

Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2020 – 10:35 AM BST

PDB ID : 4YY9

Title : The structure of hemagglutinin from a H6N1 influenza virus

(A/Taiwan/2/2013)

Authors: Wang, F.; Qi, J.; Bi, Y.; Zhang, W.; Wang, M.; Wang, M.; Liu, J.; Yan, J.;

Shi, Y.; Gao, G.F.

Deposited on : 2015-03-23

Resolution : 2.60 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 : 2.13.1

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

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove) oteins) : Engh & Huber (200

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

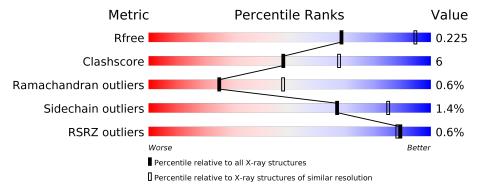
Validation Pipeline (wwPDB-VP) : 2.13.1

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 2.60 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$egin{aligned} ext{Similar resolution} \ (\# ext{Entries, resolution range}(ext{Å})) \end{aligned}$		
R_{free}	130704	3163 (2.60-2.60)		
Clashscore	141614	3518 (2.60-2.60)		
Ramachandran outliers	138981	3455 (2.60-2.60)		
Sidechain outliers	138945	3455 (2.60-2.60)		
RSRZ outliers	127900	3104 (2.60-2.60)		

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	325	84%	15%	-			
2	В	162	90%	10%				
3	С	3	67% 33%					



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4126 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 HA1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	325	Total	С	N	О	S	0	0	0
1	A	329	2568	1627	438	490	13	U	U	0

• Molecule 2 is a protein called HA2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	162	Total 1303	C 814	N 225	O 257	S 7	0	0	0

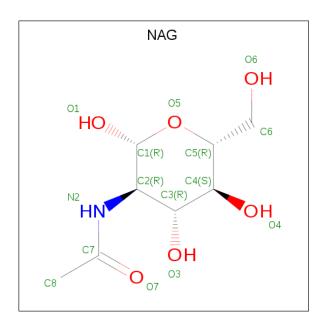
• Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	С	3	Total 39	C 22	N 2	O 15	39	0	0

• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf	
1	Λ	1	Total	С	N	О	1.4	0	
4	А	1	14	8	1	5	14		
4	Λ	1	Total	С	N	О	1.4	0	
4	A	1	14	8	1	5	14		

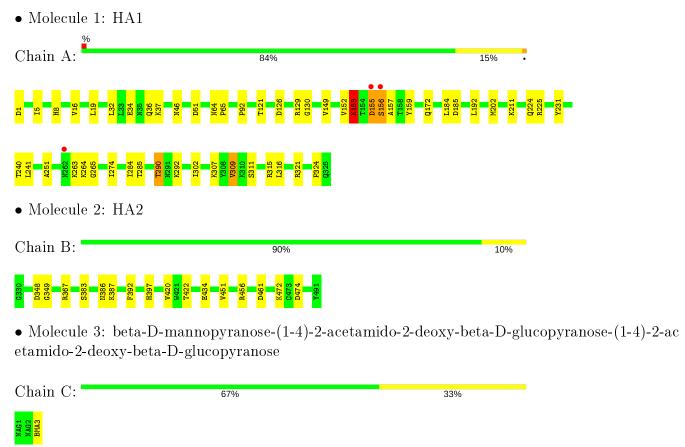
\bullet Molecule 5 is water.

Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
5	A	108	Total O 108 108	0	0
5	В	80	Total O 80 80	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.





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 63	Depositor	
Cell constants	113.90Å 113.90Å 163.84Å	Domositon	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	47.23 - 2.60	Depositor	
Resolution (A)	47.23 - 2.60	EDS	
% Data completeness	99.9 (47.23-2.60)	Depositor	
(in resolution range)	99.9 (47.23 - 2.60)	EDS	
R_{merge}	0.11	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	4.91 (at 2.61Å)	Xtriage	
Refinement program	PHENIX 1.8.3_1479	Depositor	
D D.	0.191 , 0.225	Depositor	
R, R_{free}	0.194 , 0.225	DCC	
R_{free} test set	1844 reflections (5.00%)	wwPDB-VP	
Wilson B-factor (Å ²)	42.3	Xtriage	
Anisotropy	0.326	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34 , 40.1	EDS	
L-test for twinning ²	$< L >=0.48, < L^2>=0.31$	Xtriage	
Estimated twinning fraction	0.056 for h,-h-k,-l	Xtriage	
F_o, F_c correlation	0.93	EDS	
Total number of atoms	4126	wwPDB-VP	
Average B, all atoms (Å ²)	47.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.69% 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: BMA, 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		Boı	nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.39	$1/2629 \ (0.0\%)$	0.52	0/3576	
2	В	0.35	0/1331	0.49	0/1795	
All	All	0.38	1/3960 (0.0%)	0.51	0/5371	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$Ideal(\AA)$
1	A	153	LYS	CB-CG	-6.26	1.35	1.52

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	$\mathbf{H}(\mathbf{model})$	H(added)	Clashes	Symm-Clashes
1	A	2568	0	2513	38	0
2	В	1303	0	1208	12	1
3	С	39	0	34	0	0
4	A	28	0	26	0	0
5	A	108	0	0	14	0
5	В	80	0	0	4	0
All	All	4126	0	3781	46	1



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 (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		$\operatorname{distance}\left(\mathrm{\AA}\right)$	overlap (Å)
1:A:37:LYS:NZ	5:A:701:HOH:O	1.92	1.01
1:A:315:ARG:NE	5:A:706:HOH:O	2.16	0.79
2:B:348:ASP:O	2:B:367:ARG:NH1	2.16	0.78
2:B:386:ASN:OD1	5:B:601:HOH:O	2.03	0.77
1:A:185:ASP:OD2	5:A:702:HOH:O	2.04	0.74
1:A:130:GLY:O	5:A:703:HOH:O	2.05	0.74
1:A:155:ASP:OD1	1:A:156:SER:N	2.20	0.72
1:A:240:THR:OG1	5:A:704:HOH:O	2.08	0.71
2:B:392:PHE:O	5:B:603:HOH:O	2.12	0.66
1:A:51:ASP:OD2	5:A:705:HOH:O	2.14	0.65
1:A:324:PRO:HD2	5:A:726:HOH:O	2.03	0.58
2:B:474:ASP:HB2	5:B:619:HOH:O	2.04	0.57
1:A:172:GLN:NE2	5:A:707:HOH:O	2.19	0.57
1:A:153:LYS:HB2	1:A:192:LEU:O	2.05	0.56
1:A:153:LYS:NZ	1:A:157:ALA:O	2.37	0.55
1:A:202:MET:HG2	1:A:241:LEU:HD11	1.89	0.54
1:A:32:LEU:HD11	1:A:316:LEU:HD22	1.90	0.53
1:A:315:ARG:NH1	5:A:724:HOH:O	2.41	0.53
1:A:126:ASP:OD2	1:A:129:ARG:NH1	2.42	0.52
1:A:149:VAL:HG13	1:A:251:ALA:HB3	1.92	0.52
1:A:265:GLY:H	1:A:302:ILE:HD11	1.74	0.52
1:A:309:VAL:HG13	1:A:311:SER:H	1.76	0.51
1:A:1:ASP:N	5:A:727:HOH:O	2.44	0.51
1:A:307:LYS:NZ	5:A:714:HOH:O	2.26	0.50
1:A:284:ILE:HG23	1:A:285:THR:HG23	1.95	0.48
1:A:16:VAL:HG12	1:A:315:ARG:HG2	1.96	0.48
1:A:51:ASP:HB2	1:A:274:ILE:HD12	1.97	0.47
2:B:367:ARG:HD2	2:B:367:ARG:HA	1.55	0.45
1:A:153:LYS:HE2	1:A:159:TYR:N	2.32	0.45
1:A:290:THR:HB	1:A:292:LYS:H	1.82	0.45
1:A:5:ILE:HD11	2:B:451:VAL:HG21	2.00	0.44
1:A:211:LYS:HD2	1:A:231:TYR:OH	2.18	0.43
1:A:152:VAL:HG12	1:A:153:LYS:N	2.33	0.43
1:A:321:ARG:NH2	5:A:720:HOH:O	2.32	0.43
1:A:184:LEU:HD22	1:A:225:ARG:HB2	2.01	0.42
2:B:397:HIS:ND1	5:B:602:HOH:O	2.08	0.42
1:A:19:LEU:HB2	2:B:434:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance} ({f A})$	Clash overlap (Å) 0.42 0.42 0.41 0.41 0.41 0.41 0.41 0.41 0.41
1:A:34:GLU:OE2	1:A:36:GLN:HB2	2.20	0.42
1:A:309:VAL:HG22	2:B:422:THR:HA	2.01	0.42
1:A:8:HIS:HB2	2:B:349:GLY:O	2.20	0.41
1:A:264:LYS:NZ	5:A:728:HOH:O	2.46	0.41
1:A:92:PRO:HG3	1:A:224:GLN:HB2	2.03	0.41
1:A:315:ARG:CZ	5:A:706:HOH:O	2.66	0.41
2:B:383:SER:O	2:B:387:LYS:HG2	2.21	0.41
2:B:472:LYS:HA	2:B:472:LYS:HD3	1.89	0.41
1:A:64:ASN:HA	1:A:65:PRO:HD3	1.88	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$egin{array}{c} ext{Interatomic} \ ext{distance } (ext{Å}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
2:B:456:ARG:NH2	2:B:461:ASP:O[2_565]	2.16	0.04

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	${f Allowed}$	Outliers	Perce	\mathbf{ntiles}
1	A	323/325~(99%)	306 (95%)	14 (4%)	3 (1%)	17	35
2	В	160/162~(99%)	153 (96%)	7 (4%)	0	100	100
All	All	483/487 (99%)	459 (95%)	21 (4%)	3 (1%)	25	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	SER
1	A	155	ASP
1	A	263	LYS



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	286/286 (100%)	281 (98%)	5 (2%)	60	81	
2	В	137/137 (100%)	136 (99%)	1 (1%)	84	94	
All	All	423/423 (100%)	417 (99%)	6 (1%)	67	85	

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	121	THR
1	A	153	LYS
1	A	290	THR
1	A	309	VAL
2	В	420	VAL

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)

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).

Mal	Mol Type Chain		Res	Link	Bond lengths			Bond angles		
10101	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	С	1	3,2	14,14,15	0.27	0	17,19,21	0.43	0
3	NAG	С	2	3	14,14,15	0.23	0	17,19,21	0.44	0
3	BMA	С	3	3	11,11,12	0.25	0	15,15,17	1.06	2 (13%)

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
3	NAG	С	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	С	2	3	-	3/6/23/26	0/1/1/1
3	BMA	С	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	${f Res}$	Type	${f Atoms}$	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^o)$
3	С	3	BMA	C1-C2-C3	2.23	112.41	109.67
3	С	3	BMA	C1-O5-C5	2.22	115.20	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

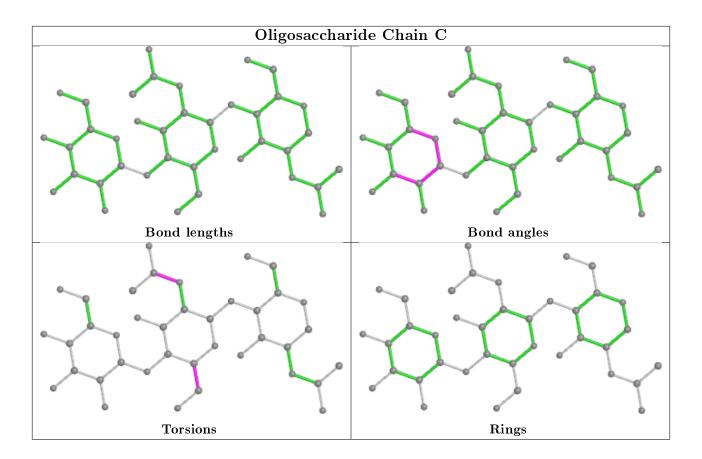
Mol	Chain	Res	Type	Atoms
3	С	2	NAG	C8-C7-N2-C2
3	С	2	NAG	O7-C7-N2-C2
3	С	2	NAG	O5-C5-C6-O6

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.





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	Bo	ond leng	ths	В	ond ang	les	
10101	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	601	1	14,14,15	0.29	0	17,19,21	0.52	0
4	NAG	A	602	1	14,14,15	0.57	0	17,19,21	0.94	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
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	NAG	A	602	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^o)$
4	A	602	NAG	C1-O5-C5	3.33	116.71	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	${f Res}$	Type	Atoms
4	A	601	NAG	O5-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	A	602	NAG	C4-C5-C6-O6
4	A	602	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	$ullet$ Analysed $ullet$ $\langle ext{RSRZ} angle ullet$ $\# ext{RSRZ} angle 2$		$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	$325/325 \; (100\%)$	-0.44	3 (0%) 84 82	24, 48, 82, 153	0
2	В	$162/162 \; (100\%)$	-0.55	0 100 100	22, 36, 62, 90	0
All	All	487/487 (100%)	-0.48	3 (0%) 89 88	22, 43, 80, 153	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	ASN	4.5
1	A	155	ASP	3.2
1	A	156	SER	2.2

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

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

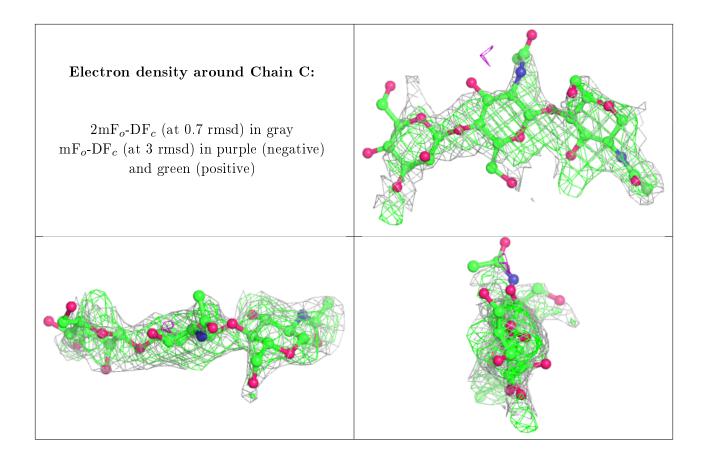
6.3 Carbohydrates (i)

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	NAG	С	1	14/15	-	-	66,71,81,88	14
3	BMA	С	3	11/12	-	-	118,128,136,138	11
3	NAG	С	2	14/15	-	-	91,102,110,114	14

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	${ m Res}$	Atoms	RSCC	RSR	$oxed{f B-factors({ m \AA}^2)}$	$\mathbf{Q}{<}0.9$
4	NAG	A	601	14/15	-	-	50,52,53,55	14
4	NAG	A	602	14/15	-	-	69,71,72,73	14

6.5 Other polymers (i)

There are no such residues in this entry.

