



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 14, 2023 – 03:21 am GMT

PDB ID : 2X0X  
Title : Ribonucleotide reductase R1 subunit of E. coli to 2.3 Å resolution  
Authors : Yokoyama, K.; Uhlin, U.; Stubbe, J.  
Deposited on : 2009-12-18  
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.

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 : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : **FAILED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

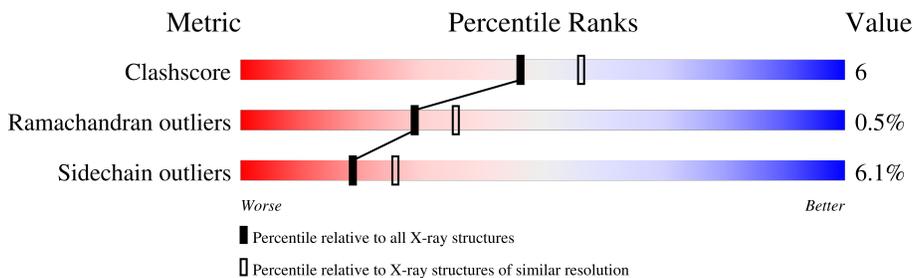
# 1 Overall quality at a glance

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)

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18869 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 RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	Total 5804	C 3688	N 995	O 1097	S 24	0	0	0
1	B	728	Total 5804	C 3688	N 995	O 1097	S 24	0	0	0
1	C	728	Total 5804	C 3688	N 995	O 1097	S 24	0	0	0

- Molecule 2 is a protein called RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	16	Total 129	C 77	N 19	O 33	0	0	0
2	E	16	Total 129	C 77	N 19	O 33	0	0	0
2	F	16	Total 129	C 77	N 19	O 33	0	0	0
2	P	3	Total 27	C 20	N 3	O 4	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	304	Total O 304 304	0	0
4	B	306	Total O 306 306	0	0
4	C	411	Total O 411 411	0	0
4	D	1	Total O 1 1	0	0
4	E	3	Total O 3 3	0	0
4	F	2	Total O 2 2	0	0
4	P	1	Total O 1 1	0	0

SEQUENCE-PLOTS INFOmissingINFO

### 3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.88Å 223.88Å 336.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	169.03 – 2.30	Depositor
% Data completeness (in resolution range)	100.0 (169.03-2.30)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.183 , 0.224	Depositor
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtrriage
Anisotropy	0.120	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	18869	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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.

## 4 Model quality

### 4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.53	0/5931	0.64	3/8033 (0.0%)
1	B	0.53	0/5931	0.64	4/8033 (0.0%)
1	C	0.63	0/5931	0.72	7/8033 (0.1%)
2	D	0.50	0/129	0.62	0/173
2	E	0.47	0/129	0.63	0/173
2	F	0.49	0/129	0.62	0/173
2	P	0.68	0/27	0.55	0/36
All	All	0.56	0/18207	0.67	14/24654 (0.1%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	216	ARG	NE-CZ-NH2	-11.86	114.37	120.30
1	C	510	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	C	216	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	B	216	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	A	216	ARG	NE-CZ-NH2	-7.18	116.71	120.30

There are no chirality outliers.

There are no planarity outliers.

### 4.2 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	5804	0	5728	82	0
1	B	5804	0	5728	58	0
1	C	5804	0	5728	82	0
2	D	129	0	111	0	0
2	E	129	0	111	1	0
2	F	129	0	111	3	0
2	P	27	0	31	5	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
4	A	304	0	0	18	0
4	B	306	0	0	12	1
4	C	411	0	0	21	1
4	D	1	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	1	0
4	P	1	0	0	2	0
All	All	18869	0	17548	224	1

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 6.

The worst 5 of 224 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:342:LEU:HG	4:A:2133:HOH:O	1.38	1.21
1:C:189:ARG:NH1	4:C:2117:HOH:O	1.87	1.07
1:A:186:ARG:HG3	1:A:186:ARG:HH11	1.25	0.99
1:B:274:PHE:HA	4:B:2117:HOH:O	1.63	0.96
1:C:450:ASN:HB2	4:C:2242:HOH:O	1.67	0.92

All (1) 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)
4:B:2006:HOH:O	4:C:2009:HOH:O[15_554]	2.16	0.04

## 4.3 Torsion angles [i](#)

### 4.3.1 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	724/761 (95%)	699 (96%)	21 (3%)	4 (1%)	25	31
1	B	724/761 (95%)	693 (96%)	28 (4%)	3 (0%)	34	42
1	C	724/761 (95%)	701 (97%)	18 (2%)	5 (1%)	22	26
2	D	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
2	E	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
2	F	14/20 (70%)	14 (100%)	0	0	100	100
2	P	1/20 (5%)	1 (100%)	0	0	100	100
All	All	2215/2363 (94%)	2134 (96%)	69 (3%)	12 (0%)	29	35

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	B	294	GLN
1	C	294	GLN
1	A	216	ARG
1	B	216	ARG

### 4.3.2 Protein sidechains [i](#)

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	626/651 (96%)	589 (94%)	37 (6%)	19	27
1	B	626/651 (96%)	592 (95%)	34 (5%)	22	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	626/651 (96%)	588 (94%)	38 (6%)	18	25
2	D	16/19 (84%)	14 (88%)	2 (12%)	4	5
2	E	16/19 (84%)	14 (88%)	2 (12%)	4	5
2	F	16/19 (84%)	12 (75%)	4 (25%)	0	0
2	P	3/19 (16%)	3 (100%)	0	100	100
All	All	1929/2029 (95%)	1812 (94%)	117 (6%)	18	25

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	364	LEU
2	D	367	THR
1	C	4	ASN
2	D	361	ILE
1	C	384	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	633	ASN
1	C	696	ASN
2	E	360	GLN
1	B	150	GLN
1	B	130	GLN

#### 4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

#### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

#### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 4.6 Ligand geometry

3 ligands are modelled in this entry.

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.

## 4.7 Other polymers

There are no such residues in this entry.

## 4.8 Polymer linkage issues

There are no chain breaks in this entry.

## 5 Fit of model and data

### 5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

### 5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers

EDS failed to run properly - this section is therefore empty.