Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2025 – 04:13 PM JST

PDB ID	:	8YYF
Title	:	RNase J2 mutant H76A
Authors	:	Singh, A.K.; Chinnasamy, K.; Gopal, B.
Deposited on	:	2024-04-03
Resolution	:	1.39 Å(reported)

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

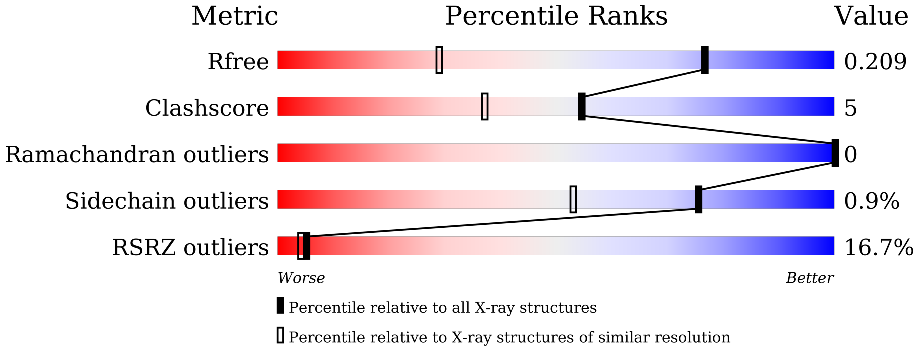
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

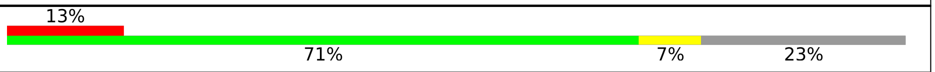
The reported resolution of this entry is 1.39 Å.

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}	164625	2247 (1.40-1.40)
Clashscore	180529	2446 (1.40-1.40)
Ramachandran outliers	177936	2398 (1.40-1.40)
Sidechain outliers	177891	2397 (1.40-1.40)
RSRZ outliers	164620	2246 (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 <=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	

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
			Total	C	N	O	S			
1	A	442	3367	2152	561	631	23	0	1	0

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

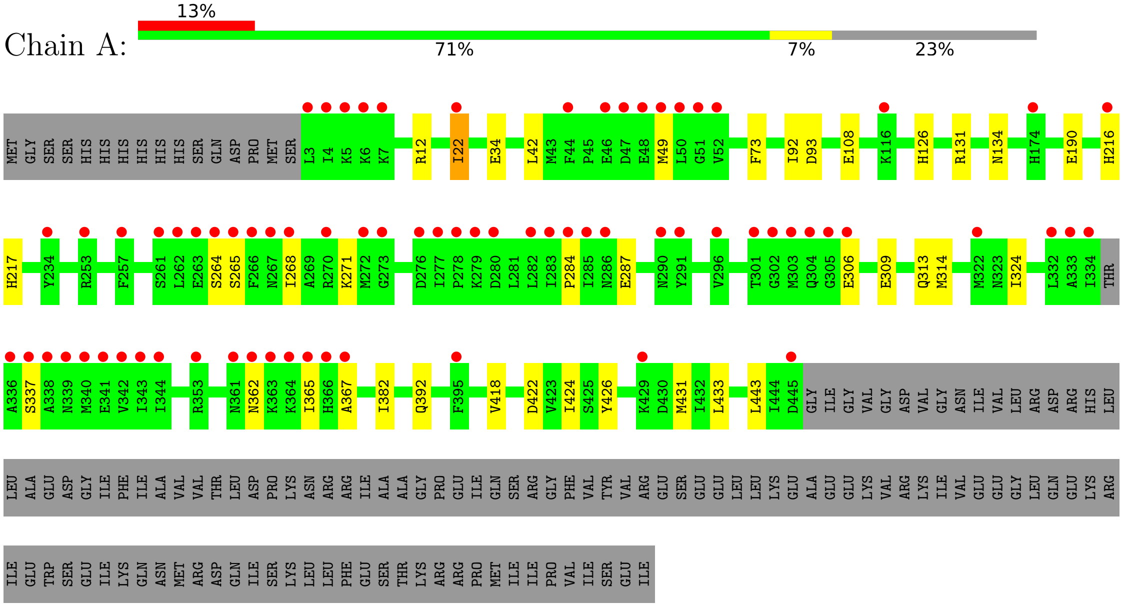
- Molecule 2 is water.

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

3 Residue-property plots ⓘ

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 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: Ribonuclease J 2



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
$< I/\sigma(I) >$ [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	4425 reflections (4.97%)	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]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	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.*

---

[1] Intensities estimated from amplitudes.

[2] 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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.55	0/3430	0.83	1/4640 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ARG	NE-CZ-NH2	-6.23	117.19	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	31	0
2	A	395	0	0	7	3
All	All	3762	0	3296	31	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 (31) 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

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
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: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:92:ILE:C	1:A:92:ILE:HD12	2.33	0.48
1:A:22:ILE:O	1:A:392:GLN:OE1	2.31	0.47
1:A:22:ILE:C	1:A:392:GLN:OE1	2.52	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:264:SER:OG	1:A:265:SER:N	2.48	0.46
1:A:217:HIS:CD2	1:A:362:ASN:ND2	2.84	0.46
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:49:MET:CE	1:A:443:LEU:HD11	2.48	0.43
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:190:GLU:OE1	2:A:601:HOH:O	2.21	0.42
1:A:42:LEU:C	1:A:42:LEU:HD12	2.41	0.41
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%)	348 (99%)	3 (1%)	75 53

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	126	HIS
1	A	306	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	208	ASN
1	A	217	HIS
1	A	438	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	1.03	74 (16%) 5 4	7, 16, 57, 411	1 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	GLY	16.0
1	A	302	GLY	11.7
1	A	4	ILE	11.3
1	A	3	LEU	11.2
1	A	303	MET	8.9
1	A	304	GLN	8.6
1	A	334	ILE	8.4
1	A	6	LYS	8.0
1	A	5	LYS	7.8
1	A	306	GLU	7.8
1	A	22	ILE	6.6
1	A	340	MET	6.6
1	A	264	SER	6.4
1	A	339	ASN	6.0
1	A	336	ALA	5.8
1	A	7	LYS	5.5
1	A	50	LEU	5.5
1	A	47	ASP	5.0
1	A	333	ALA	5.0
1	A	341	GLU	4.9
1	A	342	VAL	4.8
1	A	445	ASP	4.6
1	A	262	LEU	4.6
1	A	363	LYS	4.6
1	A	49	MET	4.4
1	A	51	GLY	4.3
1	A	353	ARG	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	338	ALA	4.1
1	A	261	SER	3.7
1	A	279	LYS	3.7
1	A	301	THR	3.6
1	A	257	PHE	3.4
1	A	365	ILE	3.4
1	A	48	GLU	3.4
1	A	270	ARG	3.3
1	A	286	ASN	3.3
1	A	367	ALA	3.3
1	A	343	ILE	3.3
1	A	267	ASN	3.2
1	A	44	PHE	3.1
1	A	395	PHE	3.1
1	A	52	VAL	3.1
1	A	332	LEU	2.9
1	A	277	ILE	2.9
1	A	361	ASN	2.9
1	A	337	SER	2.9
1	A	291	TYR	2.8
1	A	366	HIS	2.8
1	A	290	ASN	2.7
1	A	282	LEU	2.7
1	A	265	SER	2.7
1	A	266	PHE	2.7
1	A	276	ASP	2.7
1	A	278	PRO	2.7
1	A	344	ILE	2.6
1	A	234	TYR	2.6
1	A	46	GLU	2.5
1	A	296	VAL	2.5
1	A	253	ARG	2.4
1	A	283	ILE	2.4
1	A	284	PRO	2.4
1	A	362	ASN	2.4
1	A	272	MET	2.4
1	A	285	ILE	2.4
1	A	216	HIS	2.4
1	A	280	ASP	2.4
1	A	268	ILE	2.4
1	A	273	GLY	2.3
1	A	174	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	116	LYS	2.2
1	A	429	LYS	2.2
1	A	263	GLU	2.2
1	A	322	MET	2.0
1	A	364	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.