

wwPDB X-ray Structure Validation Summary Report (i)

May 26, 2020 – 08:40 pm BST

PDB ID : 299D

Title : CAPTURING THE STRUCTURE OF A CATALYTIC RNA INTERMEDI-

ATE: THE HAMMERHEAD RIBOZYME

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Deposited on : 1996-12-14

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
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467 Xtriage (Phenix) : 1.13

EDS : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

 $\begin{array}{cccc} & CCP4 & : & 7.0.044 \; (Gargrove) \\ Ideal \; geometry \; (proteins) & : & Engh \; \& \; Huber \; (2001) \end{array}$

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

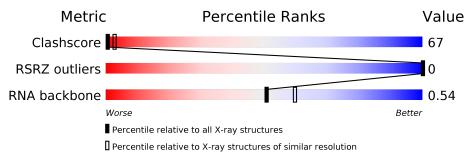
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

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	Similar resolution		
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$		
Clashscore	141614	2416 (3.00-3.00)		
RSRZ outliers	127900	1990 (3.00-3.00)		
RNA backbone	3102	1173 (3.30-2.70)		

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 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 <=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	16	25%	50%	25%
2	В	25	8%	80%	12%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 873 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 RNA HAMMERHEAD RIBOZYME.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	16	Total 342	C 153	N 62	O 112	P 15	0	0	0

• Molecule 2 is a RNA chain called RNA HAMMERHEAD RIBOZYME.

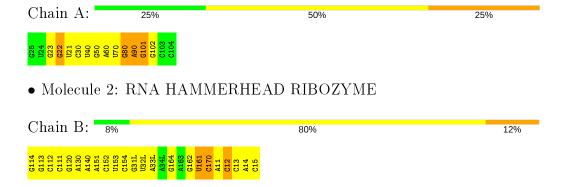
N	/Iol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
	2	В	25	Total 531	C 239	N 100	O 168	P 24	0	0	0



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 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: RNA HAMMERHEAD RIBOZYME





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	64.56Å 64.56Å 136.29Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 - 3.00	Depositor
resolution (A)	29.10 - 3.10	EDS
% Data completeness	85.4 (8.00-3.00)	Depositor
(in resolution range)	84.7 (29.10-3.10)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.40 (at 3.11Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
D D	0.216 , 0.265	Depositor
R, R_{free}	0.218 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.745	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.19 , 46.8	EDS
L-test for twinning ²	$< L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	873	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.76% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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	
WIOI	Chain	RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.67	0/382	0.81	0/595
2	В	0.62	0/594	0.76	0/924
All	All	0.64	0/976	0.78	0/1519

There are no bond length outliers.

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	342	0	174	47	0
2	В	531	0	274	61	0
All	All	873	0	448	88	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 67.

The worst 5 of 88 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{c} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{array}$	Clash overlap (Å)
1:A:90:A:H3'	1:A:101:G:C5'	1.62	1.28
1:A:90:A:C3'	1:A:101:G:H5"	1.67	1.25

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Atom-1	Atom-2	$egin{array}{c} ext{Interatomic} \ ext{distance } (ext{Å}) \end{array}$	Clash overlap (Å)
1:A:60:A:H2'	2:B:170:C:C6	1.80	1.17
1:A:23:G:C2'	1:A:22:G:H5"	1.80	1.11
1:A:23:G:H2'	1:A:22:G:H5"	1.10	1.03

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein molecules in this entry.

5.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	15/16 (93%)	3 (20%)	1 (6%)
2	В	24/25~(96%)	4 (16%)	0
All	All	39/41 (95%)	7 (17%)	1 (2%)

5 of 7 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	22	G
1	A	90	A
1	A	101	G
2	В	164	G
2	В	161	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	80	G



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 (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 $>$	$\#RSRZ{>}2$			$OWAB(A^2)$	Q<0.9
1	A	16/16 (100%)	-0.48	0	100	100	16, 32, 52, 53	0
2	В	$25/25 \; (100\%)$	-0.61	0	100	100	15, 29, 47, 55	0
All	All	41/41 (100%)	-0.56	0	100	100	15, 31, 49, 55	0

There are no RSRZ outliers to report.

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

