

wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 02:14 PM EST

PDB ID	:	5W5U
Title	:	Crystal structure of the A/Puerto Rico/8/1934 (H1N1) influenza virus hemag-
		glutinin in complex with cyclic peptide CP141037 (P4)
Authors	:	Wilson, I.A.; Kadam, R.U.
Deposited on	:	2017-06-15
Resolution	:	2.46 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

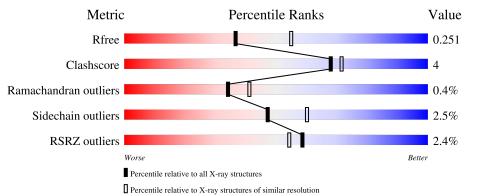
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.46 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	А	326	3%	88%		10% ••		
2	В	176	2%	91%		5% • •		
3	D	12	17%	42%	42%			
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	А	401	-	-	-	Х
5	NAG	А	403	-	-	-	Х



5W5U

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4172 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 Hemagglutinin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	300	Total	С	Ν	0	\mathbf{S}	0	0	0
	Л	322	2542	1603	443	483	13	0	0	0

• Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	171	Total 1380	C 866	N 235	0 272	S 7	0	0	0

• Molecule 3 is a protein called ACE-PH8-ORN-MLE-GLU-TYR-PHE-GLU-TRP-LEU-SER-BAL.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
3	D	12	Total 107		N 13	0 18	0	0	0

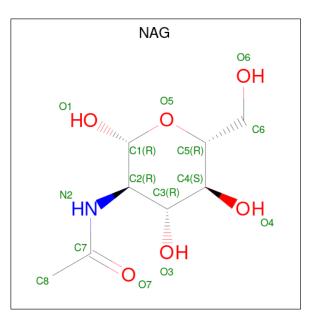
• Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



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

• 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	А	1	Total C N O 14 8 1 5	0	0
5	А	1	Total C N O 14 8 1 5	0	0
5	А	1	Total C N O 14 8 1 5	0	0
5	А	1	Total C N O 14 8 1 5	0	0

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

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

• Molecule 7 is water.

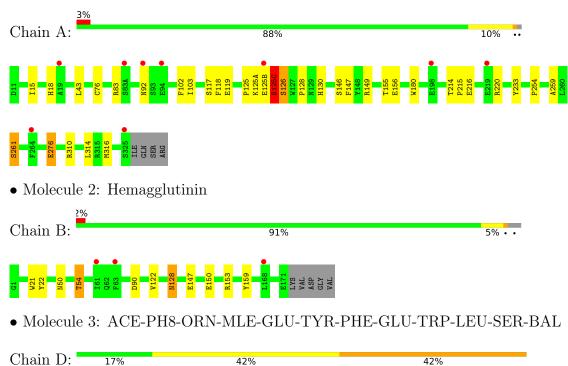
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	30	Total O 30 30	0	0
7	В	26	TotalO2626	0	0
7	D	1	Total O 1 1	0	0



opyranose

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: Hemagglutinin

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

Chain C: 50% 50%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants	161.36Å 161.36Å 161.36Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	
Resolution (Å)	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor EDS
% Data completeness	98.4 (31.65-2.46)	Depositor
(in resolution range)	98.4 (31.65-2.46)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	0.08	Depositor
$< I/\sigma(I) > 1$	2.34 (at 2.45 Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
P. P.	0.210 , 0.251	Depositor
R, R_{free}	0.215 , 0.251	DCC
R_{free} test set	1273 reflections (5.08%)	wwPDB-VP
Wilson B-factor $(Å^2)$	57.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 37.3	EDS
L-test for twinning ²	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4172	wwPDB-VP
Average B, all atoms $(Å^2)$	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: ORN, CL, BAL, NAG, MLE, ACE, PH8

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	Bo	Bond lengths		nd angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.28	0/2606	0.41	0/3544
2	В	0.29	0/1407	0.38	0/1891
3	D	3.16	12/72~(16.7%)	1.79	2/97~(2.1%)
All	All	0.50	12/4085~(0.3%)	0.46	2/5532~(0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mo	l Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	6	TYR	CB-CG	-9.04	1.38	1.51
3	D	9	TRP	CD2-CE2	-8.48	1.31	1.41
3	D	9	TRP	CG-CD2	-7.44	1.31	1.43
3	D	7	PHE	CB-CG	-7.41	1.38	1.51
3	D	10	LEU	CA-C	-7.13	1.34	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
3	D	6	TYR	CB-CG-CD2	-6.17	117.30	121.00
3	D	6	TYR	CB-CG-CD1	6.09	124.66	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
3	D	11	SER	Peptide

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	А	2542	0	2470	18	0
2	В	1380	0	1309	10	0
3	D	107	0	95	6	0
4	С	28	0	25	1	0
5	А	56	0	52	0	0
6	А	1	0	0	0	0
6	В	1	0	0	0	0
7	А	30	0	0	0	0
7	В	26	0	0	1	0
7	D	1	0	0	0	0
All	All	4172	0	3951	31	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.

The worst 5 of 31 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:ASN:O	2:B:54:THR:HG22	1.50	1.10
2:B:50:ASN:O	2:B:54:THR:CG2	2.08	1.01
3:D:2:PH8:CD1	3:D:2:PH8:HBA	2.05	0.85
1:A:125:PRO:O	1:A:126:SER:HB2	1.87	0.73
3:D:2:PH8:HBA	3:D:2:PH8:HD1	1.75	0.68

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	ntiles
1	А	320/326~(98%)	299~(93%)	19~(6%)	2(1%)	25	29
2	В	169/176~(96%)	165~(98%)	4 (2%)	0	100	100
3	D	7/12~(58%)	7 (100%)	0	0	100	100
All	All	496/514~(96%)	471 (95%)	23~(5%)	2(0%)	34	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	125(C)	SER
1	А	125(A)	LYS

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	А	285/289~(99%)	277~(97%)	8~(3%)	43 56
2	В	147/151~(97%)	144 (98%)	3~(2%)	55 67
3	D	7/7~(100%)	7 (100%)	0	100 100
All	All	439/447~(98%)	428 (98%)	11 (2%)	47 60

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type		
1	А	276	GLU		
Continued on nort nage					

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
2	В	22	TYR
2	В	128	ASN
2	В	54	THR
1	А	155	THR

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains 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)

4 non-standard protein/DNA/RNA residues 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	Bo	ond leng	\mathbf{ths}	Bond angles		
	Moi Type Chain I	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
3	MLE	D	4	3	$7,\!8,\!9$	0.33	0	6,9,11	1.14	0
3	PH8	D	2	3	12,13,14	1.59	2 (16%)	10,15,17	0.70	0
3	ORN	D	3	3	6,7,8	1.37	1 (16%)	2,7,9	0.75	0
3	BAL	D	12	3	4,4,5	0.49	0	3,3,5	1.28	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
3	MLE	D	4	3	-	1/5/8/10	-
3	PH8	D	2	3	-	2/7/8/10	0/1/1/1
3	ORN	D	3	3	-	2/5/6/8	-
3	BAL	D	12	3	-	1/1/2/3	-



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	D	2	PH8	CJ-CG	-4.85	1.37	1.51
3	D	3	ORN	CB-CA	-3.08	1.49	1.53
3	D	2	PH8	CB-CA	-2.07	1.50	1.53

All (3) bond length outliers are listed below:

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2	PH8	O-C-CA-CB
3	D	3	ORN	O-C-CA-CB
3	D	4	MLE	O-C-CA-CB
3	D	12	BAL	C-CA-CB-N
3	D	3	ORN	CA-CB-CG-CD

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	4	MLE	1	0
3	D	2	PH8	3	0
3	D	3	ORN	1	0

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		
IVIOI					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	NAG	С	1	2,4	14,14,15	0.63	0	17,19,21	1.61	3 (17%)
4	NAG	С	2	4	14,14,15	0.60	0	17,19,21	1.86	4 (23%)



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	2,4	-	1/6/23/26	0/1/1/1
4	NAG	С	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
4	С	1	NAG	C6-C5-C4	-4.76	101.86	113.00
4	С	2	NAG	C2-N2-C7	-4.67	116.25	122.90
4	С	2	NAG	O5-C5-C6	3.50	112.69	107.20
4	С	2	NAG	C4-C3-C2	-3.04	106.56	111.02
4	С	2	NAG	C3-C4-C5	-2.55	105.69	110.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	С	2	NAG	O5-C5-C6-O6
4	С	2	NAG	C8-C7-N2-C2
4	С	2	NAG	O7-C7-N2-C2
4	С	2	NAG	C4-C5-C6-O6
4	С	1	NAG	C1-C2-N2-C7

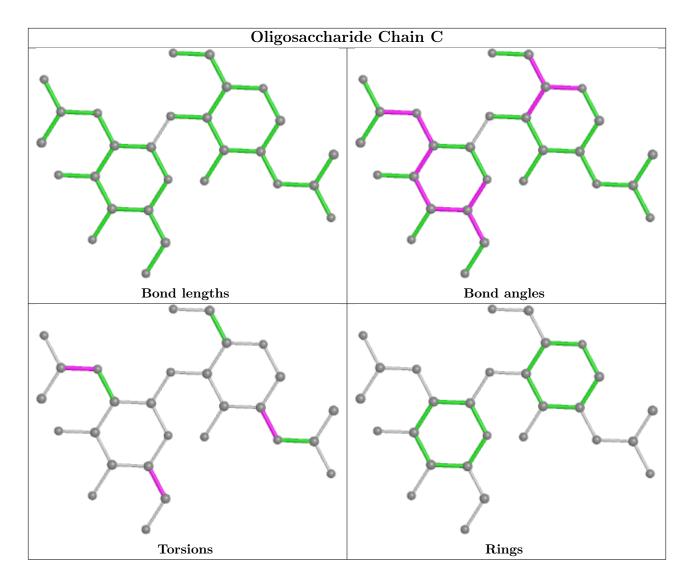
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	\mathbf{C}	2	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)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	Type	Chain	Res	Link	Bo	Bond lengths			Bond angles		
MOI	туре				Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
5	NAG	А	404	1	14,14,15	1.08	1 (7%)	$17,\!19,\!21$	1.52	3 (17%)	
5	NAG	А	402	1	14,14,15	0.61	0	17,19,21	1.08	0	
5	NAG	А	401	1	14,14,15	1.07	0	$17,\!19,\!21$	1.25	2 (11%)	



Mol Type C		Chain	Chain Res		Bog	Bog	Link	Bo	ond leng	\mathbf{ths}	Bond angles		
	Moi Type Chain R		nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2			
5	NAG	А	403	1	14,14,15	0.28	0	17,19,21	0.63	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	А	404	1	-	0/6/23/26	0/1/1/1
5	NAG	А	402	1	-	2/6/23/26	0/1/1/1
5	NAG	А	401	1	-	2/6/23/26	0/1/1/1
5	NAG	А	403	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	А	404	NAG	C2-N2	-2.14	1.42	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
5	А	404	NAG	C1-O5-C5	3.23	116.57	112.19
5	А	401	NAG	C1-O5-C5	2.98	116.23	112.19
5	А	404	NAG	C6-C5-C4	-2.88	106.25	113.00
5	А	401	NAG	O5-C1-C2	-2.18	107.85	111.29
5	А	404	NAG	O5-C1-C2	-2.18	107.85	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	А	401	NAG	C4-C5-C6-O6
5	А	402	NAG	C4-C5-C6-O6
5	А	401	NAG	O5-C5-C6-O6
5	А	403	NAG	C4-C5-C6-O6
5	А	402	NAG	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	$\langle RSRZ \rangle$	# RSRZ > 2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	322/326~(98%)	0.01	9 (2%) 53 49	42, 65, 110, 147	0
2	В	171/176~(97%)	-0.10	3 (1%) 68 65	37, 58, 90, 123	0
3	D	7/12~(58%)	-0.80	0 100 100	55, 65, 74, 87	0
All	All	500/514~(97%)	-0.04	12 (2%) 59 54	37, 62, 107, 147	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	325	SER	9.4
2	В	61	ILE	4.3
2	В	63	PHE	4.2
1	А	92	ASN	3.8
1	А	125(B)	GLU	3.5

6.2 Non-standard residues in protein, DNA, RNA chains (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	$B-factors(Å^2)$	Q < 0.9
3	BAL	D	12	5/6	0.92	0.23	83,83,85,87	0
3	ORN	D	3	8/9	0.95	0.09	$53,\!55,\!69,\!77$	0
3	PH8	D	2	13/14	0.95	0.24	55,61,77,77	0
3	MLE	D	4	9/10	0.97	0.17	42,53,62,63	0

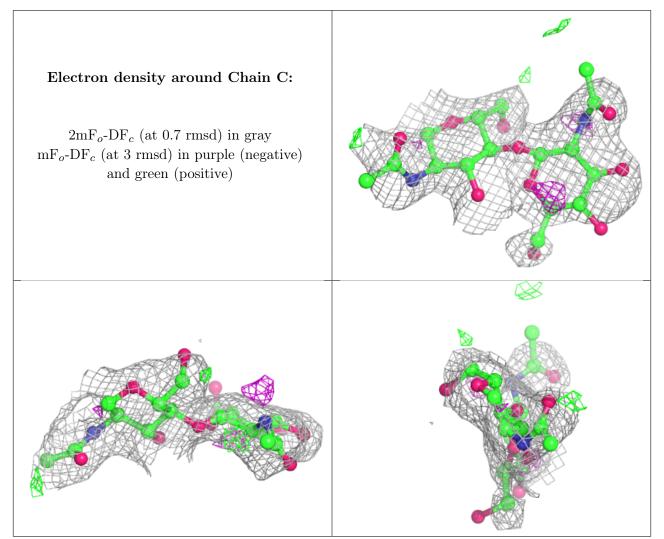


6.3 Carbohydrates (i)

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	$B-factors(Å^2)$	Q < 0.9
4	NAG	С	2	14/15	0.78	0.37	123,128,133,134	0
4	NAG	С	1	14/15	0.81	0.28	103,105,114,123	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,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q < 0.9
5	NAG	А	402	14/15	0.75	0.32	101,114,120,121	0
5	NAG	А	403	14/15	0.76	0.51	133,141,149,150	0
5	NAG	А	401	14/15	0.78	0.54	$136,\!146,\!157,\!161$	0
5	NAG	А	404	14/15	0.81	0.38	113,124,132,133	0
6	CL	А	405	1/1	0.92	0.16	83,83,83,83	0
6	CL	В	203	1/1	0.98	0.07	$65,\!65,\!65,\!65$	0

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.

6.5 Other polymers (i)

There are no such residues in this entry.

