Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2023 – 06:06 AM EDT

PDB ID	:	7N4I
Title	:	Crystal structure of SARS-CoV-2 receptor binding domain in complex with neutralizing human antibody WRAIR-2057.
Authors	:	Sankhala, R.S.; Joyce, M.G.
Deposited on	:	2021-06-04
Resolution	:	2.28 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

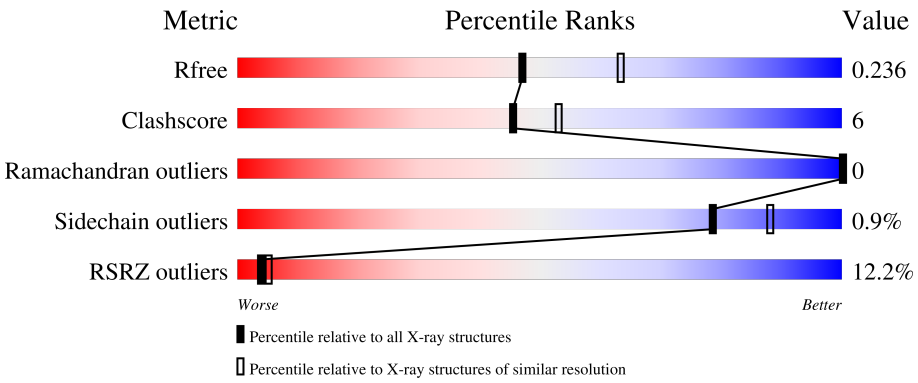
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	226	6% 90% 8% •
2	L	214	9% 87% 12% •
3	C	205	21% 81% 15% •
4	A	3	33% 33% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	2	-	-	-	X
4	BMA	A	3	-	-	-	X
5	GOL	H	301	-	-	-	X
5	GOL	L	401	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9894 atoms, of which 4734 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 WRAIR-2057 Antibody Fab Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	H	221	3283	1055	1626	266	330	6	0	0	0

- Molecule 2 is a protein called WRAIR-2057 Antibody Fab Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	L	212	3192	1008	1573	275	331	5	0	0	0

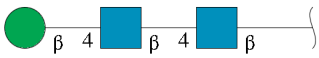
- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	199	3063	1011	1481	270	293	8	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

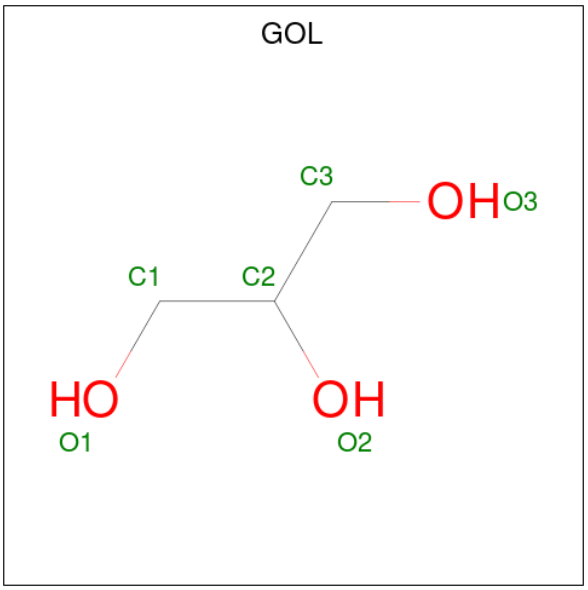
Chain	Residue	Modelled	Actual	Comment	Reference
C	528	GLY	-	expression tag	UNP P0DTC2
C	529	SER	-	expression tag	UNP P0DTC2
C	530	HIS	-	expression tag	UNP P0DTC2
C	531	HIS	-	expression tag	UNP P0DTC2
C	532	HIS	-	expression tag	UNP P0DTC2
C	533	HIS	-	expression tag	UNP P0DTC2
C	534	HIS	-	expression tag	UNP P0DTC2
C	535	HIS	-	expression tag	UNP P0DTC2

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
4	A	3	77	22	38	2	15	0	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	H	1	14	3	8	3	0	0
5	L	1	14	3	8	3	0	0

- Molecule 6 is water.

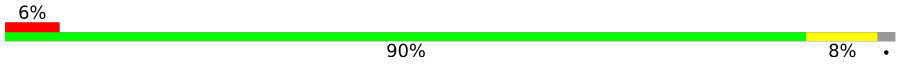
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	H	97	97	97	0	0
6	L	96	96	96	0	0
6	C	58	58	58	0	0

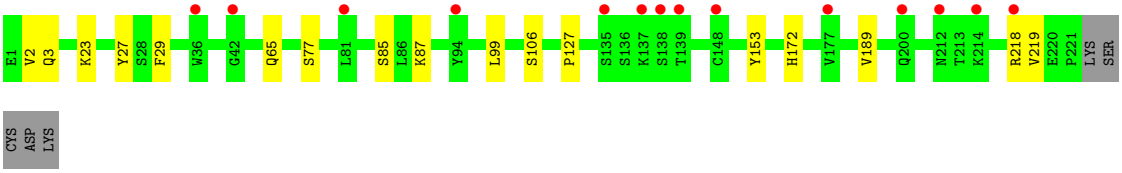
3 Residue-property plots (i)

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: WRAIR-2057 Antibody Fab Heavy Chain

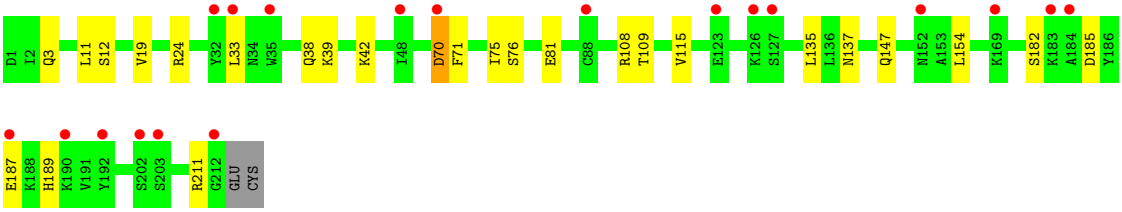
Chain H:





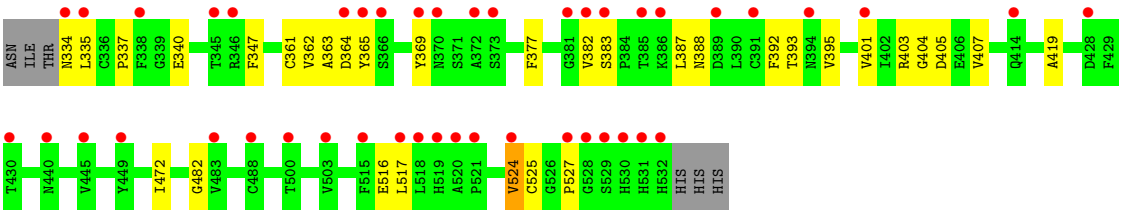
• Molecule 2: WRAIR-2057 Antibody Fab Light Chain

Chain L:



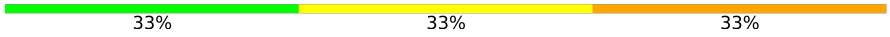
• Molecule 3: Spike protein S1

Chain C:



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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	73.93Å 73.93Å 149.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 2.28 19.87 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.87-2.28) 99.3 (19.87-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 2.28Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.200 , 0.238 0.200 , 0.236	Depositor DCC
R_{free} test set	1800 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9894	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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 (i)

5.1 Standard geometry (i)

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

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	0.32	0/1701	0.53	0/2322
2	L	0.34	0/1654	0.53	0/2248
3	C	0.30	0/1632	0.49	0/2219
All	All	0.32	0/4987	0.52	0/6789

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	H	1657	1626	1626	12	0
2	L	1619	1573	1573	24	0
3	C	1582	1481	1486	25	0
4	A	39	38	34	3	0
5	H	6	8	8	0	0
5	L	6	8	8	0	0
6	C	58	0	0	4	0
6	H	97	0	0	4	0
6	L	96	0	0	3	0
All	All	5160	4734	4735	62	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (62) 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)
6:C:658:HOH:O	4:A:2:NAG:H2	1.58	1.02
2:L:147:GLN:OE1	2:L:154:LEU:HD23	1.78	0.84
6:C:658:HOH:O	4:A:2:NAG:C1	2.37	0.71
2:L:147:GLN:CD	2:L:154:LEU:HD23	2.15	0.67
6:C:658:HOH:O	4:A:2:NAG:C2	2.29	0.64
2:L:24:ARG:NH1	2:L:70:ASP:OD1	2.32	0.63
2:L:33:LEU:HD22	2:L:71:PHE:CG	2.37	0.59
1:H:218:ARG:NH1	6:H:403:HOH:O	2.35	0.58
3:C:337:PRO:HB2	3:C:340:GLU:HB2	1.85	0.58
1:H:189:VAL:HG11	2:L:135:LEU:HD11	1.88	0.56
1:H:65:GLN:NE2	6:H:401:HOH:O	2.22	0.55
3:C:472:ILE:HD12	3:C:482:GLY:O	2.07	0.54
2:L:187:GLU:HB2	6:L:508:HOH:O	2.09	0.53
3:C:382:VAL:HG12	3:C:383:SER:H	1.74	0.52
1:H:3:GLN:NE2	6:H:408:HOH:O	2.43	0.51
3:C:383:SER:O	3:C:387:LEU:HG	2.10	0.51
3:C:335:LEU:HD12	3:C:362:VAL:O	2.12	0.49
2:L:147:GLN:CD	2:L:154:LEU:CD2	2.80	0.49
1:H:23:LYS:NZ	6:H:409:HOH:O	2.46	0.49
1:H:99:LEU:HD13	1:H:106:SER:OG	2.14	0.48
2:L:39:LYS:H	2:L:42:LYS:HG2	1.78	0.47
3:C:365:TYR:CG	3:C:387:LEU:CD1	2.97	0.47
3:C:382:VAL:HG11	3:C:387:LEU:HB3	1.97	0.47
2:L:182:SER:OG	2:L:185:ASP:OD1	2.24	0.46
3:C:404:GLY:O	3:C:407:VAL:HG22	2.15	0.46
3:C:365:TYR:CD2	3:C:387:LEU:CD1	2.99	0.46
3:C:382:VAL:HG12	3:C:383:SER:N	2.31	0.46
2:L:38:GLN:HA	2:L:42:LYS:HE2	1.98	0.45
3:C:403:ARG:NH1	3:C:405:ASP:OD1	2.49	0.45
3:C:382:VAL:CG1	3:C:387:LEU:HD23	2.45	0.45
1:H:2:VAL:HG23	1:H:27:TYR:CD1	2.51	0.45
3:C:395:VAL:HG23	3:C:524:VAL:HG21	1.99	0.45
2:L:3:GLN:NE2	6:L:506:HOH:O	2.49	0.44
3:C:363:ALA:O	3:C:527:PRO:HD3	2.17	0.44
3:C:334:ASN:O	3:C:361:CYS:HB2	2.17	0.44
1:H:219:VAL:O	1:H:219:VAL:HG23	2.17	0.44
2:L:19:VAL:CG1	2:L:75:ILE:HB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:393:THR:N	3:C:516:GLU:O	2.51	0.43
1:H:172:HIS:HD2	2:L:137:ASN:HD21	1.64	0.43
2:L:185:ASP:OD1	2:L:185:ASP:N	2.52	0.43
3:C:362:VAL:HA	3:C:525:CYS:O	2.19	0.42
1:H:85:SER:O	1:H:87:LYS:HE3	2.19	0.42
2:L:135:LEU:HD21	2:L:137:ASN:HB2	2.01	0.42
3:C:361:CYS:O	3:C:524:VAL:HA	2.19	0.42
1:H:127:PRO:HB3	1:H:153:TYR:HB3	2.00	0.42
2:L:81:GLU:H	2:L:81:GLU:CD	2.23	0.42
2:L:189:HIS:O	2:L:211:ARG:HD3	2.20	0.42
3:C:392:PHE:HA	3:C:517:LEU:HD13	2.02	0.42
2:L:19:VAL:HG13	2:L:75:ILE:HB	2.01	0.42
2:L:108:ARG:HG2	2:L:109:THR:N	2.34	0.41
2:L:39:LYS:H	2:L:42:LYS:HE2	1.86	0.41
3:C:365:TYR:HD2	3:C:388:ASN:CB	2.33	0.41
3:C:382:VAL:HG11	3:C:387:LEU:HD23	2.03	0.41
2:L:11:LEU:HD11	2:L:19:VAL:HG23	2.03	0.41
2:L:115:VAL:HA	2:L:135:LEU:O	2.20	0.41
3:C:335:LEU:HD12	3:C:362:VAL:HG13	2.03	0.41
3:C:335:LEU:HD11	3:C:364:ASP:HB2	2.03	0.41
3:C:347:PHE:HB3	3:C:401:VAL:HG23	2.02	0.41
1:H:29:PHE:CD2	1:H:77:SER:HA	2.56	0.41
2:L:11:LEU:HD23	2:L:12:SER:N	2.36	0.41
3:C:419:ALA:O	6:C:601:HOH:O	2.21	0.41
2:L:115:VAL:HG22	6:L:510:HOH:O	2.21	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	H	219/226 (97%)	208 (95%)	11 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	210/214 (98%)	199 (95%)	11 (5%)	0	100	100
3	C	198/205 (97%)	185 (93%)	13 (7%)	0	100	100
All	All	627/645 (97%)	592 (94%)	35 (6%)	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	H	189/194 (97%)	189 (100%)	0	100	100
2	L	187/189 (99%)	185 (99%)	2 (1%)	73	84
3	C	172/177 (97%)	169 (98%)	3 (2%)	60	74
All	All	548/560 (98%)	543 (99%)	5 (1%)	78	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	70	ASP
2	L	76	SER
3	C	369	TYR
3	C	377	PHE
3	C	524	VAL

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

Mol	Chain	Res	Type
1	H	172	HIS

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)

3 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	1	3,4	14,14,15	1.83	4 (28%)	17,19,21	1.68	3 (17%)
4	NAG	A	2	4	14,14,15	0.96	1 (7%)	17,19,21	0.67	0
4	BMA	A	3	4	11,11,12	0.73	0	15,15,17	0.98	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
4	NAG	A	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
4	BMA	A	3	4	-	1/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	NAG	O5-C1	-3.60	1.38	1.43
4	A	1	NAG	C1-C2	-3.34	1.47	1.52
4	A	1	NAG	C3-C2	-2.63	1.46	1.52
4	A	1	NAG	O5-C5	-2.48	1.38	1.43
4	A	2	NAG	C1-C2	-2.03	1.49	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1	NAG	C3-C4-C5	-4.88	101.54	110.24
4	A	1	NAG	O5-C1-C2	2.58	115.36	111.29
4	A	1	NAG	C1-C2-N2	2.10	114.08	110.49

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3	BMA	O5-C5-C6-O6
4	A	2	NAG	C8-C7-N2-C2
4	A	2	NAG	O7-C7-N2-C2

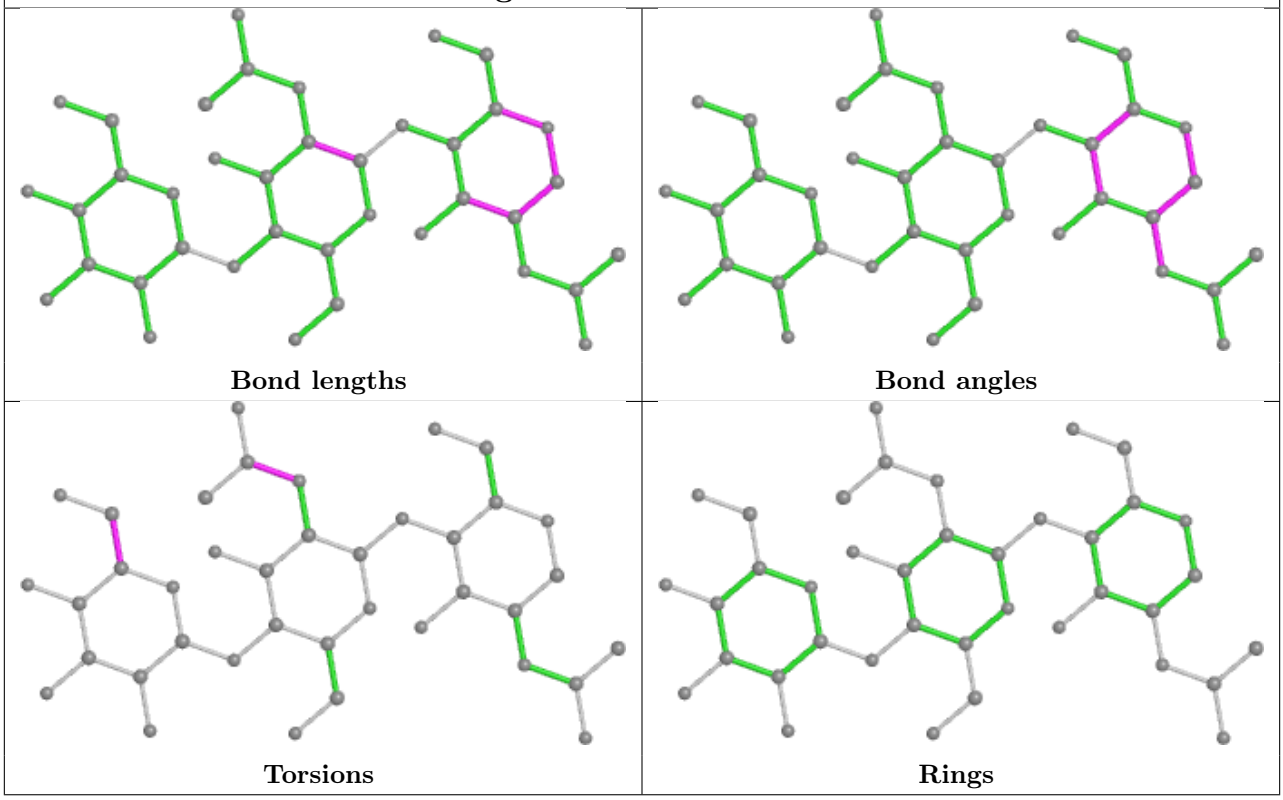
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2	NAG	3	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.

Oligosaccharide Chain A



5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	L	401	-	5,5,5	0.38	0	5,5,5	0.46	0
5	GOL	H	301	-	5,5,5	0.41	0	5,5,5	0.26	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	GOL	L	401	-	-	2/4/4/4	-
5	GOL	H	301	-	-	0/4/4/4	-

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	401	GOL	O1-C1-C2-C3
5	L	401	GOL	O1-C1-C2-O2

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	221/226 (97%)	0.47	14 (6%)	20	24	27, 42, 72, 95	0
2	L	212/214 (99%)	0.44	19 (8%)	9	12	26, 44, 77, 109	0
3	C	199/205 (97%)	1.32	44 (22%)	0	1	30, 67, 111, 142	0
All	All	632/645 (97%)	0.73	77 (12%)	4	5	26, 48, 94, 142	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	532	HIS	14.1
3	C	531	HIS	10.6
3	C	530	HIS	8.5
3	C	519	HIS	6.6
3	C	517	LEU	6.5
3	C	335	LEU	5.6
3	C	445	VAL	5.4
3	C	382	VAL	4.9
3	C	381	GLY	4.9
3	C	518	LEU	4.9
3	C	385	THR	4.8
3	C	334	ASN	4.6
3	C	483	VAL	4.5
3	C	528	GLY	4.4
3	C	527	PRO	4.4
2	L	126	LYS	4.4
3	C	383	SER	4.4
3	C	449	TYR	4.2
3	C	373	SER	4.0
3	C	365	TYR	4.0
2	L	203	SER	3.9
3	C	345	THR	3.9
1	H	218	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
3	C	430	THR	3.7
2	L	169	LYS	3.7
3	C	521	PRO	3.7
1	H	137	LYS	3.6
3	C	520	ALA	3.6
3	C	369	TYR	3.6
3	C	529	SER	3.5
3	C	401	VAL	3.5
3	C	346	ARG	3.5
2	L	187	GLU	3.5
1	H	135	SER	3.3
3	C	372	ALA	3.2
2	L	190	LYS	3.2
3	C	440	ASN	3.2
3	C	414	GLN	3.1
3	C	524	VAL	3.1
1	H	81	LEU	3.0
2	L	127	SER	3.0
2	L	202	SER	3.0
3	C	366	SER	3.0
1	H	177	VAL	2.9
1	H	36	TRP	2.9
1	H	214	LYS	2.9
3	C	488	CYS	2.9
2	L	35	TRP	2.8
3	C	428	ASP	2.7
3	C	389	ASP	2.7
2	L	183	LYS	2.6
2	L	192	TYR	2.6
1	H	138	SER	2.5
2	L	70	ASP	2.5
2	L	152	ASN	2.5
2	L	123	GLU	2.5
1	H	139	THR	2.5
2	L	184	ALA	2.4
2	L	48	ILE	2.4
2	L	33	LEU	2.4
2	L	212	GLY	2.3
2	L	88	CYS	2.3
3	C	391	CYS	2.3
3	C	500	THR	2.2
3	C	370	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	394	ASN	2.2
3	C	386	LYS	2.2
1	H	42	GLY	2.2
1	H	212	ASN	2.1
1	H	148	CYS	2.1
2	L	32	TYR	2.1
3	C	503	VAL	2.1
3	C	515	PHE	2.1
3	C	338	PHE	2.1
3	C	364	ASP	2.1
1	H	94	TYR	2.0
1	H	200	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)

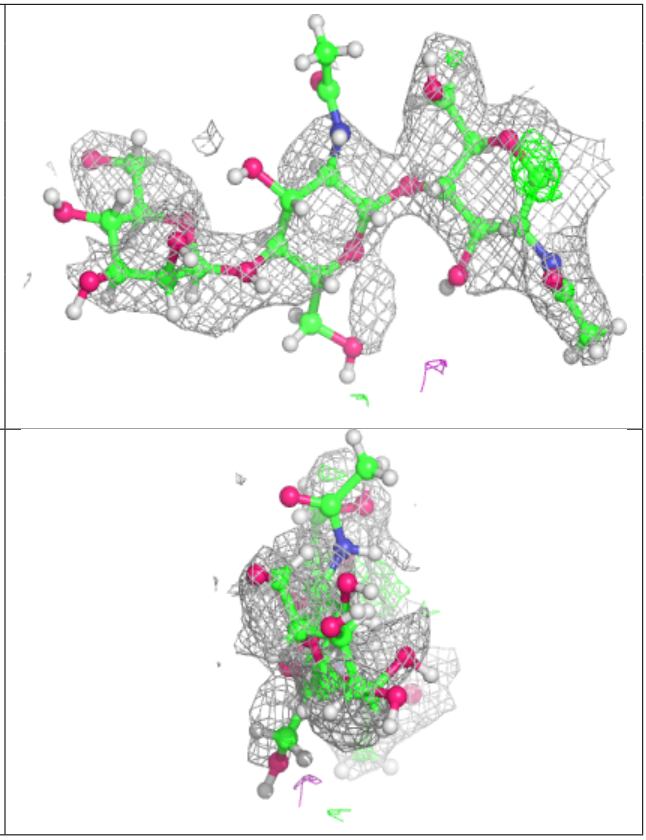
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	1	14/15	0.63	0.26	89,120,158,165	0
4	NAG	A	2	14/15	0.67	0.60	112,147,177,178	0
4	BMA	A	3	11/12	0.70	0.47	98,138,162,192	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:

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



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	GOL	H	301	6/6	0.05	1.43	239,319,382,388	0
5	GOL	L	401	6/6	0.62	0.65	72,142,252,303	0

6.5 Other polymers (i)

There are no such residues in this entry.