



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:17 AM GMT

PDB ID : 1AA7
Title : INFLUENZA VIRUS MATRIX PROTEIN CRYSTAL STRUCTURE AT PH
4.0
Authors : Sha, B.; Luo, M.
Deposited on : 1997-01-24
Resolution : 2.08 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

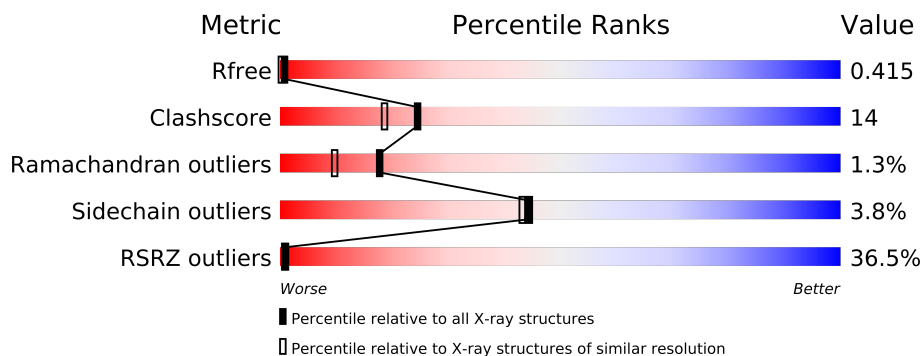
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.08 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}	66092	3396 (2.10-2.06)
Clashscore	79885	4085 (2.10-2.06)
Ramachandran outliers	78287	4045 (2.10-2.06)
Sidechain outliers	78261	4046 (2.10-2.06)
RSRZ outliers	66119	3397 (2.10-2.06)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	158	
1	B	158	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3238 atoms, of which 724 are hydrogens and 0 are deuterium.

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 INFLUENZA VIRUS MATRIX PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	158	Total	C	H	N	O	S	0	0	0
			1496	773	278	209	228	8			
1	B	157	Total	C	H	N	O	S	0	0	0
			1484	768	274	208	227	7			

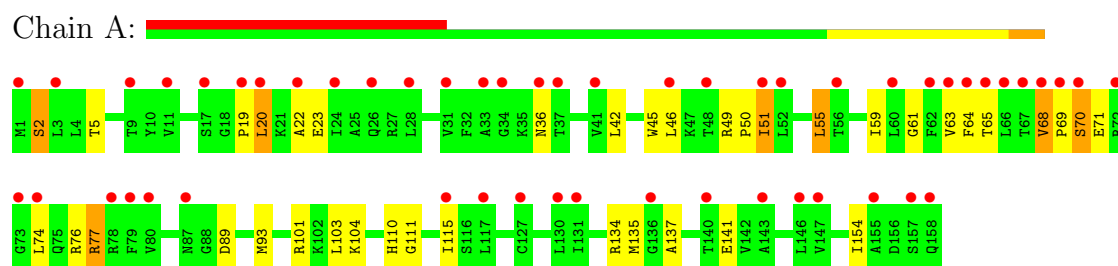
- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	49	Total	H	O	0	0
			147	98	49		
2	B	37	Total	H	O	0	0
			111	74	37		

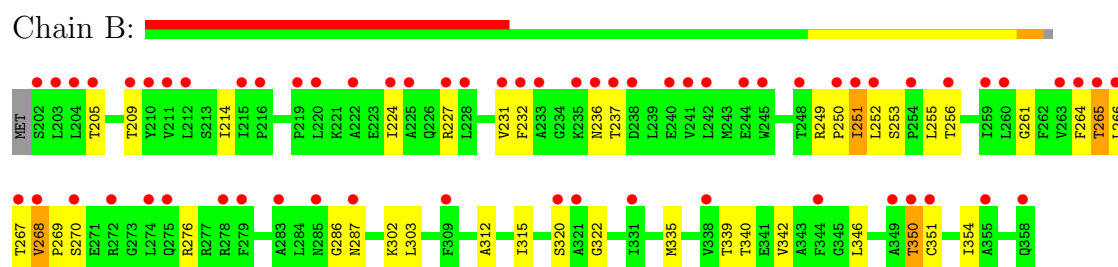
3 Residue-property plots

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 ($RSRZ > 2$). 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: INFLUENZA VIRUS MATRIX PROTEIN



• Molecule 1: INFLUENZA VIRUS MATRIX PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	66.17Å 66.17Å 135.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.08 24.47 – 2.06	Depositor EDS
% Data completeness (in resolution range)	94.7 (8.00-2.08) 91.8 (24.47-2.06)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 2.06Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.208 , 0.280 0.385 , 0.415	Depositor DCC
R_{free} test set	1904 reflections (10.51%)	DCC
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 28.9	EDS
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 20013 reflections	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	3238	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.49	0/1236	0.66	0/1668
1	B	0.52	0/1228	0.69	0/1658
All	All	0.50	0/2464	0.67	0/3326

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1218	278	981	38	2
1	B	1210	274	973	32	1
2	A	49	98	0	15	2
2	B	37	74	0	6	1
All	All	2514	724	1954	69	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (69) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:303:LEU:HD23	1:B:315:ILE:HD11	1.56	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:103:LEU:HD23	1:A:115:ILE:HD11	1.59	0.83
1:A:134:ARG:HH11	2:A:530:HOH:H2	1.28	0.81
1:B:261:GLY:O	1:B:265:THR:HG23	1.80	0.81
1:B:253:SER:HB3	1:B:256:THR:HG23	1.63	0.79
1:A:101:ARG:HH12	2:A:522:HOH:H2	1.31	0.74
1:A:61:GLY:O	1:A:65:THR:HG23	1.89	0.72
1:A:77:ARG:HH11	1:A:77:ARG:HG2	1.53	0.72
1:A:77:ARG:NH1	2:A:506:HOH:H2	1.89	0.70
1:A:74:LEU:HD13	2:A:506:HOH:O	1.91	0.69
1:B:250:PRO:O	1:B:251:ILE:HG12	1.94	0.68
1:B:232:PHE:HE1	1:B:267:THR:HG21	1.60	0.65
1:B:214:ILE:HD11	1:B:354:ILE:HB	1.76	0.65
1:A:36:ASN:HA	1:A:69:PRO:HG2	1.80	0.64
2:A:557:HOH:H1	1:B:335:MET:HG2	1.62	0.63
1:A:77:ARG:NH1	1:A:77:ARG:HG2	2.12	0.63
1:A:69:PRO:HG3	2:A:567:HOH:O	2.00	0.62
1:A:50:PRO:O	1:A:51:ILE:HG12	1.99	0.61
1:A:110:HIS:HE1	2:A:501:HOH:H1	1.50	0.60
1:A:65:THR:HG21	2:A:508:HOH:O	2.02	0.59
1:A:5:THR:HG22	2:A:505:HOH:H1	1.66	0.59
1:A:2:SER:OG	1:A:5:THR:HG23	2.03	0.58
1:B:227:ARG:HH21	2:B:536:HOH:H1	1.51	0.57
1:A:103:LEU:CD2	1:A:115:ILE:HD11	2.33	0.57
1:B:232:PHE:CE1	1:B:267:THR:HG21	2.39	0.56
1:B:339:THR:OG1	1:B:342:VAL:HG23	2.04	0.56
1:A:141:GLU:HB2	2:A:527:HOH:H2	1.72	0.55
1:B:320:SER:H	2:B:539:HOH:H2	1.52	0.55
1:B:231:VAL:HG22	1:B:236:ASN:HB3	1.90	0.54
1:B:214:ILE:CD1	1:B:354:ILE:HB	2.38	0.54
1:A:59:ILE:O	1:A:63:VAL:HG23	2.08	0.54
1:B:276:ARG:H	2:B:517:HOH:H2	1.54	0.53
1:B:346:LEU:O	1:B:350:THR:HG23	2.09	0.53
1:A:135:MET:SD	1:B:335:MET:SD	3.07	0.52
1:A:5:THR:HG22	2:A:505:HOH:O	2.10	0.52
1:A:76:ARG:H	2:A:515:HOH:H1	1.56	0.51
1:B:227:ARG:O	1:B:231:VAL:HG23	2.11	0.51
1:A:77:ARG:NH1	2:A:506:HOH:O	2.43	0.50
1:B:224:ILE:HD11	1:B:252:LEU:HD11	1.92	0.50
1:B:205:THR:O	1:B:209:THR:HG23	2.12	0.49
1:B:312:ALA:HB2	1:B:342:VAL:HG13	1.94	0.49
1:B:266:LEU:HG	1:B:340:THR:HG23	1.95	0.48
1:A:71:GLU:O	1:A:74:LEU:HG	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:20:LEU:HA	1:A:23:GLU:OE1	2.13	0.48
1:B:302:LYS:NZ	2:B:548:HOH:O	2.43	0.47
1:B:227:ARG:NH2	2:B:536:HOH:H2	2.13	0.46
1:B:264:PHE:O	1:B:268:VAL:HB	2.16	0.46
1:B:249:ARG:HA	1:B:249:ARG:NE	2.29	0.46
1:B:269:PRO:HG2	1:B:270:SER:H	1.80	0.46
1:B:214:ILE:HD11	1:B:351:CYS:O	2.16	0.46
1:A:46:LEU:HD11	1:A:64:PHE:HD2	1.81	0.45
1:A:111:GLY:O	1:A:115:ILE:HG23	2.16	0.45
1:B:253:SER:HB3	1:B:256:THR:CG2	2.42	0.45
1:B:214:ILE:HA	1:B:214:ILE:HD13	1.75	0.45
1:B:346:LEU:O	1:B:350:THR:CG2	2.65	0.44
1:A:5:THR:HG23	2:A:566:HOH:H1	1.83	0.44
1:B:256:THR:HG21	2:B:561:HOH:H1	1.83	0.43
1:A:46:LEU:HD11	1:A:64:PHE:CD2	2.54	0.42
1:A:45:TRP:O	1:A:49:ARG:HG2	2.20	0.42
1:A:19:PRO:O	1:A:22:ALA:HB3	2.19	0.42
1:A:36:ASN:CA	1:A:69:PRO:HG2	2.46	0.42
1:B:286:GLY:O	1:B:287:ASN:OD1	2.38	0.42
1:A:89:ASP:O	1:A:93:MET:HG3	2.20	0.41
1:A:55:LEU:HD13	1:A:154:ILE:HD13	2.02	0.41
1:A:36:ASN:HA	1:A:69:PRO:CG	2.49	0.41
1:A:64:PHE:O	1:A:68:VAL:HB	2.20	0.41
1:A:104:LYS:NZ	1:A:137:ALA:O	2.53	0.41
1:A:5:THR:CG2	2:A:566:HOH:H1	2.33	0.41
1:A:77:ARG:HH11	1:A:77:ARG:CG	2.25	0.40

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	Distance(Å)	Clash(Å)
1:A:70:SER:OG	2:A:529:HOH:O[5_665]	2.01	0.19
1:B:322:GLY:N	2:B:580:HOH:O[4_546]	2.13	0.07
1:A:70:SER:CB	2:A:529:HOH:O[5_665]	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	156/158 (99%)	152 (97%)	2 (1%)	2 (1%)	18	10
1	B	155/158 (98%)	149 (96%)	4 (3%)	2 (1%)	18	10
All	All	311/316 (98%)	301 (97%)	6 (2%)	4 (1%)	18	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	ILE
1	A	2	SER
1	B	237	THR
1	A	51	ILE

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	133/133 (100%)	127 (96%)	6 (4%)	38	35
1	B	132/133 (99%)	128 (97%)	4 (3%)	53	55
All	All	265/266 (100%)	255 (96%)	10 (4%)	44	43

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	42	LEU
1	A	55	LEU
1	A	68	VAL
1	A	70	SER
1	A	77	ARG
1	B	255	LEU
1	B	265	THR
1	B	268	VAL
1	B	350	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	HIS
1	B	292	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	158/158 (100%)	1.69	52 (32%) 1 1	6, 17, 38, 56	0
1	B	157/158 (99%)	2.06	63 (40%) 1 1	5, 18, 50, 71	0
All	All	315/316 (99%)	1.87	115 (36%) 1 1	5, 17, 47, 71	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.1
1	B	248	THR	5.9
1	B	270	SER	5.8
1	B	222	ALA	5.6
1	B	241	VAL	5.6
1	B	251	ILE	5.6
1	B	235	LYS	5.4
1	A	52	LEU	5.2
1	B	252	LEU	4.8
1	B	219	PRO	4.6
1	B	355	ALA	4.5
1	A	51	ILE	4.3
1	B	202	SER	4.2
1	B	203	LEU	4.1
1	A	63	VAL	4.1
1	B	260	LEU	4.0
1	B	268	VAL	4.0
1	B	274	LEU	4.0
1	B	279	PHE	3.8
1	B	250	PRO	3.7
1	A	20	LEU	3.7
1	A	70	SER	3.6
1	B	254	PRO	3.6
1	B	238	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	272	ARG	3.5
1	B	220	LEU	3.4
1	A	65	THR	3.4
1	A	78	ARG	3.4
1	B	204	LEU	3.4
1	B	256	THR	3.3
1	A	64	PHE	3.3
1	A	37	THR	3.3
1	B	264	PHE	3.3
1	A	67	THR	3.2
1	A	31	VAL	3.2
1	A	155	ALA	3.2
1	B	265	THR	3.2
1	B	240	GLU	3.1
1	B	349	ALA	3.1
1	A	158	GLN	3.1
1	A	46	LEU	3.1
1	B	350	THR	3.1
1	A	79	PHE	3.0
1	B	331	ILE	3.0
1	A	73	GLY	3.0
1	A	131	ILE	3.0
1	B	285	ASN	3.0
1	B	266	LEU	3.0
1	A	48	THR	2.9
1	B	351	CYS	2.9
1	A	22	ALA	2.9
1	A	74	LEU	2.9
1	B	245	TRP	2.9
1	A	19	PRO	2.8
1	B	263	VAL	2.8
1	B	267	THR	2.7
1	B	283	ALA	2.7
1	B	321	ALA	2.7
1	B	287	ASN	2.7
1	B	344	PHE	2.7
1	B	259	ILE	2.7
1	A	143	ALA	2.6
1	A	34	GLY	2.6
1	A	147	VAL	2.6
1	B	209	THR	2.6
1	B	309	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	232	PHE	2.5
1	A	80	VAL	2.5
1	A	24	ILE	2.5
1	B	228	LEU	2.5
1	B	224	ILE	2.5
1	B	236	ASN	2.5
1	A	72	ARG	2.5
1	B	211	VAL	2.5
1	A	26	GLN	2.5
1	A	36	ASN	2.4
1	B	225	ALA	2.4
1	B	242	LEU	2.4
1	A	68	VAL	2.4
1	B	338	VAL	2.4
1	B	244	GLU	2.4
1	A	41	VAL	2.4
1	A	130	LEU	2.3
1	B	278	ARG	2.3
1	A	127	CYS	2.3
1	A	117	LEU	2.3
1	A	87	ASN	2.3
1	A	140	THR	2.3
1	A	3	LEU	2.3
1	B	275	GLN	2.2
1	A	60	LEU	2.2
1	B	358	GLN	2.2
1	A	28	LEU	2.2
1	A	66	LEU	2.2
1	A	17	SER	2.2
1	A	62	PHE	2.2
1	A	115	ILE	2.2
1	A	146	LEU	2.2
1	B	212	LEU	2.2
1	A	11	VAL	2.2
1	B	237	THR	2.2
1	A	33	ALA	2.1
1	A	9	THR	2.1
1	A	56	THR	2.1
1	B	233	ALA	2.1
1	A	157	SER	2.1
1	B	227	ARG	2.1
1	A	69	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	320	SER	2.1
1	A	136	GLY	2.1
1	B	205	THR	2.1
1	B	216	PRO	2.1
1	B	231	VAL	2.0
1	B	210	TYR	2.0
1	B	215	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.