



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 9, 2016 – 10:22 AM EST

PDB ID : 5F6C  
Title : The structure of E. coli RNase E catalytically inactive mutant with RNA bound  
Authors : Bandyra, K.J.; Luisi, B.F.  
Deposited on : 2015-12-05  
Resolution : 3.00 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.

---

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

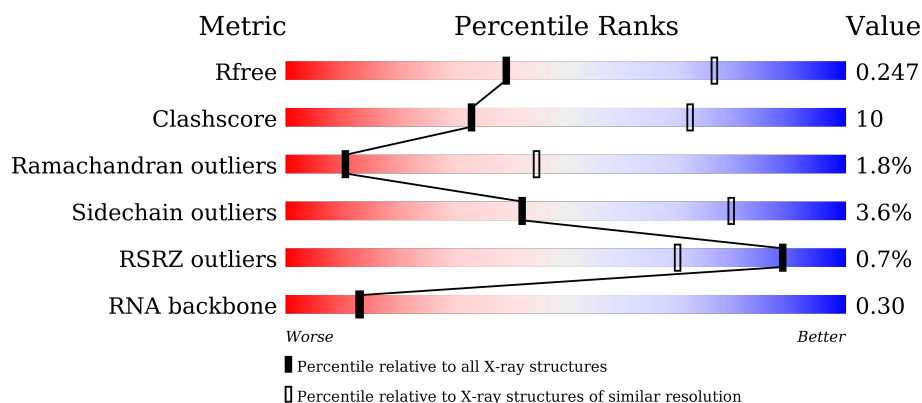
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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	512	<div> <div></div> <div>71%</div> <div>26%</div> <div>.</div> </div>
2	B	513	<div> <div>%</div> <div>74%</div> <div>22%</div> <div>..</div> </div>
3	C	2	<div> <div>50%</div> <div>50%</div> </div>
4	E	3	<div> <div>67%</div> <div>33%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	B	601	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16149 atoms, of which 8061 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 Ribonuclease E.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	512	Total	C	H	N	O	S	0	0	0
			7999	2498	4009	739	741	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	expression tag	UNP P21513
A	0	HIS	-	expression tag	UNP P21513
A	303	ARG	ASP	engineered mutation	UNP P21513
A	346	ARG	ASP	engineered mutation	UNP P21513

- Molecule 2 is a protein called Ribonuclease E.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	510	Total	C	H	N	O	S	0	0	0
			7980	2492	3997	734	746	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	ARG	-	expression tag	UNP P21513
B	0	HIS	-	expression tag	UNP P21513
B	303	ARG	ASP	engineered mutation	UNP P21513
B	346	ARG	ASP	engineered mutation	UNP P21513

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	2	Total	C	H	N	O	P	0	0	0
			66	19	22	7	16	2			

- Molecule 4 is a RNA chain called RNA (5'-R(P\*GP\*UP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	3	Total	C	H	N	O	P	0	0
			100	29	33	12	23	3		0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		

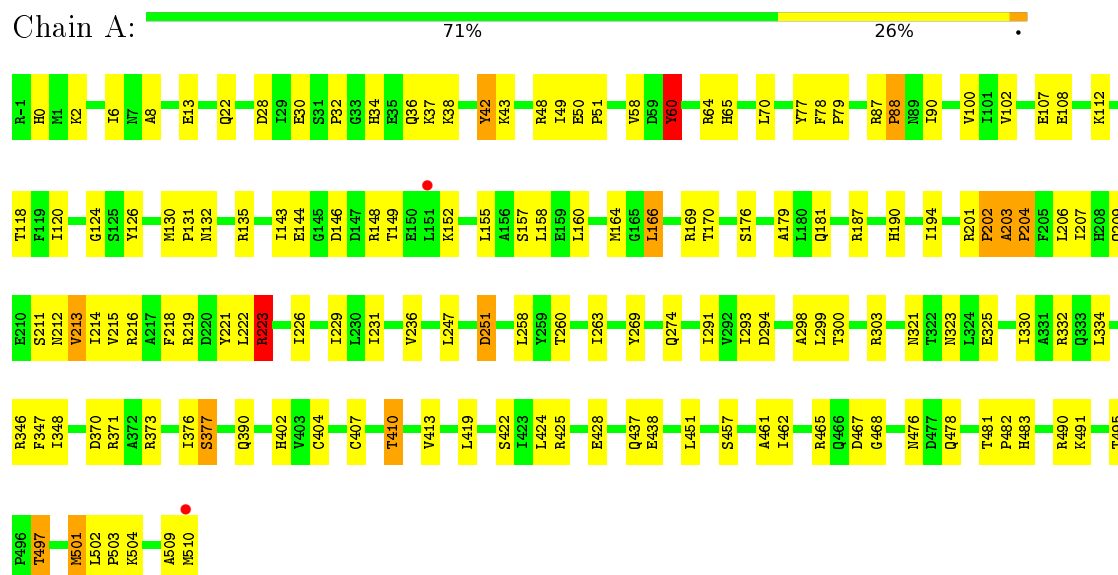
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		

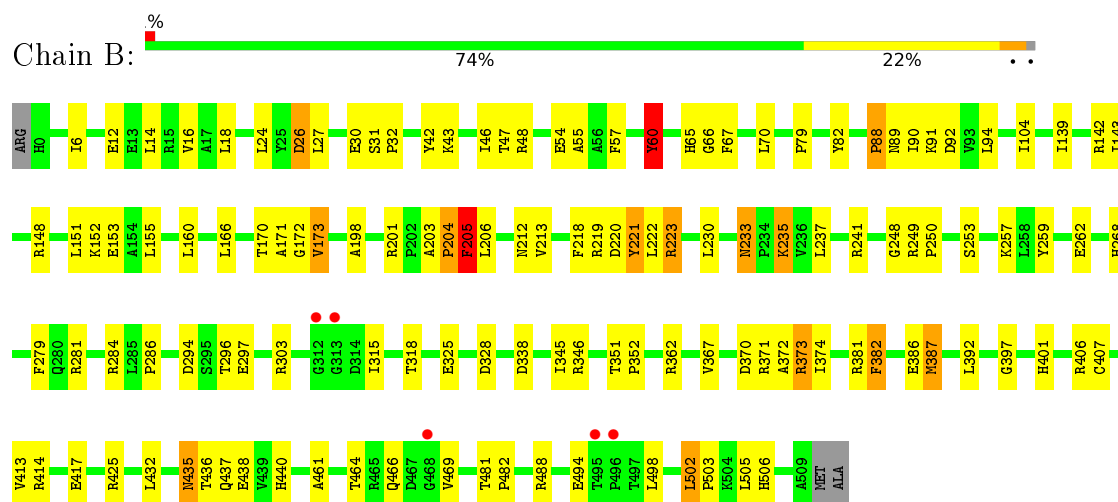
### 3 Residue-property plots

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: Ribonuclease E



#### • Molecule 2: Ribonuclease E



#### • Molecule 3: RNA (5'-R(P\*GP\*U)-3')



01  
02

- Molecule 4: RNA (5'-R(P\*GP\*UP\*G)-3')

Chain E:  67% 33%

02  
03  
04

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.62Å 122.56Å 122.19Å 90.00° 99.77° 90.00°	Depositor
Resolution (Å)	54.62 – 3.00 54.62 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (54.62-3.00) 94.0 (54.62-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.175 , 0.250 0.175 , 0.247	Depositor DCC
$R_{free}$ test set	1274 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.0	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 92.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16149	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.72	3/4056 (0.1%)	0.92	8/5483 (0.1%)
2	B	0.72	1/4049 (0.0%)	0.92	8/5475 (0.1%)
3	C	1.96	1/48 (2.1%)	2.22	3/71 (4.2%)
4	E	1.54	1/74 (1.4%)	1.78	4/112 (3.6%)
All	All	0.74	6/8227 (0.1%)	0.94	23/11141 (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
2	B	0	4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	G	OP3-P	-10.85	1.48	1.61
3	C	1	G	OP3-P	-8.98	1.50	1.61
1	A	213	VAL	CB-CG2	-6.25	1.39	1.52
1	A	404	CYS	CB-SG	-5.32	1.73	1.81
2	B	91	LYS	CD-CE	5.24	1.64	1.51

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	60	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	A	223	ARG	NE-CZ-NH2	-6.61	117.00	120.30
2	B	294	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	501	MET	CG-SD-CE	6.30	110.28	100.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	294	ASP	CB-CG-OD2	-6.12	112.80	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	203	ALA	Peptide
2	B	435	ASN	Peptide
2	B	60	TYR	Sidechain
2	B	88	PRO	Peptide

## 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	3990	4009	4008	94	0
2	B	3983	3997	3999	80	0
3	C	44	22	22	1	0
4	E	67	33	33	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
All	All	8088	8061	8062	166	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.

The worst 5 of 166 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:258:LEU:CD2	1:A:260:THR:HG23	2.21	0.71
1:A:251:ASP:OD1	1:A:251:ASP:N	2.21	0.69
2:B:43:LYS:NZ	2:B:198:ALA:O	2.24	0.69
2:B:142:ARG:NH2	3:C:1:G:OP1	2.26	0.68
1:A:410:THR:HG22	2:B:281:ARG:HD2	1.77	0.66

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	510/512 (100%)	463 (91%)	37 (7%)	10 (2%)	9	41
2	B	508/513 (99%)	451 (89%)	49 (10%)	8 (2%)	12	48
All	All	1018/1025 (99%)	914 (90%)	86 (8%)	18 (2%)	11	45

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ALA
2	B	482	PRO
1	A	157	SER
2	B	406	ARG
2	B	498	LEU

### 5.3.2 Protein sidechains [i](#)

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	419/436 (96%)	407 (97%)	12 (3%)	50	84
2	B	421/436 (97%)	403 (96%)	18 (4%)	35	75
All	All	840/872 (96%)	810 (96%)	30 (4%)	42	79

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	30	GLU
2	B	54	GLU
2	B	417	GLU
2	B	32	PRO
2	B	60	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
2	B	466	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	1/2 (50%)	0	0
4	E	2/3 (66%)	0	0
All	All	3/5 (60%)	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](#)

Of 3 ligands modelled in this entry, 3 are 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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	512/512 (100%)	-0.16	2 (0%) 93 80	53, 92, 146, 188	0
2	B	510/513 (99%)	-0.18	5 (0%) 84 60	52, 86, 141, 221	0
3	C	2/2 (100%)	0.23	0 100 100	107, 107, 107, 144	0
4	E	3/3 (100%)	-0.38	0 100 100	103, 103, 110, 120	0
All	All	1027/1030 (99%)	-0.17	7 (0%) 89 70	52, 88, 145, 221	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	312	GLY	3.0
2	B	468	GLY	2.5
2	B	313	GLY	2.5
1	A	151	LEU	2.4
2	B	495	THR	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	B	601	1/1	0.82	0.55	14.13	99,99,99,99	0
5	MG	A	601	1/1	0.98	0.23	0.68	53,53,53,53	0
6	ZN	A	602	1/1	0.99	0.17	-0.33	90,90,90,90	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.