



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2025 – 12:11 PM EDT

PDB ID : 9CPP / pdb\_00009cpp  
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with antibodies M22-17 and CC12.3  
Authors : Feng, Z.; Wilson, I.A.  
Deposited on : 2024-07-18  
Resolution : 3.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

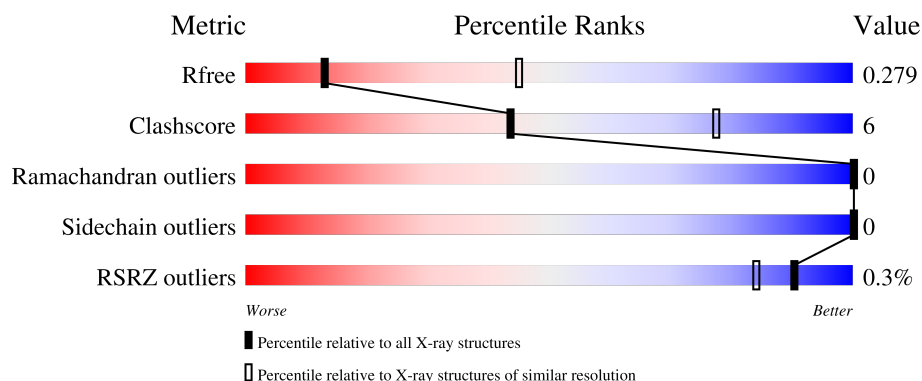
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*






The reported resolution of this entry is 3.19 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.



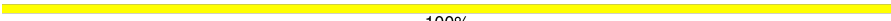
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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	 80% 14% 5%
2	F	220	 76% 20% .
3	G	214	 82% 17% .
4	H	222	 87% 10% .
5	L	220	 87% 12% .

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Mol	Chain	Length	Quality of chain
6	B	3	 100%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8111 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	194	Total	C	N	O	S	0	0	0
			1536	985	256	287	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	212	Total	C	N	O	S	0	0	0
			1591	1010	262	313	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			

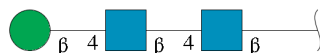
- Molecule 4 is a protein called M22-17 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	215	Total	C	N	O	S	0	0	0
			1605	1024	260	313	8			

- Molecule 5 is a protein called M22-17 Fab light chain.

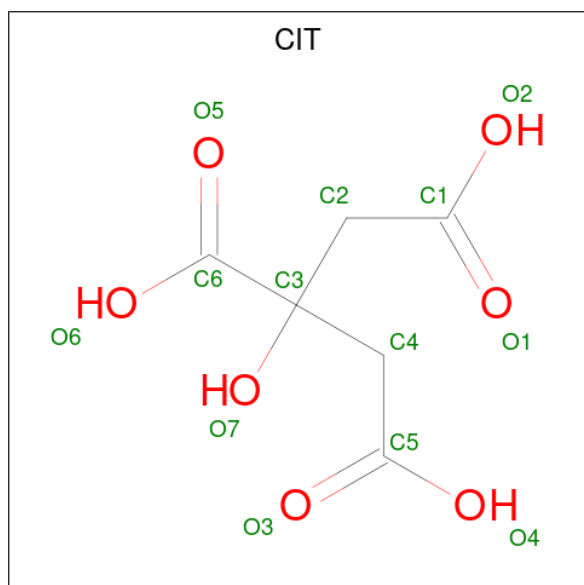
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	217	Total	C	N	O	S	0	0	0
			1692	1064	280	344	4			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-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	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

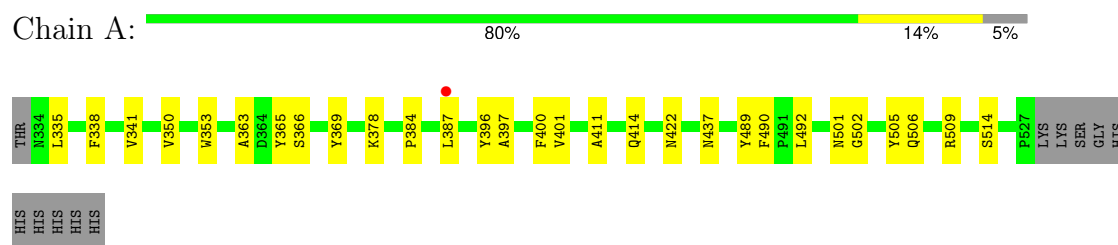


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	6	7		
7	A	1	Total	C	O	0	0
			13	6	7		

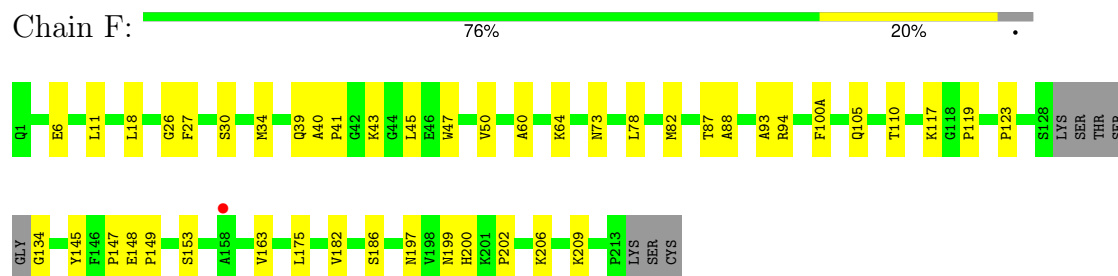
### 3 Residue-property plots [i](#)

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.

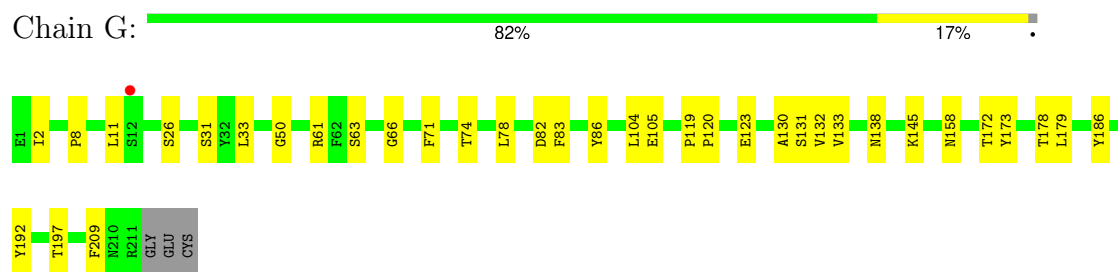
- Molecule 1: Spike protein S1



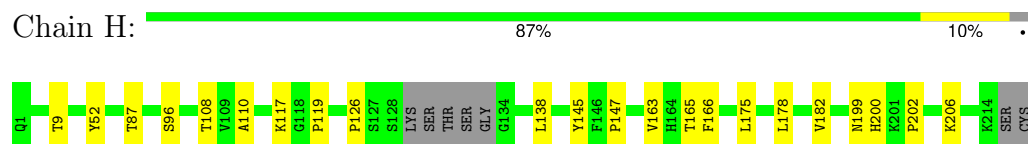
- Molecule 2: CC12.3 Fab heavy chain



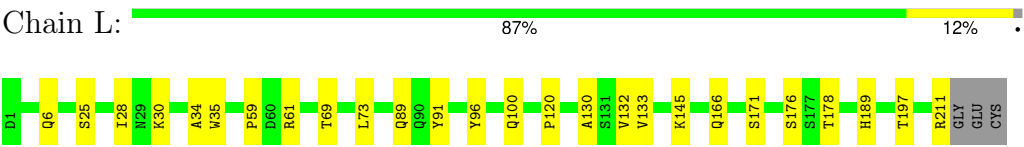
- Molecule 3: CC12.3 Fab light chain



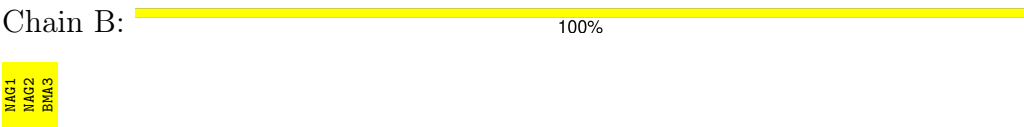
- Molecule 4: M22-17 Fab heavy chain



● Molecule 5: M22-17 Fab light chain



● Molecule 6: beta-D-mannopyranose-(1-4)-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 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.27Å 110.27Å 225.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.31 – 3.19 49.31 – 3.19	Depositor EDS
% Data completeness (in resolution range)	94.2 (49.31-3.19) 94.3 (49.31-3.19)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.82 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5127: ???)	Depositor
R, $R_{free}$	0.232 , 0.279 0.232 , 0.279	Depositor DCC
$R_{free}$ test set	1213 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.4	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 16.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8111	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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: NAG, BMA, CIT

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	0/1580	0.23	0/2151
2	F	0.08	0/1630	0.24	0/2220
3	G	0.08	0/1657	0.27	0/2249
4	H	0.09	0/1647	0.27	0/2243
5	L	0.07	0/1730	0.24	0/2353
All	All	0.08	0/8244	0.25	0/11216

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	1536	0	1452	25	0
2	F	1591	0	1547	27	0
3	G	1622	0	1583	22	0
4	H	1605	0	1581	14	0
5	L	1692	0	1642	14	0
6	B	39	0	34	0	0
7	A	26	0	10	2	0
All	All	8111	0	7849	96	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.

All (96) 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:A:384:PRO:HA	1:A:387:LEU:HD13	1.32	1.12
2:F:134:GLY:N	2:F:186:SER:HG	1.81	0.78
1:A:384:PRO:CA	1:A:387:LEU:HD13	2.13	0.76
5:L:6:GLN:O	5:L:100:GLN:NE2	2.21	0.73
1:A:489:TYR:OH	2:F:94:ARG:NH2	2.24	0.70
2:F:11:LEU:HB2	2:F:147:PRO:HG3	1.77	0.66
7:A:1201:CIT:H21	2:F:26:GLY:H	1.61	0.65
3:G:8:PRO:HD2	3:G:11:LEU:HD11	1.79	0.65
3:G:186:TYR:O	3:G:192:TYR:OH	2.15	0.64
1:A:384:PRO:HA	1:A:387:LEU:CD1	2.20	0.63
2:F:199:ASN:HD22	2:F:206:LYS:HG2	1.65	0.62
4:H:199:ASN:HD22	4:H:206:LYS:HG2	1.66	0.61
5:L:145:LYS:HB3	5:L:197:THR:HB	1.83	0.60
4:H:87:THR:HG23	4:H:110:ALA:HA	1.81	0.60
4:H:126:PRO:HG3	4:H:138:LEU:HB3	1.84	0.60
3:G:2:ILE:HG13	3:G:26:SER:HB3	1.84	0.58
3:G:82:ASP:O	3:G:86:TYR:OH	2.20	0.58
3:G:11:LEU:HB2	3:G:104:LEU:HD12	1.85	0.57
1:A:365:TYR:CD1	1:A:387:LEU:HB3	2.40	0.57
2:F:6:GLU:H	2:F:105:GLN:HE22	1.52	0.57
2:F:119:PRO:HB3	2:F:145:TYR:HB3	1.86	0.56
5:L:120:PRO:HD3	5:L:132:VAL:HG22	1.87	0.56
2:F:40:ALA:HB3	2:F:43:LYS:HB2	1.87	0.56
2:F:93:ALA:HB1	2:F:100(A):PHE:HB3	1.88	0.55
2:F:209:LYS:NZ	3:G:123:GLU:OE1	2.35	0.55
3:G:63:SER:OG	3:G:74:THR:OG1	2.24	0.55
1:A:365:TYR:CD2	1:A:387:LEU:HD23	2.42	0.55
4:H:165:THR:HG23	4:H:178:LEU:HD21	1.88	0.54
2:F:148:GLU:HB2	2:F:149:PRO:HA	1.91	0.53
2:F:153:SER:HB2	2:F:197:ASN:HB2	1.91	0.53
3:G:133:VAL:HG22	3:G:178:THR:HG22	1.92	0.51
2:F:18:LEU:HB3	2:F:82:MET:HE3	1.93	0.51
3:G:66:GLY:HA3	3:G:71:PHE:HA	1.91	0.51
3:G:31:SER:OG	3:G:50:GLY:O	2.29	0.50
5:L:189:HIS:O	5:L:211:ARG:NH2	2.44	0.50
2:F:200:HIS:CD2	2:F:202:PRO:HD2	2.47	0.50
2:F:87:THR:HG23	2:F:110:THR:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:120:PRO:HB3	3:G:131:SER:H	1.78	0.49
3:G:145:LYS:HB3	3:G:197:THR:HB	1.95	0.49
4:H:119:PRO:HB3	4:H:145:TYR:HB3	1.96	0.48
3:G:105:GLU:OE1	3:G:173:TYR:OH	2.29	0.48
2:F:47:TRP:HZ2	2:F:50:VAL:HG12	1.78	0.48
3:G:78:LEU:HD13	3:G:83:PHE:HZ	1.78	0.48
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.95	0.48
1:A:338:PHE:HE2	1:A:363:ALA:HB1	1.79	0.48
4:H:200:HIS:CD2	4:H:202:PRO:HD2	2.49	0.47
2:F:163:VAL:HG22	2:F:182:VAL:HG12	1.95	0.47
3:G:138:ASN:HA	3:G:172:THR:HB	1.94	0.47
2:F:123:PRO:HD3	2:F:209:LYS:HZ3	1.79	0.47
4:H:163:VAL:HG22	4:H:182:VAL:HG12	1.96	0.47
4:H:9:THR:HG23	4:H:108:THR:HB	1.97	0.47
1:A:335:LEU:HD23	1:A:335:LEU:H	1.80	0.46
1:A:411:ALA:HB3	1:A:414:GLN:HG3	1.98	0.46
5:L:34:ALA:HB2	5:L:91:TYR:HE1	1.79	0.46
3:G:120:PRO:HD3	3:G:132:VAL:HG22	1.98	0.46
2:F:39:GLN:HB2	2:F:45:LEU:HD23	1.98	0.46
3:G:33:LEU:HD22	3:G:71:PHE:CG	2.50	0.46
3:G:61:ARG:NE	3:G:82:ASP:OD2	2.47	0.46
5:L:89:GLN:HE21	5:L:96:TYR:HB3	1.81	0.45
3:G:78:LEU:HB3	3:G:83:PHE:CE1	2.50	0.45
1:A:365:TYR:CG	1:A:387:LEU:HD23	2.50	0.45
2:F:119:PRO:HD3	2:F:200:HIS:ND1	2.31	0.45
3:G:158:ASN:HB2	3:G:179:LEU:HD12	1.97	0.45
5:L:166:GLN:HG2	5:L:171:SER:HA	1.98	0.45
7:A:1201:CIT:H21	2:F:26:GLY:N	2.30	0.45
1:A:396:TYR:HB2	1:A:514:SER:HB3	1.98	0.44
3:G:120:PRO:HG3	3:G:130:ALA:HB1	1.99	0.44
1:A:350:VAL:HA	1:A:400:PHE:HB2	1.99	0.44
2:F:117:LYS:HD3	2:F:175:LEU:HD21	2.00	0.44
5:L:35:TRP:CE2	5:L:73:LEU:HB2	2.53	0.44
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.52	0.44
4:H:117:LYS:HD3	4:H:175:LEU:HD21	2.00	0.44
5:L:28:ILE:HG23	5:L:30:LYS:HB2	2.00	0.44
2:F:27:PHE:CE1	2:F:94:ARG:HD2	2.54	0.43
4:H:166:PHE:CZ	5:L:176:SER:HB3	2.54	0.43
1:A:502:GLY:O	1:A:506:GLN:HG3	2.19	0.43
2:F:41:PRO:HD3	2:F:88:ALA:HA	2.01	0.43
1:A:401:VAL:HG22	1:A:509:ARG:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:60:ALA:O	2:F:64:LYS:HG3	2.19	0.42
1:A:341:VAL:HG11	1:A:397:ALA:HB1	2.02	0.42
1:A:378:LYS:HG2	4:H:52:TYR:CZ	2.54	0.42
1:A:384:PRO:O	1:A:387:LEU:HB2	2.20	0.42
2:F:34:MET:HB3	2:F:78:LEU:HD22	2.02	0.42
2:F:30:SER:HB3	2:F:73:ASN:OD1	2.19	0.42
5:L:25:SER:HB3	5:L:69:THR:HA	2.02	0.42
1:A:384:PRO:HD2	4:H:96:SER:HB3	2.01	0.42
1:A:501:ASN:HB3	1:A:505:TYR:HB2	2.02	0.41
4:H:147:PRO:HG2	4:H:202:PRO:HG2	2.02	0.41
1:A:437:ASN:ND2	1:A:506:GLN:OE1	2.48	0.41
1:A:353:TRP:CD1	1:A:353:TRP:H	2.38	0.41
5:L:133:VAL:HG22	5:L:178:THR:HG22	2.02	0.41
1:A:384:PRO:HG2	4:H:96:SER:HB3	2.03	0.41
5:L:59:PRO:HB2	5:L:61:ARG:HG2	2.02	0.41
3:G:119:PRO:HB3	3:G:209:PHE:CE2	2.55	0.41
1:A:366:SER:HA	1:A:369:TYR:CZ	2.56	0.40
5:L:120:PRO:HG3	5:L:130:ALA:HB1	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	192/205 (94%)	186 (97%)	6 (3%)	0	100	100
2	F	208/220 (94%)	204 (98%)	4 (2%)	0	100	100
3	G	209/214 (98%)	199 (95%)	10 (5%)	0	100	100
4	H	211/222 (95%)	205 (97%)	6 (3%)	0	100	100
5	L	215/220 (98%)	208 (97%)	7 (3%)	0	100	100
All	All	1035/1081 (96%)	1002 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	167/177 (94%)	167 (100%)	0	100	100
2	F	179/186 (96%)	179 (100%)	0	100	100
3	G	183/185 (99%)	183 (100%)	0	100	100
4	H	180/186 (97%)	180 (100%)	0	100	100
5	L	194/196 (99%)	194 (100%)	0	100	100
All	All	903/930 (97%)	903 (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. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	ASN
2	F	164	HIS
2	F	199	ASN
3	G	137	ASN
4	H	199	ASN
5	L	6	GLN
5	L	42	GLN
5	L	89	GLN
5	L	124	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

3 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	6,1	14,14,15	0.81	0	17,19,21	1.16	1 (5%)
6	NAG	B	2	6	14,14,15	0.69	0	17,19,21	0.89	1 (5%)
6	BMA	B	3	6	11,11,12	0.80	0	15,15,17	1.74	1 (6%)

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	6,1	-	1/6/23/26	0/1/1/1
6	NAG	B	2	6	-	1/6/23/26	0/1/1/1
6	BMA	B	3	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	3	BMA	C1-O5-C5	5.13	119.06	112.19
6	B	1	NAG	C2-N2-C7	3.07	127.01	122.90
6	B	2	NAG	O5-C1-C2	-2.01	108.17	111.29

There are no chirality outliers.

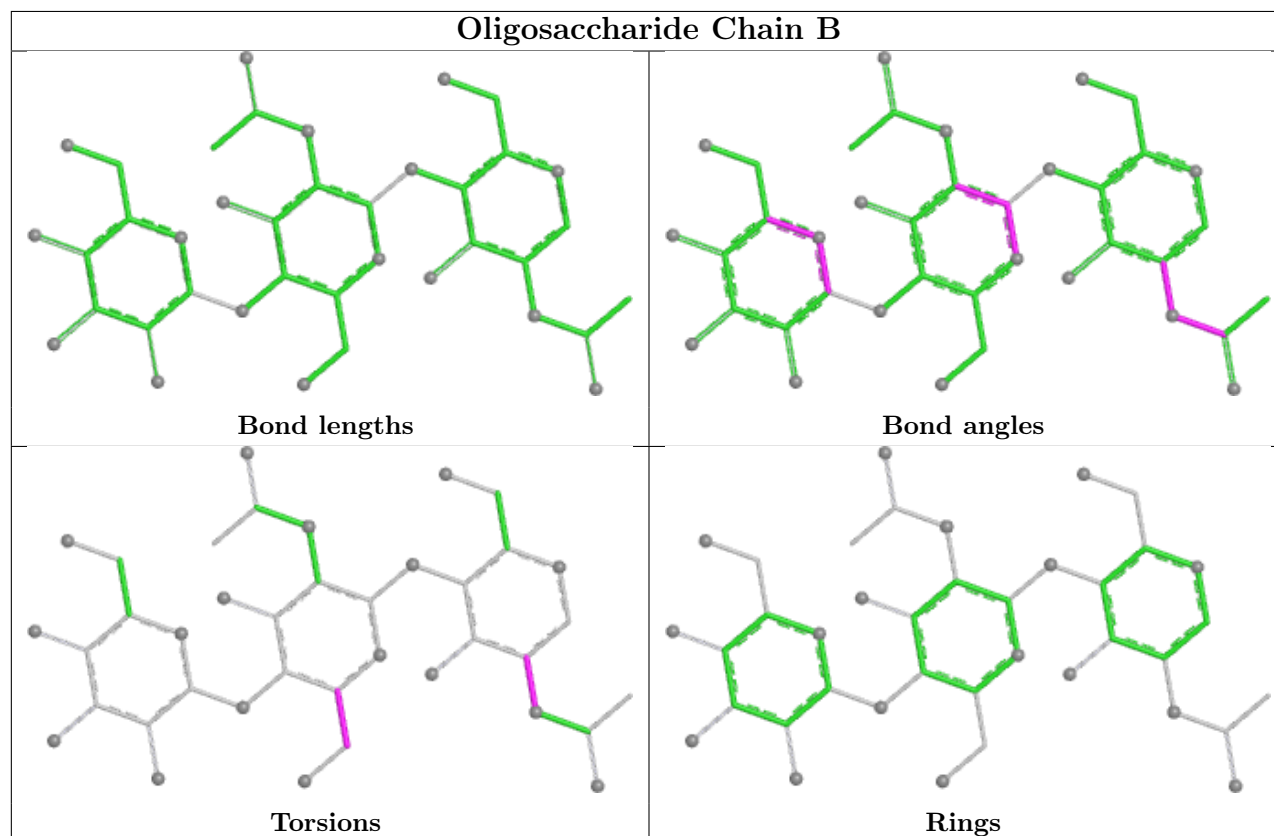
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	2	NAG	O5-C5-C6-O6
6	B	1	NAG	C3-C2-N2-C7

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 [i](#)

2 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	A	1201	-	12,12,12	1.44	1 (8%)	17,17,17	1.62	3 (17%)
7	CIT	A	1202	-	12,12,12	1.36	1 (8%)	17,17,17	1.49	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	A	1201	-	-	4/16/16/16	-
7	CIT	A	1202	-	-	8/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1201	CIT	C3-C6	3.33	1.56	1.53
7	A	1202	CIT	C3-C6	2.95	1.56	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1202	CIT	O5-C6-C3	-3.54	115.24	122.09
7	A	1201	CIT	O5-C6-C3	-3.49	115.33	122.09
7	A	1201	CIT	O6-C6-C3	3.19	119.25	113.14
7	A	1202	CIT	O6-C6-C3	2.97	118.83	113.14
7	A	1201	CIT	O7-C3-C6	2.83	112.97	108.96
7	A	1202	CIT	O7-C3-C6	2.20	112.08	108.96

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1201	CIT	O7-C3-C6-O5
7	A	1201	CIT	O7-C3-C6-O6
7	A	1201	CIT	C4-C3-C6-O5
7	A	1201	CIT	C4-C3-C6-O6
7	A	1202	CIT	C2-C3-C6-O5
7	A	1202	CIT	C2-C3-C6-O6
7	A	1202	CIT	O7-C3-C6-O5
7	A	1202	CIT	O7-C3-C6-O6
7	A	1202	CIT	C2-C3-C4-C5
7	A	1202	CIT	C6-C3-C4-C5
7	A	1202	CIT	C4-C3-C6-O5
7	A	1202	CIT	C4-C3-C6-O6

There are no ring outliers.



1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1201	CIT	2	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	194/205 (94%)	-0.08	1 (0%) 87 78	41, 57, 100, 132	0
2	F	212/220 (96%)	-0.14	1 (0%) 87 78	38, 57, 103, 120	0
3	G	211/214 (98%)	0.03	1 (0%) 87 78	47, 70, 96, 110	0
4	H	215/222 (96%)	-0.20	0 100 100	43, 60, 86, 101	0
5	L	217/220 (98%)	-0.23	0 100 100	42, 61, 78, 88	0
All	All	1049/1081 (97%)	-0.13	3 (0%) 90 84	38, 61, 96, 132	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	158	ALA	2.5
1	A	387	LEU	2.3
3	G	12	SER	2.1

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

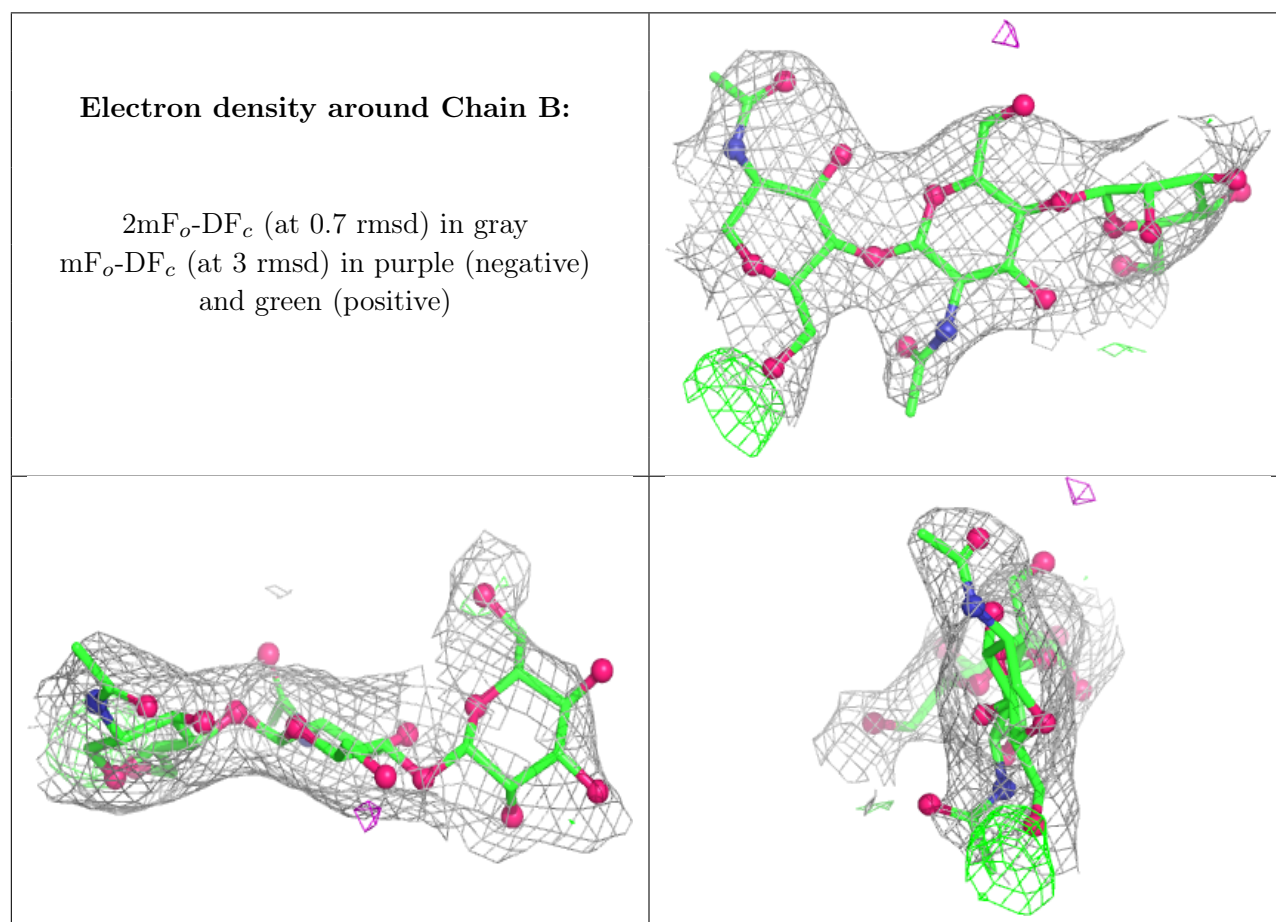
There are no non-standard protein/DNA/RNA residues in this entry.

### 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	-	-	53,68,77,78	0
6	NAG	B	2	14/15	-	-	68,81,90,94	0
6	BMA	B	3	11/12	-	-	88,99,103,104	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](#)

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
7	CIT	A	1202	13/13	0.75	0.15	68,78,89,102	0
7	CIT	A	1201	13/13	0.84	0.10	65,72,84,85	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.