

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

May 16, 2022 – 04:09 pm BST

PDB ID : 7PCR

Title : Helicobacter pylori RNase J

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Deposited on : 2021-08-03

Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 2.28.1

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

Refmac: 5.8.0267

CCP4 : 7.1.010 (Gargrove)

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

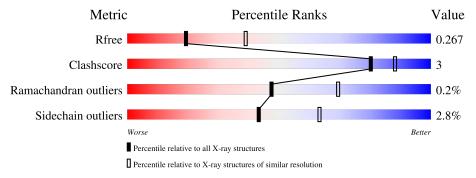
Validation Pipeline (wwPDB-VP) : 2.28.1

## 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 2.75 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
1,13,113	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)

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%

Mol	Chain	Length	Quality of chain			
1	A	553	91%	8%		



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7943 atoms, of which 3869 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 J.

Mo	Chain	Residues			Atom	ıs			ZeroOcc	AltConf	Trace
1	A	553	Total 7933	C 2584	H 3869	N 701	O 767	S 12	0	1	0

• Molecule 2 is water.

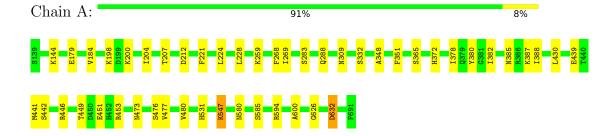
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	10	Total O 10 10	0	0



## 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.

• Molecule 1: Ribonuclease J





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants	158.49Å 158.49Å 214.26Å	Denesites
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	56.03 - 2.75	Depositor
Resolution (A)	56.03 - 2.75	EDS
% Data completeness	99.2 (56.03-2.75)	Depositor
(in resolution range)	99.2 (56.03-2.75)	EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.16	Depositor
$< I/\sigma(I) > 1$	1.53 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
D D	0.245 , $0.267$	Depositor
$R, R_{free}$	0.246 , $0.267$	DCC
$R_{free}$ test set	1805 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.8	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.48, < L^2> = 0.31$	Xtriage
	0.020  for  -1/2 *h + 1/2 *k - 1/2 *l, 1/2 *h - 1/2 *k - 1	
Estimated twinning fraction	$\begin{array}{c} 1/2*\text{l,-h-k} \\ 0.027 \text{ for -}1/2*\text{h}1/2*\text{k}+1/2*\text{l,-}1/2*\text{h}1/2*\text{k} \end{array}$	Xtriage
220111111111111111111111111111111111111	0.027 for $-1/2$ *h $-1/2$ *k $+1/2$ *l $-1/2$ *h $-1/2$ *k $-1/2$ *k $-1/2$ *h $-1/2$ *k $-1/2$ *k $-1/2$ *h $-1/2$ *k $-1/2$ *h $-1/2$ *h $-1/2$ *k $-1/2$ *h $-1$	110110.80
E E completion	1/2*l,h-k	EDC
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7943	wwPDB-VP
Average B, all atoms $(\mathring{A}^2)$	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.43	0/4147	0.62	$1/5627 \ (0.0\%)$	

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
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

	Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
ſ	1	A	632	ASP	O-C-N	-5.18	114.41	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	632	ASP	Mainchain

#### 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	4064	3869	3869	21	1

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	Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
	2	A	10	0	0	0	0
Ī	All	All	4074	3869	3869	21	1

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 3.

All (21) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ ({\rm \AA})$	$overlap (\AA)$
1:A:388:ILE:HD12	1:A:430:LEU:HD23	1.81	0.63
1:A:473:ASN:O	1:A:477:VAL:HG23	2.00	0.61
1:A:547:LYS:H	1:A:547:LYS:HE2	1.69	0.57
1:A:378:ILE:HG12	1:A:388:ILE:HG21	1.90	0.53
1:A:269:ILE:HB	1:A:288:GLN:HB2	1.91	0.52
1:A:332:SER:O	1:A:531:HIS:HB3	2.11	0.51
1:A:476:SER:O	1:A:480:VAL:HG23	2.10	0.51
1:A:441:MET:HB3	1:A:480:VAL:HG21	1.95	0.49
1:A:221:PHE:HA	1:A:224:LEU:O	2.13	0.48
1:A:378:ILE:O	1:A:382:ILE:HG23	2.14	0.47
1:A:439:GLU:OE2	1:A:580:ASN:ND2	2.43	0.47
1:A:453:ARG:HA	1:A:453:ARG:CZ	2.45	0.47
1:A:179:GLU:HB2	1:A:184:VAL:HG12	1.96	0.46
1:A:204:ILE:HB	1:A:228:LEU:HD23	1.98	0.45
1:A:268:PHE:O	1:A:269:ILE:HD13	2.18	0.43
1:A:442:SER:O	1:A:446:ARG:HG3	2.19	0.43
1:A:348:ALA:HB1	1:A:380:TYR:OH	2.18	0.43
1:A:449:THR:HG22	1:A:451:GLU:HG3	2.01	0.42
1:A:259:LYS:HE2	1:A:283:SER:OG	2.20	0.41
1:A:200:LYS:HE3	1:A:200:LYS:HB3	1.92	0.40
1:A:385:ASN:O	1:A:385:ASN:ND2	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:594:ARG:NE	1:A:626:GLY:O[16_445]	1.72	0.48



#### 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	552/553 (100%)	531 (96%)	20 (4%)	1 (0%)	47 69

#### All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	600	ALA

#### 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	398/475 (84%)	387 (97%)	11 (3%)	43 63

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	LYS
1	A	198	LYS
1	A	207	THR
1	A	212	ASP
1	A	309	ASN
1	A	351	PHE
1	A	365	SER
1	A	372	HIS
1	A	387	LYS
1	A	547	LYS

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	•	-	- 0
Mol	Chain	Res	Type
1	A	585	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

#### 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 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

