



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 22, 2021 – 06:03 PM EST

PDB ID : 7RKS  
Title : Structure of the SARS-CoV receptor binding domain in complex with the human neutralizing antibody Fab fragment, C118  
Authors : Jette, C.A.; Bjorkman, P.J.; Barnes, C.O.  
Deposited on : 2021-07-22  
Resolution : 2.70 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)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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	:	2.25
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)	:	2.25

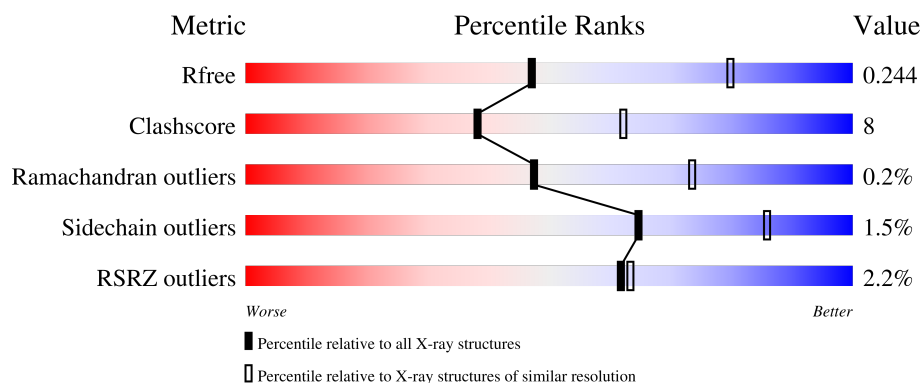
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	238	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>8%</div> </div> </div>
1	I	238	<div> <div></div> <div>79%</div> <div>14%</div> <div>7%</div> </div>
2	L	214	<div> <div>9%</div> <div></div> <div>82%</div> <div>18%</div> </div>
2	M	214	<div> <div>%</div> <div></div> <div>82%</div> <div>18%</div> </div>
3	R	196	<div> <div>%</div> <div></div> <div>75%</div> <div>16%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
3	S	196	
4	A	2	
5	B	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	2	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9582 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 C118 Antibody Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	220	Total	C	N	O	S	0	0	0
			1673	1061	281	325	6			
1	I	222	Total	C	N	O	S	0	0	0
			1685	1067	283	329	6			

- Molecule 2 is a protein called C118 Antibody Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1594	996	268	325	5			
2	M	214	Total	C	N	O	S	0	0	0
			1598	998	269	326	5			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	182	Total	C	N	O	S	0	0	0
			1465	948	238	271	8			
3	S	187	Total	C	N	O	S	0	0	0
			1501	972	244	277	8			

There are 12 discrepancies between the modelled and reference sequences:

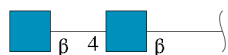
Chain	Residue	Modelled	Actual	Comment	Reference
R	511	HIS	-	expression tag	UNP P59594
R	512	HIS	-	expression tag	UNP P59594
R	513	HIS	-	expression tag	UNP P59594
R	514	HIS	-	expression tag	UNP P59594
R	515	HIS	-	expression tag	UNP P59594
R	516	HIS	-	expression tag	UNP P59594
S	511	HIS	-	expression tag	UNP P59594
S	512	HIS	-	expression tag	UNP P59594

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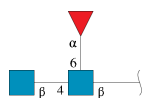
Chain	Residue	Modelled	Actual	Comment	Reference
S	513	HIS	-	expression tag	UNP P59594
S	514	HIS	-	expression tag	UNP P59594
S	515	HIS	-	expression tag	UNP P59594
S	516	HIS	-	expression tag	UNP P59594

- Molecule 4 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
4	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

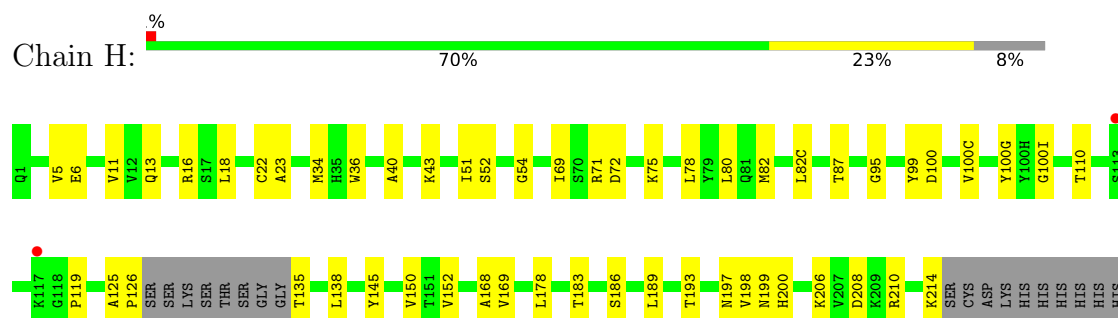


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	B	3	Total	C	N	O	0	0	0
			38	22	2	14			

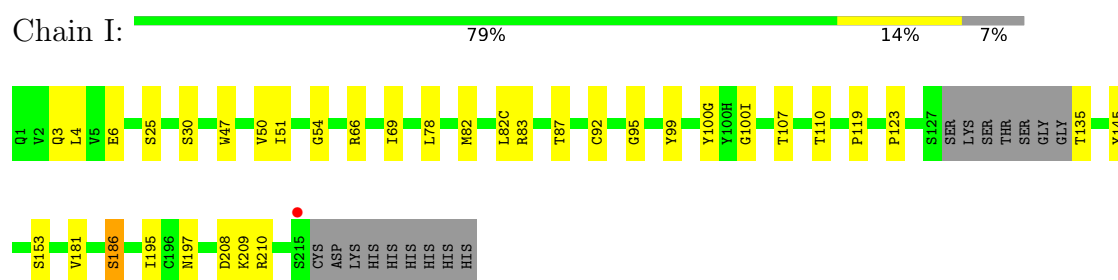
### 3 Residue-property plots

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.

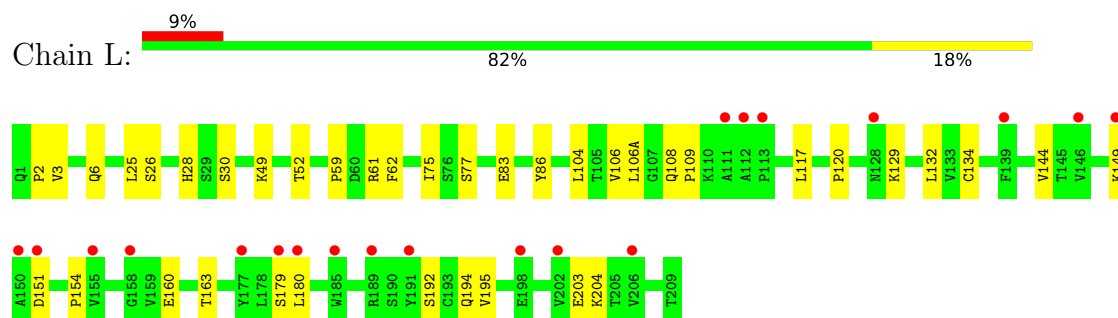
#### • Molecule 1: C118 Antibody Fab Heavy Chain



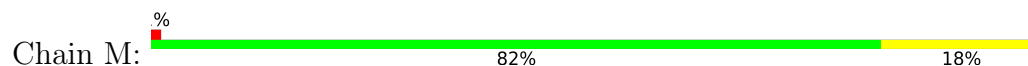
#### • Molecule 1: C118 Antibody Fab Heavy Chain

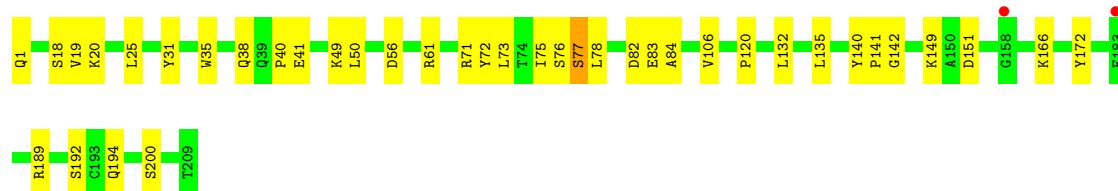


#### • Molecule 2: C118 Antibody Fab Light Chain

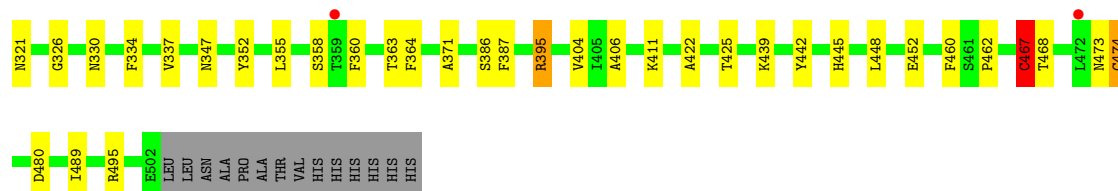
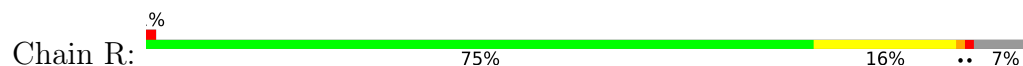


#### • Molecule 2: C118 Antibody Fab Light Chain

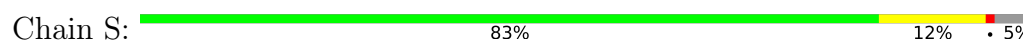




- Molecule 3: Spike protein S1



- Molecule 3: Spike protein S1



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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.92Å 89.99Å 93.86Å 90.00° 113.33° 90.00°	Depositor
Resolution (Å)	46.61 – 2.70 46.61 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.7 (46.61-2.70) 87.4 (46.61-2.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.60 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.195 , 0.247 0.191 , 0.244	Depositor DCC
$R_{free}$ test set	1821 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.2	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9582	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5459e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 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	0.48	0/1715	0.68	0/2337
1	I	0.52	0/1727	0.70	0/2353
2	L	0.40	0/1633	0.65	0/2226
2	M	0.48	0/1637	0.70	0/2231
3	R	0.56	0/1512	0.75	2/2062 (0.1%)
3	S	0.58	1/1549 (0.1%)	0.74	0/2114
All	All	0.50	1/9773 (0.0%)	0.70	2/13323 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	467	CYS	CB-SG	-5.71	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	474	CYS	CA-CB-SG	-9.23	97.39	114.00
3	R	467	CYS	CA-CB-SG	-6.58	102.16	114.00

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	H	1673	0	1622	41	0
1	I	1685	0	1632	21	0
2	L	1594	0	1545	26	0
2	M	1598	0	1551	27	0
3	R	1465	0	1384	23	0
3	S	1501	0	1424	13	0
4	A	28	0	25	1	0
5	B	38	0	34	0	0
All	All	9582	0	9217	143	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 8.

The worst 5 of 143 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:I:135:THR:N	1:I:186:SER:HG	1.36	1.23
1:H:135:THR:N	1:H:186:SER:HG	1.49	1.10
3:S:467:CYS:SG	3:S:468:THR:N	2.39	0.96
2:M:142:GLY:HA3	2:M:172:TYR:HD2	1.31	0.92
3:R:358:SER:HB3	3:R:360:PHE:CE1	2.07	0.90

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	216/238 (91%)	209 (97%)	7 (3%)	0	100	100
1	I	218/238 (92%)	212 (97%)	6 (3%)	0	100	100
2	L	212/214 (99%)	201 (95%)	9 (4%)	2 (1%)	17	40
2	M	212/214 (99%)	199 (94%)	12 (6%)	1 (0%)	29	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	R	180/196 (92%)	164 (91%)	16 (9%)	0	100	100
3	S	185/196 (94%)	171 (92%)	14 (8%)	0	100	100
All	All	1223/1296 (94%)	1156 (94%)	64 (5%)	3 (0%)	47	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	106(A)	LEU
2	L	151	ASP
2	M	151	ASP

### 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	H	184/200 (92%)	184 (100%)	0	100	100
1	I	186/200 (93%)	184 (99%)	2 (1%)	73	90
2	L	178/179 (99%)	176 (99%)	2 (1%)	73	90
2	M	179/179 (100%)	175 (98%)	4 (2%)	52	79
3	R	160/172 (93%)	156 (98%)	4 (2%)	47	76
3	S	164/172 (95%)	160 (98%)	4 (2%)	49	77
All	All	1051/1102 (95%)	1035 (98%)	16 (2%)	65	86

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	S	433	THR
3	S	426	ARG
3	R	364	PHE
3	S	364	PHE
2	M	200	SER

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 ⓘ

5 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	1.23	1 (7%)	17,19,21	1.35	1 (5%)
4	NAG	A	2	4	14,14,15	0.37	0	17,19,21	0.98	1 (5%)
5	NAG	B	1	5,3	14,14,15	0.35	0	17,19,21	0.55	0
5	NAG	B	2	5	14,14,15	0.36	0	17,19,21	0.64	0
5	FUC	B	3	5	10,10,11	1.09	1 (10%)	14,14,16	1.04	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	3,4	-	1/6/23/26	0/1/1/1
4	NAG	A	2	4	-	3/6/23/26	0/1/1/1
5	NAG	B	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	B	2	5	-	0/6/23/26	0/1/1/1
5	FUC	B	3	5	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	NAG	C1-C2	4.01	1.58	1.52
5	B	3	FUC	C1-C2	2.70	1.58	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	NAG	C2-N2-C7	4.48	129.28	122.90
4	A	2	NAG	C2-N2-C7	2.80	126.89	122.90
5	B	3	FUC	O2-C2-C1	2.74	114.76	109.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

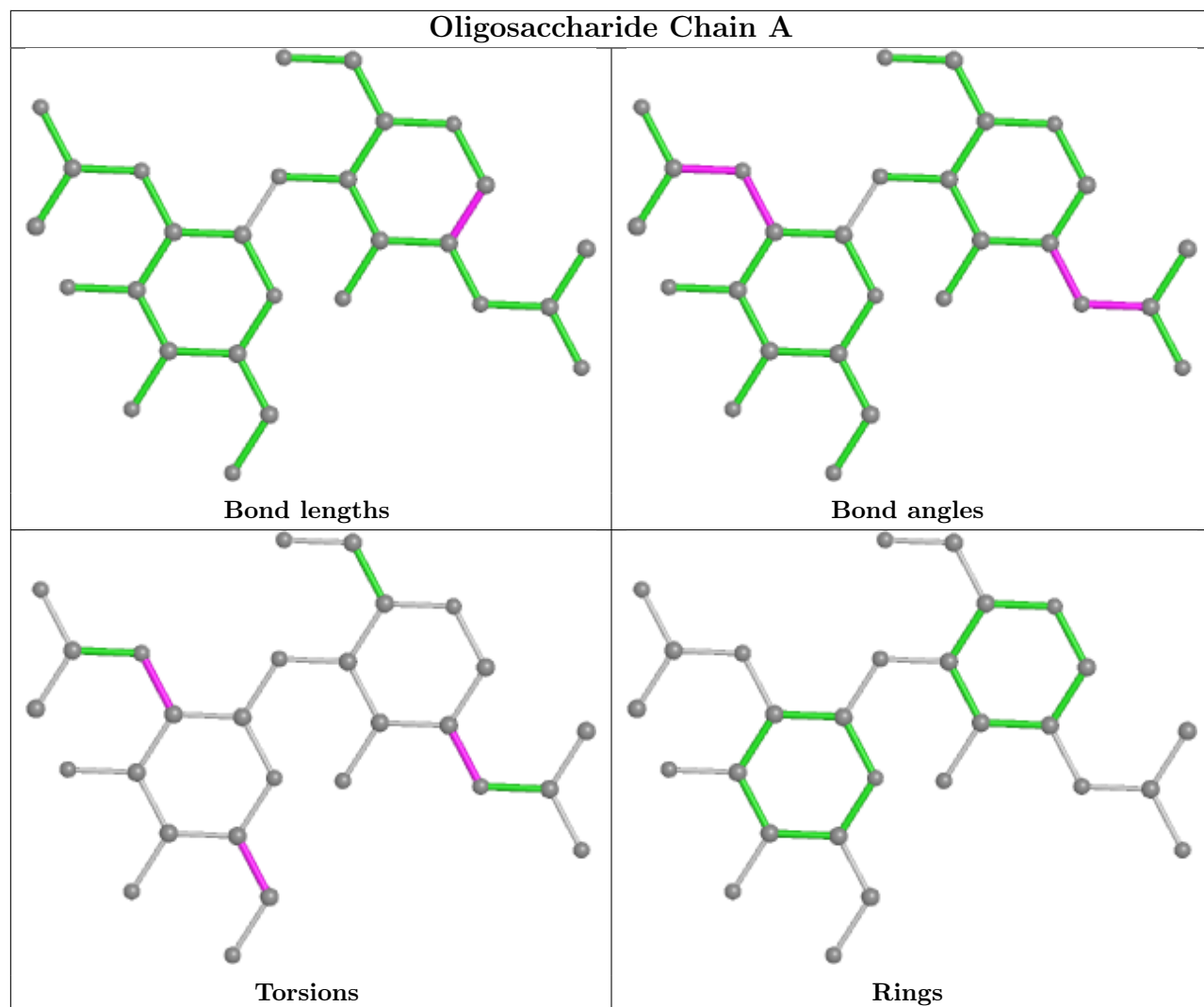
Mol	Chain	Res	Type	Atoms
4	A	1	NAG	C3-C2-N2-C7
4	A	2	NAG	C1-C2-N2-C7
4	A	2	NAG	O5-C5-C6-O6
4	A	2	NAG	C4-C5-C6-O6

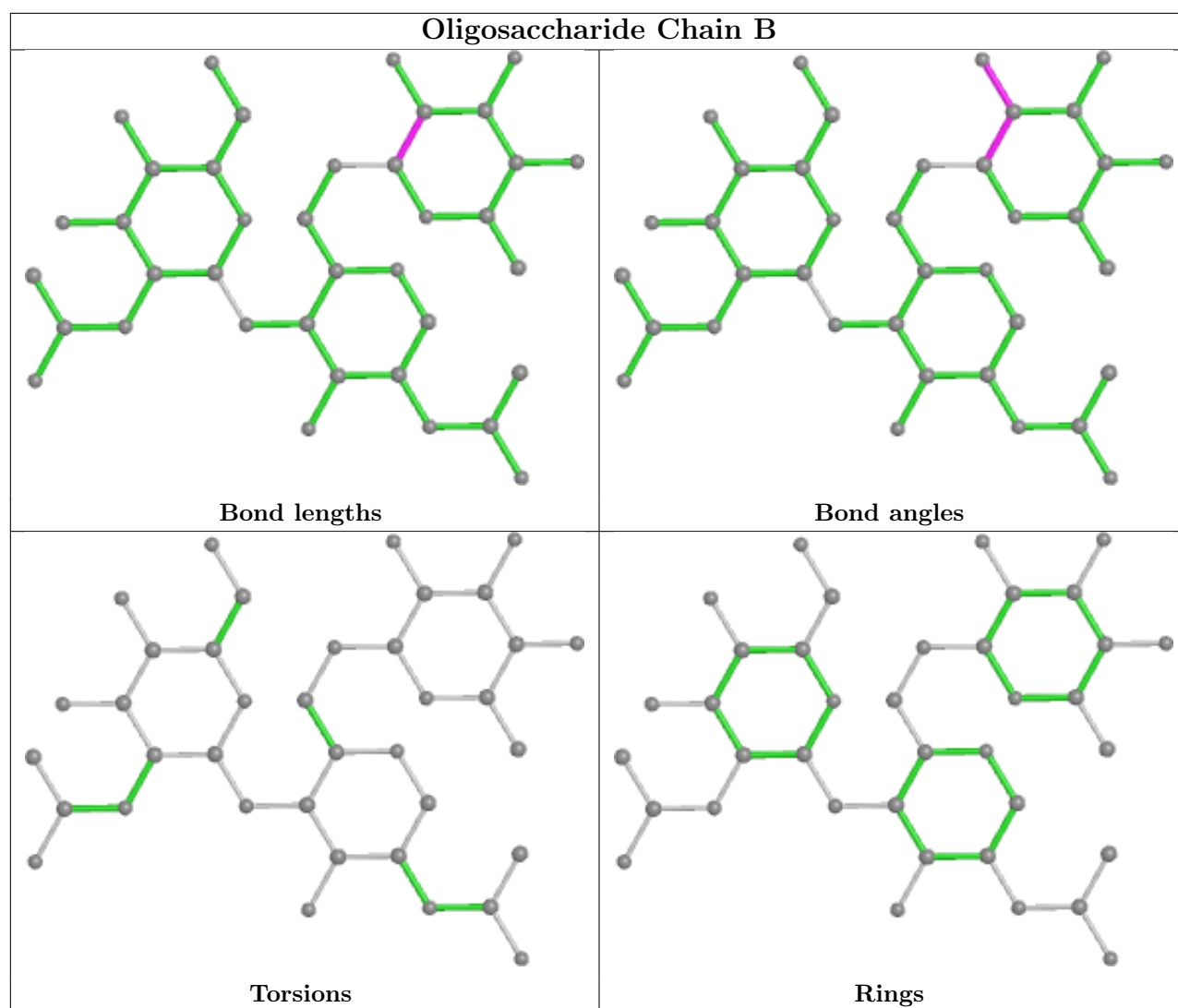
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	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 [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	220/238 (92%)	0.26	2 (0%) 84 85	45, 65, 79, 99	0
1	I	222/238 (93%)	0.15	1 (0%) 91 92	37, 55, 78, 90	0
2	L	214/214 (100%)	0.55	20 (9%) 8 6	48, 82, 114, 122	0
2	M	214/214 (100%)	0.17	2 (0%) 84 85	37, 62, 83, 95	0
3	R	182/196 (92%)	0.06	2 (1%) 80 82	39, 56, 82, 90	0
3	S	187/196 (95%)	-0.07	0 100 100	35, 48, 70, 82	0
All	All	1239/1296 (95%)	0.20	27 (2%) 62 63	35, 61, 92, 122	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	111	ALA	3.8
2	L	191	TYR	3.5
3	R	472	LEU	3.1
2	L	139	PHE	3.0
2	L	189	ARG	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.

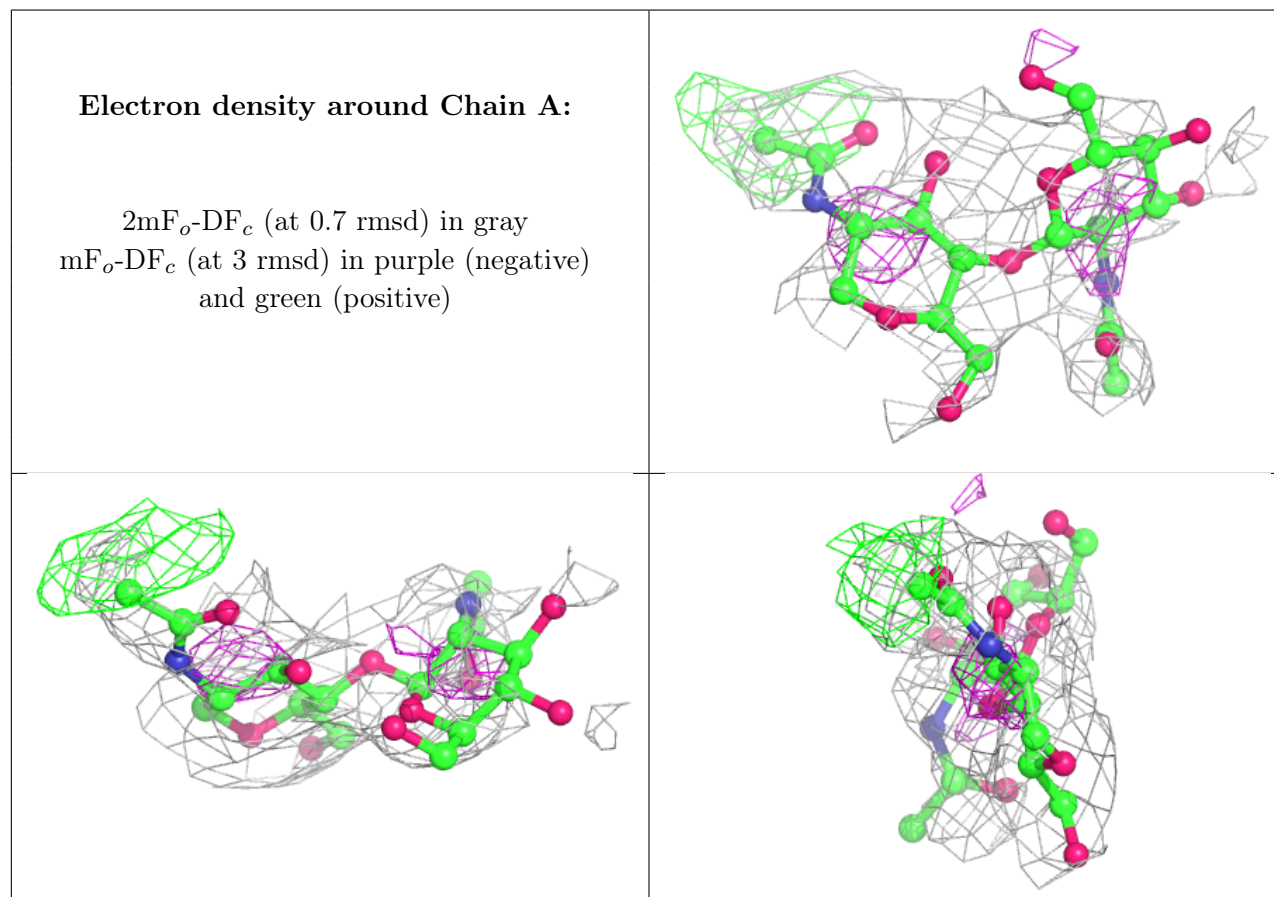
### 6.3 Carbohydrates [i](#)

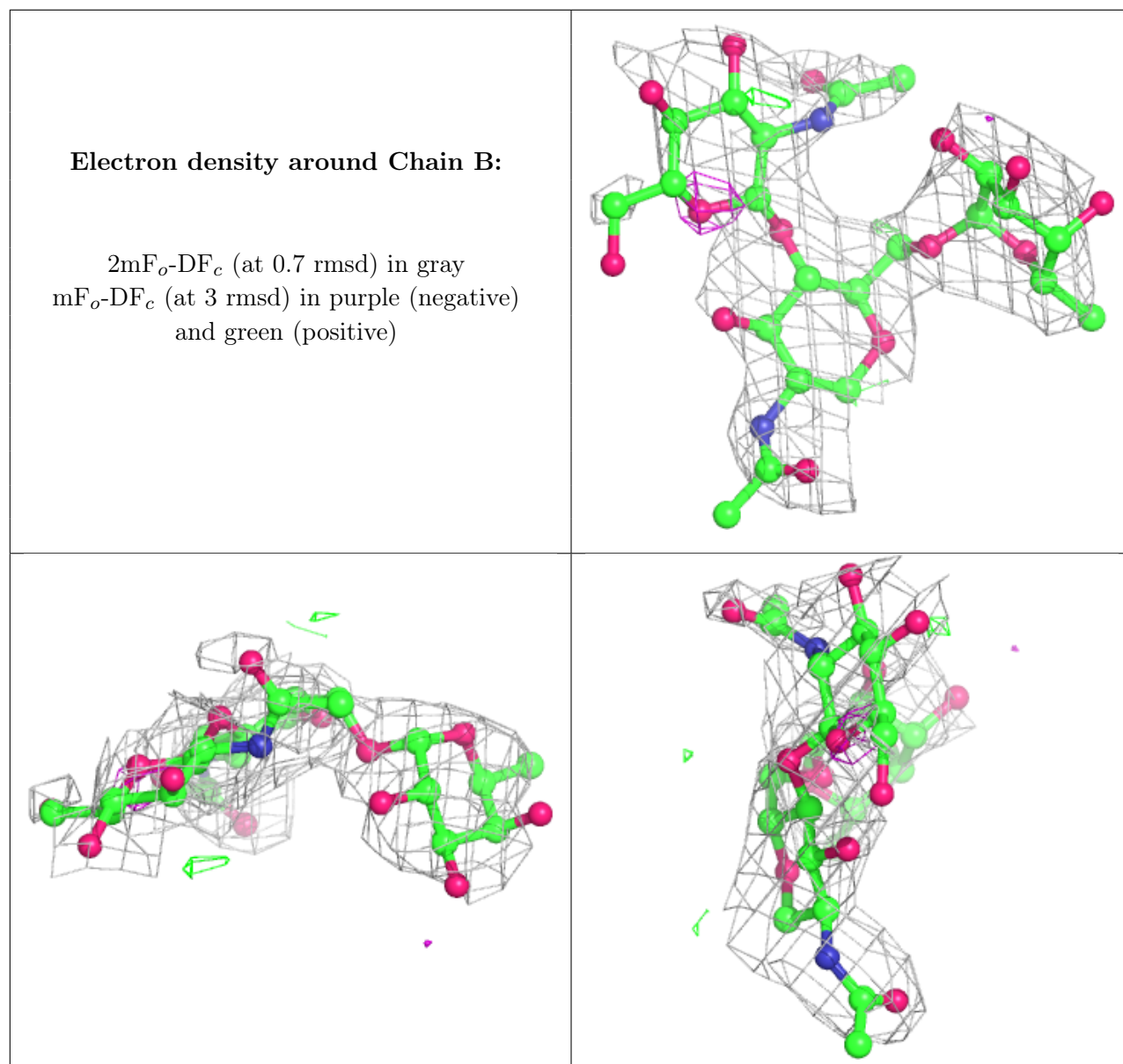
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	1	14/15	0.61	0.25	67,90,99,104	0
4	NAG	A	2	14/15	0.62	0.42	90,108,115,116	0
5	NAG	B	2	14/15	0.64	0.39	94,109,119,119	0
5	NAG	B	1	14/15	0.86	0.32	83,91,101,101	0
5	FUC	B	3	10/11	0.87	0.33	76,88,98,98	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.