Full wwPDB EM Validation Report ⓘ

Feb 20, 2025 – 12:06 pm GMT

PDB ID	:	9F0J
EMDB ID	:	EMD-50111
Title	:	Cryo-EM structure of the I923V MDA5-dsRNA filament without nucleotide
Authors	:	Singh, R.; Herrero del Valle, A.; Modis, Y.
Deposited on	:	2024-04-16
Resolution	:	3.35 Å(reported)
Based on initial model	:	7BKQ

This is a Full wwPDB EM Validation 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:

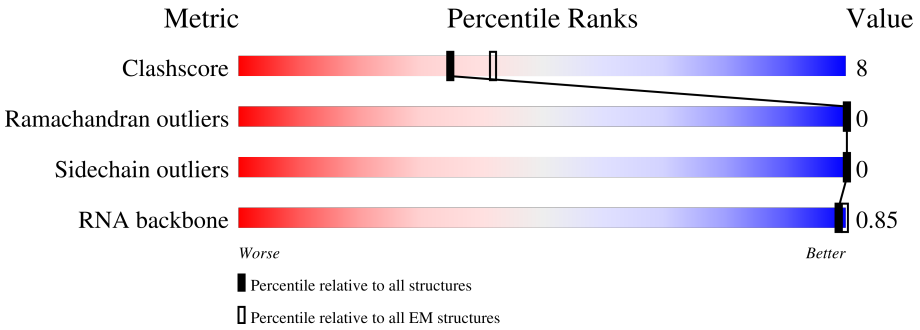
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.35 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	1028	49% 13% 38%
2	X	15	93% 7%
3	Z	15	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11368 atoms, of which 5586 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 Interferon-induced helicase C domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	640	10403	3273	5261	888	948	33	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q8R5F7
A	-19	GLY	-	expression tag	UNP Q8R5F7
A	-18	SER	-	expression tag	UNP Q8R5F7
A	-17	SER	-	expression tag	UNP Q8R5F7
A	-16	HIS	-	expression tag	UNP Q8R5F7
A	-15	HIS	-	expression tag	UNP Q8R5F7
A	-14	HIS	-	expression tag	UNP Q8R5F7
A	-13	HIS	-	expression tag	UNP Q8R5F7
A	-12	HIS	-	expression tag	UNP Q8R5F7
A	-11	HIS	-	expression tag	UNP Q8R5F7
A	-10	SER	-	expression tag	UNP Q8R5F7
A	-9	SER	-	expression tag	UNP Q8R5F7
A	-8	GLY	-	expression tag	UNP Q8R5F7
A	-7	ARG	-	expression tag	UNP Q8R5F7
A	-6	GLU	-	expression tag	UNP Q8R5F7
A	-5	ASN	-	expression tag	UNP Q8R5F7
A	-4	LEU	-	expression tag	UNP Q8R5F7
A	-3	TYR	-	expression tag	UNP Q8R5F7
A	-2	PHE	-	expression tag	UNP Q8R5F7
A	-1	GLN	-	expression tag	UNP Q8R5F7
A	0	GLY	-	expression tag	UNP Q8R5F7
A	1	HIS	-	expression tag	UNP Q8R5F7
A	2	MET	-	expression tag	UNP Q8R5F7
A	?	-	ASP	deletion	UNP Q8R5F7
A	?	-	LYS	deletion	UNP Q8R5F7
A	?	-	SER	deletion	UNP Q8R5F7
A	?	-	ASP	deletion	UNP Q8R5F7
A	?	-	ASP	deletion	UNP Q8R5F7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP Q8R5F7
A	?	-	ALA	deletion	UNP Q8R5F7
A	?	-	SER	deletion	UNP Q8R5F7
A	?	-	SER	deletion	UNP Q8R5F7
A	?	-	CYS	deletion	UNP Q8R5F7
A	?	-	ASN	deletion	UNP Q8R5F7
A	?	-	ASP	deletion	UNP Q8R5F7
A	?	-	GLN	deletion	UNP Q8R5F7
A	?	-	LEU	deletion	UNP Q8R5F7
A	?	-	LYS	deletion	UNP Q8R5F7
A	?	-	GLY	deletion	UNP Q8R5F7
A	?	-	ASP	deletion	UNP Q8R5F7
A	?	-	VAL	deletion	UNP Q8R5F7
A	923	VAL	ILE	engineered mutation	UNP Q8R5F7

- Molecule 2 is a RNA chain called RNA (5'-UCCAUGCGCAUGACG-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
2	X	15	Total	C	H	N	O	P	0	0
			480	142	162	56	105	15		

- Molecule 3 is a RNA chain called RNA (5'-CGUCAUGCGCAUGGA-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
3	Z	15	Total	C	H	N	O	P	0	0
			484	143	163	58	105	15		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

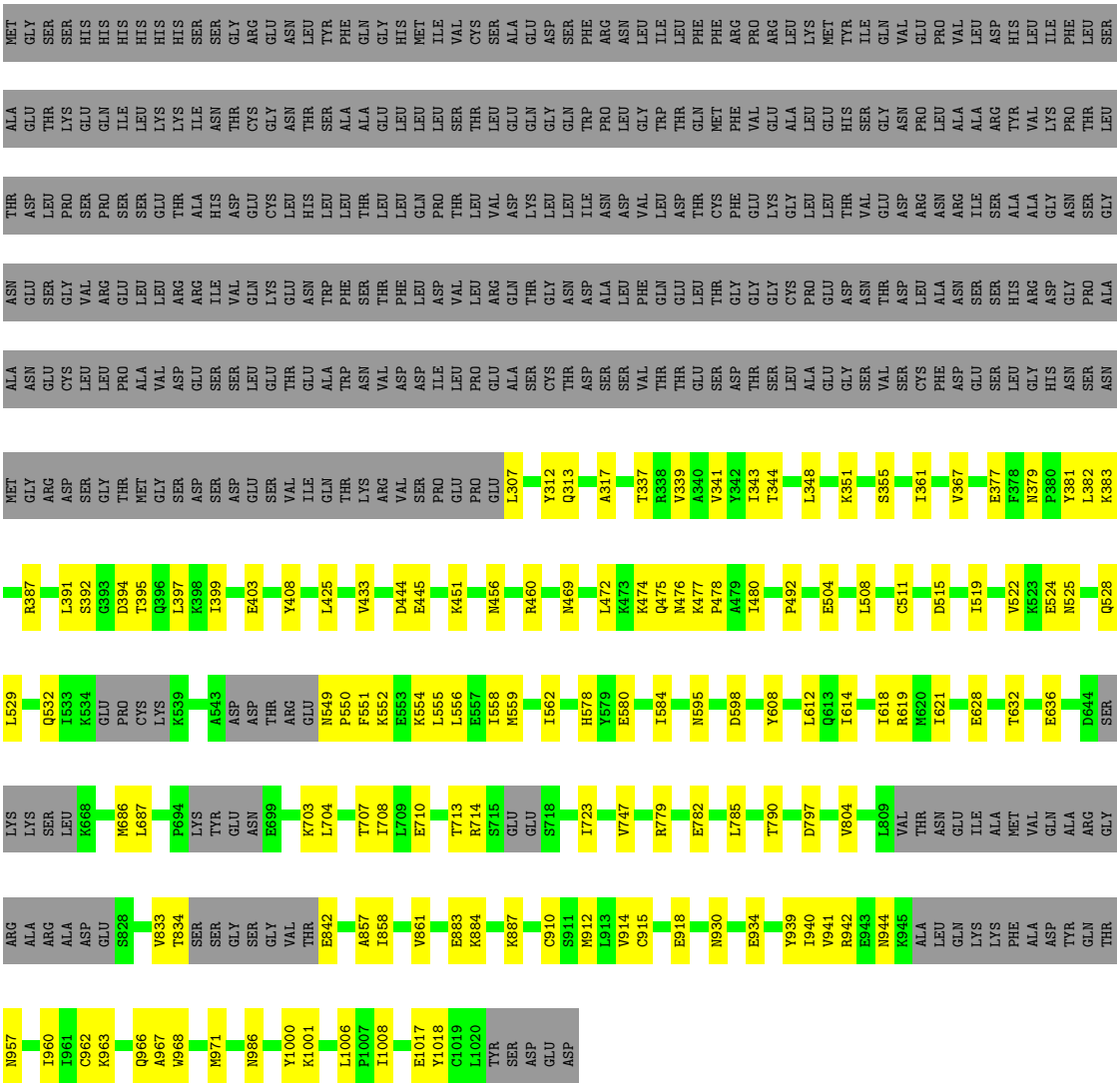
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

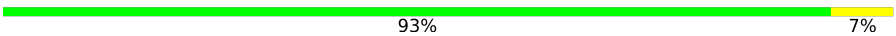
- Molecule 1: Interferon-induced helicase C domain-containing protein 1

Chain A:



- Molecule 2: RNA (5'-UCCAUGCGCAUGACG-3')

Chain X:



• Molecule 3: RNA (5'-CGUCAUGCGCAUGGA-3')

Chain Z: 100%

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=91.63°, rise=44.84 Å, axial sym=C1	Depositor
Number of segments used	547562	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 ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	0.28	0/5222	0.46	0/7011
2	X	0.39	0/354	0.76	0/549
3	Z	0.41	0/358	0.80	0/556
All	All	0.30	0/5934	0.52	0/8116

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

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	5142	5261	5261	89	0
2	X	318	162	163	1	0
3	Z	321	163	163	0	0
4	A	1	0	0	0	0
All	All	5782	5586	5587	89	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 8.

All (89) 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:779:ARG:NH2	1:A:797:ASP:OD1	2.08	0.87
1:A:960:ILE:HD11	1:A:971:MET:SD	2.29	0.72
1:A:703:LYS:O	1:A:707:THR:HG23	1.91	0.71
1:A:511:CYS:SG	1:A:519:ILE:HD11	2.31	0.70
1:A:472:LEU:O	1:A:476:ASN:N	2.26	0.68
1:A:934:GLU:N	1:A:934:GLU:OE1	2.27	0.68
1:A:782:GLU:N	1:A:782:GLU:OE1	2.28	0.67
1:A:469:ASN:ND2	1:A:480:ILE:O	2.29	0.66
1:A:1006:LEU:HD13	1:A:1008:ILE:CG1	2.25	0.66
1:A:957:ASN:N	1:A:971:MET:O	2.30	0.65
1:A:710:GLU:O	1:A:713:THR:HG22	1.98	0.64
1:A:967:ALA:O	1:A:986:ASN:ND2	2.31	0.64
1:A:714:ARG:O	1:A:714:ARG:NH1	2.32	0.62
1:A:842:GLU:N	1:A:842:GLU:OE1	2.33	0.62
1:A:399:ILE:HD11	1:A:403:GLU:HB3	1.83	0.61
1:A:1006:LEU:HD13	1:A:1008:ILE:HG12	1.82	0.60
1:A:551:PHE:CE1	1:A:687:LEU:HD22	2.36	0.60
1:A:524:GLU:OE2	1:A:525:ASN:ND2	2.35	0.60
1:A:361:ILE:O	1:A:361:ILE:HG23	2.03	0.59
1:A:351:LYS:O	1:A:355:SER:N	2.36	0.58
1:A:559:MET:SD	1:A:612:LEU:HD11	2.45	0.56
1:A:554:LYS:HE3	1:A:558:ILE:HD11	1.86	0.56
1:A:1006:LEU:HD12	1:A:1006:LEU:O	2.05	0.56
1:A:723:ILE:HD12	1:A:785:LEU:HD21	1.88	0.56
1:A:522:VAL:O	1:A:522:VAL:HG13	2.07	0.54
1:A:1006:LEU:HD13	1:A:1008:ILE:HG13	1.88	0.54
1:A:1017:GLU:OE1	1:A:1017:GLU:N	2.39	0.54
1:A:337:THR:O	1:A:341:VAL:HG23	2.09	0.53
1:A:475:GLN:N	1:A:475:GLN:OE1	2.41	0.53
1:A:532:GLN:O	1:A:532:GLN:NE2	2.37	0.53
1:A:555:LEU:HD23	1:A:555:LEU:O	2.09	0.53
1:A:552:LYS:O	1:A:556:LEU:HD13	2.08	0.53
1:A:918:GLU:N	1:A:918:GLU:OE1	2.42	0.53
1:A:504:GLU:O	1:A:508:LEU:HD23	2.09	0.52
1:A:915:CYS:SG	1:A:930:ASN:ND2	2.79	0.52
1:A:790:THR:HG22	1:A:790:THR:O	2.09	0.52
1:A:307:LEU:HD13	1:A:381:TYR:CE2	2.45	0.51
1:A:312:TYR:HB2	1:A:522:VAL:HG21	1.93	0.51
1:A:614:ILE:O	1:A:618:ILE:N	2.44	0.50
1:A:460:ARG:HE	1:A:884:LYS:HD2	1.77	0.49
1:A:636:GLU:OE1	1:A:942:ARG:NH2	2.45	0.49
1:A:833:VAL:O	1:A:834:THR:OG1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:TYR:O	1:A:382:LEU:HD12	2.13	0.48
1:A:621:ILE:H	1:A:621:ILE:HD12	1.78	0.48
1:A:492:PRO:CG	1:A:858:ILE:HD11	2.44	0.48
1:A:704:LEU:O	1:A:708:ILE:HG22	2.14	0.47
1:A:492:PRO:HG3	1:A:858:ILE:HD11	1.97	0.47
1:A:394:ASP:OD1	1:A:395:THR:N	2.48	0.47
1:A:962:CYS:SG	1:A:963:LYS:N	2.88	0.47
1:A:636:GLU:OE1	1:A:944:ASN:ND2	2.48	0.46
1:A:559:MET:O	1:A:562:ILE:HG22	2.16	0.46
1:A:1018:TYR:CD1	1:A:1018:TYR:O	2.69	0.46
1:A:939:TYR:CD1	1:A:960:ILE:HG23	2.51	0.46
1:A:962:CYS:N	1:A:966:GLN:O	2.44	0.46
1:A:555:LEU:HD21	1:A:608:TYR:CD1	2.51	0.45
1:A:313:GLN:HB3	1:A:339:VAL:HG22	1.98	0.45
1:A:344:THR:O	1:A:348:LEU:HD13	2.17	0.45
1:A:425:LEU:HD22	1:A:433:VAL:O	2.17	0.45
1:A:528:GLN:OE1	1:A:528:GLN:N	2.41	0.45
1:A:628:GLU:O	1:A:632:THR:HG23	2.18	0.44
1:A:444:ASP:OD1	1:A:445:GLU:N	2.51	0.44
1:A:910:CYS:O	1:A:912:MET:N	2.50	0.43
1:A:394:ASP:OD1	1:A:395:THR:HG23	2.18	0.43
1:A:595:ASN:ND2	1:A:598:ASP:OD2	2.51	0.43
1:A:337:THR:HG21	1:A:377:GLU:HG3	2.00	0.43
1:A:474:LYS:HB3	1:A:475:GLN:OE1	2.17	0.43
1:A:804:VAL:O	1:A:804:VAL:HG13	2.17	0.43
1:A:399:ILE:HG12	1:A:403:GLU:HB2	2.01	0.43
1:A:387:ARG:HB2	1:A:408:TYR:HA	2.01	0.42
1:A:857:ALA:O	1:A:861:VAL:HG23	2.19	0.42
1:A:1000:TYR:O	1:A:1001:LYS:HB2	2.19	0.42
1:A:307:LEU:HD13	1:A:381:TYR:HE2	1.83	0.42
1:A:578:HIS:CD2	2:X:15:G:H4'	2.55	0.42
1:A:914:VAL:HG13	1:A:968:TRP:CH2	2.54	0.42
1:A:391:LEU:CD1	1:A:397:LEU:HD22	2.50	0.42
1:A:367:VAL:HG23	1:A:392:SER:HB3	2.02	0.42
1:A:580:GLU:O	1:A:584:ILE:HG12	2.20	0.42
1:A:747:VAL:HG12	1:A:747:VAL:O	2.20	0.41
1:A:883:GLU:O	1:A:887:LYS:HG2	2.21	0.41
1:A:549:ASN:N	1:A:550:PRO:HD2	2.35	0.41
1:A:451:LYS:O	1:A:456:ASN:HB3	2.21	0.41
1:A:686:MET:SD	1:A:687:LEU:N	2.93	0.41
1:A:522:VAL:HG11	1:A:529:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:940:ILE:HG22	1:A:941:VAL:N	2.35	0.41
1:A:618:ILE:HG22	1:A:619:ARG:N	2.35	0.41
1:A:317:ALA:HB1	1:A:343:ILE:HD11	2.02	0.41
1:A:379:ASN:O	1:A:383:LYS:HG3	2.20	0.41
1:A:511:CYS:O	1:A:515:ASP:N	2.53	0.41
1:A:477:LYS:HB2	1:A:478:PRO:HD3	2.03	0.40

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	A	622/1028 (60%)	590 (95%)	32 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	A	572/918 (62%)	572 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	ASN
1	A	476	ASN
1	A	578	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	X	14/15 (93%)	0	0
3	Z	14/15 (93%)	0	0
All	All	28/30 (93%)	0	0

There are no RNA backbone outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.