

# Full wwPDB X-ray Structure Validation Report (i)

#### Nov 2, 2023 – 11:25 PM EDT

PDB ID : 3W9E

Title : Structure of Human Monoclonal Antibody E317 Fab Complex with HSV-2 gD

Authors: Lee, C.C.; Lin, L.L.; Wang, A.H.J.

Deposited on : 2013-04-03

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 : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

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

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

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

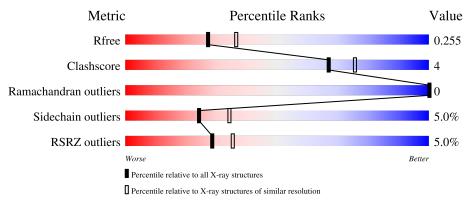
Validation Pipeline (wwPDB-VP) : 2.36

# 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
$R_{free}$	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	С	306	65%	8% •	25%					
2	A	222	87%		9%					
3	В	214	89%		7% ••					
4	D	4	50%	50%						



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5355 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 Envelope glycoprotein D.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	С	229	Total 1819	C 1170	N 310	O 329	S 10	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual Comment		Reference
С	276	HIS	-	expression tag	UNP Q69467
С	277	HIS	-	expression tag	UNP Q69467
С	278	HIS	-	expression tag	UNP Q69467
С	279	HIS	-	expression tag	UNP Q69467
С	280	HIS	-	expression tag	UNP Q69467
С	281	HIS	-	expression tag	UNP Q69467

• Molecule 2 is a protein called Antibody Fab heavy chain.

$\mathbf{Mol}$	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	215	Total 1614	C 1021	N 267	O 320	S 6	0	0	0

• Molecule 3 is a protein called Antibody Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	В	211	Total 1606	C 1000	N 275	O 327	S 4	0	0	0

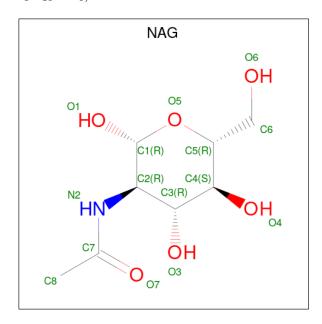
• Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	4	Total 50	C 28	N 2	O 20	0	0	0

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



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

• Molecule 6 is water.

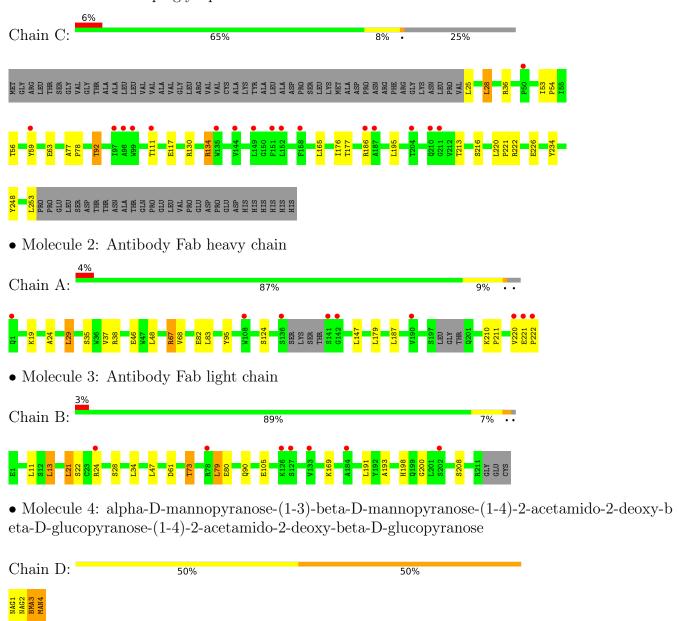
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	С	87	Total O 87 87	0	0
6	A	90	Total O 90 90	0	0
6	В	75	Total O 75 75	0	0



# 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: Envelope glycoprotein D





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	69.03Å 91.09Å 141.54Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.78 - 2.30	Depositor
rtesolution (A)	29.76 - 2.30	EDS
% Data completeness	98.5 (29.78-2.30)	Depositor
(in resolution range)	98.4 (29.76-2.30)	EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.66 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
D D.	0.203 , 0.255	Depositor
$R, R_{free}$	0.206 , $0.255$	DCC
$R_{free}$ test set	2007 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.1	Xtriage
Anisotropy	0.756	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.32, 48.0	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5355	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities 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, 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	lengths	Bond angles		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	С	0.47	0/1874	0.69	$1/2564 \ (0.0\%)$	
2	A	0.45	0/1651	0.65	$1/2250 \ (0.0\%)$	
3	В	0.43	0/1639	0.65	0/2225	
All	All	0.45	0/5164	0.67	$2/7039 \ (0.0\%)$	

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	С	134	ARG	NE-CZ-NH1	6.94	123.77	120.30
2	A	67	ARG	NE-CZ-NH2	-5.02	117.79	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	С	1819	0	1799	20	0
2	A	1614	0	1593	10	0
3	В	1606	0	1568	7	0
4	D	50	0	43	2	0
5	С	14	0	13	0	0
6	A	90	0	0	1	0



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	В	75	0	0	1	0
6	С	87	0	0	6	0
All	All	5355	0	5016	39	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 4.

All (39) 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)
6:C:487:HOH:O	4:D:4:MAN:O4	1.82	0.96
1:C:56:THR:HG23	1:C:177:THR:HG23	1.66	0.76
2:A:68:VAL:HG22	2:A:83:LEU:HD13	1.78	0.66
1:C:25:LEU:HD21	1:C:234:TYR:CD2	2.32	0.65
2:A:147:LEU:HD13	2:A:220:VAL:HG21	1.81	0.62
1:C:25:LEU:HD21	1:C:234:TYR:CE2	2.34	0.61
2:A:24:ALA:HB2	2:A:29:LEU:HD22	1.82	0.61
1:C:165:LEU:HD21	1:C:176:ILE:HG23	1.85	0.59
1:C:134:ARG:HD3	6:C:418:HOH:O	2.07	0.55
3:B:21:LEU:HD23	3:B:21:LEU:N	2.24	0.53
3:B:198:HIS:CD2	3:B:200:GLY:H	2.27	0.52
3:B:13:LEU:HD23	3:B:79:LEU:HD21	1.92	0.51
3:B:193:ALA:HB2	3:B:208:SER:HB3	1.93	0.50
1:C:28:LEU:HD23	1:C:226:GLU:CG	2.42	0.49
1:C:28:LEU:HD23	1:C:226:GLU:HG3	1.93	0.49
1:C:111:THR:HA	1:C:134:ARG:O	2.12	0.49
3:B:11:LEU:HD12	3:B:21:LEU:HD22	1.94	0.49
1:C:25:LEU:N	6:C:448:HOH:O	2.47	0.48
6:C:465:HOH:O	4:D:3:BMA:H61	2.14	0.47
1:C:63:GLU:HB2	1:C:248:TYR:CZ	2.51	0.46
1:C:213:THR:OG1	1:C:216:SER:HB3	2.16	0.46
1:C:92:THR:CG2	6:C:414:HOH:O	2.63	0.46
1:C:165:LEU:CD2	1:C:176:ILE:HG23	2.45	0.46
1:C:92:THR:HG23	6:C:414:HOH:O	2.16	0.46
2:A:187:LEU:C	2:A:187:LEU:HD12	2.36	0.46
2:A:221:GLU:HA	2:A:222:PRO:C	2.36	0.45
3:B:13:LEU:HD23	3:B:79:LEU:CD2	2.47	0.45
1:C:59:TYR:HB2	1:C:253:LEU:HD13	1.99	0.43
2:A:37:VAL:HG23	2:A:46:GLU:O	2.18	0.43
2:A:68:VAL:CG2	2:A:83:LEU:HD13	2.46	0.43
3:B:73:THR:HG23	6:B:322:HOH:O	2.19	0.43



Continued from previous page...

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	$\operatorname{distance}\left(\mathrm{\AA}\right)$	overlap (Å)
1:C:36:ARG:HA	1:C:130:ARG:O	2.18	0.43
1:C:53:ILE:HB	1:C:54:PRO:CD	2.50	0.42
2:A:19:LYS:HE2	6:A:312:HOH:O	2.20	0.42
1:C:92:THR:CG2	1:C:117:GLU:HA	2.49	0.42
1:C:221:PRO:O	1:C:222:ARG:HD2	2.21	0.41
1:C:77:ALA:HB3	1:C:78:PRO:HD3	2.01	0.41
2:A:210:LYS:N	2:A:211:PRO:CD	2.84	0.40
2:A:37:VAL:HG13	2:A:95:TYR:HB2	2.03	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	С	227/306 (74%)	219 (96%)	8 (4%)	0	100 100
2	A	209/222 (94%)	201 (96%)	8 (4%)	0	100 100
3	В	209/214 (98%)	204 (98%)	5 (2%)	0	100 100
All	All	645/742 (87%)	624 (97%)	21 (3%)	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	Rotameric Outliers	
1	$\mathbf{C}$	199/263~(76%)	194 (98%)	5 (2%)	47 65
2	A	183/189 (97%)	175 (96%)	8 (4%)	28 39
3	В	182/184 (99%)	167 (92%)	15 (8%)	11 14
All	All	564/636 (89%)	536 (95%)	28 (5%)	24 34

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	28	LEU
1	С	92	THR
1	С	186	ARG
1	C C C A A A A A A A A B	195	LEU
1	С	220	LEU
2	A	29	LEU
2 2 2 2 2 2 2 2 2	A	35	SER
2	A	38	ARG
2	A	48	LEU
2	A	67	ARG
2	A	82	GLU
2	A	124	SER
2	A	179	LEU
3		13	LEU
3	В	21	LEU
3	В	22	SER
3	В	24	ARG
3	В	28	SER
3	В	34	LEU
3	В	47	LEU
3	В	61	ASP
3	В	73	THR
3	В	79	LEU
3	В	80	GLU
3	В	90	GLN
3	В	105	GLU
3	В	169	LYS
3	В	191	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such side chains are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	С	27	GLN



Continued from previous page...

Mol	Chain	Res	Type
1	С	148	ASN
2	A	164	ASN
3	В	33	GLN
3	В	90	GLN
3	В	138	ASN
3	В	198	HIS

#### 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)

4 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		pe Chain		Link	Bond lengths			Bond angles					
MIOI	Type	Chain	nes	ries	nes	Res	res   Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	D	1	1,4	14,14,15	0.73	0	17,19,21	1.03	1 (5%)			
4	NAG	D	2	4	14,14,15	0.65	0	17,19,21	1.32	2 (11%)			
4	BMA	D	3	4	11,11,12	0.55	0	15,15,17	1.58	2 (13%)			
4	MAN	D	4	4	11,11,12	0.67	0	15,15,17	1.30	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
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
4	D	3	BMA	O3-C3-C4	4.09	119.80	110.35
4	D	3	BMA	C1-C2-C3	-3.48	105.39	109.67
4	D	4	MAN	C1-C2-C3	3.34	113.78	109.67
4	D	2	NAG	C8-C7-N2	2.97	121.13	116.10
4	D	4	MAN	O5-C5-C6	2.47	111.07	107.20
4	D	2	NAG	C3-C4-C5	2.30	114.34	110.24
4	D	1	NAG	C3-C4-C5	2.01	113.83	110.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	3	BMA	C4-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6

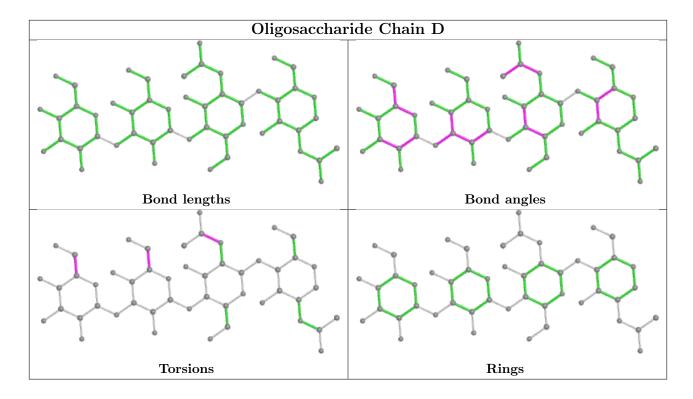
There are no ring outliers.

2 monomers are involved in 2 short contacts:

$\mathbf{Mol}$	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3	BMA	1	0
4	D	4	MAN	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)

#### 1 ligand is 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	Bond lengths			Bond angles		
				nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
	5	NAG	С	305	1	14,14,15	0.53	0	17,19,21	1.07	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
5	NAG	С	305	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	С	305	NAG	C1-O5-C5	3.28	116.64	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	С	305	NAG	C3-C2-N2-C7

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 $>$	$\#\mathrm{RSRZ}{>}2$		$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9	
1	С	$229/306 \ (74\%)$	0.22	17 (7%)	14	19	30, 48, 76, 125	0
2	A	215/222 (96%)	0.05	9 (4%)	36	43	30, 49, 89, 127	0
3	В	211/214 (98%)	0.12	7 (3%)	46	53	36, 54, 77, 94	0
All	All	655/742 (88%)	0.13	33 (5%)	28	35	30, 50, 78, 127	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	142	GLY	6.8
1	С	186	ARG	5.7
2	A	141	SER	4.5
2	A	222	PRO	4.4
3	В	126	LYS	4.0
1	С	59	TYR	4.0
2	A	220	VAL	3.8
2	A	1	GLN	3.6
1	С	111	THR	3.3
1	С	50	PRO	3.3
1	С	187	ALA	3.2
1	С	135	TRP	2.9
3	В	202	SER	2.8
1	С	144	VAL	2.8
1	С	149	LEU	2.7
2	A	221	GLU	2.6
1	С	210	GLN	2.6
1	С	98	ALA	2.6
3	В	133	VAL	2.6
2	A	190	VAL	2.5
1	С	97	ILE	2.5
3	В	78	ARG	2.4
2	A	136	SER	2.4



Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	С	151	PHE	2.4
3	В	127	SER	2.3
1	С	158	PHE	2.3
1	С	152	LEU	2.2
1	С	99	TRP	2.1
1	С	211	GLY	2.1
3	В	24	ARG	2.1
2	A	108	TRP	2.1
1	С	204	THR	2.0
3	В	184	ALA	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.

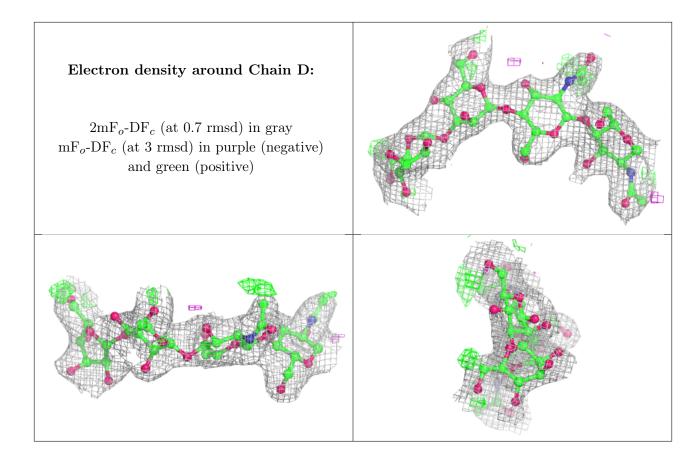
#### 6.3 Carbohydrates (i)

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	$\operatorname{Res}$	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{ ilde{A}}^2)$	Q<0.9
4	BMA	D	3	11/12	0.79	0.31	88,97,101,104	0
4	MAN	D	4	11/12	0.79	0.30	89,99,104,107	0
4	NAG	D	2	14/15	0.90	0.24	72,76,85,95	0
4	NAG	D	1	14/15	0.93	0.14	52,57,60,65	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	С	305	14/15	0.84	0.30	84,93,102,103	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

