



wwPDB EM Model Validation Summary Report ⓘ

Apr 2, 2020 – 12:50 PM EDT

PDB ID : 6V5C
EMDB ID : EMD-21052
Title : Human Drosha and DGCR8 in complex with Primary MicroRNA (MP/RNA complex) - partially docked state
Authors : Partin, A.; Zhang, K.; Jeong, B.; Herrell, E.; Li, S.; Chiu, W.; Nam, Y.
Deposited on : 2019-12-04
Resolution : 4.40 Å(reported)

This is a wwPDB EM 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

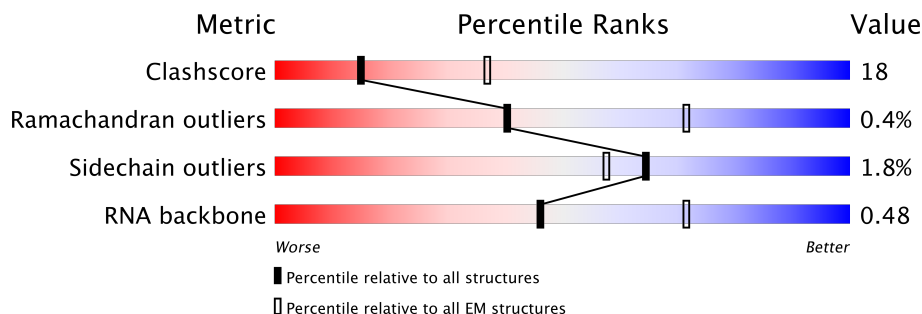
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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 on 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	1016	
2	B	532	
2	C	532	
3	D	105	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12251 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 Ribonuclease 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	903	7371	4696	1301	1325	49	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	GLY	-	expression tag	UNP Q9NRR4
A	351	SER	-	expression tag	UNP Q9NRR4
A	352	GLY	-	expression tag	UNP Q9NRR4
A	1045	GLN	GLU	engineered mutation	UNP Q9NRR4
A	1222	GLN	GLU	engineered mutation	UNP Q9NRR4

- Molecule 2 is a protein called Microprocessor complex subunit DGCR8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	217	1747	1104	312	321	10	0	0
2	B	216	1739	1099	308	322	10	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	220	GLY	-	expression tag	UNP Q8WYQ5
C	221	SER	-	expression tag	UNP Q8WYQ5
C	222	GLY	-	expression tag	UNP Q8WYQ5
B	220	GLY	-	expression tag	UNP Q8WYQ5
B	221	SER	-	expression tag	UNP Q8WYQ5
B	222	GLY	-	expression tag	UNP Q8WYQ5

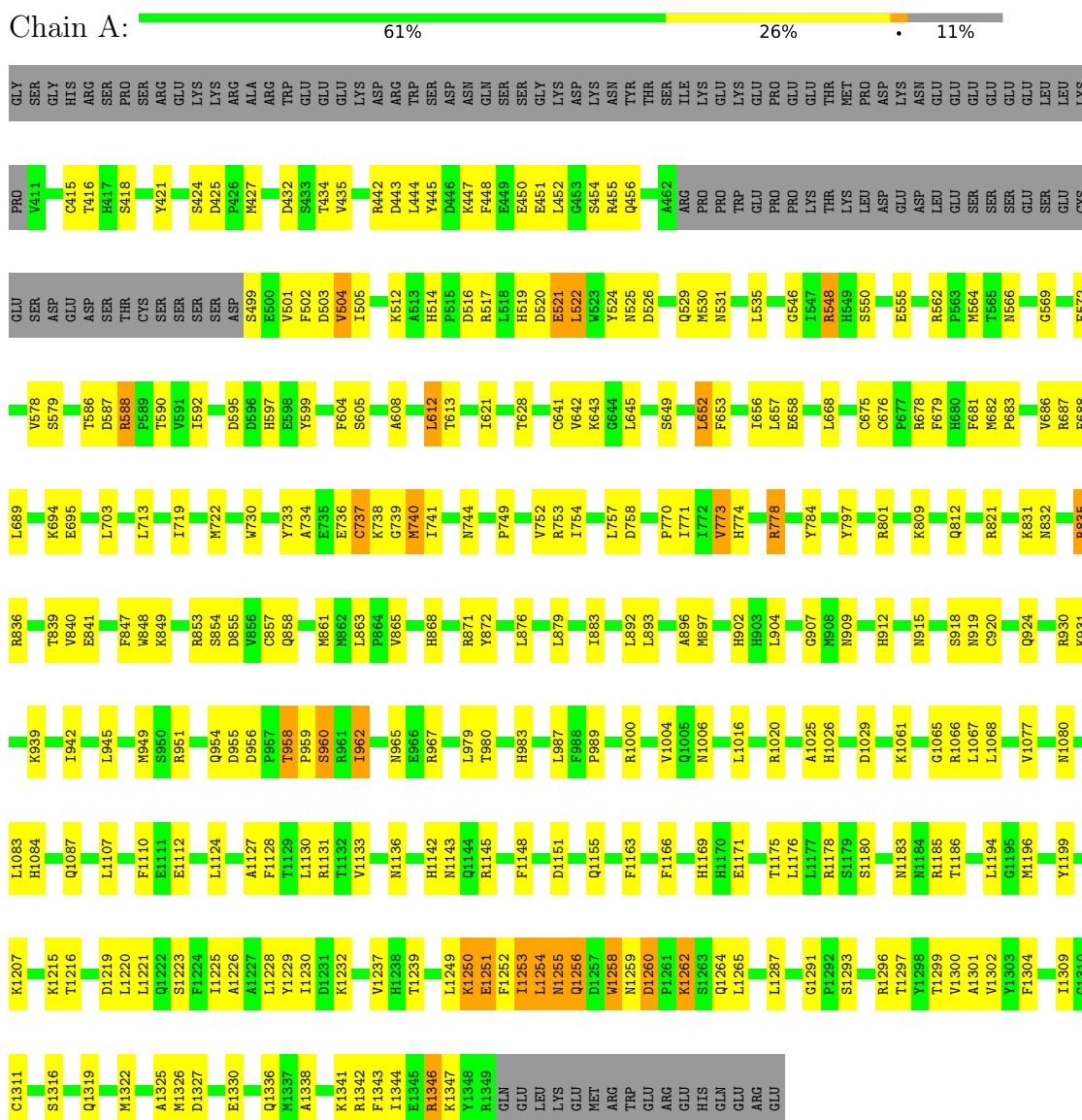
- Molecule 3 is a RNA chain called Pri-miR-16-2 (66-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	66	Total	C	N	O	P	0	0
			1394	624	237	467	66		

3 Residue-property plots

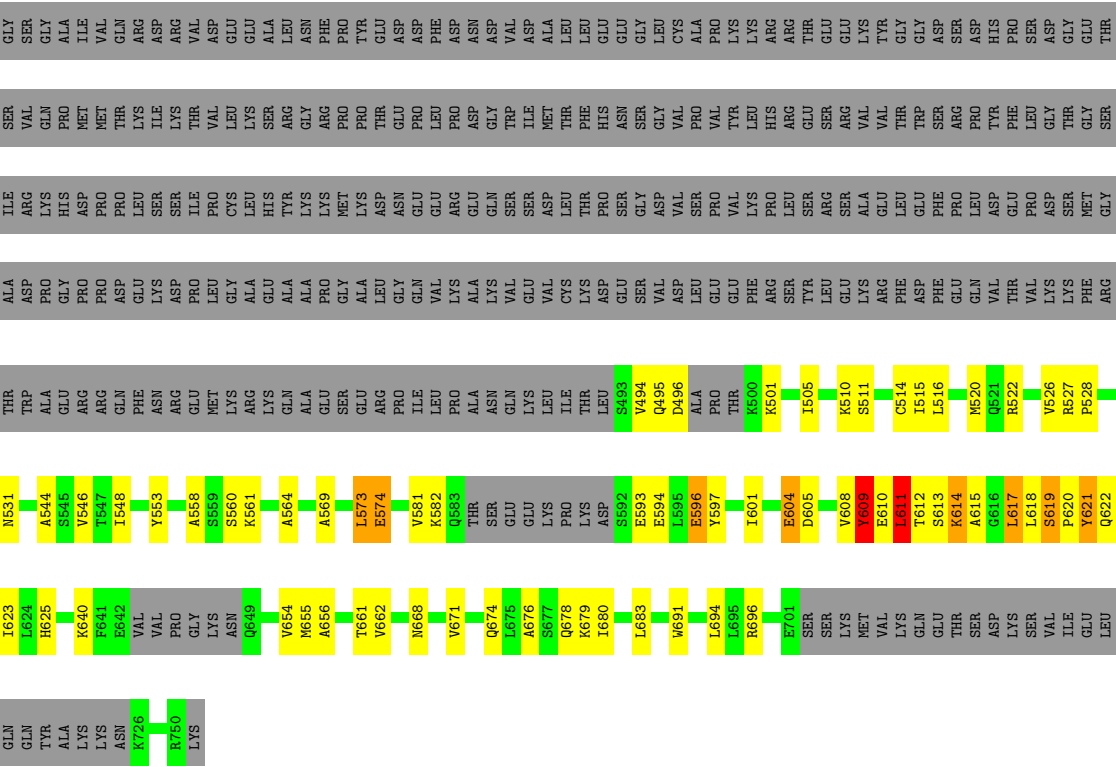
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: Ribonuclease 3

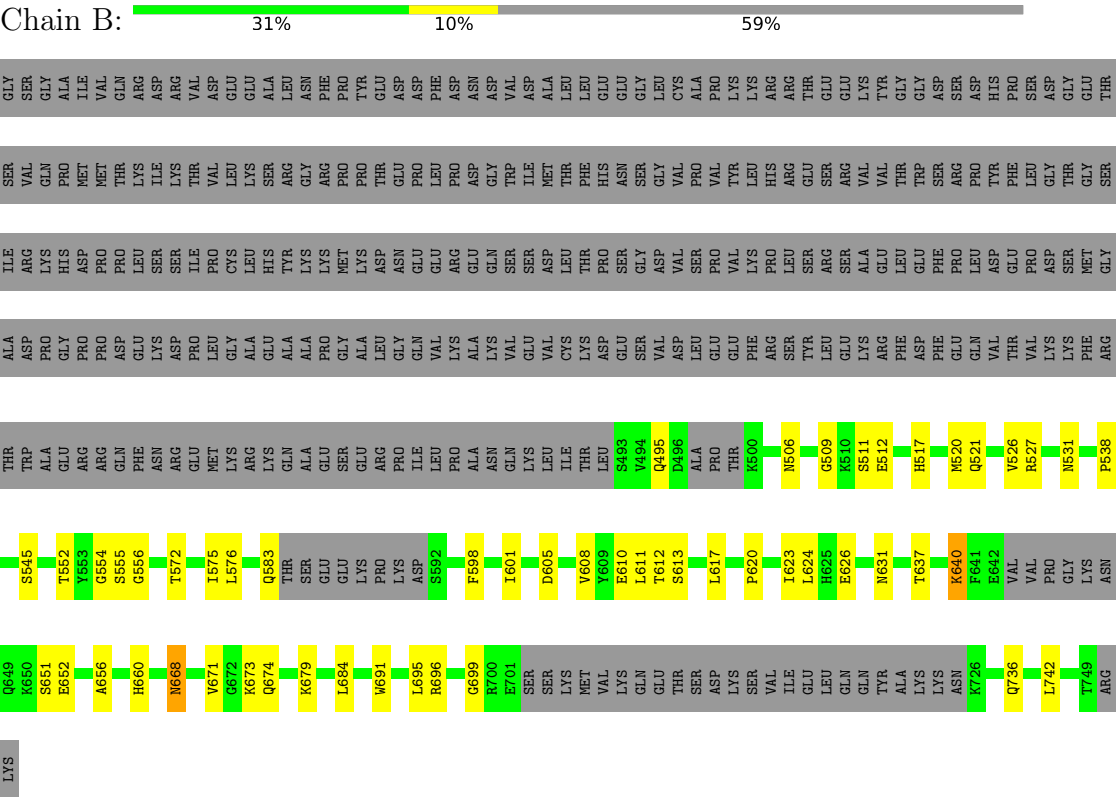


• Molecule 2: Microprocessor complex subunit DGCR8

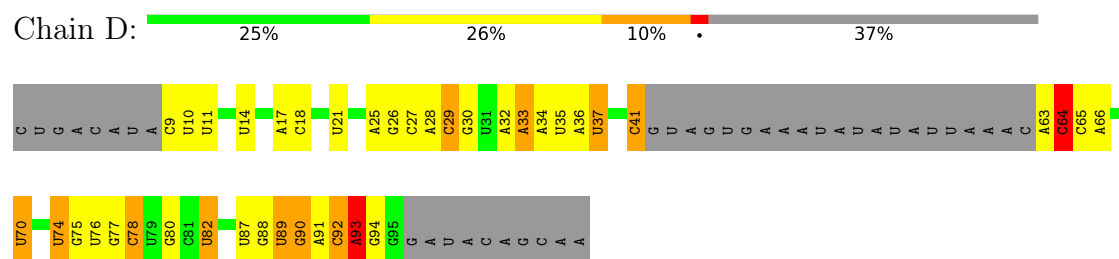




● Molecule 2: Microprocessor complex subunit DGCR8



● Molecule 3: Pri-miR-16-2 (66-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	381468	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 ($e^-/\text{\AA}^2$)	46.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (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	0.40	0/7555	0.68	15/10217 (0.1%)
2	B	0.30	0/1769	0.58	0/2369
2	C	0.40	0/1777	0.70	7/2379 (0.3%)
3	D	0.58	0/1554	1.27	15/2414 (0.6%)
All	All	0.41	0/12655	0.78	37/17379 (0.2%)

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	A	0	5
2	B	0	2
2	C	0	2
All	All	0	9

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	904	LEU	CA-CB-CG	8.18	134.12	115.30
1	A	1124	LEU	CA-CB-CG	7.78	133.18	115.30
1	A	736	GLU	O-C-N	7.61	134.87	122.70
2	C	608	VAL	N-CA-C	7.34	130.83	111.00
1	A	736	GLU	C-N-CA	7.15	139.56	121.70

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	521	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	522	LEU	Peptide
1	A	773	VAL	Peptide
1	A	778	ARG	Peptide
1	A	983	HIS	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	A	7371	0	7304	259	0
2	B	1739	0	1753	36	0
2	C	1747	0	1764	123	0
3	D	1394	0	707	25	0
All	All	12251	0	11528	431	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 18.

The worst 5 of 431 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:C:495:GLN:HB2	2:C:582:LYS:CG	1.39	1.50
2:C:495:GLN:CB	2:C:582:LYS:HG2	1.36	1.49
1:A:740:MET:HE1	1:A:920:CYS:CB	1.52	1.37
1:A:740:MET:CE	1:A:920:CYS:HB3	1.52	1.36
1:A:738:LYS:HA	1:A:754:ILE:CD1	1.56	1.35

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	899/1016 (88%)	753 (84%)	144 (16%)	2 (0%)	49	84
2	B	206/532 (39%)	192 (93%)	13 (6%)	1 (0%)	31	73
2	C	207/532 (39%)	182 (88%)	23 (11%)	2 (1%)	17	58
All	All	1312/2080 (63%)	1127 (86%)	180 (14%)	5 (0%)	40	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1260	ASP
2	B	611	LEU
2	C	609	TYR
2	C	619	SER
1	A	959	PRO

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	807/916 (88%)	790 (98%)	17 (2%)	56	78
2	B	193/475 (41%)	193 (100%)	0	100	100
2	C	193/475 (41%)	188 (97%)	5 (3%)	49	73
All	All	1193/1866 (64%)	1171 (98%)	22 (2%)	64	82

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1250	LYS
1	A	1254	LEU
2	C	617	LEU
1	A	1251	GLU
1	A	1253	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	964	HIS
1	A	1080	ASN
2	C	632	HIS
1	A	924	GLN
1	A	954	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	64/105 (60%)	20 (31%)	0

5 of 20 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	D	11	U
3	D	17	A
3	D	18	C
3	D	21	U
3	D	25	A

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 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 ⓘ

There are no chain breaks in this entry.