



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 5, 2026 – 03:10 AM UTC

PDB ID : 9D09 / pdb\_00009d09  
Title : Crystal structure of IgG1 FC M252H at pH 5.6  
Authors : Reddem, E.R.; Shapiro, L.  
Deposited on : 2024-08-06  
Resolution : 2.92 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.

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

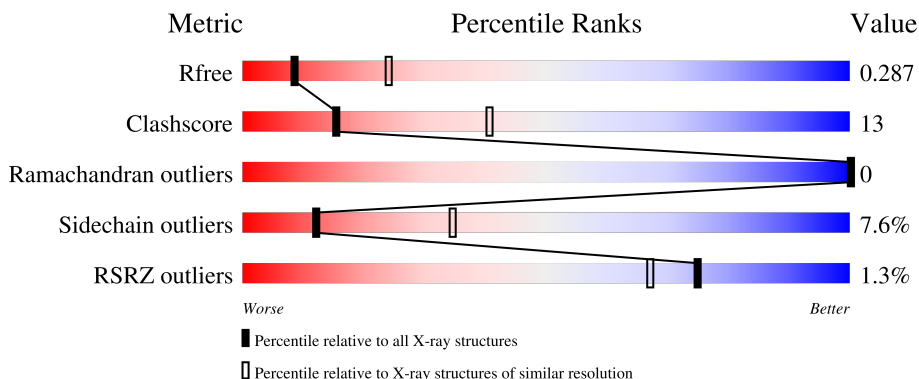
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.92 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))
$R_{free}$	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	A	231	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 60%; height: 10px; background-color: green;"></div> <div style="width: 26%; height: 10px; background-color: yellow;"></div> <div style="width: 10%; height: 10px; background-color: orange;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>60%</span> <span>26%</span> <span>• 10%</span> </div> </div>
1	B	231	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 27%; height: 10px; background-color: green;"></div> <div style="width: 18%; height: 10px; background-color: yellow;"></div> <div style="width: 55%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>27%</span> <span>18%</span> <span>55%</span> </div> </div>
2	C	7	<div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>71%</span> <span>29%</span> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2574 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 Immunoglobulin gamma-1 heavy chain Fc Fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1666	1060	282	319	5			
1	B	104	Total	C	N	O	S	0	0	0
			826	521	139	163	3			

There are 40 discrepancies between the modelled and reference sequences:

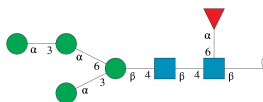
Chain	Residue	Modelled	Actual	Comment	Reference
A	217	MET	-	initiating methionine	UNP P0DOX5
A	218	GLY	-	expression tag	UNP P0DOX5
A	219	TRP	-	expression tag	UNP P0DOX5
A	220	SER	-	expression tag	UNP P0DOX5
A	221	CYS	-	expression tag	UNP P0DOX5
A	222	ILE	-	expression tag	UNP P0DOX5
A	223	ILE	-	expression tag	UNP P0DOX5
A	224	LEU	-	expression tag	UNP P0DOX5
A	225	PHE	-	expression tag	UNP P0DOX5
A	226	LEU	-	expression tag	UNP P0DOX5
A	227	VAL	-	expression tag	UNP P0DOX5
A	228	ALA	-	expression tag	UNP P0DOX5
A	229	THR	-	expression tag	UNP P0DOX5
A	230	ALA	-	expression tag	UNP P0DOX5
A	231	THR	-	expression tag	UNP P0DOX5
A	232	GLY	-	expression tag	UNP P0DOX5
A	233	VAL	-	expression tag	UNP P0DOX5
A	234	HIS	-	expression tag	UNP P0DOX5
A	235	SER	-	expression tag	UNP P0DOX5
A	252	HIS	MET	engineered mutation	UNP P0DOX5
B	217	MET	-	initiating methionine	UNP P0DOX5
B	218	GLY	-	expression tag	UNP P0DOX5
B	219	TRP	-	expression tag	UNP P0DOX5
B	220	SER	-	expression tag	UNP P0DOX5
B	221	CYS	-	expression tag	UNP P0DOX5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	222	ILE	-	expression tag	UNP P0DOX5
B	223	ILE	-	expression tag	UNP P0DOX5
B	224	LEU	-	expression tag	UNP P0DOX5
B	225	PHE	-	expression tag	UNP P0DOX5
B	226	LEU	-	expression tag	UNP P0DOX5
B	227	VAL	-	expression tag	UNP P0DOX5
B	228	ALA	-	expression tag	UNP P0DOX5
B	229	THR	-	expression tag	UNP P0DOX5
B	230	ALA	-	expression tag	UNP P0DOX5
B	231	THR	-	expression tag	UNP P0DOX5
B	232	GLY	-	expression tag	UNP P0DOX5
B	233	VAL	-	expression tag	UNP P0DOX5
B	234	HIS	-	expression tag	UNP P0DOX5
B	235	SER	-	expression tag	UNP P0DOX5
B	252	HIS	MET	engineered mutation	UNP P0DOX5

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
2	C	7	Total	C	N	O	0	0	0
			82	46	2	34			



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.41Å 111.56Å 63.74Å 90.00° 96.07° 90.00°	Depositor
Resolution (Å)	33.52 – 2.92 33.52 – 2.92	Depositor EDS
% Data completeness (in resolution range)	73.0 (33.52-2.92) 73.0 (33.52-2.92)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.203 , 0.283 0.206 , 0.287	Depositor DCC
$R_{free}$ test set	348 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.9	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 29.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	2574	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.07% 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: MAN, 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	A	0.54	0/1713	0.66	0/2335
1	B	0.48	0/849	0.62	0/1156
All	All	0.52	0/2562	0.65	0/3491

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	1666	0	1628	43	0
1	B	826	0	784	27	0
2	C	82	0	70	2	0
All	All	2574	0	2482	68	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 13.

The worst 5 of 68 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:B:373:TYR:HD1	1:B:374:PRO:HA	1.40	0.86
1:B:413:ASP:HB2	1:B:416:ARG:HG3	1.59	0.85
1:B:373:TYR:CD1	1:B:374:PRO:HA	2.19	0.77
1:A:278:TYR:HD1	1:A:320:LYS:HD2	1.50	0.76
1:B:415:SER:O	1:B:419:GLN:HG3	1.86	0.75

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	A	206/231 (89%)	195 (95%)	11 (5%)	0	100	100
1	B	102/231 (44%)	95 (93%)	7 (7%)	0	100	100
All	All	308/462 (67%)	290 (94%)	18 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	194/211 (92%)	178 (92%)	16 (8%)	10	31
1	B	96/211 (46%)	90 (94%)	6 (6%)	16	43
All	All	290/422 (69%)	268 (92%)	22 (8%)	12	34



5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	397	VAL
1	B	370	LYS
1	B	356	ASP
1	B	375	SER
1	A	314	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	285	HIS
1	A	384	ASN
1	B	362	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 ⓘ

7 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	$\# Z  > 2$
2	NAG	C	1	2,1	14,14,15	0.68	1 (7%)	17,19,21	0.68	0
2	NAG	C	2	2	14,14,15	0.51	0	17,19,21	0.74	1 (5%)
2	BMA	C	3	2	11,11,12	2.65	5 (45%)	15,15,17	1.80	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAN	C	4	2	11,11,12	1.78	4 (36%)	15,15,17	1.46	3 (20%)
2	MAN	C	5	2	11,11,12	1.81	4 (36%)	15,15,17	1.94	2 (13%)
2	MAN	C	6	2	11,11,12	1.88	3 (27%)	15,15,17	0.96	0
2	FUC	C	7	2	10,10,11	1.75	3 (30%)	14,14,16	1.40	2 (14%)

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
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	2/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	FUC	C	7	2	-	-	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	BMA	C2-C3	5.05	1.60	1.52
2	C	3	BMA	C4-C5	4.75	1.63	1.53
2	C	6	MAN	C4-C5	3.53	1.60	1.53
2	C	7	FUC	O5-C5	3.45	1.50	1.43
2	C	5	MAN	C1-C2	3.05	1.59	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	MAN	C1-O5-C5	5.20	119.16	112.19
2	C	3	BMA	C1-O5-C5	3.19	116.46	112.19
2	C	3	BMA	C1-C2-C3	3.06	114.10	109.64
2	C	7	FUC	O2-C2-C1	2.94	115.96	109.22
2	C	7	FUC	C1-C2-C3	-2.82	105.54	109.64

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

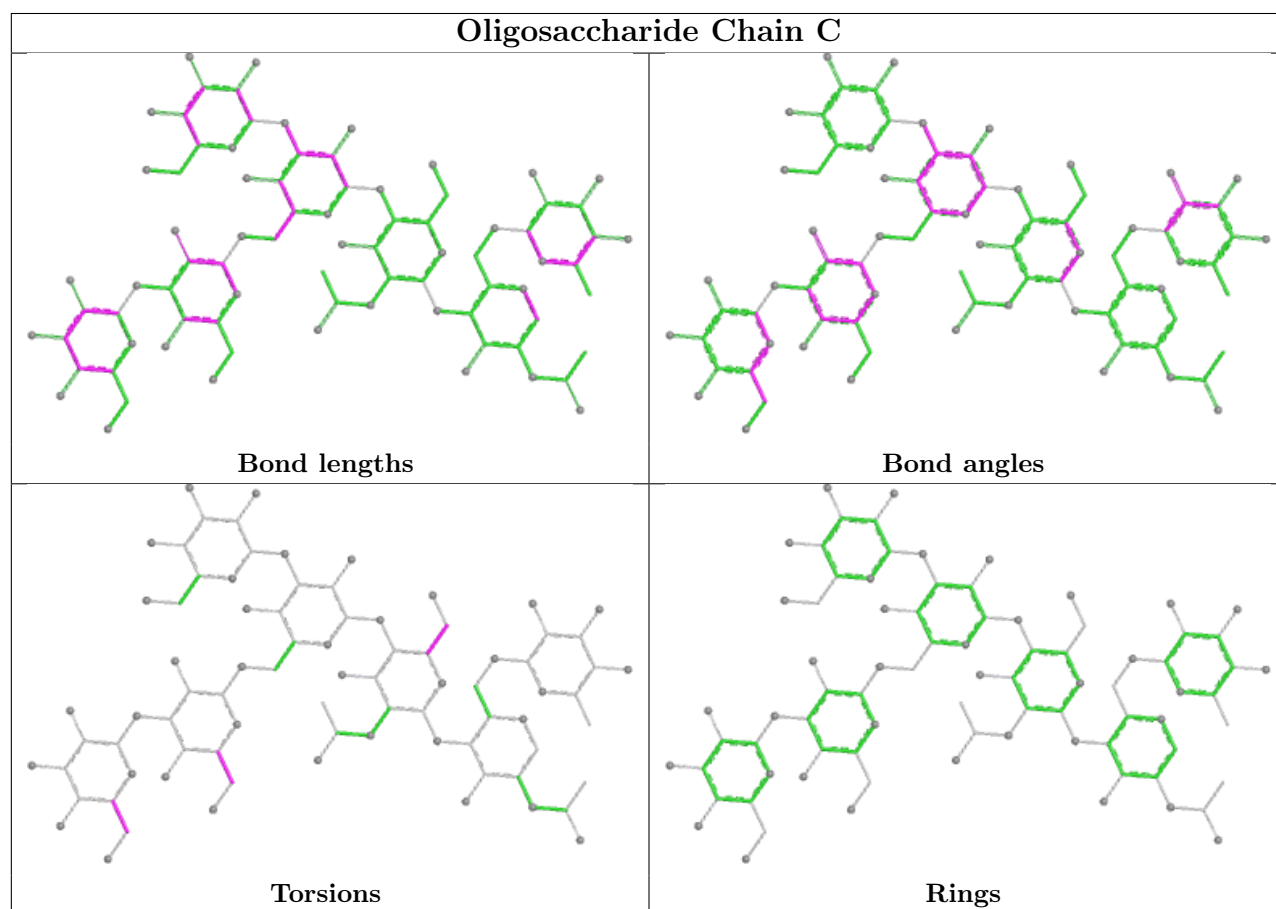
Mol	Chain	Res	Type	Atoms
2	C	5	MAN	O5-C5-C6-O6
2	C	5	MAN	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	2	0
2	C	4	MAN	2	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 ⓘ

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	A	208/231 (90%)	-0.04	2 (0%) 79 72	23, 39, 60, 75	0
1	B	104/231 (45%)	0.25	2 (1%) 66 58	28, 51, 73, 84	0
All	All	312/462 (67%)	0.06	4 (1%) 75 67	23, 42, 69, 84	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	SER	2.9
1	B	433	HIS	2.4
1	A	273	VAL	2.1
1	B	389	ASN	2.0

### 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.

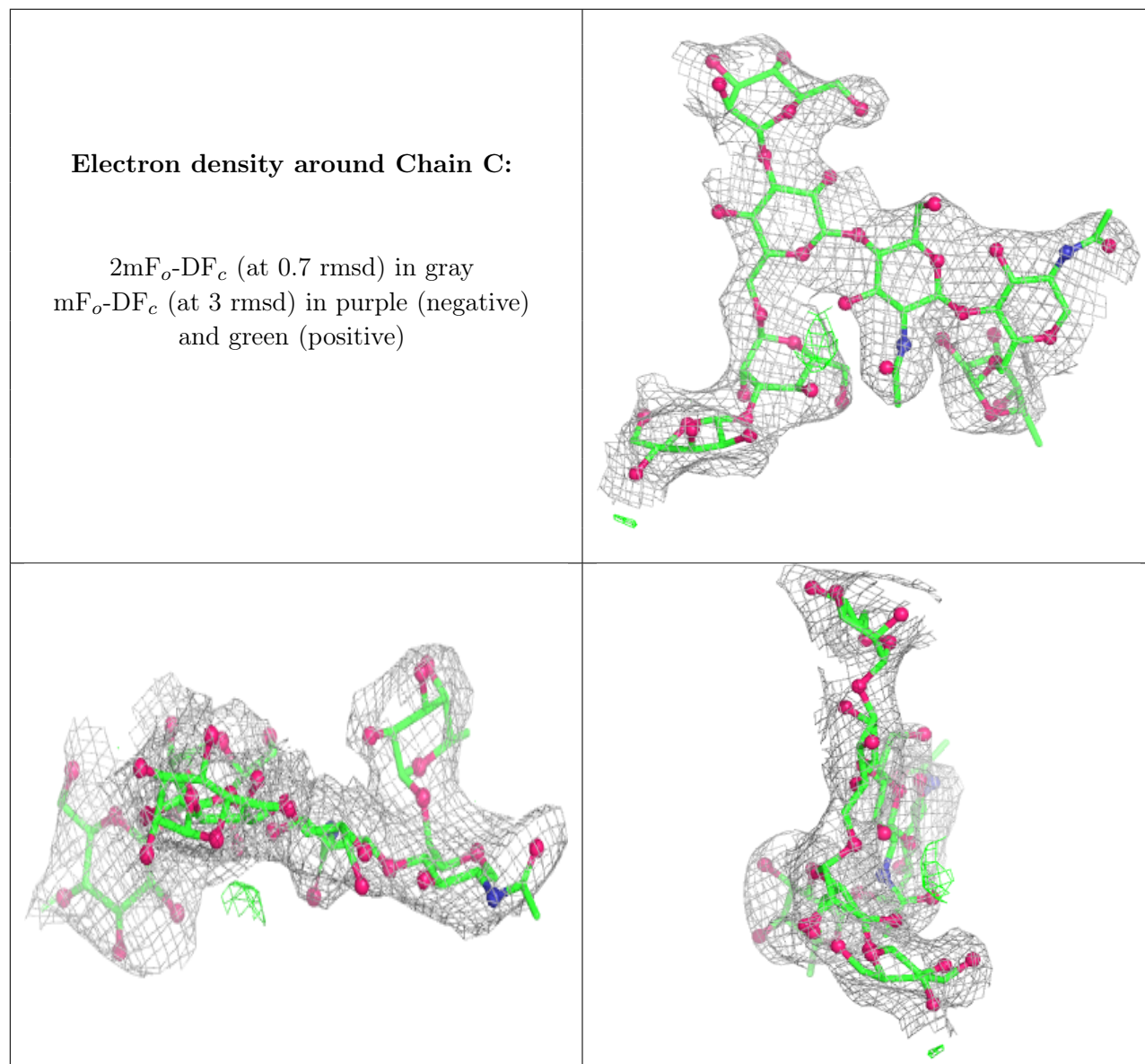
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAN	C	6	11/12	0.74	0.11	49,67,72,74	0
2	MAN	C	5	11/12	0.80	0.12	48,59,64,65	0
2	FUC	C	7	10/11	0.82	0.12	65,71,74,75	0
2	BMA	C	3	11/12	0.87	0.10	48,57,63,65	0
2	MAN	C	4	11/12	0.88	0.09	55,62,66,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	1	14/15	0.90	0.10	57,64,68,69	0
2	NAG	C	2	14/15	0.93	0.10	56,61,66,67	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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.