

Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 02:59 PM EDT

PDB ID : 5EN2

Title: Molecular basis for antibody-mediated neutralization of New World hemor-

rhagic fever mammarenaviruses

Authors: Mahmutovic, S.; Clark, L.; Levis, S.; Briggiler, A.; Enria, D.; Harrison, S.C.;

Abraham, J.

Deposited on : 2015-11-09

Resolution : 1.82 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35.1

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

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

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

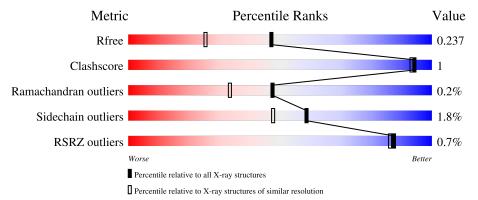
Validation Pipeline (wwPDB-VP) : 2.35.1

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 1.82 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	224	96%	•••
2	В	212	95%	·
3	С	141	92%	8%
4	D	7	57%	43%
5	Е	2	50%	50%



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
7	NAG	С	610	-	-	-	X



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5473 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 GD01 heavy chain.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	A	219	Total 1671	C 1061	N 277	O 327	S 6	0	1	0

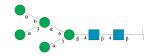
• Molecule 2 is a protein called GD01 light chain.

Mol	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace
2	В	212	Total 1646	C 1025	N 276	O 337	S 8	0	0	0

• Molecule 3 is a protein called Pre-glycoprotein polyprotein GP complex.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
3	С	141	Total 1145	C 739	N 189	O 207	S 10	0	0	0

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



Mol	Chain	Residues	1	Ator	ns	ZeroOcc	AltConf	Trace
4	D	7	Total 82		N 2	0	0	0

• Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



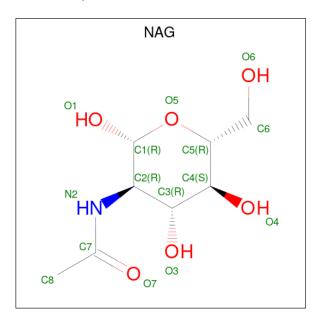


Mol	Chain	Residues	A	Lton	\mathbf{ns}		ZeroOcc	AltConf	Trace
5	Е	2	Total 28	C 16	N 2	O 10	0	0	0

• Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total Cl 1 1	0	0

 \bullet Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\rm C_8H_{15}NO_6).$



Mol	Chain	Residues	A	Atoms				AltConf
7	С	1	Total 14	C 8	N 1	O 5	0	0

• Molecule 8 is water.

\mathbf{M}	ol	Chain	Residues	Atoms	ZeroOcc	AltConf
8		A	356	Total O 356 356	0	0
8		В	341	Total O 341 341	0	0

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Mol	Chain	Residues	Atom	ıs	ZeroOcc	AltConf
8	С	189	Total 189	O 189	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 21 21 21	Depositor
Cell constants	52.11Å 74.79Å 177.64Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.93 - 1.82	Depositor
Resolution (A)	68.93 - 1.82	EDS
% Data completeness	99.7 (68.93-1.82)	Depositor
(in resolution range)	99.9 (68.93-1.82)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$< I/\sigma(I) > 1$	1.37 (at 1.82Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.10.2	Depositor
P. P.	0.180 , 0.224	Depositor
R, R_{free}	0.190 , 0.237	DCC
R_{free} test set	3168 reflections (5.03%)	wwPDB-VP
Wilson B-factor $(Å^2)$	17.5	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 54.2	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5473	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.95% 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, CL, NAG, 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	lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.50	0/1717	0.66	0/2339	
2	В	0.54	0/1681	0.66	0/2279	
3	С	0.49	0/1181	0.60	0/1604	
All	All	0.51	0/4579	0.64	0/6222	

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	1671	0	1638	1	0
2	В	1646	0	1579	6	0
3	С	1145	0	1100	6	0
4	D	82	0	68	0	0
5	Ε	28	0	25	0	0
6	В	1	0	0	0	0
7	С	14	0	13	0	0
8	A	356	0	0	0	0
8	В	341	0	0	0	0
8	С	189	0	0	0	0
All	All	5473	0	4423	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 1.

All (12) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance } (\text{\AA}) \end{array}$	Clash overlap (Å)
2:B:196:ALA:HB3	2:B:205:ILE:CG2	2.25	0.67
2:B:196:ALA:HB3	2:B:205:ILE:HG22	1.80	0.62
3:C:127:GLN:HG2	3:C:161:PRO:HB3	1.86	0.56
2:B:136:LEU:CD2	2:B:196:ALA:HB2	2.38	0.52
2:B:93:SER:HB3	3:C:116:ALA:HB3	1.96	0.48
2:B:195:GLU:HG2	2:B:206:VAL:HG22	1.99	0.45
3:C:182:THR:HB	3:C:210:GLY:HA2	1.98	0.45
2:B:136:LEU:HD21	2:B:196:ALA:HB2	1.99	0.44
3:C:178:ASN:HA	3:C:214:LEU:HD23	2.01	0.43
3:C:116:ALA:HA	3:C:214:LEU:HD13	1.99	0.42
1:A:33:TRP:CE2	1:A:52:TYR:HB2	2.56	0.40
3:C:153:GLY:O	3:C:191:LYS:HE2	2.21	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	Perce	$_{ m ntiles}$
1	A	$216/224\ (96\%)$	213 (99%)	3 (1%)	0	100	100
2	В	210/212 (99%)	205 (98%)	4 (2%)	1 (0%)	29	15
3	С	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
All	All	565/577 (98%)	552 (98%)	12 (2%)	1 (0%)	47	33

All (1) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
2	В	8	GLN

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	Perce	ntiles
1	A	186/189 (98%)	183 (98%)	3 (2%)	62	53
2	В	188/188 (100%)	184 (98%)	4 (2%)	53	41
3	С	128/128 (100%)	126 (98%)	2 (2%)	62	53
All	All	502/505 (99%)	493 (98%)	9 (2%)	59	48

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	134	SER
1	A	196	ASN
2	В	8	GLN
2	В	78	MET
2	В	80	SER
2	В	105	GLU
3	С	88	LEU
3	С	140	ASP

Sometimes 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)

9 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	Tuna	Chain	Res	Link	Вс	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	D	1	3,4	14,14,15	0.26	0	17,19,21	0.58	0
4	NAG	D	2	4	14,14,15	0.23	0	17,19,21	0.53	0
4	BMA	D	3	4	11,11,12	0.32	0	15,15,17	0.43	0
4	MAN	D	4	4	11,11,12	0.38	0	15,15,17	0.88	2 (13%)
4	MAN	D	5	4	11,11,12	0.43	0	15,15,17	0.90	1 (6%)
4	MAN	D	6	4	10,10,12	0.40	0	13,13,17	0.64	0
4	MAN	D	7	4	11,11,12	0.35	0	15,15,17	0.83	1 (6%)
5	NAG	Е	1	3,5	14,14,15	0.31	0	17,19,21	0.70	1 (5%)
5	NAG	E	2	5	14,14,15	0.32	0	17,19,21	0.54	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
4	NAG	D	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	MAN	D	5	4	-	1/2/19/22	1/1/1/1
4	MAN	D	6	4	-	0/2/16/22	0/1/1/1
4	MAN	D	7	4	-	0/2/19/22	0/1/1/1
5	NAG	Е	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	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	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	D	5	MAN	C1-O5-C5	3.10	116.39	112.19
4	D	7	MAN	C1-O5-C5	2.67	115.80	112.19
5	Ε	1	NAG	C1-O5-C5	2.60	115.72	112.19
4	D	4	MAN	C1-C2-C3	2.21	112.38	109.67
4	D	4	MAN	C1-O5-C5	2.09	115.03	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	5	MAN	O5-C5-C6-O6

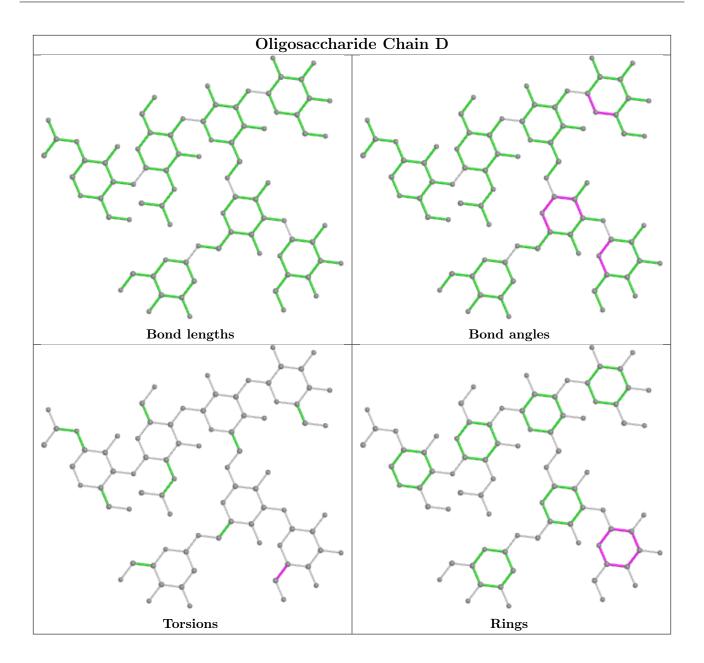
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	5	MAN	C1-C2-C3-C4-C5-O5

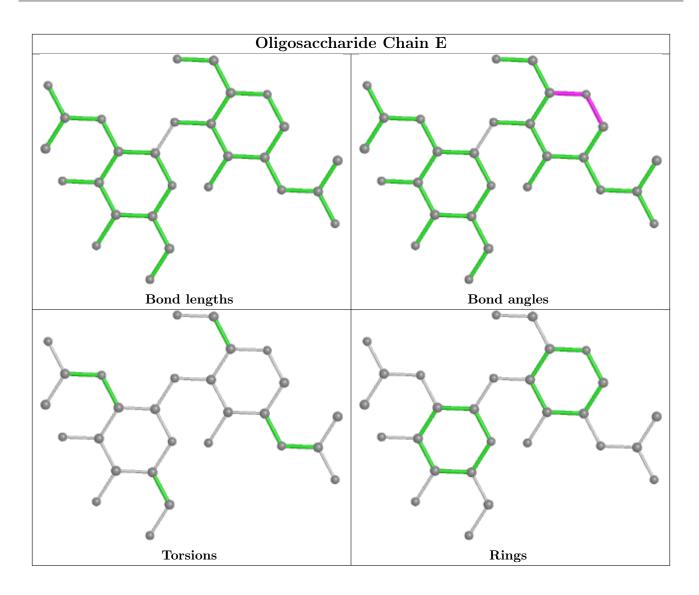
No monomer is involved in short contacts.

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)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	Trunc	Type Chain Res L			Bo	Bond lengths			Bond angles		
	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
7	NAG	С	610	3	14,14,15	0.33	0	17,19,21	0.86	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
7	NAG	С	610	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
7	С	610	NAG	C1-C2-N2	2.59	114.92	110.49

There are no chirality outliers.

There are no torsion outliers.

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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(\AA^2)$	Q < 0.9
1	A	219/224 (97%)	-0.46	1 (0%) 91 89	9, 19, 38, 47	0
2	В	212/212 (100%)	-0.39	0 100 100	9, 18, 39, 54	0
3	С	141/141 (100%)	-0.22	3 (2%) 63 59	10, 23, 43, 69	0
All	All	572/577 (99%)	-0.37	4 (0%) 87 86	9, 20, 40, 69	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	GLY	2.9
3	С	88	LEU	2.7
3	С	201	ARG	2.2
3	С	157	TYR	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
4	MAN	D	5	11/12	0.48	0.39	77,80,82,82	0
5	NAG	Ε	2	14/15	0.57	0.29	61,65,70,71	0
4	MAN	D	6	10/12	0.70	0.28	84,86,87,88	0
4	MAN	D	7	11/12	0.75	0.24	57,60,62,64	0

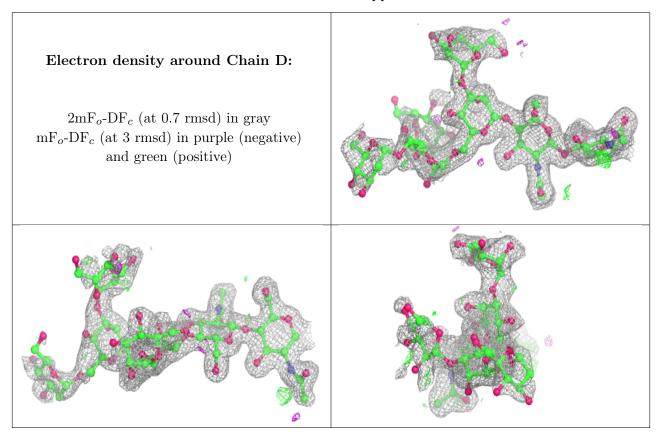
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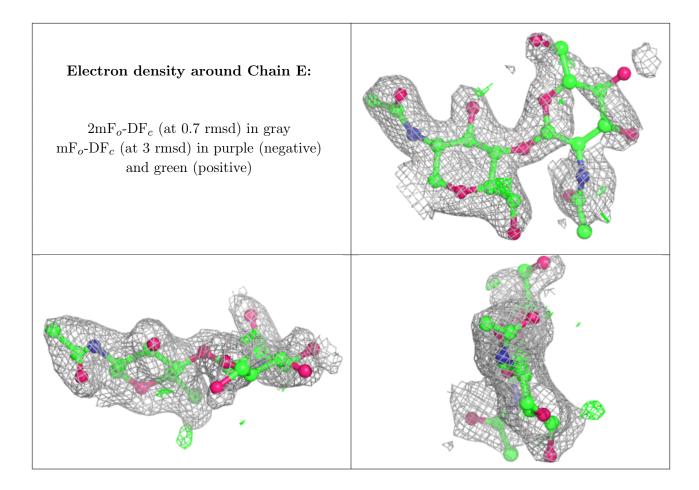
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	MAN	D	4	11/12	0.83	0.19	59,66,75,80	0
5	NAG	Е	1	14/15	0.90	0.13	30,37,47,54	0
4	BMA	D	3	11/12	0.92	0.11	31,38,50,51	0
4	NAG	D	2	14/15	0.96	0.08	19,21,28,32	0
4	NAG	D	1	14/15	0.96	0.09	16,19,25,25	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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
7	NAG	С	610	14/15	0.64	0.43	94,97,100,101	0
6	CL	В	301	1/1	0.99	0.07	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.

