



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1EA3
Title : Influenza virus M1 protein
Authors : Arzt, S.
Deposited on : 2000-11-03
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

PERCENTILES INFOmissingINFO

1 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2499 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 MATRIX PROTEIN M1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	157	1209	768	208	226	7	32	0	0
1	B	157	1209	768	208	226	7	32	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	43	43	43	0	0
2	B	38	38	38	0	0

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	36.86Å 44.15Å 47.69Å 77.10° 67.83° 77.60°	Depositor
Resolution (Å)	14.98 – 2.30 33.19 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.7 (14.98-2.30) 94.7 (33.19-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.20Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.242 , 0.313 0.246 , 0.258	Depositor DCC
R_{free} test set	1307 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtrriage
Anisotropy	0.379	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2499	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 81.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3254e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

3 Model quality i

3.1 Standard geometry i

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	0.36	0/1227	0.59	0/1658
1	B	0.35	0/1227	0.59	0/1658
All	All	0.35	0/2454	0.59	0/3316

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

3.2 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	1209	0	1247	63	0
1	B	1209	0	1247	65	0
2	A	43	0	0	2	0
2	B	38	0	0	4	0
All	All	2499	0	2494	126	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 26.

The worst 5 of 126 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:B:37:THR:HG22	1:B:38:ASP:H	1.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ASN:O	1:A:94:ASP:N	2.06	0.89
1:A:68:VAL:HA	2:A:2017:HOH:O	1.82	0.79
1:A:82:ASN:HA	1:A:87:ASN:HD21	1.50	0.76
1:B:37:THR:HG22	1:B:38:ASP:N	2.05	0.71

There are no symmetry-related clashes.

3.3 Torsion angles [i](#)

3.3.1 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	155/164 (94%)	133 (86%)	13 (8%)	9 (6%)	1	0
1	B	155/164 (94%)	135 (87%)	9 (6%)	11 (7%)	1	0
All	All	310/328 (94%)	268 (86%)	22 (7%)	20 (6%)	1	0

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	51	ILE
1	A	70	SER
1	A	89	ASP
1	B	3	LEU

3.3.2 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	132/139 (95%)	128 (97%)	4 (3%)	41	57
1	B	132/139 (95%)	126 (96%)	6 (4%)	27	39
All	All	264/278 (95%)	254 (96%)	10 (4%)	33	47

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	76	ARG
1	B	126	SER
1	B	158	GLN
1	A	126	SER
1	B	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	92	ASN
1	B	82	ASN
1	B	87	ASN
1	B	133	ASN

3.3.3 RNA [i](#)

There are no RNA molecules in this entry.

3.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

3.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

3.6 Ligand geometry [i](#)

There are no ligands in this entry.

3.7 Other polymers

There are no such residues in this entry.

3.8 Polymer linkage issues

There are no chain breaks in this entry.

4 Fit of model and data [i](#)

4.1 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	153/164 (93%)	0.23	8 (5%) 27 34	18, 38, 75, 84	0
1	B	153/164 (93%)	0.21	5 (3%) 46 53	19, 39, 68, 83	0
All	All	306/328 (93%)	0.22	13 (4%) 36 43	18, 39, 72, 84	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	91	ASN	4.3
1	A	158	GLN	3.6
1	A	69	PRO	3.4
1	B	69	PRO	3.3
1	A	87	ASN	2.9

4.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.4 Ligands [i](#)

There are no ligands in this entry.

4.5 Other polymers [i](#)

There are no such residues in this entry.