



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 05:37 PM BST

PDB ID : 5XL2  
Title : The structure of hemagglutinin from a swine-origin H4N6 influenza virus  
Authors : Song, H.; Qi, J.; Gao, G.F.  
Deposited on : 2017-05-10  
Resolution : 2.30 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](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1  
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) : 2.13.1

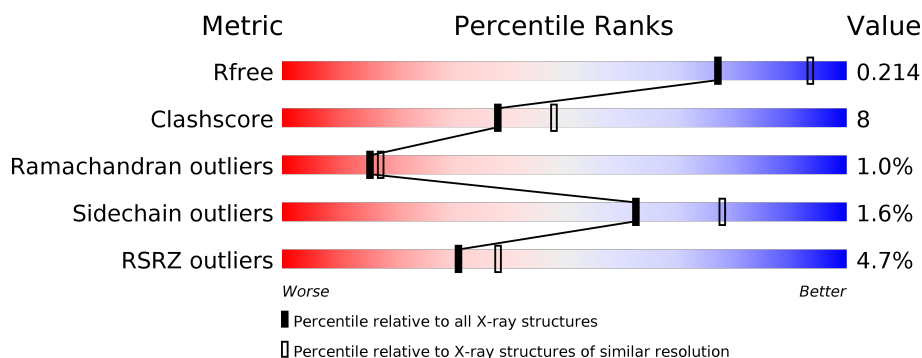
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	503	<div> <div>85%</div> <div>10% . .</div> </div>
1	B	503	<div> <div>5%</div> <div>82%</div> <div>14% . .</div> </div>
1	C	503	<div> <div>9%</div> <div>79%</div> <div>15% . . .</div> </div>

## 2 Entry composition [i](#)

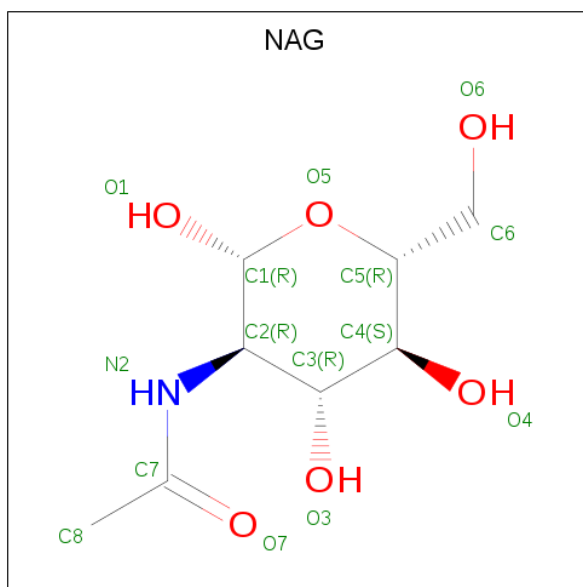
There are 3 unique types of molecules in this entry. The entry contains 12325 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	A	486	Total	C	N	O	S	0	0	0
			3841	2398	680	748	15			
1	B	486	Total	C	N	O	S	0	0	0
			3843	2400	680	748	15			
1	C	484	Total	C	N	O	S	0	0	0
			3830	2391	678	746	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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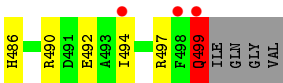
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	274	Total	O	0	0
			274	274		
3	B	240	Total	O	0	0
			240	240		
3	C	213	Total	O	0	0
			213	213		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.42Å 120.56Å 132.28Å 90.00° 92.29° 90.00°	Depositor
Resolution (Å)	35.57 – 2.30 35.57 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.57-2.30) 99.5 (35.57-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.09 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.184 , 0.213 0.186 , 0.214	Depositor DCC
$R_{free}$ test set	4559 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	1.122	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12325	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 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	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.32	0/3923	0.52	1/5323 (0.0%)
1	B	0.33	0/3925	0.52	1/5327 (0.0%)
1	C	0.34	0/3912	0.51	3/5309 (0.1%)
All	All	0.33	0/11760	0.52	5/15959 (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.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	239	LEU	CA-CB-CG	6.04	129.20	115.30
1	A	160	LEU	CA-CB-CG	5.68	128.37	115.30
1	B	365	LEU	CA-CB-CG	-5.67	102.26	115.30
1	C	499	GLN	CA-CB-CG	5.46	125.40	113.40
1	C	339	ASN	N-CA-C	-5.14	97.12	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	384	GLU	Peptide



## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3841	0	3690	47	0
1	B	3843	0	3698	55	0
1	C	3830	0	3682	76	0
2	A	28	0	26	0	0
2	B	28	0	26	0	0
2	C	28	0	26	2	0
3	A	274	0	0	6	0
3	B	240	0	0	11	0
3	C	213	0	0	11	0
All	All	12325	0	11148	173	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 8.

The worst 5 of 173 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)
1:C:137:ARG:NE	1:C:142:ASP:OD2	1.57	1.36
1:C:499:GLN:HE21	1:C:499:GLN:HA	1.21	1.02
1:B:439:ASP:OD1	3:B:702:HOH:O	1.89	0.91
1:A:244:THR:HG21	1:A:248:LEU:HB2	1.53	0.90
1:C:122:GLN:OE1	3:C:701:HOH:O	1.90	0.89

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	Percentiles	
1	A	482/503 (96%)	463 (96%)	17 (4%)	2 (0%)	34	42
1	B	482/503 (96%)	454 (94%)	25 (5%)	3 (1%)	25	31
1	C	480/503 (95%)	448 (93%)	23 (5%)	9 (2%)	8	7
All	All	1444/1509 (96%)	1365 (94%)	65 (4%)	14 (1%)	15	17

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	472	ASP
1	B	386	PRO
1	C	6	ASN
1	C	338	GLU

### 5.3.2 Protein sidechains ⓘ

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	425/437 (97%)	419 (99%)	6 (1%)	67	81
1	B	425/437 (97%)	419 (99%)	6 (1%)	67	81
1	C	424/437 (97%)	416 (98%)	8 (2%)	57	73
All	All	1274/1311 (97%)	1254 (98%)	20 (2%)	62	78

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	342	GLN
1	B	365	LEU
1	C	336	PHE
1	B	90	VAL
1	B	239	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	339	ASN
1	B	342	GLN
1	C	339	ASN
1	B	14	HIS
1	C	139	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](#)

There are no monosaccharides in this entry.

## 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	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	C	602	1	14,14,15	0.68	0	17,19,21	0.46	0
2	NAG	A	601	1	14,14,15	0.51	0	17,19,21	0.50	0
2	NAG	C	601	1	14,14,15	0.32	0	17,19,21	0.59	0
2	NAG	A	602	1	14,14,15	0.46	0	17,19,21	0.44	0
2	NAG	B	602	1	14,14,15	0.52	0	17,19,21	0.51	0
2	NAG	B	601	1	14,14,15	0.26	0	17,19,21	0.42	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
2	NAG	C	602	1	-	0/6/23/26	0/1/1/1
2	NAG	A	601	1	-	2/6/23/26	0/1/1/1
2	NAG	C	601	1	-	2/6/23/26	0/1/1/1
2	NAG	A	602	1	-	2/6/23/26	0/1/1/1
2	NAG	B	602	1	-	0/6/23/26	0/1/1/1
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAG	O5-C5-C6-O6
2	A	602	NAG	O5-C5-C6-O6
2	C	601	NAG	C8-C7-N2-C2
2	C	601	NAG	O7-C7-N2-C2
2	A	601	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	NAG	1	0
2	C	601	NAG	1	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, 95<sup>th</sup> 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	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	486/503 (96%)	-0.25	2 (0%) 92 95	15, 30, 64, 105	0
1	B	486/503 (96%)	-0.07	23 (4%) 31 38	16, 32, 78, 146	0
1	C	484/503 (96%)	0.25	43 (8%) 9 13	19, 37, 97, 147	0
All	All	1456/1509 (96%)	-0.02	68 (4%) 31 38	15, 34, 83, 147	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	335	GLY	17.7
1	B	322	PRO	8.5
1	C	336	PHE	8.2
1	B	387	ASN	6.9
1	C	499	GLN	5.9

### 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](#)

There are no monosaccharides in this entry.

### 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	602	14/15	0.87	0.20	31,37,40,45	0
2	NAG	B	601	14/15	0.89	0.21	68,73,77,80	0
2	NAG	C	602	14/15	0.90	0.17	42,48,57,58	0
2	NAG	B	602	14/15	0.90	0.15	38,45,54,54	0
2	NAG	A	601	14/15	0.90	0.14	39,43,51,53	0
2	NAG	C	601	14/15	0.94	0.14	34,40,46,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.