

wwPDB X-ray Structure Validation Summary Report (i)

Oct 13, 2020 - 10:12 AM BST

PDB ID	:	$6 \mathrm{TJW}$
Title	:	Crystal structure of the haemagglutinin mutant (Gln226Leu, Del228) from an
		H10N7 seal influenza virus isolated in Germany
Authors	:	Zhang, J.; Xiong, X.; Purkiss, A.; Walker, P.; Gamblin, S.; Skehel, J.J.
Deposited on		
$\operatorname{Resolution}$:	2.31 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 following versions of software and data (see references (1)) were used in the production of this report:

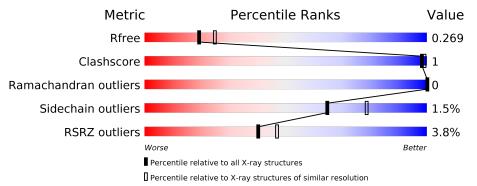
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 2.31 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R_{free}	130704	5974(2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523(2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855(2.34-2.30)

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 on 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		204	2%	
	A	324	94%	••
	G	224	2%	
1	С	324	94%	• •
			10%	
1	Е	324	96%	••
	- D		% •	
2	В	177	96%	••
_	-		2%	
2	D	177	93%	• • •
			3%	
2	F	177	95%	• •



Continued from previous page...

Mol	Chain	Length	Quality	v of chain
3	G	2	50%	50%



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12274 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	Δ	317	Total	С	Ν	Ο	\mathbf{S}	0	1	0	
	A	517	2429	1508	438	467	16	0	T	0	
1	C	311	Total	С	Ν	Ο	S	0	9	0	
		311	2397	1488	432	461	16	0	2		
1	Е	319	Total	С	Ν	Ο	S	0	0	0	
		519	2441	1515	442	468	16	0	0	0	

• Molecule 1 is a protein called Hemagglutinin HA1.

There are 9	discrepancies	between	the modelled	and	reference sequences:
THOIC GIU D	anserepaneres	Deemeen	une modened	ana	reference bequences.

Chain	Residue	Modelled	Actual	Comment	Reference
А	0	ASP	-	expression tag	UNP A0A0A7HR51
А	1	PRO	-	expression tag	UNP A0A0A7HR51
A	?	-	GLY	deletion	UNP A0A0A7HR51
С	0	ASP	-	expression tag	UNP A0A0A7HR51
С	1	PRO	-	expression tag	UNP A0A0A7HR51
C	?	-	GLY	deletion	UNP A0A0A7HR51
Е	0	ASP	-	expression tag	UNP A0A0A7HR51
Е	1	PRO	-	expression tag	UNP A0A0A7HR51
Е	?	-	GLY	deletion	UNP A0A0A7HR51

• Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
2	В	172	Total	С	Ν	Ο	S	0	0	0	
2	D	112	1386	857	241	280	8	0	0	0	
0	П	172	Total	С	Ν	Ο	S	0	0	0	
		172	1386	857	241	280	8	0	0	0	
0	F	172	Total	С	Ν	Ο	S	0	0	0	
	L L	172	1386	857	241	280	8	0	0	U	

There are 3 discrepancies between the modelled and reference sequences:



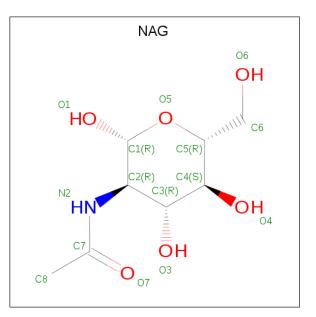
Chain	Residue	Modelled	Actual	Comment	Reference
В	177	LYS	-	expression tag	UNP A0A0A7HR51
D	177	LYS	-	expression tag	UNP A0A0A7HR51
F	177	LYS	-	expression tag	UNP A0A0A7HR51

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



Mo	l Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
3	G	2	Total 28	C 16	N 2	O 10	0	0	0

• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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



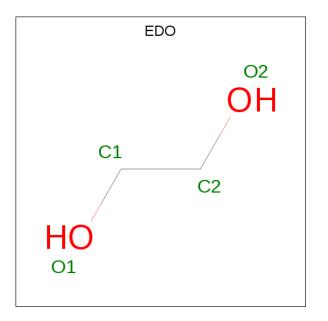
Continued from previous page...

Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
4	Б	1	Total	С	Ν	Ο	0	0
4	Г	L	14	8	1	5	0	0

• Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues			ZeroOcc	AltConf
5	В	1	Total Ca 1 1	ı	0	0

• Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
6	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
6	Е	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
6	F	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	190	Total O 190 190	0	0



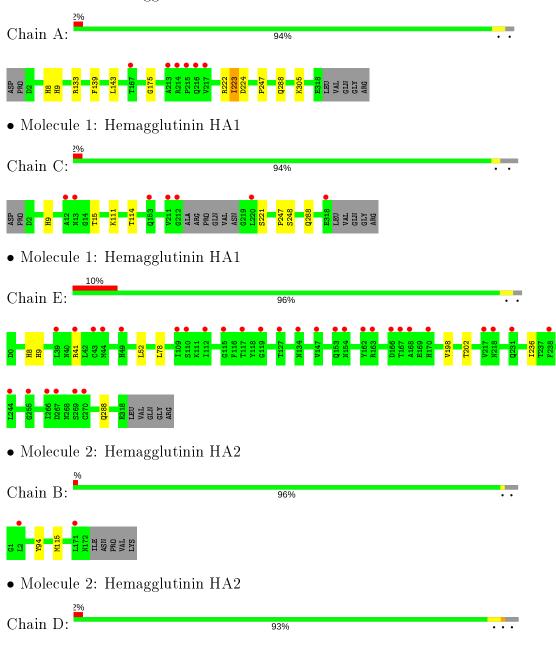
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	114	Total O 114 114	0	0
7	С	160	Total O 160 160	0	0
7	D	97	Total O 97 97	0	0
7	Е	80	Total O 80 80	0	0
7	F	93	Total O 93 93	0	0



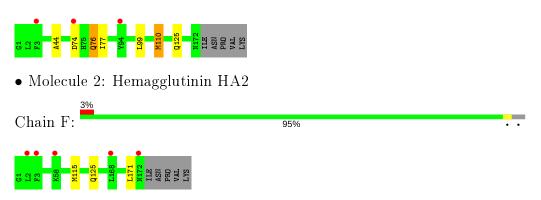
3 Residue-property plots (i)

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: Hemagglutinin HA1





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:	50%	50%
NAG 1 NAG 2		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	69.29Å 210.46 Å 82.75 Å	Depositor
a, b, c, α , β , γ	90.00° 101.40° 90.00°	Depositor
Resolution (Å)	41.60 - 2.31	Depositor
Resolution (A)	41.60 - 2.31	EDS
% Data completeness	99.8 (41.60-2.31)	Depositor
(in resolution range)	99.8 (41.60-2.31)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.90 (at 2.32 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
D D.	0.239 , 0.281	Depositor
R, R_{free}	0.227 , 0.269	DCC
R_{free} test set	4952 reflections $(4.90%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	35.4	Xtriage
Anisotropy	0.899	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31, 34.9	EDS
L-test for twinning ²	$ \langle L \rangle = 0.48, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12274	wwPDB-VP
Average B, all atoms $(Å^2)$	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.66% 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: CA, NAG, EDO

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		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.35	0/2478	0.58	0/3357	
1	С	0.35	0/2444	0.57	0/3307	
1	Е	0.37	0/2491	0.55	0/3375	
2	В	0.37	0/1411	0.55	0/1903	
2	D	0.38	0/1411	0.56	0/1903	
2	F	0.37	0/1411	0.56	0/1903	
All	All	0.36	0/11646	0.56	0/15748	

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	А	2429	0	2384	5	0
1	С	2397	0	2353	1	0
1	Е	2441	0	2404	3	0
2	В	1386	0	1291	2	0
2	D	1386	0	1291	4	0
2	F	1386	0	1291	1	0
3	G	28	0	25	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	А	14	0	13	0	0
4	С	14	0	13	0	0
4	D	14	0	13	0	0
4	Е	14	0	13	0	0
4	F	14	0	13	0	0
5	В	1	0	0	0	0
6	С	8	0	12	0	0
6	Е	4	0	6	0	0
6	F	4	0	6	0	0
7	А	190	0	0	0	0
7	В	114	0	0	0	0
7	С	160	0	0	0	0
7	D	97	0	0	0	0
7	Е	80	0	0	0	0
7	F	93	0	0	0	0
All	All	12274	0	11128	13	0

Continued from previous page...

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.

The worst 5 of 13 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:D:44:ALA:HA	2:D:110:MET:HE3	1.86	0.57
1:A:175:GLY:HA3	1:A:223:ILE:HD11	1.88	0.54
2:D:74:ASP:HB2	2:D:77:ILE:HG22	1.90	0.53
1:E:52:LEU:HD21	1:E:78:LEU:HD11	1.95	0.47
1:E:8:HIS:HB3	2:F:115:MET:CE	2.44	0.47

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	316/324~(98%)	309~(98%)	7(2%)	0	100	100
1	С	309/324~(95%)	301 (97%)	8 (3%)	0	100	100
1	Ε	317/324~(98%)	307~(97%)	10 (3%)	0	100	100
2	В	170/177~(96%)	164 (96%)	6 (4%)	0	100	100
2	D	170/177~(96%)	165~(97%)	5(3%)	0	100	100
2	F	170/177~(96%)	165~(97%)	5(3%)	0	100	100
All	All	1452/1503~(97%)	1411 (97%)	41 (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	Outliers	Percentiles
1	А	269/275~(98%)	265~(98%)	4 (2%)	65 79
1	С	266/275~(97%)	260~(98%)	6 (2%)	50 66
1	Ε	271/275~(98%)	267~(98%)	4 (2%)	65 79
2	В	146/151~(97%)	146~(100%)	0	100 100
2	D	146/151~(97%)	143~(98%)	3 (2%)	53 70
2	F	146/151~(97%)	144~(99%)	2 (1%)	67 80
All	All	1244/1278~(97%)	1225~(98%)	19 (2%)	65 79

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	248	SER
2	D	76	GLN
1	Ε	202	THR
1	С	221	SER
1	Е	288	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:



Mol	Chain	Res	Type
2	D	95	GLN
2	F	105	GLN
1	Е	231	GLN
2	В	95	GLN
1	Е	268	ASN

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 C	Chain Re	Res	Link	Bond lengths			Bond angles		
intor Type Cha	Unam			Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	NAG	G	1	3,2,5	14, 14, 15	0.40	0	$17,\!19,\!21$	0.95	1 (5%)
3	NAG	G	2	3	14, 14, 15	0.36	0	$17,\!19,\!21$	0.76	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	NAG	G	1	3,2,5	-	0/6/23/26	0/1/1/1
3	NAG	G	2	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	Z	$Observed(^{o})$	$Ideal(^{o})$
3	G	1	NAG	C1-O5-C5	2.19	115.15	112.19

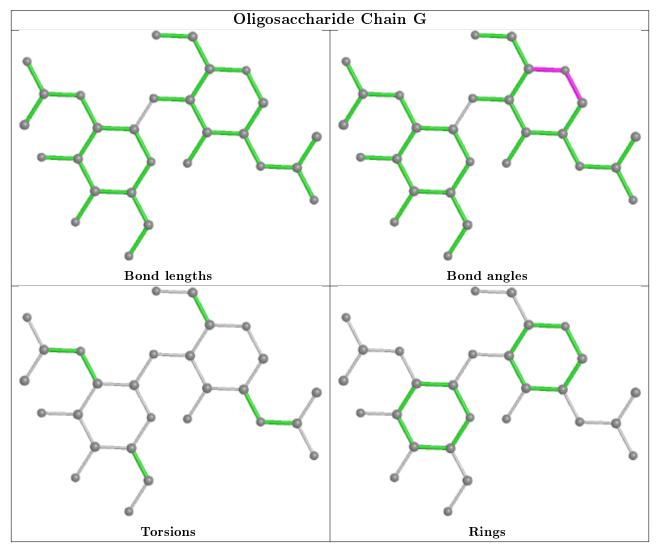
There are no chirality outliers.

There are no torsion outliers.

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)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.



 $6 \mathrm{TJW}$

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	Turne	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
IVIOI	Type	Cham	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
6	EDO	С	403	-	3,3,3	0.44	0	2,2,2	0.35	0
6	EDO	Е	402	-	$3,\!3,\!3$	0.41	0	2,2,2	0.37	0
4	NAG	Е	401	1	14,14,15	0.48	0	$17,\!19,\!21$	0.83	1(5%)
4	NAG	D	201	2	14, 14, 15	0.39	0	$17,\!19,\!21$	1.05	1(5%)
4	NAG	А	401	1	14, 14, 15	0.45	0	$17,\!19,\!21$	0.77	0
4	NAG	С	401	1	14, 14, 15	0.38	0	$17,\!19,\!21$	1.17	2 (11%)
4	NAG	F	201	2	14,14,15	0.48	0	$17,\!19,\!21$	1.02	1(5%)
6	EDO	F	202	-	$3,\!3,\!3$	0.46	0	2,2,2	0.34	0
6	EDO	С	402	-	3,3,3	0.52	0	2,2,2	0.14	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	\mathbf{Res}	\mathbf{Link}	Chirals	Torsions	Rings
6	EDO	С	403	-	-	0/1/1/1	-
6	EDO	Е	402	-	-	0/1/1/1	-
4	NAG	Е	401	1	-	0/6/23/26	0/1/1/1
4	NAG	D	201	2	-	2/6/23/26	0/1/1/1
4	NAG	А	401	1	-	1/6/23/26	0/1/1/1
4	NAG	С	401	1	-	2/6/23/26	0/1/1/1
4	NAG	F	201	2	-	0/6/23/26	0/1/1/1
6	EDO	F	202	-	-	1/1/1/1	-
6	EDO	С	402	_	_	1/1/1/1	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	D	201	NAG	C1-O5-C5	2.98	116.23	112.19
4	F	201	NAG	C1-O5-C5	2.88	116.10	112.19
4	С	401	NAG	C2-N2-C7	2.58	126.57	122.90



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
4	С	401	NAG	C8-C7-N2	2.46	120.27	116.10
4	Е	401	NAG	O5-C5-C6	2.36	110.91	107.20

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	201	NAG	O5-C5-C6-O6
4	D	201	NAG	C4-C5-C6-O6
4	С	401	NAG	C8-C7-N2-C2
4	С	401	NAG	O7-C7-N2-C2
6	F	202	EDO	O1-C1-C2-O2

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 > 2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	$\mathbf{Q}{<}0.9$
1	А	317/324~(97%)	0.05	6 (1%) 66 73	31, 45, 73, 144	0
1	С	311/324~(95%)	-0.01	7 (2%) 60 67	31, 46, 85, 108	0
1	Ε	319/324~(98%)	0.63	32 (10%) 7 10	34, 74, 101, 119	0
2	В	172/177~(97%)	0.14	2 (1%) 79 83	27, 44, 60, 78	0
2	D	172/177~(97%)	0.28	3 (1%) 70 76	30, 48, 68, 86	0
2	F	172/177~(97%)	0.47	5 (2%) 51 59	31, 48, 83, 98	0
All	All	1463/1503~(97%)	0.25	55 (3%) 40 47	27, 49, 90, 144	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	Е	218	ASN	5.6
1	Е	270	CYS	5.0
1	Е	167	THR	4.4
1	С	212	GLY	4.3
1	Е	168	ALA	4.3

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

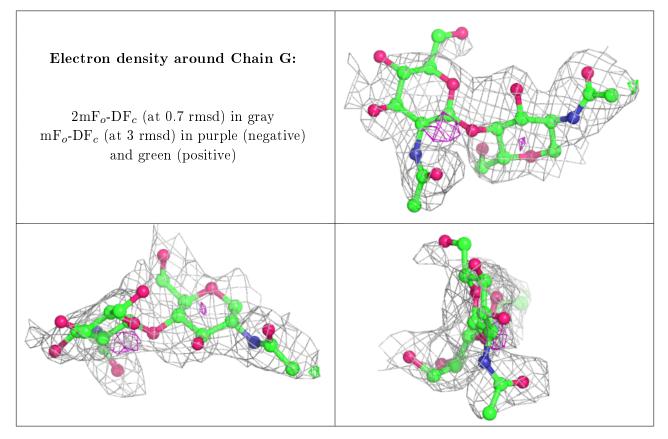
6.3 Carbohydrates (i)

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	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	$Q{<}0.9$
3	NAG	G	2	14/15	0.80	0.30	$86,\!96,\!99,\!99$	0
3	NAG	G	1	14/15	0.84	0.16	74,80,85,91	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	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
4	NAG	А	401	14/15	0.66	0.27	$81,\!86,\!89,\!92$	0
4	NAG	Е	401	14/15	0.80	0.22	$84,\!88,\!93,\!93$	0
4	NAG	С	401	14/15	0.80	0.24	81,88,91,92	0
6	EDO	С	402	4/4	0.82	0.32	$57,\!58,\!59,\!59$	0
4	NAG	D	201	14/15	0.85	0.18	70,73,75,76	0
6	EDO	F	202	4/4	0.86	0.31	$64,\!67,\!68,\!70$	0
4	NAG	F	201	14/15	0.87	0.24	74,78,82,83	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	$Q{<}0.9$
5	CA	В	203	1/1	0.87	0.08	$83,\!83,\!83,\!83$	0
6	EDO	Е	402	4/4	0.92	0.28	$51,\!52,\!53,\!55$	0
6	EDO	С	403	4/4	0.96	0.16	$45,\!46,\!47,\!48$	0

Continued from previous page...

6.5 Other polymers (i)

There are no such residues in this entry.

