



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Jan 21, 2018 – 01:30 PM EST

PDB ID : 6BUA
EMDB ID: : EMD-7291
Title : Drosophila Dicer-2 apo homology model (helicase, Platform-PAZ, RNaseIII domains)
Authors : Shen, P.S.; Sinha, N.K.; Bass, B.L.
Deposited on : 2017-12-09
Resolution : 7.10 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation 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) : rb-20030736

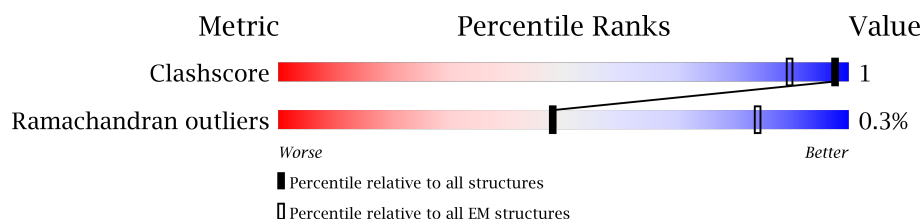
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.10 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

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	A	1724	<div> <div style="width: 54%; background-color: green;"></div> <div style="width: 45%; background-color: grey;"></div> <div style="width: 1%; background-color: yellow;"></div> <div style="width: 0%; background-color: orange;"></div> <div style="width: 0%; background-color: red;"></div> </div> <div>54% . 45%</div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4670 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 Dicer-2, isoform A.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	942	Total	C	N	O	0	0
			4670	2786	942	942		

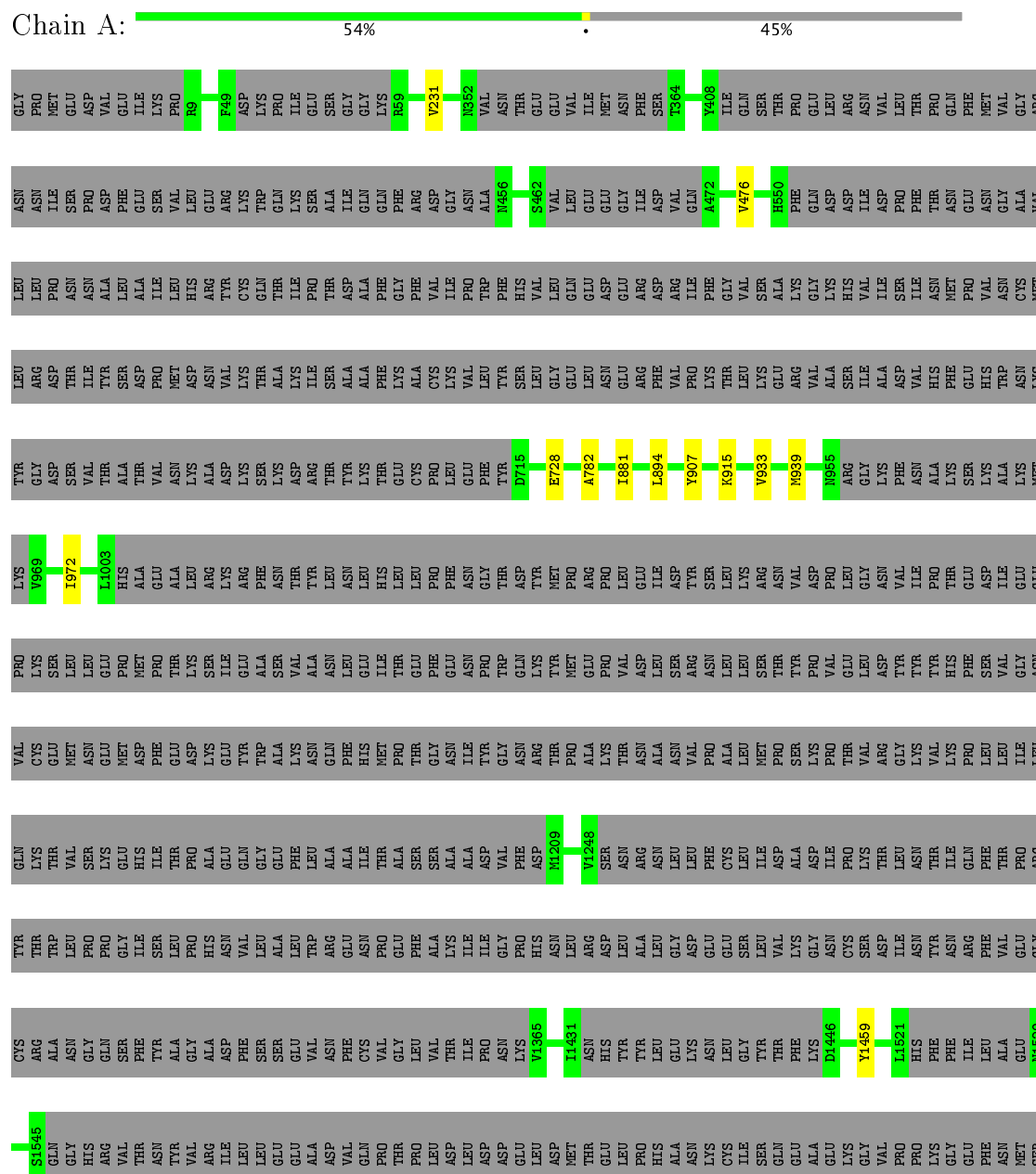
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A1ZAW0
A	0	PRO	-	expression tag	UNP A1ZAW0
A	1217	ALA	ASP	conflict	UNP A1ZAW0
A	1476	ALA	ASP	conflict	UNP A1ZAW0

3 Residue-property plots [i](#)

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: Dicer-2, isoform A



THR	LYS
ASN	HIS
VAL	ALA
ASP	LYS
VAL	PRO
PRO	VAL
LYS	PHE
ALA	SER
LEU	SER
GLY	PRO
ASP	ILE
VAL	VAL
LEU	GLU
GLU	GLY
ALA	GLU
LEU	THR
ILE	VAL
ALA	MET
ALA	VAL
VAL	SER
TYR	CYS
LEU	GLN
ASP	PHE
CYS	THR
ARG	CYS
ASP	MET
LEU	GLU
GLN	LYS
ARG	THR
THR	ILE
TRP	LYS
GLU	VAL
VAL	TYR
ILE	GLY
PHE	PHE
ASN	GLY
LEU	SER
PHE	ASN
GLU	LYS
PRO	ASP
GLU	GLN
LEU	ALA
GLN	LYS
GLU	LEU
PHE	SER
THR	ALA
ARG	ALA
LYS	LYS
VAL	HIS
PRO	ALA
ILE	LEU
ASN	GLN
HIS	GLN
ILE	LEU
ILE	SER
ARG	LYS
GLN	CYS
LEU	ASP
VAL	ALA
GLU	
HIS	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	85119	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.2	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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	A	0.24	1/4659 (0.0%)	0.41	0/6481

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1459	TYR	C-N	5.76	1.45	1.34

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	4670	0	2025	4	0
All	All	4670	0	2025	4	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 1.

All (4) 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:881:ILE:HA	1:A:894:LEU:HA	1.81	0.61
1:A:939:MET:HA	1:A:972:ILE:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:TYR:HA	1:A:915:LYS:HA	1.97	0.47
1:A:728:GLU:N	1:A:782:ALA:O	2.53	0.41

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	920/1724 (53%)	829 (90%)	88 (10%)	3 (0%)	44 81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	933	VAL
1	A	231	VAL
1	A	476	VAL

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.