



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2022 – 06:05 PM EST

PDB ID : 7LM9  
Title : Crystal structure of SARS-CoV spike protein receptor-binding domain in complex with a cross-neutralizing antibody CV38-142 Fab isolated from COVID-19 patient  
Authors : Liu, H.; Yuan, M.; Zhu, X.; Wilson, I.A.  
Deposited on : 2021-02-05  
Resolution : 1.53 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.

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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 : 2.26  
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) : 2.26

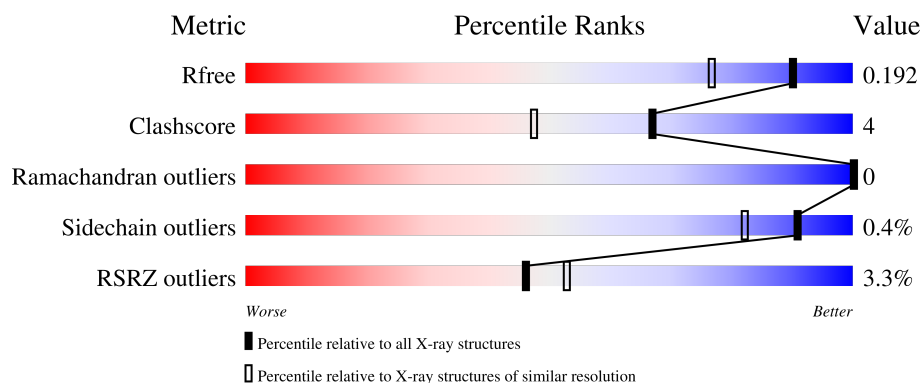
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.53 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	230	<div> <div>7%</div> <div> <div></div> <div>76%</div> <div>8%</div> <div>17%</div> </div> </div>
2	H	226	<div> <div></div> <div>93%</div> <div>7%</div> </div>
3	L	217	<div> <div>%</div> <div>93%</div> <div>6%</div> </div>
4	B	4	<div> <div>50%</div> <div>50%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5619 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 glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	2	0
			1532	990	251	282	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	528	SER	-	expression tag	UNP D2E265
A	529	GLY	-	expression tag	UNP D2E265
A	530	HIS	-	expression tag	UNP D2E265
A	531	HIS	-	expression tag	UNP D2E265
A	532	HIS	-	expression tag	UNP D2E265
A	533	HIS	-	expression tag	UNP D2E265
A	534	HIS	-	expression tag	UNP D2E265
A	535	HIS	-	expression tag	UNP D2E265

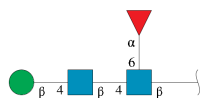
- Molecule 2 is a protein called CV38-142 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	226	Total	C	N	O	S	0	6	0
			1721	1089	281	343	8			

- Molecule 3 is a protein called CV38-142 Fab light chain.

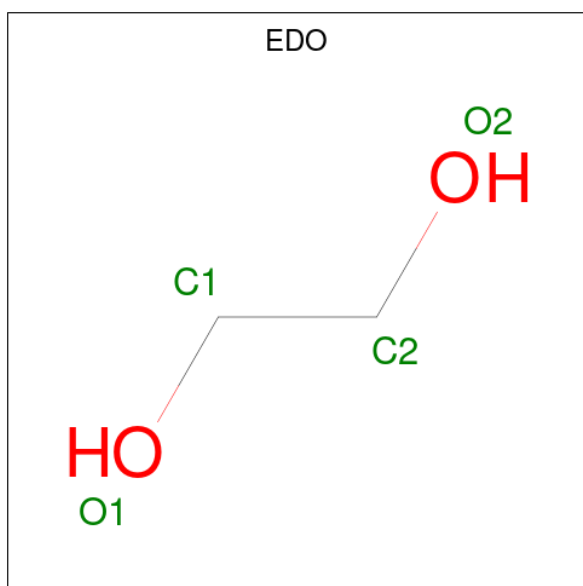
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	216	Total	C	N	O	S	0	1	0
			1659	1036	278	339	6			

- 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	B	4	Total	C	N	O	0	2	0
			74	42	3	29			

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		

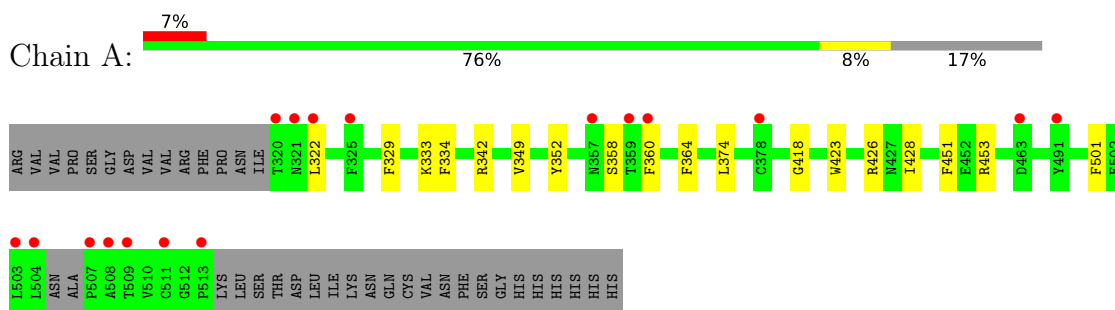
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	145	Total	O	0	0
			145	145		
6	H	232	Total	O	0	0
			232	232		
6	L	216	Total	O	0	0
			216	216		

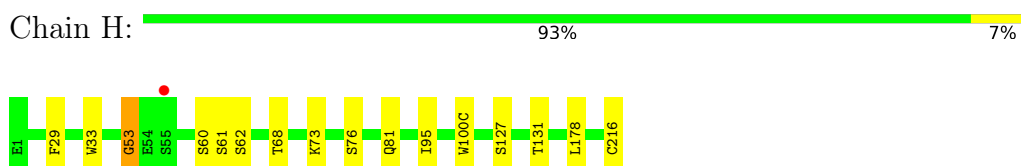
### 3 Residue-property plots [i](#)

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.

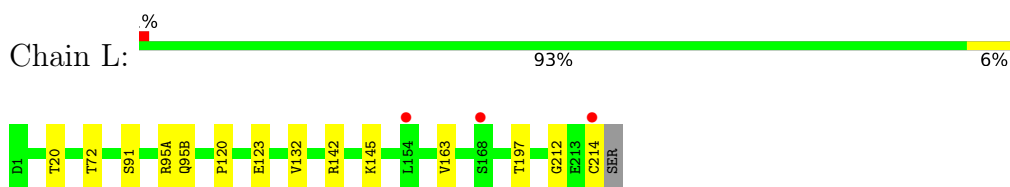
- Molecule 1: Spike glycoprotein



- Molecule 2: CV38-142 Fab heavy chain



- Molecule 3: CV38-142 Fab light chain



- 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	238.00Å 71.88Å 49.24Å 90.00° 90.78° 90.00°	Depositor
Resolution (Å)	49.24 – 1.53 49.24 – 1.53	Depositor EDS
% Data completeness (in resolution range)	95.6 (49.24-1.53) 95.6 (49.24-1.53)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 1.52Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.170 , 0.192 0.170 , 0.192	Depositor DCC
$R_{free}$ test set	6011 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.2	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5619	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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: BMA, FUC, NAG, EDO

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	0/1586	0.68	0/2165
2	H	0.59	0/1775	0.74	0/2414
3	L	0.56	0/1698	0.72	0/2306
All	All	0.56	0/5059	0.72	0/6885

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
2	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	53	GLY	Peptide

### 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	1532	0	1447	15	0
2	H	1721	0	1682	11	0
3	L	1659	0	1604	14	0
4	B	74	0	65	3	0
5	A	16	0	24	5	0
5	H	8	0	12	0	0
5	L	16	0	24	3	0
6	A	145	0	0	3	0
6	H	232	0	0	1	0
6	L	216	0	0	1	0
All	All	5619	0	4858	39	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 4.

All (39) 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:L:212:GLY:H	5:L:303:EDO:H11	1.55	0.72
4:B:2[B]:NAG:H5	4:B:4:FUC:O2	1.93	0.68
3:L:123:GLU:OE1	6:L:401:HOH:O	2.14	0.66
3:L:212:GLY:H	5:L:303:EDO:C1	2.13	0.61
1:A:428[B]:ILE:HG23	6:A:818:HOH:O	2.03	0.58
2:H:53:GLY:HA2	2:H:73:LYS:HD3	1.86	0.56
3:L:142:ARG:NH2	3:L:163:VAL:HG11	2.21	0.55
2:H:127:SER:O	2:H:131[B]:THR:HG23	2.07	0.55
1:A:342:ARG:HH22	5:A:604:EDO:H21	1.72	0.55
2:H:60:SER:HA	3:L:95(A):ARG:HA	1.92	0.52
1:A:322:LEU:HD13	1:A:349:VAL:O	2.09	0.52
1:A:333:LYS:HD3	6:A:706:HOH:O	2.11	0.51
1:A:360:PHE:HZ	1:A:423:TRP:CD1	2.31	0.48
6:H:588:HOH:O	3:L:95(A):ARG:HD2	2.12	0.48
1:A:329:PHE:HB2	4:B:1:NAG:H82	1.95	0.48
3:L:20:THR:HG23	3:L:72:THR:CG2	2.44	0.47
3:L:145:LYS:HB3	3:L:197:THR:OG1	2.14	0.47
2:H:53:GLY:CA	2:H:73:LYS:HD3	2.44	0.47
1:A:360:PHE:HE2	5:A:602:EDO:H21	1.80	0.46
3:L:95(A):ARG:NH2	3:L:95(B):GLN:HE21	2.13	0.45
1:A:360:PHE:CZ	1:A:423:TRP:CD1	3.04	0.45
2:H:33:TRP:HB2	2:H:95:ILE:HB	1.98	0.45
1:A:342:ARG:NH2	5:A:604:EDO:H21	2.31	0.45
3:L:212:GLY:N	5:L:303:EDO:H11	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:GLY:HA2	1:A:501:PHE:CD2	2.52	0.45
3:L:120:PRO:HD3	3:L:132:VAL:HG22	2.00	0.44
2:H:61:SER:OG	2:H:62:SER:N	2.51	0.43
1:A:352:TYR:CD2	1:A:374:LEU:HB3	2.54	0.43
2:H:29:PHE:CD2	2:H:76:SER:HA	2.54	0.43
2:H:216:CYS:SG	3:L:214:CYS:HB3	2.58	0.42
5:A:603:EDO:H12	4:B:1:NAG:H3	2.01	0.42
2:H:100(C):TRP:HB2	3:L:91:SER:HB2	2.02	0.42
1:A:426[B]:ARG:NH2	6:A:704:HOH:O	2.52	0.42
1:A:451:PHE:CE2	5:A:604:EDO:H22	2.55	0.42
1:A:333:LYS:HE2	1:A:334:PHE:O	2.20	0.41
1:A:453:ARG:HH11	1:A:453:ARG:HD3	1.73	0.41
2:H:68:THR:HB	2:H:81:GLN:HG2	2.04	0.40
2:H:178:LEU:HD12	2:H:178:LEU:C	2.42	0.40
3:L:20:THR:HG23	3:L:72:THR:HG23	2.03	0.40

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	190/230 (83%)	184 (97%)	6 (3%)	0	100	100
2	H	230/226 (102%)	224 (97%)	6 (3%)	0	100	100
3	L	215/217 (99%)	210 (98%)	5 (2%)	0	100	100
All	All	635/673 (94%)	618 (97%)	17 (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	167/203 (82%)	165 (99%)	2 (1%)	71	47
2	H	196/190 (103%)	196 (100%)	0	100	100
3	L	190/192 (99%)	190 (100%)	0	100	100
All	All	553/585 (94%)	551 (100%)	2 (0%)	91	82

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	358	SER
1	A	364	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	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](#)

6 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	B	1	4,1	14,14,15	0.45	0	17,19,21	0.92	0
4	NAG	B	2[A]	4	14,14,15	0.46	0	17,19,21	0.63	0
4	NAG	B	2[B]	4	14,14,15	1.00	1 (7%)	17,19,21	0.79	0
4	BMA	B	3[A]	4	11,11,12	0.72	0	15,15,17	0.77	0
4	BMA	B	3[B]	4	11,11,12	0.86	0	15,15,17	0.86	1 (6%)
4	FUC	B	4	4	10,10,11	1.52	2 (20%)	14,14,16	1.14	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
4	NAG	B	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	B	2[A]	4	-	0/6/23/26	0/1/1/1
4	NAG	B	2[B]	4	-	2/6/23/26	0/1/1/1
4	BMA	B	3[A]	4	-	2/2/19/22	0/1/1/1
4	BMA	B	3[B]	4	-	2/2/19/22	0/1/1/1
4	FUC	B	4	4	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4	FUC	O5-C1	-3.51	1.38	1.43
4	B	2[B]	NAG	C1-C2	3.22	1.57	1.52
4	B	4	FUC	O2-C2	-2.06	1.39	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4	FUC	C1-O5-C5	2.51	118.48	112.78
4	B	3[B]	BMA	O2-C2-C3	-2.31	105.50	110.14
4	B	4	FUC	C3-C4-C5	-2.06	106.56	109.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

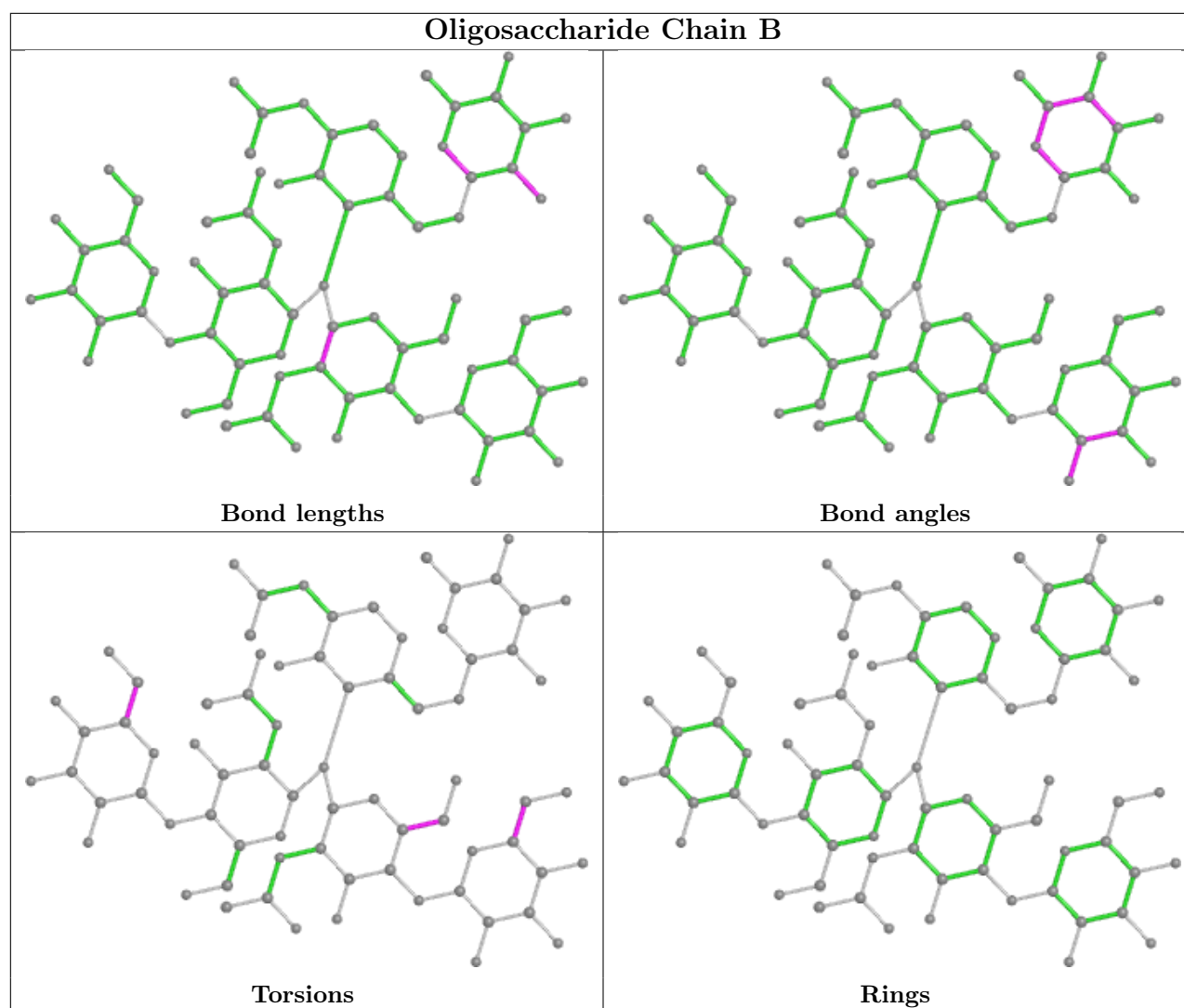
Mol	Chain	Res	Type	Atoms
4	B	2[B]	NAG	C4-C5-C6-O6
4	B	3[A]	BMA	O5-C5-C6-O6
4	B	3[A]	BMA	C4-C5-C6-O6
4	B	2[B]	NAG	O5-C5-C6-O6
4	B	3[B]	BMA	O5-C5-C6-O6
4	B	3[B]	BMA	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	NAG	2	0
4	B	2[B]	NAG	1	0
4	B	4	FUC	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](#)

10 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	$\# Z  > 2$
5	EDO	A	603	-	3,3,3	0.51	0	2,2,2	0.20	0
5	EDO	L	303	-	3,3,3	0.35	0	2,2,2	0.43	0
5	EDO	H	302	-	3,3,3	0.40	0	2,2,2	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	601	-	3,3,3	0.41	0	2,2,2	0.72	0
5	EDO	A	604	-	3,3,3	0.44	0	2,2,2	0.17	0
5	EDO	A	602	-	3,3,3	0.47	0	2,2,2	0.47	0
5	EDO	L	302	-	3,3,3	0.54	0	2,2,2	0.28	0
5	EDO	L	301	-	3,3,3	0.83	0	2,2,2	0.37	0
5	EDO	H	301	-	3,3,3	0.72	0	2,2,2	0.30	0
5	EDO	L	304	-	3,3,3	0.52	0	2,2,2	0.41	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
5	EDO	A	603	-	-	0/1/1/1	-
5	EDO	L	303	-	-	0/1/1/1	-
5	EDO	H	302	-	-	1/1/1/1	-
5	EDO	A	601	-	-	0/1/1/1	-
5	EDO	A	604	-	-	0/1/1/1	-
5	EDO	A	602	-	-	0/1/1/1	-
5	EDO	L	302	-	-	1/1/1/1	-
5	EDO	L	301	-	-	0/1/1/1	-
5	EDO	H	301	-	-	0/1/1/1	-
5	EDO	L	304	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	302	EDO	O1-C1-C2-O2
5	H	302	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	603	EDO	1	0
5	L	303	EDO	3	0

*Continued on next page...*

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	EDO	3	0
5	A	602	EDO	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

### 6.1 Protein, DNA and RNA chains

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	192/230 (83%)	0.58	17 (8%) 9 11	15, 28, 52, 77	0
2	H	226/226 (100%)	-0.02	1 (0%) 92 94	14, 22, 36, 56	0
3	L	216/217 (99%)	-0.01	3 (1%) 75 79	14, 22, 41, 68	0
All	All	634/673 (94%)	0.17	21 (3%) 46 53	14, 23, 45, 77	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	320	THR	7.9
1	A	504	LEU	7.8
1	A	508	ALA	6.2
1	A	360	PHE	6.2
1	A	503	LEU	4.3
1	A	507	PRO	4.3
1	A	359	THR	4.3
1	A	322	LEU	4.2
1	A	321	ASN	4.0
1	A	513	PRO	3.8
1	A	509	THR	3.6
1	A	378	CYS	3.6
1	A	511	CYS	3.5
3	L	214	CYS	3.4
1	A	491	TYR	3.3
1	A	463	ASP	2.9
1	A	357	ASN	2.4
3	L	154	LEU	2.2
2	H	55	SER	2.2
1	A	325	PHE	2.1
3	L	168	SER	2.0

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

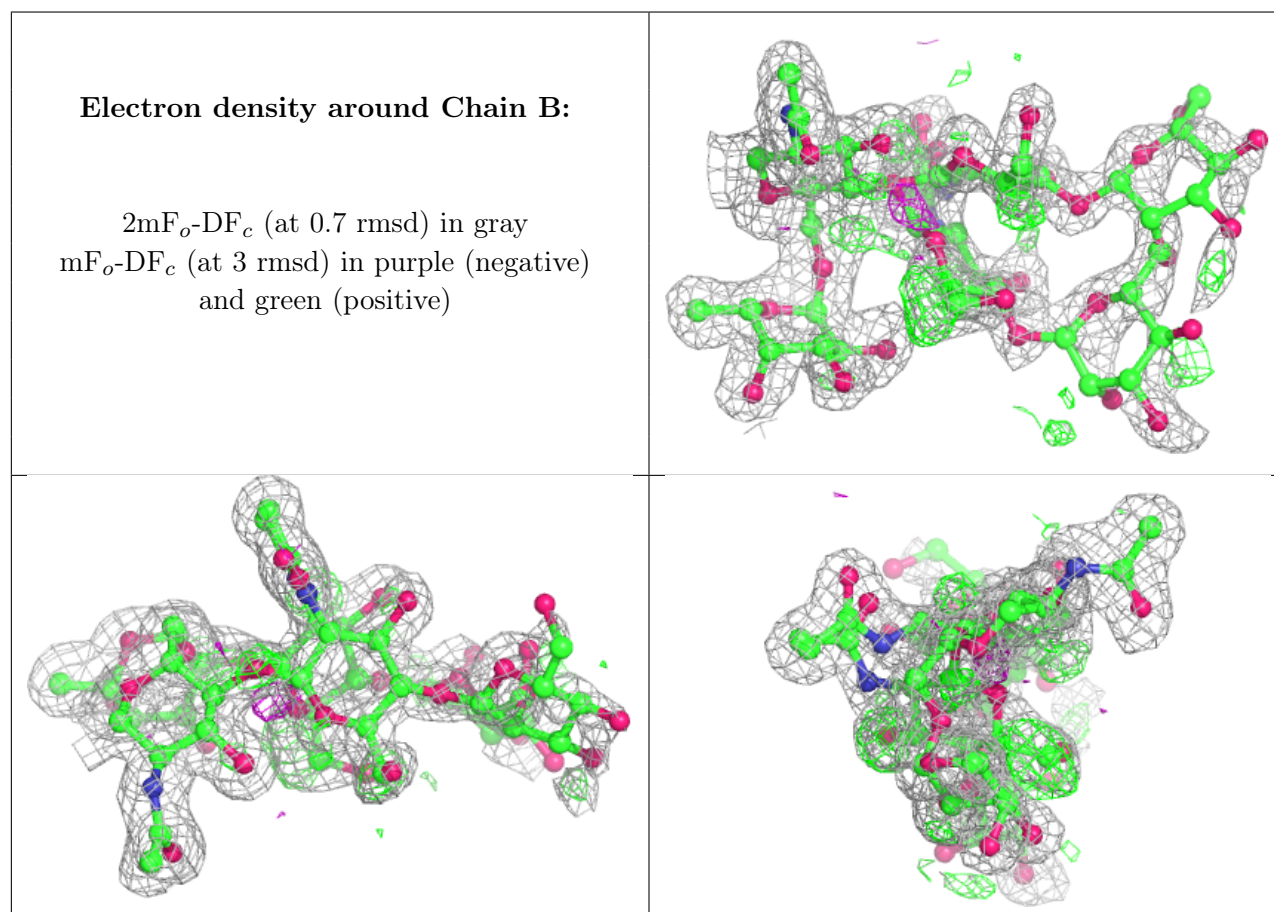
There are no non-standard protein/DNA/RNA residues in this entry.

## 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( $\text{\AA}^2$ )	Q<0.9
4	BMA	B	3[A]	11/12	0.69	0.25	32,45,48,49	11
4	BMA	B	3[B]	11/12	0.69	0.25	39,46,49,51	11
4	FUC	B	4	10/11	0.77	0.17	23,32,38,41	0
4	NAG	B	2[B]	14/15	0.79	0.19	17,27,36,37	14
4	NAG	B	2[A]	14/15	0.79	0.19	18,23,30,31	14
4	NAG	B	1	14/15	0.91	0.09	19,26,33,34	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
5	EDO	L	302	4/4	0.67	0.16	51,54,54,56	0
5	EDO	A	604	4/4	0.83	0.19	45,47,48,52	0
5	EDO	A	603	4/4	0.86	0.10	58,58,60,60	0
5	EDO	L	304	4/4	0.86	0.16	43,48,54,56	0
5	EDO	L	301	4/4	0.88	0.13	20,29,34,35	0
5	EDO	H	302	4/4	0.89	0.25	46,49,54,56	0
5	EDO	A	601	4/4	0.92	0.12	32,32,33,34	0
5	EDO	H	301	4/4	0.92	0.12	21,27,27,34	0
5	EDO	L	303	4/4	0.94	0.10	36,38,44,55	0
5	EDO	A	602	4/4	0.95	0.12	26,33,40,43	0

## 6.5 Other polymers

There are no such residues in this entry.