



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8YYF / pdb_00008yyf
Title : RNase J2 mutant H76A
Authors : Singh, A.K.; Chinnasamy, K.; Gopal, B.
Deposited on : 2024-04-03
Resolution : 1.39 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

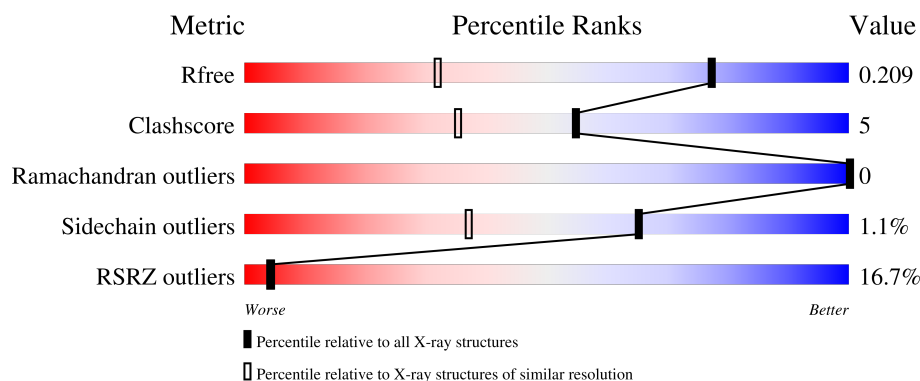
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.39 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}	180053	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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 $\leq 5\%$. 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	571	13% 69% 8% 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3762 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 J 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	1	0
			3367	2152	561	631	23			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q5HPR6
A	-12	GLY	-	expression tag	UNP Q5HPR6
A	-11	SER	-	expression tag	UNP Q5HPR6
A	-10	SER	-	expression tag	UNP Q5HPR6
A	-9	HIS	-	expression tag	UNP Q5HPR6
A	-8	HIS	-	expression tag	UNP Q5HPR6
A	-7	HIS	-	expression tag	UNP Q5HPR6
A	-6	HIS	-	expression tag	UNP Q5HPR6
A	-5	HIS	-	expression tag	UNP Q5HPR6
A	-4	HIS	-	expression tag	UNP Q5HPR6
A	-3	SER	-	expression tag	UNP Q5HPR6
A	-2	GLN	-	expression tag	UNP Q5HPR6
A	-1	ASP	-	expression tag	UNP Q5HPR6
A	0	PRO	-	expression tag	UNP Q5HPR6
A	76	ALA	HIS	engineered mutation	UNP Q5HPR6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	395	Total	O	0	0
			395	395		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.04Å 72.43Å 106.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.89 – 1.39 42.89 – 1.39	Depositor EDS
% Data completeness (in resolution range)	90.4 (42.89-1.39) 90.4 (42.89-1.39)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 1.39Å)	Xtriage
Refinement program	REFMAC 5.8.0350	Depositor
R, R_{free}	0.165 , 0.205 0.198 , 0.209	Depositor DCC
R_{free} test set	4005 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3762	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.77	4/3430 (0.1%)	1.06	6/4640 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	HIS	CE1-NE2	7.95	1.40	1.32
1	A	370	HIS	CE1-NE2	6.22	1.38	1.32
1	A	357	HIS	CE1-NE2	5.75	1.38	1.32
1	A	401	HIS	CE1-NE2	5.60	1.38	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ILE	N-CA-C	7.12	119.18	111.77
1	A	141	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	413	GLU	CB-CG-CD	5.29	121.60	112.60
1	A	166	GLU	CB-CA-C	5.28	118.46	109.53
1	A	394	GLU	CB-CG-CD	5.14	121.34	112.60
1	A	122	TYR	CB-CA-C	-5.10	102.92	110.62

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	3367	0	3296	32	0
2	A	395	0	0	7	3
All	All	3762	0	3296	32	3

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 5.

All (32) 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:93:ASP:CB	2:A:938:HOH:O	2.33	0.76
1:A:49:MET:HE2	1:A:443:LEU:HD11	1.74	0.69
1:A:426:TYR:CD1	1:A:431[B]:MET:HG2	2.28	0.69
1:A:22:ILE:O	1:A:22:ILE:HG23	1.96	0.65
1:A:284:PRO:HG2	1:A:287:GLU:HG3	1.79	0.64
1:A:367:ALA:HA	2:A:887:HOH:O	2.07	0.54
1:A:92:ILE:C	1:A:92:ILE:HD12	2.33	0.53
1:A:22:ILE:C	1:A:392:GLN:OE1	2.52	0.52
1:A:309:GLU:OE1	1:A:313:GLN:NE2	2.44	0.50
1:A:382:ILE:HG13	2:A:816:HOH:O	2.12	0.48
1:A:131:ARG:NH1	2:A:609:HOH:O	2.46	0.48
1:A:22:ILE:O	1:A:392:GLN:OE1	2.31	0.47
1:A:22:ILE:HG21	1:A:337:SER:HB3	1.96	0.47
1:A:426:TYR:HD1	1:A:431[B]:MET:HG2	1.74	0.46
1:A:217:HIS:CD2	1:A:362:ASN:HD22	2.34	0.46
1:A:217:HIS:CD2	1:A:362:ASN:ND2	2.84	0.46
1:A:264:SER:OG	1:A:265:SER:N	2.48	0.45
1:A:42:LEU:HD12	1:A:42:LEU:C	2.41	0.45
1:A:422:ASP:HB3	1:A:433:LEU:HD11	1.98	0.45
1:A:22:ILE:O	1:A:22:ILE:CG2	2.65	0.45
1:A:22:ILE:HD12	1:A:22:ILE:HA	1.72	0.45
1:A:108:GLU:HG2	1:A:268:ILE:HD11	1.98	0.45
1:A:418:VAL:HG11	1:A:424:ILE:HD11	2.00	0.43
1:A:271:LYS:CB	2:A:945:HOH:O	2.66	0.43
1:A:216:HIS:HB3	2:A:915:HOH:O	2.19	0.43
1:A:314:MET:HB3	1:A:324:ILE:HG12	2.01	0.43
1:A:128:SER:HB3	1:A:130:MET:HE3	2.01	0.42
1:A:190:GLU:OE1	2:A:601:HOH:O	2.21	0.42
1:A:73:PHE:CD1	1:A:73:PHE:N	2.89	0.41
1:A:217:HIS:CG	1:A:365:ILE:HD11	2.55	0.40
1:A:426:TYR:HB2	1:A:431[B]:MET:SD	2.60	0.40
1:A:34:GLU:OE1	1:A:134:ASN:HB2	2.21	0.40

All (3) 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	Interatomic distance (Å)	Clash overlap (Å)
2:A:659:HOH:O	2:A:745:HOH:O[4_455]	1.93	0.27
2:A:745:HOH:O	2:A:762:HOH:O[4_555]	2.05	0.15
2:A:620:HOH:O	2:A:713:HOH:O[4_455]	2.07	0.13

5.3 Torsion angles

5.3.1 Protein backbone

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	439/571 (77%)	429 (98%)	10 (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	
1	A	351/495 (71%)	347 (99%)	4 (1%)	65	37

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	282	LEU
1	A	340	MET
1	A	443	LEU

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

Mol	Chain	Res	Type
1	A	134	ASN
1	A	217	HIS
1	A	313	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	A	442/571 (77%)	1.05	74 (16%) 4 4	7, 16, 57, 411	1 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	GLY	16.3
1	A	302	GLY	11.9
1	A	4	ILE	11.4
1	A	3	LEU	11.2
1	A	303	MET	8.8
1	A	304	GLN	8.6
1	A	334	ILE	8.5
1	A	6	LYS	8.0
1	A	306	GLU	7.8
1	A	5	LYS	7.8
1	A	22	ILE	6.7
1	A	264	SER	6.5
1	A	340	MET	6.5
1	A	339	ASN	6.1
1	A	336	ALA	5.9
1	A	50	LEU	5.6
1	A	7	LYS	5.5
1	A	333	ALA	5.1
1	A	47	ASP	5.0
1	A	341	GLU	4.9
1	A	342	VAL	4.9
1	A	445	ASP	4.7
1	A	262	LEU	4.6
1	A	363	LYS	4.5
1	A	51	GLY	4.4
1	A	49	MET	4.3
1	A	338	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	353	ARG	4.1
1	A	261	SER	3.8
1	A	301	THR	3.7
1	A	279	LYS	3.6
1	A	257	PHE	3.5
1	A	365	ILE	3.5
1	A	48	GLU	3.4
1	A	367	ALA	3.4
1	A	270	ARG	3.3
1	A	286	ASN	3.3
1	A	343	ILE	3.3
1	A	267	ASN	3.3
1	A	44	PHE	3.2
1	A	52	VAL	3.2
1	A	395	PHE	3.2
1	A	277	ILE	3.0
1	A	332	LEU	3.0
1	A	337	SER	2.9
1	A	361	ASN	2.9
1	A	291	TYR	2.9
1	A	290	ASN	2.8
1	A	265	SER	2.8
1	A	282	LEU	2.8
1	A	278	PRO	2.7
1	A	266	PHE	2.7
1	A	276	ASP	2.7
1	A	366	HIS	2.7
1	A	344	ILE	2.7
1	A	234	TYR	2.6
1	A	296	VAL	2.5
1	A	46	GLU	2.5
1	A	284	PRO	2.5
1	A	253	ARG	2.5
1	A	283	ILE	2.5
1	A	362	ASN	2.4
1	A	285	ILE	2.4
1	A	280	ASP	2.4
1	A	268	ILE	2.4
1	A	272	MET	2.4
1	A	273	GLY	2.3
1	A	216	HIS	2.3
1	A	263	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	116	LYS	2.2
1	A	429	LYS	2.2
1	A	174	HIS	2.1
1	A	252	ASN	2.0
1	A	322	MET	2.0

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 oligosaccharides 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.