

wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2023 – 01:59 PM EDT

PDB ID	:	8CWJ
Title	:	Fab arms of antibodies 4C12-B12 and CR3022 bound to pangolin receptor
		binding domain (pRBD)
Authors	:	Langley, D.B.; Christ, D.
Deposited on	:	2022-05-19
Resolution	:	2.45 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	:	2.32.2
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)	:	2.32.2

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 2.45 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.



Motrie	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	٨	020	3%		
	A	230	84%	10%	5%
			8%		
1	Н	230	86%	8%	6%
			8%		
2	В	220	82%	16%	••
			2%		
2	L	220	94%		6%
			2%		
3	G	204	91%	(5% •



Conti	nueu jion	i previous	paye	
Mol	Chain	Length	Quality of chain	
			.%	
3	Ι	204	91%	6% •
	_		2%	
4	J	230	85%	8% 7%
		222	10%	
4	U	230	87%	6% 7%
-	τ.	015	5%	
5	K	215	94%	5%
-	X 7	015	10%	_
5	V	215	88%	10% ••
C	C	Ð		
0	C	3	33% 33% 33%	•
G	Л	າ		
0	U	3	67% 339	%
6	Б	9		
U	Ľ	3	67% 339	%

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	D	1	-	-	-	Х
6	NAG	D	2	-	-	-	Х
6	FUC	Е	3	-	-	-	Х

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2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 16808 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 Heavy chain of CR3022 antibody Fab.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
1	ц	217	Total	С	Ν	0	S	0	1	0
	11	211	1601	1016	259	318	8	0	L	0
1	Δ	218	Total	С	Ν	0	S	0	7	0
	А	210	1662	1057	269	327	9	0	1	0

• Molecule 2 is a protein called Light chain of CR3022 antibody Fab.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	т	220	Total	С	Ν	0	S	0	1	0
		220	1705	1068	281	351	5	0	L	U
0	D	010	Total	С	Ν	0	S	0	0	0
	D	210	1652	1035	272	341	4	0	0	0

• Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	C	107	Total	С	Ν	0	S	0	1	0
0	G	197	1555	994	259	294	8	0	1	0
2	т	107	Total	С	Ν	0	S	0	1	0
0	1	197	1552	994	259	291	8	0	1	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	420	GLY	ASP	conflict	UNP A0A7D6TQ96
G	529	GLY	-	expression tag	UNP A0A7D6TQ96
G	530	SER	-	expression tag	UNP A0A7D6TQ96
G	531	HIS	-	expression tag	UNP A0A7D6TQ96
G	532	HIS	-	expression tag	UNP A0A7D6TQ96
G	533	HIS	-	expression tag	UNP A0A7D6TQ96
G	534	HIS	-	expression tag	UNP A0A7D6TQ96
G	535	HIS	_	expression tag	UNP A0A7D6TQ96



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Chain	Residue	Modelled	Actual	Comment	Reference
G	536	HIS	-	expression tag	UNP A0A7D6TQ96
Ι	420	GLY	ASP	conflict	UNP A0A7D6TQ96
Ι	529	GLY	-	expression tag	UNP A0A7D6TQ96
Ι	530	SER	-	expression tag	UNP A0A7D6TQ96
Ι	531	HIS	-	expression tag	UNP A0A7D6TQ96
Ι	532	HIS	-	expression tag	UNP A0A7D6TQ96
Ι	533	HIS	-	expression tag	UNP A0A7D6TQ96
Ι	534	HIS	-	expression tag	UNP A0A7D6TQ96
Ι	535	HIS	-	expression tag	UNP A0A7D6TQ96
Ι	536	HIS	-	expression tag	UNP A0A7D6TQ96

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• Molecule 4 is a protein called Heavy chain of 4C12-B12 antibody Fab.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
4	т	012	Total	С	Ν	Ο	S	0	2	0
4	4 J	213	1600	1005	268	321	6	0	2	0
4	II	214	Total	С	Ν	0	S	0	2	0
4	U	214	1607	1010	269	322	6		ა	

• Molecule 5 is a protein called Light chain of 4C12-B12 antibody Fab.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
5	K	214	Total	С	Ν	0	S	0	4	0
0	5 K	214	1668	1039	278	344	7	0	4	0
5	V	012	Total	С	Ν	0	S	0	0	0
	v	213	1615	1009	269	331	6		U	U

• 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	Atoms	ZeroOcc	AltConf	Trace
6	С	3	Total C N O 38 22 2 14	0	0	0
6	D	3	Total C N O 38 22 2 14	0	0	0
6	Е	3	Total C N O 38 22 2 14	0	0	0



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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	G	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
7	Ι	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
7	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	J	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
7	J	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
7	К	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	U	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	V	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	V	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	V	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	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	A	tor	ns		ZeroOcc	AltConf
8	G	1	Total 14	C 8	N 1	O 5	0	0

• Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	3	Total Cl 3 3	0	0
9	Ι	4	Total Cl 4 4	0	0
9	J	1	Total Cl 1 1	0	0
9	K	1	Total Cl 1 1	0	0
9	U	1	Total Cl 1 1	0	0

• Molecule 10 is water.



0	\cap	٢X	T	Т
0	U	V	V	J

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	Н	50	Total O 50 50	0	0
10	L	18	Total O 18 18	0	0
10	G	58	Total O 58 58	0	0
10	А	49	Total O 49 49	0	0
10	В	6	Total O 6 6	0	0
10	Ι	43	Total O 43 43	0	0
10	J	44	Total O 44 44	0	0
10	K	29	Total O 29 29	0	0
10	U	44	Total O 44 44	0	0
10	V	22	TotalO2222	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: Heavy chain of CR3022 antibody Fab





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

Chain C: 33% 33% 33%

NAG1 NAG2 FUC3

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

Chain D:	67%	33%
NAG1 NGC2 FUC3		

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

Chain E:	67%	33%

NAG1 NAG2 FUC3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	157.43Å 144.10 Å 168.84 Å	Deperitor
a, b, c, α , β , γ	90.00° 117.51° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	48.69 - 2.45	Depositor
Resolution (A)	48.69 - 2.45	EDS
% Data completeness	99.9 (48.69-2.45)	Depositor
(in resolution range)	$100.0 \ (48.69-2.45)$	EDS
R _{merge}	0.11	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.75 (at 2.45 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.11.1	Depositor
D D.	0.196 , 0.230	Depositor
Π, Π_{free}	0.196 , 0.230	DCC
R_{free} test set	6037 reflections $(4.92%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	54.5	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.30 , 42.7	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.006 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16808	wwPDB-VP
Average B, all atoms $(Å^2)$	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.15% 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: NAG, CL, FUC, GOL

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		
WIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.26	0/1703	0.50	0/2323	
1	Н	0.27	0/1642	0.50	0/2242	
2	В	0.25	0/1690	0.47	0/2310	
2	L	0.25	0/1743	0.46	0/2374	
3	G	0.27	0/1599	0.47	0/2179	
3	Ι	0.27	0/1596	0.46	0/2175	
4	J	0.26	0/1638	0.50	0/2234	
4	U	0.25	0/1645	0.50	0/2245	
5	Κ	0.26	0/1702	0.48	0/2312	
5	V	0.25	0/1649	0.48	0/2244	
All	All	0.26	0/16607	0.48	0/22638	

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	1662	0	1624	14	0
1	Н	1601	0	1546	13	0
2	В	1652	0	1538	19	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1705	0	1624	8	0
3	G	1555	0	1459	7	0
3	Ι	1552	0	1459	7	0
4	J	1600	0	1531	11	0
4	U	1607	0	1534	6	0
5	Κ	1668	0	1595	7	0
5	V	1615	0	1542	16	0
6	С	38	0	34	1	0
6	D	38	0	34	1	0
6	Е	38	0	34	0	0
7	G	12	0	16	0	0
7	Н	6	0	8	0	0
7	Ι	30	0	40	0	0
7	J	12	0	16	1	0
7	Κ	6	0	8	1	0
7	U	6	0	8	0	0
7	V	18	0	24	3	0
8	G	14	0	13	2	0
9	G	3	0	0	0	0
9	Ι	4	0	0	0	0
9	J	1	0	0	0	0
9	Κ	1	0	0	0	0
9	U	1	0	0	0	0
10	А	49	0	0	0	0
10	В	6	0	0	0	0
10	G	58	0	0	0	0
10	Н	50	0	0	0	0
10	Ι	43	0	0	0	0
10	J	44	0	0	0	0
10	K	29	0	0	0	0
10	L	18	0	0	0	0
10	U	44	0	0	0	0
10	V	22	0	0	0	0
All	All	16808	0	15687	101	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 3.

The worst 5 of 101 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)
4:J:141:THR:N	4:J:192:SER:HG	1.90	0.68
4:U:52:ASP:O	4:U:72:ARG:NH2	2.27	0.68
2:B:119:PRO:HB3	2:B:145:PHE:HB3	1.78	0.65
4:J:66:GLY:H	7:J:302:GOL:H12	1.64	0.63
1:H:129:PRO:HD3	1:H:215:LYS:HE3	1.82	0.60

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	entiles
1	А	221/230~(96%)	212 (96%)	8 (4%)	1 (0%)	29	34
1	Н	214/230~(93%)	200 (94%)	11 (5%)	3 (1%)	11	10
2	В	216/220~(98%)	199 (92%)	14 (6%)	3 (1%)	11	10
2	L	219/220~(100%)	211 (96%)	8 (4%)	0	100	100
3	G	196/204~(96%)	190 (97%)	6 (3%)	0	100	100
3	Ι	196/204~(96%)	190 (97%)	6 (3%)	0	100	100
4	J	211/230~(92%)	207 (98%)	4 (2%)	0	100	100
4	U	213/230~(93%)	202 (95%)	10 (5%)	1 (0%)	29	34
5	К	216/215~(100%)	209 (97%)	7 (3%)	0	100	100
5	V	211/215~(98%)	201 (95%)	10 (5%)	0	100	100
All	All	2113/2198 (96%)	2021 (96%)	84 (4%)	8 (0%)	34	41

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Н	194	SER
1	Н	192	SER
4	U	194	SER



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Mol	Chain	Res	Type
1	Н	199	THR
2	В	159	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.

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	neric Outliers		Percentiles		
1	А	187/194~(96%)	183~(98%)	4 (2%)	53	66		
1	Η	178/194~(92%)	178 (100%)	0	100	100		
2	В	182/195~(93%)	177~(97%)	5(3%)	44	57		
2	L	193/195~(99%)	190~(98%)	3~(2%)	62	74		
3	G	169/176~(96%)	168~(99%)	1 (1%)	86	91		
3	Ι	168/176~(96%)	166~(99%)	2(1%)	71	81		
4	J	177/192~(92%)	175~(99%)	2(1%)	73	83		
4	U	177/192~(92%)	176~(99%)	1 (1%)	86	91		
5	Κ	189/188~(100%)	187~(99%)	2(1%)	73	83		
5	V	181/188~(96%)	176 (97%)	5(3%)	43	56		
All	All	1801/1890~(95%)	1776 (99%)	25 (1%)	67	78		

5 of 25 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
3	Ι	514	SER
5	Κ	81	GLU
5	V	181	LEU
4	J	197	THR
5	Κ	147	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



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)

9 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	Turne	Chain	Deg Link		Bo	ond leng	\mathbf{ths}	В	ond ang	les
WIOI	туре		nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
6	NAG	C	1	6,3	14,14,15	0.24	0	17,19,21	0.73	1 (5%)
6	NAG	С	2	6	14,14,15	0.21	0	17,19,21	0.44	0
6	FUC	C	3	6	10,10,11	0.92	1 (10%)	14,14,16	0.84	0
6	NAG	D	1	6,3	14,14,15	0.25	0	17,19,21	0.99	1 (5%)
6	NAG	D	2	6	14,14,15	0.28	0	17,19,21	0.46	0
6	FUC	D	3	6	10,10,11	0.80	0	14,14,16	0.79	0
6	NAG	E	1	6,3	14,14,15	0.34	0	17,19,21	0.58	0
6	NAG	E	2	6	14,14,15	0.34	0	17,19,21	0.44	0
6	FUC	E	3	6	10,10,11	1.05	1 (10%)	14,14,16	1.02	1 (7%)

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
6	NAG	С	1	6,3	-	3/6/23/26	0/1/1/1
6	NAG	С	2	6	-	4/6/23/26	0/1/1/1
6	FUC	С	3	6	-	-	0/1/1/1
6	NAG	D	1	6,3	-	2/6/23/26	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
6	FUC	D	3	6	-	-	0/1/1/1
6	NAG	Е	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	Е	2	6	-	0/6/23/26	0/1/1/1
6	FUC	Е	3	6	-	-	0/1/1/1

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All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
6	Е	3	FUC	O5-C1	-2.50	1.39	1.43
6	С	3	FUC	O5-C1	-2.11	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	D	1	NAG	C1-O5-C5	3.12	116.42	112.19
6	Е	3	FUC	O2-C2-C1	2.45	114.16	109.15
6	С	1	NAG	C1-O5-C5	2.09	115.02	112.19

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	2	NAG	O5-C5-C6-O6
6	D	2	NAG	C4-C5-C6-O6
6	С	2	NAG	C8-C7-N2-C2
6	С	2	NAG	O7-C7-N2-C2
6	С	1	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1	NAG	1	0
6	С	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)

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 for Mogul analysis.

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	Dog	Tink	Bo	ond leng	ths	Bond angles		
WIOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	G	602	3	14,14,15	1.01	1 (7%)	17,19,21	1.90	3 (17%)
7	GOL	Ι	605	-	5,5,5	0.36	0	$5,\!5,\!5$	0.22	0
7	GOL	G	603	-	$5,\!5,\!5$	0.37	0	$5,\!5,\!5$	0.30	0



Mal	Turne	Chain	Dec	Tiple	Bo	ond leng	$_{\rm ths}$	В	ond ang	les
INIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
7	GOL	Ι	604	-	$5,\!5,\!5$	0.37	0	$5,\!5,\!5$	0.31	0
7	GOL	K	301	-	$5,\!5,\!5$	0.36	0	$5,\!5,\!5$	0.41	0
7	GOL	Ι	603	-	$5,\!5,\!5$	0.38	0	$5,\!5,\!5$	0.29	0
7	GOL	U	301	-	$5,\!5,\!5$	0.37	0	$5,\!5,\!5$	0.32	0
7	GOL	V	302	-	$5,\!5,\!5$	0.35	0	$5,\!5,\!5$	0.42	0
7	GOL	Н	301	-	$5,\!5,\!5$	0.37	0	$5,\!5,\!5$	0.30	0
7	GOL	Ι	601	-	$5,\!5,\!5$	0.37	0	$5,\!5,\!5$	0.31	0
7	GOL	J	301	-	$5,\!5,\!5$	0.36	0	$5,\!5,\!5$	0.31	0
7	GOL	J	302	-	$5,\!5,\!5$	0.34	0	$5,\!5,\!5$	0.39	0
7	GOL	V	303	-	$5,\!5,\!5$	0.34	0	$5,\!5,\!5$	0.32	0
7	GOL	G	601	-	$5,\!5,\!5$	0.38	0	$5,\!5,\!5$	0.28	0
7	GOL	Ι	602	-	$5,\!5,\!5$	0.37	0	$5,\!5,\!5$	0.27	0
7	GOL	V	301	-	$5,\!5,\!5$	0.37	0	5, 5, 5	0.33	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	G	602	3	-	2/6/23/26	0/1/1/1
7	GOL	Ι	605	-	-	2/4/4/4	-
7	GOL	G	603	-	-	2/4/4/4	-
7	GOL	Ι	604	-	-	2/4/4/4	-
7	GOL	К	301	-	-	0/4/4/4	-
7	GOL	Ι	603	-	-	2/4/4/4	-
7	GOL	U	301	-	-	0/4/4/4	-
7	GOL	V	302	-	-	0/4/4/4	-
7	GOL	Н	301	-	-	2/4/4/4	-
7	GOL	Ι	601	-	-	4/4/4/4	-
7	GOL	J	301	-	-	0/4/4/4	-
7	GOL	J	302	-	-	2/4/4/4	-
7	GOL	V	303	-	-	2/4/4/4	-
7	GOL	G	601	-	-	2/4/4/4	-
7	GOL	Ι	602	-	-	0/4/4/4	-
7	GOL	V	301	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	602	NAG	O5-C1	2.72	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
8	G	602	NAG	C1-O5-C5	6.16	120.53	112.19
8	G	602	NAG	C1-C2-N2	2.45	114.67	110.49
8	G	602	NAG	O5-C5-C4	2.21	116.20	110.83

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	601	GOL	O1-C1-C2-C3
7	Ι	601	GOL	O1-C1-C2-O2
7	Ι	605	GOL	O1-C1-C2-C3
7	V	303	GOL	O1-C1-C2-C3
8	G	602	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	602	NAG	2	0
7	K	301	GOL	1	0
7	V	302	GOL	2	0
7	J	302	GOL	1	0
7	V	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>	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	218/230~(94%)	0.01	6 (2%) 53 49	43, 63, 103, 141	0
1	Н	217/230~(94%)	0.27	18 (8%) 11 8	42, 63, 126, 156	0
2	В	218/220~(99%)	0.47	17 (7%) 13 10	52, 87, 130, 142	0
2	L	220/220~(100%)	0.08	4 (1%) 68 64	45, 76, 100, 125	0
3	G	197/204~(96%)	0.24	4 (2%) 65 61	35, 49, 84, 114	0
3	Ι	197/204~(96%)	0.21	2 (1%) 82 81	35, 51, 90, 124	0
4	J	213/230~(92%)	0.05	4 (1%) 66 63	35, 56, 120, 145	0
4	U	214/230~(93%)	0.38	22 (10%) 6 4	36, 63, 124, 151	0
5	Κ	214/215~(99%)	0.18	10 (4%) 31 29	36, 65, 107, 133	0
5	V	213/215~(99%)	0.42	22 (10%) 6 4	39, 74, 119, 145	0
All	All	2121/2198 (96%)	0.23	109 (5%) 28 25	35, 67, 118, 156	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Н	197	THR	7.9
5	V	181	LEU	6.2
2	В	154	TRP	5.9
4	U	134	SER	5.5
1	А	222	CYS	5.1

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, 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
6	FUC	D	3	10/11	0.55	0.30	164,166,166,166	0
6	NAG	D	2	14/15	0.65	0.47	142,153,156,158	0
6	FUC	Е	3	10/11	0.69	0.47	129,136,140,140	0
6	NAG	D	1	14/15	0.70	0.44	151,164,168,168	0
6	NAG	С	2	14/15	0.79	0.29	115,124,128,131	0
6	NAG	Е	2	14/15	0.81	0.41	114,125,131,134	0
6	NAG	С	1	14/15	0.83	0.28	77,98,117,121	0
6	NAG	Ē	1	14/15	0.85	0.27	75,92,114,122	0
6	FUC	С	3	10/11	0.90	0.22	128,131,133,134	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	$B-factors(Å^2)$	Q<0.9
7	GOL	J	301	6/6	0.55	0.33	82,84,86,86	0
7	GOL	U	301	6/6	0.71	0.24	$95,\!95,\!96,\!96$	0
8	NAG	G	602	14/15	0.72	0.29	126,135,139,140	0
7	GOL	Н	301	6/6	0.74	0.22	89,93,95,95	0
9	CL	J	303	1/1	0.75	0.14	97,97,97,97	0
7	GOL	Ι	605	6/6	0.76	0.29	77,80,81,83	0
7	GOL	Ι	602	6/6	0.78	0.31	81,82,83,84	0
7	GOL	V	301	6/6	0.80	0.26	78,80,82,84	0
7	GOL	Ι	604	6/6	0.80	0.30	83,87,88,92	0



Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	RSR	$B-factors(A^2)$	Q < 0.9	
7	GOL	Ι	603	6/6	0.80	0.23	86,91,91,95	0	
7	GOL	V	303	6/6	0.81	0.26	83,90,93,93	0	
9	CL	Ι	609	1/1	0.85	0.34	87,87,87,87	0	
7	GOL	G	603	6/6	0.85	0.31	87,89,92,99	0	
9	CL	Κ	302	1/1	0.85	0.13	105,105,105,105	0	
7	GOL	Ι	601	6/6	0.86	0.50	71,77,81,84	0	
9	CL	U	302	1/1	0.86	0.12	101,101,101,101	0	
9	CL	Ι	607	1/1	0.87	0.38	96,96,96,96	0	
7	GOL	G	601	6/6	0.88	0.21	82,84,84,85	0	
9	CL	G	604	1/1	0.89	0.46	97,97,97,97	0	
7	GOL	V	302	6/6	0.89	0.18	72,82,84,85	0	
9	CL	G	605	1/1	0.90	0.31	93,93,93,93	0	
7	GOL	K	301	6/6	0.90	0.25	68,80,80,84	0	
7	GOL	J	302	6/6	0.91	0.32	67,80,82,83	0	
9	CL	Ι	606	1/1	0.94	0.17	91,91,91,91	0	
9	CL	G	606	1/1	0.96	0.20	115,115,115,115	0	
9	CL	Ι	608	1/1	0.96	0.16	88,88,88,88	0	

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6.5 Other polymers (i)

There are no such residues in this entry.

