

wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2020 – 11:30 PM BST

PDB ID : 4DJ6

> Title : Structure of the hemagglutinin from a highly pathogenic H7N7 influenza virus

Authors : Yang, H.; Carney, P.J.; Donis, R.O.; Stevens, J.

2012-02-01 Deposited on

2.61 Å(reported) Resolution

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

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.13.1

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

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4 Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

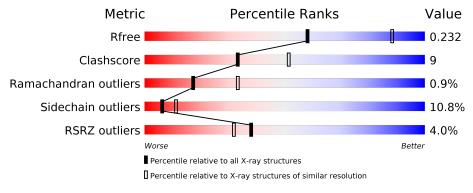
Validation Pipeline (wwPDB-VP) 2.13.1

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 2.61 Å.

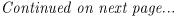
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	A	327	76%	17%		•	-		
1	С	327	78%	15%			-		
1	Е	327	78%	17%		•	.		
2	В	177	71%	18%	7%				
2	D	177	9%	21%	6%		-		
2	F	177	71%	19%	5%	59	— %		





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Mol	Chain	Length	Quality of chain
3	G	2	100%

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
4	NAG	С	402	X	_	_	_



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11804 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					ZeroOcc	AltConf	Trace	
1	Λ	316	Total	С	N	О	S	6	0	0
1	A	310	2422	1502	435	471	14	0	0	
1	С	316	Total	С	N	О	S	0	0	0
1		310	2422	1502	435	471	14	0		
1	E	317	Total	С	N	О	S	4	0	0
1	E	317	2426	1504	436	472	14	4		U

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	_	expression tag	UNP Q6VMK1
A	-2	ASP	-	expression tag	UNP Q6VMK1
A	-1	PRO	_	expression tag	UNP Q6VMK1
A	0	GLY	_	expression tag	UNP Q6VMK1
С	-3	ALA	-	expression tag	UNP Q6VMK1
С	-2	ASP	_	expression tag	UNP Q6VMK1
С	-1	PRO	_	expression tag	UNP Q6VMK1
С	0	GLY	_	expression tag	UNP Q6VMK1
Е	-3	ALA	_	expression tag	UNP Q6VMK1
Е	-2	ASP	-	expression tag	UNP Q6VMK1
Е	-1	PRO	-	expression tag	UNP Q6VMK1
Е	0	GLY	-	expression tag	UNP Q6VMK1

• Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	R	170	Total	С	N	О	S	4	0	0
	Ъ	170	1380	851	243	279	7	4	U	
2	D	171	Total	С	N	О	S	0	0	0
	ע	111	1388	857	244	280	7	0		
2	F	169	Total	С	N	О	S	0	0	0
	I'	109	1369	845	239	278	7	0		U



There are 0	discrepancies	hetween	the modelled	and	reference	segmences.
There are 9	discrepancies	Detween	the modelied	anu	reference	sequences.

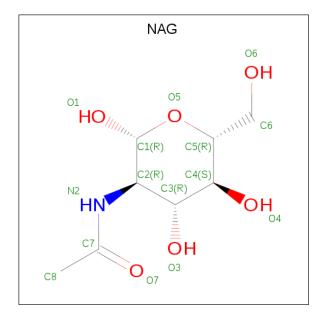
Chain	Residue	Modelled	Actual	Comment	Reference
В	175	SER	-	expression tag	UNP Q6VMK1
В	176	GLY	_	expression tag	UNP Q6VMK1
В	177	ARG	-	expression tag	UNP Q6VMK1
D	175	SER	_	expression tag	UNP Q6VMK1
D	176	GLY	_	expression tag	UNP Q6VMK1
D	177	ARG	-	expression tag	UNP Q6VMK1
F	175	SER	_	expression tag	UNP Q6VMK1
F	176	GLY	=	expression tag	UNP Q6VMK1
F	177	ARG	-	expression tag	UNP Q6VMK1

• 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	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	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	В	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	С	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
4	E	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0

• Molecule 5 is water.

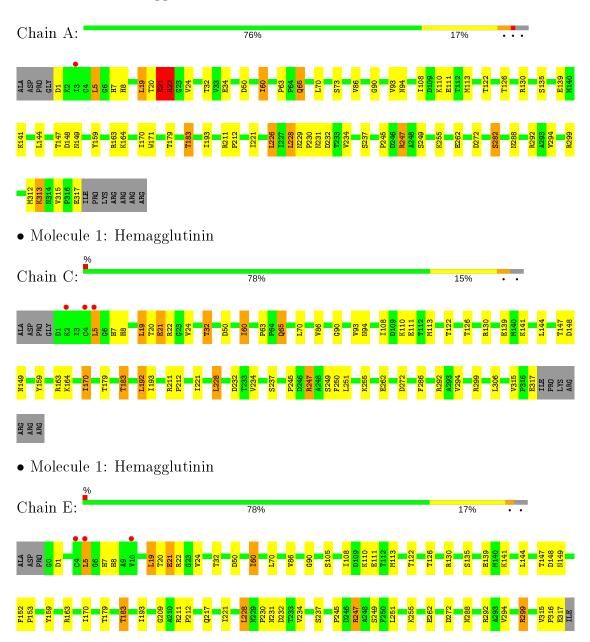
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	59	Total O 59 59	0	0
5	В	12	Total O 12 12	0	0
5	С	59	Total O 59 59	0	0
5	D	13	Total O 13 13	0	0
5	E	54	Total O 54 54	0	0
5	F	18	Total O 18 18	0	0



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.

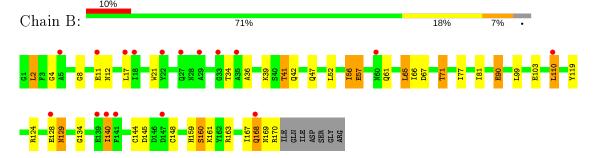
• Molecule 1: Hemagglutinin



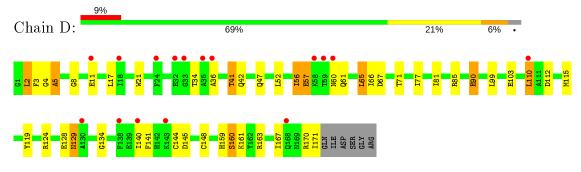


PRO LYS ARG ARG ARG ARG

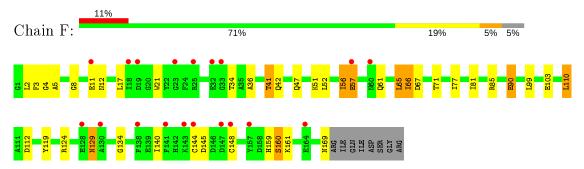
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



 $\bullet \ \, \text{Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2$

Chain G: 100%

NAG1 NAG2



Data and refinement statistics (i) 4

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	201.95Å 116.57Å 117.32Å	D : 4
a, b, c, α , β , γ	90.00° 124.92° 90.00°	Depositor
Resolution (Å)	49.85 - 2.61	Depositor
Resolution (A)	49.85 - 2.61	EDS
% Data completeness	99.0 (49.85-2.61)	Depositor
(in resolution range)	99.0 (49.85-2.61)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) > 1$	2.74 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
D D	0.203 , 0.236	Depositor
R, R_{free}	0.200 , 0.232	DCC
R_{free} test set	3421 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33 , 30.3	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	$\begin{array}{c} 0.015 \; \text{for} \; -1/2*\text{h}-3/2*\text{k}-\text{l},-1/2*\text{h}+1/2*\text{k}-\text{l},1/2 \\ & *\text{h}+1/2*\text{k} \\ 0.009 \; \text{for} \; 1/2*\text{h}+1/2*\text{k}+2*\text{l},1/2*\text{h}+1/2*\text{k},-1 \\ & /2*\text{h}+1/2*\text{k}-\text{l} \\ 0.019 \; \text{for} \; 1/2*\text{h}-1/2*\text{k}+2*\text{l},-1/2*\text{h}+1/2*\text{k},-1 \\ & /2*\text{h}-1/2*\text{k}-\text{l} \\ 0.015 \; \text{for} \; -1/2*\text{h}+3/2*\text{k}-\text{l},1/2*\text{h}+1/2*\text{k}+\text{l},1 \\ & /2*\text{h}-1/2*\text{k} \\ 0.005 \; \text{for} \; -\text{h}-\text{k}-\text{l},\text{l},\text{k} \\ 0.021 \; \text{for} \; -\text{h}-\text{k}-\text{l},\text{l},\text{k} \\ 0.021 \; \text{for} \; -\text{h}+\text{k}-\text{l},\text{-l},\text{-k} \\ 0.008 \; \text{for} \; -1/2*\text{h}-1/2*\text{k}+\text{l},-1/2*\text{h}-1/2*\text{k}-\text{l},1/2 \\ & *\text{h}-1/2*\text{k} \\ 0.019 \; \text{for} \; -1/2*\text{h}+1/2*\text{k}+\text{l},1/2*\text{h}-1/2*\text{k}+\text{l},1 \\ & /2*\text{h}+1/2*\text{k} \\ 0.457 \; \text{for} \; 1/2*\text{h}-3/2*\text{k},-1/2*\text{h}-1/2*\text{k},-1/2*\text{h} \\ & +1/2*\text{k}-\text{l} \\ 0.457 \; \text{for} \; 1/2*\text{h}+3/2*\text{k},1/2*\text{h}-1/2*\text{k},-1/2*\text{h}-1/2*\text{k} \\ 0.017 \; \text{for} \; -\text{h}-2*\text{l},-\text{k},\text{l} \\ \end{array}$	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11804	wwPDB-VP
Average B, all atoms $(Å^2)$	66.0	wwPDB-VP

¹Intensities estimated from amplitudes.

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.



Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.



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

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		ond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	1.36	$2/2468 \; (0.1\%)$	2.84	4/3337~(0.1%)
1	С	0.48	0/2468	0.57	0/3337
1	E	0.45	0/2472	0.56	0/3342
2	В	0.39	0/1404	0.53	1/1892~(0.1%)
2	D	0.37	0/1412	0.46	0/1903
2	F	0.36	0/1393	0.47	0/1878
All	All	0.73	2/11617~(0.0%)	1.39	$5/15689 \ (0.0\%)$

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	С	0	1
1	E	0	1
2	В	0	1
2	D	0	1
2	F	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	A	22	ARG	NE-CZ	63.21	2.15	1.33
1	A	21	GLU	CG-CD	-7.53	1.40	1.51

All (5) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	22	ARG	NE-CZ-NH1	-134.49	53.05	120.30
1	A	22	ARG	NE-CZ-NH2	83.86	162.23	120.30
1	A	22	ARG	CD-NE-CZ	-23.50	90.69	123.60
1	A	21	GLU	CG-CD-OE1	-14.06	90.18	118.30
2	В	39	LYS	CA-CB-CG	-11.02	89.15	113.40

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	LEU	Peptide
1	A	21	GLU	Sidechain
1	A	22	ARG	Sidechain
2	В	56	ILE	Peptide
1	С	19	LEU	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	Α	2422	0	2369	45	0
1	С	2422	0	2369	42	0
1	E	2426	0	2372	40	0
2	В	1380	0	1283	31	0
2	D	1388	0	1294	33	0
2	F	1369	0	1270	26	0
3	G	28	0	25	0	0
4	A	28	0	26	0	0
4	В	14	0	13	0	0
4	С	42	0	39	3	0
4	D	14	0	13	0	0
4	Ε	42	0	39	0	0
4	F	14	0	13	0	0
5	A	59	0	0	0	0
5	В	12	0	0	1	0
5	С	59	0	0	0	0
5	D	13	0	0	2	0
5	E	54	0	0	1	0

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Mol	Chain	Non-H	$\mathbf{H}(\mathbf{model})$	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
5	F	18	0	0	2	0
All	All	11804	0	11125	194	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 9.

The worst 5 of 194 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	Clash overlap (Å)
4:C:403:NAG:C6	4:C:403:NAG:O6	1.69	1.40
2:D:60:ASN:HB2	5:D:301:HOH:O	1.53	1.08
1:C:60:ILE:HG21	1:C:170:ILE:HD13	1.08	1.06
1:C:60:ILE:CG2	1:C:170:ILE:HD13	1.91	1.00
1:C:5:LEU:HD22	1:C:5:LEU:H	1.33	0.93

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	A	$314/327 \ (96\%)$	296 (94%)	18 (6%)	0	100	100
1	С	314/327 (96%)	296 (94%)	18 (6%)	0	100	100
1	E	315/327~(96%)	298 (95%)	16 (5%)	1 (0%)	41	62
2	В	168/177 (95%)	148 (88%)	16 (10%)	4 (2%)	6	9
2	D	169/177~(96%)	150 (89%)	15 (9%)	4 (2%)	6	9
2	F	167/177 (94%)	147 (88%)	16 (10%)	4 (2%)	6	9
All	All	1447/1512 (96%)	1335 (92%)	99 (7%)	13 (1%)	17	33

5 of 13 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
2	В	57	GLU
2	D	57	GLU
2	F	57	GLU
2	D	119	TYR
2	F	119	TYR

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	$268/277 \; (97\%)$	236 (88%)	32 (12%)	5 8
1	С	268/277~(97%)	238 (89%)	30 (11%)	6 10
1	E	$268/277 \; (97\%)$	242 (90%)	26 (10%)	8 15
2	В	$145/151\ (96\%)$	130 (90%)	15 (10%)	7 12
2	D	$146/151 \; (97\%)$	131 (90%)	15 (10%)	7 12
2	F	$144/151 \; (95\%)$	128 (89%)	16 (11%)	6 10
All	All	1239/1284~(96%)	1105 (89%)	134 (11%)	6 11

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	130	ARG
1	С	315	VAL
2	F	57	GLU
1	С	144	LEU
1	С	237	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

\mathbf{Mol}	Chain	${f Res}$	\mathbf{Type}	
1	Ε	94	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).

Mol	Mol Type Chain Res Link		Bo	Bond lengths			Bond angles			
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	G	1	1,3	14,14,15	0.64	0	17,19,21	2.38	7 (41%)
3	NAG	G	2	3	14,14,15	0.65	0	17,19,21	1.14	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	${f Res}$	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
3	G	1	NAG	O4-C4-C3	5.38	122.78	110.35
3	G	1	NAG	C4-C3-C2	-4.31	104.70	111.02
3	G	1	NAG	C3-C4-C5	-3.64	103.75	110.24
3	G	1	NAG	O5-C5-C6	2.95	111.84	107.20
3	G	2	NAG	C4-C3-C2	2.92	115.30	111.02



There are no chirality outliers.

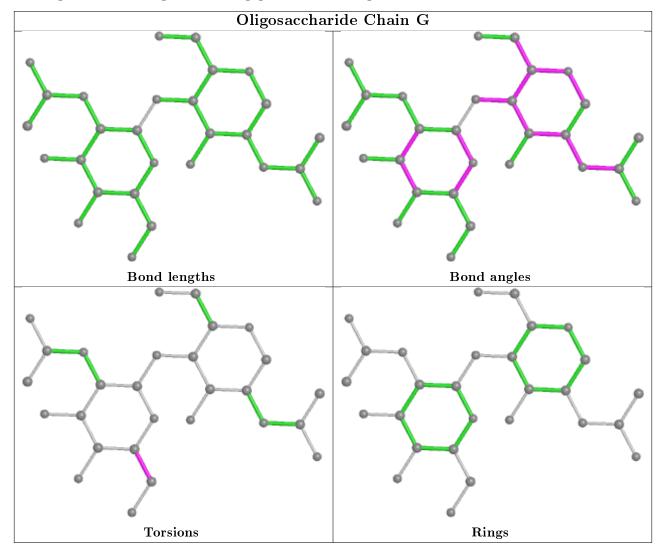
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-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)

11 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).

Mal	Т	Chair	Dag	T : 1.	Во	ond leng	ths	В	ond ang	les
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	В	201	2	14,14,15	0.53	0	17,19,21	1.01	1 (5%)
4	NAG	D	201	2	14,14,15	0.57	0	17,19,21	1.00	0
4	NAG	F	201	2	14,14,15	0.58	0	17,19,21	1.39	1 (5%)
4	NAG	С	401	1	14,14,15	0.50	0	17,19,21	1.52	3 (17%)
4	NAG	Е	402	1	14,14,15	0.46	0	17,19,21	0.99	1 (5%)
4	NAG	Е	401	1	14,14,15	0.57	0	17,19,21	1.56	3 (17%)
4	NAG	С	402	1	14,14,15	0.75	0	17,19,21	2.16	4 (23%)
4	NAG	С	403	1	14,14,15	1.83	1 (7%)	17,19,21	1.34	2 (11%)
4	NAG	Е	403	1	14,14,15	0.66	0	17,19,21	1.25	2 (11%)
4	NAG	A	403	1	14,14,15	0.55	0	17,19,21	1.12	2 (11%)
4	NAG	A	404	1	14,14,15	0.62	0	17,19,21	1.49	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	В	201	2	-	0/6/23/26	0/1/1/1
4	NAG	D	201	2	-	0/6/23/26	0/1/1/1
4	NAG	F	201	2	-	2/6/23/26	0/1/1/1
4	NAG	С	401	1	-	2/6/23/26	0/1/1/1
4	NAG	Е	402	1	-	0/6/23/26	0/1/1/1
4	NAG	Е	401	1	-	0/6/23/26	0/1/1/1
4	NAG	С	402	1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	С	403	1	-	2/6/23/26	0/1/1/1
4	NAG	Е	403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	403	1	-	0/6/23/26	0/1/1/1
4	NAG	A	404	1	_	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$Ideal(\AA)$
4	С	403	NAG	O6-C6	6.51	1.69	1.42

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
4	С	402	NAG	C1-O5-C5	-5.62	104.58	112.19
4	С	402	NAG	O5-C5-C6	4.18	113.75	107.20
4	F	201	NAG	O5-C5-C6	4.09	113.62	107.20
4	A	404	NAG	O5-C1-C2	3.72	117.17	111.29
4	Е	401	NAG	C3-C4-C5	-3.67	103.70	110.24

All (1) chirality outliers are listed below:

Mol	Chain	${f Res}$	Type	Atom
4	С	402	NAG	C1

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	201	NAG	O5-C5-C6-O6
4	С	403	NAG	O5-C5-C6-O6
4	E	403	NAG	O5-C5-C6-O6
4	F	201	NAG	C4-C5-C6-O6
4	E	403	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	С	403	NAG	3	0

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, 95th 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>	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	$316/327 \ (96\%)$	-0.03	1 (0%) 94 93	27, 43, 79, 135	2 (0%)
1	С	$316/327 \ (96\%)$	-0.03	3 (0%) 84 82	27, 43, 85, 146	0
1	E	317/327 (96%)	-0.02	3 (0%) 84 82	26, 43, 84, 143	1 (0%)
2	В	170/177 (96%)	0.71	17 (10%) 7 4	20, 94, 161, 167	1 (0%)
2	D	171/177 (96%)	0.71	16 (9%) 8 5	22, 94, 161, 167	0
2	F	$169/177 \; (95\%)$	0.77	19 (11%) 5 3	21, 93, 161, 166	0
All	All	$1459/1512 \ (96\%)$	0.24	59 (4%) 38 32	20, 49, 157, 167	4 (0%)

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	18	ILE	6.6
2	D	60	ASN	5.8
2	F	33	GLY	4.6
2	В	147	ASP	4.6
2	F	60	ASN	3.8

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

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

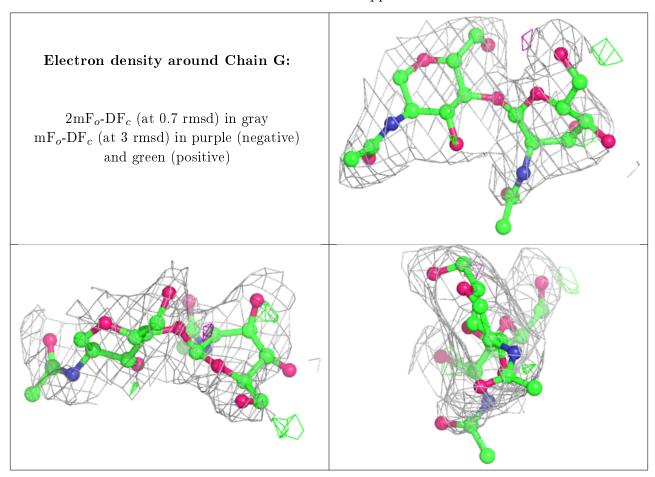
6.3 Carbohydrates (i)

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	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
3	NAG	G	2	14/15	0.79	0.23	124,148,158,158	0
3	NAG	G	1	14/15	0.89	0.15	87,104,117,132	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
4	NAG	Ε	403	14/15	0.35	0.33	130,162,170,170	0
4	NAG	С	403	14/15	0.43	0.29	123,156,172,172	0
4	NAG	A	404	14/15	0.59	0.27	129,154,165,166	0
4	NAG	F	201	14/15	0.72	0.18	93,107,116,121	0
4	NAG	A	403	14/15	0.73	0.22	125,143,153,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B\text{-}factors}({f A}^2)$	Q < 0.9
4	NAG	С	402	14/15	0.76	0.29	131,148,152,153	0
4	NAG	D	201	14/15	0.77	0.20	77,110,117,122	0
4	NAG	Ε	402	14/15	0.81	0.23	121,142,162,163	0
4	NAG	В	201	14/15	0.82	0.16	87,106,112,121	0
4	NAG	Ε	401	14/15	0.86	0.14	88,99,117,119	0
4	NAG	С	401	14/15	0.90	0.18	84,101,111,114	0

6.5 Other polymers (i)

There are no such residues in this entry.

