

# wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID : 1DZA

Title : 3-D structure of a HP-RNase

Authors: Pous, J.; Canals, A.; Terzyan, S.S.; Guasch, A.; Benito, A.; Ribo, M.; Vilanova,

M.; Coll, M.

Deposited on : 2000-02-21

Resolution : 1.65 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED

EDS : NOT EXECUTED

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

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

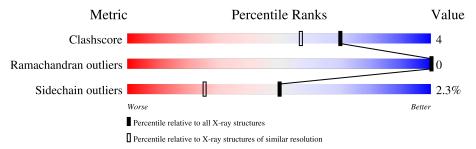
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 1.65 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	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)

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 of 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	A	129	76%	16%	• 6%
1	В	129	81%	12%	•• 6%



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2182 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 RIBONUCLEASE 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	121	Total	С	N	О	S	18	0	0
1 A	121	957	579	181	183	14	10	U		
1	B	121	Total	С	N	О	S	43	0	0
1	D	121	952	574	180	185	13	40	U	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	FME	GLY	engineered mutation	UNP P07998
A	104	ALA	ARG	engineered mutation	UNP P07998
A	106	ALA	LYS	engineered mutation	UNP P07998
A	109	GLU	GLN	engineered mutation	UNP P07998
A	116	GLY	ASP	engineered mutation	UNP P07998
A	117	ASN	SER	engineered mutation	UNP P07998
A	150	SER	PRO	engineered mutation	UNP P07998
В	100	FME	GLY	engineered mutation	UNP P07998
В	104	ALA	ARG	engineered mutation	UNP P07998
В	106	ALA	LYS	engineered mutation	UNP P07998
В	109	GLU	GLN	engineered mutation	UNP P07998
В	116	GLY	ASP	engineered mutation	UNP P07998
В	117	ASN	SER	engineered mutation	UNP P07998
В	150	SER	PRO	engineered mutation	UNP P07998

#### • Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	151	Total O 151 151	0	0
2	В	122	Total O 122 122	0	0

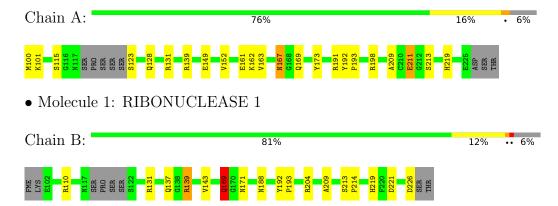


# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

Note EDS was not executed.

• Molecule 1: RIBONUCLEASE 1





# 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	27.85Å 67.42Å 114.14Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	19.90 - 1.65	Depositor	
% Data completeness	96.6 (19.90-1.65)	Depositor	
(in resolution range)	30.0 (13.30 1.00)	Depositor	
$R_{merge}$	0.13	Depositor	
$R_{sym}$	0.11	Depositor	
Refinement program	REFMAC	Depositor	
$R, R_{free}$	0.185 , $0.236$	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	2182	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP	



## 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: FME

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	Bo	nd lengths	Bond angles		
Moi Chain		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.87	4/964 (0.4%)	1.30	11/1295~(0.8%)	
1	В	0.78	4/969 (0.4%)	1.42	11/1303 (0.8%)	
All	All	0.83	8/1933 (0.4%)	1.36	$22/2598 \; (0.8\%)$	

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(Å)	$\operatorname{Ideal}(\text{\AA})$
1	A	211	GLU	CG-CD	17.91	1.78	1.51
1	В	169	GLN	CG-CD	-12.91	1.21	1.51
1	A	101	LYS	CG-CD	-8.78	1.22	1.52
1	В	226	ASP	CB-CG	-7.45	1.36	1.51
1	A	128	GLN	CG-CD	-6.42	1.36	1.51

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
1	В	204	ARG	CD-NE-CZ	16.18	146.25	123.60
1	В	169	GLN	CB-CG-CD	12.04	142.90	111.60
1	В	204	ARG	NE-CZ-NH1	11.88	126.24	120.30
1	A	131	ARG	CD-NE-CZ	9.03	136.25	123.60
1	A	101	LYS	CB-CG-CD	9.02	135.05	111.60

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	957	0	908	8	0
1	В	952	0	893	5	0
2	A	151	0	0	3	0
2	В	122	0	0	1	0
All	All	2182	0	1801	13	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 4.

The worst 5 of 13 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:B:169:GLN:HG3	1:B:171:ASN:OD1	2.05	0.57
1:B:209:ALA:HB3	1:B:219:HIS:HB3	1.90	0.54
1:A:167:ASN:ND2	1:A:169:GLN:H	2.08	0.51
1:B:213:SER:HA	1:B:214:PRO:C	2.29	0.51
1:A:219:HIS:HB2	2:A:2142:HOH:O	2.10	0.51

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	Chain Analysed Favoured Allowed		Outliers	Perce	ntiles	
1	A	117/129 (91%)	112 (96%)	5 (4%)	0	100	100
1	В	117/129 (91%)	113 (97%)	4 (3%)	0	100	100
All	All	234/258 (91%)	225 (96%)	9 (4%)	0	100	100

There are no Ramachandran outliers to report.



#### 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	108/116 (93%)	106 (98%)	2 (2%)	57 34			
1	В	109/116 (94%)	106 (97%)	3 (3%)	43 18			
All	All	217/232 (94%)	212 (98%)	5 (2%)	50 25			

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Iol   Chain   Res		Type
1	A	167	ASN
1	A	213	SER
1	В	139	ARG
1	В	169	GLN
1	1 B		ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	HIS
1	В	180	HIS
1	В	188	ASN
1	A	167	ASN
1	A	137	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

#### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue 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 Chai		Res	Link	Bond lengths			Bond angles		
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	FME	A	100	1	8,9,10	0.70	0	7,9,11	1.90	2 (28%)

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
1	FME	A	100	1	-	1/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\mathrm{Ideal}(^{o})$
1	A	100	FME	CA-N-CN	-3.83	116.94	122.82
1	A	100	FME	O1-CN-N	-2.35	119.09	125.27

There are no chirality outliers.

All (1) torsion outliers are listed below:

$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type	${f Atoms}$
1	A	100	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

### 5.5 Carbohydrates (i)

There are no monosaccharides 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

#### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

#### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

