



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2025 – 12:07 AM JST

PDB ID : 9IIZ  
EMDB ID : EMD-60610  
Title : Cryo-EM Structure of EfPiwi-piRNA-target (25-nt, comma)  
Authors : Li, Z.Q.; Xu, Q.K.; Wu, J.P.; Shen, E.Z.  
Deposited on : 2024-06-21  
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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) : 2.41.2

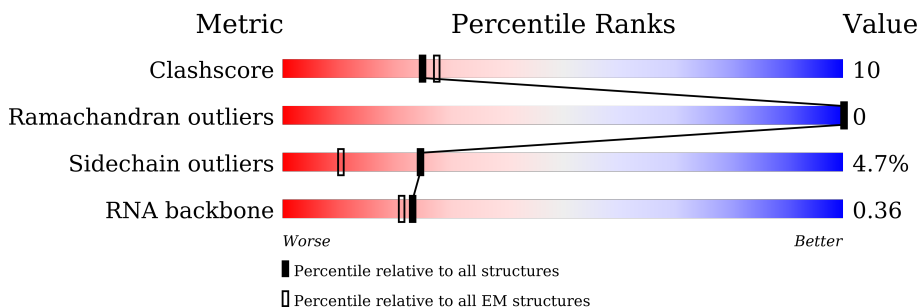
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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  $\geq 3$ , 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	987	27% 10% 62%
2	B	25	16% 28% 40% 16%
3	C	24	50% 46%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4080 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 Piwi.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	377	Total	C	N	O	S	0	0
			3043	1949	528	546	20		

- Molecule 2 is a RNA chain called RNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	25	Total	C	N	O	P	0	0
			529	237	92	175	25		

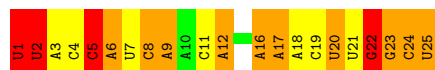
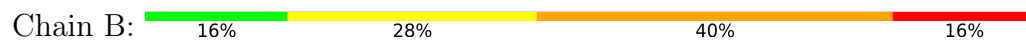
- Molecule 3 is a RNA chain called RNA (5'-R(P\*AP\*GP\*CP\*CP\*AP\*AP\*GP\*UP\*UP\*UP\*CP\*CP\*AP\*UP\*GP\*UP\*UP\*GP\*AP\*UP\*GP\*GP\*UP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	24	Total	C	N	O	P	0	0
			508	228	88	168	24		

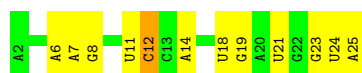




• Molecule 2: RNA (25-MER)



• Molecule 3: RNA (5'-R(P\*AP\*GP\*CP\*CP\*AP\*AP\*GP\*UP\*UP\*UP\*CP\*CP\*AP\*UP\*GP\*UP\*UP\*GP\*AP\*UP\*GP\*GP\*UP\*A)-3')



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67583	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor

## 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	0.30	0/3114	0.74	11/4213 (0.3%)
2	B	0.70	1/590 (0.2%)	1.39	7/914 (0.8%)
3	C	0.38	0/567	1.20	3/879 (0.3%)
All	All	0.39	1/4271 (0.0%)	0.94	21/6006 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	U	OP3-P	-10.63	1.48	1.61

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	967	LEU	CA-CB-CG	8.34	134.49	115.30
1	A	982	ASP	CB-CG-OD1	7.92	125.43	118.30
3	C	12	C	C2-N1-C1'	7.62	127.19	118.80
1	A	803	LEU	CA-CB-CG	7.48	132.51	115.30
1	A	736	MET	CA-CB-CG	7.44	125.95	113.30
2	B	1	U	OP2-P-O3'	6.93	120.44	105.20
2	B	1	U	P-O3'-C3'	6.70	127.73	119.70
2	B	5	C	C2-N1-C1'	6.63	126.10	118.80
1	A	739	LYS	CA-CB-CG	6.62	127.97	113.40
3	C	12	C	N1-C2-O2	6.31	122.68	118.90
1	A	736	MET	CB-CG-SD	6.30	131.31	112.40
1	A	694	ASP	CB-CG-OD1	6.09	123.78	118.30
2	B	2	U	O5'-P-OP2	-5.47	100.78	105.70
3	C	12	C	C6-N1-C1'	-5.43	114.28	120.80
1	A	714	LEU	CA-CB-CG	5.27	127.43	115.30
2	B	22	G	OP2-P-O3'	5.27	116.79	105.20
1	A	817	MET	CA-CB-CG	5.27	122.25	113.30
1	A	751	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	953	ARG	C-N-CA	5.19	134.68	121.70
2	B	8	C	C5-C6-N1	5.16	123.58	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	C	C5-C6-N1	5.10	123.55	121.00

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	3043	0	3073	64	0
2	B	529	0	269	16	0
3	C	508	0	257	0	0
All	All	4080	0	3599	79	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 10.

All (79) 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:760:ASP:OD1	1:A:830:ASP:HB2	1.73	0.87
1:A:638:PHE:O	1:A:641:MET:HB3	1.80	0.82
2:B:23:G:H3'	2:B:24:C:H6	1.55	0.71
1:A:760:ASP:OD1	1:A:830:ASP:CB	2.42	0.68
2:B:1:U:H4'	2:B:2:U:H5''	1.77	0.66
1:A:793:GLN:NE2	1:A:795:GLN:O	2.29	0.66
1:A:714:LEU:HB2	2:B:2:U:H5'	1.77	0.65
1:A:712:GLN:NE2	1:A:735:GLN:OE1	2.31	0.62
2:B:23:G:H3'	2:B:24:C:C6	2.34	0.62
2:B:24:C:H2'	2:B:25:U:C6	2.37	0.59
1:A:829:ARG:HH21	1:A:867:VAL:HG22	1.70	0.57
1:A:932:ASP:OD1	1:A:935:GLN:NE2	2.38	0.57
1:A:674:ARG:HE	1:A:702:LEU:HD11	1.69	0.57
1:A:908:GLN:NE2	1:A:909:HIS:O	2.38	0.57
1:A:957:PRO:HA	1:A:960:TYR:HB2	1.86	0.56
2:B:8:C:H2'	2:B:9:A:H8	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:HIS:HA	1:A:804:LYS:HE2	1.87	0.55
1:A:634:LYS:NZ	1:A:722:GLN:OE1	2.36	0.55
1:A:610:LEU:HD22	1:A:730:GLN:HG2	1.89	0.54
1:A:624:ALA:HA	1:A:657:LYS:H	1.73	0.53
1:A:762:TYR:HB2	1:A:965:ALA:HB1	1.90	0.52
1:A:632:GLN:O	1:A:635:ALA:HB3	2.09	0.52
1:A:937:LEU:O	1:A:941:LEU:N	2.42	0.52
1:A:631:ASP:O	1:A:635:ALA:N	2.42	0.51
1:A:693:ASP:OD1	1:A:693:ASP:N	2.43	0.51
2:B:8:C:H2'	2:B:9:A:C8	2.46	0.51
1:A:934:LEU:O	1:A:938:THR:OG1	2.26	0.50
1:A:604:ASP:OD1	1:A:604:ASP:N	2.41	0.50
2:B:21:U:C2	2:B:22:G:H1'	2.46	0.50
1:A:975:ASP:OD1	1:A:975:ASP:N	2.44	0.50
2:B:17:A:H2'	2:B:18:A:H8	1.76	0.50
2:B:16:A:H2'	2:B:17:A:C8	2.46	0.49
1:A:780:ASN:N	1:A:780:ASN:OD1	2.46	0.48
1:A:863:LEU:H	1:A:926:LYS:HB2	1.78	0.48
1:A:848:PHE:HD2	1:A:863:LEU:HD13	1.78	0.48
2:B:17:A:H2'	2:B:18:A:C8	2.48	0.48
1:A:954:THR:OG1	1:A:959:ASN:OD1	2.31	0.48
2:B:11:C:H2'	2:B:12:A:C8	2.48	0.48
1:A:755:MET:HA	1:A:783:PHE:HE1	1.79	0.47
1:A:760:ASP:OD1	1:A:830:ASP:OD2	2.32	0.47
1:A:900:SER:OG	1:A:922:VAL:O	2.33	0.46
1:A:625:VAL:HG12	1:A:685:VAL:HB	1.97	0.46
1:A:820:SER:OG	1:A:821:LEU:N	2.49	0.46
1:A:938:THR:HA	1:A:941:LEU:HD12	1.98	0.46
1:A:667:GLU:HA	1:A:670:LEU:HD12	1.98	0.46
1:A:943:HIS:HB3	1:A:944:MET:HE3	1.98	0.46
1:A:638:PHE:O	1:A:641:MET:CB	2.59	0.45
1:A:609:CYS:HA	1:A:612:GLU:HG3	1.99	0.45
1:A:668:SER:HB2	1:A:671:ARG:HH21	1.83	0.45
1:A:634:LYS:HE2	1:A:634:LYS:HB2	1.81	0.44
1:A:866:VAL:HG22	1:A:922:VAL:HG13	1.99	0.44
2:B:5:C:H2'	2:B:6:A:C8	2.53	0.44
1:A:619:SER:O	1:A:682:GLN:NE2	2.51	0.44
2:B:19:C:H2'	2:B:20:U:C6	2.53	0.43
1:A:663:ASN:OD1	1:A:663:ASN:N	2.46	0.43
1:A:915:VAL:HG13	1:A:917:PRO:HD3	2.00	0.43
1:A:869:GLN:HB2	1:A:919:TYR:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:PHE:HA	1:A:687:VAL:HG23	2.00	0.43
1:A:778:SER:HA	1:A:786:TRP:HA	2.01	0.43
1:A:636:THR:HA	1:A:639:VAL:HG22	2.01	0.42
1:A:702:LEU:HD12	1:A:702:LEU:HA	1.87	0.42
1:A:830:ASP:O	1:A:830:ASP:OD1	2.37	0.42
1:A:967:LEU:HD21	1:A:986:PHE:HB2	2.02	0.42
1:A:734:LEU:HG	1:A:744:LEU:HD13	2.01	0.42
1:A:751:LEU:HB2	1:A:824:ARG:HH12	1.85	0.42
1:A:941:LEU:HA	1:A:943:HIS:CE1	2.55	0.41
2:B:19:C:H2'	2:B:20:U:H6	1.85	0.41
1:A:963:LYS:O	1:A:967:LEU:HD23	2.20	0.41
1:A:760:ASP:OD1	1:A:830:ASP:CG	2.59	0.41
1:A:866:VAL:HA	1:A:922:VAL:HA	2.02	0.41
2:B:7:U:H2'	2:B:8:C:C6	2.56	0.41
1:A:586:PRO:HA	1:A:587:PRO:HD3	1.82	0.41
1:A:592:PHE:CZ	1:A:745:TRP:HB3	2.55	0.41
1:A:620:LEU:H	1:A:651:MET:HE2	1.86	0.41
1:A:673:LEU:HD23	1:A:677:ILE:HG13	2.02	0.40
1:A:845:VAL:O	1:A:849:ASN:ND2	2.54	0.40
1:A:673:LEU:HA	1:A:677:ILE:HG13	2.02	0.40
1:A:869:GLN:HB2	1:A:919:TYR:HB3	2.04	0.40
1:A:968:VAL:HA	1:A:972:LEU:HB2	2.02	0.40

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	373/987 (38%)	338 (91%)	35 (9%)	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	339/872 (39%)	323 (95%)	16 (5%)	22	46

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	623	TRP
1	A	636	THR
1	A	669	TYR
1	A	671	ARG
1	A	674	ARG
1	A	687	VAL
1	A	694	ASP
1	A	714	LEU
1	A	792	MET
1	A	803	LEU
1	A	812	LYS
1	A	839	TYR
1	A	843	PHE
1	A	959	ASN
1	A	960	TYR
1	A	966	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	25/25 (100%)	13 (52%)	1 (4%)
3	C	23/24 (95%)	12 (52%)	0
All	All	48/49 (97%)	25 (52%)	1 (2%)

All (25) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	U
2	B	3	A
2	B	5	C
2	B	6	A
2	B	9	A
2	B	12	A
2	B	16	A
2	B	17	A
2	B	20	U
2	B	22	G
2	B	23	G
2	B	24	C
2	B	25	U
3	C	6	A
3	C	7	A
3	C	8	G
3	C	11	U
3	C	12	C
3	C	14	A
3	C	18	U
3	C	19	G
3	C	21	U
3	C	23	G
3	C	24	U
3	C	25	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1	U

## 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 oligosaccharides 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.