



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 11:07 AM UTC

PDB ID : 1RNR / pdb_00001rnr
Title : AUTOCATALYTIC GENERATION OF DOPA IN THE ENGINEERED PROTEIN R2 F208Y FROM ESCHERICHIA COLI RIBONUCLEOTIDE REDUCTASE AND CRYSTAL STRUCTURE OF THE DOPA-208 PROTEIN
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Deposited on : 1993-04-26
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

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

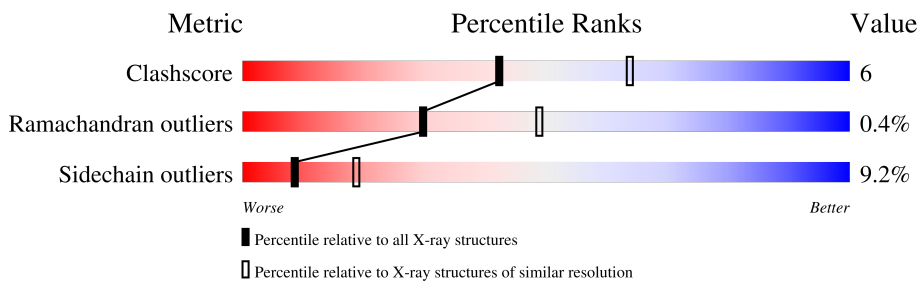
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	375	 62% 24% 6% 9%
1	B	375	 63% 21% 6% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5727 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	O	S	0	0	0
			2786	1782	463	528	13			
1	B	340	Total	C	N	O	S	0	0	0
			2786	1782	463	528	13			

There are 8 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	208	DAH	PHE	engineered mutation	UNP P69924
A	326	ASN	GLN	conflict	UNP P69924
B	7	ALA	GLN	conflict	UNP P69924
B	24	GLN	ASN	conflict	UNP P69924
B	208	DAH	PHE	engineered mutation	UNP P69924
B	326	ASN	GLN	conflict	UNP P69924

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	Hg	0	0
			6	6		
3	B	8	Total	Hg	0	0
			8	8		

- Molecule 4 is water.

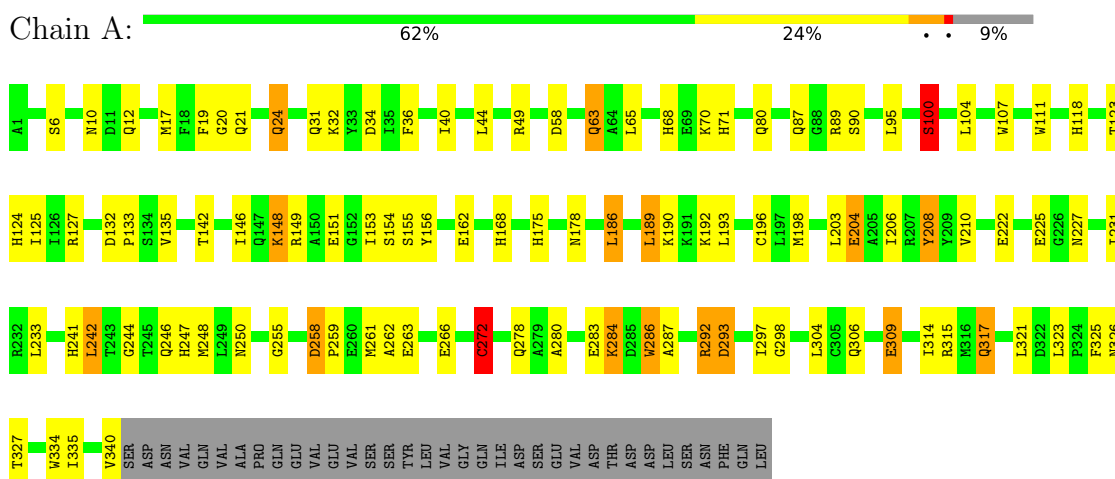
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total 72	O 72	1	0
4	B	65	Total 65	O 65	1	0

3 Residue-property plots

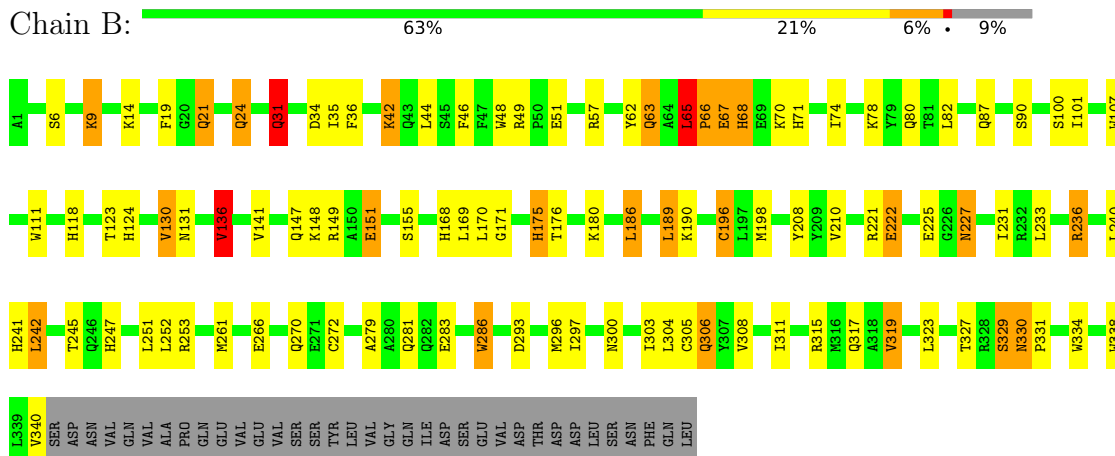
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.10Å 85.30Å 115.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5727	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: FE, DAH, HG

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	1.00	9/2835 (0.3%)	1.78	62/3845 (1.6%)
1	B	0.98	13/2835 (0.5%)	1.77	55/3845 (1.4%)
All	All	0.99	22/5670 (0.4%)	1.77	117/7690 (1.5%)

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	298	GLY	N-CA	7.46	1.56	1.45
1	B	124	HIS	CD2-NE2	-7.20	1.29	1.37
1	A	175	HIS	CD2-NE2	-7.16	1.29	1.37
1	A	118	HIS	CD2-NE2	-7.13	1.30	1.37
1	A	124	HIS	CD2-NE2	-7.06	1.30	1.37

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	319	VAL	N-CA-CB	-11.19	99.30	112.39
1	B	304	LEU	CA-C-O	-10.02	110.38	120.70
1	B	330	ASN	OD1-CG-ND2	-9.58	113.02	122.60
1	A	247	HIS	CA-CB-CG	-9.22	104.58	113.80
1	B	147	GLN	OE1-CD-NE2	-8.63	113.97	122.60

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	2786	0	2727	33	0
1	B	2786	0	2725	30	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	6	0	0	1	0
3	B	8	0	0	1	0
4	A	72	0	0	1	0
4	B	65	0	0	1	0
All	All	5727	0	5452	61	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 6.

The worst 5 of 61 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:272:CYS:CB	3:A:407:HG:HG	1.84	0.85
1:A:272:CYS:SG	1:A:321:LEU:HD21	2.25	0.77
1:B:252:LEU:HD22	1:B:261:MET:HG2	1.69	0.75
1:A:266:GLU:HG2	4:A:480:HOH:O	1.87	0.74
1:A:123:THR:HG22	1:A:127:ARG:HH11	1.53	0.73

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	Percentiles	
1	A	337/375 (90%)	331 (98%)	5 (2%)	1 (0%)	36	55
1	B	337/375 (90%)	329 (98%)	6 (2%)	2 (1%)	21	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	674/750 (90%)	660 (98%)	11 (2%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	GLU
1	B	66	PRO
1	A	153	ILE

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	305/338 (90%)	283 (93%)	22 (7%)	13	28
1	B	305/338 (90%)	271 (89%)	34 (11%)	6	12
All	All	610/676 (90%)	554 (91%)	56 (9%)	8	19

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	57	ARG
1	B	327	THR
1	B	131	ASN
1	B	319	VAL
1	B	253	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	201	ASN
1	B	330	ASN
1	A	336	ASN
1	B	10	ASN
1	B	87	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	DAH	B	208	1,2	12,13,14	0.96	1 (8%)	12,17,19	0.98	0
1	DAH	A	208	1,2	12,13,14	1.01	0	12,17,19	1.62	4 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DAH	B	208	1,2	-	1/5/6/8	0/1/1/1
1	DAH	A	208	1,2	-	2/5/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	208	DAH	CB-CA	-2.08	1.49	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	DAH	CE2-CD2-CG	-2.89	117.82	120.81
1	A	208	DAH	CE1-CZ-CE2	2.79	122.64	119.66
1	A	208	DAH	CD1-CE1-CZ	-2.59	117.91	120.50
1	A	208	DAH	CD1-CG-CD2	2.08	121.42	118.55

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	208	DAH	N-CA-CB-CG
1	A	208	DAH	C-CA-CB-CG
1	B	208	DAH	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	208	DAH	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.