



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:58 PM UTC

PDB ID : 6R1R / pdb_00006r1r
Title : RIBONUCLEOTIDE REDUCTASE E441D 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

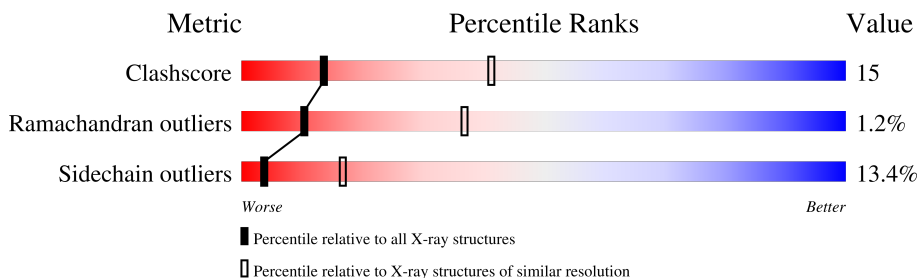
1 Overall quality at a glance

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	52% 35% 9% ..
1	B	761	54% 32% 10% ..
1	C	761	54% 32% 10% ..
2	D	20	65% 15% 10% 10%
2	E	20	60% 20% 10% 10%
2	F	20	55% 25% 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 18163 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
			5874	3728	1010	1111	25			
1	B	738	Total	C	N	O	S	0	0	0
			5874	3728	1010	1111	25			
1	C	738	Total	C	N	O	S	0	0	0
			5874	3728	1010	1111	25			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	441	ASP	GLU	engineered mutation	UNP P00452
B	441	ASP	GLU	engineered mutation	UNP P00452
C	441	ASP	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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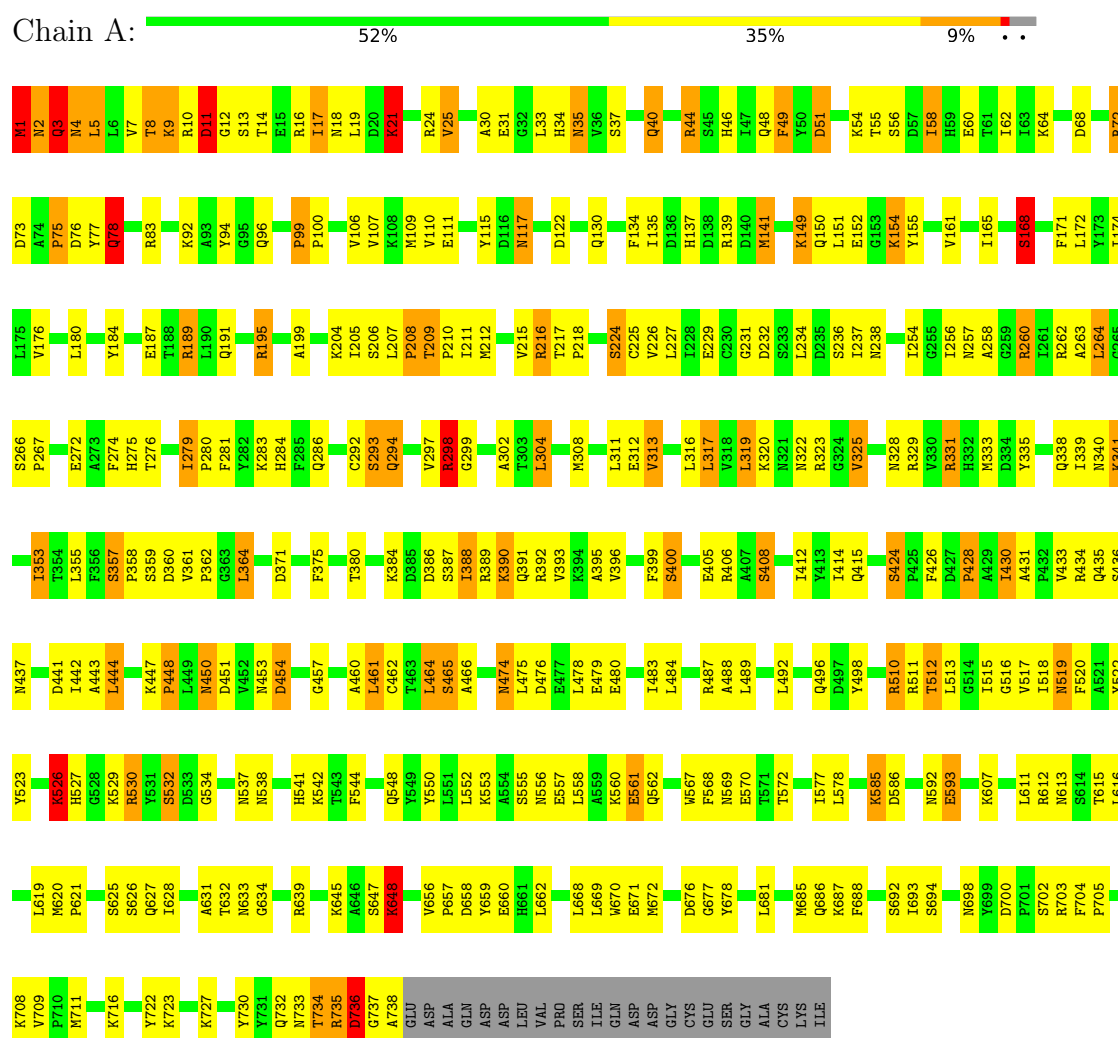
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	30	Total	O	0	0
			30	30		
3	C	32	Total	O	0	0
			32	32		

3 Residue-property plots

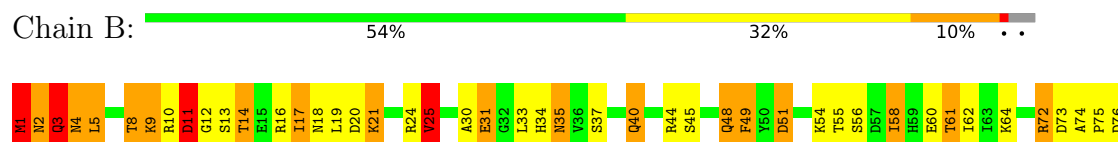
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

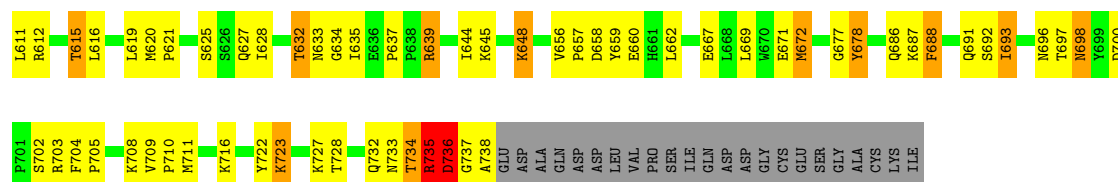


• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN





P499	H419	V325	V248	I165	S71	N1
I500	C420	N328	R251	S168	R72	N2
R510	N421	R329	G252	G253	D73	Q3
R511	S424	V330	G253	G254	A74	N4
T512	P425	R331	I254	L171	P75	N5
L513	F426	R332	G255	L172	D76	L6
G514	D427	M333	L286	T173	T77	V7
T515	P428	D334	D287	I174	Q78	T8
G516	A429	V335	D288	L175	K9	R10
V517	I430	Q338	G259	R83	R10	R10
L518	A431	Q338	G260	L180	R83	D11
N519	F432	Q338	I261	L186	G12	G12
F520	V433	K341	R262	L189	S13	S13
A521	R434	K341	A263	Y184	R89	T14
Y522	Q435	L348	L264	P185	R90	E15
K523	L438	L353	R269	R186	K91	R16
R524	C439	L353	R269	E187	K92	I17
R530	L440	S357	E272	T188	A93	N18
L531	D441	P358	A273	R189	Y94	L19
S532	I442	S359	F274	G95	Q96	K21
A443	A443	D360	D275	K194	P99	H23
L444	L444	V361	T276	R195	R24	R24
H541	K447	L364	G277	A199	V106	V25
K542	P448	K364	T278	V200	V110	A30
T543	K448	L449	I279	S201	E31	E31
F544	M450	F368	P280	T202	G32	G32
Q548	D451	F369	K283	F903	M17	L33
Y549	D451	A370	K283	K204	L120	H34
Y550	D454	E373	Q286	I205	E121	N35
S555	N455	F374	S293	S206	D122	V36
S556	N456	F375	S293	L207	Y123	S37
E557	A460	T380	Q284	P208	T124	
L558	L461	T380	V287	T209	Q40	
A559	L461	T380	R298	P210	E127	
K560	L464	K384	R298	I211	R44	
E561	S465	D385	A302	M212	S45	
Q562	A466	D386	T303	V215	I135	H46
		S387	T303	D136	I47	I47
W567	M474	L388	L304	R216	H137	Q48
F568	L475	R389	F305	R218	D138	F49
N569	L475	K390	Y306	P218	R139	Y50
E570	L478	Q391	P307	T217	D51	
T571	E479	R392	P307	D140	D51	
T572	E479	V393	H310	S223	M141	
		V393	H310	S224	K54	
I577	I483	K394	L311	C225	T55	
L578	L484	A395	E312	V226	S56	
P579	R487	V396	V313	L227	Y145	
				I228	K149	I58
K585	A488	F399	L316	E229	Q150	H59
D586	L489	S400	L317	C230	L151	E60
			V318	C231	E152	T61
		S408	L319	D232	G153	
	L492	I414	K320	S233	K154	K64
N592	L492	I414	N322	L234	Y155	
E593	Q496	Q415	R323	I244	V161	D68
	N497	D418	R323		L69	
K607	Y108	D418	R323		T70	



● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain D: 65% 15% 10% 10%



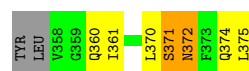
● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain E: 60% 20% 10% 10%



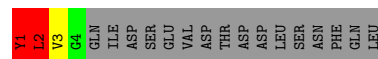
● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain F: 55% 25% 10% 10%



● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain P: 5% 5% 10% 80%



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	224.49Å 224.49Å 336.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	89.7 (20.00-3.10)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
Refinement program	TNT, REFMAC	Depositor
R, R_{free}	0.194 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18163	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.60	0/6002	1.76	128/8129 (1.6%)
1	B	0.60	0/6002	1.79	128/8129 (1.6%)
1	C	0.64	0/6002	1.81	137/8129 (1.7%)
2	D	0.44	0/140	1.44	1/188 (0.5%)
2	E	0.47	0/140	1.41	1/188 (0.5%)
2	F	0.47	0/140	1.44	0/188
2	P	0.91	0/31	2.62	3/41 (7.3%)
All	All	0.61	0/18457	1.78	398/24992 (1.6%)

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	B	0	2
1	C	0	2
All	All	0	6

There are no bond length outliers.

The worst 5 of 398 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	736	ASP	CA-CB-CG	12.37	124.97	112.60
1	C	195	ARG	CD-NE-CZ	11.91	141.07	124.40
1	B	195	ARG	CD-NE-CZ	11.30	140.22	124.40
1	B	736	ASP	CA-CB-CG	10.24	122.84	112.60
1	A	24	ARG	CD-NE-CZ	10.01	138.41	124.40

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	46	HIS	Mainchain
1	A	75	PRO	Mainchain
1	B	667	GLU	Mainchain
1	B	697	THR	Mainchain
1	C	46	HIS	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	5874	0	5797	181	0
1	B	5874	0	5797	167	0
1	C	5874	0	5797	170	0
2	D	140	0	123	4	0
2	E	140	0	123	3	0
2	F	140	0	123	5	0
2	P	31	0	34	3	0
3	A	28	0	0	3	0
3	B	30	0	0	4	0
3	C	32	0	0	3	0
All	All	18163	0	17794	525	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 15.

The worst 5 of 525 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:191:GLN:HE21	1:A:195:ARG:HH21	1.04	0.98
1:B:191:GLN:HE21	1:B:195:ARG:HH21	1.03	0.94
1:C:191:GLN:HE21	1:C:195:ARG:HH21	0.95	0.91
1:A:1:MET:H2	1:A:3:GLN:HG3	1.40	0.87
1:C:1:MET:H2	1:C:3:GLN:HG3	1.40	0.87

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%)	680 (92%)	48 (6%)	8 (1%)	11	39
1	B	736/761 (97%)	681 (92%)	47 (6%)	8 (1%)	11	39
1	C	736/761 (97%)	685 (93%)	44 (6%)	7 (1%)	12	41
2	D	16/20 (80%)	14 (88%)	1 (6%)	1 (6%)	1	6
2	E	16/20 (80%)	13 (81%)	2 (12%)	1 (6%)	1	6
2	F	16/20 (80%)	14 (88%)	1 (6%)	1 (6%)	1	6
2	P	2/20 (10%)	0	2 (100%)	0	100	100
All	All	2258/2363 (96%)	2087 (92%)	145 (6%)	26 (1%)	10	37

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	A	735	ARG
2	D	371	SER
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%)	549 (87%)	83 (13%)	4	17
1	B	632/651 (97%)	547 (87%)	85 (13%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	632/651 (97%)	546 (86%)	86 (14%)	3	16
2	D	17/19 (90%)	16 (94%)	1 (6%)	18	48
2	E	17/19 (90%)	15 (88%)	2 (12%)	5	21
2	F	17/19 (90%)	15 (88%)	2 (12%)	5	21
2	P	3/19 (16%)	1 (33%)	2 (67%)	0	0
All	All	1950/2029 (96%)	1689 (87%)	261 (13%)	4	17

5 of 261 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	465	SER
1	C	530	ARG
2	P	2	LEU
1	B	54	LYS
1	B	40	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	496	GLN
1	C	548	GLN
1	C	698	ASN
1	B	40	GLN
1	B	18	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 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.