



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 3, 2016 – 11:26 PM EDT

PDB ID : 4YY9
Title : The structure of hemagglutinin from a H6N1 influenza virus (A/Taiwan/2/2013)
Authors : Wang, F.; Qi, J.; Bi, Y.; Zhang, W.; Wang, M.; Wang, M.; Liu, J.; Yan, J.; Shi, Y.; Gao, G.F.
Deposited on : 2015-03-23
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

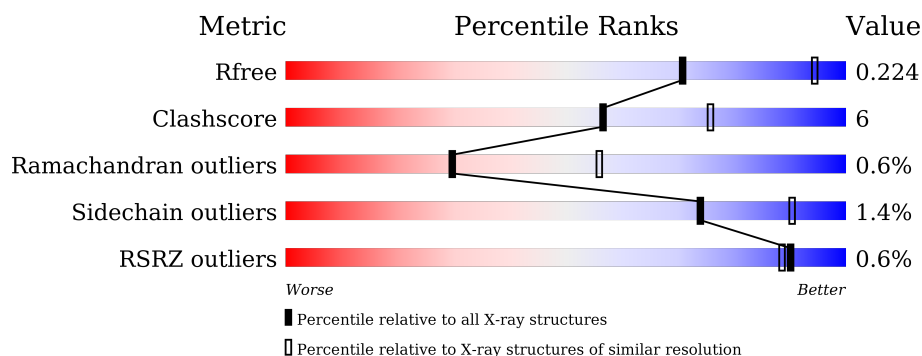
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

i

X-RAY DIFFRACTION

A.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

Mol	Chain	Length	Quality of chain
1	A	325	<div> <div></div> <div>84%</div> <div>15%</div> </div>
2	B	162	<div> <div></div> <div>90%</div> <div>10%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4126 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.

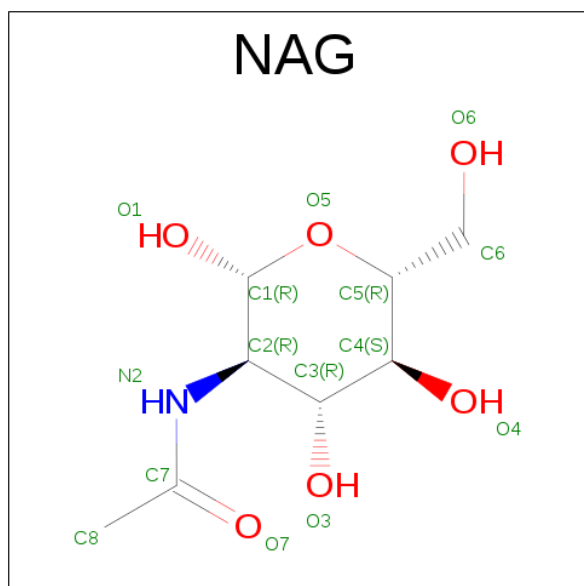
- Molecule 1 is a protein called HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2568	1627	438	490	13			

- Molecule 2 is a protein called HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	162	Total	C	N	O	S	0	0	0
			1303	814	225	257	7			

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



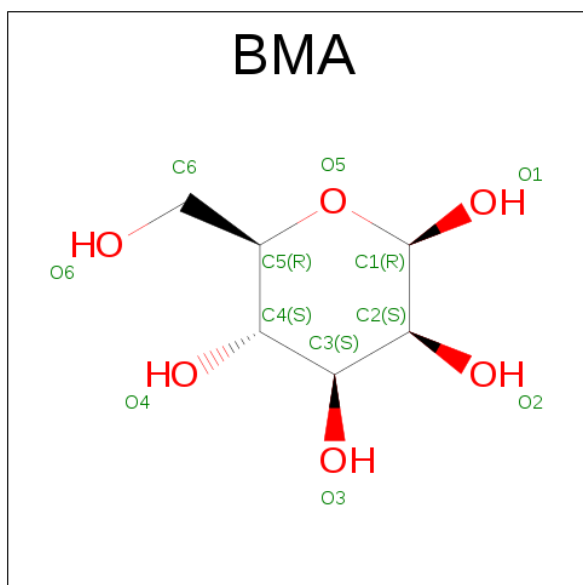
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	14	0
			14	8	1	5		
3	A	1	Total	C	N	O	14	0
			14	8	1	5		

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

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

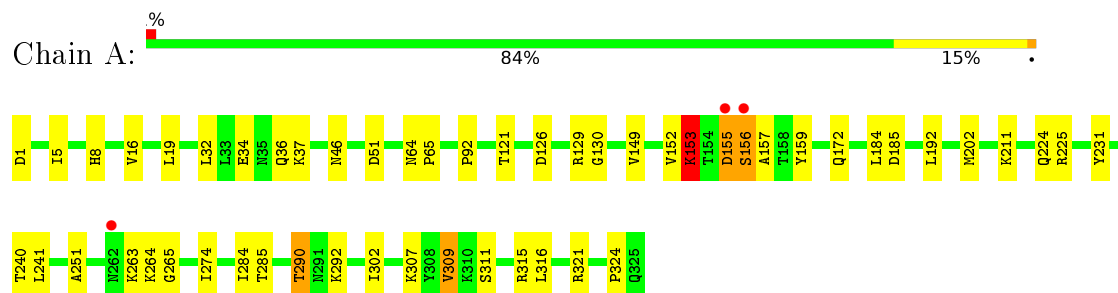
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	80	Total	O	0	0
			80	80		

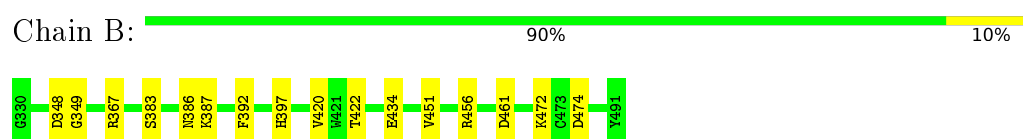
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: HA1



- Molecule 2: HA2



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	113.90Å 113.90Å 163.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.23 – 2.60 47.23 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.23-2.60) 99.9 (47.23-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.91 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.191 , 0.225 0.193 , 0.224	Depositor DCC
R_{free} test set	1845 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.1	EDS
Estimated twinning fraction	0.056 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 36907 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4126	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.39	1/2629 (0.0%)	0.52	0/3576
2	B	0.35	0/1331	0.49	0/1795
All	All	0.38	1/3960 (0.0%)	0.51	0/5371

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	LYS	CB-CG	-6.26	1.35	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2568	0	2513	38	0
2	B	1303	0	1208	12	1
3	A	28	0	26	0	0
3	B	28	0	24	0	0
4	B	11	0	10	0	0
5	A	108	0	0	14	0
5	B	80	0	0	4	0
All	All	4126	0	3781	46	1

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 6.

All (46) 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:37:LYS:NZ	5:A:701:HOH:O	1.92	1.01
1:A:315:ARG:NE	5:A:706:HOH:O	2.16	0.79
2:B:348:ASP:O	2:B:367:ARG:NH1	2.16	0.78
2:B:386:ASN:OD1	5:B:601:HOH:O	2.03	0.77
1:A:185:ASP:OD2	5:A:702:HOH:O	2.04	0.74
1:A:130:GLY:O	5:A:703:HOH:O	2.05	0.74
1:A:155:ASP:OD1	1:A:156:SER:N	2.20	0.72
1:A:240:THR:OG1	5:A:704:HOH:O	2.08	0.71
2:B:392:PHE:O	5:B:603:HOH:O	2.12	0.66
1:A:51:ASP:OD2	5:A:705:HOH:O	2.14	0.65
1:A:324:PRO:HD2	5:A:726:HOH:O	2.03	0.58
2:B:474:ASP:HB2	5:B:619:HOH:O	2.04	0.57
1:A:172:GLN:NE2	5:A:707:HOH:O	2.19	0.57
1:A:153:LYS:HB2	1:A:192:LEU:O	2.05	0.56
1:A:153:LYS:NZ	1:A:157:ALA:O	2.37	0.55
1:A:202:MET:HG2	1:A:241:LEU:HD11	1.89	0.54
1:A:32:LEU:HD11	1:A:316:LEU:HD22	1.90	0.53
1:A:315:ARG:NH1	5:A:724:HOH:O	2.41	0.53
1:A:126:ASP:OD2	1:A:129:ARG:NH1	2.42	0.52
1:A:149:VAL:HG13	1:A:251:ALA:HB3	1.92	0.52
1:A:265:GLY:H	1:A:302:ILE:HD11	1.74	0.52
1:A:309:VAL:HG13	1:A:311:SER:H	1.76	0.51
1:A:1:ASP:N	5:A:727:HOH:O	2.44	0.51
1:A:307:LYS:NZ	5:A:714:HOH:O	2.26	0.50
1:A:284:ILE:HG23	1:A:285:THR:HG23	1.95	0.48
1:A:16:VAL:HG12	1:A:315:ARG:HG2	1.96	0.48
1:A:51:ASP:HB2	1:A:274:ILE:HD12	1.97	0.47
2:B:367:ARG:HD2	2:B:367:ARG:HA	1.55	0.45
1:A:153:LYS:HE2	1:A:159:TYR:N	2.32	0.45
1:A:290:THR:HB	1:A:292:LYS:H	1.82	0.45
1:A:5:ILE:HD11	2:B:451:VAL:HG21	2.00	0.44
1:A:211:LYS:HD2	1:A:231:TYR:OH	2.18	0.43
1:A:152:VAL:HG12	1:A:153:LYS:N	2.33	0.43
1:A:321:ARG:NH2	5:A:720:HOH:O	2.32	0.43
1:A:184:LEU:HD22	1:A:225:ARG:HB2	2.01	0.42
2:B:397:HIS:ND1	5:B:602:HOH:O	2.08	0.42
1:A:19:LEU:HB2	2:B:434:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLU:OE2	1:A:36:GLN:HB2	2.20	0.42
1:A:309:VAL:HG22	2:B:422:THR:HA	2.01	0.42
1:A:8:HIS:HB2	2:B:349:GLY:O	2.20	0.41
1:A:264:LYS:NZ	5:A:728:HOH:O	2.46	0.41
1:A:92:PRO:HG3	1:A:224:GLN:HB2	2.03	0.41
1:A:315:ARG:CZ	5:A:706:HOH:O	2.66	0.41
2:B:383:SER:O	2:B:387:LYS:HG2	2.21	0.41
2:B:472:LYS:HA	2:B:472:LYS:HD3	1.89	0.41
1:A:64:ASN:HA	1:A:65:PRO:HD3	1.88	0.41

All (1) 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)
2:B:456:ARG:NH2	2:B:461:ASP:O[2_565]	2.16	0.04

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	323/325 (99%)	306 (95%)	14 (4%)	3 (1%)	21	42
2	B	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
All	All	483/487 (99%)	459 (95%)	21 (4%)	3 (1%)	30	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	SER
1	A	155	ASP
1	A	263	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	A	286/286 (100%)	281 (98%)	5 (2%)	68	88
2	B	137/137 (100%)	136 (99%)	1 (1%)	88	96
All	All	423/423 (100%)	417 (99%)	6 (1%)	74	90

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	121	THR
1	A	153	LYS
1	A	290	THR
1	A	309	VAL
2	B	420	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains 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](#)

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](#)

5 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	601	1	14,14,15	0.28	0	15,19,21	0.43	0
3	NAG	A	602	1	14,14,15	0.57	0	15,19,21	0.92	1 (6%)
3	NAG	B	501	3,2	14,14,15	0.26	0	15,19,21	0.35	0
3	NAG	B	502	3,4	14,14,15	0.22	0	15,19,21	0.34	0
4	BMA	B	503	3	11,11,12	0.24	0	15,15,17	1.01	2 (13%)

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	601	1	-	0/6/23/26	0/1/1/1
3	NAG	A	602	1	-	0/6/23/26	0/1/1/1
3	NAG	B	501	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	502	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	503	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	BMA	C1-O5-C5	2.08	115.20	112.14
4	B	503	BMA	C1-C2-C3	2.36	112.41	109.55
3	A	602	NAG	C1-O5-C5	3.11	116.71	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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>2	OWAB(Å ²)	Q<0.9
1	A	325/325 (100%)	-0.44	3 (0%) 85 83	24, 48, 82, 153	0
2	B	162/162 (100%)	-0.55	0 100 100	22, 36, 62, 90	0
All	All	487/487 (100%)	-0.48	3 (0%) 90 88	22, 43, 80, 153	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	ASN	4.6
1	A	155	ASP	3.2
1	A	156	SER	2.3

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](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	601	14/15	-	-	-	50,52,53,55	14
3	NAG	A	602	14/15	-	-	-	69,71,72,73	14
3	NAG	B	501	14/15	-	-	-	66,71,81,88	14
4	BMA	B	503	11/12	-	-	-	118,128,136,138	11
3	NAG	B	502	14/15	-	-	-	91,102,110,114	14

6.5 Other polymers [i](#)

There are no such residues in this entry.