

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

#### Mar 23, 2024 – 01:38 PM EDT

PDB ID : 3N42

Title: Crystal structures of the mature envelope glycoprotein complex (furin cleav-

age) of Chikungunya virus.

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Deposited on : 2010-05-21

Resolution : 3.00 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 : 2.36.1

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)

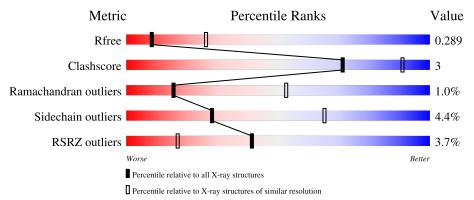
Validation Pipeline (wwPDB-VP) : 2.36.1

## 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 3.00 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	65	17% 63% 1	.4%	20%
2	В	360	5%		7% • 6%
3	F	473	74%	9%	16%
4	С	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
5	NAG	В	1001	-	-	-	X



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6205 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 E3 envelope glycoprotein.

Mol	Chain	Residues		Ato	$\mathbf{m}\mathbf{s}$			ZeroOcc	AltConf	Trace
1	A	52	Total 406	C 253	N 64	O 80	S 9	0	0	0

• Molecule 2 is a protein called E2 envelope glycoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	338	Total 2669	C 1666	N 483	O 500	S 20	0	0	0

• Molecule 3 is a protein called E1 envelope glycoprotein.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
3	F	395	Total 3000	C 1896	N 503	O 577	S 24	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

	Chain	Residue	Modelled	Actual	Comment	Reference
	F	-1	GLY	-	SEE REMARK 999	UNP Q1H8W5
Ī	F	0	GLY	-	SEE REMARK 999	UNP Q1H8W5

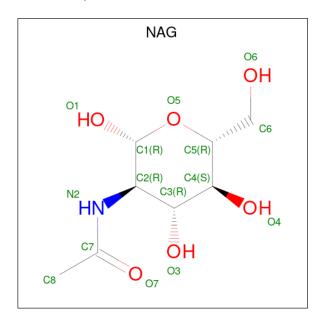
• Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	A	<b>A</b> ton	ns		ZeroOcc	AltConf	Trace
4	С	2	Total 28	C 16	N 2	O 10	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	В	1	Total 14	C 8	N 1	O 5	0	0

• Molecule 6 is water.

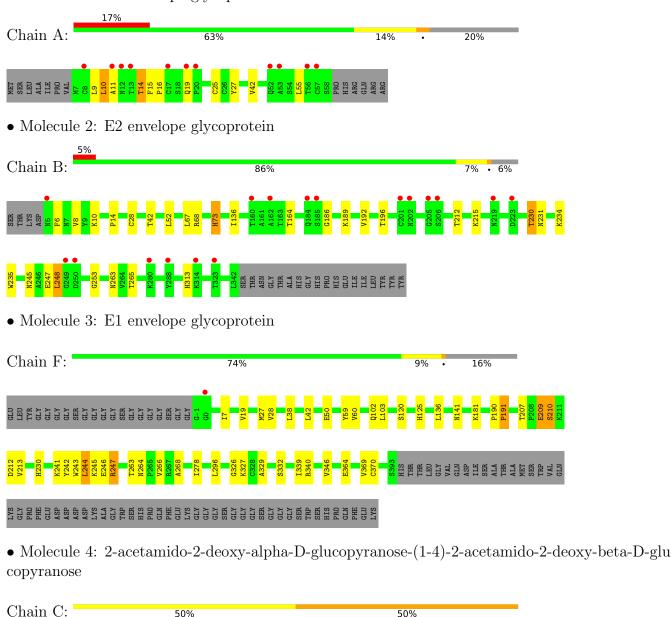
$\mathbf{Mol}$	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
6	В	26	Total O 26 26	0	0
6	F	62	Total O 62 62	0	0



## 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	58.39Å 90.68Å 178.41Å	Donositon
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.60 - 3.00	Depositor
Resolution (A)	44.60 - 3.00	EDS
% Data completeness	96.2 (44.60-3.00)	Depositor
(in resolution range)	96.1 (44.60-3.00)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$< I/\sigma(I) > 1$	1.96 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
D D.	0.247 , 0.278	Depositor
$R, R_{free}$	0.258 , $0.289$	DCC
$R_{free}$ test set	980 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.9	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.31 , 49.7	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	6205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.17% 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: NDG, 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	Bond	lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.40	0/415	0.60	0/565	
2	В	0.42	0/2741	0.61	0/3731	
3	F	0.58	0/3077	0.61	0/4197	
All	All	0.50	0/6233	0.61	0/8493	

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	406	0	386	5	0
2	В	2669	0	2588	10	0
3	F	3000	0	2903	30	0
4	С	28	0	24	1	0
5	В	14	0	13	0	0
6	В	26	0	0	0	0
6	F	62	0	0	0	0
All	All	6205	0	5914	42	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 3.



All (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:F:245:LYS:HE2	3:F:246:GLU:OE2	1.79	0.82
3:F:243:TRP:O	3:F:247:ARG:HG2	1.84	0.77
1:A:27:TYR:OH	2:B:234:LYS:NZ	2.26	0.65
3:F:42:LEU:HD11	3:F:266:VAL:HG22	1.80	0.64
2:B:14:PRO:HG3	2:B:68:ARG:HG2	1.78	0.63
3:F:190:PRO:C	3:F:191:PRO:O	2.35	0.61
2:B:245:ASN:HB3	2:B:248:LEU:HD22	1.83	0.60
2:B:10:LYS:O	2:B:234:LYS:NZ	2.34	0.59
3:F:212:ASP:C	3:F:213:VAL:CG1	2.72	0.58
3:F:263:THR:HG22	3:F:264:ASN:N	2.19	0.57
3:F:245:LYS:CE	3:F:246:GLU:OE2	2.53	0.57
3:F:326:GLY:O	3:F:346:VAL:HG22	2.06	0.56
3:F:212:ASP:C	3:F:213:VAL:HG13	2.25	0.56
3:F:209:GLU:C	3:F:210:SER:O	2.39	0.56
3:F:207:THR:OG1	3:F:210:SER:HB2	2.07	0.55
3:F:242:TYR:CE1	3:F:246:GLU:HG3	2.42	0.54
3:F:190:PRO:O	3:F:191:PRO:O	2.27	0.52
2:B:196:THR:O	2:B:230:THR:HG23	2.09	0.52
3:F:207:THR:OG1	3:F:210:SER:N	2.45	0.50
3:F:60:VAL:HG22	3:F:102:GLN:HG3	1.94	0.50
2:B:230:THR:O	2:B:230:THR:OG1	2.30	0.49
3:F:209:GLU:O	3:F:210:SER:O	2.30	0.49
3:F:38:LEU:HB2	3:F:268:ALA:HB3	1.94	0.49
3:F:263:THR:CG2	3:F:264:ASN:H	2.26	0.48
2:B:52:LEU:HD22	2:B:67:LEU:HD21	1.96	0.48
3:F:207:THR:OG1	3:F:210:SER:CB	2.63	0.47
3:F:263:THR:CG2	3:F:264:ASN:N	2.77	0.47
1:A:16:PRO:HG2	1:A:19:GLN:HB2	1.96	0.46
3:F:263:THR:HG22	3:F:264:ASN:H	1.80	0.46
2:B:42:THR:HB	2:B:136:ILE:HD11	1.98	0.45
3:F:19:VAL:HB	3:F:27:MET:HB3	1.97	0.45
3:F:50:GLU:OE1	3:F:241:LYS:HE2	2.17	0.45
3:F:243:TRP:CE3	3:F:244:LEU:HD12	2.51	0.45
1:A:42:VAL:HG11	2:B:253:GLY:HA2	1.99	0.45
3:F:28:VAL:HG23	3:F:329:ALA:HB1	1.98	0.45
3:F:59:TYR:HB3	3:F:103:LEU:HB3	2.01	0.41
3:F:141:ASN:HD22	4:C:1:NAG:H83	1.84	0.41
1:A:55:LEU:HD13	2:B:8:VAL:HA	2.03	0.41
3:F:296:LEU:HD12	3:F:369:VAL:O	2.21	0.41
3:F:332:SER:HB2	3:F:339:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
1:A:10:LEU:HB2	1:A:15:PHE:CE1	2.56	0.41
3:F:7:ILE:HG12	3:F:278:ILE:HD12	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	Perc	entiles
1	A	50/65 (77%)	46 (92%)	2 (4%)	2 (4%)	3	17
2	В	336/360 (93%)	310 (92%)	22 (6%)	4 (1%)	13	48
3	F	393/473 (83%)	378 (96%)	13 (3%)	2 (0%)	29	68
All	All	779/898 (87%)	734 (94%)	37 (5%)	8 (1%)	15	53

#### All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	6	PHE
1	A	11	ALA
3	F	210	SER
2	В	73	HIS
2	В	164	THR
2	В	186	GLY
1	A	14	THR
3	F	191	PRO

#### 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	49/61 (80%)	45 (92%)	4 (8%)	11	39	
2	В	300/319 (94%)	286 (95%)	14 (5%)	26	63	
3	F	329/378 (87%)	317 (96%)	12 (4%)	35	70	
All	All	678/758 (89%)	648 (96%)	30 (4%)	28	65	

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	10	LEU
1	A	14	THR
1	A	25	CYS
2	В	28	CYS
2	В	73	HIS
2	В	189	LYS
2	В	192	VAL
2	В	212	THR
2	В	215	LYS
2	В	230	THR
2	В	231	ASN
2	В	235	TRP GLU
2 2	В	247	GLU
2	В	248	LEU
2	В	263	ASN
2 2	В	265	THR
	В	313	HIS
3	F	120	SER
3	F	125	HIS
3	F	136	LEU
3	F	181	LYS
3	F	209	GLU
3	F	230	HIS
3	F	244	LEU
3	F	247	ARG
3	$\mathbf{F}$	327	LYS
3	F	340	ARG
3	F	364	GLU
3	F	370	CYS



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	В	184	GLN
2	В	193	ASN
2	В	236	GLN
2	В	282	GLN
3	F	373	GLN

#### 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).

Mal	Mol Type Chain		n Res	Dag	Res Link	Bo	Bond lengths			Bond angles		
MOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2		
4	NAG	С	1	4,3	14,14,15	1.16	1 (7%)	17,19,21	1.09	2 (11%)		
4	NDG	С	2	4	14,14,15	1.46	1 (7%)	17,19,21	1.26	2 (11%)		

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	С	1	4,3	-	2/6/23/26	0/1/1/1
4	NDG	С	2	4	-	0/6/23/26	0/1/1/1



#### All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
4	С	2	NDG	C1-C2	3.86	1.58	1.52
4	С	1	NAG	C1-C2	2.64	1.56	1.52

#### All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	С	2	NDG	C1-C2-N2	3.29	116.10	110.49
4	С	1	NAG	C1-O5-C5	2.63	115.76	112.19
4	С	1	NAG	C2-N2-C7	2.48	126.43	122.90
4	С	2	NDG	C4-C3-C2	2.22	114.27	111.02

There are no chirality outliers.

#### All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	С	1	NAG	C8-C7-N2-C2
4	С	1	NAG	O7-C7-N2-C2

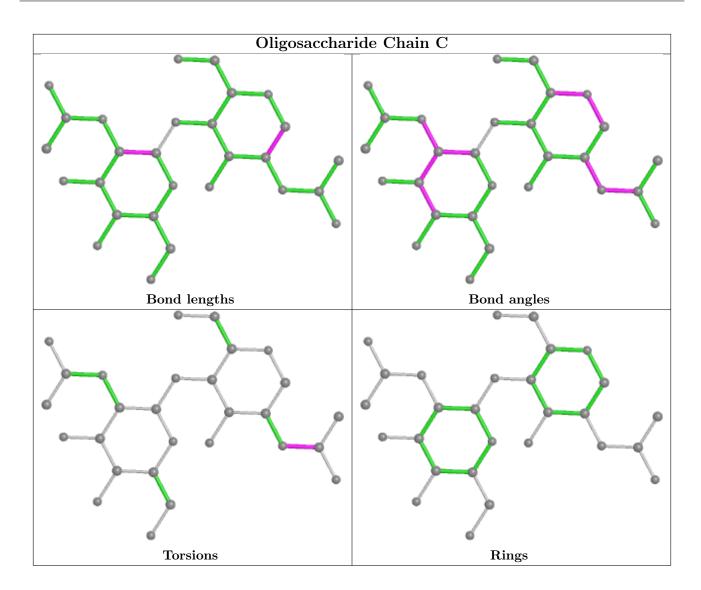
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	С	1	NAG	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	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	В	1001	2	14,14,15	1.45	1 (7%)	17,19,21	1.47	2 (11%)

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
5	NAG	В	1001	2	-	0/6/23/26	0/1/1/1

#### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
5	В	1001	NAG	C1-C2	4.03	1.58	1.52

#### All (2) bond angle outliers are listed below:

$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^o)$
5	В	1001	NAG	C1-O5-C5	3.73	117.25	112.19
5	В	1001	NAG	O5-C1-C2	2.31	114.93	111.29

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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	52/65 (80%)	1.16	11 (21%) 0 0	84, 101, 119, 126	0
2	В	338/360 (93%)	0.31	17 (5%) 28 10	33, 62, 83, 97	0
3	F	395/473 (83%)	-0.10	1 (0%) 94 84	26, 46, 80, 106	0
All	All	785/898 (87%)	0.16	29 (3%) 41 17	26, 55, 95, 126	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	THR	5.1
1	A	12	ASN	4.7
2	В	250	ASP	4.0
1	A	8	CYS	3.8
2	В	184	GLN	3.3
2	В	162	ALA	3.2
2	В	202	ASN	3.1
1	A	57	CYS	3.1
2	В	249	GLY	3.1
2	В	219	ASN	2.9
2	В	185	SER	2.9
2	В	288	TYR	2.8
1	A	56	THR	2.8
2	В	223	ASP	2.8
1	A	11	ALA	2.7
1	A	52	GLN	2.7
1	A	53	ALA	2.7
3	F	0	GLY	2.6
2	В	323	THR	2.5
2	В	206	SER	2.4
2	В	201	CYS	2.3
1	A	19	GLN	2.3
1	A	17	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	В	205	GLY	2.1
1	A	20	PRO	2.1
2	В	160	THR	2.1
2	В	314	LYS	2.1
2	В	5	ASN	2.0
2	В	280	LYS	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.

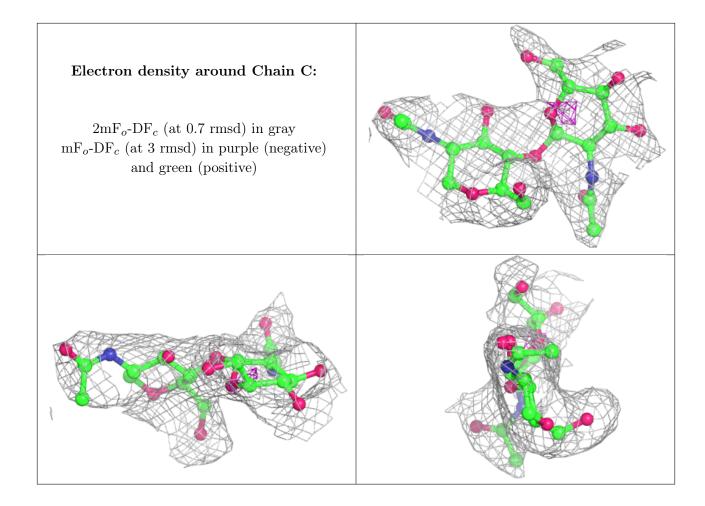
### 6.3 Carbohydrates (i)

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
4	NDG	С	2	14/15	0.78	0.28	57,61,64,64	0
4	NAG	С	1	14/15	0.89	0.22	51,54,57,57	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	В	1001	14/15	0.68	0.47	71,75,77,77	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

