

wwPDB X-ray Structure Validation Summary Report (i)

Jan 24, 2022 – 06:24 pm GMT

PDB ID : 7QA4

Title : Crystal structure of stabilized H3N2 A/Hong Kong/1/1968 Hemagglutinin at

2.2 Angstrom

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Deposited on : 2021-11-16

Resolution : 2.19 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.24

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0267

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

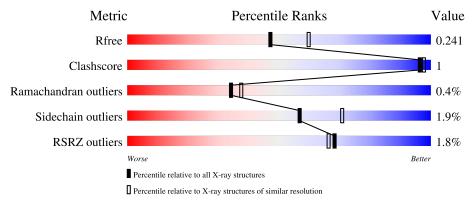
Validation Pipeline (wwPDB-VP) : 2.24

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 2.19 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	A	512	2%	1% 5% 5%				
2	В	3		100%				
3	С	5	20%	80%				
4	D	2		100%				
4	Е	2	50%	50%				



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4161 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.

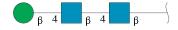
• Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	488	Total 3853	C 2408	N 678	O 748	S 19	41	2	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	TRP	HIS	conflict	UNP Q91MA7
A	380	ILE	LYS	conflict	UNP Q91MA7
A	432	ILE	GLU	conflict	UNP Q91MA7
A	506	GLY	-	expression tag	UNP Q91MA7
A	507	GLY	-	expression tag	UNP Q91MA7
A	508	SER	-	expression tag	UNP Q91MA7
A	509	GLU	-	expression tag	UNP Q91MA7
A	510	PRO	-	expression tag	UNP Q91MA7
A	511	GLU	-	expression tag	UNP Q91MA7
A	512	ALA	_	expression tag	UNP Q91MA7

• Molecule 2 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		
2	В	3	Total 39		N 2		0	0	0

• Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





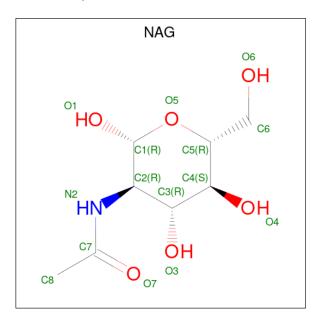
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	С	5	Total C N C 61 34 2 2	1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	D	2	Total C N O 28 16 2 10	0	0	0
4	Е	2	Total C N O 28 16 2 10	0	0	0

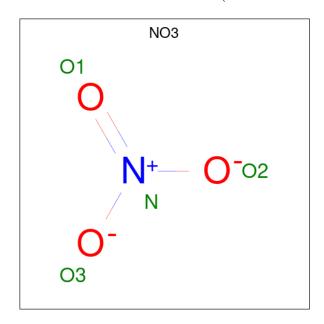
• Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	A	Atoms			ZeroOcc	AltConf	
5	Λ	1	Total	С	N	О	4	0	
5	A	1	14	8	1	5	4	U	



• Molecule 6 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
6	A	1	Total 4	N 1	O 3	0	0

• Molecule 7 is water.

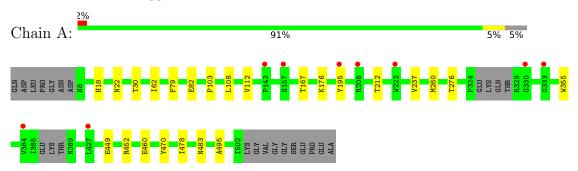
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	134	Total O 134 134	0	0



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: Hemagglutinin



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

Chain B:

NAG1 NAG2 BMA3

 $\bullet \ \, Molecule \ 3: \ alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-$

Chain C: 20% 80%

NAG1 NAG2 BMA3 MAN4 MAN5

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

Chain D: 100%

NAG1 NAG2

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



Chain E: 50% 50%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants	154.09Å 154.09Å 154.09Å	Danagitan
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	108.96 - 2.19	Depositor
Resolution (A)	108.96 - 2.19	EDS
% Data completeness	100.0 (108.96-2.19)	Depositor
(in resolution range)	100.0 (108.96-2.19)	EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) > 1$	1.62 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
D.D.	0.198 , 0.251	Depositor
R, R_{free}	0.200 , 0.241	DCC
R_{free} test set	1577 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.032 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4161	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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, NO3, MAN, BMA

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	$\mathbf{lengths}$	Bond angles		
			RMSZ	# Z > 5	RMSZ	# Z > 5	
	1	A	0.66	0/3933	0.80	0/5335	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3853	0	3718	8	0
2	В	39	0	34	0	0
3	С	61	0	52	1	0
4	D	28	0	25	0	0
4	Е	28	0	25	0	0
5	A	14	0	13	0	0
6	A	4	0	0	0	0
7	A	134	0	0	1	0
All	All	4161	0	3867	8	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.

The worst 5 of 8 close contacts within the same asymmetric unit are listed below, sorted by their



clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:470:TYR:O	1:A:495:ALA:HA	2.08	0.54
1:A:108:LEU:O	1:A:112:VAL:HG12	2.13	0.48
1:A:176:LYS:HB2	1:A:237:VAL:HG22	1.98	0.45
1:A:355:TRP:CD2	1:A:478:ILE:HG21	2.52	0.45
1:A:167:THR:HB	3:C:1:NAG:H62	2.00	0.43

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	484/512 (94%)	462 (96%)	20 (4%)	2 (0%)	34 37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	62	ILE

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	427/444 (96%)	419 (98%)	8 (2%)	57 71	



5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	460	GLU
1	A	276	THR
1	A	212	THR
1	A	195	TYR
1	A	260	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	211	GLN

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)

12 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	Trno	Chain	Res	es Link Budgets			$ ag{ths}$	Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	В	1	1,2	14,14,15	0.28	0	17,19,21	0.94	0
2	NAG	В	2	2	14,14,15	0.28	0	17,19,21	0.61	0
2	BMA	В	3	2	11,11,12	0.34	0	15,15,17	0.59	0
3	NAG	С	1	1,3	14,14,15	0.25	0	17,19,21	0.74	0
3	NAG	С	2	3	14,14,15	0.30	0	17,19,21	1.33	2 (11%)
3	BMA	С	3	3	11,11,12	0.43	0	15,15,17	1.25	0



Mol	Tuno	Chain	Res	Res Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	С	4	3	11,11,12	0.37	0	15,15,17	0.96	1 (6%)
3	MAN	С	5	3	11,11,12	0.34	0	15,15,17	1.33	1 (6%)
4	NAG	D	1	1,4	14,14,15	0.25	0	17,19,21	0.69	0
4	NAG	D	2	4	14,14,15	0.25	0	17,19,21	0.77	0
4	NAG	Е	1	1,4	14,14,15	0.30	0	17,19,21	0.78	0
4	NAG	Е	2	4	14,14,15	0.42	0	17,19,21	0.91	1 (5%)

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	В	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	В	2	2	-	0/6/23/26	0/1/1/1
2	BMA	В	3	2	-	0/2/19/22	0/1/1/1
3	NAG	С	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	С	2	3	-	0/6/23/26	0/1/1/1
3	BMA	С	3	3	-	2/2/19/22	0/1/1/1
3	MAN	С	4	3	-	1/2/19/22	0/1/1/1
3	MAN	С	5	3	-	2/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
4	NAG	Е	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Е	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	С	5	MAN	C1-O5-C5	4.82	118.72	112.19
4	Е	2	NAG	C4-C3-C2	2.35	114.47	111.02
3	С	2	NAG	C1-O5-C5	2.30	115.31	112.19
3	С	4	MAN	C1-O5-C5	2.27	115.26	112.19
3	С	2	NAG	C4-C3-C2	2.04	114.00	111.02

There are no chirality outliers.

5 of 8 torsion outliers are listed below:



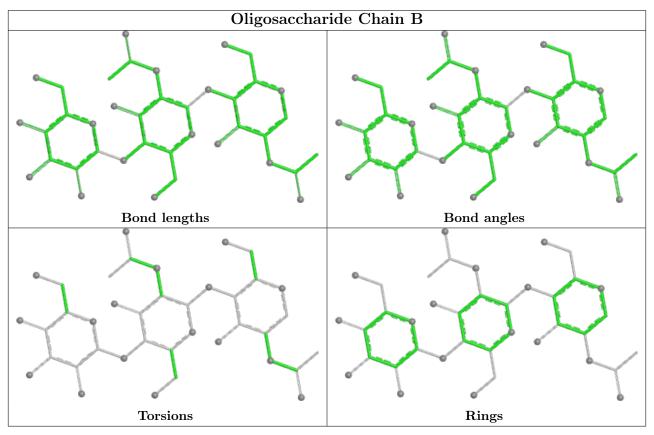
Mol	Chain	Res	Type	Atoms
3	С	5	MAN	O5-C5-C6-O6
3	С	3	BMA	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
3	С	4	MAN	O5-C5-C6-O6
3	С	5	MAN	C4-C5-C6-O6

There are no ring outliers.

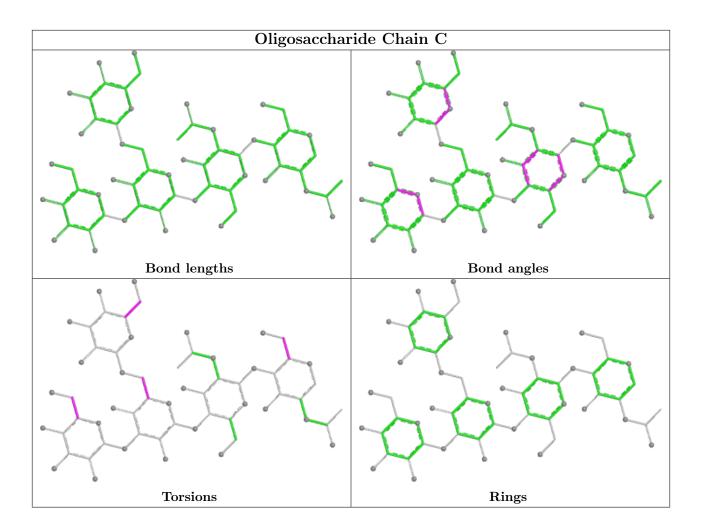
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	1	NAG	1	0

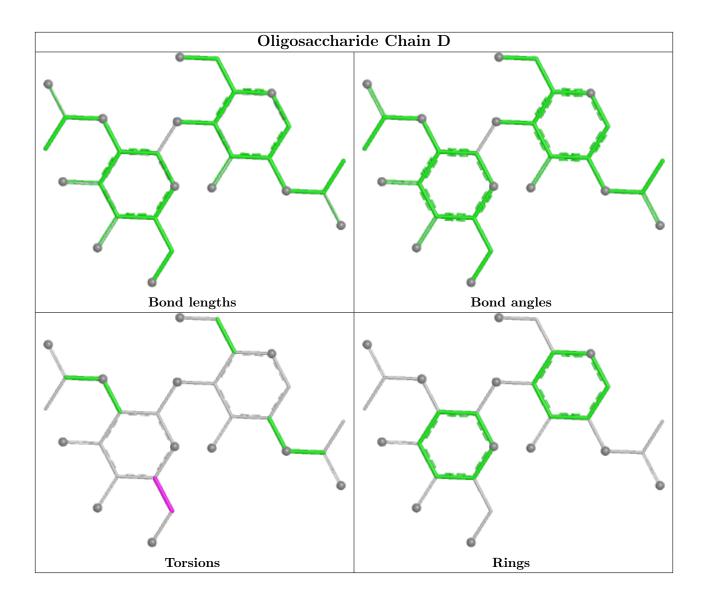
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



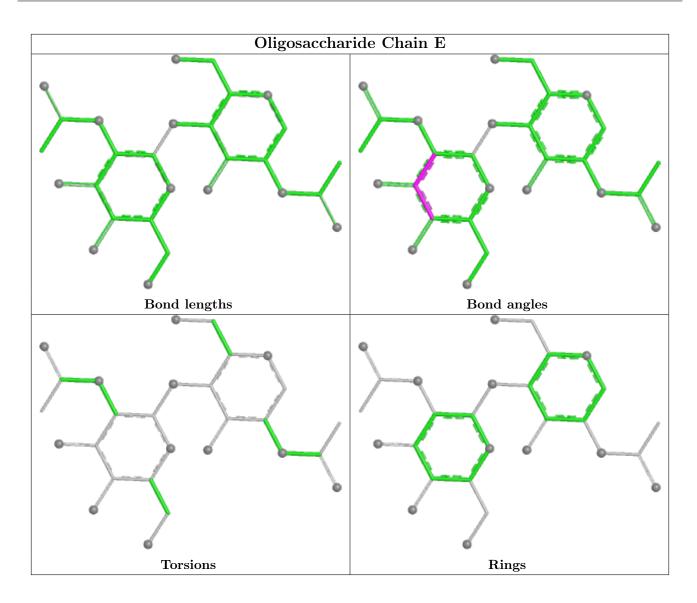












5.6 Ligand geometry (i)

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	Chain	Res	Link	Bond lengths			Bond angles		
IVIOI	туре		nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
5	NAG	A	601	1	14,14,15	0.29	0	17,19,21	0.83	1 (5%)	
6	NO3	A	602	-	1,3,3	0.26	0	0,3,3	-	-	



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	601	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
5	A	601	NAG	C2-N2-C7	2.16	125.97	122.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	NAG	O5-C5-C6-O6

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, 95^{th} 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	$OWAB(A^2)$	Q<0.9
1	A	488/512 (95%)	0.18	9 (1%) 68 66	44, 63, 92, 134	17 (3%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	PRO	4.6
1	A	330	GLY	4.6
1	A	208	ARG	2.8
1	A	333	GLY	2.5
1	A	222	TRP	2.3

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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
4	NAG	Ε	2	14/15	0.72	0.24	96,130,145,145	0
3	MAN	С	4	11/12	0.76	0.16	106,126,134,136	1
4	NAG	D	2	14/15	0.81	0.20	82,115,129,143	0
3	MAN	С	5	11/12	0.82	0.13	117,140,148,153	0
3	BMA	С	3	11/12	0.86	0.12	117,124,145,158	0
4	NAG	Ε	1	14/15	0.88	0.12	64,74,92,103	0
4	NAG	D	1	14/15	0.92	0.14	66,79,96,98	0

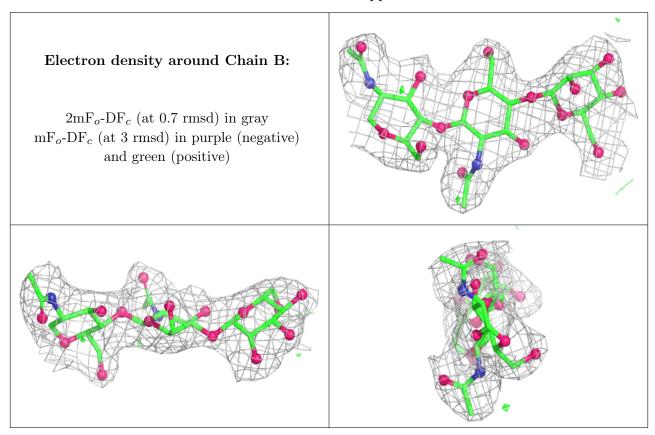
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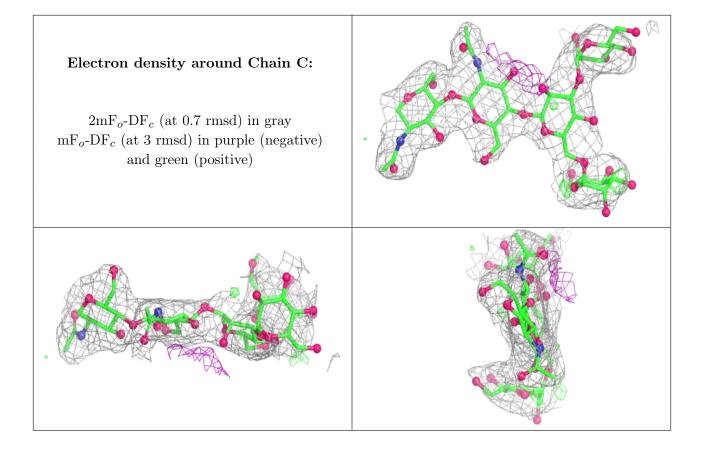
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	BMA	В	3	11/12	0.92	0.09	73,96,106,108	0
2	NAG	В	1	14/15	0.94	0.11	65,79,93,103	0
3	NAG	С	1	14/15	0.95	0.10	61,71,87,92	0
3	NAG	С	2	14/15	0.95	0.14	66,75,83,110	0
2	NAG	В	2	14/15	0.95	0.10	75,81,91,98	0

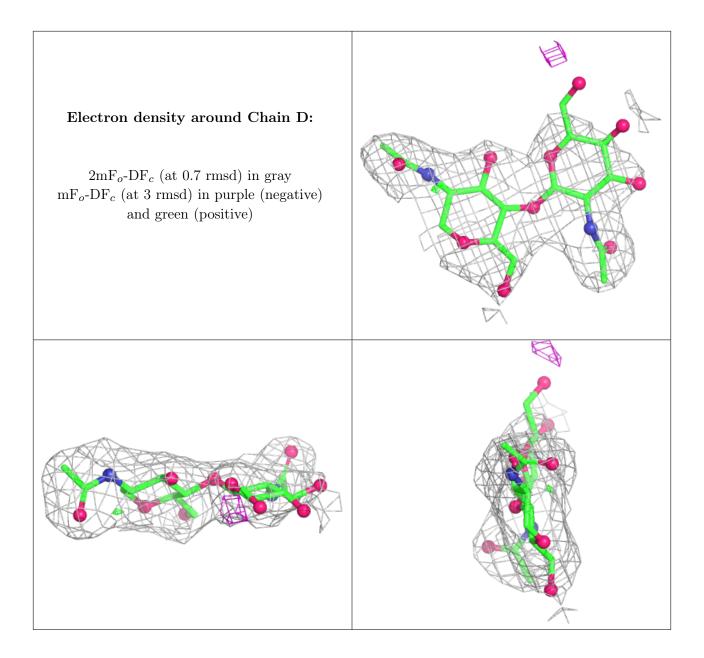
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



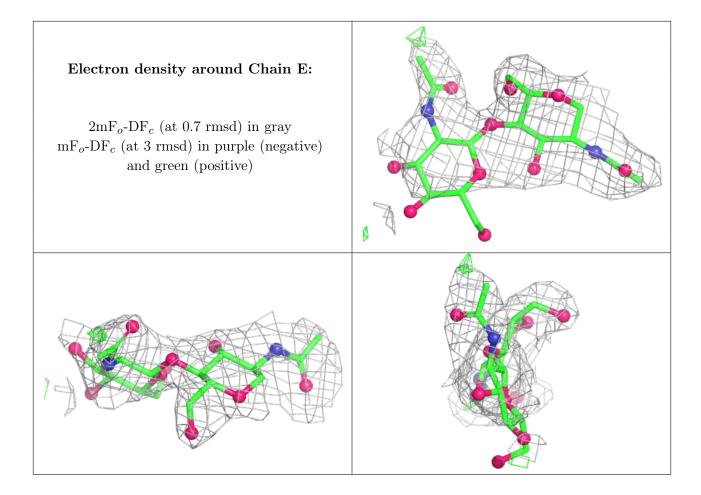












6.4 Ligands (i)

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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
5	NAG	A	601	14/15	0.83	0.20	108,127,132,135	4
6	NO3	A	602	4/4	0.98	0.14	51,68,69,69	4

6.5 Other polymers (i)

There are no such residues in this entry.

