



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:56 PM GMT

PDB ID : 1RC7
Title : Crystal structure of RNase III Mutant E110K from Aquifex Aeolicus complexed with ds-RNA at 2.15 Angstrom Resolution
Authors : Blaszczyk, J.; Gan, J.; Ji, X.
Deposited on : 2003-11-03
Resolution : 2.15 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
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 : 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

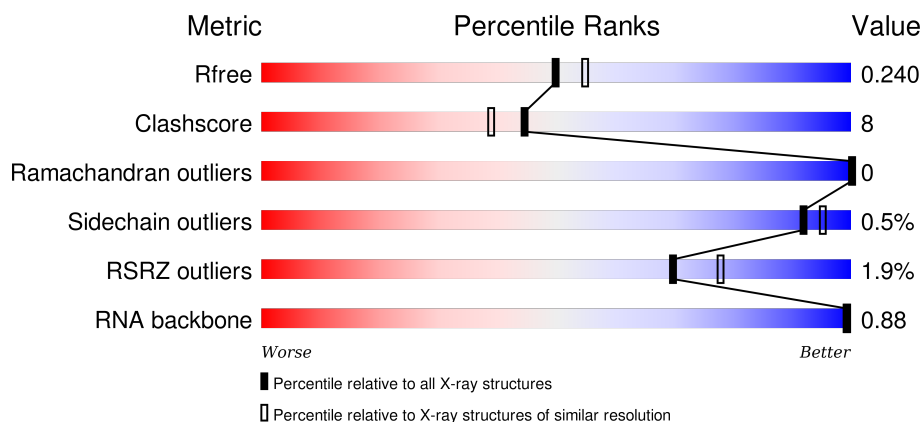
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)
RNA backbone	2183	1077 (2.80-1.52)

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 ≥ 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	B	10	<div> <div style="width: 70%;"></div> <div style="width: 30%;"></div> </div>
1	C	10	<div> <div style="width: 70%;"></div> <div style="width: 30%;"></div> </div>
1	D	10	<div> <div style="width: 60%;"></div> <div style="width: 40%;"></div> </div>
1	E	10	<div> <div style="width: 60%;"></div> <div style="width: 40%;"></div> </div>

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Mol	Chain	Length	Quality of chain
2	A	220	 A horizontal bar chart showing the quality of chain A. The bar is divided into three segments: a small red segment at the beginning labeled '2%', a large green segment in the middle labeled '81%', and a yellow segment at the end labeled '18%'. A small black dot is located at the far right end of the bar.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2930 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 RNA chain called 5'-R(*GP*GP*CP*GP*CP*GP*CP*GP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	10	Total	C	N	O	P	0	0	0
			212	95	40	68	9			
1	C	10	Total	C	N	O	P	0	0	0
			212	95	40	68	9			
1	D	10	Total	C	N	O	P	0	0	0
			212	95	40	68	9			
1	E	10	Total	C	N	O	P	0	0	0
			212	95	40	68	9			

- Molecule 2 is a protein called Ribonuclease III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	220	Total	C	N	O	S	0	0	0
			1838	1197	308	331	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	LYS	GLU	ENGINEERED	UNP O67082

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	184	Total	O	0	0
			184	184		
4	B	9	Total	O	0	0
			9	9		
4	C	22	Total	O	0	0
			22	22		
4	D	15	Total	O	0	0
			15	15		
4	E	6	Total	O	0	0
			6	6		

i

● Molecule 1: 5'-R(*GP*GP*CP*GP*CP*GP*CP*GP*CP*C)-3'

● Molecule 1: 5'-R(*GP*GP*CP*GP*CP*GP*CP*GP*CP*C)-3'

Diagram illustrating a sequence of nodes: G11, G12, C13, G16, C17, and C20. The nodes are arranged horizontally and connected by lines. Nodes G11, G12, and C20 are green, while C13, G16, and C17 are yellow.

● Molecule 1: 5'-R(*GP*GP*CP*GP*CP*GP*CP*GP*CP*C)-3'

Diagram illustrating a sequence of nodes: G21 (green), G24 (yellow), C25 (green), G26 (yellow), C29 (yellow), and C30 (yellow). G21 is connected to G24, and G26 is connected to C29.

● Molecule 1: 5'-R(*GP*GP*CP*GP*CP*GP*CP*GP*CP*C)-3'

Diagram illustrating a sequence of nodes: G31, G34, C35, G38, C39, and C40. The nodes are arranged horizontally and connected by lines. Nodes G31, G38, and C40 are green, while G34, C35, and C39 are yellow.

- Molecule 2: Ribonuclease III

I190
 R194
 T195
 E198
 K202
 K203
 E206
 Q207
 R208
 A209
 A210
 L213
 I214
 E219
 S220

K1
 K2
 Q6
 Y13
 T26
 H35
 Y36
 E37
 L66
 L55
 N61
 P66
 L67
 S68
 P69
 L70
 N81
 L82
 L83
 A84
 Q85
 D107
 K110
 A111
 L112
 W113
 L130
 F135
 R163
 W164
 K165
 E166
 R167
 E176
 H179
 H180
 K181
 K182
 A183
 F184
 E187
 A188
 K189

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	58.29Å 118.14Å 106.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.47 – 2.15 37.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.6 (28.47-2.15) 79.7 (37.33-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.192 , 0.242 0.192 , 0.240	Depositor DCC
R_{free} test set	1091 reflections (5.83%)	DCC
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 21531 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2930	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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

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	B	0.30	0/236	0.67	0/367
1	C	0.32	0/236	0.64	0/367
1	D	0.26	0/236	0.62	0/367
1	E	0.22	0/236	0.64	0/367
2	A	0.35	0/1873	0.57	1/2502 (0.0%)
All	All	0.33	0/2817	0.60	1/3970 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	113	TRP	CA-CB-CG	-5.28	103.68	113.70

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	B	212	0	112	2	0
1	C	212	0	112	2	0
1	D	212	0	112	4	0
1	E	212	0	112	2	0
2	A	1838	0	1912	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	0	12	2	0
4	A	184	0	0	3	0
4	B	9	0	0	0	0
4	C	22	0	0	1	0
4	D	15	0	0	0	0
4	E	6	0	0	0	0
All	All	2930	0	2372	40	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 8.

The worst 5 of 40 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:A:61:ASN:HB3	2:A:66:PHE:CD2	2.17	0.78
2:A:37:GLU:HB3	3:A:300:TRS:H22	1.72	0.70
2:A:202:LYS:O	2:A:206:GLU:HG3	1.93	0.67
2:A:55:LEU:HD11	2:A:70:LEU:HD23	1.78	0.64
1:D:26:G:OP1	2:A:203:LYS:HE2	1.99	0.62

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
2	A	218/220 (99%)	213 (98%)	5 (2%)	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	
2	A	197/197 (100%)	196 (100%)	1 (0%)	92	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	70	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	6	GLN
2	A	85	GLN
2	A	157	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	9/10 (90%)	0	0
1	C	9/10 (90%)	0	0
1	D	9/10 (90%)	0	0
1	E	9/10 (90%)	0	0
All	All	36/40 (90%)	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 ⓘ

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TRS	A	300	-	7,7,7	1.73	2 (28%)	9,9,9	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRS	A	300	-	-	0/9/9/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	300	TRS	C-N	-3.28	1.45	1.50
3	A	300	TRS	C3-C	2.28	1.57	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	300	TRS	2	0

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 [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, 95th 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 ²)	Q<0.9
1	B	10/10 (100%)	-0.17	0 100 100	39, 48, 69, 72	0
1	C	10/10 (100%)	-0.42	0 100 100	39, 43, 52, 54	0
1	D	10/10 (100%)	-0.30	0 100 100	48, 52, 62, 73	0
1	E	10/10 (100%)	-0.02	0 100 100	50, 58, 73, 74	0
2	A	220/220 (100%)	0.36	5 (2%) 64 72	21, 41, 64, 86	0
All	All	260/260 (100%)	0.27	5 (1%) 70 78	21, 43, 68, 86	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	163	ARG	3.5
2	A	164	TRP	2.7
2	A	46	LEU	2.5
2	A	179	HIS	2.4
2	A	219	GLU	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, 95th 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(Å ²)	Q<0.9
3	TRS	A	300	8/8	0.90	0.19	1.10	43,57,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.