



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:00 PM GMT

PDB ID : 4NGF  
Title : Structure of human Dicer Platform-PAZ-Connector Helix cassette in complex with 17-mer siRNA having 5'-p and UU-3' ends (3.1 Angstrom resolution)  
Authors : Simanshu, D.K.; Tian, Y.; Patel, D.J.  
Deposited on : 2013-11-01  
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

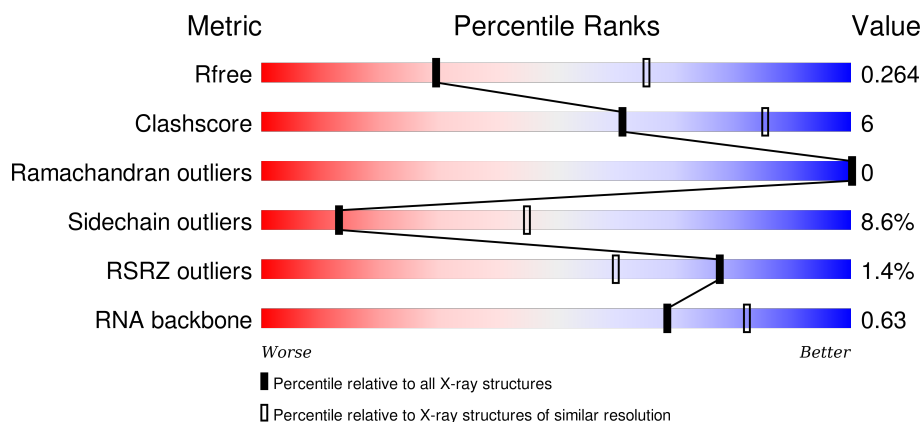
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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.



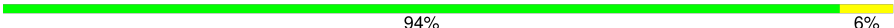

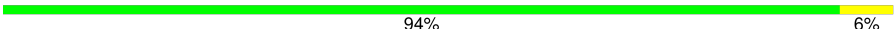
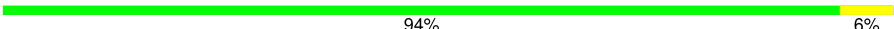
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	302	<div> <div>2%</div> <div>71% 13% • 14%</div> </div>
1	B	302	<div> <div>2%</div> <div>72% 12% • 14%</div> </div>
1	C	302	<div> <div>%</div> <div>62% 22% • 15%</div> </div>
1	D	302	<div> <div>%</div> <div>69% 16% • 14%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	17	 94%6%
2	F	17	 71%29%
2	G	17	 94%6%
2	H	17	 94%6%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9701 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Endoribonuclease Dicer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2049	1343	330	367	9			
1	B	259	Total	C	N	O	S	0	0	0
			2065	1345	336	375	9			
1	C	258	Total	C	N	O	S	0	0	0
			2103	1374	348	372	9			
1	D	260	Total	C	N	O	S	0	0	0
			2056	1344	339	365	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	754	SER	-	EXPRESSION TAG	UNP Q9UPY3
B	754	SER	-	EXPRESSION TAG	UNP Q9UPY3
C	754	SER	-	EXPRESSION TAG	UNP Q9UPY3
D	754	SER	-	EXPRESSION TAG	UNP Q9UPY3

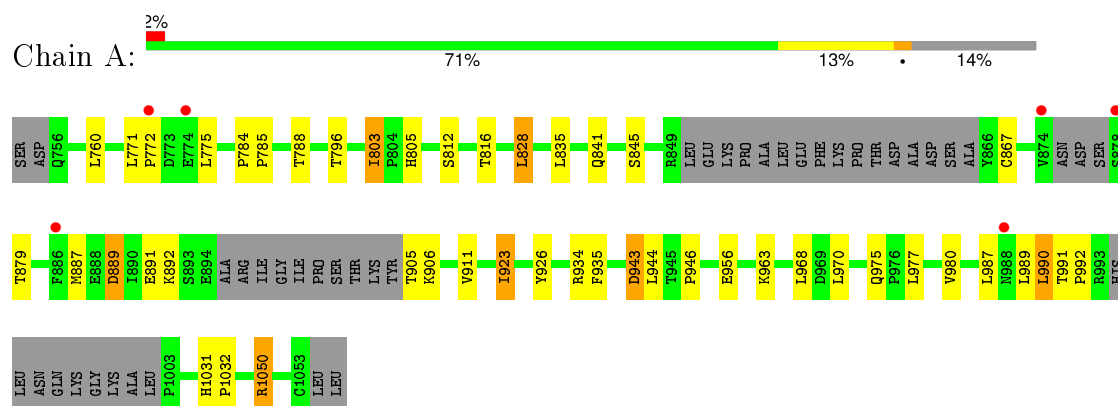
- Molecule 2 is a RNA chain called 5'-R(P\*UP\*CP\*GP\*AP\*AP\*GP\*GP\*UP\*CP\*CP\*UP\*UP\*CP\*GP\*UP\*UP\*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	17	Total	C	N	O	P	0	0	0
			357	159	56	125	17			
2	F	17	Total	C	N	O	P	0	0	0
			357	159	56	125	17			
2	G	17	Total	C	N	O	P	0	0	0
			357	159	56	125	17			
2	H	17	Total	C	N	O	P	0	0	0
			357	159	56	125	17			

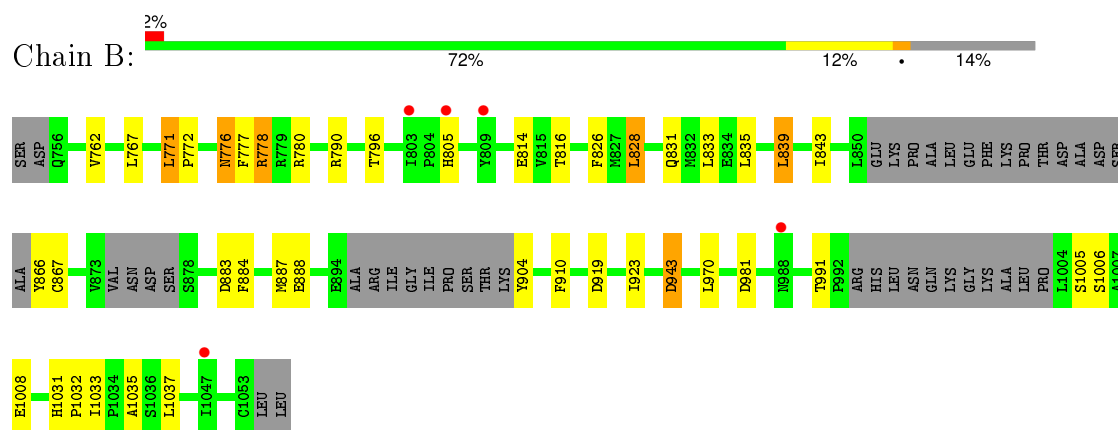
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

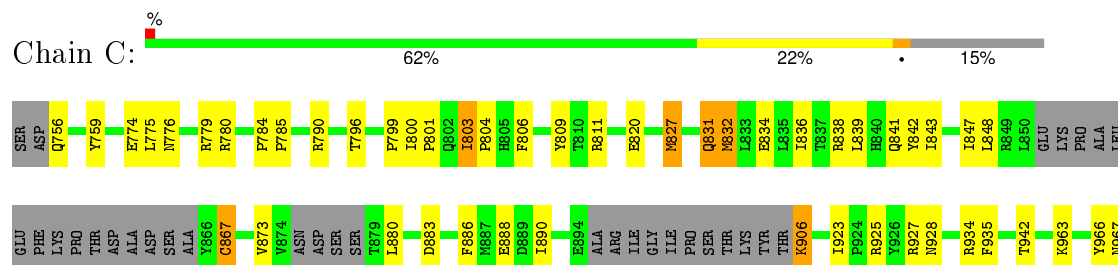
#### • Molecule 1: Endoribonuclease Dicer

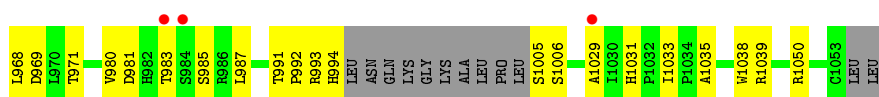


#### • Molecule 1: Endoribonuclease Dicer

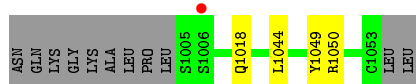


#### • Molecule 1: Endoribonuclease Dicer





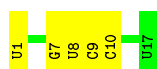
- Molecule 1: Endoribonuclease Dicer



- Molecule 2: 5'-R(P\*UP\*CP\*GP\*AP\*AP\*GP\*GP\*UP\*CP\*CP\*UP\*UP\*CP\*GP\*UP\*UP\*U)-3',



- Molecule 2: 5'-R(P\*UP\*CP\*GP\*AP\*AP\*GP\*GP\*UP\*CP\*CP\*UP\*UP\*CP\*GP\*UP\*UP\*U)-3',



- Molecule 2: 5'-R(P\*UP\*CP\*GP\*AP\*AP\*GP\*GP\*UP\*CP\*CP\*UP\*UP\*CP\*GP\*UP\*UP\*U)-3',



- Molecule 2: 5'-R(P\*UP\*CP\*GP\*AP\*AP\*GP\*GP\*UP\*CP\*CP\*UP\*UP\*CP\*GP\*UP\*UP\*U)-3',



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.25Å 104.19Å 368.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.48 – 3.10 47.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	91.1 (42.48-3.10) 88.6 (47.96-3.10)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.38 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.223 , 0.270 0.219 , 0.264	Depositor DCC
$R_{free}$ test set	1541 reflections (4.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.6	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 34.2	EDS
Estimated twinning fraction	0.050 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 32042 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	9701	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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  >5	RMSZ	# Z  >5
1	A	0.30	0/2105	0.58	1/2875 (0.0%)
1	B	0.33	0/2120	0.61	0/2891
1	C	0.36	0/2160	0.61	0/2939
1	D	0.30	0/2112	0.58	0/2887
2	E	0.61	1/396 (0.3%)	0.77	0/612
2	F	0.62	1/396 (0.3%)	0.77	0/612
2	G	0.59	1/396 (0.3%)	0.75	0/612
2	H	0.66	1/396 (0.3%)	0.76	0/612
All	All	0.39	4/10081 (0.0%)	0.63	1/14040 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	U	OP3-P	-11.17	1.47	1.61
2	E	1	U	OP3-P	-10.49	1.48	1.61
2	F	1	U	OP3-P	-10.32	1.48	1.61
2	G	1	U	OP3-P	-10.21	1.48	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	889	ASP	N-CA-C	-5.01	97.48	111.00

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	2049	0	1994	19	0
1	B	2065	0	2006	18	0
1	C	2103	0	2096	35	0
1	D	2056	0	1989	26	0
2	E	357	0	181	0	0
2	F	357	0	181	3	0
2	G	357	0	181	0	0
2	H	357	0	181	0	0
All	All	9701	0	8809	101	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 6.

The worst 5 of 101 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:B:904:TYR:HA	1:B:910:PHE:HB2	1.72	0.71
1:D:795:LEU:O	1:D:866:TYR:N	2.23	0.71
1:A:803:ILE:HG13	1:A:1050:ARG:HH22	1.58	0.68
1:B:1005:SER:HB3	1:B:1008:GLU:HB2	1.76	0.68
1:C:925:ARG:HD3	1:C:1029:ALA:HB2	1.76	0.67

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 X-ray entries followed by that with respect to entries of similar resolution.

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	250/302 (83%)	238 (95%)	12 (5%)	0	100	100
1	B	249/302 (82%)	237 (95%)	12 (5%)	0	100	100
1	C	248/302 (82%)	240 (97%)	8 (3%)	0	100	100
1	D	250/302 (83%)	238 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	997/1208 (82%)	953 (96%)	44 (4%)	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 X-ray entries followed by that with respect to entries of similar resolution.

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	222/282 (79%)	201 (90%)	21 (10%)	11	38
1	B	226/282 (80%)	207 (92%)	19 (8%)	14	46
1	C	235/282 (83%)	212 (90%)	23 (10%)	10	36
1	D	220/282 (78%)	205 (93%)	15 (7%)	20	55
All	All	903/1128 (80%)	825 (91%)	78 (9%)	13	45

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	923	ILE
1	C	820	GLU
1	D	934	ARG
1	B	943	ASP
1	B	991	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	846	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	16/17 (94%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	16/17 (94%)	0	0
2	G	16/17 (94%)	0	0
2	H	16/17 (94%)	0	0
All	All	64/68 (94%)	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 [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.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	260/302 (86%)	-0.14	6 (2%) 64 40	29, 68, 138, 185	0
1	B	259/302 (85%)	-0.06	5 (1%) 70 48	22, 62, 133, 167	0
1	C	258/302 (85%)	-0.09	3 (1%) 81 64	26, 56, 104, 199	0
1	D	260/302 (86%)	-0.03	2 (0%) 87 75	25, 71, 150, 217	0
2	E	17/17 (100%)	-0.42	0 100 100	37, 47, 56, 62	0
2	F	17/17 (100%)	-0.48	0 100 100	36, 44, 52, 58	0
2	G	17/17 (100%)	-0.65	0 100 100	41, 50, 60, 62	0
2	H	17/17 (100%)	-0.48	0 100 100	37, 44, 68, 77	0
All	All	1105/1276 (86%)	-0.11	16 (1%) 78 60	22, 62, 134, 217	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1006	SER	3.3
1	A	774	GLU	3.2
1	A	772	PRO	2.8
1	C	983	THR	2.7
1	A	886	PHE	2.7

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.