



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 1, 2022 – 02:23 PM JST

PDB ID : 7FJC
Title : Crystal structure of SARS-CoV-2 Beta RBD complexed with P36-5D2 Fab
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Deposited on : 2021-08-03
Resolution : 2.96 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 ⓘ 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 ⓘ](#)) 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	:	2.29
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)	:	2.29

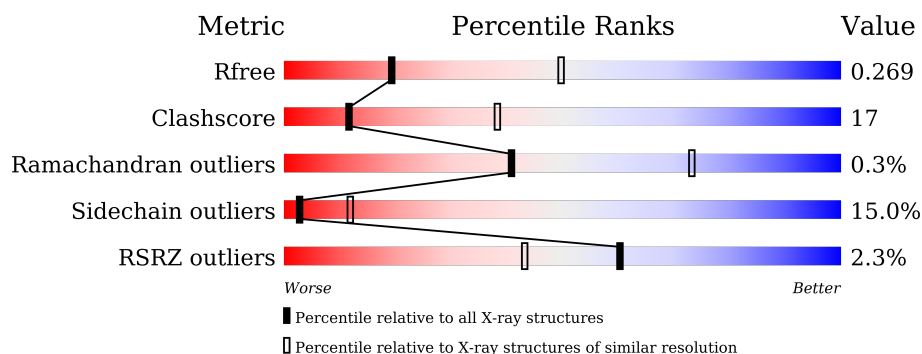
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 $\leq 5\%$. 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	H	222	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>36%</div> <div>5%</div> </div> </div>
2	L	214	<div> <div></div> <div> <div>56%</div> <div>36%</div> <div>7%</div> </div> </div>
3	E	187	<div> <div>3%</div> <div> <div></div> <div>52%</div> <div>36%</div> <div>5%</div> </div> <div>7%</div> </div>
4	A	2	<div> <div></div> <div>100%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4717 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 P36-5D2 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	216	Total	C	N	O	S	0	0	0
			1629	1029	277	316	7			

- Molecule 2 is a protein called P36-5D2 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	1	0
			1653	1036	274	336	7			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	174	Total	C	N	O	S	0	0	0
			1411	912	233	260	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	417	ASN	LYS	conflict	UNP P0DTC2
E	501	TYR	ASN	conflict	UNP P0DTC2
E	516	LEU	GLU	conflict	UNP P0DTC2

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

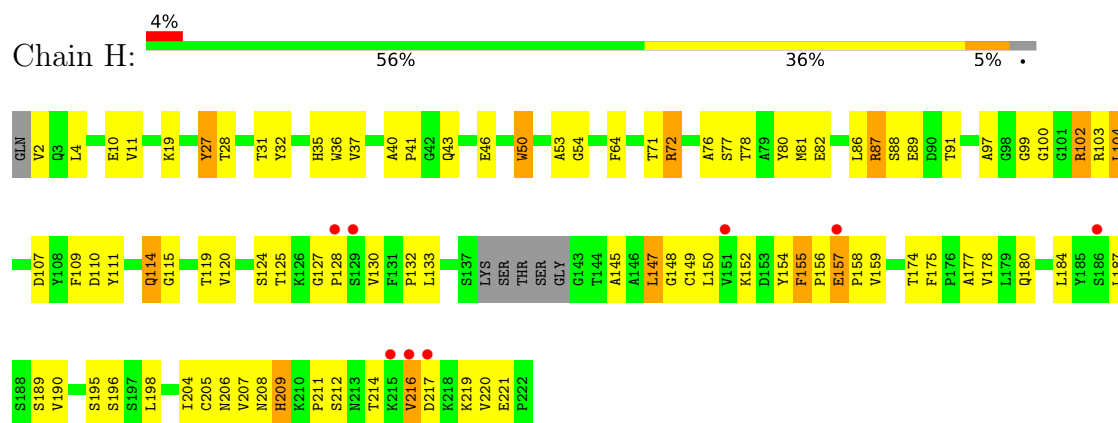


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	2	Total	C	N	O		0	0	0
			24	14	1	9				

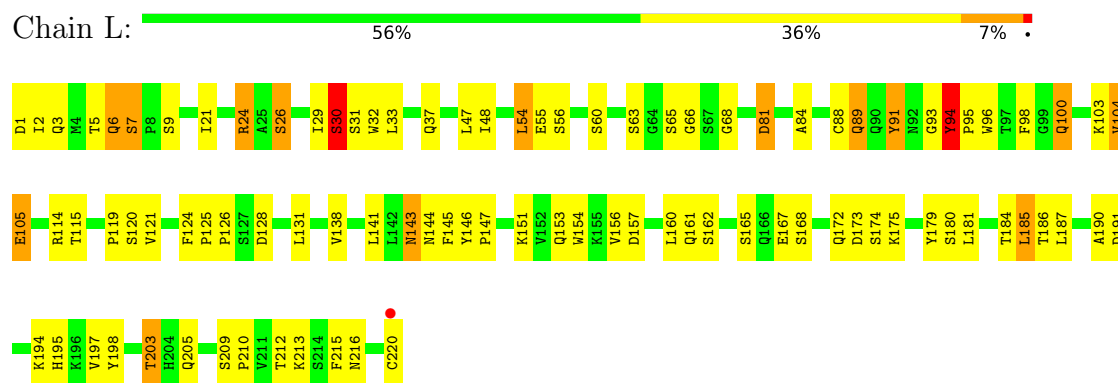
3 Residue-property plots [i](#)

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.

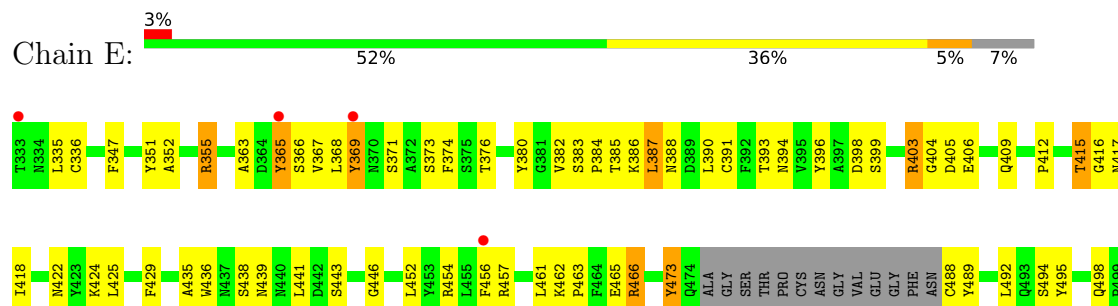
• Molecule 1: P36-5D2 heavy chain



• Molecule 2: P36-5D2 light chain




• Molecule 3: Spike protein S1





- Molecule 4: α -L-fucopyranose-(1-6)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain A:  100%

MAGI
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.11Å 42.11Å 122.09Å 90.00° 102.79° 90.00°	Depositor
Resolution (Å)	43.48 – 2.96 43.48 – 2.96	Depositor EDS
% Data completeness (in resolution range)	94.7 (43.48-2.96) 94.7 (43.48-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.212 , 0.269 0.212 , 0.269	Depositor DCC
R_{free} test set	859 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4717	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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, 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	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	H	0.44	0/1669	0.60	0/2271
2	L	0.49	0/1694	0.66	0/2302
3	E	0.61	0/1451	0.73	1/1973 (0.1%)
All	All	0.51	0/4814	0.66	1/6546 (0.0%)

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
1	H	0	1
2	L	0	3
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	466	ARG	NE-CZ-NH1	-6.31	117.15	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	155	PHE	Peptide
2	L	29	ILE	Peptide
2	L	6	GLN	Peptide
2	L	94	TYR	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	H	1629	0	1588	54	0
2	L	1653	0	1595	54	0
3	E	1411	0	1341	61	0
4	A	24	0	22	0	0
All	All	4717	0	4546	162	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 17.

The worst 5 of 162 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:E:418:ILE:HA	3:E:422:ASN:HD22	1.42	0.84
1:H:177:ALA:HA	1:H:187:LEU:HB3	1.59	0.83
2:L:143:ASN:OD1	2:L:144:ASN:ND2	2.17	0.78
3:E:415:THR:O	3:E:415:THR:OG1	2.05	0.73
1:H:88:SER:HA	1:H:120:VAL:HB	1.69	0.73

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	H	212/222 (96%)	192 (91%)	20 (9%)	0	100	100
2	L	213/214 (100%)	194 (91%)	17 (8%)	2 (1%)	17	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	170/187 (91%)	150 (88%)	20 (12%)	0	100	100
All	All	595/623 (96%)	536 (90%)	57 (10%)	2 (0%)	41	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	95	PRO
2	L	30	SER

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	H	179/184 (97%)	151 (84%)	28 (16%)	2	11
2	L	189/188 (100%)	158 (84%)	31 (16%)	2	9
3	E	154/163 (94%)	135 (88%)	19 (12%)	4	18
All	All	522/535 (98%)	444 (85%)	78 (15%)	3	12

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	209	SER
3	E	462	LYS
3	E	335	LEU
3	E	387	LEU
3	E	517	LEU

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

Mol	Chain	Res	Type
2	L	195	HIS

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$
4	NAG	A	1	3,4	14,14,15	1.12	2 (14%)	17,19,21	0.64	0
4	FUC	A	2	4	10,10,11	2.46	6 (60%)	14,14,16	1.50	4 (28%)

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	A	1	3,4	-	2/6/23/26	0/1/1/1
4	FUC	A	2	4	-	-	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2	FUC	O5-C1	5.03	1.51	1.43
4	A	2	FUC	C2-C3	3.35	1.57	1.52
4	A	1	NAG	O5-C1	2.95	1.48	1.43
4	A	1	NAG	C1-C2	2.77	1.56	1.52
4	A	2	FUC	O2-C2	2.57	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2	FUC	C1-O5-C5	3.41	120.51	112.78
4	A	2	FUC	O2-C2-C3	2.46	115.06	110.14
4	A	2	FUC	O2-C2-C1	2.22	113.69	109.15
4	A	2	FUC	O5-C1-C2	2.13	114.06	110.77

There are no chirality outliers.

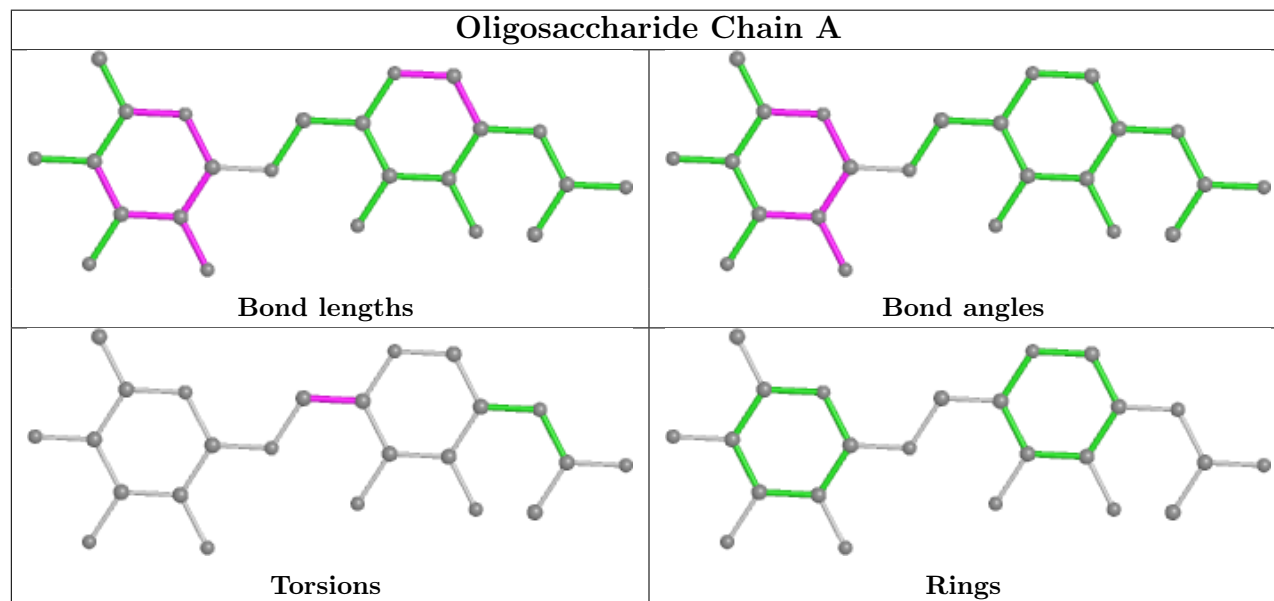
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	NAG	C4-C5-C6-O6
4	A	1	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 ⓘ

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](#)

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	H	216/222 (97%)	0.15	8 (3%) 41 27	60, 100, 129, 140	0
2	L	214/214 (100%)	-0.14	1 (0%) 91 81	56, 77, 128, 146	0
3	E	174/187 (93%)	0.20	5 (2%) 51 35	43, 65, 130, 148	0
All	All	604/623 (96%)	0.06	14 (2%) 60 43	43, 82, 129, 148	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	220	CYS	5.0
3	E	365	TYR	3.8
1	H	215	LYS	3.4
1	H	128	PRO	3.2
3	E	456	PHE	3.0

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

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

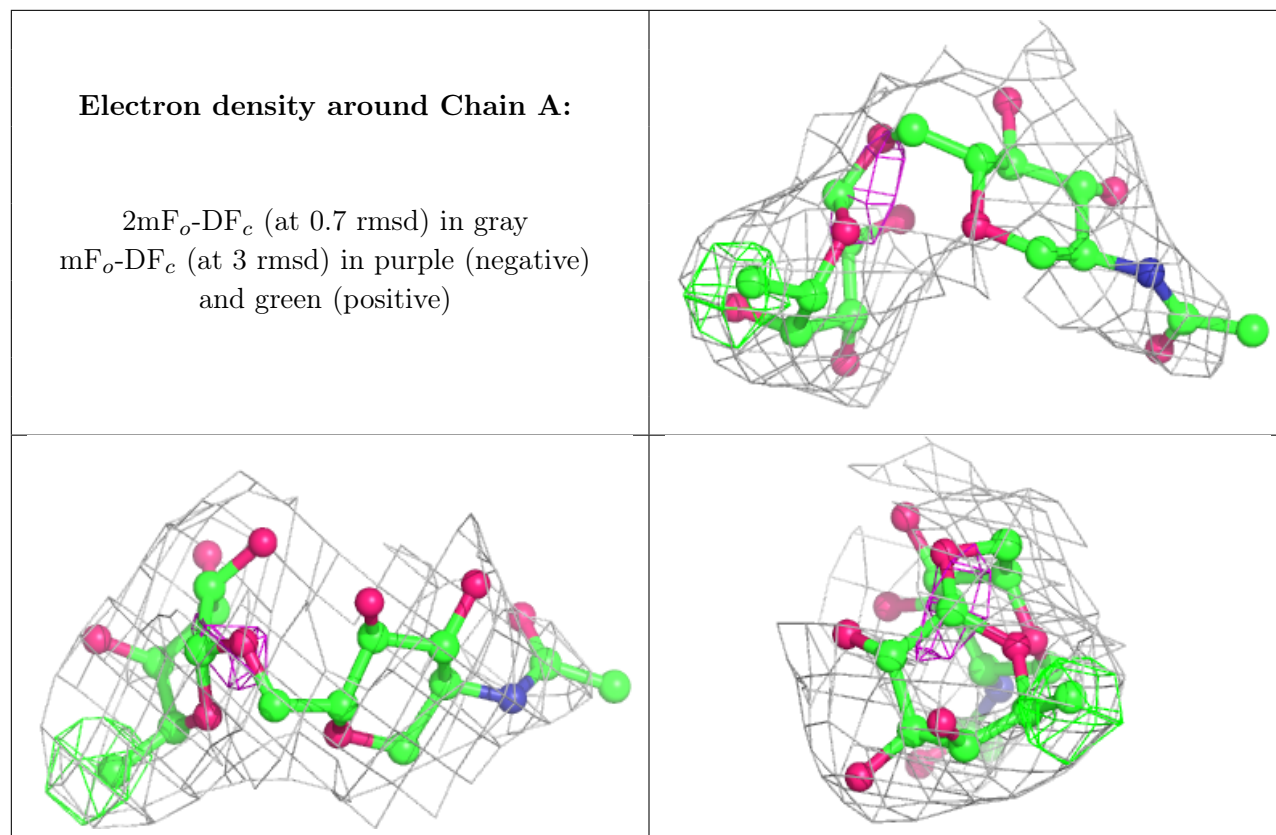
6.3 Carbohydrates [i](#)

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, 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
4	FUC	A	2	10/11	0.76	0.22	86,91,93,93	0
4	NAG	A	1	14/15	0.83	0.28	88,91,97,98	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.