Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	6Y6P
Title	:	Structure of Hantaan virus envelope glycoprotein Gn
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Deposited on	:	2020-02-27
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

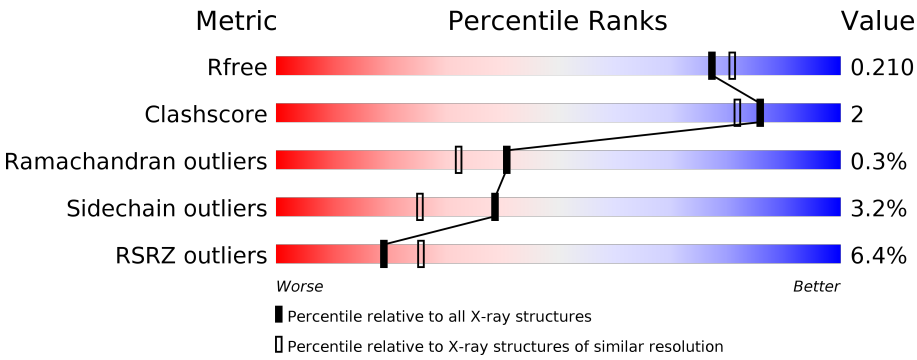
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 on 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	A	389	6% 80% 7% 12%
2	B	2	100%
2	C	2	100%

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
2	NAG	C	2	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2947 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 Envelope polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	343	2689	1708	439	518	24	0	4	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	PRO	ALA	conflict	UNP Q89839
A	293	SER	ARG	conflict	UNP Q89839
A	353	PHE	-	expression tag	UNP Q89839
A	354	GLU	-	expression tag	UNP Q89839
A	355	ASP	-	expression tag	UNP Q89839
A	356	ASP	-	expression tag	UNP Q89839
A	357	ASP	-	expression tag	UNP Q89839
A	358	ASP	-	expression tag	UNP Q89839
A	359	LYS	-	expression tag	UNP Q89839
A	360	ALA	-	expression tag	UNP Q89839
A	361	GLY	-	expression tag	UNP Q89839
A	362	TRP	-	expression tag	UNP Q89839
A	363	SER	-	expression tag	UNP Q89839
A	364	HIS	-	expression tag	UNP Q89839
A	365	PRO	-	expression tag	UNP Q89839
A	366	GLN	-	expression tag	UNP Q89839
A	367	PHE	-	expression tag	UNP Q89839
A	368	GLU	-	expression tag	UNP Q89839
A	369	LYS	-	expression tag	UNP Q89839
A	370	GLY	-	expression tag	UNP Q89839
A	371	GLY	-	expression tag	UNP Q89839
A	372	GLY	-	expression tag	UNP Q89839
A	373	SER	-	expression tag	UNP Q89839
A	374	GLY	-	expression tag	UNP Q89839
A	375	GLY	-	expression tag	UNP Q89839
A	376	GLY	-	expression tag	UNP Q89839
A	377	SER	-	expression tag	UNP Q89839

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Chain	Residue	Modelled	Actual	Comment	Reference
A	378	GLY	-	expression tag	UNP Q89839
A	379	GLY	-	expression tag	UNP Q89839
A	380	GLY	-	expression tag	UNP Q89839
A	381	SER	-	expression tag	UNP Q89839
A	382	TRP	-	expression tag	UNP Q89839
A	383	SER	-	expression tag	UNP Q89839
A	384	HIS	-	expression tag	UNP Q89839
A	385	PRO	-	expression tag	UNP Q89839
A	386	GLN	-	expression tag	UNP Q89839
A	387	PHE	-	expression tag	UNP Q89839
A	388	GLU	-	expression tag	UNP Q89839
A	389	LYS	-	expression tag	UNP Q89839

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

- Molecule 3 is water.

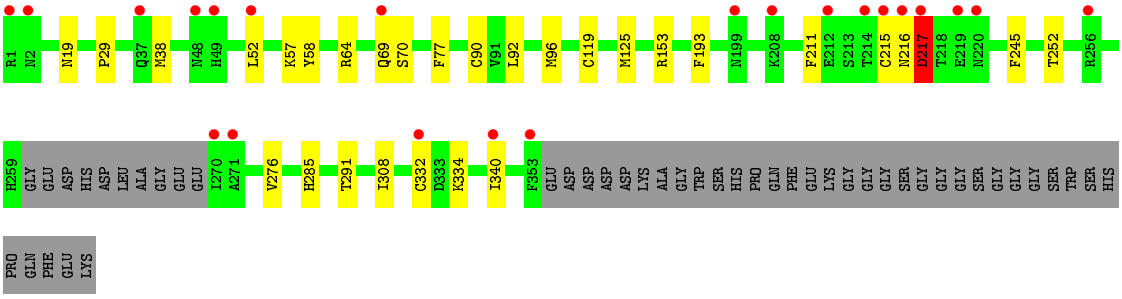
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	202	202	202	0	0

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.

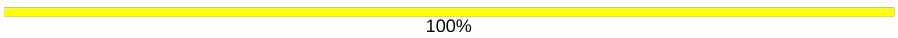
• Molecule 1: Envelope polyprotein

Chain A:



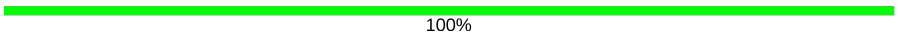
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



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

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.60Å 92.22Å 94.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.34 – 1.94 35.34 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.34-1.94) 99.6 (35.34-1.94)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.13	Depositor
R, R_{free}	0.167 , 0.211 0.167 , 0.210	Depositor DCC
R_{free} test set	1673 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2947	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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: 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	A	0.80	2/2753 (0.1%)	0.81	2/3739 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	TYR	CD2-CE2	5.84	1.48	1.39
1	A	58	TYR	CD1-CE1	5.58	1.47	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	A	64	ARG	NE-CZ-NH2	-5.58	117.51	120.30

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	2689	0	2626	12	0
2	B	28	0	25	0	0
2	C	28	0	25	0	0
3	A	202	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2947	0	2676	12	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 (12) 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)
1:A:69:GLN:O	3:A:501:HOH:O	1.94	0.84
1:A:90:CYS:HB2	1:A:340:ILE:HD11	1.62	0.80
1:A:92:LEU:HD22	1:A:96:MET:HE1	1.65	0.79
1:A:92:LEU:HD22	1:A:96:MET:CE	2.33	0.57
1:A:211:PHE:HZ	1:A:252:THR:HA	1.77	0.49
1:A:77:PHE:CE2	1:A:276:VAL:HG12	2.50	0.47
1:A:285:HIS:CD2	3:A:684:HOH:O	2.70	0.44
1:A:57:LYS:HB3	1:A:57:LYS:HE2	1.69	0.43
1:A:193:PHE:CD2	1:A:308:ILE:HD13	2.53	0.42
1:A:216:ASN:HB2	1:A:217:ASP:OD2	2.19	0.42
1:A:291:THR:O	1:A:334:LYS:HA	2.20	0.41
1:A:29:PRO:HA	1:A:119:CYS:O	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	343/389 (88%)	325 (95%)	17 (5%)	1 (0%)	41 32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	313/341 (92%)	303 (97%)	10 (3%)	39 25

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	38	MET
1	A	52	LEU
1	A	70	SER
1	A	125	MET
1	A	153	ARG
1	A	215	CYS
1	A	217	ASP
1	A	245	PHE
1	A	332	CYS

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

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)

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	$\#\|Z\| > 2$
2	NAG	B	1	1,2	14,14,15	0.69	1 (7%)	17,19,21	0.90	1 (5%)
2	NAG	B	2	2	14,14,15	0.75	1 (7%)	17,19,21	1.03	1 (5%)
2	NAG	C	1	1,2	14,14,15	0.24	0	17,19,21	0.85	0
2	NAG	C	2	2	14,14,15	0.49	0	17,19,21	0.46	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
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	2.23	1.55	1.52
2	B	2	NAG	O5-C1	-2.01	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	C1-O5-C5	-3.17	107.90	112.19
2	B	1	NAG	O3-C3-C2	-2.02	105.29	109.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

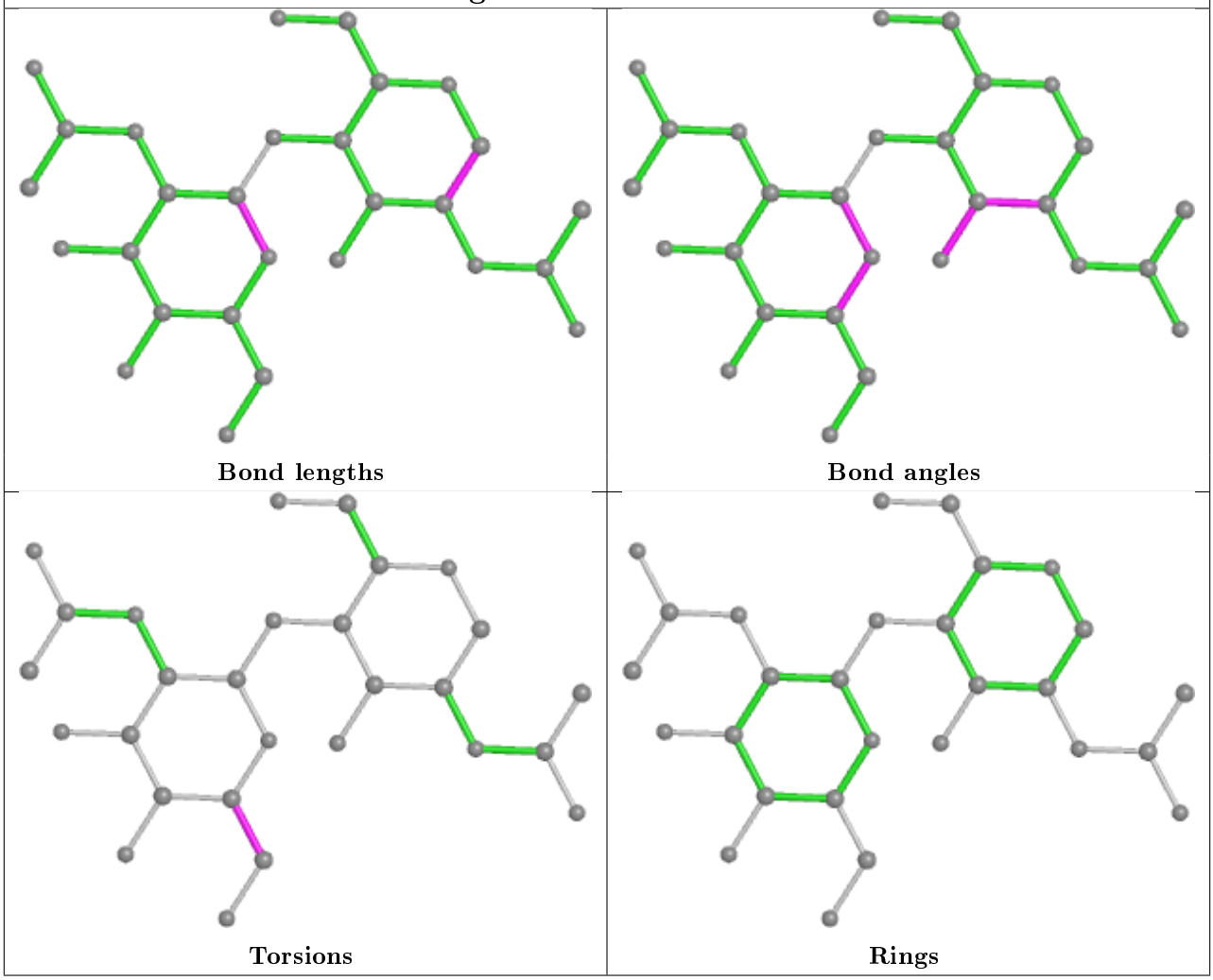
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

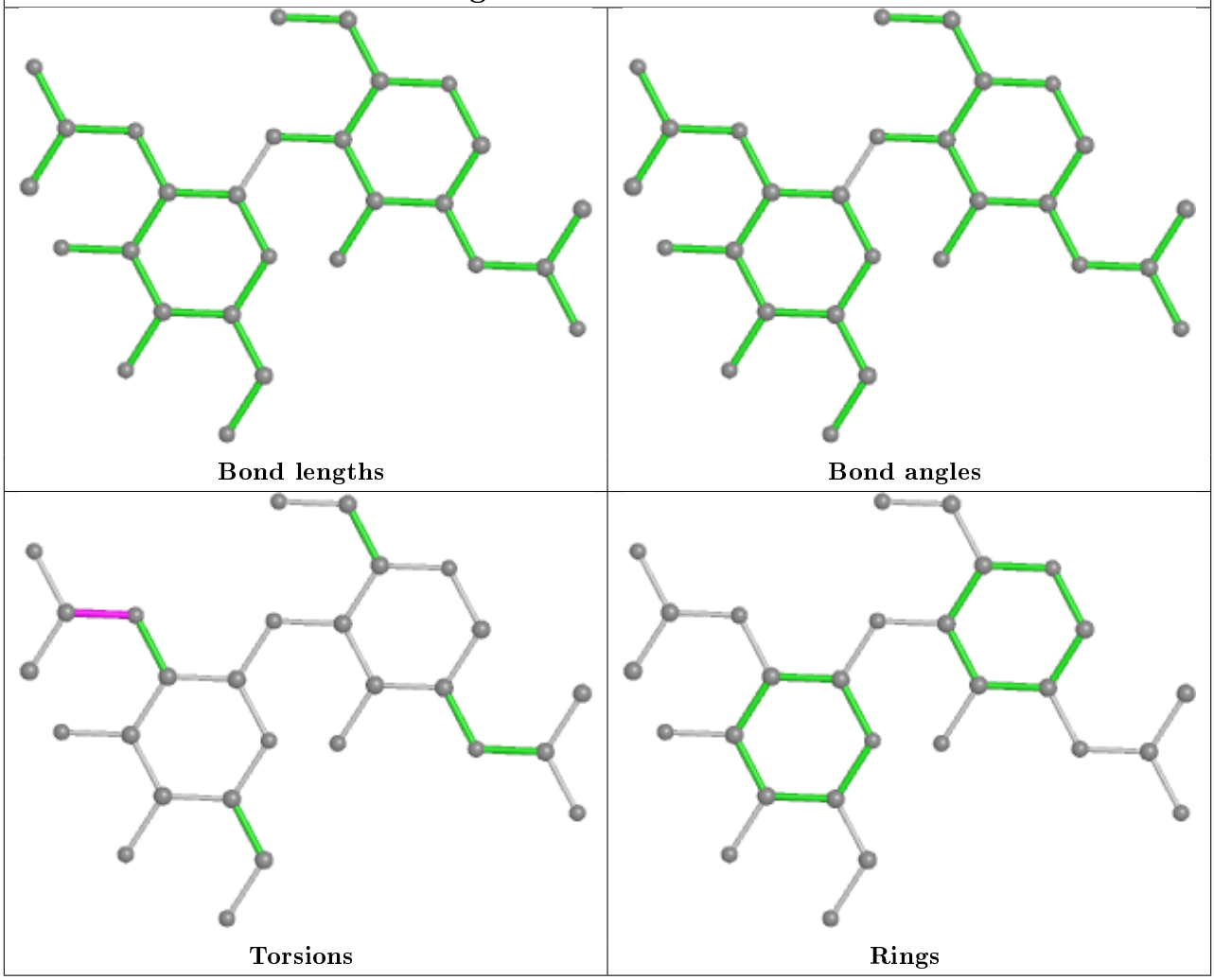
No monomer is involved in short contacts.

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 B



Oligosaccharide Chain C



5.6 Ligand geometry (i)

There are no ligands in this entry.

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	A	343/389 (88%)	0.18	22 (6%) 19 26	23, 38, 89, 133	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	ILE	6.2
1	A	219	GLU	3.7
1	A	49	HIS	3.6
1	A	1	ARG	3.4
1	A	52	LEU	3.4
1	A	212	GLU	3.3
1	A	217	ASP	3.2
1	A	214	THR	3.1
1	A	2	ASN	2.9
1	A	208	LYS	2.8
1	A	271	ALA	2.8
1	A	332	CYS	2.6
1	A	37	GLN	2.5
1	A	69	GLN	2.4
1	A	353	PHE	2.4
1	A	220	ASN	2.2
1	A	199	ASN	2.2
1	A	256	ARG	2.1
1	A	340	ILE	2.1
1	A	216	ASN	2.1
1	A	48	ASN	2.1
1	A	215	CYS	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)

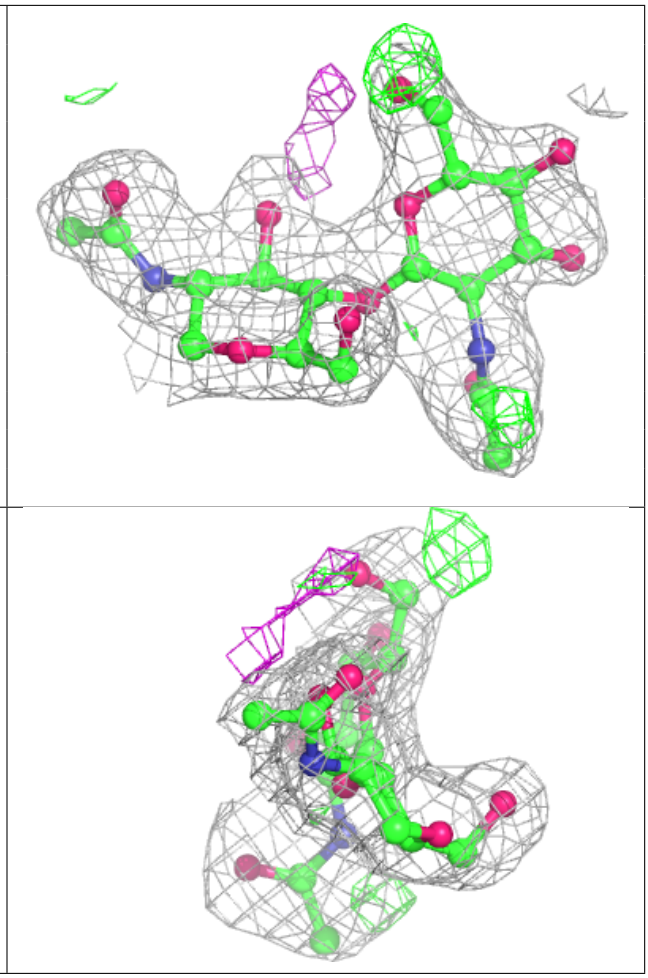
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	2	14/15	0.59	0.49	86,111,118,119	0
2	NAG	B	2	14/15	0.82	0.24	58,75,91,92	0
2	NAG	C	1	14/15	0.86	0.28	80,92,103,105	0
2	NAG	B	1	14/15	0.96	0.15	36,41,51,51	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.

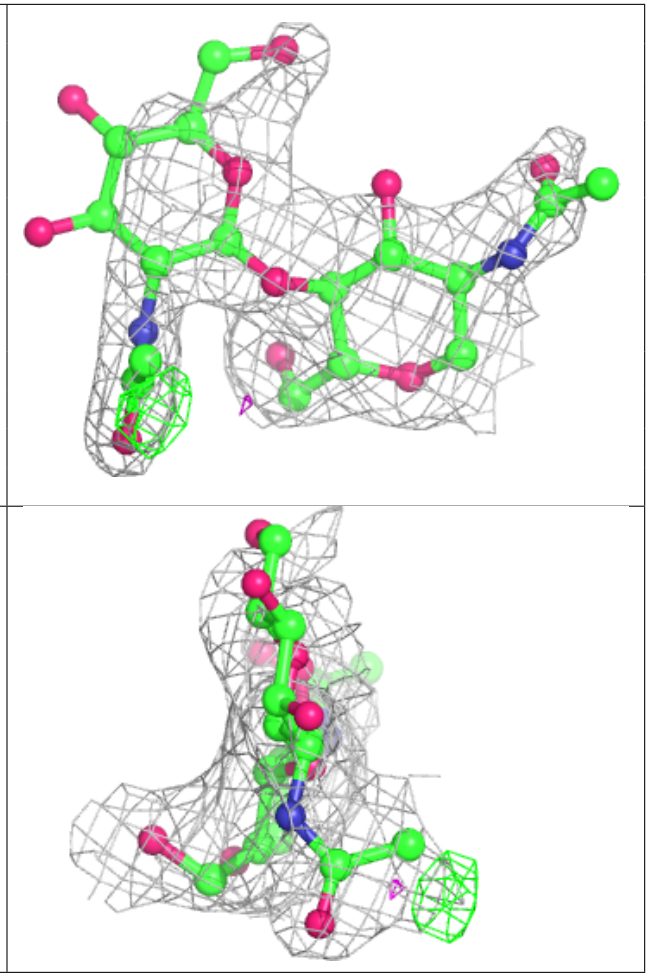
Electron density around Chain B:

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



Electron density around Chain C:

$2mF_o$-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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.