

Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 05:46 pm GMT

PDB ID : 6FRV

Title : Structure of the catalytic domain of Aspergillus niger Glucoamylase Authors : Roth, C.; Moroz, O.V.; Ariza, A.; Friis, E.P.; Davies, G.J.; Wilson, K.S.

Deposited on : 2018-02-16

Resolution : 2.30 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 (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 : 2.36

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)

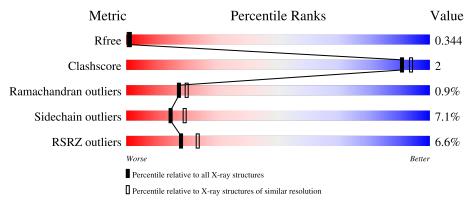
Validation Pipeline (wwPDB-VP) : 2.36

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 2.30 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	616	68%	7%	24%
2	В	2	100%		



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3633 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 Glucoamylase.

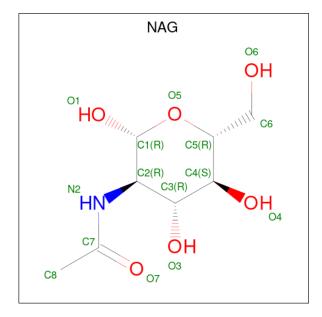
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	467	Total	С	N	О	S	0	0	0
1	A	407	3542	2221	580	732	9	0	U	0

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



Mo	l Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	В	2	Total C N O 28 16 2 10	0	0	0

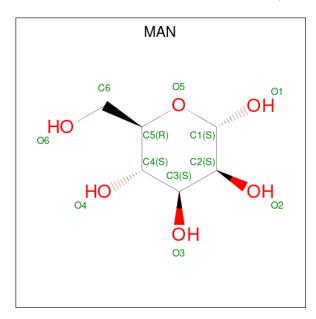
• Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
3	A	1	Total	С	N 1	O 5	0	0
0	11	_	14	8	1	5		

 \bullet Molecule 4 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $\mathrm{C_6H_{12}O_6}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0

• Molecule 5 is water.

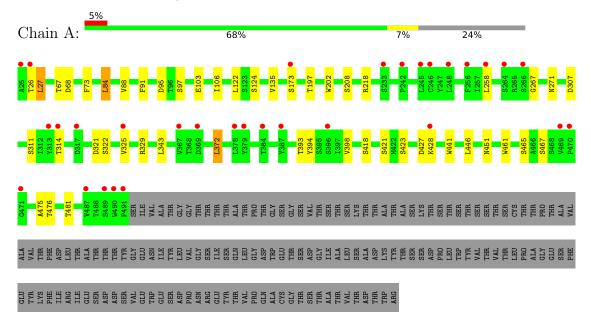
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	27	Total O 27 27	0	0



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: Glucoamylase



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

Chain B:	100%	
# 8		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	56.37Å 73.12Å 102.88Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.67 - 2.30	Depositor
Resolution (A)	44.64 - 2.30	EDS
% Data completeness	99.4 (59.67-2.30)	Depositor
(in resolution range)	99.5 (44.64-2.30)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.95 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
D D.	0.251 , 0.343	Depositor
R, R_{free}	0.254 , 0.344	DCC
R_{free} test set	972 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.820	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.39, 46.8	EDS
L-test for twinning ²	$ < L >=0.41, < L^2>=0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3633	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.68% 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: MAN, 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).

Mal	Chain	Bond	$\mathbf{lengths}$	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.47	0/3630	0.63	0/4969	

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	3542	0	3289	12	0
2	В	28	0	25	0	0
3	A	14	0	13	0	0
4	A	22	0	20	0	0
5	A	27	0	0	1	0
All	All	3633	0	3347	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	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	Clash overlap (Å)
1:A:26:THR:HG23	1:A:27:LEU:HD13	1.63	0.78
1:A:202:TRP:CD2	1:A:329:ARG:HD2	2.47	0.50
1:A:73:PHE:CE2	1:A:135:VAL:HG21	2.49	0.48
1:A:465:SER:O	5:A:801:HOH:O	2.20	0.47
1:A:343:LEU:HD22	1:A:441:TRP:CD2	2.54	0.43
1:A:84:LEU:O	1:A:88:VAL:HG23	2.19	0.42
1:A:218:ARG:HG3	1:A:461:TRP:CD2	2.54	0.42
1:A:394:TYR:O	1:A:398:VAL:HG22	2.20	0.41
1:A:258:LEU:HD23	1:A:267:GLY:HA3	2.02	0.41
1:A:103:GLU:O	1:A:106:ILE:N	2.54	0.40
1:A:91:PHE:HA	1:A:95:ASP:O	2.22	0.40
1:A:73:PHE:HE2	1:A:135:VAL:HG21	1.87	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	A	465/616 (76%)	439 (94%)	22 (5%)	4 (1%)	17 20	

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type		
1	A	372	LEU		
1	A	475	ALA		
1	A	427	ASP		
1	A	271	ASN		

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	381/508 (75%)	354 (93%)	27 (7%)	14 19	

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type	
1	A	27	LEU	
1	A	67	THR	
1	A	68	ASP	
1	A	84	LEU	
1	A A	97	SER	
1	A	122	LEU	
1	A	124	SER	
1	A	173	SER	
1	A	197	THR	
1	A	208	SER	
1	A	307	ASP	
1	A A	311	SER	
1	A	314	THR	
1	A	321	ASP	
1	A	322	SER	
1	A	325	VAL	
1	A	372	LEU	
1	A	393	THR	
1	A A	418	SER	
1	A	421	SER	
1	A	423	SER	
1	A	428	LYS	
1	A	446	LEU	
1	A	451	ASN	
1	A	467	SER	
1	A	476	THR	
1	A	481	THR	

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type	
1	A	33	ASN	
1	A	109	GLN	

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Mol	Chain	Res	Type		
1	A	339	ASN		
1	A	451	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)

2 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		
MIOI	Type		nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	В	1	2,1	14,14,15	0.56	0	17,19,21	1.62	3 (17%)
2	NAG	В	2	2	14,14,15	0.41	0	17,19,21	1.49	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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	В	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	В	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
2	В	1	NAG	O5-C1-C2	-4.12	104.79	111.29
2	В	1	NAG	C1-O5-C5	4.10	117.74	112.19
2	В	2	NAG	O5-C1-C2	-3.39	105.94	111.29
2	В	2	NAG	C1-O5-C5	2.56	115.66	112.19
2	В	1	NAG	C1-C2-N2	2.44	114.65	110.49
2	В	2	NAG	O4-C4-C5	2.03	114.34	109.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

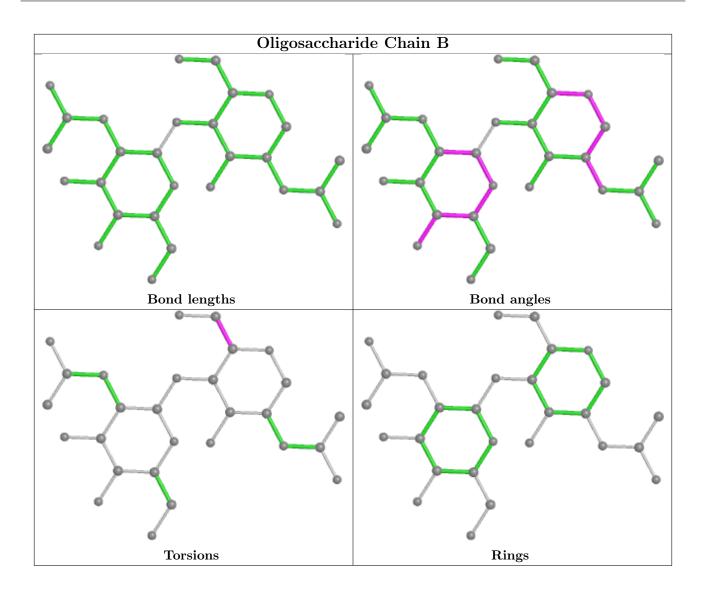
Mol	Chain	Res	Type	Atoms
2	В	1	NAG	O5-C5-C6-O6
2	В	1	NAG	C4-C5-C6-O6

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.





5.6 Ligand geometry (i)

3 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		
MIOI	Type				Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	A	705	1	11,11,12	0.26	0	15,15,17	0.89	1 (6%)
4	MAN	A	704	1	11,11,12	0.40	0	15,15,17	1.06	1 (6%)
3	NAG	A	703	1	14,14,15	0.36	0	17,19,21	1.40	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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	705	1	-	0/2/19/22	0/1/1/1
4	MAN	A	704	1	-	2/2/19/22	0/1/1/1
3	NAG	A	703	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
4	A	705	MAN	C1-O5-C5	2.78	115.96	112.19
3	A	703	NAG	C2-N2-C7	2.59	126.59	122.90
4	A	704	MAN	O5-C5-C6	2.20	110.65	107.20
3	A	703	NAG	C8-C7-N2	2.12	119.68	116.10
3	A	703	NAG	O5-C5-C6	2.05	110.42	107.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	NAG	C8-C7-N2-C2
3	A	703	NAG	O7-C7-N2-C2
4	A	704	MAN	C4-C5-C6-O6
3	A	703	NAG	O5-C5-C6-O6
4	A	704	MAN	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>	# RSRZ > 2		$OWAB(Å^2)$	Q<0.9
1	A	467/616 (75%)	0.52	31 (6%)	18 23	28, 56, 81, 120	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	471	GLY	6.7
1	A	490	TRP	5.1
1	A	387	TYR	4.9
1	A	258	LEU	4.6
1	A	25	ALA	4.1
1	A	379	TYR	3.9
1	A	367	VAL	3.9
1	A	491	PRO	3.8
1	A	369	ASP	3.8
1	A	378	LEU	3.7
1	A	384	THR	3.4
1	A	256	PHE	3.3
1	A	233	SER	3.3
1	A	487	VAL	3.0
1	A	26	THR	2.9
1	A	266	SER	2.9
1	A	314	THR	2.9
1	A	317	ASP	2.7
1	A	469	VAL	2.7
1	A	470	PRO	2.5
1	A	242	PRO	2.4
1	A	428	LYS	2.3
1	A	246	CYS	2.3
1	A	325	VAL	2.2
1	A	248	LEU	2.2
1	A	396	SER	2.2
1	A	245	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	264	SER	2.2
1	A	173	SER	2.1
1	A	489	SER	2.1
1	A	313	TYR	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.

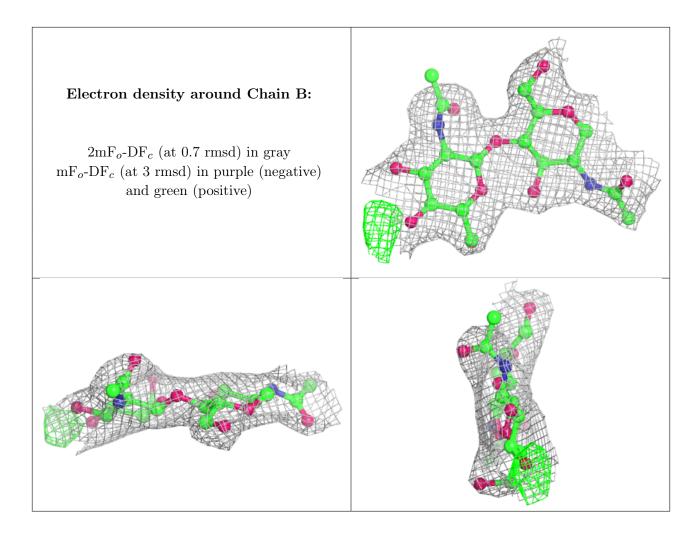
6.3 Carbohydrates (i)

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, 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
2	NAG	В	2	14/15	0.90	0.20	53,57,67,68	0
2	NAG	В	1	14/15	0.95	0.15	48,50,55,58	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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{ ilde{A}}^2)$	Q<0.9
3	NAG	A	703	14/15	0.90	0.17	63,66,73,74	0
4	MAN	A	704	11/12	0.94	0.13	53,58,61,63	0
4	MAN	A	705	11/12	0.95	0.19	57,63,66,66	0

6.5 Other polymers (i)

There are no such residues in this entry.

