Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2025 – 04:09 PM JST

PDB ID	:	8YYH
Title	:	RNase J2 mutant H144A
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Deposited on	:	2024-04-03
Resolution	:	1.12 Å(reported)

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

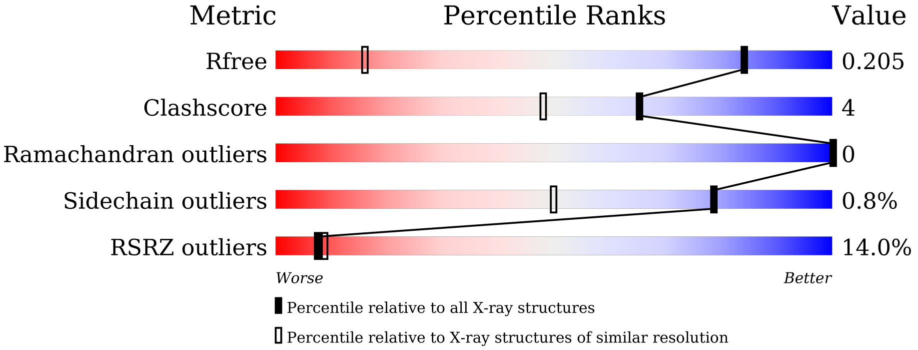
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance

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

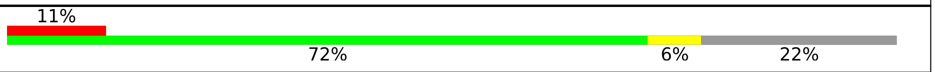
The reported resolution of this entry is 1.12 Å.

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	1652 (1.14-1.10)
Clashscore	180529	1870 (1.14-1.10)
Ramachandran outliers	177936	1828 (1.14-1.10)
Sidechain outliers	177891	1824 (1.14-1.10)
RSRZ outliers	164620	1652 (1.14-1.10)

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 3660 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	443	3387	2167	563	635	22	0	2	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	144	ALA	HIS	engineered mutation	UNP Q5HPR6

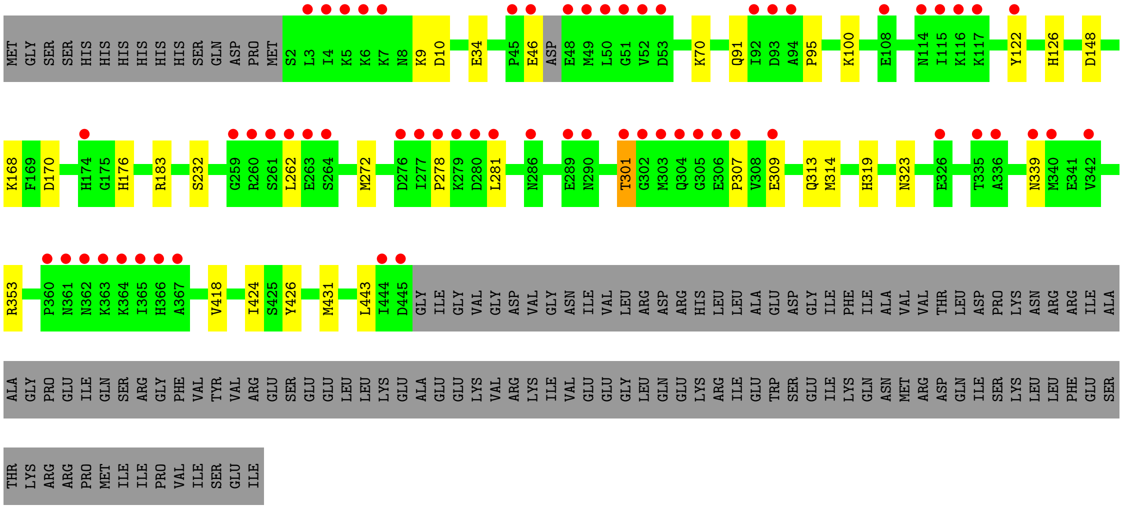
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	273	273	273	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	56.52Å 71.95Å 106.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.19 – 1.12 53.19 – 1.12	Depositor EDS
% Data completeness (in resolution range)	95.0 (53.19-1.12) 94.9 (53.19-1.12)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 1.12Å)	Xtriage
Refinement program	REFMAC 5.8.0350	Depositor
R, R_{free}	0.178 , 0.204 0.180 , 0.205	Depositor DCC
R_{free} test set	8161 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	12.5	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3660	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.58	1/3455 (0.0%)	0.87	2/4677 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	GLU	CD-OE1	-5.09	1.20	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	353	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	353	ARG	NE-CZ-NH1	5.15	122.88	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	3387	0	3330	25	0
2	A	273	0	0	2	0
All	All	3660	0	3330	25	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.

All (25) 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:183:ARG:HD3	2:A:629:HOH:O	1.60	1.02
1:A:319:HIS:H	1:A:323:ASN:HD21	1.26	0.81
1:A:278:PRO:HG2	1:A:281:LEU:HD22	1.70	0.72
1:A:100:LYS:HG2	1:A:272:MET:CE	2.25	0.66
1:A:9:LYS:HD3	1:A:10:ASP:CG	2.21	0.60
1:A:319:HIS:N	1:A:323:ASN:HD21	1.98	0.60
1:A:100:LYS:HG2	1:A:272:MET:HE1	1.84	0.59
1:A:278:PRO:CG	1:A:281:LEU:HD22	2.36	0.56
1:A:443:LEU:HD12	1:A:443:LEU:N	2.21	0.55
1:A:426:TYR:HB2	1:A:431[B]:MET:SD	2.47	0.55
1:A:309:GLU:OE2	1:A:313:GLN:NE2	2.41	0.52
1:A:314:MET:HA	1:A:323:ASN:HD22	1.75	0.51
1:A:95:PRO:HB3	1:A:122:TYR:CE2	2.47	0.49
1:A:148:ASP:OD1	1:A:176:HIS:HD2	1.95	0.49
1:A:262:LEU:HB2	1:A:301:THR:CG2	2.43	0.49
1:A:70:LYS:HE3	2:A:627:HOH:O	2.14	0.47
1:A:232:SER:OG	1:A:307:PRO:HB2	2.15	0.47
1:A:100:LYS:HE3	1:A:272:MET:HE2	1.97	0.45
1:A:46:GLU:CA	1:A:339:ASN:OD1	2.65	0.45
1:A:418:VAL:HG11	1:A:424:ILE:HD11	1.98	0.44
1:A:262:LEU:HB2	1:A:301:THR:HG21	2.01	0.43
1:A:9:LYS:HD3	1:A:10:ASP:OD2	2.19	0.42
1:A:168:LYS:HE2	1:A:170:ASP:HB2	2.01	0.42
1:A:9:LYS:HD3	1:A:10:ASP:OD1	2.19	0.42
1:A:443:LEU:N	1:A:443:LEU:CD1	2.83	0.41

There are no symmetry-related clashes.

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	441/571 (77%)	433 (98%)	8 (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	356/495 (72%)	353 (99%)	3 (1%)	79	50

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

Mol	Chain	Res	Type
1	A	91	GLN
1	A	126	HIS
1	A	301	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	HIS
1	A	176	HIS
1	A	323	ASN
1	A	381	ASN
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	443/571 (77%)	0.98	62 (13%) 7 9	8, 15, 90, 208	2 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365	ILE	17.4
1	A	262	LEU	15.8
1	A	305	GLY	10.9
1	A	336	ALA	10.9
1	A	7	LYS	10.2
1	A	50	LEU	10.1
1	A	335	THR	10.1
1	A	290	ASN	10.0
1	A	94	ALA	8.9
1	A	261	SER	8.6
1	A	93	ASP	8.3
1	A	280	ASP	8.2
1	A	364	LYS	7.9
1	A	51	GLY	7.9
1	A	278	PRO	7.6
1	A	264	SER	7.6
1	A	363	LYS	7.6
1	A	302	GLY	7.2
1	A	306	GLU	7.1
1	A	304	GLN	7.1
1	A	279	LYS	7.0
1	A	307	PRO	6.6
1	A	303	MET	6.5
1	A	263	GLU	6.4
1	A	445	ASP	6.4
1	A	6	LYS	6.2
1	A	366	HIS	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	260	ARG	5.9
1	A	301	THR	5.8
1	A	116	LYS	5.6
1	A	53	ASP	5.6
1	A	52	VAL	5.4
1	A	46	GLU	5.2
1	A	289	GLU	5.0
1	A	48	GLU	4.6
1	A	277	ILE	4.6
1	A	92	ILE	4.4
1	A	117	LYS	4.1
1	A	3	LEU	4.1
1	A	45	PRO	4.0
1	A	281	LEU	3.8
1	A	49	MET	3.8
1	A	286	ASN	3.7
1	A	259	GLY	3.6
1	A	5	LYS	3.4
1	A	361	ASN	2.8
1	A	108	GLU	2.8
1	A	276	ASP	2.5
1	A	340	MET	2.5
1	A	114	ASN	2.5
1	A	339	ASN	2.4
1	A	122	TYR	2.4
1	A	360	PRO	2.4
1	A	326	GLU	2.4
1	A	115	ILE	2.3
1	A	444	ILE	2.2
1	A	174	HIS	2.2
1	A	4	ILE	2.1
1	A	367	ALA	2.1
1	A	362	ASN	2.1
1	A	342	VAL	2.1
1	A	309	GLU	2.1

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.