



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2022 – 06:07 PM EST

PDB ID : 7LM8
Title : Crystal structure of SARS-CoV-2 spike protein receptor-binding domain in complex with two cross-neutralizing antibodies CV38-142 and COVA1-16 Fabs isolated from COVID-19 patients
Authors : Liu, H.; Wilson, I.A.
Deposited on : 2021-02-05
Resolution : 1.94 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

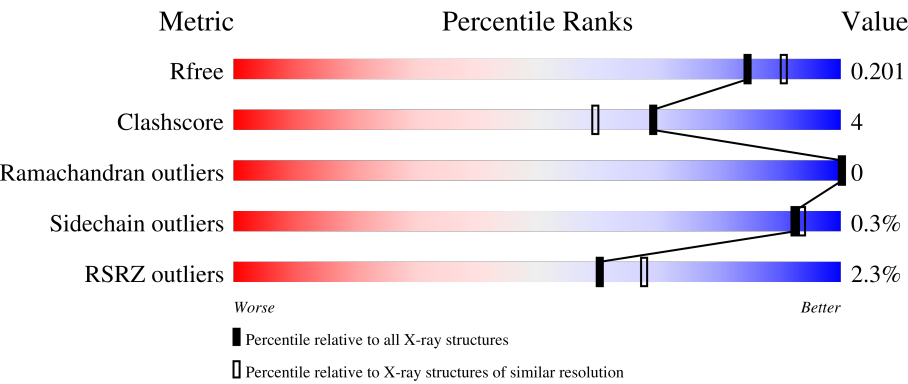
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 ≥ 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>5%</div><div><div></div><div>79%</div><div>6%</div><div>15%</div></div></div>
2	H	232	<div><div>%</div><div><div></div><div>95%</div><div></div><div></div></div><div></div></div>
3	L	215	<div><div>%</div><div><div></div><div>90%</div><div>9%</div><div></div></div><div></div></div>
4	M	226	<div><div>2%</div><div><div></div><div>88%</div><div>8%</div><div></div></div><div></div></div>
5	N	217	<div><div>%</div><div><div></div><div>98%</div><div></div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
6	B	4	 25% 75%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9315 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	196	Total	C	N	O	S	0	0	0
			1539	986	256	289	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	SER	-	expression tag	UNP P0DTC2
A	543	GLY	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
A	548	HIS	-	expression tag	UNP P0DTC2
A	549	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called COVA1-16 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	226	Total	C	N	O	S	0	0	0
			1719	1083	293	335	8			

- Molecule 3 is a protein called COVA1-16 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1632	1019	272	337	4			

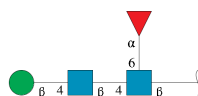
- Molecule 4 is a protein called CV38-142 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	219	Total	C	N	O	S	0	0	0
			1639	1044	268	320	7			

- Molecule 5 is a protein called CV38-142 Fab light chain.

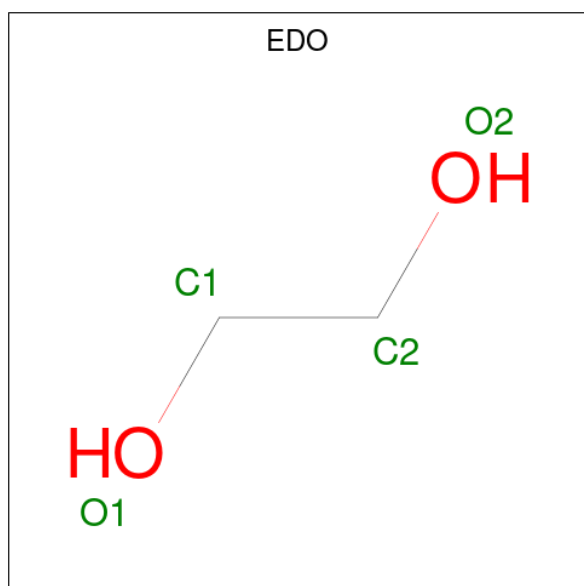
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	N	217	Total	C	N	O	S	3	1	0
			1666	1038	279	343	6			

- Molecule 6 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
6	B	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

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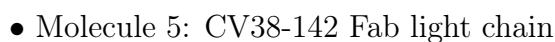
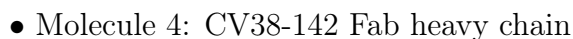
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	H	1	Total C O 4 2 2	0	0
7	L	1	Total C O 4 2 2	0	0
7	L	1	Total C O 4 2 2	0	0
7	M	1	Total C O 4 2 2	0	0
7	M	1	Total C O 4 2 2	0	0
7	M	1	Total C O 4 2 2	0	0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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	171	Total O 171 171	0	0
8	H	213	Total O 213 213	0	0
8	L	198	Total O 198 198	0	0
8	M	184	Total O 184 184	0	0
8	N	241	Total O 241 241	0	0

- Molecule 1: Spike protein S1





- Molecule 6: 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

Chain B: 25% 75%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.66Å 148.23Å 162.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.71 – 1.94 33.71 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.0 (33.71-1.94) 99.1 (33.71-1.94)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.169 , 0.201 0.169 , 0.201	Depositor DCC
R_{free} test set	5355 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9315	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: EDO, BMA, NAG, FUC

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	0.58	0/1582	0.63	0/2153
2	H	0.53	0/1763	0.64	0/2400
3	L	0.59	0/1667	0.70	0/2269
4	M	0.54	0/1683	0.62	0/2293
5	N	0.59	0/1705	0.67	0/2315
All	All	0.57	0/8400	0.65	0/11430

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	1539	0	1444	12	0
2	H	1719	0	1661	4	0
3	L	1632	0	1566	12	0
4	M	1639	0	1589	29	0
5	N	1666	0	1604	5	0
6	B	49	0	43	1	0
7	A	24	0	36	5	0
7	H	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	8	0	12	1	0
7	M	16	0	24	6	0
7	N	12	0	18	0	0
8	A	171	0	0	0	0
8	H	213	0	0	1	0
8	L	198	0	0	3	0
8	M	184	0	0	1	0
8	N	241	0	0	4	0
All	All	9315	0	8003	60	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 (60) 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)
4:M:83:LYS:HD3	4:M:85:SER:H	1.11	1.15
4:M:83:LYS:CD	4:M:85:SER:H	1.87	0.88
4:M:83:LYS:HD3	4:M:85:SER:N	1.90	0.86
4:M:210:LYS:HZ2	4:M:212:GLU:CG	2.02	0.72
4:M:210:LYS:HD3	4:M:210:LYS:C	2.12	0.70
4:M:11:VAL:HB	4:M:147:PRO:HG3	1.72	0.69
3:L:83:ILE:HD11	3:L:105:GLU:HA	1.75	0.69
5:N:197:THR:HG21	8:N:620:HOH:O	1.93	0.68
3:L:39:ARG:NH2	8:L:402:HOH:O	2.30	0.64
4:M:210:LYS:NZ	4:M:212:GLU:CG	2.63	0.62
5:N:197:THR:HG23	8:N:502:HOH:O	2.02	0.59
4:M:94:ARG:HH22	7:M:302:EDO:H21	1.67	0.59
4:M:210:LYS:NZ	4:M:211:VAL:O	2.34	0.59
1:A:388:ASN:HB3	1:A:528:LYS:HD3	1.85	0.59
4:M:83:LYS:HE2	4:M:84:ALA:HB3	1.85	0.58
3:L:24:GLN:NE2	8:L:403:HOH:O	2.39	0.56
4:M:210:LYS:NZ	8:M:402:HOH:O	2.39	0.56
3:L:57:GLY:C	7:L:302:EDO:H12	2.27	0.55
7:A:603:EDO:H11	2:H:99:TYR:HA	1.87	0.55
1:A:381:GLY:H	7:A:603:EDO:H12	1.72	0.54
5:N:21:ILE:HG23	8:N:408:HOH:O	2.07	0.54
4:M:83:LYS:HD3	4:M:85:SER:CB	2.38	0.53
1:A:472:ILE:HD12	1:A:484:GLU:HG2	1.91	0.53
4:M:83:LYS:CE	4:M:85:SER:H	2.22	0.52
4:M:149:PRO:HG2	7:M:304:EDO:H22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:6:GLN:HB3	8:N:408:HOH:O	2.09	0.52
4:M:201:LYS:HD2	7:M:304:EDO:H12	1.92	0.51
3:L:145:LYS:HB3	3:L:197:THR:OG1	2.11	0.50
1:A:493:GLN:NE2	1:A:494:SER:H	2.11	0.49
3:L:80:PRO:HA	3:L:106:ILE:CD1	2.44	0.48
4:M:33:TRP:HB2	4:M:95:ILE:HB	1.95	0.48
4:M:83:LYS:CD	4:M:85:SER:CB	2.93	0.47
1:A:347:PHE:O	7:A:605:EDO:H22	2.13	0.47
4:M:100(C):TRP:HB2	5:N:91:SER:HB2	1.97	0.47
3:L:55:GLU:HG3	3:L:56:THR:N	2.30	0.46
4:M:210:LYS:HZ2	4:M:212:GLU:CA	2.29	0.45
3:L:94:PRO:HA	3:L:95:PRO:C	2.37	0.45
1:A:342:PHE:HB2	6:B:1:NAG:H82	1.99	0.45
1:A:406:GLU:OE2	7:A:606:EDO:H12	2.17	0.44
4:M:210:LYS:HD3	4:M:211:VAL:N	2.32	0.44
4:M:52:TYR:HD1	4:M:54:GLU:HB2	1.81	0.44
4:M:84:ALA:HA	4:M:111:VAL:HB	2.00	0.44
1:A:346:ARG:CZ	7:A:605:EDO:H21	2.47	0.44
1:A:493:GLN:HE21	1:A:494:SER:H	1.65	0.44
4:M:83:LYS:HD3	4:M:85:SER:HB3	1.99	0.44
4:M:145:TYR:CE2	4:M:150:VAL:HG13	2.52	0.44
1:A:365:TYR:CD2	1:A:387:LEU:HB3	2.53	0.43
3:L:35:TRP:CE2	3:L:73:PHE:HB2	2.53	0.43
3:L:161:GLU:OE2	8:L:401:HOH:O	2.20	0.43
1:A:378:LYS:HE3	2:H:99:TYR:CZ	2.54	0.43
4:M:94:ARG:HH22	7:M:302:EDO:C2	2.32	0.42
1:A:528:LYS:N	1:A:528:LYS:HD2	2.34	0.42
4:M:210:LYS:NZ	4:M:211:VAL:C	2.73	0.41
2:H:143:LYS:NZ	2:H:171:GLN:OE1	2.54	0.41
4:M:210:LYS:HD2	4:M:212:GLU:CG	2.50	0.41
3:L:149:LYS:HG2	3:L:154:LEU:HD12	2.01	0.41
3:L:40:PRO:HB3	3:L:165:GLU:HG3	2.02	0.41
2:H:68:THR:HG23	8:H:496:HOH:O	2.20	0.40
4:M:94:ARG:NH2	7:M:302:EDO:H21	2.35	0.40
4:M:149:PRO:HG2	7:M:304:EDO:C2	2.52	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	194/231 (84%)	188 (97%)	6 (3%)	0	100	100
2	H	222/232 (96%)	217 (98%)	5 (2%)	0	100	100
3	L	211/215 (98%)	206 (98%)	5 (2%)	0	100	100
4	M	215/226 (95%)	212 (99%)	3 (1%)	0	100	100
5	N	216/217 (100%)	209 (97%)	7 (3%)	0	100	100
All	All	1058/1121 (94%)	1032 (98%)	26 (2%)	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	165/203 (81%)	165 (100%)	0	100	100
2	H	190/198 (96%)	188 (99%)	2 (1%)	73	67
3	L	186/190 (98%)	186 (100%)	0	100	100
4	M	181/190 (95%)	181 (100%)	0	100	100
5	N	191/192 (100%)	190 (100%)	1 (0%)	88	88
All	All	913/973 (94%)	910 (100%)	3 (0%)	92	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	71	ARG
2	H	127	SER
5	N	214	CYS

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	334	ASN
1	A	493	GLN
3	L	53	ASN
3	L	93	ASN

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 ⓘ

4 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	0.24	0	17,19,21	0.72	0
6	NAG	B	2	6	14,14,15	0.44	0	17,19,21	0.32	0
6	BMA	B	3	6	11,11,12	1.15	1 (9%)	15,15,17	0.78	0
6	FUC	B	4	6	10,10,11	1.70	2 (20%)	14,14,16	0.79	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	6,1	-	0/6/23/26	0/1/1/1
6	NAG	B	2	6	-	0/6/23/26	0/1/1/1
6	BMA	B	3	6	-	0/2/19/22	0/1/1/1
6	FUC	B	4	6	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	4	FUC	O5-C1	-3.18	1.38	1.43
6	B	4	FUC	C2-C3	2.93	1.56	1.52
6	B	3	BMA	C2-C3	2.16	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

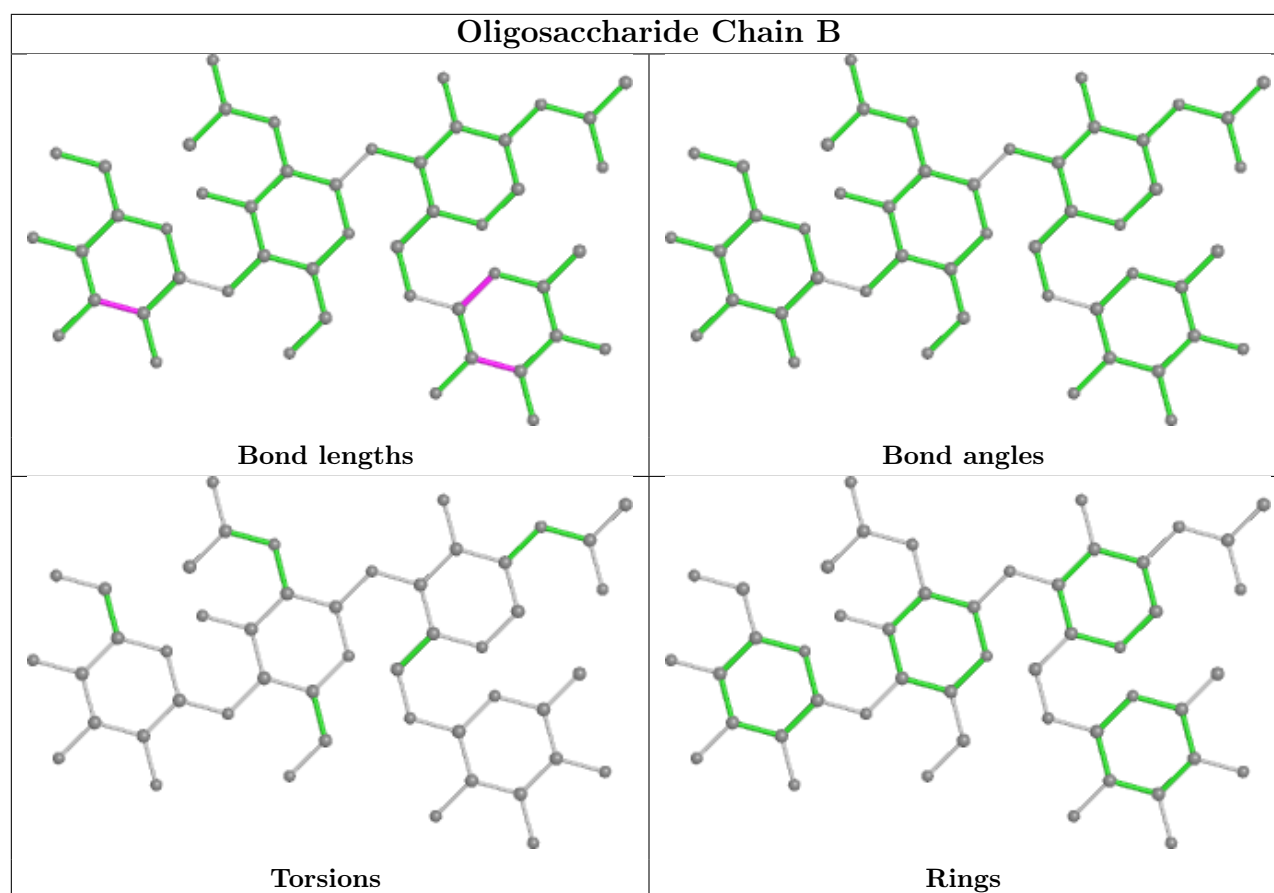
There are no torsion outliers.

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](#)

16 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	EDO	N	302	-	3,3,3	0.70	0	2,2,2	0.06	0
7	EDO	M	304	-	3,3,3	0.58	0	2,2,2	0.38	0
7	EDO	M	301	-	3,3,3	0.44	0	2,2,2	0.17	0
7	EDO	L	302	-	3,3,3	0.56	0	2,2,2	0.50	0
7	EDO	M	302	-	3,3,3	0.50	0	2,2,2	0.25	0
7	EDO	H	301	-	3,3,3	0.51	0	2,2,2	0.19	0
7	EDO	A	604	-	3,3,3	0.65	0	2,2,2	0.16	0
7	EDO	A	602	-	3,3,3	0.47	0	2,2,2	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	N	301	-	3,3,3	0.65	0	2,2,2	0.44	0
7	EDO	A	603	-	3,3,3	0.41	0	2,2,2	0.52	0
7	EDO	A	601	-	3,3,3	0.57	0	2,2,2	0.42	0
7	EDO	A	606	-	3,3,3	0.63	0	2,2,2	0.17	0
7	EDO	N	303	-	3,3,3	0.55	0	2,2,2	0.34	0
7	EDO	L	301	-	3,3,3	0.64	0	2,2,2	0.33	0
7	EDO	A	605	-	3,3,3	0.51	0	2,2,2	0.25	0
7	EDO	M	303	-	3,3,3	0.47	0	2,2,2	0.22	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
7	EDO	N	302	-	-	0/1/1/1	-
7	EDO	M	304	-	-	0/1/1/1	-
7	EDO	M	301	-	-	0/1/1/1	-
7	EDO	L	302	-	-	1/1/1/1	-
7	EDO	M	302	-	-	0/1/1/1	-
7	EDO	H	301	-	-	0/1/1/1	-
7	EDO	A	604	-	-	1/1/1/1	-
7	EDO	A	602	-	-	0/1/1/1	-
7	EDO	N	301	-	-	0/1/1/1	-
7	EDO	A	603	-	-	0/1/1/1	-
7	EDO	A	601	-	-	0/1/1/1	-
7	EDO	A	606	-	-	1/1/1/1	-
7	EDO	N	303	-	-	0/1/1/1	-
7	EDO	L	301	-	-	0/1/1/1	-
7	EDO	A	605	-	-	1/1/1/1	-
7	EDO	M	303	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	606	EDO	O1-C1-C2-O2
7	L	302	EDO	O1-C1-C2-O2
7	A	605	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	A	604	EDO	O1-C1-C2-O2
7	M	303	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	304	EDO	3	0
7	L	302	EDO	1	0
7	M	302	EDO	3	0
7	A	603	EDO	2	0
7	A	606	EDO	1	0
7	A	605	EDO	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

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, 95th 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 ²)	Q<0.9
1	A	196/231 (84%)	0.10	12 (6%) 21 27	10, 20, 49, 70	0
2	H	226/232 (97%)	-0.29	3 (1%) 77 81	11, 20, 33, 58	0
3	L	213/215 (99%)	-0.23	3 (1%) 75 80	10, 18, 35, 65	0
4	M	219/226 (96%)	-0.09	4 (1%) 68 74	11, 22, 45, 63	0
5	N	217/217 (100%)	-0.24	3 (1%) 75 80	10, 19, 38, 60	0
All	All	1071/1121 (95%)	-0.16	25 (2%) 60 67	10, 20, 39, 70	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	477	SER	4.9
1	A	476	GLY	4.8
1	A	481	ASN	4.2
2	H	215	SER	4.2
2	H	133	GLY	3.9
1	A	478	THR	3.9
1	A	482	GLY	3.3
3	L	212	GLY	3.3
5	N	214	CYS	3.2
1	A	486	PHE	3.0
1	A	479	PRO	2.9
4	M	190	GLY	2.9
4	M	134	GLY	2.7
1	A	489	TYR	2.6
1	A	335	LEU	2.6
3	L	185	ASP	2.5
1	A	487	ASN	2.4
4	M	189	LEU	2.4
3	L	213	GLU	2.3
1	A	485	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	1	GLN	2.3
5	N	1	ASP	2.2
1	A	471	GLU	2.2
5	N	215	SER	2.1
4	M	204	ASN	2.1

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

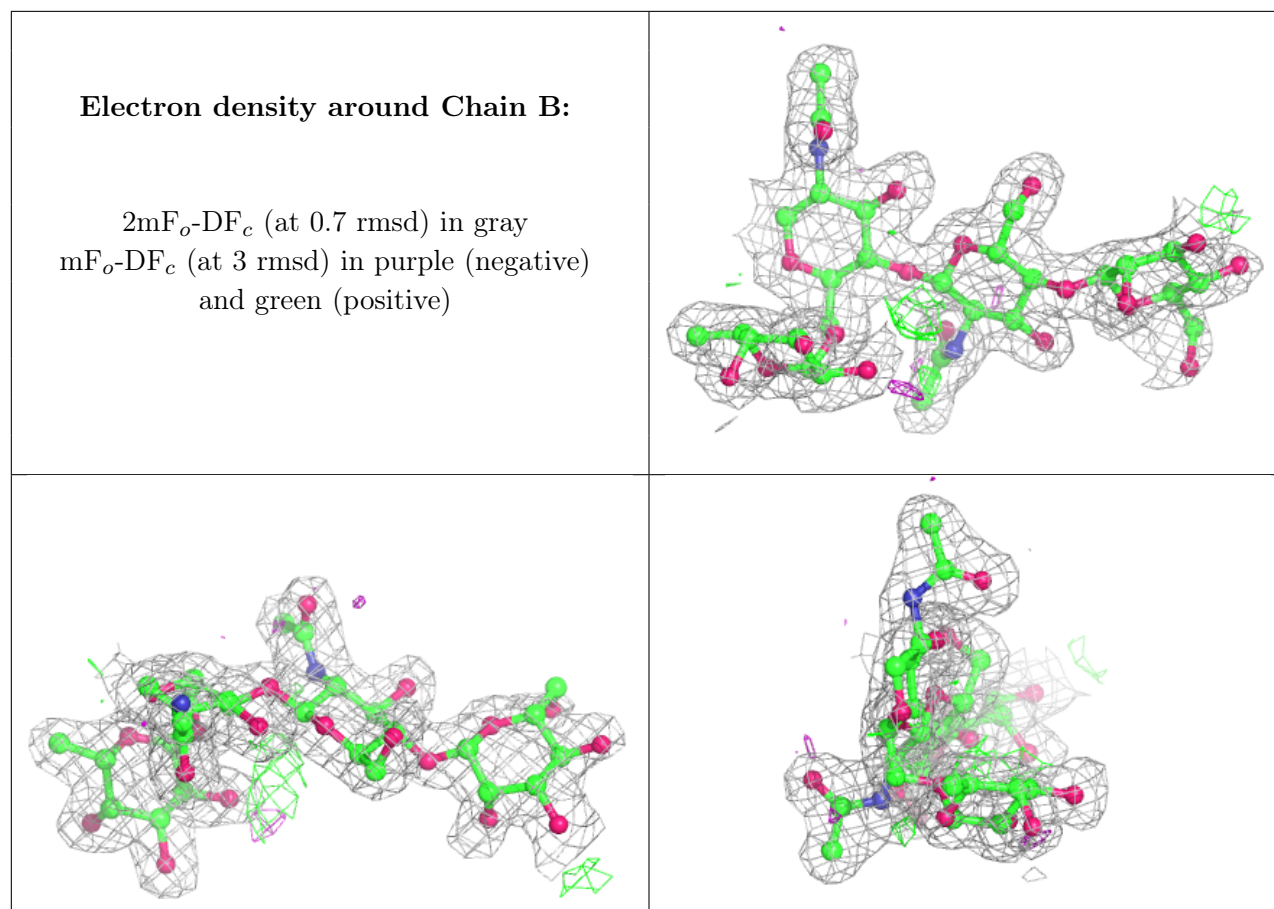
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th 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 ²)	Q<0.9
6	BMA	B	3	11/12	0.81	0.31	48,54,60,61	0
6	NAG	B	2	14/15	0.90	0.16	21,27,33,41	0
6	FUC	B	4	10/11	0.92	0.14	19,27,28,28	0
6	NAG	B	1	14/15	0.95	0.10	15,19,26,27	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, 95th 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 ²)	Q<0.9
7	EDO	A	605	4/4	0.77	0.19	41,42,44,45	0
7	EDO	A	606	4/4	0.79	0.21	39,42,47,48	0
7	EDO	M	301	4/4	0.86	0.11	39,42,45,46	0
7	EDO	M	304	4/4	0.87	0.18	32,36,40,42	0
7	EDO	M	303	4/4	0.89	0.29	36,40,44,45	0
7	EDO	A	604	4/4	0.89	0.21	28,32,37,40	0
7	EDO	L	302	4/4	0.90	0.22	42,44,46,47	0
7	EDO	M	302	4/4	0.92	0.30	31,34,37,39	0
7	EDO	N	302	4/4	0.92	0.11	28,30,30,31	0
7	EDO	A	603	4/4	0.94	0.14	34,37,40,43	0
7	EDO	A	601	4/4	0.96	0.14	19,22,25,25	0
7	EDO	A	602	4/4	0.96	0.09	19,19,19,23	0
7	EDO	H	301	4/4	0.96	0.16	27,28,31,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	EDO	N	301	4/4	0.97	0.09	17,24,26,29	0
7	EDO	L	301	4/4	0.97	0.07	16,19,19,21	0
7	EDO	N	303	4/4	0.97	0.10	20,26,31,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.