



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1XSM  
Title : PROTEIN R2 OF RIBONUCLEOTIDE REDUCTASE FROM MOUSE  
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Deposited on : 1996-07-03  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

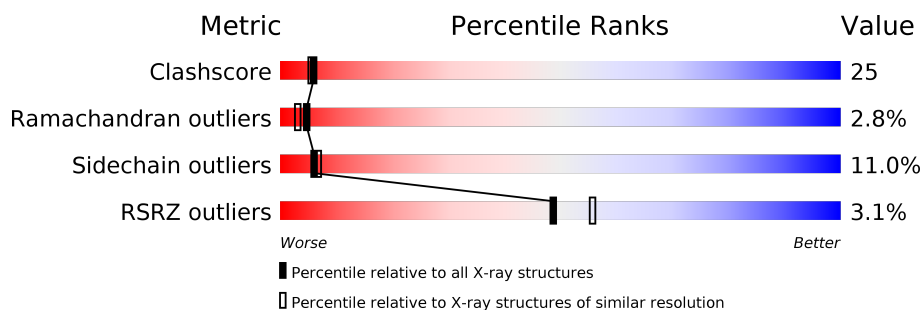
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on the lower 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  $\leq 5\%$ . 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	390	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2467 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 RIBONUCLEOTIDE REDUCTASE R2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2376	1540	394	427	15			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

Chain A:

39% 25% 8% 26%

Q323	D217	F135	LYS
Y324	A136	A143	ALA
I325	K218	E144	PRO
E326	E219	D139	THR
D330	Y222	R143	P66
R331	G223	E144	S67
L334	E224	N145	V68
K340	R225	L146	D69
R343	V226	V147	D70
E344	G239	E148	F71
E345	V246	R149	F72
K346	E253	E153	L73
P347	M263	V154	L74
F348	M260	Q155	R75
D349	E261	Q155	E76
E352	R265	E158	M77
ASN	D266	Q166	F78
ILE	E267	Q166	R79
SER	D272	M176	R80
LEU	L281	Y177	V82
GLY	L281	S178	V83
LYS	K284	L179	F84
THR	P285	L180	R86
ASN	A286	I181	E87
PHE	E287	D182	D90
GLU	R291	T183	I91
LYS	R291	Y184	Q93
ARG	VAL	I185	K96
VAL	T295	K186	Y96
GLY	R299	D187	E99
GLU	T300	P188	D109
TYR	I300	K189	L110
GLN	Q301	E190	SER
ARG	E302	R191	THR
MET	E303	E192	S111
GLY	F304	Y193	K112
VAL	L305	I114	D113
MET	T306	N196	I114
SER	E307	A197	Q115
ASN	A308	I198	H116
SER	L309	E199	W117
THR	P310	T200	E118
GLU	V311	R201	A119
ASN	K312	P202	L120
PHE	L313	C203	K121
PHE	I314	V204	P122
THR	G315	K205	D123
LEU	M316	K206	E124
ASP	T319	K207	R125
ALA	L320	A208	I128
ASP	M321	D209	L132
PHE	T322	E212	L133
		E213	F134

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.08 Å 108.93 Å 92.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 29.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (25.00-2.30) 96.5 (29.80-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.79 (at 2.31 Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.191 , 0.250 0.186 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 93.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2467	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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	1.33	20/2438 (0.8%)	1.61	42/3293 (1.3%)

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	GLU	CD-OE1	8.13	1.34	1.25
1	A	287	GLU	CD-OE2	7.38	1.33	1.25
1	A	148	GLU	CD-OE2	7.08	1.33	1.25
1	A	303	GLU	CD-OE1	6.93	1.33	1.25
1	A	153	GLU	CD-OE2	6.71	1.33	1.25

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	225	ARG	NE-CZ-NH2	-16.05	112.28	120.30
1	A	225	ARG	NE-CZ-NH1	15.90	128.25	120.30
1	A	343	ARG	NE-CZ-NH1	11.37	125.98	120.30
1	A	266	ASP	CB-CG-OD2	-8.47	110.67	118.30
1	A	182	ASP	CB-CG-OD2	-8.35	110.78	118.30

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	2376	0	2324	117	1
2	A	1	0	0	0	0
3	A	90	0	0	5	1
All	All	2467	0	2324	117	2

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 25.

The worst 5 of 117 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:246:TRP:HD1	1:A:314:ILE:HD12	1.27	0.97
1:A:197:ALA:HA	1:A:201:MET:HG3	1.53	0.90
1:A:246:TRP:CD1	1:A:314:ILE:HD12	2.05	0.90
1:A:120:LEU:HD23	1:A:125:ARG:HG2	1.56	0.88
1:A:201:MET:HB2	1:A:204:VAL:HG12	1.59	0.84

All (2) 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)
3:A:850:HOH:O	3:A:850:HOH:O[3_756]	1.73	0.47
1:A:121:LYS:NZ	1:A:219:GLU:OE2[8_466]	1.98	0.22

## 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	286/390 (73%)	260 (91%)	18 (6%)	8 (3%)	<b>5</b> <b>3</b>

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	GLU
1	A	81	PHE
1	A	113	ASP
1	A	66	PRO
1	A	77	ASN

### 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	254/345 (74%)	226 (89%)	28 (11%)	6 7

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	MET
1	A	198	ILE
1	A	319	THR
1	A	179	LEU
1	A	180	LEU

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

Mol	Chain	Res	Type
1	A	77	ASN
1	A	116	HIS
1	A	126	HIS
1	A	143	ASN
1	A	196	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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 ⓘ

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	288/390 (73%)	-0.35	9 (3%) 49 56	9, 30, 76, 99	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	ARG	4.8
1	A	65	ASN	4.5
1	A	77	ASN	4.5
1	A	81	PHE	4.4
1	A	66	PRO	3.7

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FE	A	401	1/1	0.96	0.11	42,42,42,42	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.