



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 16, 2018 – 09:50 pm GMT

PDB ID : 1JSN
Title : STRUCTURE OF AVIAN H5 HAEMAGGLUTININ COMPLEXED WITH
LSTA RECEPTRO ANALOG
Authors : Ha, Y.; Stevens, D.J.; Skehel, J.J.; Wiley, D.C.
Deposited on : 2001-08-17
Resolution : 2.40 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

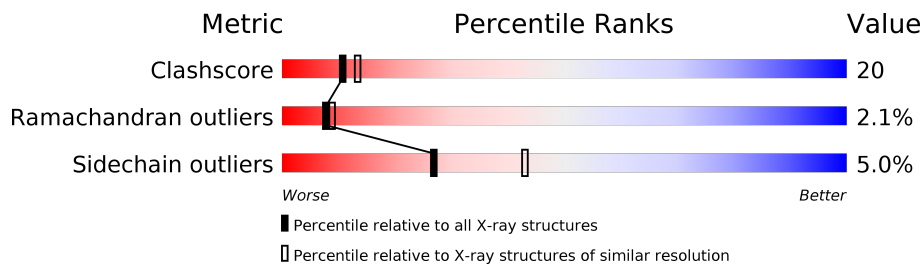
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	122078	3953 (2.40-2.40)
Ramachandran outliers	120005	3894 (2.40-2.40)
Sidechain outliers	119972	3895 (2.40-2.40)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	325	
2	B	176	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4096 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.

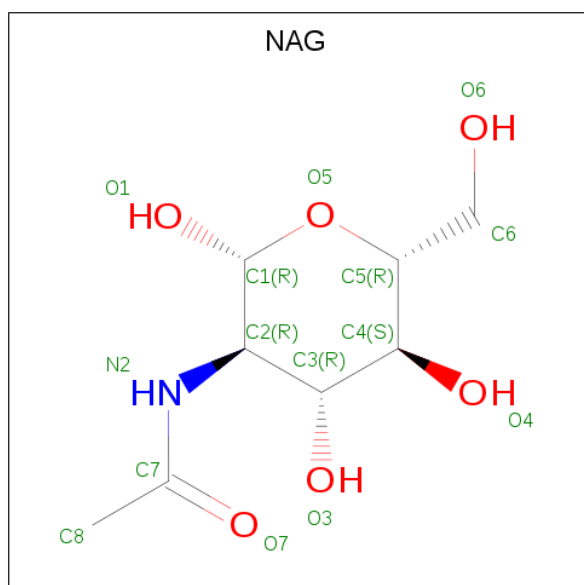
- Molecule 1 is a protein called HAEMAGGLUTININ (HA1 CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2509	1581	439	474	15			

- Molecule 2 is a protein called HAEMAGGLUTININ (HA2 CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1227	766	211	242	8			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



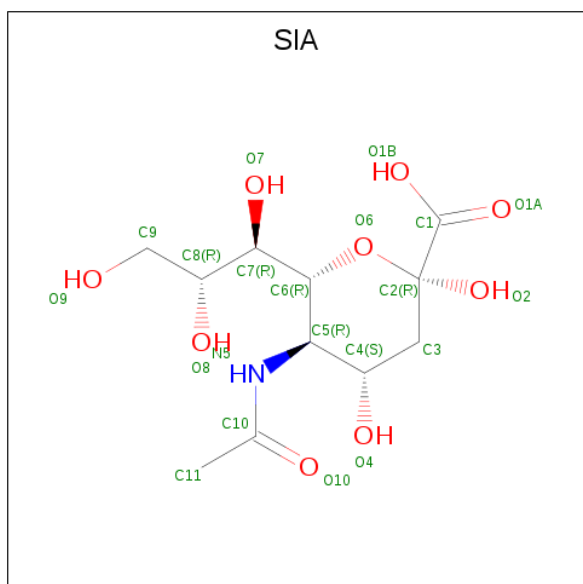
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			15	8	1	6		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is O-SIALIC ACID (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 5 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).

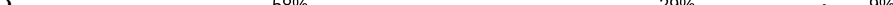



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	168	Total	O	0	0
			168	168		
6	B	48	Total	O	0	0
			48	48		

Note EDS was not executed.

- Chain B:  58% 29% 9%
- 

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	131.63Å 131.63Å 254.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.296	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4096	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

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: SIA, GAL, 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	0.50	1/2572 (0.0%)	0.74	0/3501
2	B	0.55	1/1251 (0.1%)	0.65	1/1688 (0.1%)
All	All	0.52	2/3823 (0.1%)	0.71	1/5189 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	GLU	CB-CG	-5.37	1.42	1.52
2	B	11	GLU	CB-CG	-5.12	1.42	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	160	PRO	N-CA-CB	5.56	109.97	103.30

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	A	2509	0	2417	98	1
2	B	1227	0	1083	54	1
3	A	85	0	78	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	25	5	0
4	A	20	0	17	2	0
5	A	11	0	9	0	0
6	A	168	0	0	27	0
6	B	48	0	0	9	1
All	All	4096	0	3629	147	3

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 20.

The worst 5 of 147 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:A:55:CYS:HB3	6:A:346:HOH:O	1.54	1.05
3:B:177:NAG:H3	3:B:178:NAG:HN2	1.31	0.96
1:A:121:SER:HB3	1:A:162:ARG:HH22	1.38	0.88
2:B:146:ASN:HD22	2:B:146:ASN:N	1.70	0.87
1:A:209:SER:HB2	6:A:445:HOH:O	1.74	0.87

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:180:HOH:O	6:B:180:HOH:O[11_446]	1.08	1.12
2:B:142:HIS:NE2	2:B:142:HIS:NE2[11_446]	2.11	0.09
1:A:206:ASN:OD1	1:A:216:ARG:NH1[3_655]	2.13	0.07

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	Percentiles	
1	A	319/325 (98%)	292 (92%)	23 (7%)	4 (1%)	13	18
2	B	158/176 (90%)	138 (87%)	14 (9%)	6 (4%)	3	3
All	All	477/501 (95%)	430 (90%)	37 (8%)	10 (2%)	8	9

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	GLU
1	A	260	GLY
2	B	159	TYR
2	B	158	ASP
1	A	263	ALA

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	279/289 (96%)	268 (96%)	11 (4%)	35	54
2	B	118/150 (79%)	109 (92%)	9 (8%)	14	22
All	All	397/439 (90%)	377 (95%)	20 (5%)	27	43

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

Mol	Chain	Res	Type
1	A	299	ILE
1	A	317	LEU
2	B	133	LEU
1	A	280	THR
1	A	293	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	ASN

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Mol	Chain	Res	Type
1	A	293	ASN
2	B	30	GLN
1	A	207	GLN
2	B	26	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
3	NAG	A	326	1	14,14,15	0.58	0	17,19,21	0.88	1 (5%)
3	NAG	A	327	1	14,14,15	0.49	0	17,19,21	0.72	0
3	NAG	A	328	1,3	14,14,15	0.60	0	17,19,21	0.99	1 (5%)
3	NAG	A	329	3	14,14,15	0.63	0	17,19,21	0.61	0
3	NAG	A	331	1	14,14,15	0.65	0	17,19,21	0.85	1 (5%)
4	SIA	A	332	5	17,20,21	0.69	0	19,28,31	0.65	0
5	GAL	A	333	3,4	11,11,12	0.69	0	15,15,17	0.70	1 (6%)
3	NAG	A	334	5	15,15,15	0.69	0	21,21,21	0.60	0
3	NAG	B	177	3,2	14,14,15	0.94	1 (7%)	17,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	178	3	14,14,15	0.80	1 (7%)	17,19,21	0.72	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	A	326	1	-	0/6/23/26	0/1/1/1
3	NAG	A	327	1	-	0/6/23/26	0/1/1/1
3	NAG	A	328	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	329	3	-	0/6/23/26	0/1/1/1
3	NAG	A	331	1	-	0/6/23/26	0/1/1/1
4	SIA	A	332	5	-	0/14/34/38	0/1/1/1
5	GAL	A	333	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	334	5	-	0/6/26/26	0/1/1/1
3	NAG	B	177	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	178	3	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	178	NAG	C1-C2	2.28	1.55	1.52
3	B	177	NAG	C1-C2	2.59	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	328	NAG	C2-N2-C7	-2.94	118.65	122.94
3	A	331	NAG	C2-N2-C7	-2.20	119.73	122.94
3	A	326	NAG	C2-N2-C7	-2.16	119.80	122.94
5	A	333	GAL	C1-C2-C3	2.13	112.35	109.66

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	178	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	332	SIA	2	0
3	B	177	NAG	5	0
3	B	178	NAG	5	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.