Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2022 – 06:40 am GMT

|		
PDB ID	:	8BH5
Title	:	SARS-CoV-2 BA.2.12.1 RBD in complex with Beta-27 Fab and C1 nanobody
Authors	:	Huo, J.; Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on	:	2022-10-29
Resolution	:	2.38 Å(reported)

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 2.38 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.
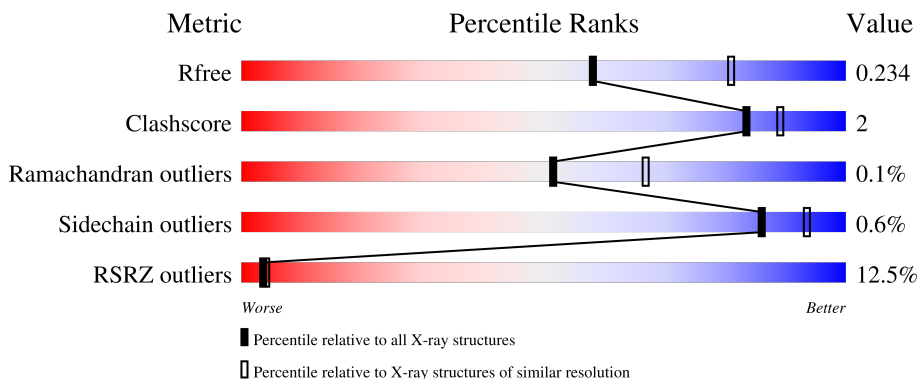
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 <=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	H	222	7% / 92% / 6% ·
2	L	214	5% / 93% / 6%
3	E	202	17% / 87% / 6% / 7%
4	C	131	24% / 85% / 9% / 5%
5	A	2	100%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 5982 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 Beta-27 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	218	Total 1617	C 1017	N 274	O 318	S 8	0	0	0

- Molecule 2 is a protein called Beta-27 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total 1622	C 1010	N 275	O 332	S 5	0	1	0

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	187	Total 1519	C 980	N 256	O 275	S 8	0	3	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	327	HIS	-	expression tag	UNP P0DTC2
E	328	HIS	-	expression tag	UNP P0DTC2
E	329	HIS	-	expression tag	UNP P0DTC2
E	330	HIS	-	expression tag	UNP P0DTC2
E	331	HIS	-	expression tag	UNP P0DTC2
E	332	HIS	-	expression tag	UNP P0DTC2
E	339	ASP	GLY	variant	UNP P0DTC2
E	371	PHE	SER	variant	UNP P0DTC2
E	373	PRO	SER	engineered mutation	UNP P0DTC2
E	375	PHE	SER	variant	UNP P0DTC2
E	376	ALA	THR	variant	UNP P0DTC2
E	405	ASN	ASP	variant	UNP P0DTC2
E	408	SER	ARG	variant	UNP P0DTC2
E	417	ASN	LYS	variant	UNP P0DTC2

Continued on next page...

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	440	LYS	ASN	variant	UNP P0DTC2
E	452	GLN	LEU	variant	UNP P0DTC2
E	477	ASN	SER	variant	UNP P0DTC2
E	478	LYS	THR	variant	UNP P0DTC2
E	484	ALA	GLU	variant	UNP P0DTC2
E	493	ARG	GLN	variant	UNP P0DTC2
E	498	ARG	GLN	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	505	HIS	TYR	variant	UNP P0DTC2
E	527	LYS	PRO	engineered mutation	UNP P0DTC2

- Molecule 4 is a protein called Nanobody C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	124	965	605	167	189	4	0	0	0

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	A	2	24	14	1	9	0	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1 C2

HO

O1

OH

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total 6	C 3	O 3	0	0
6	H	1	Total 6	C 3	O 3	0	0
6	H	1	Total 6	C 3	O 3	0	0
6	H	1	Total 6	C 3	O 3	0	0
6	L	1	Total 6	C 3	O 3	0	0
6	L	1	Total 6	C 3	O 3	0	0
6	L	1	Total 6	C 3	O 3	0	0
6	E	1	Total 6	C 3	O 3	0	0
6	E	1	Total 6	C 3	O 3	0	0
6	E	1	Total 6	C 3	O 3	0	0
6	E	1	Total 6	C 3	O 3	0	0
6	C	1	Total 6	C 3	O 3	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O⁻

O2 O⁻ — P == O O1

P

O⁻

O4

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total 5	O 4	P 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	54	Total 54	O 54	0	0
8	L	55	Total 55	O 55	0	0
8	E	38	Total 38	O 38	0	0
8	C	11	Total 11	O 11	0	0

3 Residue-property plots ⓘ

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: Beta-27 heavy chain
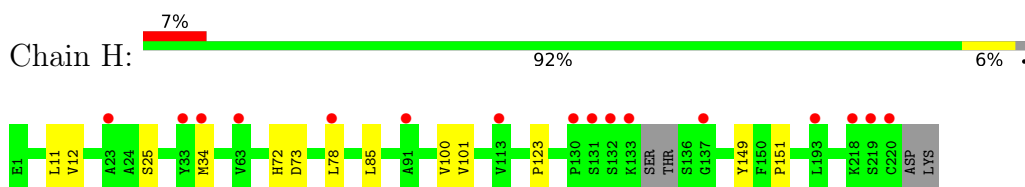
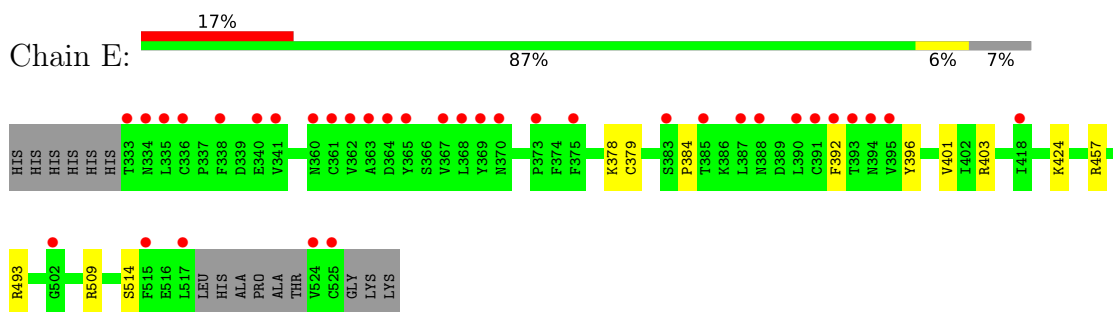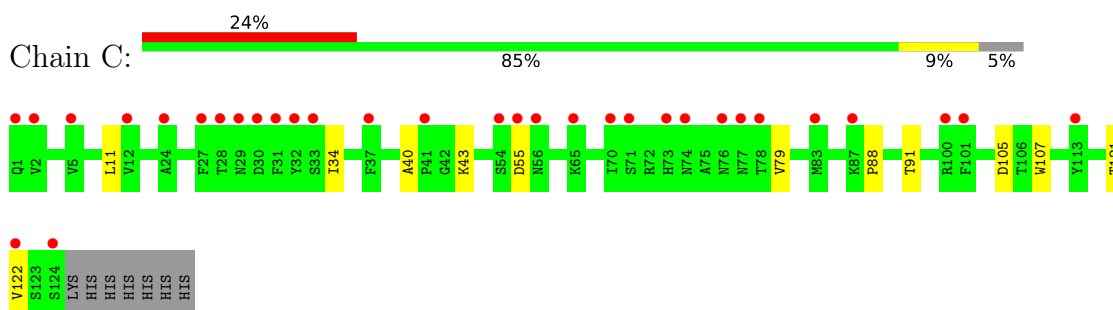Chain H:

• Molecule 2: Beta-27 light chain
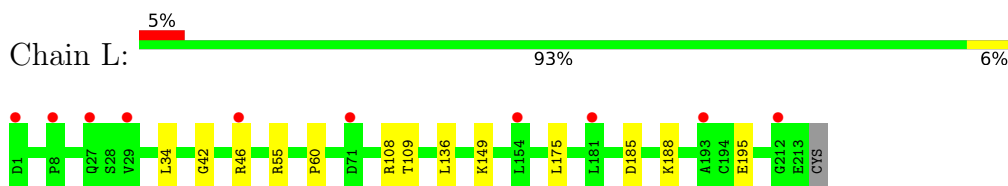
Chain L:

• Molecule 3: Spike protein S1

Chain E:

• Molecule 4: Nanobody C1

Chain C:

• Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:

100%

NAG1 FUC2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	186.85Å　99.99Å　56.49Å 90.00°　104.11°　90.00°	Depositor
Resolution (Å)	54.78　–　2.38 54.78　–　2.38	Depositor EDS
% Data completeness (in resolution range)	91.3 (54.78-2.38) 91.4 (54.78-2.38)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.186　,　0.233 0.186　,　0.234	Depositor DCC
R_{free} test set	1842 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	48.2	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5982	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GOL, FUC, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	H	0.25	0/1652	0.51	0/2249
2	L	0.25	0/1659	0.48	0/2250
3	E	0.26	0/1572	0.48	0/2134
4	C	0.25	0/990	0.50	0/1347
All	All	0.25	0/5873	0.49	0/7980

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 ⓘ

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	H	1617	0	1592	7	0
2	L	1622	0	1573	7	0
3	E	1519	0	1446	7	0
4	C	965	0	906	8	0
5	A	24	0	22	0	0
6	C	6	0	8	1	0
6	E	24	0	32	1	0
6	H	24	0	32	2	0
6	L	18	0	24	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	5	0	0	0	0
8	C	11	0	0	0	0
8	E	38	0	0	1	0
8	H	54	0	0	0	0
8	L	55	0	0	1	0
All	All	5982	0	5635	27	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 2.

All (27) 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:E:457:ARG:HH12	6:E:701:GOL:H12	1.65	0.62
1:H:11:LEU:HD11	1:H:151:PRO:HG3	1.82	0.61
4:C:34:ILE:HG13	4:C:79:VAL:HG21	1.83	0.59
1:H:123:PRO:HB3	1:H:149:TYR:HB3	1.85	0.58
2:L:149:LYS:NZ	2:L:195:GLU:OE1	2.38	0.57
2:L:42:GLY:H	6:L:403:GOL:H2	1.71	0.55
4:C:91:THR:HG23	4:C:121:THR:HA	1.89	0.54
2:L:46:ARG:NH2	8:L:502:HOH:O	2.39	0.54
2:L:185:ASP:HA	2:L:188:LYS:HD3	1.89	0.54
4:C:55:ASP:OD1	4:C:55:ASP:N	2.43	0.51
2:L:108:ARG:NH1	2:L:109:THR:O	2.44	0.50
1:H:12:VAL:HG11	1:H:85:LEU:HD12	1.95	0.49
1:H:101:VAL:HG21	3:E:493:ARG:HD2	1.94	0.48
3:E:396:TYR:HB2	3:E:514[A]:SER:OG	2.14	0.48
3:E:378:LYS:HD3	4:C:105:ASP:HB2	1.96	0.48
2:L:55:ARG:HD2	2:L:60:PRO:O	2.15	0.47
3:E:403:ARG:NH2	8:E:801:HOH:O	2.49	0.46
4:C:107:TRP:CE3	6:C:201:GOL:H31	2.51	0.46
1:H:34:MET:HB3	1:H:78:LEU:HD22	1.97	0.45
1:H:73:ASP:H	6:H:302:GOL:H31	1.83	0.44
1:H:72:HIS:HA	6:H:302:GOL:H2	1.99	0.44
2:L:136:LEU:HB2	2:L:175:LEU:HB3	2.00	0.44
3:E:379:CYS:SG	3:E:384:PRO:HG3	2.58	0.43
4:C:40:ALA:HB3	4:C:43:LYS:HB2	2.01	0.42
4:C:88:PRO:HA	4:C:122:VAL:HB	2.01	0.42
4:C:11:LEU:HD13	4:C:121:THR:HB	2.02	0.42
3:E:401:VAL:HG22	3:E:509:ARG:HG2	2.02	0.41

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	H	214/222 (96%)	209 (98%)	4 (2%)	1 (0%)	29	39
2	L	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
3	E	186/202 (92%)	179 (96%)	7 (4%)	0	100	100
4	C	122/131 (93%)	118 (97%)	4 (3%)	0	100	100
All	All	734/769 (95%)	713 (97%)	20 (3%)	1 (0%)	51	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	100	VAL

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	H	182/187 (97%)	181 (100%)	1 (0%)	88	95
2	L	184/184 (100%)	183 (100%)	1 (0%)	88	95
3	E	165/174 (95%)	163 (99%)	2 (1%)	71	84
4	C	103/110 (94%)	103 (100%)	0	100	100
All	All	634/655 (97%)	630 (99%)	4 (1%)	86	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	25	SER
2	L	34	LEU
3	E	392	PHE
3	E	424	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	$\#|Z| > 2$
5	NAG	A	1	5,3	14,14,15	0.33	0	17,19,21	0.52	0
5	FUC	A	2	5	10,10,11	0.85	0	14,14,16	0.81	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	NAG	A	1	5,3	-	<mark>2/6/23/26</mark>	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FUC	A	2	5	-	-	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	A	1	NAG	O5-C5-C6-O6
5	A	1	NAG	C4-C5-C6-O6

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.

Oligosaccharide Chain A

Bond lengths

Bond angles

Torsions

Rings
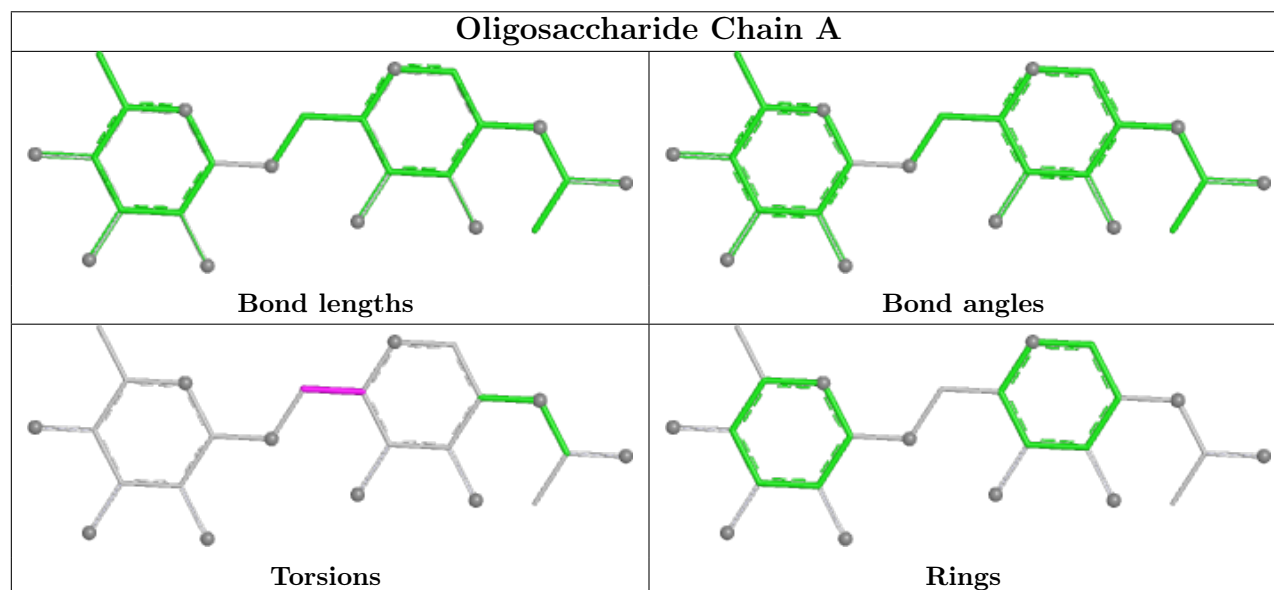
5.6 Ligand geometry ⓘ

13 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	$\#|Z| > 2$
6	GOL	E	704	-	5,5,5	1.01	0	5,5,5	0.86	0
6	GOL	C	201	-	5,5,5	0.97	0	5,5,5	0.93	0
6	GOL	L	402	-	5,5,5	0.92	0	5,5,5	0.97	0
6	GOL	H	302	-	5,5,5	0.89	0	5,5,5	1.00	0
6	GOL	H	303	-	5,5,5	0.89	0	5,5,5	1.03	0
7	PO4	H	305	-	4,4,4	0.90	0	6,6,6	0.43	0
6	GOL	E	701	-	5,5,5	0.90	0	5,5,5	1.00	0
6	GOL	H	301	-	5,5,5	0.92	0	5,5,5	0.99	0
6	GOL	E	703	-	5,5,5	0.92	0	5,5,5	1.01	0
6	GOL	L	401	-	5,5,5	0.95	0	5,5,5	0.87	0
6	GOL	L	403	-	5,5,5	0.92	0	5,5,5	0.99	0
6	GOL	H	304	-	5,5,5	0.91	0	5,5,5	0.98	0
6	GOL	E	702	-	5,5,5	0.89	0	5,5,5	1.01	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	GOL	E	704	-	-	1/4/4/4	-
6	GOL	C	201	-	-	2/4/4/4	-
6	GOL	L	402	-	-	1/4/4/4	-
6	GOL	H	302	-	-	0/4/4/4	-
6	GOL	H	303	-	-	0/4/4/4	-
6	GOL	E	701	-	-	3/4/4/4	-
6	GOL	H	301	-	-	2/4/4/4	-
6	GOL	E	703	-	-	2/4/4/4	-
6	GOL	L	401	-	-	2/4/4/4	-
6	GOL	L	403	-	-	0/4/4/4	-
6	GOL	H	304	-	-	0/4/4/4	-
6	GOL	E	702	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	401	GOL	O1-C1-C2-C3
6	E	701	GOL	C1-C2-C3-O3
6	E	703	GOL	C1-C2-C3-O3
6	E	701	GOL	O2-C2-C3-O3
6	C	201	GOL	O1-C1-C2-C3
6	L	401	GOL	O1-C1-C2-O2
6	E	703	GOL	O2-C2-C3-O3
6	E	701	GOL	O1-C1-C2-C3
6	E	702	GOL	O2-C2-C3-O3
6	E	704	GOL	O2-C2-C3-O3
6	H	301	GOL	C1-C2-C3-O3
6	C	201	GOL	C1-C2-C3-O3
6	H	301	GOL	O2-C2-C3-O3
6	L	402	GOL	C1-C2-C3-O3
6	E	702	GOL	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	201	GOL	1	0
6	H	302	GOL	2	0
6	E	701	GOL	1	0
6	L	403	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	H	218/222 (98%)	1.13	16 (7%)	15	16	38, 46, 75, 127	0
2	L	213/214 (99%)	0.98	10 (4%)	31	34	40, 52, 73, 128	0
3	E	187/202 (92%)	1.65	35 (18%)	1	1	39, 51, 115, 142	0
4	C	124/131 (94%)	1.59	32 (25%)	0	0	46, 67, 97, 115	0
All	All	742/769 (96%)	1.30	93 (12%)	3	4	38, 52, 102, 142	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	335	LEU	12.0
3	E	334	ASN	10.1
3	E	333	THR	8.9
1	H	220	CYS	7.9
3	E	392	PHE	7.3
3	E	367	VAL	7.1
4	C	24	ALA	6.1
3	E	524	VAL	6.0
2	L	1	ASP	5.9
3	E	360	ASN	5.8
3	E	391	CYS	5.6
1	H	132	SER	5.4
3	E	390	LEU	5.4
3	E	365	TYR	4.9
4	C	77	ASN	4.9
4	C	31	PHE	4.7
4	C	73	HIS	4.7
3	E	368	LEU	4.6
3	E	338	PHE	4.6
3	E	373	PRO	4.6
3	E	362	VAL	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	525	CYS	4.5
3	E	385	THR	4.3
4	C	65	LYS	4.0
4	C	76	ASN	4.0
4	C	32	TYR	3.9
4	C	1	GLN	3.8
1	H	218	LYS	3.8
4	C	5	VAL	3.8
4	C	28	THR	3.7
3	E	363	ALA	3.7
1	H	219	SER	3.7
3	E	336	CYS	3.7
3	E	361	CYS	3.7
4	C	41	PRO	3.7
4	C	29	ASN	3.6
4	C	56	ASN	3.6
3	E	388	ASN	3.6
3	E	517	LEU	3.5
4	C	70	ILE	3.5
3	E	387	LEU	3.5
3	E	341	VAL	3.3
1	H	131	SER	3.2
2	L	27	GLN	3.2
4	C	74	ASN	3.1
3	E	393	THR	3.0
4	C	100	ARG	3.0
3	E	340	GLU	3.0
1	H	137	GLY	3.0
2	L	212	GLY	2.9
4	C	30	ASP	2.9
3	E	370	ASN	2.9
4	C	78	THR	2.7
4	C	27	PHE	2.7
1	H	193	LEU	2.7
4	C	71	SER	2.7
4	C	12	VAL	2.7
3	E	375	PHE	2.6
4	C	124	SER	2.6
3	E	395	VAL	2.5
3	E	394	ASN	2.5
3	E	364	ASP	2.5
2	L	46	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	C	55	ASP	2.4
2	L	181	LEU	2.4
4	C	2	VAL	2.4
1	H	133	LYS	2.4
1	H	113	VAL	2.4
4	C	101	PHE	2.4
1	H	78	LEU	2.3
1	H	63	VAL	2.3
4	C	113	TYR	2.3
3	E	502	GLY	2.3
4	C	33	SER	2.2
2	L	71	ASP	2.2
2	L	8	PRO	2.2
2	L	29	VAL	2.2
1	H	91	ALA	2.2
2	L	154	LEU	2.2
4	C	54	SER	2.1
4	C	122	VAL	2.1
3	E	369	TYR	2.1
3	E	515	PHE	2.1
4	C	37	PHE	2.1
1	H	130	PRO	2.1
1	H	23	ALA	2.1
4	C	83	MET	2.1
3	E	383	SER	2.1
1	H	34	MET	2.0
1	H	33	TYR	2.0
3	E	418	ILE	2.0
2	L	193	ALA	2.0
4	C	87	LYS	2.0

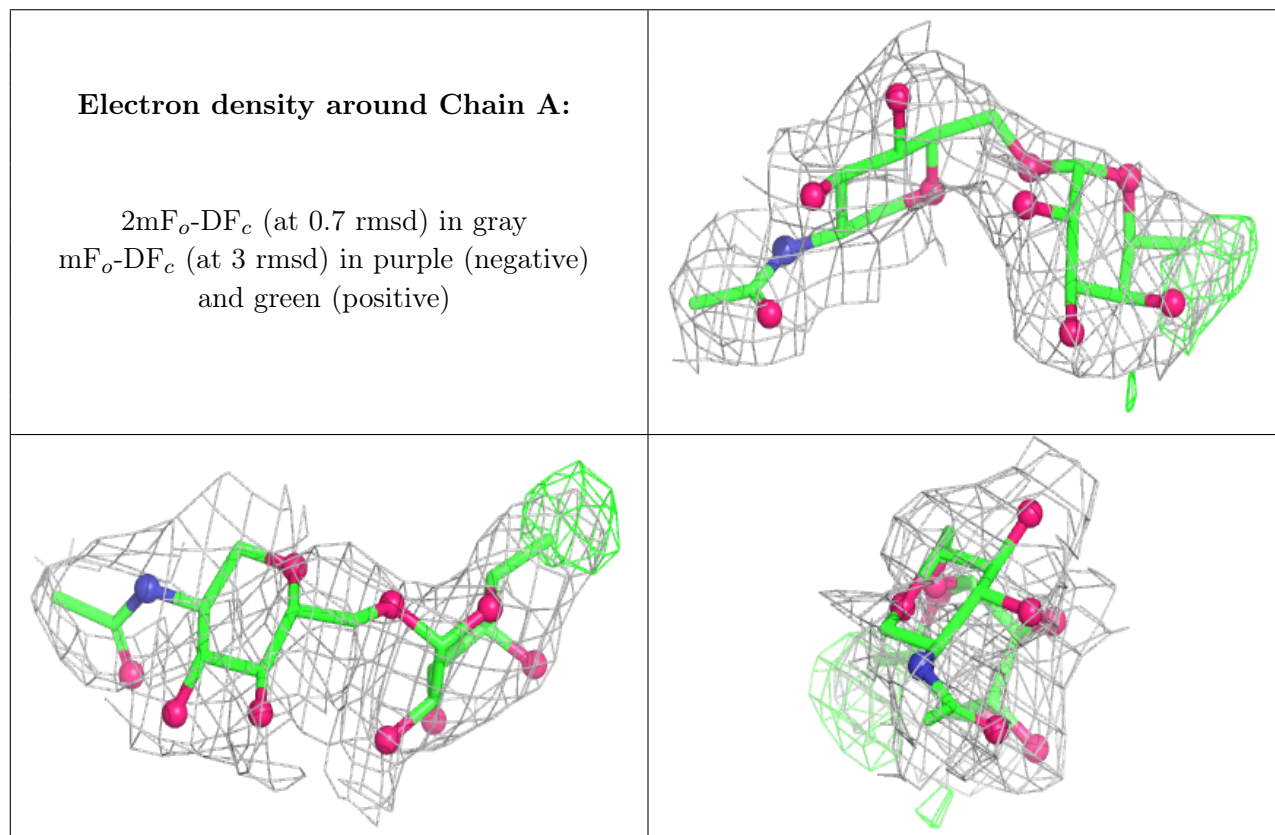## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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
5	FUC	A	2	10/11	0.63	0.30	84,99,103,103	0
5	NAG	A	1	14/15	0.68	0.27	82,95,102,103	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.

Electron density around Chain A:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

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
6	GOL	E	704	6/6	0.73	0.29	60,65,70,70	0
6	GOL	C	201	6/6	0.76	0.24	51,58,68,73	0
6	GOL	L	403	6/6	0.77	0.24	56,63,66,67	0
6	GOL	E	703	6/6	0.78	0.19	52,65,72,73	0
6	GOL	L	402	6/6	0.81	0.18	53,57,61,63	0
6	GOL	H	303	6/6	0.84	0.21	52,62,65,67	0
6	GOL	E	702	6/6	0.85	0.41	71,75,82,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
6	GOL	L	401	6/6	0.85	0.30	63,73,76,78	0
6	GOL	H	304	6/6	0.86	0.26	54,59,62,62	0
6	GOL	H	302	6/6	0.86	0.18	68,73,75,78	0
6	GOL	E	701	6/6	0.87	0.16	55,63,64,68	0
7	PO4	H	305	5/5	0.90	0.21	74,76,90,97	0
6	GOL	H	301	6/6	0.92	0.19	46,53,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.