



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2021 – 12:50 PM EDT

PDB ID : 7R6W
Title : SARS-CoV-2 spike receptor-binding domain (RBD) in complex with S2X35 Fab and S309 Fab
Authors : Snell, G.; Czudnochowski, N.; Hernandez, P.; Nix, J.C.; Croll, T.I.; Corti, D.; Cameroni, E.; Pinto, D.; Beltramello, M.
Deposited on : 2021-06-23
Resolution : 1.83 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 : 2.23.1
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) : 2.23.1

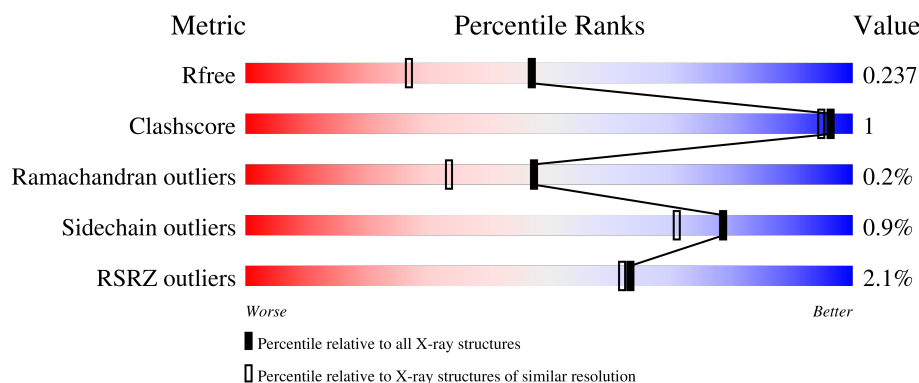
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

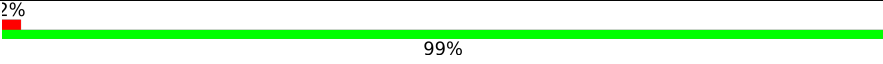
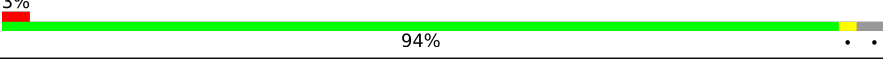
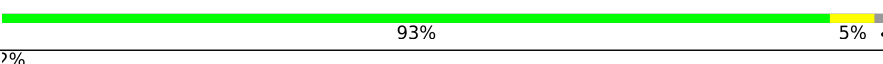
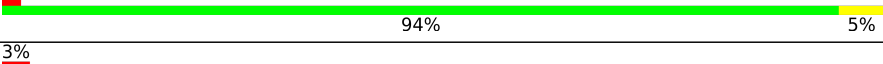

The reported resolution of this entry is 1.83 Å.

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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	B	214	
2	A	230	
3	L	219	
4	H	231	
5	R	216	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	C	2	 100%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 8911 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 Light Chain of Fab domain of monoclonal antibody S309.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	213	Total	C	N	O	S	0	0	0
			1624	1011	277	332	4			

- Molecule 2 is a protein called Heavy Chain of Fab domain of monoclonal antibody S309.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	221	Total	C	N	O	S	0	0	0
			1671	1057	282	325	7			

- Molecule 3 is a protein called Light Chain of Fab domain of monoclonal antibody S2X35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	0	0
			1582	987	264	327	4			

- Molecule 4 is a protein called Heavy Chain of Fab domain of monoclonal antibody S2X35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	230	Total	C	N	O	S	0	0	0
			1735	1099	287	341	8			

- Molecule 5 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	R	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	324	GLU	-	expression tag	UNP P0DTC2
R	325	THR	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

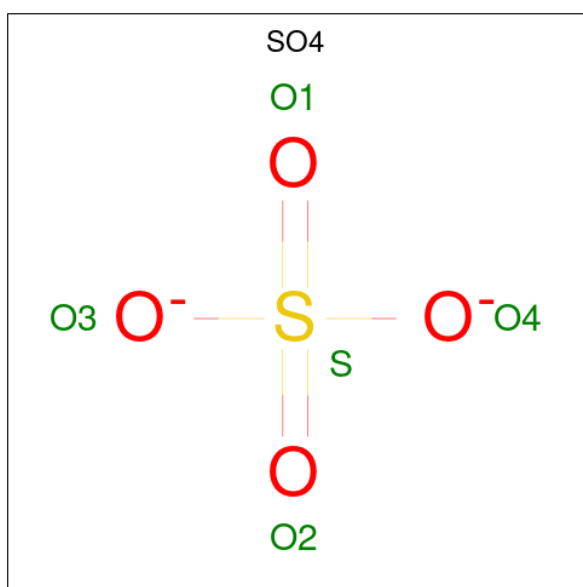
Chain	Residue	Modelled	Actual	Comment	Reference
R	326	GLY	-	expression tag	UNP P0DTC2
R	327	THR	-	expression tag	UNP P0DTC2
R	532	HIS	-	expression tag	UNP P0DTC2
R	533	HIS	-	expression tag	UNP P0DTC2
R	534	HIS	-	expression tag	UNP P0DTC2
R	535	HIS	-	expression tag	UNP P0DTC2
R	536	HIS	-	expression tag	UNP P0DTC2
R	537	HIS	-	expression tag	UNP P0DTC2
R	538	HIS	-	expression tag	UNP P0DTC2
R	539	HIS	-	expression tag	UNP P0DTC2

- 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	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



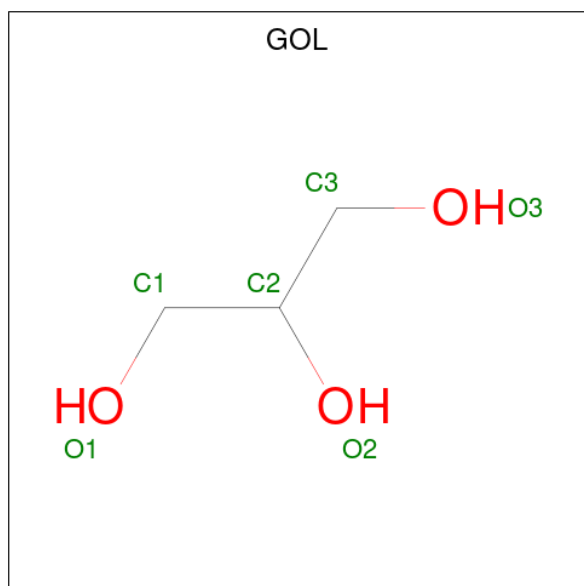
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	L	1	Total O S 5 4 1	0	0
7	L	1	Total O S 5 4 1	0	0
7	L	1	Total O S 5 4 1	0	0
7	L	1	Total O S 5 4 1	0	0
7	L	1	Total O S 5 4 1	0	0
7	L	1	Total O S 5 4 1	0	0
7	L	1	Total O S 5 4 1	0	0
7	H	1	Total O S 5 4 1	0	0
7	H	1	Total O S 5 4 1	0	0
7	R	1	Total O S 5 4 1	0	0
7	R	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	R	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

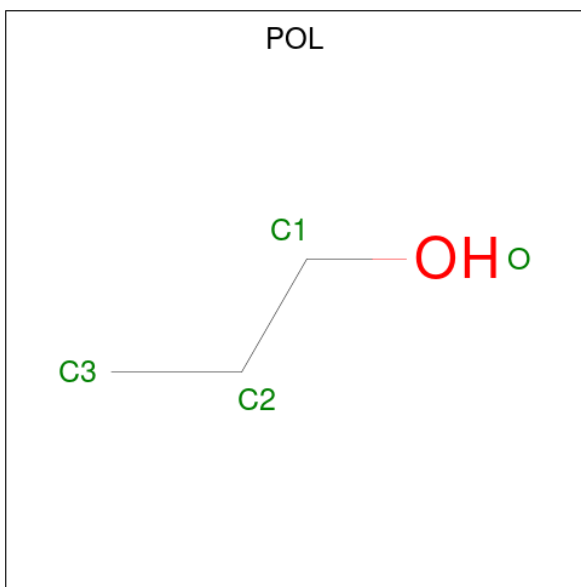


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		
9	H	1	Total	Cl	0	0
			1	1		
9	R	1	Total	Cl	0	0
			1	1		

- Molecule 10 is N-PROPANOL (three-letter code: POL) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	R	1	Total	C	O	0	0
			4	3	1		
10	R	1	Total	C	O	0	0
			4	3	1		

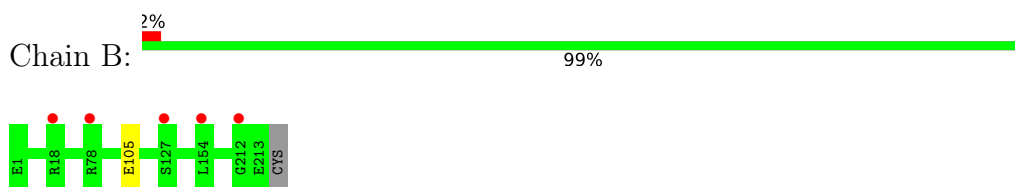
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	122	Total	O	0	0
			122	122		
11	A	108	Total	O	0	0
			108	108		
11	L	113	Total	O	0	0
			113	113		
11	H	125	Total	O	0	0
			125	125		
11	R	116	Total	O	0	0
			116	116		

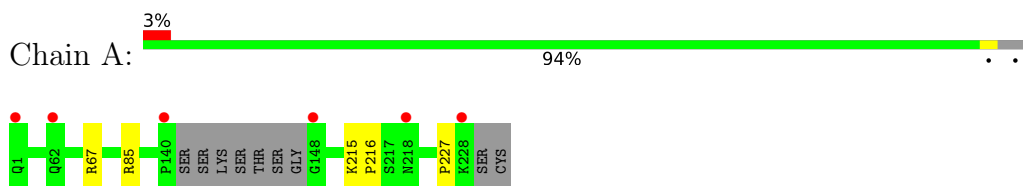
3 Residue-property plots [i](#)

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.

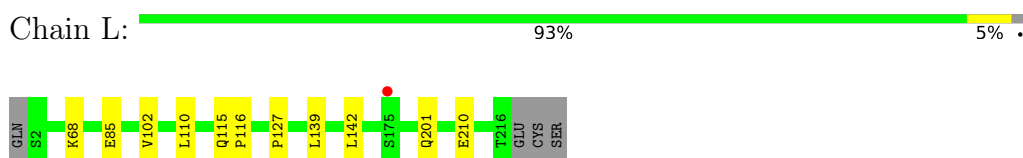
- Molecule 1: Light Chain of Fab domain of monoclonal antibody S309



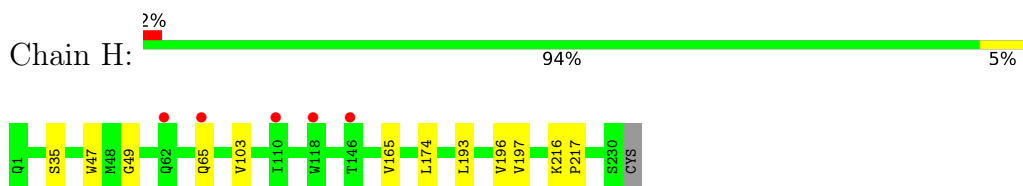
- Molecule 2: Heavy Chain of Fab domain of monoclonal antibody S309



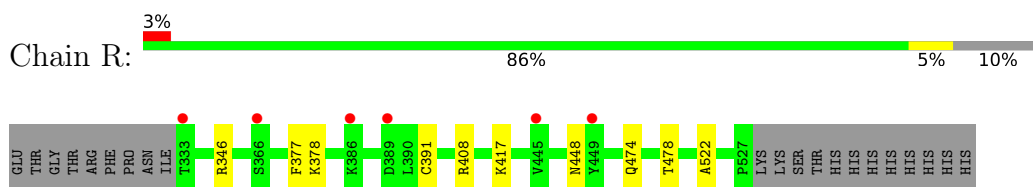
- Molecule 3: Light Chain of Fab domain of monoclonal antibody S2X35



- Molecule 4: Heavy Chain of Fab domain of monoclonal antibody S2X35



- Molecule 5: Spike protein S1



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

100%

M61
M62

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	106.27Å 239.37Å 129.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.91 – 1.83 38.88 – 1.83	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.91-1.83) 98.3 (38.88-1.83)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.211 , 0.232 0.218 , 0.237	Depositor DCC
R_{free} test set	7049 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8911	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: SO4, NAG, CL, GOL, POL

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	B	0.64	0/1657	0.75	0/2250
2	A	0.64	0/1713	0.74	0/2334
3	L	0.65	0/1620	0.73	0/2214
4	H	0.64	0/1779	0.74	0/2426
5	R	0.62	0/1587	0.74	0/2161
All	All	0.64	0/8356	0.74	0/11385

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	B	1624	0	1582	0	0
2	A	1671	0	1629	2	0
3	L	1582	0	1530	6	0
4	H	1735	0	1697	7	0
5	R	1543	0	1459	4	0
6	C	28	0	25	0	0
7	A	25	0	0	0	0
7	B	30	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	10	0	0	0	0
7	L	35	0	0	0	0
7	R	15	0	0	0	0
8	A	6	0	8	0	0
8	B	12	0	16	0	0
9	A	1	0	0	0	0
9	H	1	0	0	0	0
9	R	1	0	0	0	0
10	R	8	0	16	0	0
11	A	108	0	0	0	0
11	B	122	0	0	0	0
11	H	125	0	0	0	0
11	L	113	0	0	0	0
11	R	116	0	0	1	0
All	All	8911	0	7962	16	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 1.

All (16) 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:H:47:TRP:CZ2	4:H:49:GLY:HA2	2.40	0.56
4:H:103:VAL:HG21	5:R:378:LYS:HB2	1.88	0.53
4:H:193:LEU:C	4:H:193:LEU:HD12	2.29	0.52
3:L:142:LEU:CD1	4:H:196:VAL:HG11	2.39	0.52
5:R:417:LYS:NZ	11:R:701:HOH:O	2.41	0.52
3:L:127:PRO:HD3	3:L:139:LEU:CD2	2.44	0.48
2:A:67:ARG:HG2	2:A:85:ARG:NH1	2.28	0.48
4:H:174:LEU:HD21	4:H:197:VAL:HG21	1.95	0.47
5:R:391:CYS:HB3	5:R:522:ALA:HB1	1.99	0.43
3:L:201:GLN:NE2	3:L:210:GLU:OE1	2.36	0.43
3:L:102:VAL:HB	4:H:47:TRP:CG	2.54	0.42
2:A:215:LYS:N	2:A:216:PRO:CD	2.82	0.42
5:R:474:GLN:NE2	5:R:478:THR:O	2.35	0.42
4:H:216:LYS:N	4:H:217:PRO:CD	2.83	0.41
3:L:115:GLN:HB2	3:L:116:PRO:HD2	2.02	0.41
3:L:85:GLU:HG3	3:L:110:LEU:O	2.22	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	B	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
2	A	217/230 (94%)	213 (98%)	3 (1%)	1 (0%)	29	15
3	L	213/219 (97%)	207 (97%)	6 (3%)	0	100	100
4	H	228/231 (99%)	222 (97%)	5 (2%)	1 (0%)	34	20
5	R	193/216 (89%)	186 (96%)	7 (4%)	0	100	100
All	All	1062/1110 (96%)	1033 (97%)	27 (2%)	2 (0%)	47	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	65	GLN
2	A	227	PRO

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	B	184/185 (100%)	183 (100%)	1 (0%)	88	85
2	A	184/192 (96%)	184 (100%)	0	100	100
3	L	178/182 (98%)	177 (99%)	1 (1%)	86	82
4	H	193/194 (100%)	191 (99%)	2 (1%)	76	68
5	R	168/188 (89%)	164 (98%)	4 (2%)	49	32
All	All	907/941 (96%)	899 (99%)	8 (1%)	78	71

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	105	GLU
3	L	68	LYS
4	H	35	SER
4	H	165	VAL
5	R	346	ARG
5	R	377	PHE
5	R	408	ARG
5	R	448	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	27	GLN
2	A	3	GLN
3	L	81	GLN
4	H	102	GLN
5	R	498	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 ⓘ

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	C	1	6,5	14,14,15	0.41	0	17,19,21	0.62	0
6	NAG	C	2	6	14,14,15	0.27	0	17,19,21	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	C	1	6,5	-	0/6/23/26	0/1/1/1
6	NAG	C	2	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

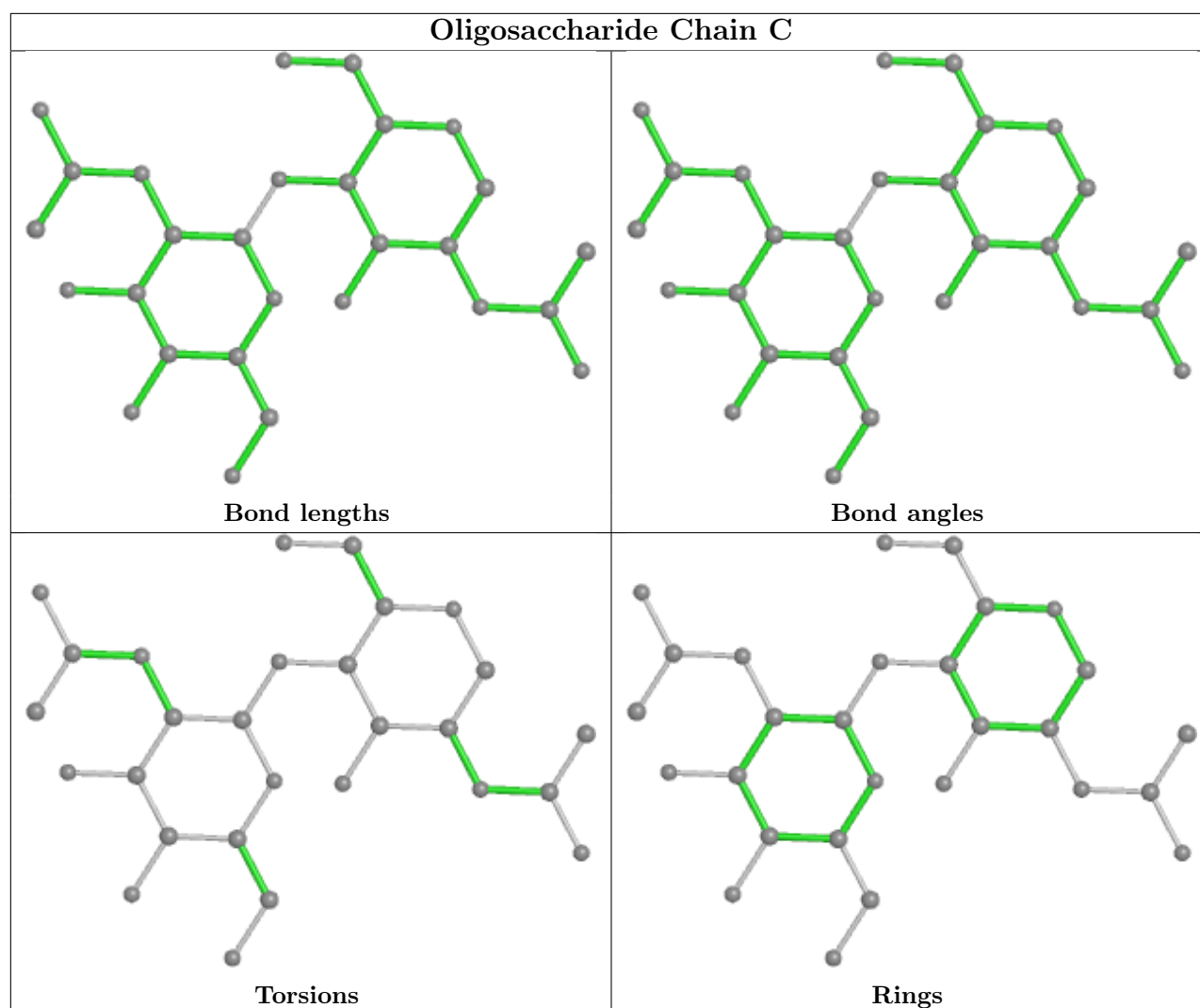
There are no chirality outliers.

There are no torsion outliers.

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](#)

Of 31 ligands modelled in this entry, 3 are monoatomic - leaving 28 for Mogul analysis.

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	SO4	B	302	-	4,4,4	0.39	0	6,6,6	0.04	0
8	GOL	B	307	-	5,5,5	0.10	0	5,5,5	0.27	0
7	SO4	B	303	-	4,4,4	0.38	0	6,6,6	0.05	0
7	SO4	L	304	-	4,4,4	0.37	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	B	304	-	4,4,4	0.38	0	6,6,6	0.04	0
7	SO4	A	307	-	4,4,4	0.38	0	6,6,6	0.04	0
7	SO4	L	303	-	4,4,4	0.38	0	6,6,6	0.05	0
8	GOL	A	302	-	5,5,5	0.07	0	5,5,5	0.25	0
7	SO4	H	302	-	4,4,4	0.37	0	6,6,6	0.05	0
7	SO4	R	601	-	4,4,4	0.39	0	6,6,6	0.05	0
8	GOL	B	306	-	5,5,5	0.10	0	5,5,5	0.28	0
7	SO4	L	302	-	4,4,4	0.38	0	6,6,6	0.05	0
7	SO4	B	305	-	4,4,4	0.38	0	6,6,6	0.05	0
7	SO4	L	306	-	4,4,4	0.38	0	6,6,6	0.05	0
7	SO4	L	305	-	4,4,4	0.38	0	6,6,6	0.05	0
10	POL	R	603	-	3,3,3	0.24	0	2,2,2	0.15	0
7	SO4	A	303	-	4,4,4	0.39	0	6,6,6	0.05	0
7	SO4	R	606	-	4,4,4	0.36	0	6,6,6	0.05	0
7	SO4	B	301	-	4,4,4	0.37	0	6,6,6	0.05	0
7	SO4	L	307	-	4,4,4	0.39	0	6,6,6	0.05	0
7	SO4	L	301	-	4,4,4	0.38	0	6,6,6	0.04	0
7	SO4	A	306	-	4,4,4	0.37	0	6,6,6	0.06	0
7	SO4	H	303	-	4,4,4	0.40	0	6,6,6	0.06	0
7	SO4	R	602	-	4,4,4	0.39	0	6,6,6	0.05	0
7	SO4	A	304	-	4,4,4	0.38	0	6,6,6	0.05	0
7	SO4	A	305	-	4,4,4	0.38	0	6,6,6	0.05	0
7	SO4	B	308	-	4,4,4	0.38	0	6,6,6	0.04	0
10	POL	R	604	-	3,3,3	0.26	0	2,2,2	0.14	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
8	GOL	B	307	-	-	2/4/4/4	-
10	POL	R	603	-	-	0/1/1/1	-
8	GOL	A	302	-	-	0/4/4/4	-
8	GOL	B	306	-	-	4/4/4/4	-
10	POL	R	604	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	306	GOL	O1-C1-C2-C3
8	B	306	GOL	C1-C2-C3-O3
8	B	307	GOL	C1-C2-C3-O3
8	B	307	GOL	O2-C2-C3-O3
8	B	306	GOL	O1-C1-C2-O2
8	B	306	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	B	213/214 (99%)	-0.11	5 (2%) 60 58	30, 39, 51, 63	0
2	A	221/230 (96%)	0.11	6 (2%) 54 52	29, 40, 58, 79	0
3	L	215/219 (98%)	-0.12	1 (0%) 91 91	28, 38, 53, 62	0
4	H	230/231 (99%)	0.08	5 (2%) 62 60	27, 38, 55, 75	0
5	R	195/216 (90%)	0.29	6 (3%) 49 46	27, 36, 54, 64	1 (0%)
All	All	1074/1110 (96%)	0.05	23 (2%) 63 62	27, 38, 55, 79	1 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	65	GLN	4.2
5	R	333	THR	4.0
2	A	1	GLN	4.0
5	R	449	TYR	3.8
5	R	445	VAL	3.6
3	L	175	SER	3.5
5	R	366	SER	2.9
2	A	228	LYS	2.9
1	B	78	ARG	2.8
1	B	154	LEU	2.7
2	A	218	ASN	2.6
5	R	389	ASP	2.6
5	R	386	LYS	2.5
1	B	212	GLY	2.4
4	H	146	THR	2.4
2	A	148	GLY	2.4
4	H	118	TRP	2.2
2	A	140	PRO	2.2
1	B	127	SER	2.1
4	H	110	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	18	ARG	2.0
2	A	62	GLN	2.0
4	H	62	GLN	2.0

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

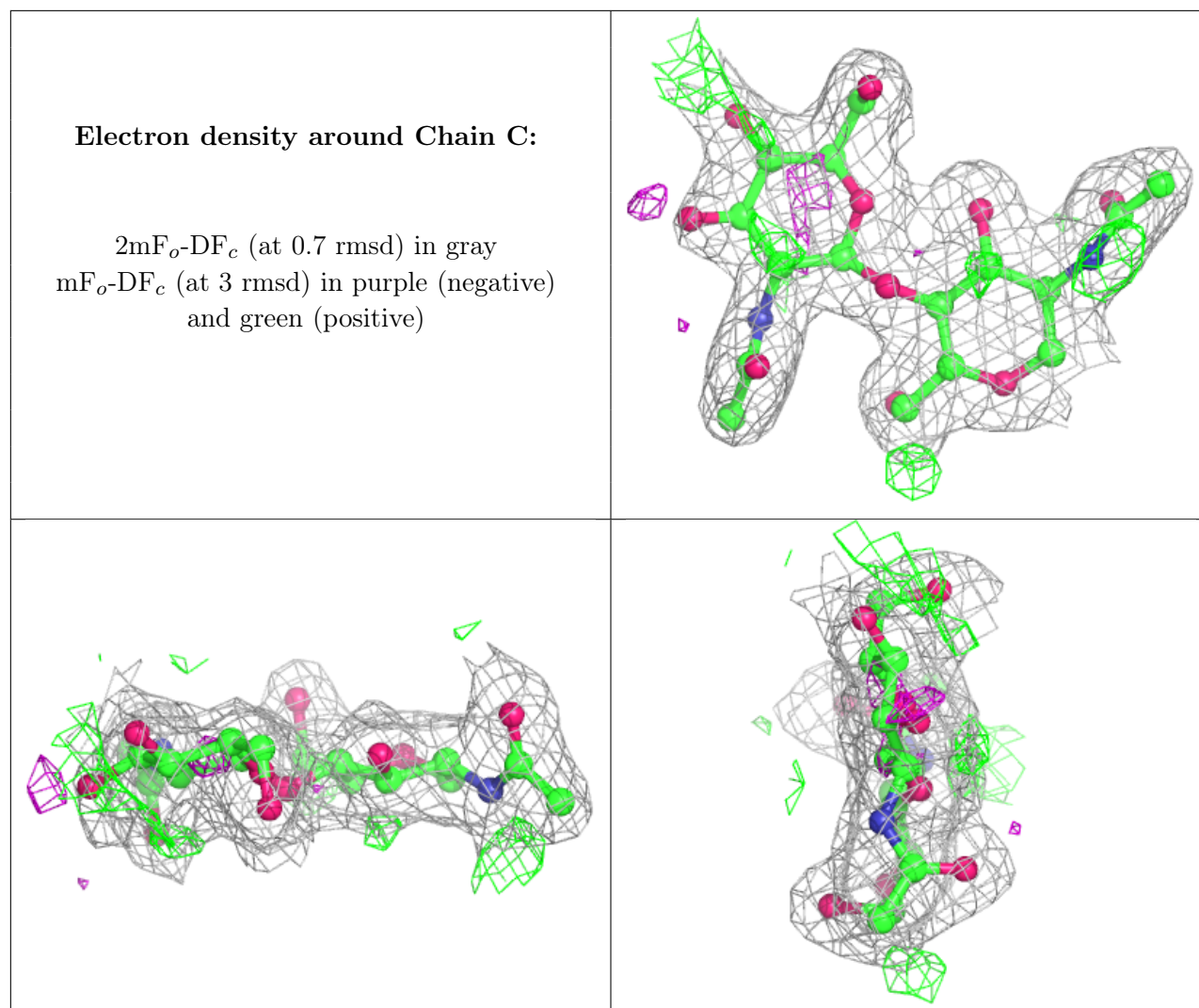
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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(\AA^2)	Q<0.9
6	NAG	C	2	14/15	0.75	0.17	48,53,55,56	0
6	NAG	C	1	14/15	0.92	0.10	35,39,43,46	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	SO4	R	606	5/5	0.56	0.26	90,93,96,97	0
8	GOL	B	306	6/6	0.67	0.19	62,66,67,70	0
7	SO4	H	302	5/5	0.69	0.29	90,90,91,94	0
7	SO4	H	303	5/5	0.71	0.34	118,119,121,122	0
7	SO4	A	306	5/5	0.73	0.20	81,82,86,88	0
7	SO4	B	301	5/5	0.82	0.18	84,87,88,90	0
9	CL	H	301	1/1	0.83	0.09	75,75,75,75	0
7	SO4	B	305	5/5	0.84	0.23	99,100,101,101	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	SO4	L	307	5/5	0.85	0.25	104,105,106,106	0
7	SO4	B	304	5/5	0.85	0.25	92,94,96,96	0
8	GOL	A	302	6/6	0.86	0.20	49,49,50,51	0
8	GOL	B	307	6/6	0.88	0.16	36,38,38,38	0
10	POL	R	604	4/4	0.88	0.23	45,50,51,52	0
7	SO4	A	304	5/5	0.89	0.23	88,90,90,91	0
7	SO4	B	303	5/5	0.90	0.23	99,101,102,102	0
7	SO4	L	301	5/5	0.90	0.24	102,103,103,104	0
7	SO4	L	304	5/5	0.90	0.22	88,89,89,92	0
7	SO4	A	305	5/5	0.91	0.17	95,97,98,98	0
7	SO4	A	307	5/5	0.92	0.16	81,85,85,85	0
7	SO4	B	302	5/5	0.92	0.28	99,99,100,100	0
7	SO4	L	302	5/5	0.94	0.19	81,82,83,83	0
10	POL	R	603	4/4	0.94	0.27	40,42,42,42	0
9	CL	A	301	1/1	0.94	0.08	63,63,63,63	0
7	SO4	A	303	5/5	0.95	0.20	68,69,73,73	0
7	SO4	L	306	5/5	0.96	0.21	95,95,96,97	0
7	SO4	B	308	5/5	0.96	0.23	77,78,78,79	0
7	SO4	L	303	5/5	0.97	0.20	68,68,69,70	0
7	SO4	L	305	5/5	0.97	0.13	73,74,74,75	0
7	SO4	R	601	5/5	0.98	0.13	55,57,58,61	0
7	SO4	R	602	5/5	0.98	0.11	60,60,61,62	0
9	CL	R	605	1/1	1.00	0.13	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.