



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:59 PM GMT

PDB ID : 1RLR
Title : STRUCTURE OF RIBONUCLEOTIDE REDUCTASE PROTEIN R1
Authors : Uhlin, U.; Eklund, H.
Deposited on : 1994-08-12
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

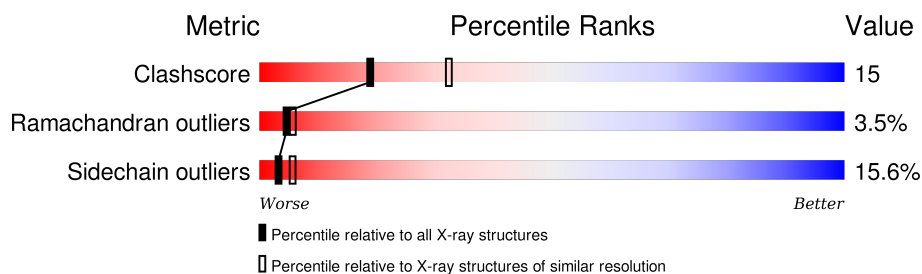
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	761	 55% 28% 10% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5875 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 PROTEIN R1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	737	Total	C	N	O	S	0	0	0
			5875	3729	1007	1115	24			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	479	ASP	GLU	CONFLICT	UNP P00452
A	526	LYS	ASN	CONFLICT	UNP P00452
A	527	HIS	ASP	CONFLICT	UNP P00452
A	739	ASP	GLY	CONFLICT	UNP P00452
A	740	ILE	ALA	CONFLICT	UNP P00452
A	741	ASP	GLU	CONFLICT	UNP P00452
A	743	LEU	ALA	CONFLICT	UNP P00452
A	744	SER	GLN	CONFLICT	UNP P00452
A	745	ASN	ASP	CONFLICT	UNP P00452
A	746	PHE	ASP	CONFLICT	UNP P00452
A	747	GLN	LEU	CONFLICT	UNP P00452
A	748	LEU	VAL	CONFLICT	UNP P00452

4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	226.00Å 226.00Å 341.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5875	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.26	33/6003 (0.5%)	2.08	233/8130 (2.9%)

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	5

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	ALA	C-N	19.95	1.79	1.34
1	A	200	VAL	CA-CB	16.46	1.89	1.54
1	A	176	VAL	CA-CB	13.38	1.82	1.54
1	A	12	GLY	N-CA	10.42	1.61	1.46
1	A	17	ILE	N-CA	10.40	1.67	1.46

The worst 5 of 233 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	GLY	O-C-N	-27.57	78.59	122.70
1	A	12	GLY	C-N-CA	-16.06	81.56	121.70
1	A	12	GLY	CA-C-N	14.76	149.66	117.20
1	A	264	LEU	O-C-N	-14.18	99.09	123.20
1	A	406	ARG	NE-CZ-NH2	-13.65	113.48	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	GLY	Mainchain
1	A	16	ARG	Peptide
1	A	264	LEU	Mainchain
1	A	361	VAL	Peptide
1	A	79	TYR	Sidechain

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	5875	0	5774	178	1
All	All	5875	0	5774	178	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 15.

The worst 5 of 178 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:176:VAL:CA	1:A:176:VAL:CB	1.82	1.57
1:A:200:VAL:CA	1:A:200:VAL:CB	1.89	1.50
1:A:273:ALA:C	1:A:274:PHE:N	1.79	1.35
1:A:264:LEU:HD23	1:A:389:ARG:NH1	1.66	1.09
1:A:249:SER:HB3	1:A:292:CYS:HB2	1.31	1.08

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)
1:A:276:THR:OG1	1:A:293:SER:O[18_655]	1.19	1.01

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	733/761 (96%)	661 (90%)	46 (6%)	26 (4%)	4 6

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	216	ARG
1	A	250	GLN
1	A	267	PRO
1	A	276	THR

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	633/654 (97%)	534 (84%)	99 (16%)	3 6

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	SER
1	A	394	LYS
1	A	681	LEU
1	A	313	VAL
1	A	329	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	321	ASN
1	A	322	ASN
1	A	596	HIS
1	A	250	GLN
1	A	686	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.