



## Full wwPDB EM Validation Report ⓘ

Apr 16, 2026 – 10:12 am BST

PDB ID : 9SJX / pdb\_00009sjx  
Title : Serial electron diffraction (SerialED) structure of Y122F mutant Ribonucleotide reductase R2 from E. coli in its oxidised (met) form (re-oxidised)  
Authors : Pacoste, L.; Kumar, R.; Hongyi, X.; Hofer, G.; Hogbom, M.; Zou, X.  
Deposited on : 2025-09-01  
Resolution : 2.00 Å(reported)  
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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>.

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

MolProbity : 4-5-2 with Phenix2.0  
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

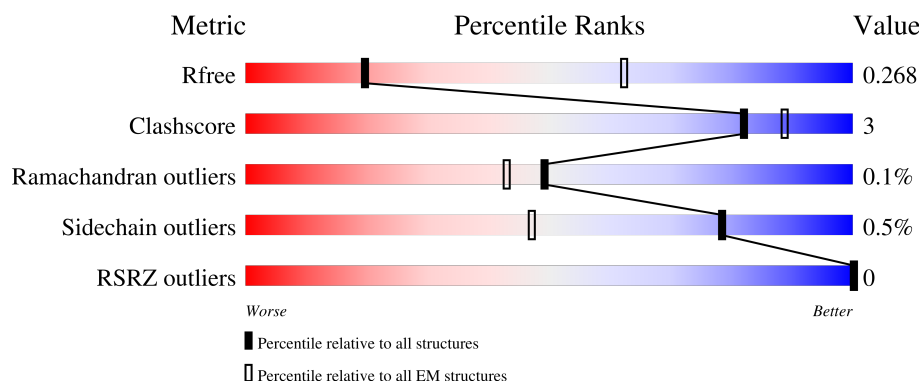
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON CRYSTALLOGRAPHY*

The reported resolution of this entry is 2.00 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)	EM structures (#Entries)
$R_{free}$	180332	208
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RSRZ outliers	180361	209

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	375	
1	B	375	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11633 atoms, of which 5664 are hydrogens and 0 are deuteriums.

In the tables below, 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 Ribonucleoside-diphosphate reductase 1 subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	341	Total	C	H	N	O	S	8	0
			5603	1808	2773	476	532	14		
1	B	340	Total	C	H	N	O	S	30	0
			5808	1860	2891	491	550	16		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	PHE	TYR	engineered mutation	UNP P69924
B	122	PHE	TYR	engineered mutation	UNP P69924

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total	Fe	0
			2	2	
2	B	2	Total	Fe	0
			2	2	

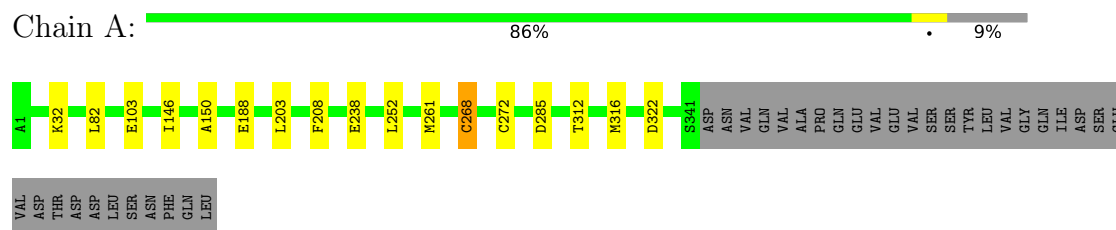
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	114	Total	O	0
			114	114	
3	B	104	Total	O	0
			104	104	

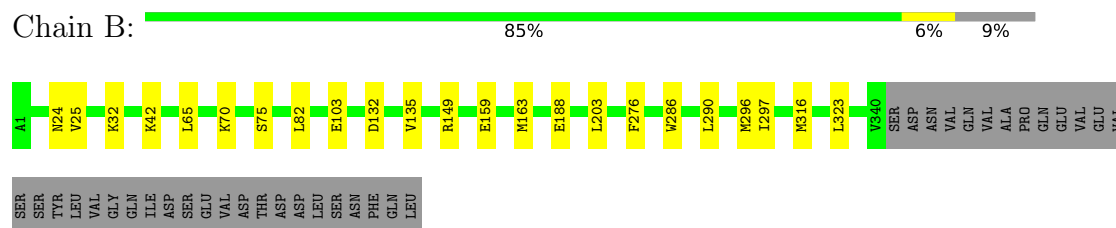
### 3 Residue-property plots [i](#)

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: Ribonucleoside-diphosphate reductase 1 subunit beta



- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.95Å 76.54Å 145.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.00 19.93 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.1 (19.93-2.00) 73.5 (19.93-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	-0.30 (at 1.40Å)	Xtriage
Refinement program	unknown	Depositor
R, $R_{free}$	0.247 , 0.285 0.240 , 0.268	Depositor DCC
$R_{free}$ test set	2011 reflections (1.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.4	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.147 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11633	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE

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	0.08	0/2927	0.21	0/3969
1	B	0.08	0/3112	0.22	0/4212
All	All	0.08	0/6039	0.22	0/8181

There are no bond length outliers.

There are no bond angle outliers.

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	2830	2773	2736	11	0
1	B	2917	2891	2758	18	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	114	0	0	2	0
3	B	104	0	0	1	0
All	All	5969	5664	5494	29	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 3.

All (29) 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:B:75[A]:SER:OG	1:B:290:LEU:HD11	1.84	0.76
1:A:238:GLU:OE2	3:A:501:HOH:O	2.16	0.60
1:B:149:ARG:HD3	1:B:286:TRP:CE3	2.36	0.60
1:A:82:LEU:HD22	1:A:146:ILE:HG22	1.86	0.57
1:B:149:ARG:HD2	1:B:286:TRP:HB3	1.88	0.55
1:B:75[B]:SER:HB2	1:B:290:LEU:HD11	1.89	0.53
1:A:82:LEU:HD22	1:A:146:ILE:CG2	2.40	0.51
1:B:42:LYS:NZ	3:B:513:HOH:O	2.46	0.48
1:A:268:CYS:O	1:A:272:CYS:N	2.35	0.47
1:A:203:LEU:C	1:A:203:LEU:HD23	2.40	0.47
1:B:32:LYS:N	1:B:103:GLU:OE2	2.48	0.47
1:B:65:LEU:O	1:B:70:LYS:NZ	2.43	0.45
1:B:276:PHE:HB2	1:B:316:MET:HE3	1.97	0.45
1:A:32:LYS:N	1:A:103:GLU:OE2	2.50	0.45
1:A:312:THR:O	1:A:316:MET:HG3	2.17	0.44
1:B:323:LEU:N	1:B:323:LEU:HD23	2.32	0.43
1:A:82:LEU:HD21	1:A:150:ALA:HB2	2.00	0.42
1:B:203:LEU:HD23	1:B:203:LEU:C	2.44	0.42
1:A:188:GLU:OE1	3:A:502:HOH:O	2.21	0.42
1:B:297:ILE:C	1:B:297:ILE:HD12	2.44	0.42
1:B:163[B]:MET:HE1	1:B:188[B]:GLU:HB3	2.01	0.41
1:A:252:LEU:HD22	1:A:261:MET:HG3	2.02	0.41
1:A:285:ASP:OD1	1:A:285:ASP:N	2.53	0.41
1:B:132:ASP:OD2	1:B:135:VAL:HG13	2.21	0.41
1:B:286:TRP:HE1	1:B:290:LEU:HD13	1.85	0.41
1:B:82:LEU:C	1:B:82:LEU:HD23	2.46	0.40
1:B:24:ASN:OD1	1:B:25:VAL:N	2.45	0.40
1:B:75[A]:SER:CB	1:B:290:LEU:HD11	2.51	0.40

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 PDB entries followed by that with respect to all EM entries.

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	347/375 (92%)	343 (99%)	4 (1%)	0	100	100
1	B	370/375 (99%)	360 (97%)	9 (2%)	1 (0%)	36	35
All	All	717/750 (96%)	703 (98%)	13 (2%)	1 (0%)	49	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	296	MET

### 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 PDB entries followed by that with respect to all EM entries.

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	316/340 (93%)	313 (99%)	3 (1%)	70	78
1	B	338/340 (99%)	338 (100%)	0	100	100
All	All	654/680 (96%)	651 (100%)	3 (0%)	78	87

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

Mol	Chain	Res	Type
1	A	208	PHE
1	A	268	CYS
1	A	322	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	124	HIS
1	A	278	GLN
1	A	326	GLN
1	B	68	HIS
1	B	246	GLN
1	B	326	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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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.