



wwPDB EM Validation Summary Report ⓘ

Oct 22, 2023 – 12:07 AM JST

PDB ID : 8JSM
EMDB ID : EMD-36623
Title : The structure of EBOV L-VP35-RNA complex (conformation 1)
Authors : Qi, P.; Yi, S.
Deposited on : 2023-06-20
Resolution : 3.30 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

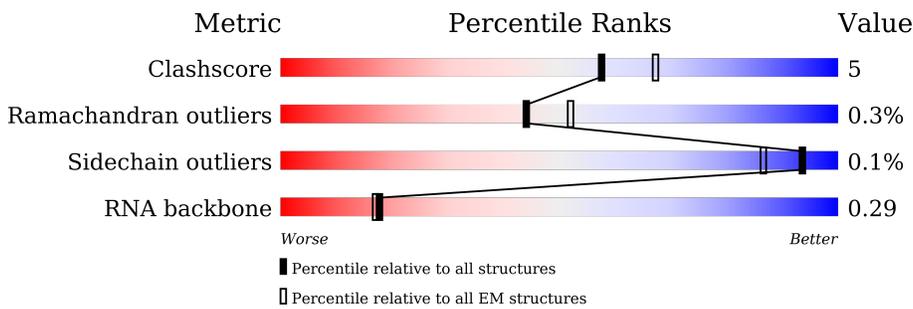
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	A	2212	55% (green), 7% (yellow), 38% (grey)
2	B	340	62% (green), 15% (yellow), 24% (grey)
2	C	340	26% (green), 71% (grey)
2	D	340	14% (green), 5% (yellow), 80% (grey)
2	E	340	16% (green), 80% (grey)
3	G	18	33% (green), 22% (yellow), 44% (grey)

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 14856 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-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1362	10897	7002	1853	1986	56	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	759	ASP	GLY	conflict	UNP A0A1C4HDB0

- Molecule 2 is a protein called Polymerase cofactor VP35.

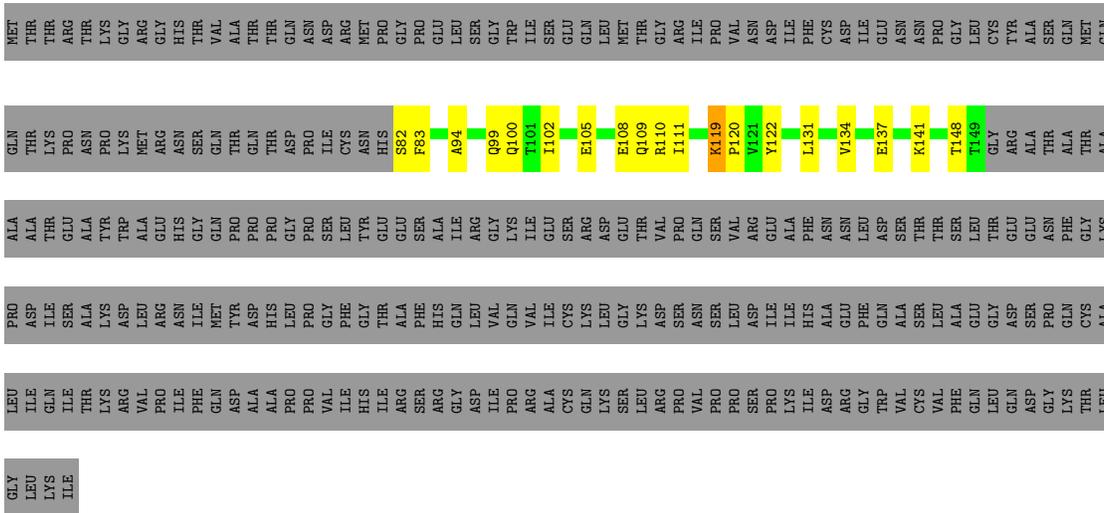
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	260	1989	1247	342	391	9	1	0
2	C	99	737	460	119	154	4	0	0
2	D	68	511	321	80	106	4	0	0
2	E	67	509	318	84	104	3	0	0

- Molecule 3 is a RNA chain called The leader sequence of EBOV genome..

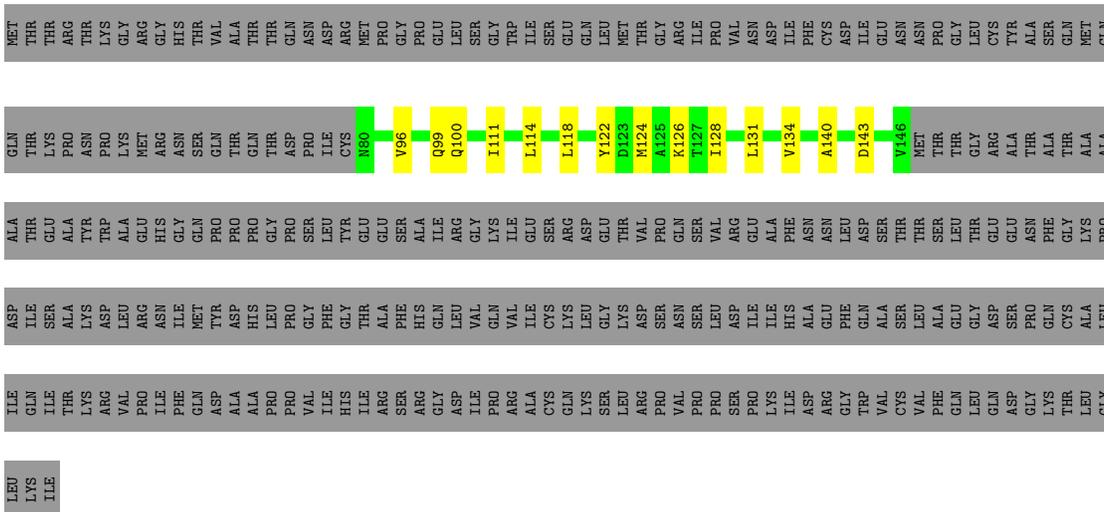
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	G	10	212	94	34	74	10	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

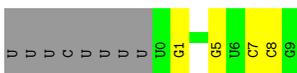
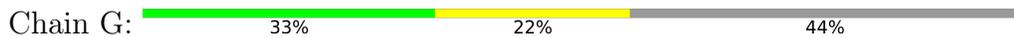
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	



• Molecule 2: Polymerase cofactor VP35



• Molecule 3: The leader sequence of EBOV genome.



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	197788	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

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:
ZN

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	0.25	0/11168	0.47	0/15169
2	B	0.26	0/2028	0.48	0/2759
2	C	0.26	0/750	0.44	0/1027
2	D	0.24	0/514	0.43	0/698
2	E	0.24	0/513	0.49	0/697
3	G	0.18	0/235	0.71	0/364
All	All	0.25	0/15208	0.48	0/20714

There are no bond length outliers.

There are no bond angle outliers.

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	10897	0	10861	94	0
2	B	1989	0	1963	33	0
2	C	737	0	704	8	0
2	D	511	0	519	13	0
2	E	509	0	509	11	0
3	G	212	0	107	3	0
4	A	1	0	0	0	0
All	All	14856	0	14663	147	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 5.

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)
2:E:99:GLN:NE2	2:E:100:GLN:OE1	2.05	0.90
1:A:1153:CYS:SG	1:A:1347:HIS:CE1	2.68	0.86
1:A:959:ASN:O	1:A:959:ASN:ND2	2.21	0.74
1:A:905:VAL:HG13	1:A:911:GLY:HA3	1.69	0.73
1:A:1218:GLU:OE1	1:A:1247:ARG:NH2	2.27	0.68

There are no symmetry-related clashes.

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 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	A	1354/2212 (61%)	1266 (94%)	83 (6%)	5 (0%)	34	66
2	B	259/340 (76%)	245 (95%)	14 (5%)	0	100	100
2	C	97/340 (28%)	93 (96%)	4 (4%)	0	100	100
2	D	66/340 (19%)	63 (96%)	2 (3%)	1 (2%)	10	38
2	E	65/340 (19%)	63 (97%)	2 (3%)	0	100	100
All	All	1841/3572 (52%)	1730 (94%)	105 (6%)	6 (0%)	44	71

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	LEU
1	A	751	VAL
1	A	851	THR
1	A	1174	VAL
1	A	829	ILE

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 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	A	1210/1994 (61%)	1209 (100%)	1 (0%)	93	97
2	B	219/294 (74%)	219 (100%)	0	100	100
2	C	79/294 (27%)	79 (100%)	0	100	100
2	D	59/294 (20%)	58 (98%)	1 (2%)	60	78
2	E	58/294 (20%)	58 (100%)	0	100	100
All	All	1625/3170 (51%)	1623 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	959	ASN
2	D	119	LYS

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	307	GLN
1	A	795	HIS
1	A	1321	ASN
2	E	99	GLN
2	E	100	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	G	9/18 (50%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	G	1	G

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Mol	Chain	Res	Type
3	G	8	C

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.