

# wwPDB X-ray Structure Validation Summary Report (i)

#### May 18, 2023 – 04:06 PM EDT

PDB ID : 8GB6

Title: Crystal structure of SARS-CoV-2 receptor binding domain in complex with

neutralizing antibody 21B6

Authors: Yuan, M.; Wilson, I.A.

Deposited on : 2023-02-24

Resolution : 1.75 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$ 

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)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

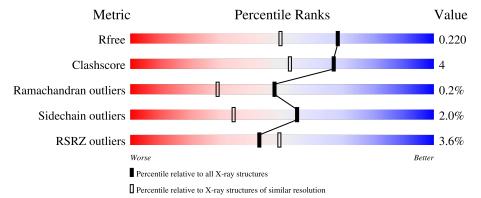
Validation Pipeline (wwPDB-VP) : 2.32.2

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	Whole archive	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	A	205	8%	8% • 5%
2	Н	226	93%	6% •
3	L	214	89%	8% •
4	В	3	67%	33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	$\operatorname{Res}$	Chirality	Geometry	Clashes	Electron density
4	FUC	В	3	-	-	=	X



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5523 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 Spike protein S1.

$\mathbf{Mol}$	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total 1543	C 989	N 257	O 289	S 8	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	531	GLY	-	expression tag	UNP P0DTC2
A	532	HIS	-	expression tag	UNP P0DTC2
A	533	HIS	-	expression tag	UNP P0DTC2
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2
A	536	HIS	-	expression tag	UNP P0DTC2
A	537	HIS	-	expression tag	UNP P0DTC2

• Molecule 2 is a protein called 21B6 Heavy chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	Н	226	Total 1681	C 1063	N 286	O 326	S 6	0	0	0

• Molecule 3 is a protein called 21B6 Light chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	L	213	Total 1634	C 1021	N 272	O 336	S 5	0	0	0

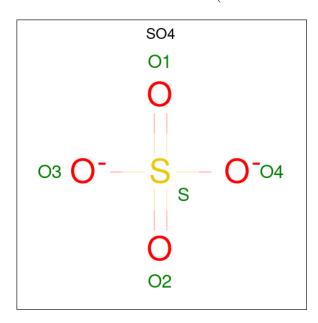
• Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[al pha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
4	В	3	Total 38	C 22	N 2	O 14	0	0	0

 $\bullet$  Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $\mathrm{O_4S}).$ 



Mol	Chain	Residues	Atoms	5	ZeroOcc	AltConf	
5	A	1	Total O	S	0	0	
	Λ	1	5 4	1	U	U	
5	A	1	Total O	$\mathbf{S}$	0	0	
	Λ	1	5 4	1	0	U	
5	Н	1	Total O	$\mathbf{S}$	0	0	
	11	1	5 4	1	0	U	
5	Н	1	Total O	$\mathbf{S}$	0	0	
	11	1	5   4	1	0	J	
5	H	1	Total O	$\mathbf{S}$	0	0	
5	11	1	5 4	1	0	U	
5	Н	1	Total O	$\mathbf{S}$	0	0	
	11	1	5   4	1	0	0	
5	L	1	Total O	S	0	0	
	ь	1	5   4	1		0	
5	L	1	Total O	S	0	0	
5	ь	1	5   4	1	0	0	

• Molecule 6 is water.

$\mathbf{Mol}$	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	173	Total O 173 173	0	0



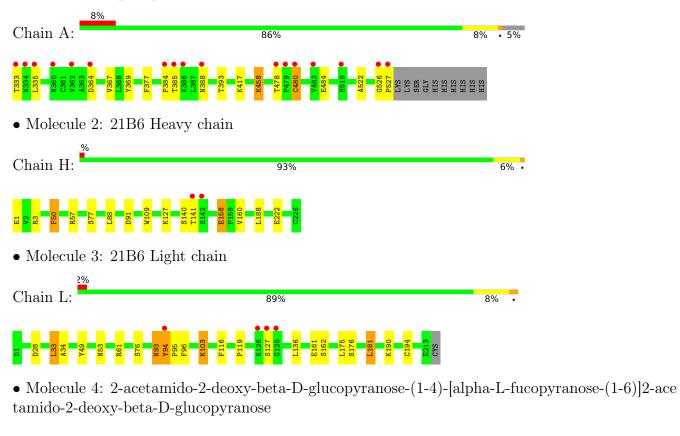
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Н	211	Total O 211 211	0	0
6	L	203	Total O 203 203	0	0



# 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



67%



Chain B:



33%

# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	72.65Å 78.83Å 131.81Å	Donogitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.50 - 1.75	Depositor
rtesolution (A)	41.50 - 1.75	EDS
% Data completeness	97.4 (41.50-1.75)	Depositor
(in resolution range)	97.4 (41.50-1.75)	EDS
$R_{merge}$	0.99	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.49  (at  1.75Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
P. P.	0.182 , 0.221	Depositor
$R, R_{free}$	0.181 , $0.220$	DCC
$R_{free}$ test set	2000 reflections $(2.65\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.35, 48.4	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.47, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5523	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities 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, SO4, 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).

Mol	Chain	Bo	nd lengths	Bond angles	
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.81	1/1587 (0.1%)	0.84	2/2161 (0.1%)
2	Н	0.81	$2/1723 \ (0.1\%)$	0.93	3/2349 (0.1%)
3	L	0.76	$2/1671 \ (0.1\%)$	0.87	7/2272 (0.3%)
All	All	0.80	5/4981 (0.1%)	0.88	$12/6782 \ (0.2\%)$

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
2	Н	0	1
3	L	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	Ideal(A)
1	A	480	CYS	CB-SG	-7.13	1.70	1.82
3	L	194	CYS	CB-SG	-7.12	1.70	1.82
2	Н	158	GLU	CD-OE1	7.06	1.33	1.25
3	L	162	SER	CB-OG	-6.58	1.33	1.42
2	Н	109	TRP	CE3-CZ3	5.10	1.47	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
1	A	480	CYS	CA-CB-SG	-9.19	97.45	114.00
3	L	33	LEU	CA-CB-CG	-7.05	99.07	115.30
3	L	94	TYR	CA-CB-CG	6.78	126.27	113.40



Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	L	181	LEU	CA-CB-CG	6.69	130.68	115.30
3	L	28	ASP	CB-CG-OD1	6.58	124.22	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Н	141	THR	Peptide
3	L	93	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	A	1543	0	1459	14	0
2	Н	1681	0	1652	9	0
3	L	1634	0	1570	16	0
4	В	38	0	34	0	0
5	A	10	0	0	1	0
5	Н	20	0	0	0	0
5	L	10	0	0	0	0
6	A	173	0	0	6	0
6	Н	211	0	0	5	0
6	L	203	0	0	4	0
All	All	5523	0	4715	38	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 4.

The worst 5 of 38 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)
3:L:103:LYS:NZ	6:L:401:HOH:O	2.04	0.88
1:A:527:PRO:O	6:A:701:HOH:O	2.01	0.78
1:A:333:THR:HB	1:A:335:LEU:HD23	1.66	0.78



Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
3:L:103:LYS:HD2	3:L:103:LYS:H	1.50	0.76
1:A:364:ASP:OD1	6:A:703:HOH:O	2.07	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.

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	A	193/205~(94%)	186 (96%)	6 (3%)	1 (0%)	29	12
2	Н	224/226 (99%)	212 (95%)	12 (5%)	0	100	100
3	L	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
All	All	628/645 (97%)	602 (96%)	25 (4%)	1 (0%)	47	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	GLU

#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	168/177 (95%)	166 (99%)	2 (1%)	71 56
2	Н	186/186 (100%)	182 (98%)	4 (2%)	52 29



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	187/188 (100%)	182 (97%)	5 (3%)	44	22
All	All	541/551 (98%)	530 (98%)	11 (2%)	55	34

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	127	SER
3	L	176	SER
3	L	190	LYS
3	L	181	LEU
2	Н	160	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	53	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)

3 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).

Mol	Type	Chain	Res	Link	Bond lengths			В	ond ang	les
IVIOI	туре	Chain	rtes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	В	1	1,4	14,14,15	0.50	0	17,19,21	0.71	0



Mol	Trino	Chain	Res	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	В	2	4	14,14,15	0.45	0	17,19,21	0.42	0
4	FUC	В	3	4	10,10,11	1.65	3 (30%)	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
4	NAG	В	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	В	2	4	-	2/6/23/26	0/1/1/1
4	FUC	В	3	4	-	-	0/1/1/1

#### All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\mathring{\mathbf{A}})$	Ideal(A)
4	В	3	FUC	C1-C2	3.13	1.59	1.52
4	В	3	FUC	C4-C5	2.13	1.57	1.52
4	В	3	FUC	O5-C5	2.02	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	В	3	FUC	C1-O5-C5	2.79	119.09	112.78
4	В	3	FUC	C1-C2-C3	2.46	112.69	109.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

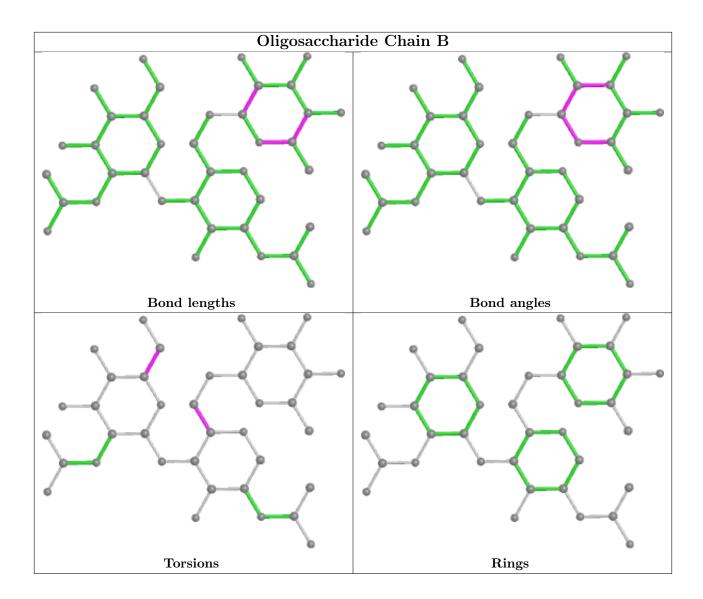
Mol	Chain	Res	Type	Atoms
4	В	1	NAG	C4-C5-C6-O6
4	В	1	NAG	O5-C5-C6-O6
4	В	2	NAG	C4-C5-C6-O6
4	В	2	NAG	O5-C5-C6-O6

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)

8 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
WIOI	туре	Chain	rtes	Lilik	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
5	SO4	A	601	-	4,4,4	0.40	0	6,6,6	0.64	0
5	SO4	Н	302	-	4,4,4	0.15	0	6,6,6	0.34	0
5	SO4	L	302	-	4,4,4	0.20	0	6,6,6	0.19	0



Mol	Trino	Chain	Dag	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	Н	303	-	4,4,4	0.12	0	6,6,6	0.36	0
5	SO4	L	301	-	4,4,4	0.23	0	6,6,6	0.27	0
5	SO4	Н	301	-	4,4,4	0.28	0	6,6,6	0.49	0
5	SO4	A	602	-	4,4,4	0.24	0	6,6,6	1.15	0
5	SO4	Н	304	-	4,4,4	0.29	0	6,6,6	0.58	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	SO4	1	0

#### 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

#### 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	# RSRZ > 2	$OWAB(Å^2)$	Q < 0.9
1	A	$195/205\ (95\%)$	0.26	17 (8%) 10 13	18, 28, 55, 89	0
2	Н	226/226 (100%)	-0.10	2 (0%) 84 89	18, 26, 46, 72	0
3	L	213/214 (99%)	-0.11	4 (1%) 66 74	20, 29, 44, 66	0
All	All	634/645 (98%)	0.01	23 (3%) 42 49	18, 28, 50, 89	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	333	THR	13.5
2	Н	141	THR	7.0
1	A	334	ASN	6.8
3	L	94	TYR	6.2
1	A	335	LEU	5.7

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

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

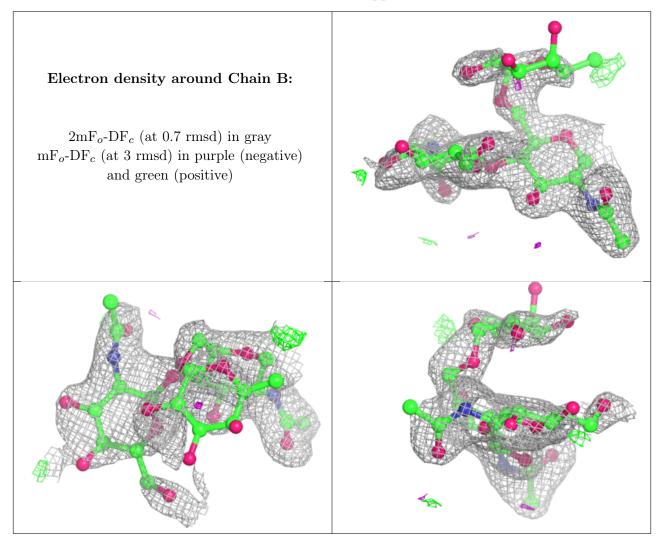
### 6.3 Carbohydrates (i)

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	FUC	В	3	10/11	0.65	0.57	75,79,91,94	0
4	NAG	В	2	14/15	0.77	0.29	65,74,85,91	0
4	NAG	В	1	14/15	0.91	0.15	30,41,60,74	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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
5	SO4	L	301	5/5	0.92	0.23	59,62,76,88	0
5	SO4	Н	301	5/5	0.94	0.22	46,64,71,79	0
5	SO4	Н	302	5/5	0.95	0.18	61,66,68,69	0
5	SO4	L	302	5/5	0.95	0.17	57,57,71,77	0
5	SO4	Н	303	5/5	0.96	0.16	45,58,64,76	0
5	SO4	Н	304	5/5	0.96	0.19	50,52,61,62	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
5	SO4	A	601	5/5	0.99	0.06	35,37,39,48	0
5	SO4	A	602	5/5	0.99	0.08	41,41,46,47	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

