



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Feb 9, 2017 – 11:02 am GMT

PDB ID : 5H0R
EMDB ID: : EMD-9564
Title : RNA dependent RNA polymerase ,vp4,dsRNA
Authors : Li, X.; Zhou, N.; Chen, W.; Zhu, B.; Wang, X.; Xu, B.; Wang, J.; Liu, H.;
Cheng, L.
Deposited on : 2016-10-06
Resolution : 3.90 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28906

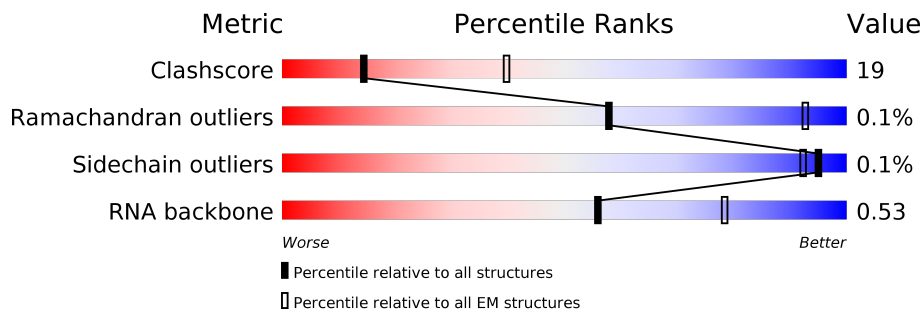
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	F	1225	61% 35% .
2	G	561	49% 34% . 16%
3	H	42	33% 57% 10%
4	I	42	21% 69% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15037 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	1183	Total	C	N	O	S	0	0
			9474	6022	1635	1781	36		

- Molecule 2 is a protein called VP4 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	473	Total	C	N	O	S	0	0
			3799	2432	635	716	16		

- Molecule 3 is a RNA chain called RNA (42-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	42	Total	C	N	O	P	0	0
			924	420	210	252	42		

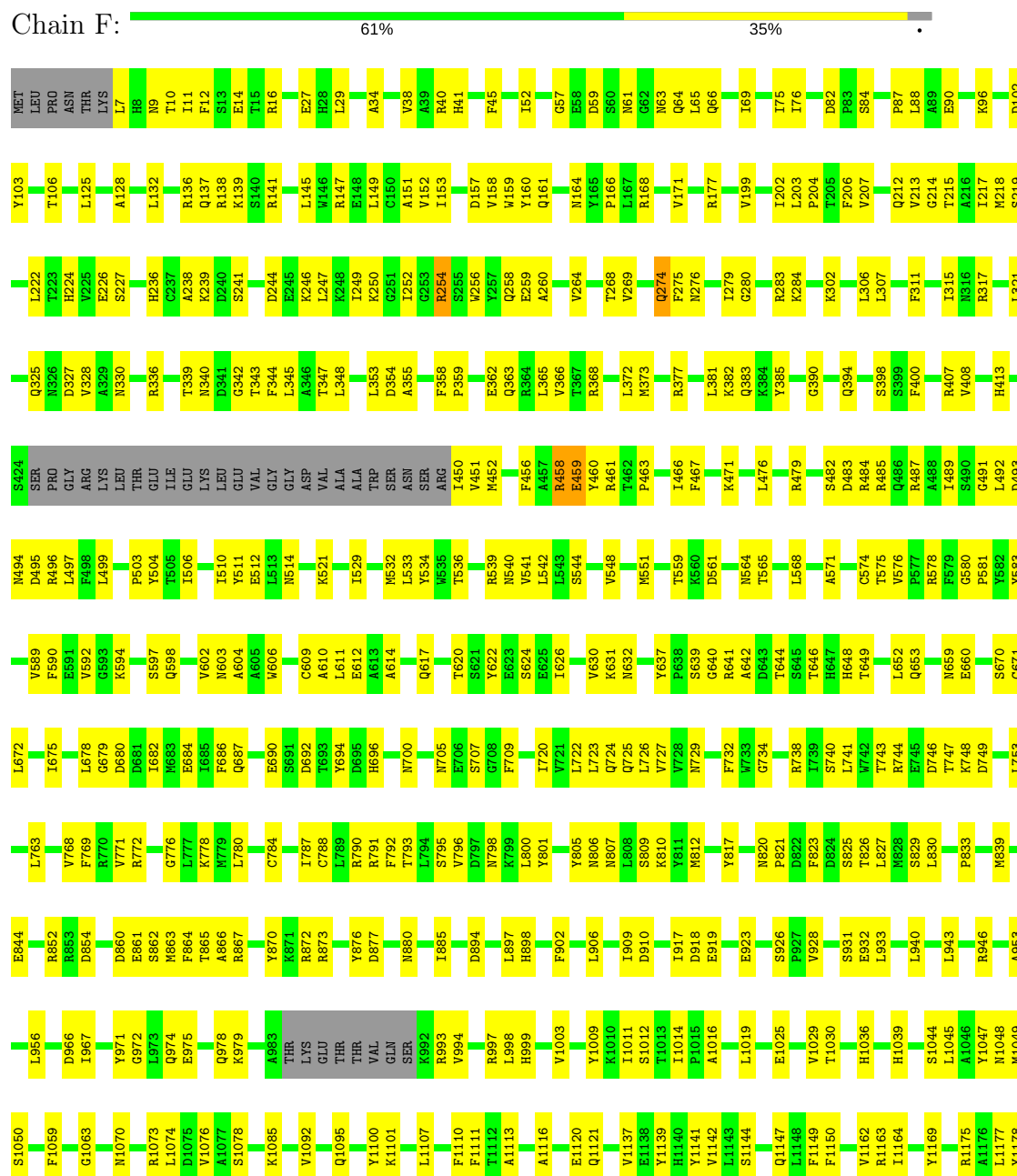
- Molecule 4 is a RNA chain called RNA (42-MER).

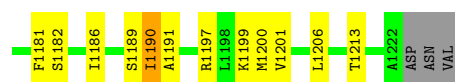
Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	42	Total	C	N	O	P	0	0
			840	378	84	336	42		

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

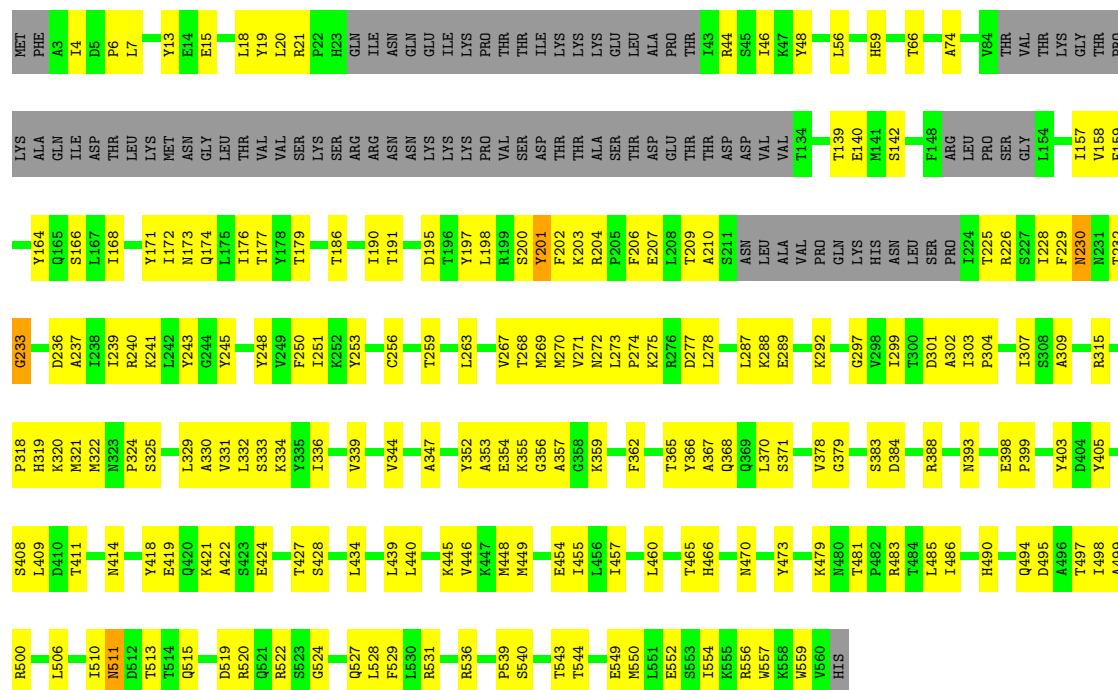
- Molecule 1: RNA-dependent RNA polymerase





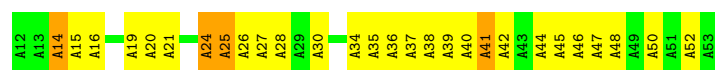
- Molecule 2: VP4 protein

Chain G:



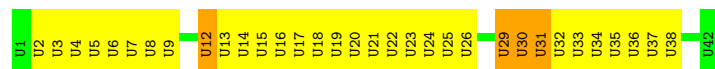
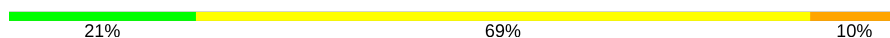
- Molecule 3: RNA (42-MER)

Chain H:



- Molecule 4: RNA (42-MER)

Chain I:



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	27000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality [i](#)

5.1 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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	F	0.35	0/9678	0.51	2/13098 (0.0%)
2	G	0.85	6/3879 (0.2%)	0.54	0/5253
3	H	0.29	0/1049	0.80	0/1634
4	I	0.24	0/923	0.83	0/1424
All	All	0.51	6/15529 (0.0%)	0.57	2/21409 (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	F	0	3
2	G	0	5
All	All	0	8

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	201	TYR	CD1-CE1	25.56	1.77	1.39
2	G	201	TYR	CD2-CE2	25.50	1.77	1.39
2	G	201	TYR	CE2-CZ	18.43	1.62	1.38
2	G	201	TYR	CE1-CZ	18.32	1.62	1.38
2	G	201	TYR	CG-CD1	14.88	1.58	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	458	ARG	N-CA-C	6.58	128.76	111.00
1	F	458	ARG	C-N-CA	5.28	134.89	121.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	254	ARG	Peptide
1	F	459	GLU	Peptide
1	F	926	SER	Peptide
2	G	230	ASN	Peptide
2	G	233	GLY	Peptide

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	F	9474	0	9361	327	0
2	G	3799	0	3780	188	0
3	H	924	0	463	31	0
4	I	840	0	421	36	0
All	All	15037	0	14025	562	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 19.

The worst 5 of 562 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)
2:G:46:ILE:CD1	2:G:201:TYR:CD1	1.75	1.66
2:G:201:TYR:CD2	2:G:201:TYR:CE2	1.77	1.64
2:G:46:ILE:CG1	2:G:201:TYR:CD1	1.77	1.64
2:G:201:TYR:CE1	2:G:201:TYR:CD1	1.77	1.61
2:G:46:ILE:CD1	2:G:201:TYR:CG	1.80	1.58

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 PDB entries followed by that with respect to all EM entries.

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	F	1177/1225 (96%)	1078 (92%)	97 (8%)	2 (0%)	51	84
2	G	463/561 (82%)	421 (91%)	42 (9%)	0	100	100
All	All	1640/1786 (92%)	1499 (91%)	139 (8%)	2 (0%)	58	88

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	451	VAL
1	F	1190	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 PDB entries followed by that with respect to all EM entries.

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	F	1026/1063 (96%)	1025 (100%)	1 (0%)	94	97
2	G	416/500 (83%)	416 (100%)	0	100	100
All	All	1442/1563 (92%)	1441 (100%)	1 (0%)	95	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	274	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	820	ASN
1	F	1121	GLN
2	G	494	GLN
1	F	1084	HIS
1	F	1095	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	H	41/42 (97%)	7 (17%)	0
4	I	41/42 (97%)	6 (14%)	0
All	All	82/84 (97%)	13 (15%)	0

5 of 13 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	H	14	A
3	H	24	A
3	H	25	A
3	H	41	A
3	H	42	A

There are no RNA pucker outliers to report.

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.