



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2025 – 12:11 PM EDT

PDB ID : 9CPS / pdb\_00009cps  
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with antibodies M22-91 and CC12.3  
Authors : Feng, Z.; Wilson, I.A.  
Deposited on : 2024-07-18  
Resolution : 3.03 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 Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

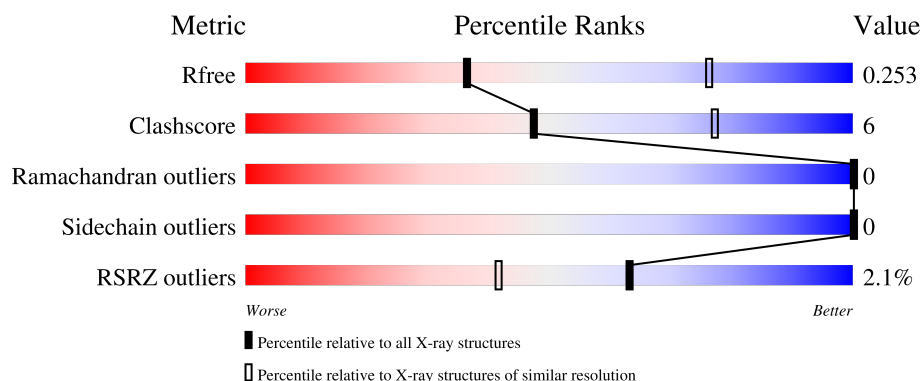
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.03 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))
$R_{free}$	164625	3418 (3.08-3.00)
Clashscore	180529	3811 (3.08-3.00)
Ramachandran outliers	177936	3656 (3.08-3.00)
Sidechain outliers	177891	3658 (3.08-3.00)
RSRZ outliers	164620	3430 (3.08-3.00)

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	205	
2	F	220	
3	G	214	
4	H	222	
5	L	220	

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Mol	Chain	Length	Quality of chain
6	B	2	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8030 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1528	981	254	285	8			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	531	GLY	-	expression tag	UNP P0DTC2
A	532	HIS	-	expression tag	UNP P0DTC2
A	533	HIS	-	expression tag	UNP P0DTC2
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2
A	536	HIS	-	expression tag	UNP P0DTC2
A	537	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called CC12.3 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	213	Total	C	N	O	S	0	0	0
			1600	1016	264	314	6			

- Molecule 3 is a protein called CC12.3 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	211	Total	C	N	O	S	0	0	0
			1622	1014	277	327	4			

- Molecule 4 is a protein called M22-91 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	209	Total	C	N	O	S	0	0	0
			1565	998	254	306	7			

- Molecule 5 is a protein called M22-91 Fab light chain.

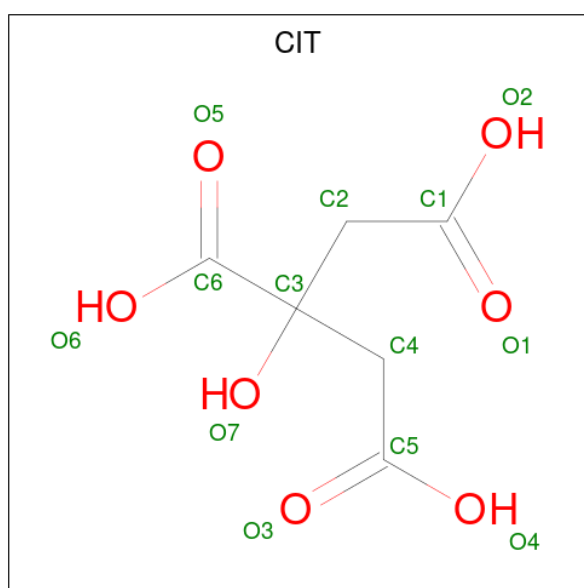
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	204	Total	C	N	O	S	0	0	0
			1583	998	258	323	4			

- Molecule 6 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
6	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is CITRIC ACID (CCD ID: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			13	6	7		
7	F	1	Total	C	O	0	0
			13	6	7		
7	F	1	Total	C	O	0	0
			13	6	7		
7	F	1	Total	C	O	0	0
			13	6	7		

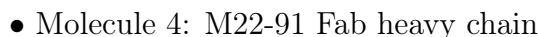
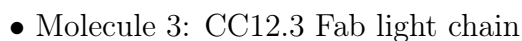
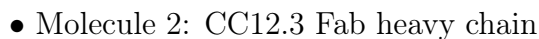
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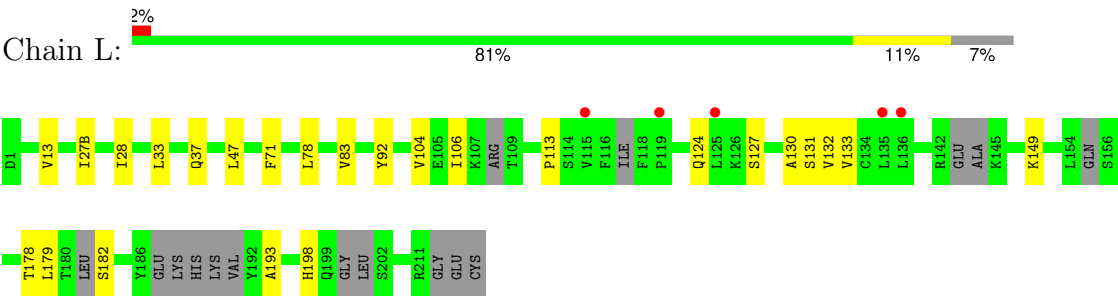
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	C	O	0	0
			13	6	7		
7	G	1	Total	C	O	0	0
			13	6	7		
7	H	1	Total	C	O	0	0
			13	6	7		
7	H	1	Total	C	O	0	0
			13	6	7		



- Molecule 1: Spike protein S1



● Molecule 5: M22-91 Fab light chain



● Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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, $\alpha$ , $\beta$ , $\gamma$	55.64Å 103.32Å 135.53Å 90.00° 99.59° 90.00°	Depositor
Resolution (Å)	48.02 – 3.03 48.02 – 3.03	Depositor EDS
% Data completeness (in resolution range)	84.2 (48.02-3.03) 84.2 (48.02-3.03)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5127: ???)	Depositor
R, $R_{free}$	0.215 , 0.253 0.215 , 0.253	Depositor DCC
$R_{free}$ test set	1479 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.2	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8030	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: CIT, 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	0.08	0/1572	0.24	0/2140
2	F	0.08	0/1639	0.24	0/2231
3	G	0.07	0/1657	0.24	0/2249
4	H	0.08	0/1603	0.25	0/2176
5	L	0.07	0/1613	0.23	0/2185
All	All	0.07	0/8084	0.24	0/10981

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	A	1528	0	1446	24	0
2	F	1600	0	1560	21	0
3	G	1622	0	1583	15	0
4	H	1565	0	1542	18	0
5	L	1583	0	1522	16	0
6	B	28	0	25	1	0
7	F	52	0	20	1	0
7	G	26	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	26	0	10	0	0
All	All	8030	0	7718	87	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 6.

The worst 5 of 87 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:G:103:LYS:HD2	7:G:302:CIT:H21	1.66	0.78
2:F:126:PRO:HG3	2:F:138:LEU:HB3	1.66	0.76
1:A:489:TYR:OH	2:F:94:ARG:NH2	2.20	0.74
1:A:378:LYS:NZ	4:H:56:GLU:OE1	2.23	0.70
3:G:33:LEU:HD22	3:G:71:PHE:CG	2.27	0.70

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	191/205 (93%)	185 (97%)	6 (3%)	0	100	100
2	F	209/220 (95%)	205 (98%)	4 (2%)	0	100	100
3	G	209/214 (98%)	203 (97%)	6 (3%)	0	100	100
4	H	199/222 (90%)	190 (96%)	9 (4%)	0	100	100
5	L	188/220 (86%)	180 (96%)	8 (4%)	0	100	100
All	All	996/1081 (92%)	963 (97%)	33 (3%)	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	166/177 (94%)	166 (100%)	0	100	100
2	F	180/186 (97%)	180 (100%)	0	100	100
3	G	183/185 (99%)	183 (100%)	0	100	100
4	H	177/186 (95%)	177 (100%)	0	100	100
5	L	181/194 (93%)	181 (100%)	0	100	100
All	All	887/928 (96%)	887 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	189	HIS
5	L	31	ASN
5	L	166	GLN
2	F	73	ASN
1	A	370	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

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	$\# Z  > 2$
6	NAG	B	1	1,6	14,14,15	0.70	0	17,19,21	0.94	1 (5%)
6	NAG	B	2	6	14,14,15	0.73	0	17,19,21	0.80	0

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
6	NAG	B	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	2	6	-	0/6/23/26	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(°)
6	B	1	NAG	O5-C1-C2	-2.27	107.78	111.29

There are no chirality outliers.

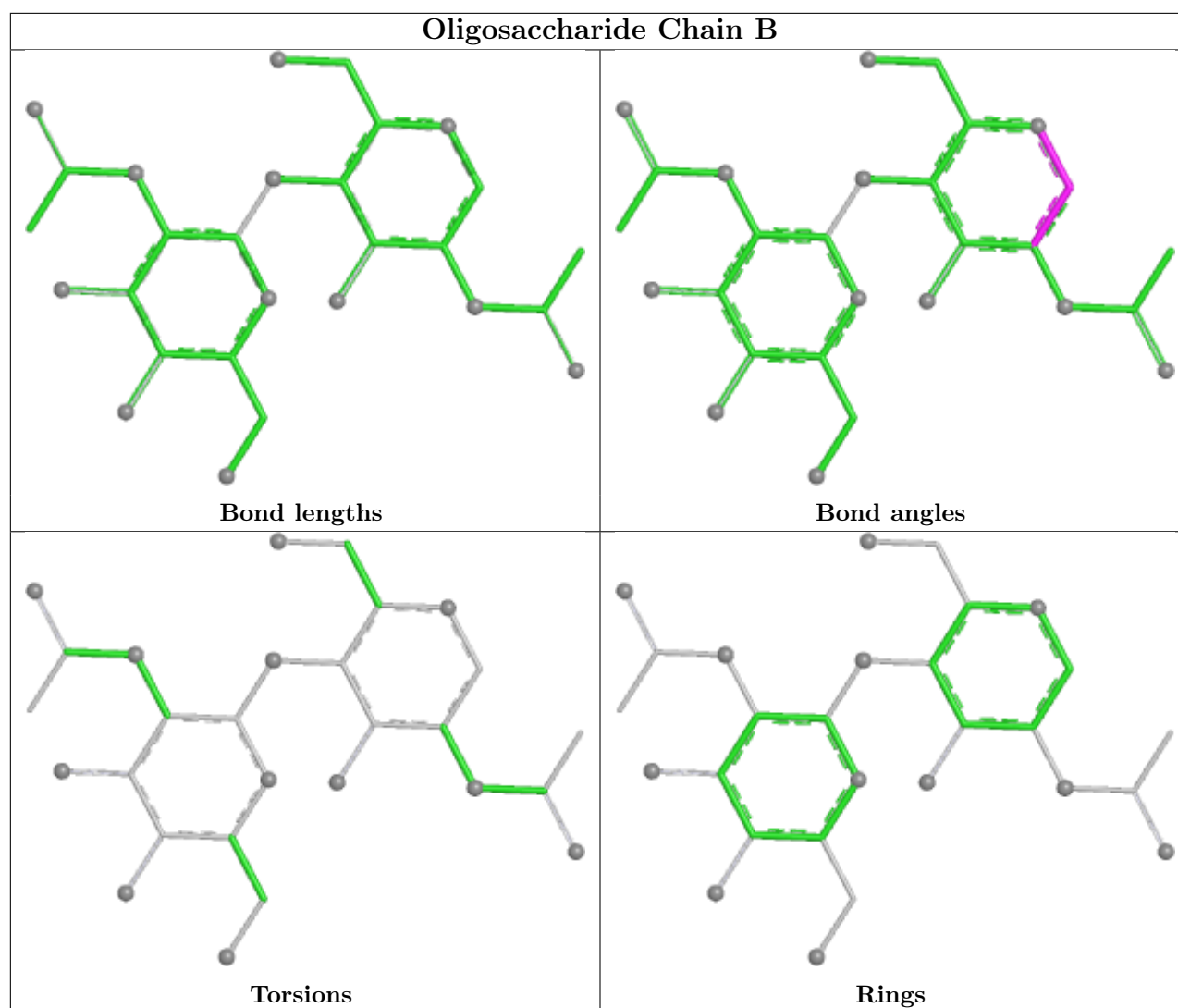
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	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](#)

8 ligands 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	$\# Z  > 2$
7	CIT	F	1203	-	12,12,12	1.40	1 (8%)	17,17,17	1.46	3 (17%)
7	CIT	F	1202	-	12,12,12	1.36	1 (8%)	17,17,17	1.46	3 (17%)
7	CIT	G	302	-	12,12,12	1.39	1 (8%)	17,17,17	1.45	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	CIT	H	302	-	12,12,12	1.40	1 (8%)	17,17,17	1.50	3 (17%)
7	CIT	G	301	-	12,12,12	1.36	1 (8%)	17,17,17	1.49	4 (23%)
7	CIT	H	301	-	12,12,12	1.38	1 (8%)	17,17,17	1.46	3 (17%)
7	CIT	F	1201	-	12,12,12	1.45	1 (8%)	17,17,17	1.52	2 (11%)
7	CIT	F	1204	-	12,12,12	1.37	1 (8%)	17,17,17	1.44	3 (17%)

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
7	CIT	F	1203	-	-	3/16/16/16	-
7	CIT	F	1202	-	-	3/16/16/16	-
7	CIT	G	302	-	-	10/16/16/16	-
7	CIT	H	302	-	-	7/16/16/16	-
7	CIT	G	301	-	-	4/16/16/16	-
7	CIT	H	301	-	-	6/16/16/16	-
7	CIT	F	1201	-	-	1/16/16/16	-
7	CIT	F	1204	-	-	9/16/16/16	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	1201	CIT	C3-C6	3.21	1.56	1.53
7	H	302	CIT	C3-C6	3.18	1.56	1.53
7	G	302	CIT	C3-C6	3.14	1.56	1.53
7	F	1203	CIT	C3-C6	3.11	1.56	1.53
7	H	301	CIT	C3-C6	3.04	1.56	1.53

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	1201	CIT	O5-C6-C3	-3.51	115.30	122.09
7	G	301	CIT	O5-C6-C3	-3.44	115.42	122.09
7	F	1203	CIT	O5-C6-C3	-3.35	115.61	122.09
7	H	302	CIT	O5-C6-C3	-3.31	115.69	122.09
7	F	1201	CIT	O6-C6-C3	3.30	119.46	113.14

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	1204	CIT	O7-C3-C6-O5
7	F	1204	CIT	O7-C3-C6-O6
7	F	1204	CIT	C4-C3-C6-O5
7	F	1204	CIT	C4-C3-C6-O6
7	G	302	CIT	C2-C3-C6-O5

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	302	CIT	2	0
7	F	1201	CIT	1	0

## 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	193/205 (94%)	-0.19	0 <span>100</span> <span>100</span>	41, 64, 110, 124	0
2	F	213/220 (96%)	-0.47	1 (0%) <span>87</span> <span>74</span>	33, 53, 86, 118	0
3	G	211/214 (98%)	-0.42	2 (0%) <span>81</span> <span>63</span>	38, 58, 81, 89	0
4	H	209/222 (94%)	0.39	14 (6%) <span>25</span> <span>14</span>	57, 108, 146, 160	0
5	L	204/220 (92%)	0.42	5 (2%) <span>58</span> <span>37</span>	76, 124, 157, 175	0
All	All	1030/1081 (95%)	-0.06	22 (2%) <span>63</span> <span>42</span>	33, 72, 145, 175	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	151	THR	4.2
4	H	180	SER	4.0
4	H	181	VAL	3.2
3	G	171	SER	3.1
4	H	182	VAL	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.

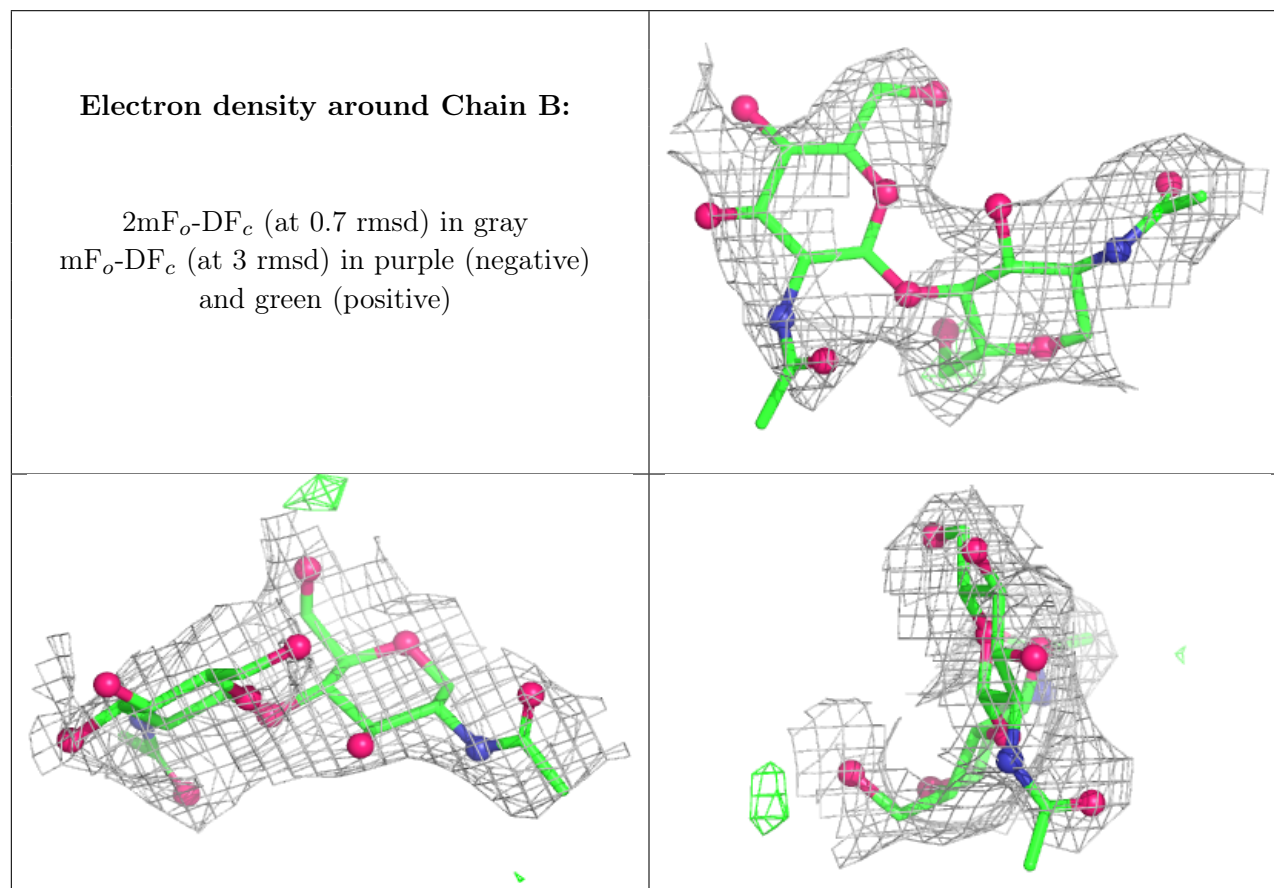
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	B	1	14/15	-	-	84,123,135,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	B	2	14/15	-	-	106,131,140,140	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 ⓘ

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
7	CIT	H	302	13/13	0.63	0.14	80,110,125,126	0
7	CIT	F	1204	13/13	0.67	0.10	87,105,118,127	0
7	CIT	G	301	13/13	0.72	0.18	84,101,118,121	0
7	CIT	F	1203	13/13	0.74	0.18	91,108,142,146	0
7	CIT	H	301	13/13	0.76	0.13	90,107,120,125	0
7	CIT	F	1201	13/13	0.83	0.14	67,84,92,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CIT	G	302	13/13	0.85	0.11	58,82,114,137	0
7	CIT	F	1202	13/13	0.88	0.12	71,86,102,105	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.