	expression tag	UNP P0DTC2
D	528	GLY	-	expression tag	UNP P0DTC2
D	529	SER	-	expression tag	UNP P0DTC2

• Molecule 2 is a protein called Nanobody 2.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9		120	Total	С	Ν	Ο	\mathbf{S}	0	1	0
	Ľ	150	1002	628	171	197	6	0	1	0
9	2 F	120	Total	С	Ν	0	S	0	0	0
		130	987	620	166	195	6	0		
9	С	131	Total	С	Ν	0	S	0	1	0
	Z G		1006	631	171	198	6	0		0
2	2 H	130	Total	С	Ν	Ο	S	0	0	0
			990	622	167	195	6	0	U	U





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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	Ι	4	Total C N O 49 28 2 19	0	0	0
3	K	4	Total C N O 49 28 2 19	0	0	0

• Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alp ha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Aton	ns	ZeroOcc	AltConf	Trace
4	J	6	TotalC7442	N O 3 29	0	0	0

• Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	А	1	Total 11	С 6	O 5	0	0

• Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total 14	C 8	N 1	O 5	0	0

• Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	Е	1	Total 8	${ m C}{5}$	O 3	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf		
8	В	10	Total O	0	0		
0	D	13	19 19	0	0		
8	Δ	10	Total O	0	0		
0	11	15	19 19	0	0		
8	С	31	Total O	0	0		
0	U	51	31 31	0	0		
8	8 D	17	Total O	0	0		
0	D		17 17	0	U		
8	F	10	Total O	0	0		
0	Ľ	Ľ	Ľ		19 19	0	0
8	F	18	Total O	0	0		
0	Ľ	10	18 18	0	0		
8	C	28	Total O	0	0		
0	G	20	28 28	0	0		
8	н	13	Total O	0	0		
0	11	10	13 13		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 glycoprotein





 $\bullet \ Molecule \ 3: \ beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[bet a-L-fucopyranose-(1-6)] 2-acetamido-2-deoxy-beta-D-glucopyranose$

Chain I:	50%	50%
NAG1 NAG2 BMA3 FUL4		

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

Chain K:

100%

NAG1 NAG2 BMA3 FUL4

 $\label{eq:2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose$







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	73.12Å 88.51Å 107.49Å	Deperitor
a, b, c, α , β , γ	90.00° 90.40° 90.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	45.94 - 2.36	Depositor
Resolution (A)	45.94 - 2.36	EDS
% Data completeness	99.9 (45.94-2.36)	Depositor
(in resolution range)	99.9 (45.94 - 2.36)	EDS
R _{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.93 (at 2.37 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
B B.	0.210 , 0.268	Depositor
Space groupCell constantsa, b, c, α , β , γ Resolution (Å)% Data completeness(in resolution range) R_{merge} R_{sym} $< I/\sigma(I) > 1$ Refinement program R, R_{free} R_{free} test setWilson B-factor (Ų)Anisotropyulk solvent $k_{sol}(e/Å^3), B_{sol}(Ų)$ L-test for twinning²Estimated twinning fraction F_o, F_c correlationTotal number of atomsAverage B, all atoms (Ų)	0.216 , 0.273	DCC
R_{free} test set	2750 reflections $(4.87%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	52.4	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.29, 33.8	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10429	wwPDB-VP
Average B, all atoms $(Å^2)$	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.45% 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, FUL, PG4, 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	Bond	angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.31	0/1562	0.47	0/2124
1	В	0.31	0/1609	0.49	0/2189
1	С	0.28	0/1551	0.45	0/2108
1	D	0.33	0/1519	0.49	0/2064
2	Е	0.28	0/1026	0.47	0/1387
2	F	0.30	0/1011	0.47	0/1368
2	G	0.27	0/1031	0.47	0/1395
2	Н	0.28	0/1014	0.47	0/1372
All	All	0.30	0/10323	0.47	0/14007

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	1520	0	1430	17	0
1	В	1567	0	1486	24	0
1	С	1510	0	1425	12	0
1	D	1478	0	1397	17	0
2	Е	1002	0	942	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	987	0	924	9	0
2	G	1006	0	938	7	0
2	Н	990	0	927	15	0
3	Ι	49	0	43	1	0
3	K	49	0	43	6	0
4	J	74	0	64	4	0
5	А	11	0	10	0	0
6	D	14	0	13	1	0
7	Е	8	0	8	2	0
8	А	19	0	0	2	0
8	В	19	0	0	0	0
8	С	31	0	0	0	0
8	D	17	0	0	0	0
8	Ε	19	0	0	0	0
8	F	18	0	0	1	0
8	G	28	0	0	1	0
8	Н	13	0	0	0	0
All	All	10429	0	9650	111	0

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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 6.

The worst 5 of 111 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:517:LEU:HD22	1:D:517:LEU:O	1.48	1.11
1:D:336:CYS:SG	1:D:363:ALA:HB2	2.03	0.97
1:A:393:THR:HB	1:A:516:GLU:HG3	1.65	0.77
1:A:465:GLU:OE2	3:K:4:FUL:H5	1.88	0.73
2:H:84:PRO:HA	2:H:124:VAL:CG2	2.19	0.72

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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	189/199~(95%)	177 (94%)	10 (5%)	2(1%)	14 13
1	В	195/199~(98%)	185~(95%)	10 (5%)	0	100 100
1	С	187/199~(94%)	178 (95%)	9~(5%)	0	100 100
1	D	183/199~(92%)	171 (93%)	10 (6%)	2(1%)	14 13
2	Е	129/131~(98%)	128 (99%)	1 (1%)	0	100 100
2	F	128/131~(98%)	125~(98%)	3 (2%)	0	100 100
2	G	130/131~(99%)	128 (98%)	2(2%)	0	100 100
2	Н	128/131 (98%)	127 (99%)	1 (1%)	0	100 100
All	All	1269/1320~(96%)	1219 (96%)	46 (4%)	4 (0%)	41 47

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

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	481	ASN
1	D	481	ASN
1	А	482	GLY
1	D	360	ASN

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
1	А	165/171~(96%)	162~(98%)	3~(2%)	59	70
1	В	$171/171 \ (100\%)$	166~(97%)	5(3%)	42	52
1	С	164/171~(96%)	160 (98%)	4 (2%)	49	59
1	D	160/171~(94%)	159 (99%)	1 (1%)	86	93
2	Е	104/104~(100%)	100 (96%)	4 (4%)	33	41
2	F	102/104~(98%)	99~(97%)	3~(3%)	42	52
2	G	104/104~(100%)	103~(99%)	1 (1%)	76	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles						
2	Н	102/104~(98%)	101 (99%)	1 (1%)	76 85						
All	All	1072/1100~(98%)	1050 (98%)	22 (2%)	55 65						

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5 of 22 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
2	Ε	25	SER
2	F	7	SER
2	Е	111	ASP
2	F	17	SER
1	А	359	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	331	ASN
1	А	481	ASN
1	D	354	ASN
1	D	360	ASN
2	Н	5	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)

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	Type	Chain	Dec	Res Link	Bo	ond leng	$_{\rm ths}$	Bond angles		
MOI	туре	Unain	1005		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	NAG	Ι	1	3,1	14,14,15	1.05	1 (7%)	17,19,21	1.01	1 (5%)
3	NAG	Ι	2	3	14,14,15	0.30	0	17,19,21	0.95	1 (5%)
3	BMA	Ι	3	3	11,11,12	0.29	0	15,15,17	0.64	0
3	FUL	Ι	4	3	10,10,11	0.30	0	14,14,16	0.79	0
4	NAG	J	1	4,1	14,14,15	0.75	1 (7%)	17,19,21	1.21	1 (5%)
4	NAG	J	2	4	14,14,15	0.20	0	17,19,21	0.38	0
4	MAN	J	3	4	11,11,12	0.32	0	15,15,17	1.18	3 (20%)
4	MAN	J	4	4	11,11,12	0.24	0	15,15,17	1.51	3 (20%)
4	NAG	J	5	4	14,14,15	0.36	0	17,19,21	0.96	1 (5%)
4	FUL	J	6	4	10,10,11	0.41	0	14,14,16	1.15	2 (14%)
3	NAG	K	1	3,1	14,14,15	0.84	1 (7%)	17,19,21	1.05	1 (5%)
3	NAG	К	2	3	14,14,15	0.38	0	17,19,21	1.09	2 (11%)
3	BMA	K	3	3	11,11,12	0.25	0	15,15,17	0.91	1 (6%)
3	FUL	K	4	3	10,10,11	0.40	0	14,14,16	1.37	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Ι	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Ι	2	3	-	1/6/23/26	0/1/1/1
3	BMA	Ι	3	3	-	2/2/19/22	0/1/1/1
3	FUL	Ι	4	3	-	-	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	MAN	J	3	4	-	2/2/19/22	0/1/1/1
4	MAN	J	4	4	-	1/2/19/22	0/1/1/1
4	NAG	J	5	4	-	3/6/23/26	0/1/1/1
4	FUL	J	6	4	-	-	0/1/1/1
3	NAG	Κ	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	К	2	3	_	3/6/23/26	0/1/1/1
3	BMA	К	3	3	-	2/2/19/22	0/1/1/1
3	FUL	K	4	3	-	-	0/1/1/1

All (3) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	Ι	1	NAG	C1-C2	3.52	1.57	1.52
3	Κ	1	NAG	C1-C2	2.92	1.56	1.52
4	J	1	NAG	C1-C2	2.53	1.56	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	J	4	MAN	C1-O5-C5	3.58	117.05	112.19
3	Κ	4	FUL	C1-C2-C3	3.49	113.96	109.67
3	Κ	1	NAG	C1-O5-C5	2.99	116.24	112.19
4	J	1	NAG	C1-O5-C5	2.91	116.14	112.19
4	J	3	MAN	C1-O5-C5	2.90	116.13	112.19

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	5	NAG	C3-C2-N2-C7
4	J	5	NAG	C8-C7-N2-C2
4	J	5	NAG	O7-C7-N2-C2
3	K	1	NAG	O5-C5-C6-O6
3	K	2	NAG	C8-C7-N2-C2

There are no ring outliers.

12 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Ι	1	NAG	1	0
4	J	5	NAG	1	0
3	Κ	4	FUL	4	0
4	J	2	NAG	1	0
3	Κ	3	BMA	1	0
4	J	6	FUL	1	0
4	J	3	MAN	1	0
4	J	4	MAN	1	0
3	Κ	1	NAG	2	0
4	J	1	NAG	1	0
3	Κ	2	NAG	2	0
3	Ι	2	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)

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	ol Type	Chain	Res	Link	Bo	ond leng	$_{\rm sths}$	Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	А	601	-	11,11,12	1.09	1 (9%)	15,15,17	1.83	5 (33%)
6	NAG	D	600	-	14,14,15	0.39	0	17,19,21	1.29	2 (11%)
7	PG4	E	201	-	7,7,12	0.44	0	6,6,11	0.29	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	MAN	А	601	-	-	1/2/19/22	0/1/1/1
6	NAG	D	600	-	-	5/6/23/26	0/1/1/1
7	PG4	Е	201	-	-	1/5/5/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
5	А	601	MAN	C1-C2	2.66	1.58	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
6	D	600	NAG	C2-N2-C7	4.36	129.11	122.90
5	А	601	MAN	C1-O5-C5	3.94	117.54	112.19
5	А	601	MAN	O5-C1-C2	3.40	116.02	110.77
5	А	601	MAN	C3-C4-C5	-2.42	105.92	110.24
5	А	601	MAN	O2-C2-C3	-2.21	105.72	110.14

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	600	NAG	O5-C5-C6-O6
6	D	600	NAG	C4-C5-C6-O6
6	D	600	NAG	C8-C7-N2-C2
6	D	600	NAG	O7-C7-N2-C2
7	Е	201	PG4	O2-C3-C4-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	600	NAG	1	0
7	Е	201	PG4	2	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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	193/199~(96%)	0.16	3 (1%) 72 80	37, 54, 80, 91	0
1	В	198/199~(99%)	0.14	6 (3%) 50 61	44, 60, 89, 101	0
1	С	191/199~(95%)	0.24	9 (4%) 31 44	40, 54, 91, 111	0
1	D	184/199~(92%)	0.62	20 (10%) 5 9	44, 60, 96, 115	0
2	Ε	130/131~(99%)	0.02	3 (2%) 60 70	39, 50, 73, 81	0
2	F	130/131~(99%)	0.15	3 (2%) 60 70	42, 53, 70, 82	0
2	G	131/131~(100%)	-0.02	1 (0%) 86 91	42, 55, 73, 96	0
2	Н	130/131~(99%)	0.53	7 (5%) 25 37	46, 62, 81, 101	0
All	All	1287/1320~(97%)	0.24	52 (4%) 38 51	37, 56, 89, 115	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
2	Н	2	VAL	5.2
1	D	368	LEU	5.1
2	Н	27	PHE	4.1
1	В	529	SER	4.1
1	В	521	PRO	4.1

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,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
4	NAG	J	5	14/15	0.47	0.30	84,111,116,118	0
3	BMA	Ι	3	11/12	0.54	0.42	30,30,30,30	0
4	MAN	J	3	11/12	0.64	0.31	100,109,115,116	0
4	MAN	J	4	11/12	0.68	0.19	107,115,117,121	0
3	BMA	K	3	11/12	0.68	0.32	30,30,30,30	0
4	NAG	J	2	14/15	0.71	0.30	104,112,117,119	0
4	NAG	J	1	14/15	0.71	0.22	66,93,102,105	0
4	FUL	J	6	10/11	0.73	0.42	30,30,30,30	0
3	NAG	К	2	14/15	0.78	0.26	102,107,113,117	0
3	FUL	Ι	4	10/11	0.78	0.36	30,30,30,30	0
3	NAG	Ι	1	14/15	0.84	0.15	79,97,106,111	0
3	NAG	Ι	2	14/15	0.85	0.19	91,100,103,104	0
3	FUL	Κ	4	10/11	0.85	0.38	30,30,30,30	0
3	NAG	K	1	14/15	0.88	0.13	55,81,90,100	0

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.

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
5	MAN	А	601	11/12	0.72	0.33	93,99,105,110	0
6	NAG	D	600	14/15	0.75	0.30	81,100,108,112	0
7	PG4	Е	201	8/13	0.82	0.32	39,52,56,61	0

6.5 Other polymers (i)

There are no such residues in this entry.

