

# wwPDB X-ray Structure Validation Summary Report (i)

Feb 4, 2024 – 12:39 PM EST

PDB ID : 1RIB

Title : STRUCTURE AND FUNCTION OF THE ESCHERICHIA COLI RIBONU-

CLEOTIDE REDUCTASE PROTEIN R2

Authors : Eklund, H. Deposited on : 1993-01-19

Resolution : 2.20 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*A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

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)

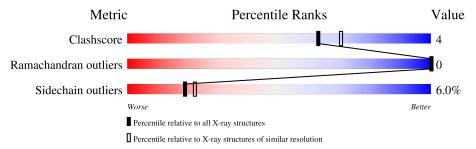
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.20 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain				
1	A	375	74%	14%		9%	
1	В	375	71%	14%	5% •	9%	



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5899 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.

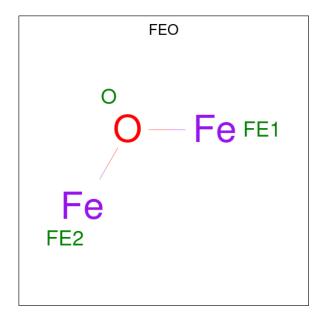
• Molecule 1 is a protein called RIBONUCLEOTIDE REDUCTASE R1 PROTEIN.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	340	Total	C	N 462	0	S	0	0	0
			2784	1782	463	526	13			
1	R	340	Total	$\mathbf{C}$	N	O	$\mathbf{S}$	0		0
1	Ъ	340	2784	1782	463	526	13	0	0	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	GLN	conflict	UNP P69924
A	24	GLN	ASN	conflict	UNP P69924
A	326	ASN	$\operatorname{GLN}$	conflict	UNP P69924
В	7	ALA	GLN	conflict	UNP P69924
В	24	GLN	ASN	conflict	UNP P69924
В	326	ASN	GLN	conflict	UNP P69924

• Molecule 2 is MU-OXO-DIIRON (three-letter code: FEO) (formula: Fe<sub>2</sub>O).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe O 3 2 1	0	0
2	В	1	Total Fe O 3 2 1	0	0

## $\bullet\,$ Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	161	Total O 161 161	0	0
3	В	164	Total O 164 164	0	0

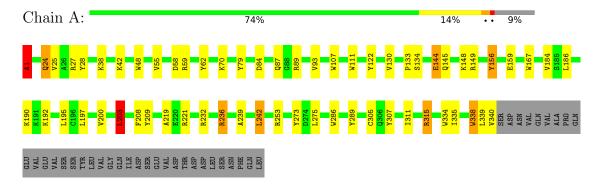


# 3 Residue-property plots (i)

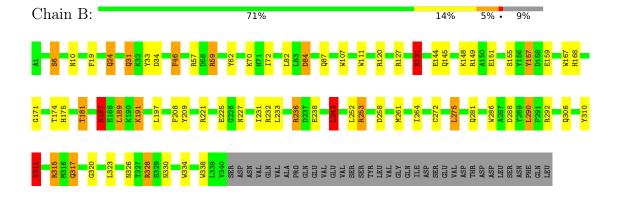
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN



• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN





# 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	74.30Å 85.50Å 115.70Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	7.00 - 2.20	Depositor	
% Data completeness	(Not available) (7.00-2.20)	Depositor	
(in resolution range)	(1.00 available) (1.00 2.20)	Depositor	
$R_{merge}$	(Not available)	Depositor	
$R_{sym}$	(Not available)	Depositor	
Refinement program	X-PLOR	Depositor	
$R, R_{free}$	0.175 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	5899	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP	



# 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: FEO

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		Bo	nd lengths	Bond angles		
IVIOI	Chain	Chain RMSZ #		RMSZ	# Z >5	
1	A	0.83	$2/2848 \; (0.1\%)$	1.52	56/3864 (1.4%)	
1	В	0.77	0/2848	1.50	44/3864 (1.1%)	
All	All	0.80	$2/5696 \ (0.0\%)$	1.51	100/7728 (1.3%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	В	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	$\operatorname{Ideal}( ext{\AA})$
1	A	1	ALA	N-CA	-13.10	1.20	1.46
1	A	1	ALA	CA-CB	-5.04	1.41	1.52

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	1	ALA	N-CA-CB	-11.07	94.61	110.10
1	В	236	ARG	NE-CZ-NH2	-10.63	114.98	120.30
1	A	286	TRP	CD1-CG-CD2	9.34	113.77	106.30
1	A	338	TRP	CD1-CG-CD2	8.84	113.37	106.30
1	A	1	ALA	CA-C-O	-8.73	101.77	120.10

There are no chirality outliers.



All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	Mainchain
1	A	156	TYR	Sidechain
1	В	131	ASN	Peptide
1	В	157	TYR	Sidechain

#### 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	2784	0	2731	20	0
1	В	2784	0	2731	27	0
2	A	3	0	0	0	0
2	В	3	0	0	0	0
3	A	161	0	0	7	0
3	В	164	0	0	6	0
All	All	5899	0	5462	47	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.

The worst 5 of 47 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$	
1:A:305:CYS:SG	3:A:668:HOH:O	2.48	0.71	
1:A:209:TYR:OH	1:A:340:VAL:HG21	1.96	0.65	
1:B:306:GLN:HG3	1:B:328:ARG:HD3	1.81	0.62	
1:B:252:LEU:HD22	1:B:261:MET:HG3	1.84	0.58	
1:B:317:GLN:HB2	1:B:323:LEU:HD21	1.85	0.58	

There are no symmetry-related clashes.



### 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	Perce	ntiles
1	A	338/375 (90%)	331 (98%)	7 (2%)	0	100	100
1	В	338/375~(90%)	332 (98%)	6 (2%)	0	100	100
All	All	$676/750 \; (90\%)$	663 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 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	306/339 (90%)	294 (96%)	12 (4%)	32 41		
1	В	306/339 (90%)	281 (92%)	25 (8%)	11 11		
All	All	612/678 (90%)	575 (94%)	37 (6%)	19 22		

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	242	LEU
1	В	326	ASN
1	В	253	ARG
1	В	290	LEU
1	В	6	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:



Mol	Chain	Res	Type
1	В	168	HIS
1	В	175	HIS
1	В	330	ASN
1	A	227	ASN
1	В	10	ASN

#### 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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles	
IVIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	$\mid \text{RMSZ} \mid \# Z  > 2$
2	FEO	A	401	3,1	0,2,2	-	-	-	
2	FEO	В	402	3,1	0,2,2	-	-	-	

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.



## 6 Fit of model and data (i)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

#### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

#### 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

