



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 5, 2022 – 10:25 PM JST

PDB ID : 7X2M  
Title : Crystal structure of nanobody 1-2C7 with SARS-CoV-2 RBD  
Authors : Wang, X.Q.; Zhang, L.Q.; Ren, Y.F.; Li, M.X.  
Deposited on : 2022-02-25  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) 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	:	2.31.3
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)	:	2.31.3

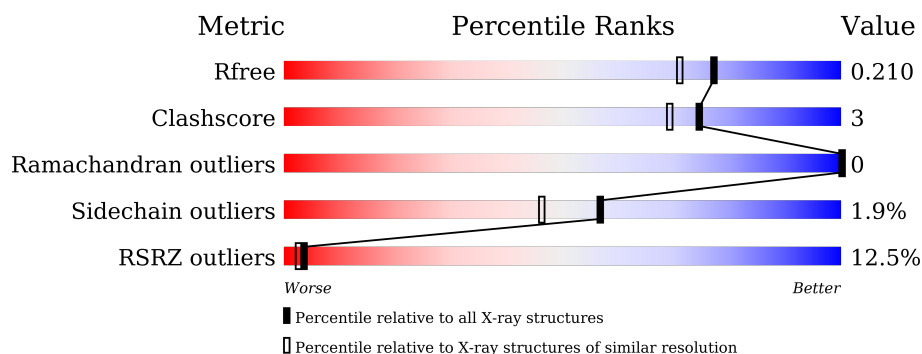
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	E	203	<div> <div></div> <div>92%</div> <div>5%</div> <div></div> </div>
2	B	124	<div> <div>30%</div> <div>82%</div> <div>18%</div> </div>
3	A	3	<div> <div>67%</div> <div>33%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2771 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	196	Total	C	N	O	S	0	1	0
			1560	1002	260	290	8			

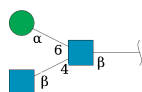
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	417	ASN	LYS	variant	UNP P0DTC2
E	484	LYS	GLU	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	530	HIS	-	expression tag	UNP P0DTC2
E	531	HIS	-	expression tag	UNP P0DTC2
E	532	HIS	-	expression tag	UNP P0DTC2
E	533	HIS	-	expression tag	UNP P0DTC2
E	534	HIS	-	expression tag	UNP P0DTC2
E	535	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called 1-2C7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	124	Total	C	N	O	S	0	1	0
			947	582	168	192	5			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



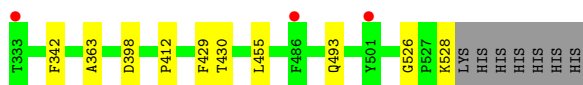
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	3	Total	C	N	O	0	0	0
			39	22	2	15			

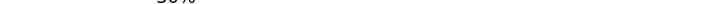
- Molecule 4 is water.

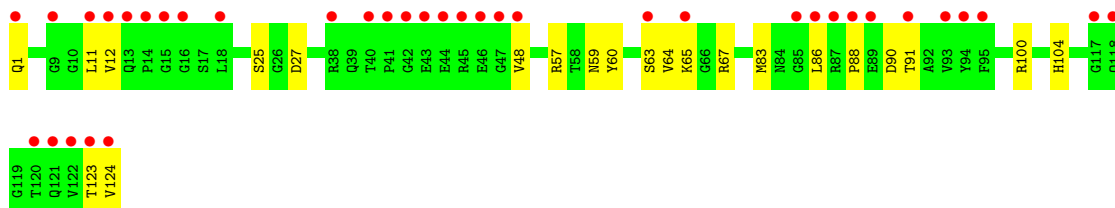
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	179	Total 179	O 179	0	0
4	B	46	Total 46	O 46	0	0



- Molecule 1: Spike protein S1



- Chain B:  30% 82% 18%



- Chain A:  67% 33%



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.62Å 143.62Å 143.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.39 – 1.80 45.42 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.39-1.80) 100.0 (45.42-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.180 , 0.207 0.180 , 0.210	Depositor DCC
$R_{free}$ test set	2201 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2771	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG

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	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	E	0.39	0/1608	0.58	0/2189
2	B	0.34	0/971	0.55	0/1318
All	All	0.37	0/2579	0.57	0/3507

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

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	E	1560	0	1481	6	0
2	B	947	0	886	10	0
3	A	39	0	34	1	0
4	B	46	0	0	1	0
4	E	179	0	0	1	0
All	All	2771	0	2401	16	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (16) 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:E:430:THR:O	4:E:601:HOH:O	2.09	0.70
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.84	0.60
2:B:91:THR:HG23	2:B:123:THR:HA	1.86	0.57
2:B:88:PRO:HA	2:B:124:VAL:HB	1.91	0.51
2:B:67:ARG:NH2	2:B:90:ASP:OD2	2.47	0.48
1:E:363:ALA:O	1:E:526:GLY:HA2	2.14	0.47
2:B:1:GLN:HG2	2:B:100:ARG:NH2	2.30	0.45
2:B:48:VAL:HG13	2:B:64:VAL:HG21	1.98	0.45
1:E:412:PRO:HG3	1:E:429:PHE:HB3	1.99	0.45
1:E:342:PHE:HB2	3:A:1:NAG:H82	2.02	0.41
2:B:57:ARG:HG3	2:B:104:HIS:O	2.21	0.41
2:B:59:ASN:ND2	4:B:201:HOH:O	2.54	0.41
2:B:63:SER:O	2:B:67:ARG:NH1	2.52	0.41
2:B:60:TYR:HB2	2:B:65:LYS:HD3	2.03	0.41
1:E:455:LEU:HD22	1:E:493:GLN:HG3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	195/203 (96%)	189 (97%)	6 (3%)	0	100	100
2	B	123/124 (99%)	120 (98%)	3 (2%)	0	100	100
All	All	318/327 (97%)	309 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	E	170/176 (97%)	169 (99%)	1 (1%)	86	84
2	B	102/101 (101%)	98 (96%)	4 (4%)	32	17
All	All	272/277 (98%)	267 (98%)	5 (2%)	57	48

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	528	LYS
2	B	11	LEU
2	B	12	VAL
2	B	25	SER
2	B	27	ASP

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

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			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	1	1,3	14,14,15	0.32	0	17,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	2	3	14,14,15	0.33	0	17,19,21	0.39	0
3	MAN	A	3	3	11,11,12	0.96	0	15,15,17	1.03	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	A	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	0/6/23/26	0/1/1/1
3	MAN	A	3	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

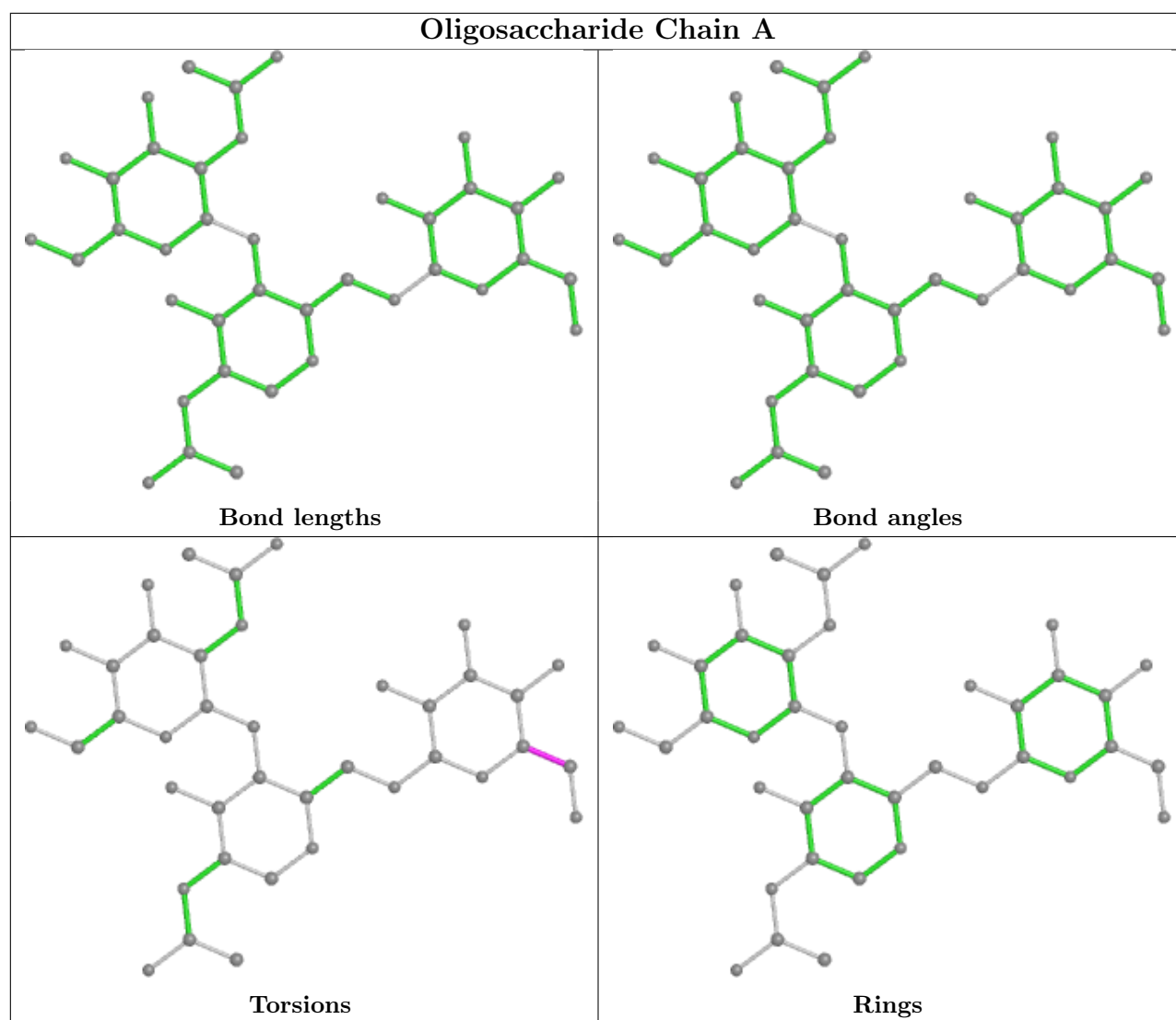
Mol	Chain	Res	Type	Atoms
3	A	3	MAN	C4-C5-C6-O6
3	A	3	MAN	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	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](#)

There are no ligands in this entry.

## 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

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	E	196/203 (96%)	0.12	3 (1%) 73 70	25, 36, 58, 67	0
2	B	124/124 (100%)	1.18	37 (29%) 0 0	27, 56, 81, 92	0
All	All	320/327 (97%)	0.53	40 (12%) 3 2	25, 40, 74, 92	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	41	PRO	7.2
2	B	11	LEU	5.5
2	B	88	PRO	5.1
2	B	87	ARG	5.0
1	E	333	THR	4.9
2	B	1	GLN	4.7
2	B	93	VAL	4.7
2	B	13	GLN	4.6
2	B	40	THR	4.2
2	B	12	VAL	4.0
1	E	486	PHE	3.9
2	B	42	GLY	3.9
2	B	86	LEU	3.8
2	B	14	PRO	3.7
2	B	89	GLU	3.7
2	B	118	GLN	3.7
2	B	16	GLY	3.6
2	B	123	THR	3.4
2	B	46	GLU	3.1
2	B	63	SER	3.0
2	B	117	GLY	2.9
2	B	43	GLU	2.7
2	B	47	GLY	2.7
2	B	91	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	120	THR	2.6
2	B	45	ARG	2.5
2	B	122	VAL	2.5
2	B	94	TYR	2.5
1	E	501	TYR	2.5
2	B	44	GLU	2.4
2	B	9	GLY	2.4
2	B	38	ARG	2.2
2	B	65	LYS	2.2
2	B	95	PHE	2.2
2	B	48	VAL	2.2
2	B	121	GLN	2.2
2	B	124	VAL	2.1
2	B	18	LEU	2.1
2	B	15	GLY	2.1
2	B	85	GLY	2.1

## 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](#)

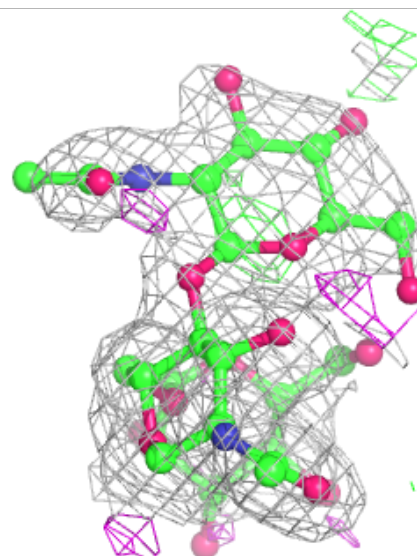
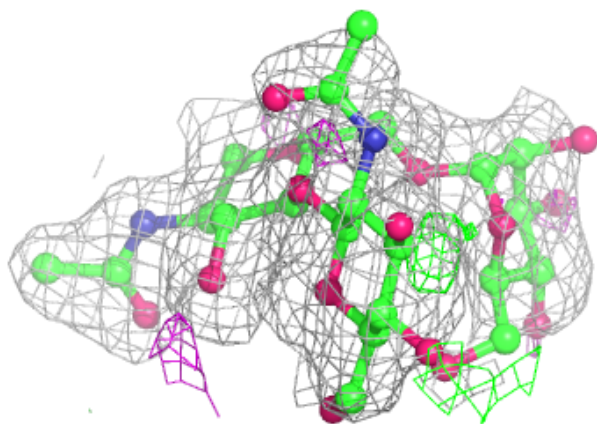
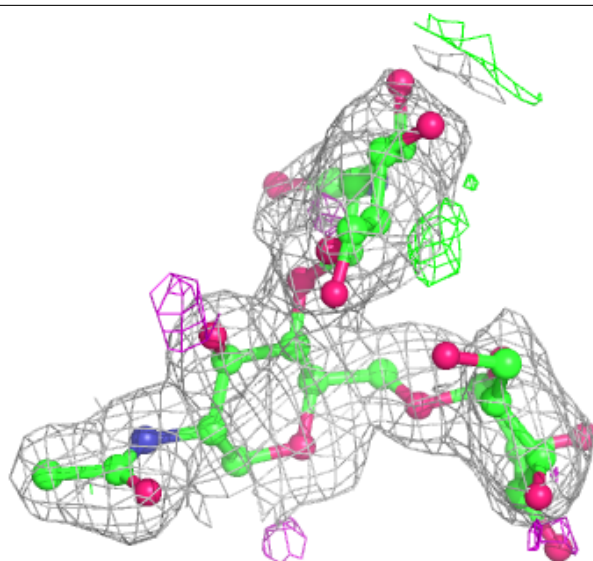
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	2	14/15	0.86	0.17	70,73,78,79	0
3	MAN	A	3	11/12	0.88	0.30	70,76,79,79	0
3	NAG	A	1	14/15	0.91	0.10	39,49,62,65	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.

**Electron density around Chain A:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.