

Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 08:29 AM EDT

PDB ID : 3N40

Title : Crystal structure of the immature envelope glycoprotein complex of Chikun-

gunya virus.

Authors: Voss, J.; Vaney, M.C.; Duquerroy, S.; Rey, F.A.

Deposited on : 2010-05-21

Resolution : 2.17 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

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)

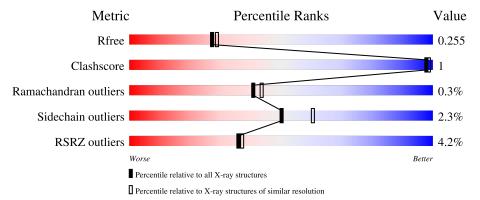
Validation Pipeline (wwPDB-VP) : 2.35

1 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 2.17 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	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	Р	401	7% 95%
2	F	393	96%
3	A	2	100%
4	В	2	100%



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6669 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 P62 envelope glycoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Р	401	Total 3168	C 1973	N 568	O 598	S 29	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Р	64	GLU	ARG	engineered mutation	UNP Q1H8W5

• Molecule 2 is a protein called E1 envelope glycoprotein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	F	393	Total 2995	C 1893	N 502	O 576	S 24	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	${f Comment}$	Reference
F	-1	GLY	-	SEE REMARK 999	UNP Q1H8W5
F	0	GLY	-	SEE REMARK 999	UNP Q1H8W5

• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
3	A	2	Total 28	C N 16 2	O 10	0	0	0

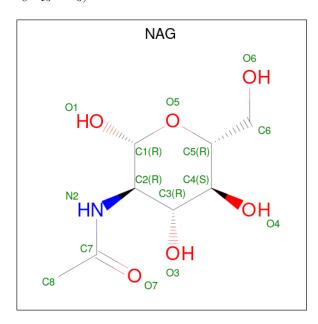


• Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
4	В	2	Total 28	C 16	_	O 10	0	0	0

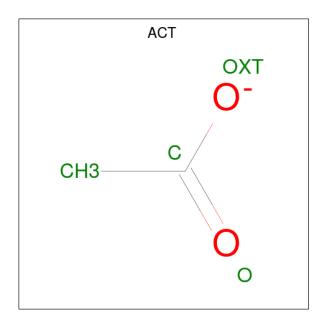
 \bullet Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\rm C_8H_{15}NO_6).$



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

• Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Р	1	Total C O 4 2 2	0	0
6	Р	1	Total C O 4 2 2	0	0
6	Р	1	Total C O 4 2 2	0	0
6	Р	1	Total C O 4 2 2	0	0
6	F	1	Total C O 4 2 2	0	0

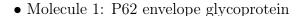
• Molecule 7 is water.

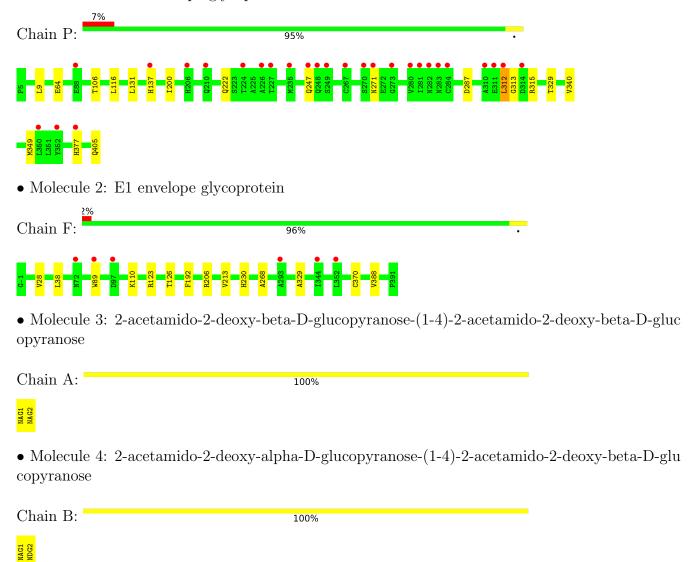
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	Р	193	Total O 193 193	0	0
7	F	223	Total O 223 223	0	0



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	58.74Å 90.01Å 179.03Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.10 - 2.17	Depositor
Resolution (A)	49.11 - 2.17	EDS
% Data completeness	99.4 (49.10-2.17)	Depositor
(in resolution range)	99.3 (49.11-2.17)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) > 1$	1.87 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
D D.	0.208 , 0.239	Depositor
R, R_{free}	0.222 , 0.255	DCC
R_{free} test set	2582 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 41.5	EDS
L-test for twinning ²	$ < L > = 0.46, < L^2> = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6669	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.03% 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: NDG, NAG, ACT

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		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	Р	0.35	0/3253	0.58	0/4428	
2	F	0.33	0/3072	0.57	0/4190	
All	All	0.34	0/6325	0.58	0/8618	

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	Р	3168	0	3063	4	0
2	F	2995	0	2897	5	0
3	A	28	0	25	0	0
4	В	28	0	24	0	0
5	Р	14	0	13	0	0
6	F	4	0	3	0	0
6	Р	16	0	12	0	0
7	F	223	0	0	0	0
7	Р	193	0	0	0	0
All	All	6669	0	6037	9	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 (9) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance} ({ m \AA})$	overlap (Å)
2:F:206:ARG:HG3	2:F:206:ARG:HH11	1.69	0.56
1:P:116:LEU:HD22	1:P:131:LEU:HD21	1.87	0.55
1:P:340:VAL:HG22	1:P:349:MET:HG2	1.93	0.51
2:F:38:LEU:HB2	2:F:268:ALA:HB3	1.93	0.50
2:F:110:LYS:HG3	2:F:213:VAL:HG11	1.93	0.49
2:F:28:VAL:HG23	2:F:329:ALA:HB1	1.96	0.46
1:P:312:LEU:HD13	1:P:315:ARG:HB2	1.99	0.44
2:F:192:PHE:CE1	2:F:206:ARG:HG2	2.52	0.44
1:P:106:THR:HB	1:P:200:ILE:HD11	2.04	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	\mathbf{ntiles}
1	Р	399/401 (100%)	379 (95%)	19 (5%)	1 (0%)	41	43
2	F	$392/393\ (100\%)$	383 (98%)	8 (2%)	1 (0%)	41	43
All	All	791/794 (100%)	762 (96%)	27 (3%)	2 (0%)	41	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	126	THR
1	Р	313	GLY



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	Р	360/360 (100%)	349 (97%)	11 (3%)	40 4	18	
2	F	329/328 (100%)	324 (98%)	5 (2%)	65 7	6	
All	All	689/688 (100%)	673 (98%)	16 (2%)	50 6	0	

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Р	9	LEU
1	Р	64	GLU
1	Р	137	HIS
1	Р	222	GLN
1	Р	247	GLN
1	Р	271	ASN
1	Р	287	ASP
1	Р	312	LEU
1	Р	329	THR
1	Р	377	HIS
1	Р	405	GLN
2	F	89	TRP
2	F	123	ARG
2	F	230	HIS
2	F	370	CYS
2	F	388	VAL

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)

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	Tuno	Chain	Res	Link	Вс	ond leng	ths	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	1	1,3	14,14,15	1.19	1 (7%)	17,19,21	1.37	3 (17%)
3	NAG	A	2	3	14,14,15	1.24	1 (7%)	17,19,21	0.85	0
4	NAG	В	1	2,4	14,14,15	1.03	1 (7%)	17,19,21	0.88	0
4	NDG	В	2	4	14,14,15	1.50	1 (7%)	17,19,21	1.22	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	\mathbf{Type}	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	A	2	3	-	0/6/23/26	0/1/1/1
4	NAG	В	1	2,4	-	0/6/23/26	0/1/1/1
4	NDG	В	2	4	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
4	В	2	NDG	C1-C2	3.99	1.58	1.52
3	A	2	NAG	C1-C2	3.11	1.57	1.52
3	A	1	NAG	C1-C2	2.68	1.56	1.52
4	В	1	NAG	C1-C2	2.57	1.56	1.52

All (4) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	В	2	NDG	C1-C2-N2	3.55	116.55	110.49
3	A	1	NAG	C4-C3-C2	3.18	115.67	111.02
3	A	1	NAG	O5-C5-C6	2.22	110.68	107.20
3	A	1	NAG	O4-C4-C3	-2.11	105.48	110.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

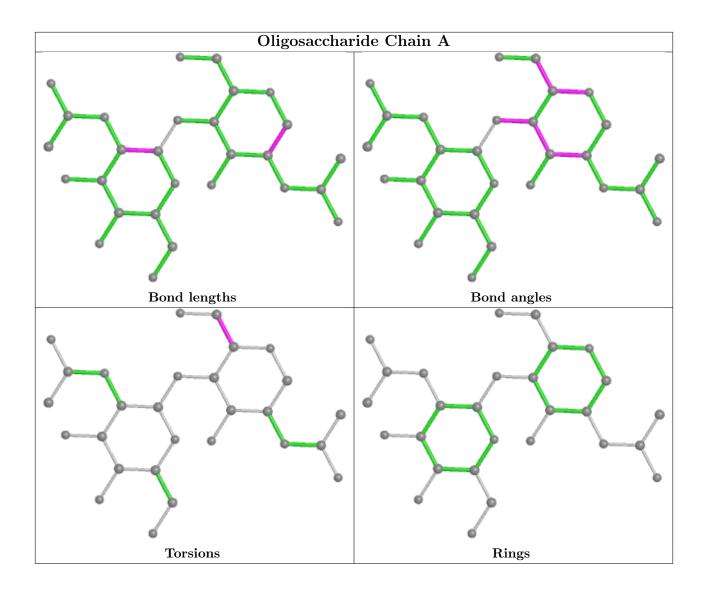
Mol	Chain	Res	Type	Atoms
3	A	1	NAG	C4-C5-C6-O6
4	В	2	NDG	O5-C5-C6-O6

There are no ring outliers.

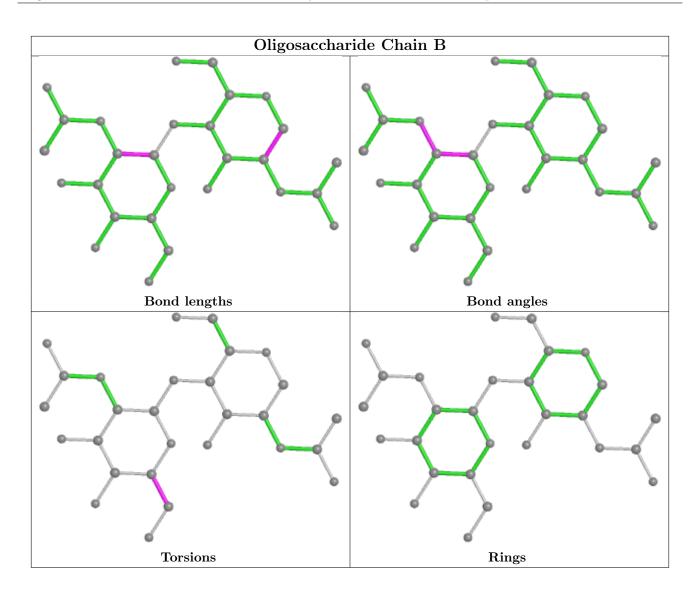
No monomer is involved in short contacts.

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)

6 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	s Link	Bond lengths			Bond angles		
			nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	Р	2001	1	14,14,15	1.29	1 (7%)	17,19,21	1.03	2 (11%)
6	ACT	Р	2	-	3,3,3	1.07	0	3,3,3	0.78	0
6	ACT	P	3	-	3,3,3	1.05	0	3,3,3	0.79	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
MIOI	Moi Type			LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACT	P	1	-	3,3,3	1.08	0	3,3,3	0.77	0
6	ACT	P	406	-	3,3,3	1.05	0	3,3,3	0.89	0
6	ACT	F	392	-	3,3,3	1.12	0	3,3,3	0.74	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
5	NAG	Р	2001	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
5	Р	2001	NAG	C1-C2	3.16	1.57	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
5	P	2001	NAG	C1-C2-N2	2.16	114.19	110.49
5	Р	2001	NAG	C1-O5-C5	2.14	115.09	112.19

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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	Р	401/401 (100%)	0.58	27 (6%) 17 18	23, 38, 66, 80	0
2	F	393/393 (100%)	0.38	6 (1%) 73 74	22, 35, 58, 71	0
All	All	794/794 (100%)	0.48	33 (4%) 36 37	22, 36, 62, 80	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Р	283	ASN	7.0
1	Р	249	SER	4.9
1	Р	281	ILE	4.5
1	Р	280	VAL	4.3
1	Р	226	ALA	4.2
1	Р	227	THR	4.1
1	Р	282	ASN	3.9
1	Р	312	LEU	3.7
1	Р	310	ALA	3.1
1	Р	311	GLU	3.1
2	F	293	ALA	3.1
1	Р	377	HIS	3.0
1	Р	352	TYR	2.9
2	F	89	TRP	2.9
1	Р	206	HIS	2.9
1	Р	247	GLN	2.8
1	Р	88	GLU	2.8
1	Р	271	ASN	2.7
2	F	352	LEU	2.6
1	Р	314	ASP	2.6
1	Р	270	SER	2.3
2	F	344	ILE	2.3
1	Р	350	LEU	2.3
1	Р	235	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	Р	273	GLY	2.2
1	Р	284	CYS	2.2
1	Р	267	CYS	2.2
1	Р	224	THR	2.2
2	F	97	ASP	2.1
1	Р	210	GLN	2.1
1	Р	248	GLN	2.1
1	Р	137	HIS	2.0
2	F	72	ASN	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.

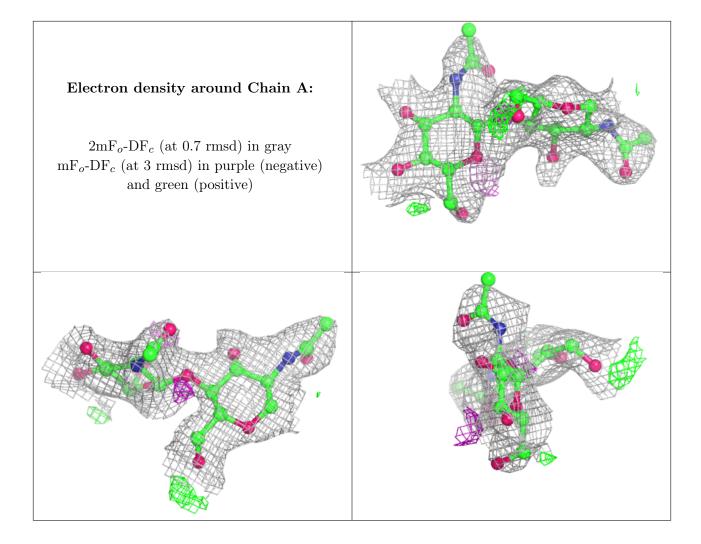
6.3 Carbohydrates (i)

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.

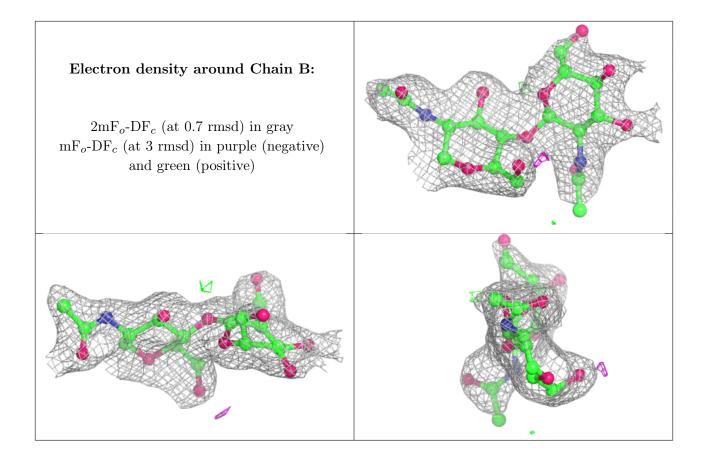
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	NAG	A	1	14/15	0.72	0.21	62,66,68,68	0
3	NAG	A	2	14/15	0.79	0.23	68,72,75,75	0
4	NDG	В	2	14/15	0.88	0.29	51,55,57,57	0
4	NAG	В	1	14/15	0.95	0.14	43,47,49,50	0

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	B -factors (\mathring{A}^2)	Q<0.9
6	ACT	Р	2	4/4	0.62	0.29	65,65,65,65	0
5	NAG	P	2001	14/15	0.71	0.38	62,65,68,68	0
6	ACT	Р	406	4/4	0.83	0.19	62,62,62,62	0
6	ACT	F	392	4/4	0.91	0.16	44,44,44,45	0
6	ACT	Р	1	4/4	0.93	0.16	54,54,54,54	0
6	ACT	Р	3	4/4	0.94	0.16	54,54,54,55	0

6.5 Other polymers (i)

There are no such residues in this entry.

