



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2025 – 04:45 PM JST

PDB ID : 8Z2E / pdb\_00008z2e  
Title : Crystal structure of nanobody Tnb04-1 with antibody 1F11 fab and SARS-CoV-2 RBD  
Authors : Wang, X.Q.; Zhang, L.Q.; Chen, J.; Dong, H.D.  
Deposited on : 2024-04-12  
Resolution : 2.30 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)	:	2.0rc1
EDS	:	<b>FAILED</b>
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

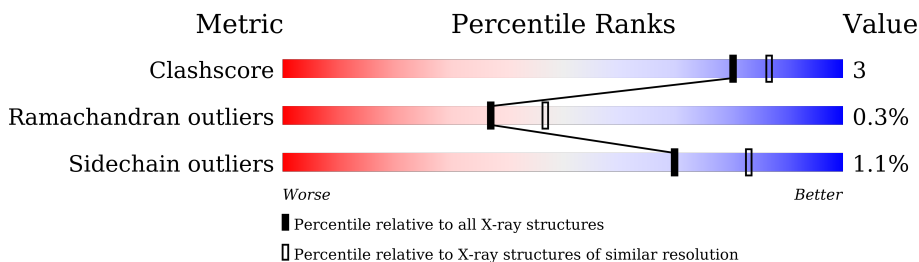
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)

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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	B	116	 96%
2	E	217	 82% 7% 10%
3	H	217	 90% 8%
4	L	214	 93% 7%
5	A	2	 50% 50%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5963 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 Tnb04-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	116	Total	C	N	O	S	0	0	0
			889	558	154	173	4			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 3 is a protein called 1F11-H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	212	Total	C	N	O	S	0	0	0
			1567	985	265	310	7			

- Molecule 4 is a protein called 1F11-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	214	Total	C	N	O	S	0	0	0
			1636	1021	277	333	5			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	22	Total	O	0	0
			22	22		
6	E	71	Total	O	0	0
			71	71		
6	H	113	Total	O	0	0
			113	113		
6	L	94	Total	O	0	0
			94	94		

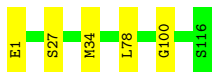
### 3 Residue-property plots [i](#)

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. 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. 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.


Note EDS failed to run properly.

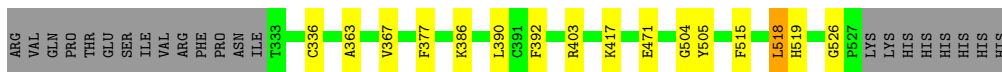
- Molecule 1: Tnb04-1

Chain B:  96%



- Molecule 2: Spike protein S1

Chain E:  82% 7% 10%



- Molecule 3: 1F11-H

Chain H:  90% 8%



- Molecule 4: 1F11-L

Chain L:  93% 7%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:  50% 50%



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.14Å 89.75Å 127.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.36 – 2.30	Depositor
% Data completeness (in resolution range)	99.5 (73.36-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, $R_{free}$	0.195 , 0.234	Depositor
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.383	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
Total number of atoms	5963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	B	0.42	0/906	0.63	0/1224
2	E	0.52	0/1587	0.68	0/2161
3	H	0.51	0/1601	0.67	0/2183
4	L	0.47	0/1671	0.64	0/2268
All	All	0.49	0/5765	0.66	0/7836

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	B	889	0	869	4	0
2	E	1543	0	1459	9	0
3	H	1567	0	1540	7	0
4	L	1636	0	1589	9	0
5	A	28	0	25	0	0
6	B	22	0	0	0	0
6	E	71	0	0	0	0
6	H	113	0	0	0	0
6	L	94	0	0	1	0
All	All	5963	0	5482	28	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 (28) 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:H:4:LEU:HD21	3:H:27:ILE:HD11	1.82	0.60
4:L:34:LEU:HD13	4:L:72:PHE:CG	2.37	0.59
1:B:34:MET:HB3	1:B:78:LEU:HD22	1.85	0.59
2:E:386:LYS:HG3	2:E:390:LEU:HD21	1.86	0.57
3:H:12:VAL:HG11	3:H:85:LEU:HD13	1.87	0.55
2:E:403:ARG:HG2	2:E:504:GLY:O	2.11	0.51
4:L:56:ALA:HB3	4:L:59:ILE:HG12	1.95	0.47
3:H:11:LEU:HD23	3:H:114:THR:HB	1.96	0.46
2:E:403:ARG:CG	2:E:505:TYR:HA	2.45	0.45
2:E:363:ALA:O	2:E:526:GLY:HA2	2.16	0.45
3:H:20:LEU:HD11	3:H:82:MET:HE1	1.97	0.45
4:L:82:GLU:OE2	4:L:82:GLU:N	2.40	0.45
4:L:147:GLN:NE2	4:L:195:GLU:OE1	2.51	0.44
1:B:1:GLU:CG	1:B:27:SER:HB3	2.46	0.44
3:H:143:GLY:HA2	3:H:158:TRP:CH2	2.53	0.44
2:E:336:CYS:HB2	2:E:363:ALA:HB2	2.00	0.43
2:E:417:LYS:HD3	6:L:305:HOH:O	2.18	0.43
2:E:403:ARG:HD2	2:E:505:TYR:HA	2.00	0.43
4:L:78:ARG:HG2	4:L:78:ARG:HH11	1.83	0.43
4:L:62:ARG:CZ	4:L:80:GLU:HG3	2.50	0.42
4:L:125:LEU:O	4:L:183:LYS:HD2	2.18	0.42
2:E:392:PHE:CE2	2:E:515:PHE:HB3	2.56	0.41
4:L:60:PRO:HG2	4:L:63:PHE:HE2	1.86	0.41
1:B:100:GLY:HA3	2:E:367:VAL:HG21	2.03	0.41
3:H:192:SER:O	3:H:196:GLN:HB2	2.21	0.41
1:B:1:GLU:HG3	1:B:27:SER:HB3	2.04	0.40
4:L:77:SER:O	4:L:78:ARG:HG3	2.21	0.40
3:H:67:PHE:HA	3:H:81:GLN:O	2.21	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	B	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
2	E	193/217 (89%)	180 (93%)	12 (6%)	1 (0%)	25	32
3	H	208/217 (96%)	202 (97%)	5 (2%)	1 (0%)	25	32
4	L	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
All	All	727/764 (95%)	700 (96%)	25 (3%)	2 (0%)	37	47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	100	VAL
2	E	518	LEU

### 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	B	94/94 (100%)	94 (100%)	0	100	100
2	E	168/190 (88%)	164 (98%)	4 (2%)	44	61
3	H	177/182 (97%)	175 (99%)	2 (1%)	70	83
4	L	185/185 (100%)	184 (100%)	1 (0%)	86	93
All	All	624/651 (96%)	617 (99%)	7 (1%)	70	83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	377	PHE
2	E	471	GLU
2	E	518	LEU
2	E	519	HIS

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Mol	Chain	Res	Type
3	H	153	PRO
3	H	154	VAL
4	L	92	TYR

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

Mol	Chain	Res	Type
2	E	360	ASN

### 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	$\# Z  > 2$
5	NAG	A	1	2,5	14,14,15	0.53	0	17,19,21	0.60	0
5	NAG	A	2	5	14,14,15	0.31	0	17,19,21	0.83	1 (5%)

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	NAG	A	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	A	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2	NAG	C1-O5-C5	2.82	116.01	112.19

There are no chirality outliers.

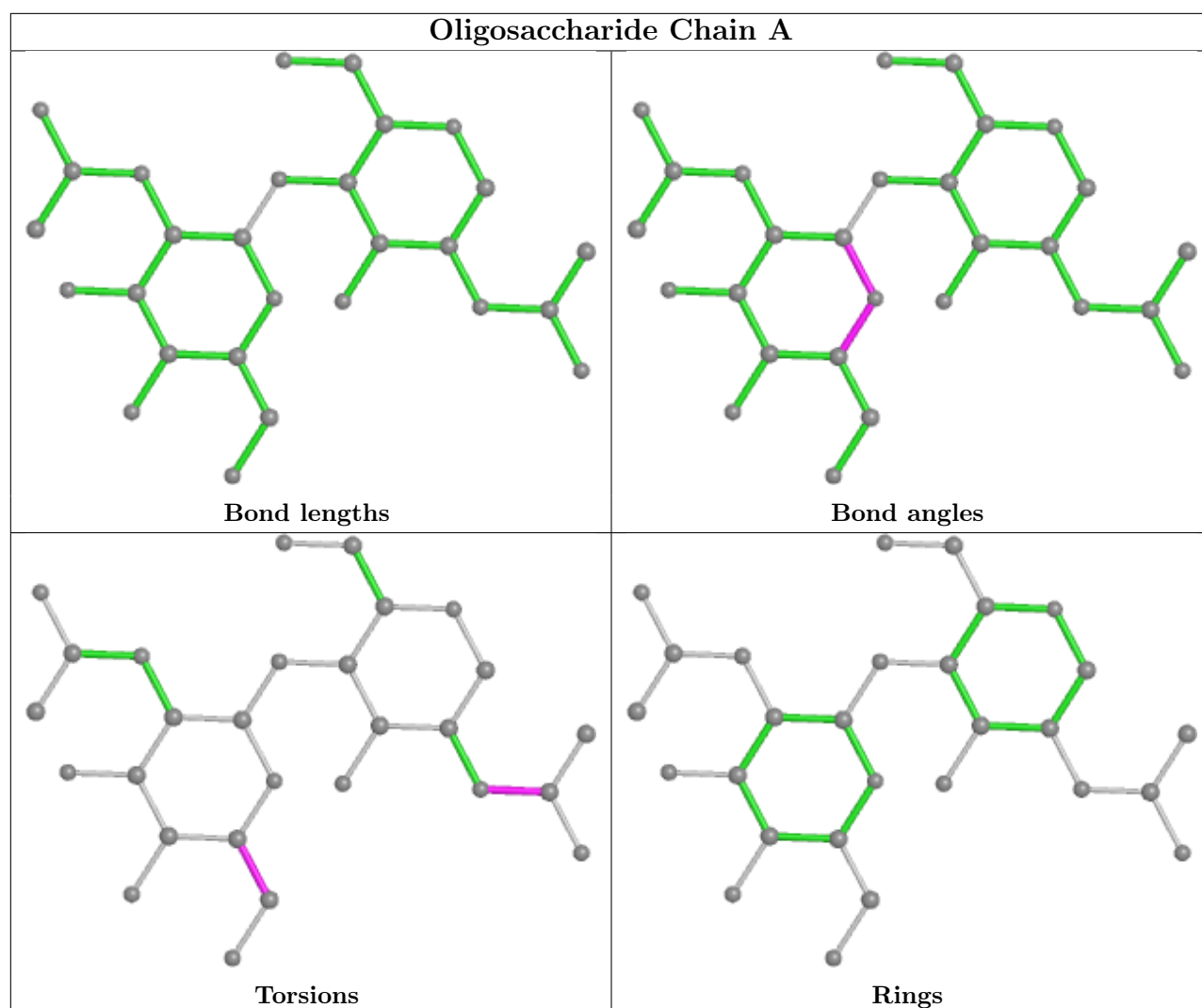
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1	NAG	C8-C7-N2-C2
5	A	1	NAG	O7-C7-N2-C2
5	A	2	NAG	C4-C5-C6-O6
5	A	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](#)

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 [i](#)

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

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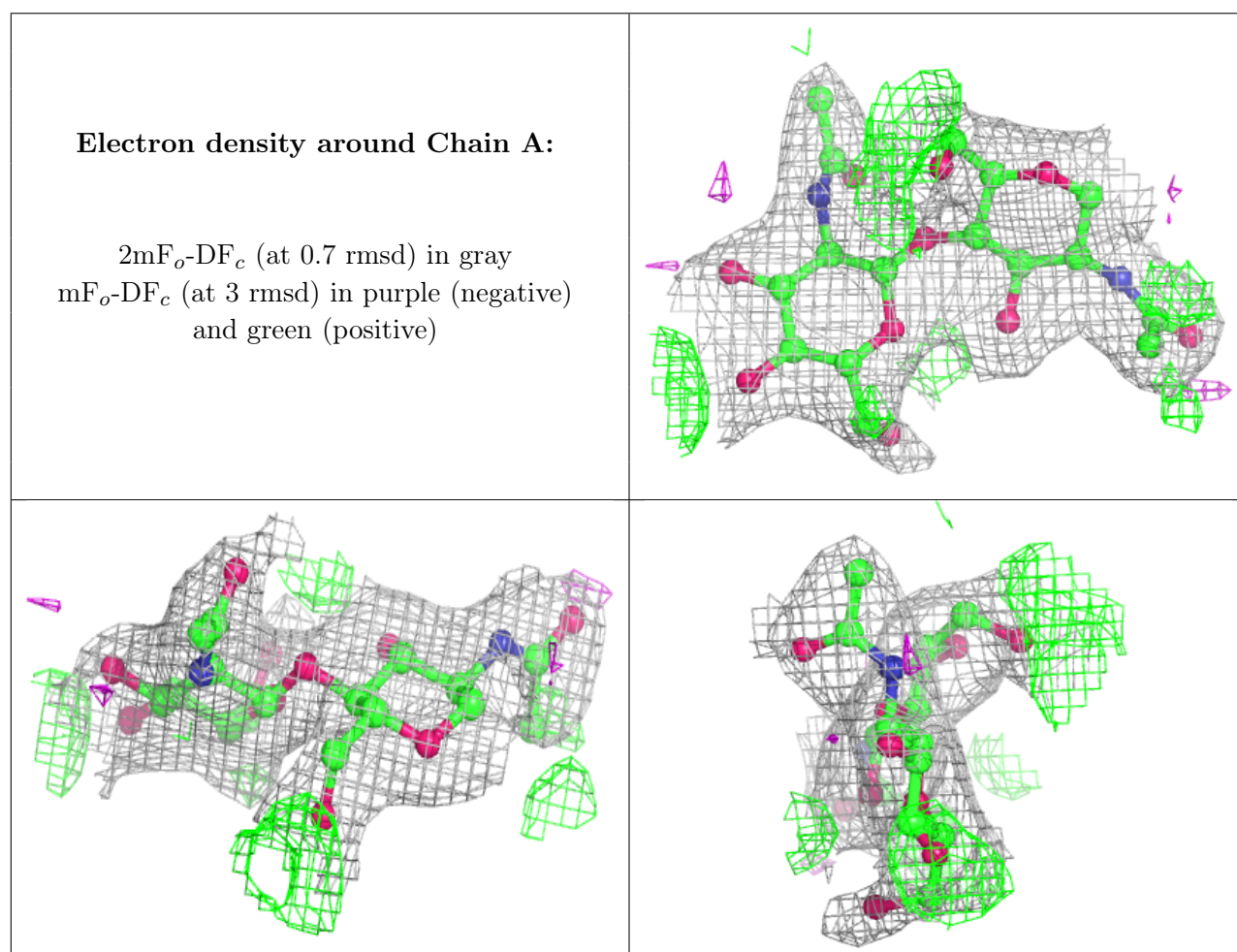
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

## 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.