



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:57 AM UTC

PDB ID : 7R1R / pdb_00007r1r
Title : RIBONUCLEOTIDE REDUCTASE E441Q MUTANT R1 PROTEIN FROM
ESCHERICHIA COLI
Authors : Eriksson, M.; Eklund, H.
Deposited on : 1997-09-17
Resolution : 3.10 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
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

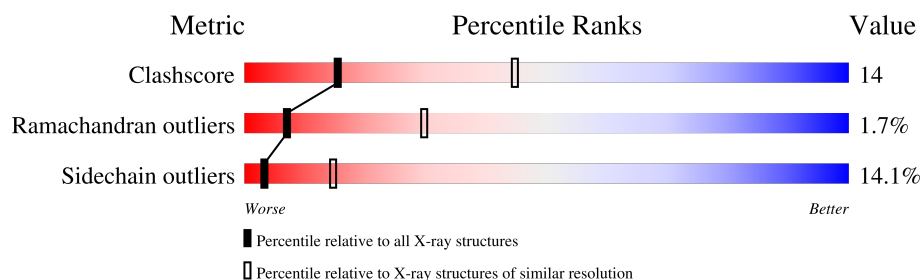
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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	761	53% 33% 9% . .
1	B	761	55% 31% 10% . .
1	C	761	54% 32% 10% . .
2	D	20	65% 10% 10% 5% 10%
2	E	20	55% 25% 10% 10%
2	F	20	50% 30% 10% 10%
2	P	20	5% 5% 10% 80%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18166 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	738	Total	C	N	O	S	0	0	0
			5875	3729	1011	1110	25			
1	B	738	Total	C	N	O	S	0	0	0
			5875	3729	1011	1110	25			
1	C	738	Total	C	N	O	S	0	0	0
			5875	3729	1011	1110	25			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	441	GLN	GLU	engineered mutation	UNP P00452
B	441	GLN	GLU	engineered mutation	UNP P00452
C	441	GLN	GLU	engineered mutation	UNP P00452

- Molecule 2 is a protein called RIBONUCLEOTIDE REDUCTASE R2 PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	18	Total	C	N	O	0	0	0
			140	84	21	35			
2	E	18	Total	C	N	O	0	0	0
			140	84	21	35			
2	F	18	Total	C	N	O	0	0	0
			140	84	21	35			
2	P	4	Total	C	N	O	0	0	0
			31	22	4	5			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		

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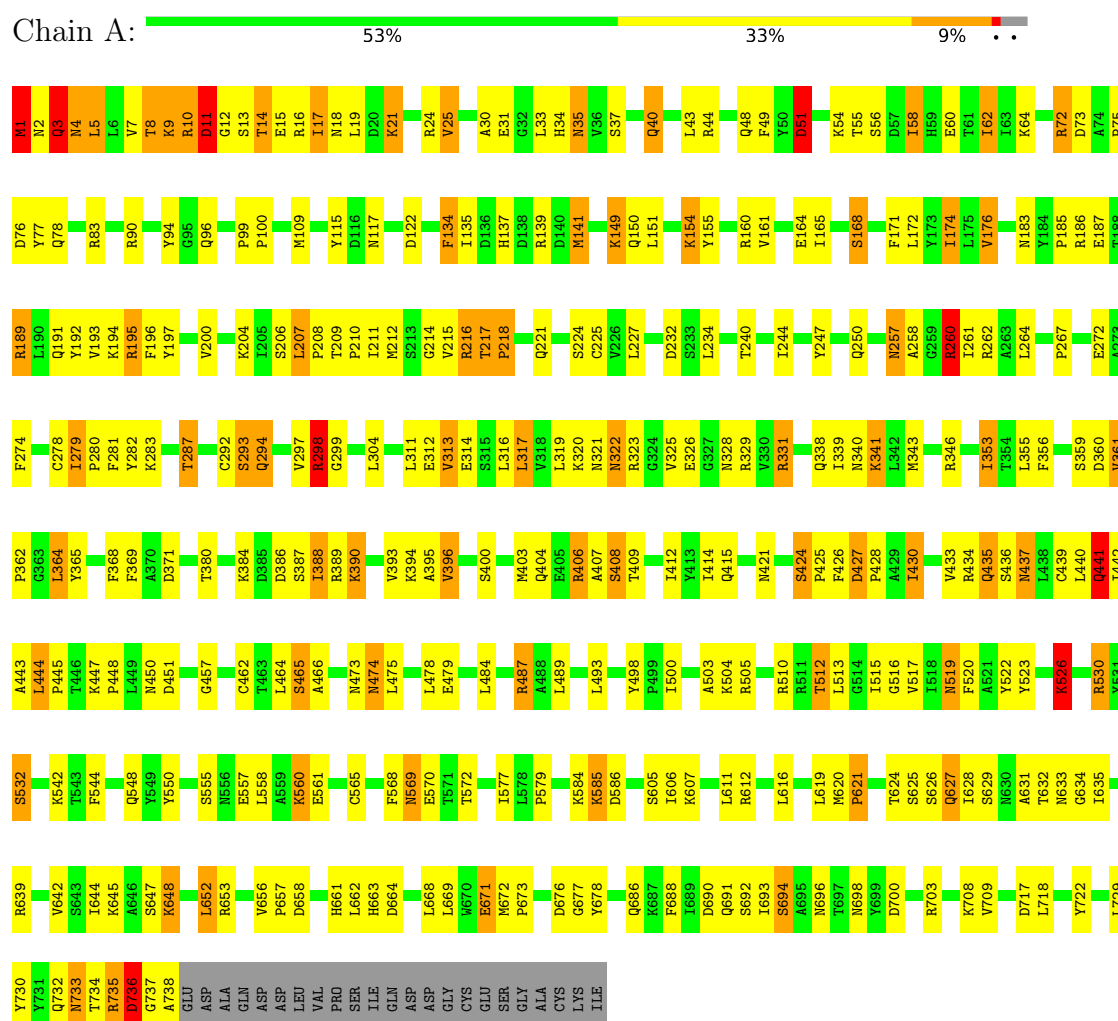
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	30	Total	O	0	0
			30	30		
3	C	32	Total	O	0	0
			32	32		

3 Residue-property plots

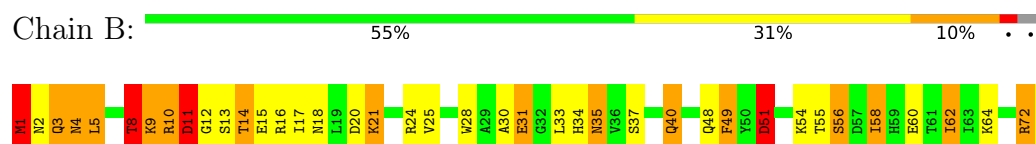
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

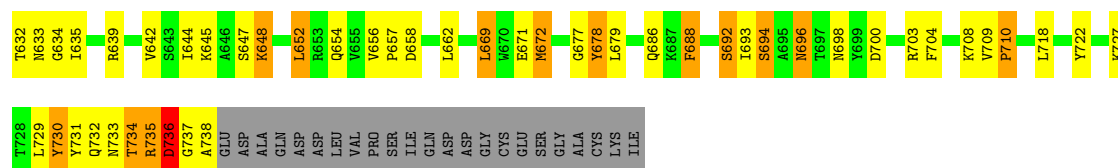


• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN





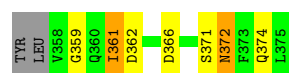
R530	L438	L355	R262	L180	P75	R1
C439	C439	F356	A263	N183	D76	N2
S532	L440	S357	L264		Y77	Q3
	Q441	P358			Q78	N4
N538	L442	S359	E272	E187	Y79	L5
	A443	D360	A273	T188	L50	
	L444	V361	F274	R189		T8
K542		P362			R83	K9
T543	N450	G363	I279	L190		R10
E545		L364	P280	Q191	R90	D11
	D454			K194		G12
Q548		A370	K283	R195	Y94	S13
Y549	G457		H284		G95	T14
Y550		T380	F285	V200	Q96	S13
	L461				F97	R16
S555	T463	K384	V289	F203	E98	I17
N556	L464	D386	S293	K204	P99	N18
E557	S465	S387	Q294	T205		
A558	A466	I388		S206	V106	K21
N559		R389	V297	L207		
K560		K390	R298	T209	M109	R24
E561	N473		G299	P210	V110	V25
	N474			I211		
N569	L475	V393		M212	Y115	W28
E570	D476	K394	L304		A29	A29
T571	E477	A395			E31	A30
T572	L478	V396	P307	V215	N117	
	E479		M308	R216		G32
		F399	W309	T217	E121	L33
I577	L484	S400	H310	P218	D122	H34
L578			L311	T219		
P579		M403	E312	R220	F134	N36
K584	R487	Q404	V313	Q221	I135	V36
K585	L489	E405		F222	D136	I38
D586		R406	L316	S223	H137	S39
	L492	A407	L317	S224	D138	Q40
N592		S408	L318	C225	R139	
E593	Q496	T409	L319	V226	D140	R44
	D497	G410	K320	L227	M141	
S605	Y498	R411	N321			I47
I606	P499	I412	N322	C230	K149	Q48
K607	I600	Y413	R323	Q150	Q150	F49
T608	P501	I414	G324	L234	L151	Y50
			V325			D51
L611	R510	M421	N328	T240	K154	
R612	R511	S424	R329	I244	Y155	K54
	T512	P425	V330			T55
L616	L513	F426	R331	Q250	R160	S56
	G514	D427		V161		D57
L619	I515	P428	Y335	R251	I165	H59
M620	G516	M428		A252	I165	E60
P621	V517	A429		G253		T61
	I518	I430	I339	T254	S168	
S625	N519	A431	N340	G255		I62
S626	F520	P432	K341	I256	L172	K64
Q627	P433	V432	L348	N257	Y173	G64
I628	R434	R434		A258	I174	
S629	Y522			G259	L175	R72
		Q435		R260	V176	D73
N630	K526	N436	L353	T261		W74
E631		V127				



● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



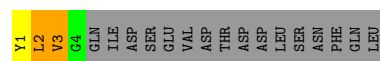
● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	224.56 Å 224.56 Å 335.45 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	91.2 (20.00-3.10)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.200 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18166	wwPDB-VP
Average B, all atoms (Å ²)	54.0	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	0.63	0/6003	1.78	135/8130 (1.7%)
1	B	0.60	0/6003	1.80	137/8130 (1.7%)
1	C	0.65	0/6003	1.83	140/8130 (1.7%)
2	D	0.48	0/140	1.49	1/188 (0.5%)
2	E	0.46	0/140	1.45	1/188 (0.5%)
2	F	0.51	0/140	1.55	1/188 (0.5%)
2	P	1.14	0/31	2.86	4/41 (9.8%)
All	All	0.62	0/18460	1.80	419/24995 (1.7%)

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	1
1	B	0	2
1	C	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 419 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	736	ASP	CA-CB-CG	12.84	125.44	112.60
1	C	195	ARG	CD-NE-CZ	12.77	142.27	124.40
1	B	736	ASP	CA-CB-CG	11.22	123.82	112.60
1	B	703	ARG	NE-CZ-NH2	-10.74	109.54	119.20
1	B	195	ARG	CD-NE-CZ	10.54	139.15	124.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	579	PRO	Mainchain
1	B	620	MET	Mainchain
1	B	697	THR	Mainchain
1	C	579	PRO	Mainchain

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	5801	165	0
1	B	5875	0	5801	154	0
1	C	5875	0	5801	164	0
2	D	140	0	123	3	0
2	E	140	0	123	3	0
2	F	140	0	123	3	0
2	P	31	0	34	4	0
3	A	28	0	0	2	0
3	B	30	0	0	3	0
3	C	32	0	0	3	0
All	All	18166	0	17806	485	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 14.

The worst 5 of 485 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:B:619:LEU:HD12	1:B:693:ILE:HG12	1.46	0.96
1:B:191:GLN:HE21	1:B:195:ARG:HH21	1.11	0.94
1:A:191:GLN:HE21	1:A:195:ARG:HH21	1.12	0.93
1:C:441:GLN:NE2	1:C:620:MET:HB3	1.85	0.92
1:C:441:GLN:HE21	1:C:620:MET:HB3	1.34	0.92

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	736/761 (97%)	675 (92%)	51 (7%)	10 (1%)	9	34
1	B	736/761 (97%)	678 (92%)	46 (6%)	12 (2%)	7	30
1	C	736/761 (97%)	679 (92%)	47 (6%)	10 (1%)	9	34
2	D	16/20 (80%)	13 (81%)	2 (12%)	1 (6%)	1	6
2	E	16/20 (80%)	13 (81%)	1 (6%)	2 (12%)	0	1
2	F	16/20 (80%)	13 (81%)	1 (6%)	2 (12%)	0	1
2	P	2/20 (10%)	0	1 (50%)	1 (50%)	0	0
All	All	2258/2363 (96%)	2071 (92%)	149 (7%)	38 (2%)	7	30

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	A	735	ARG
1	B	14	THR
1	B	294	GLN
1	B	735	ARG

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	632/651 (97%)	545 (86%)	87 (14%)	3	15
1	B	632/651 (97%)	543 (86%)	89 (14%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	632/651 (97%)	544 (86%)	88 (14%)	3	15
2	D	17/19 (90%)	14 (82%)	3 (18%)	2	9
2	E	17/19 (90%)	14 (82%)	3 (18%)	2	9
2	F	17/19 (90%)	13 (76%)	4 (24%)	1	3
2	P	3/19 (16%)	2 (67%)	1 (33%)	0	0
All	All	1950/2029 (96%)	1675 (86%)	275 (14%)	3	15

5 of 275 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	387	SER
1	C	424	SER
1	C	644	ILE
1	B	17	ILE
1	B	10	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	453	ASN
1	C	548	GLN
1	C	696	ASN
1	B	18	ASN
1	B	3	GLN

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 oligosaccharides 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

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.