

wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2020 – 02:51 AM BST

PDB ID : 7NN9

Title : NATIVE INFLUENZA VIRUS NEURAMINIDASE SUBTYPE N9 (TERN)

Authors: Varghese, J.N.; Colman, P.M.

Deposited on : 1995-03-15

Resolution : 2.00 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 : 1.8.5 (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) roteins) : Engh & Huber (2001)

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

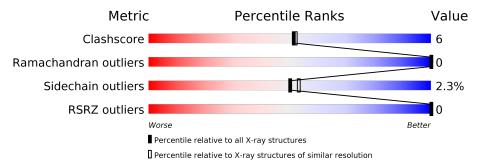
Validation Pipeline (wwPDB-VP) : 2.13.1

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 2.00 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$egin{aligned} ext{Similar resolution} \ (\# ext{Entries}, ext{resolution range}(ext{Å})) \end{aligned}$
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	388	88%	11%	-			
2	В	7	86%	14%	_			

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	\mathbf{Type}	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	В	3	X	-	_	-



2 Entry composition (i)

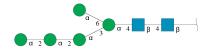
There are 5 unique types of molecules in this entry. The entry contains 3400 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NEURAMINIDASE N9.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	388	Total 3067	C 1914	N 538	O 592	S 23	31	0	0

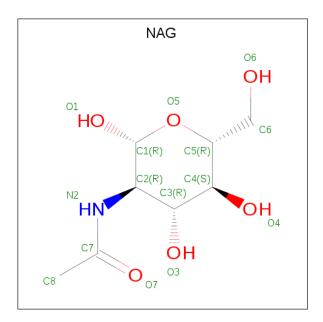
• Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	В	7	Total 83	C 46	N 2	O 35	0	0	0

• Molecule 3 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	
3	Δ	1	Total	С	N	О	0	0	
		1	14	8	1	5	U		
2	Λ.	1	Total	С	Ν	Ο	0	0	
)	A	1	14	8	1	5	0	0	

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0

• Molecule 5 is water.

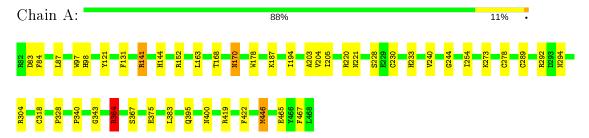
\mathbf{Mol}	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
5	A	221	Total O 221 221	0	0



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: NEURAMINIDASE N9



• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 86% 14%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants	182.80Å 182.80Å 182.80Å	Danagitan
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 - 2.00	Depositor
Resolution (A)	5.92 - 2.19	EDS
% Data completeness	(Not available) (6.00-2.00)	Depositor
(in resolution range)	68.9 (5.92-2.19)	EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR	Depositor
D D	0.152 , (Not available)	Depositor
R, R_{free}	0.149 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 56.4	EDS
L-test for twinning ¹	$ < L >=0.37, < L^2>=0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3400	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.

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: CA, NAG, MAN

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		
IVIOI		RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.55	0/3150	0.80	2/4290 (0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}(^{o})$
1	A	364	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	364	ARG	NE-CZ-NH2	-5.12	117.74	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	3067	0	2893	34	0
2	В	83	0	70	2	0
3	A	28	0	26	0	0
4	A	1	0	0	0	0
5	A	221	0	0	2	2
All	All	3400	0	2989	34	2

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.



The worst 5 of 34 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	Clash overlap (Å)
1:A:87:LEU:H	1:A:233:HIS:HD2	1.31	0.78
1:A:292:ARG:HH21	1:A:294:ASN:ND2	1.83	0.75
1:A:98:HIS:HE1	1:A:419:ARG:HH11	1.34	0.74
1:A:168:THR:H	1:A:170:ASN:HD21	1.35	0.73
1:A:98:HIS:CE1	1:A:419:ARG:HH11	2.12	0.67

All (2) 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	$egin{array}{ll} ext{Interatomic} \ ext{distance} \ (ext{\AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
5:A:775:HOH:O	5:A:777:HOH:O[48_555]	0.54	1.66
5:A:785:HOH:O	5:A:785:HOH:O[48_555]	1.35	0.85

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	Perce	\mathbf{ntiles}
1	A	386/388 (100%)	366 (95%)	20 (5%)	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	A	341/341 (100%)	333 (98%)	8 (2%)	50 53

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

Mol	Chain	Res	Type
1	A	204	VAL
1	A	446	MET
1	A	304	ARG
1	A	170	ASN
1	A	230	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	${f Res}$	Type
1	A	233	HIS
1	A	294	ASN
1	A	392	GLN
1	A	221	ASN
1	A	346	ASN

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)

7 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	Tune	Chain	Res	Link	Во	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	В	1	1,2	14,14,15	1.68	3 (21%)	17,19,21	1.80	3 (17%)
2	NAG	В	2	2	14,14,15	1.32	2 (14%)	17,19,21	2.06	6 (35%)
2	MAN	В	3	2	11,11,12	1.33	1 (9%)	15,15,17	1.46	2 (13%)
2	MAN	В	4	2	11,11,12	1.39	1 (9%)	15,15,17	1.97	5 (33%)
2	MAN	В	5	2	11,11,12	0.91	0	15,15,17	1.31	3 (20%)
2	MAN	В	6	2	11,11,12	1.38	2 (18%)	15,15,17	1.35	2 (13%)
2	MAN	В	7	2	11,11,12	1.94	3 (27%)	15,15,17	3.09	8 (53%)

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	MAN	В	3	2	1/1/4/5	1/2/19/22	0/1/1/1
2	MAN	В	4	2	-	0/2/19/22	0/1/1/1
2	MAN	В	5	2	-	0/2/19/22	0/1/1/1
2	MAN	В	6	2	-	0/2/19/22	0/1/1/1
2	MAN	В	7	2	-	0/2/19/22	1/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	${f Observed(\AA)}$	$\operatorname{Ideal}(ext{\AA})$
2	В	7	MAN	C4-C5	-4.98	1.42	1.53
2	В	1	NAG	C1-C2	4.20	1.58	1.52
2	В	3	MAN	C4-C5	-3.42	1.45	1.53
2	В	4	MAN	C4-C5	-3.32	1.46	1.53
2	В	1	NAG	C4-C5	2.88	1.59	1.53

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
2	В	7	MAN	C1-O5-C5	7.35	122.15	112.19
2	В	1	NAG	C1-C2-N2	-5.83	100.52	110.49
2	В	4	MAN	C1-O5-C5	4.60	118.43	112.19
2	В	7	MAN	O2-C2-C1	-4.37	100.22	109.15
2	В	2	NAG	C8-C7-N2	4.09	123.03	116.10



All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	В	3	MAN	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	3	MAN	C4-C5-C6-O6

All (1) ring outliers are listed below:

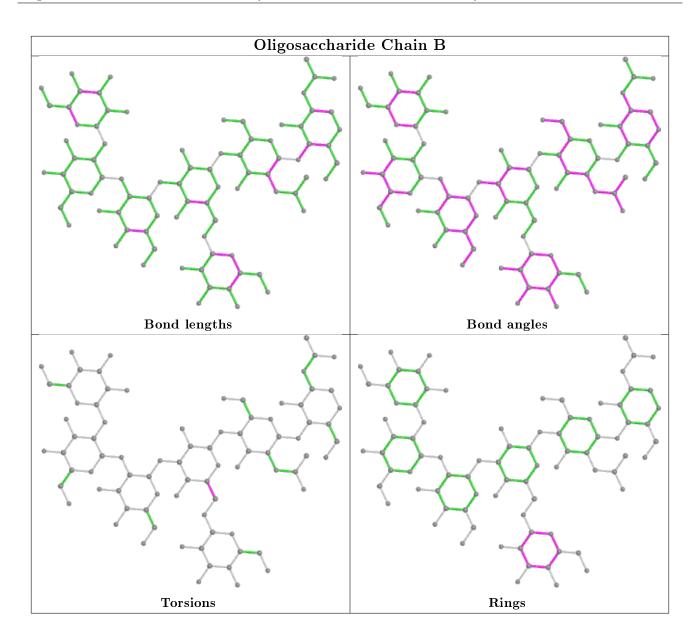
Mol	Chain	Res	Type	Atoms
2	В	7	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1	NAG	2	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)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	Tuno	Type Chain	Res	Link	Bond lengths			Bond angles		
IVIOI	Type		ites	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	477(A)	1	14,14,15	1.34	1 (7%)	17,19,21	2.18	6 (35%)



<u> </u>	Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
L.				nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
	3	NAG	A	476(A)	1	14,14,15	1.08	1 (7%)	17,19,21	1.75	3 (17%)

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.

Mo	l Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	477(A)	1	-	2/6/23/26	0/1/1/1
3	NAG	A	476(A)	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(\text{\AA})$
3	A	477(A)	NAG	C1-C2	-4.21	1.46	1.52
3	A	476(A)	NAG	O5-C1	-2.09	1.40	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}(^{o})$
3	A	477(A)	NAG	C6-C5-C4	4.66	123.93	113.00
3	A	477(A)	NAG	C2-N2-C7	-4.48	116.53	122.90
3	A	476(A)	NAG	C4-C3-C2	-3.56	105.80	111.02
3	A	476(A)	NAG	O5-C1-C2	-3.47	105.81	111.29
3	A	476(A)	NAG	C6-C5-C4	-3.35	105.15	113.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	477(A)	NAG	C4-C5-C6-O6
3	A	477(A)	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		$OWAB(m \AA^2)$	Q < 0.9
1	A	388/388 (100%)	-0.82	0 100	100	10, 17, 28, 38	8 (2%)

There are no RSRZ outliers to report.

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

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

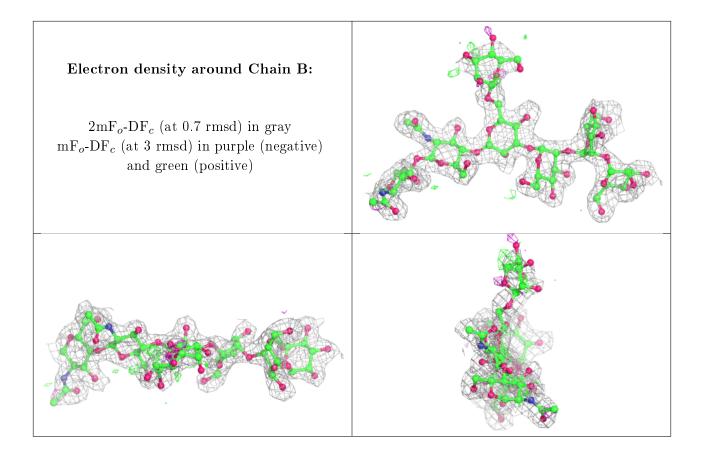
6.3 Carbohydrates (i)

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	${f B-factors}({f A}^2)$	Q < 0.9
2	MAN	В	7	11/12	0.70	0.36	48,52,55,55	0
2	MAN	В	4	11/12	0.92	0.12	27,28,29,31	0
2	NAG	В	1	14/15	0.95	0.12	21,22,25,25	0
2	MAN	В	5	11/12	0.95	0.10	25,26,27,28	0
2	NAG	В	2	14/15	0.95	0.10	21,23,26,27	0
2	MAN	В	3	11/12	0.96	0.09	27,29,35,42	0
2	MAN	В	6	11/12	0.96	0.09	23,24,25,25	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	${f B-factors}({f \AA}^2)$	Q < 0.9
3	NAG	A	477(A)	14/15	0.89	0.16	37,40,41,42	0
3	NAG	A	476(A)	14/15	0.94	0.12	28,30,32,33	0
4	CA	A	600	1/1	0.99	0.03	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.

