Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 08:23 AM JST

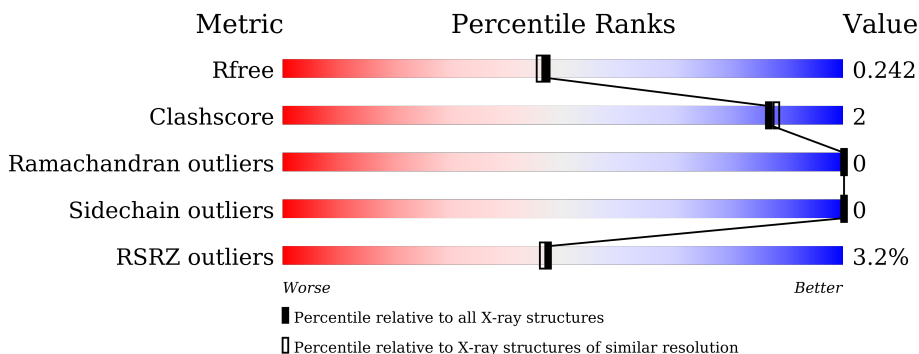|		
PDB ID	:	7FAT
Title	:	Structure Determination of the RBD-NB1A7
Authors	:	Geng, Y.; Shi, Z.Z.; Li, X.Y.; Wang, L.; Sun, Z.C.; Zhang, H.W.; Chen, X.C.
Deposited on	:	2021-07-07
Resolution	:	1.99 Å(reported)

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 1.99 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	Percentile Ranks	Value
Rfree		0.242
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0
RSRZ outliers		3.2%

Worse ← → *Better*

▌ Percentile relative to all X-ray structures

❘ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	219	2% / 78% / 6% / 16%
2	B	138	4% / 93% / · ·
3	C	2	50% / 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2711 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	A	184	Total	C	N	O	S	0	0	0
			1466	939	244	275	8			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	318	MET	-	expression tag	UNP P0DTC2
A	319	PHE	-	expression tag	UNP P0DTC2
A	320	VAL	-	expression tag	UNP P0DTC2
A	321	PHE	-	expression tag	UNP P0DTC2
A	322	LEU	-	expression tag	UNP P0DTC2
A	323	VAL	-	expression tag	UNP P0DTC2
A	324	LEU	-	expression tag	UNP P0DTC2
A	325	LEU	-	expression tag	UNP P0DTC2
A	326	PRO	-	expression tag	UNP P0DTC2
A	327	LEU	-	expression tag	UNP P0DTC2
A	328	VAL	-	expression tag	UNP P0DTC2
A	329	SER	-	expression tag	UNP P0DTC2
A	330	SER	-	expression tag	UNP P0DTC2
A	331	GLN	-	expression tag	UNP P0DTC2
A	332	CYS	-	expression tag	UNP P0DTC2
A	524	SER	-	expression tag	UNP P0DTC2
A	525	ARG	-	expression tag	UNP P0DTC2
A	526	ALA	-	expression tag	UNP P0DTC2
A	527	ALA	-	expression tag	UNP P0DTC2
A	528	ALA	-	expression tag	UNP P0DTC2
A	529	ASP	-	expression tag	UNP P0DTC2
A	530	TYR	-	expression tag	UNP P0DTC2
A	531	LYS	-	expression tag	UNP P0DTC2
A	532	ASP	-	expression tag	UNP P0DTC2
A	533	ASP	-	expression tag	UNP P0DTC2
A	534	ASP	-	expression tag	UNP P0DTC2
A	535	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	536	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called nb_1A7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	132	972	602	164	199	7	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
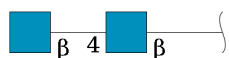
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	2	28	16	2	10	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	143	143	143	0	0
4	B	102	102	102	0	0

3 Residue-property plots ⓘ

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

Chain A:

• Molecule 2: nb_1A7

Chain B:

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

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	110.66Å 183.79Å 42.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.72 – 1.99 19.72 – 1.99	Depositor EDS
% Data completeness (in resolution range)	87.7 (19.72-1.99) 87.0 (19.72-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 1.99Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.193 , 0.242 0.193 , 0.242	Depositor DCC
R_{free} test set	1994 reflections (7.19%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.5	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.026 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2711	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.54	0/1507	0.65	0/2049
2	B	0.57	0/991	0.72	0/1338
All	All	0.55	0/2498	0.68	0/3387

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	A	1466	0	1381	8	0
2	B	972	0	914	2	0
3	C	28	0	25	1	0
4	A	143	0	0	2	0
4	B	102	0	0	0	0
All	All	2711	0	2320	10	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 2.

All (10) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ALA:O	4:A:601:HOH:O	2.18	0.52
2:B:61:ASP:OD1	2:B:64:LYS:HE3	2.09	0.52
2:B:6:GLU:OE2	2:B:126:THR:HG22	2.12	0.49
1:A:342:PHE:HB2	3:C:1:NAG:H82	1.94	0.49
1:A:378:LYS:HE3	4:A:658:HOH:O	2.13	0.46
1:A:484:GLU:HG3	1:A:488:CYS:O	2.17	0.45
1:A:386:LYS:HG2	1:A:515:PHE:CZ	2.52	0.45
1:A:408:ARG:O	1:A:414:GLN:HG3	2.21	0.41
1:A:502:GLY:O	1:A:506:GLN:HG3	2.21	0.41
1:A:382:VAL:HG13	1:A:430:THR:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	182/219 (83%)	173 (95%)	9 (5%)	0	100	100
2	B	130/138 (94%)	130 (100%)	0	0	100	100
All	All	312/357 (87%)	303 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	160/190 (84%)	160 (100%)	0	100	100
2	B	101/108 (94%)	101 (100%)	0	100	100
All	All	261/298 (88%)	261 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	493	GLN

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 ⓘ

2 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	C	1	1,3	14,14,15	0.49	0	17,19,21	0.70	0
3	NAG	C	2	3	14,14,15	0.26	0	17,19,21	0.42	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	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	<mark>2/6/23/26</mark>	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	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	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.

Oligosaccharide Chain C
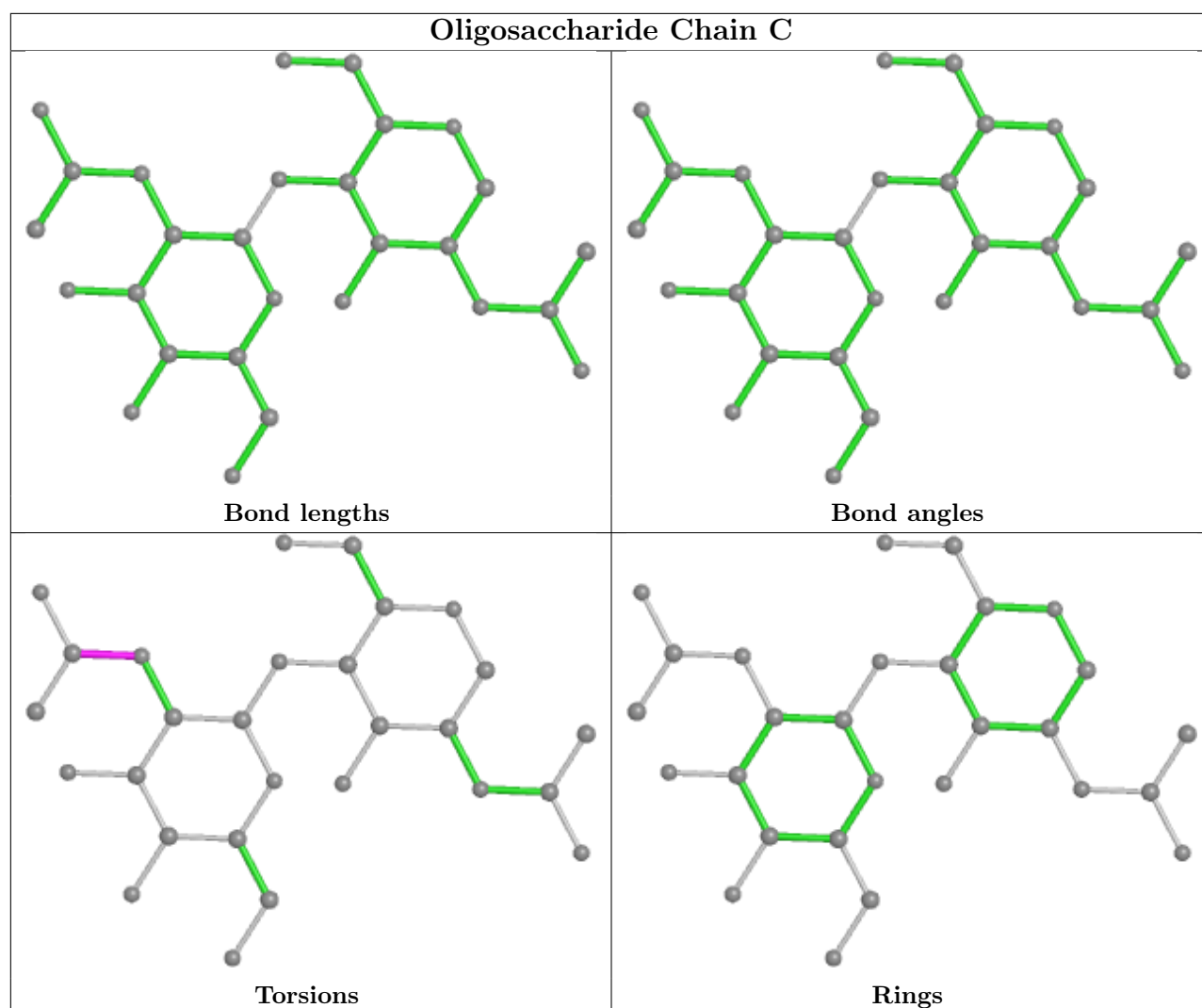
5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	A	184/219 (84%)	0.24	5 (2%) 54	53	15, 27, 45, 57	0
2	B	132/138 (95%)	0.25	5 (3%) 40	39	12, 26, 44, 66	0
All	All	316/357 (88%)	0.24	10 (3%) 47	46	12, 26, 45, 66	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	42	GLY	4.0
2	B	43	LYS	3.7
1	A	392	PHE	3.5
1	A	333	THR	3.4
1	A	478	THR	2.9
1	A	445	VAL	2.8
2	B	44	GLU	2.8
2	B	132	SER	2.7
1	A	479	PRO	2.5
2	B	41	PRO	2.4

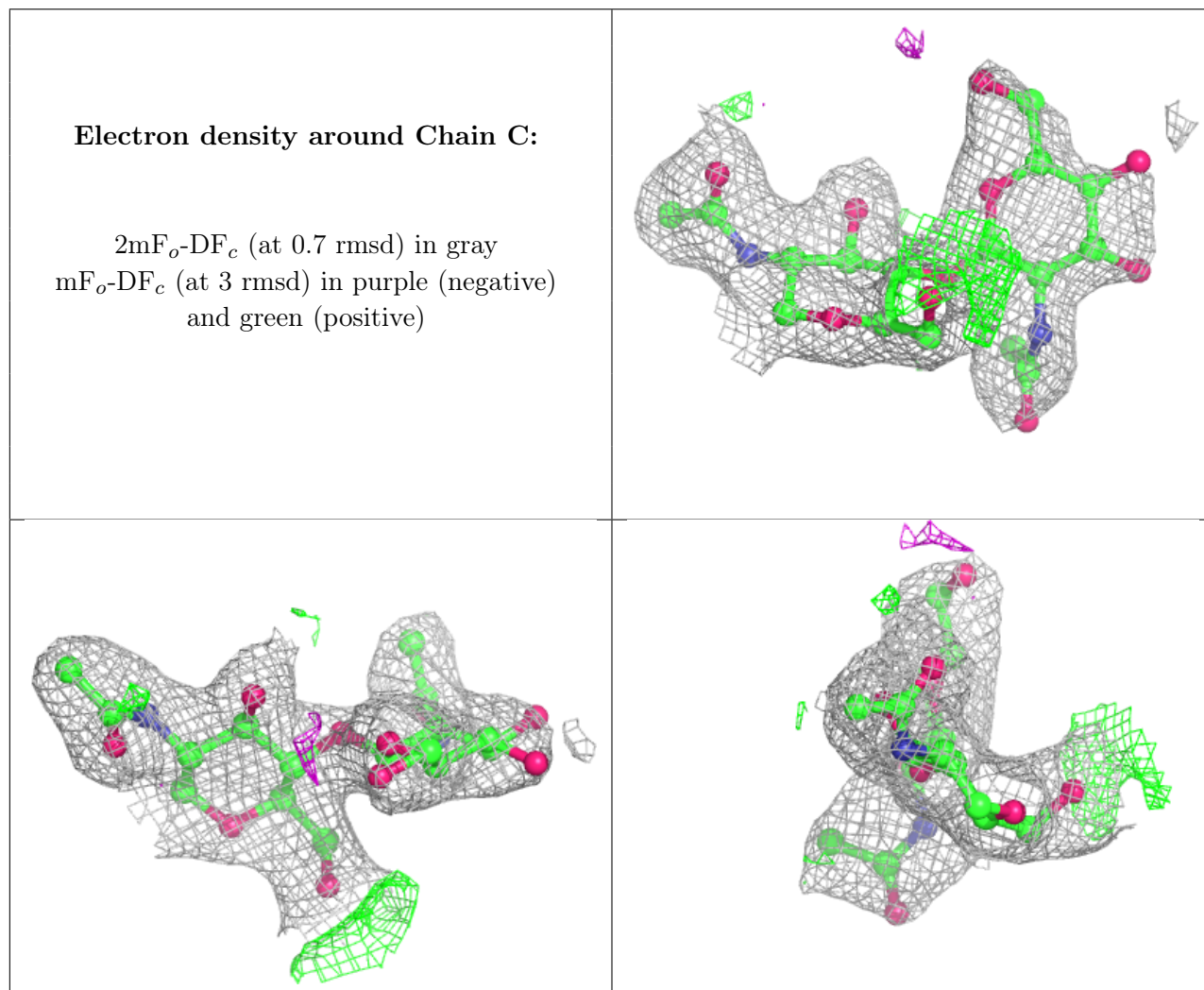## 6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3   Carbohydrates ⓘ

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, 95th 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
3	NAG	C	2	14/15	0.80	0.34	57,63,73,80	0
3	NAG	C	1	14/15	0.84	0.16	26,41,51,62	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 C:

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

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.