



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 20, 2022 – 12:24 PM JST

PDB ID : 7Y0V  
Title : The co-crystal structure of BA.1-RBD with Fab-5549  
Authors : Xiao, J.Y.; Zhang, Y.  
Deposited on : 2022-06-06  
Resolution : 2.48 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](mailto:validation@mail.wwpdb.org)

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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	:	2.30
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)	:	2.30

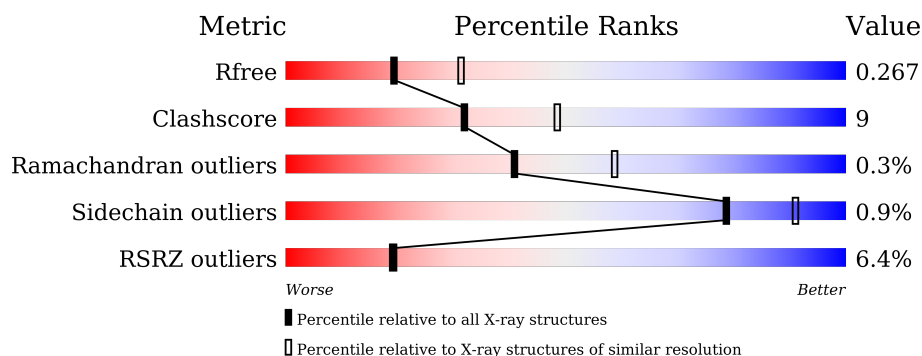
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.48 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	H	233	 7% 73% 21% . .
2	L	213	 5% 77% 21% .
3	R	225	 6% 71% 13% . 14%
4	A	4	 75% 25%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4838 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 5549-Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	223	Total	C	N	O	S	0	0	0
			1663	1059	272	327	5			

- Molecule 2 is a protein called 5549-Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	210	Total	C	N	O	S	0	0	0
			1571	984	257	326	4			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	193	Total	C	N	O	S	0	0	0
			1551	1000	262	281	8			

There are 25 discrepancies between the modelled and reference sequences:

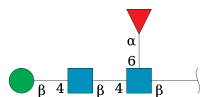
Chain	Residue	Modelled	Actual	Comment	Reference
R	339	ASP	GLY	variant	UNP P0DTC2
R	371	LEU	SER	variant	UNP P0DTC2
R	373	PRO	SER	variant	UNP P0DTC2
R	375	PHE	SER	variant	UNP P0DTC2
R	417	ASN	LYS	variant	UNP P0DTC2
R	440	LYS	ASN	variant	UNP P0DTC2
R	446	SER	GLY	variant	UNP P0DTC2
R	477	ASN	SER	variant	UNP P0DTC2
R	478	LYS	THR	variant	UNP P0DTC2
R	484	ALA	GLU	variant	UNP P0DTC2
R	493	ARG	GLN	variant	UNP P0DTC2
R	496	SER	GLY	variant	UNP P0DTC2
R	498	ARG	GLN	variant	UNP P0DTC2
R	501	TYR	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
R	505	HIS	TYR	variant	UNP P0DTC2
R	520	PRO	ALA	variant	UNP P0DTC2
R	521	ALA	PRO	variant	UNP P0DTC2
R	542	HIS	-	expression tag	UNP P0DTC2
R	543	HIS	-	expression tag	UNP P0DTC2
R	544	HIS	-	expression tag	UNP P0DTC2
R	545	HIS	-	expression tag	UNP P0DTC2
R	546	HIS	-	expression tag	UNP P0DTC2
R	547	HIS	-	expression tag	UNP P0DTC2
R	548	HIS	-	expression tag	UNP P0DTC2
R	549	HIS	-	expression tag	UNP P0DTC2

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	A	4	Total	C	N	O	0	0	0
			49	28	2	19			

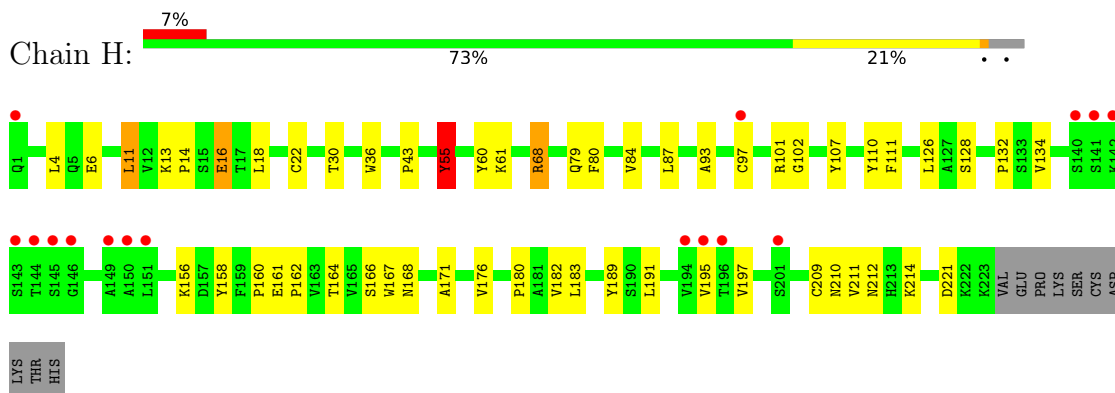
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	2	Total	O	0	0
			2	2		
5	L	1	Total	O	0	0
			1	1		
5	R	1	Total	O	0	0
			1	1		

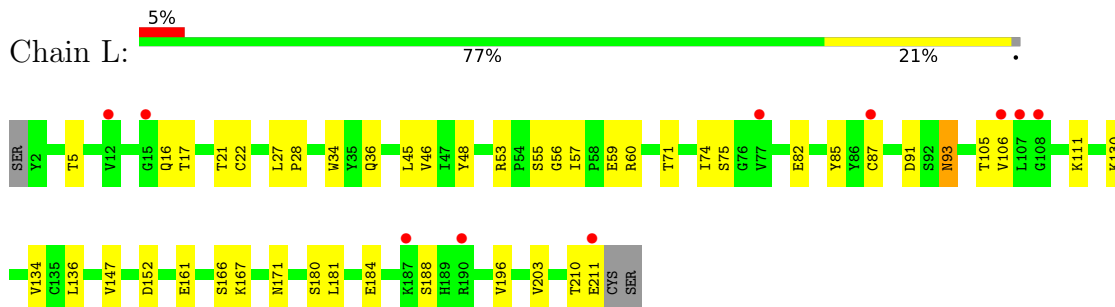
### 3 Residue-property plots [i](#)

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.

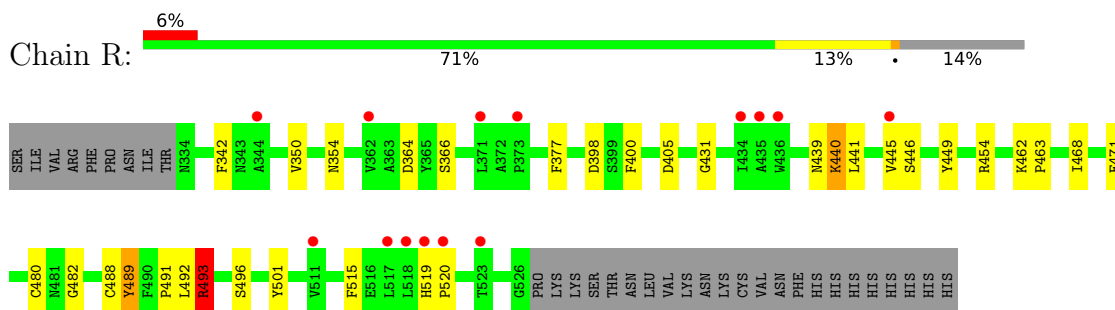
- Molecule 1: 5549-Fab



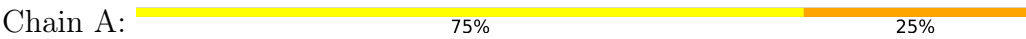
- Molecule 2: 5549-Fab



- Molecule 3: Spike protein S1



- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



MG1
MG2
MG3
FUC4

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.77Å 138.91Å 178.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.09 – 2.48 34.09 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.09-2.48) 99.9 (34.09-2.48)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.211 , 0.268 0.211 , 0.267	Depositor DCC
$R_{free}$ test set	1999 reflections (6.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.1	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 58.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4838	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: FUC, BMA, 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	H	0.56	0/1709	0.83	6/2336 (0.3%)
2	L	0.56	0/1611	0.76	2/2210 (0.1%)
3	R	0.66	3/1597 (0.2%)	0.83	3/2173 (0.1%)
All	All	0.59	3/4917 (0.1%)	0.81	11/6719 (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
3	R	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	489	TYR	CD1-CE1	-7.39	1.28	1.39
3	R	489	TYR	CB-CG	-6.12	1.42	1.51
3	R	489	TYR	CD2-CE2	-6.00	1.30	1.39

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	68	ARG	CB-CG-CD	7.91	132.16	111.60
3	R	493	ARG	CD-NE-CZ	6.68	132.95	123.60
1	H	68	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	H	68	ARG	CG-CD-NE	-6.36	98.44	111.80
3	R	493	ARG	NE-CZ-NH2	-6.36	117.12	120.30

There are no chirality outliers.



All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	R	493	ARG	Sidechain

## 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	H	1663	0	1641	42	0
2	L	1571	0	1507	27	0
3	R	1551	0	1481	23	1
4	A	49	0	43	2	0
5	H	2	0	0	2	0
5	L	1	0	0	0	0
5	R	1	0	0	0	0
All	All	4838	0	4672	85	1

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 9.

The worst 5 of 85 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:R:480:CYS:HB3	3:R:488:CYS:SG	2.13	0.88
1:H:18:LEU:HB2	1:H:87:LEU:HD11	1.55	0.84
1:H:61:LYS:NZ	5:H:301:HOH:O	2.15	0.80
2:L:21:THR:HG22	2:L:71:THR:HG22	1.69	0.74
1:H:156:LYS:NZ	2:L:130:LYS:HE3	2.12	0.64

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:489:TYR:OH	3:R:493:ARG:NH2[3_855]	2.12	0.08

## 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	221/233 (95%)	206 (93%)	15 (7%)	0	100	100
2	L	208/213 (98%)	189 (91%)	18 (9%)	1 (0%)	29	46
3	R	191/225 (85%)	175 (92%)	15 (8%)	1 (0%)	29	46
All	All	620/671 (92%)	570 (92%)	48 (8%)	2 (0%)	41	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	R	440	LYS
2	L	152	ASP

### 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	190/200 (95%)	188 (99%)	2 (1%)	73	88
2	L	177/180 (98%)	175 (99%)	2 (1%)	73	88
3	R	168/200 (84%)	167 (99%)	1 (1%)	86	94
All	All	535/580 (92%)	530 (99%)	5 (1%)	78	91

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

Mol	Chain	Res	Type
1	H	55	TYR

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Mol	Chain	Res	Type
1	H	128	SER
2	L	105	THR
2	L	111	LYS
3	R	377	PHE

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 ⓘ

4 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	4,3	14,14,15	1.04	1 (7%)	17,19,21	0.73	1 (5%)
4	NAG	A	2	4	14,14,15	0.50	0	17,19,21	0.49	0
4	BMA	A	3	4	11,11,12	1.61	4 (36%)	15,15,17	0.91	0
4	FUC	A	4	4	10,10,11	0.64	0	14,14,16	0.96	1 (7%)

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	4,3	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	1/6/23/26	0/1/1/1
4	BMA	A	3	4	-	2/2/19/22	0/1/1/1
4	FUC	A	4	4	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	NAG	O5-C1	-3.73	1.37	1.43
4	A	3	BMA	C4-C5	2.95	1.59	1.53
4	A	3	BMA	O5-C1	2.36	1.47	1.43
4	A	3	BMA	C4-C3	2.20	1.57	1.52
4	A	3	BMA	C2-C3	2.18	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	NAG	C1-O5-C5	2.08	115.01	112.19
4	A	4	FUC	O3-C3-C4	-2.05	105.62	110.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

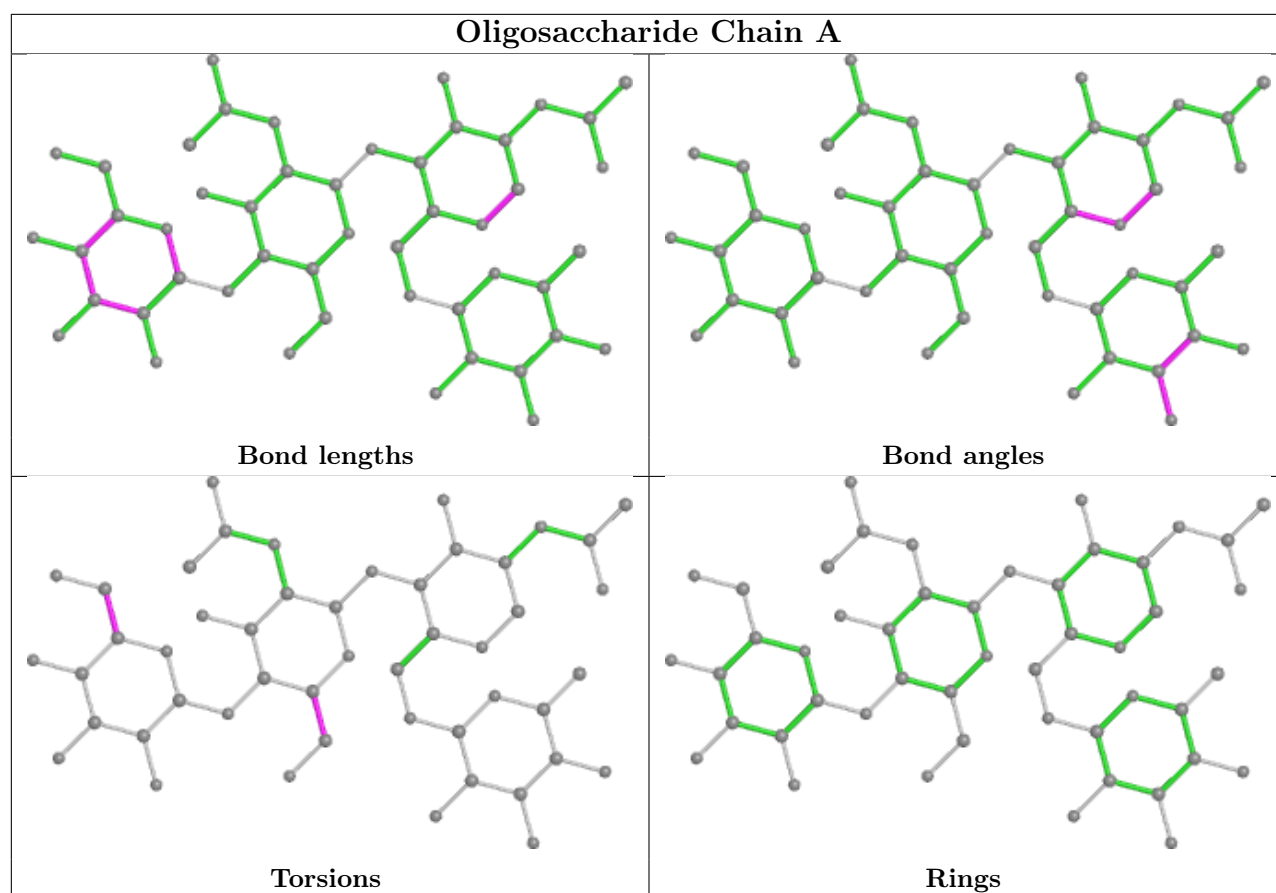
Mol	Chain	Res	Type	Atoms
4	A	3	BMA	O5-C5-C6-O6
4	A	3	BMA	C4-C5-C6-O6
4	A	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	NAG	1	0
4	A	2	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 [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<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	H	223/233 (95%)	0.35	16 (7%) 15 15	62, 80, 119, 151	0
2	L	210/213 (98%)	0.38	10 (4%) 30 32	61, 84, 105, 143	0
3	R	193/225 (85%)	0.41	14 (7%) 15 14	60, 79, 116, 141	0
All	All	626/671 (93%)	0.38	40 (6%) 19 19	60, 81, 112, 151	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	143	SER	6.0
1	H	145	SER	5.5
2	L	107	LEU	5.0
2	L	211	GLU	4.7
3	R	517	LEU	4.7

### 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<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.

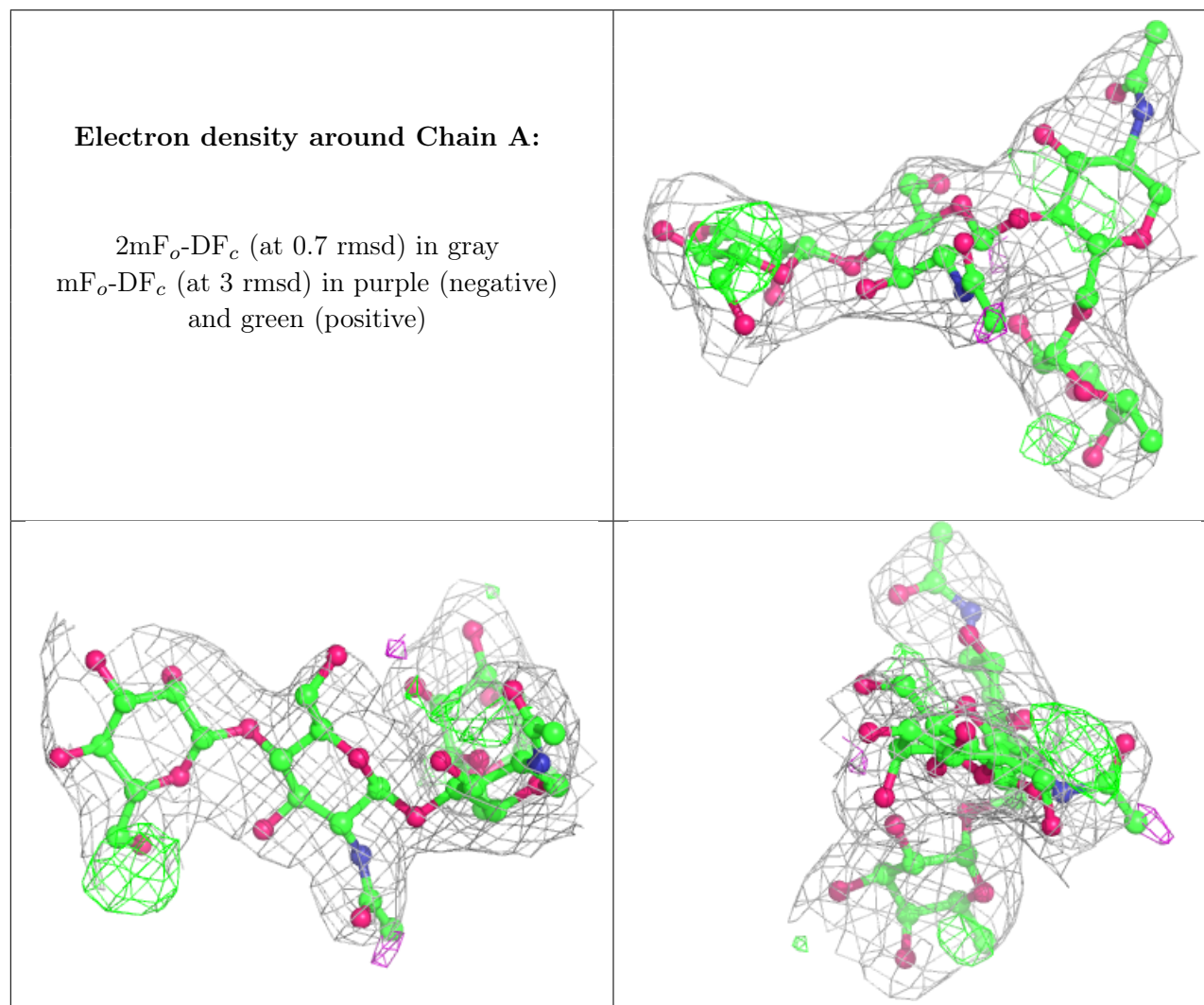
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	BMA	A	3	11/12	0.81	0.15	100,102,106,111	0
4	NAG	A	2	14/15	0.94	0.14	72,82,93,96	0
4	NAG	A	1	14/15	0.95	0.20	63,75,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FUC	A	4	10/11	0.98	0.17	64,69,73,74	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.