WORLD WIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:38 am GMT

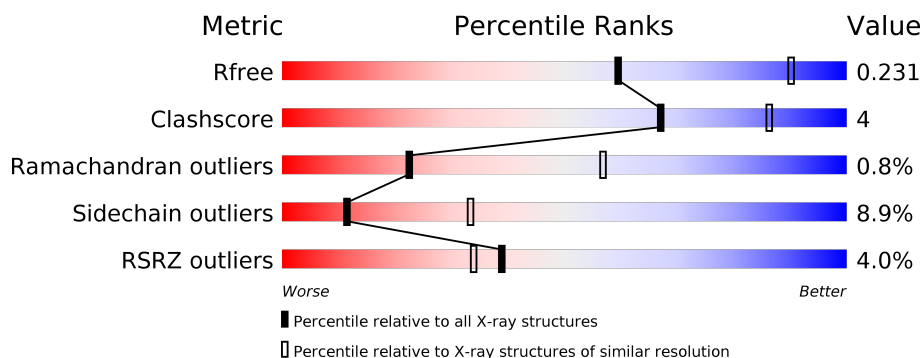|		
PDB ID	:	1R1R
Title	:	RIBONUCLEOTIDE REDUCTASE R1 PROTEIN MUTANT Y730F WITH A REDUCED ACTIVE SITE FROM ESCHERICHIA COLI
Authors	:	Eriksson, M.; Eklund, H.
Deposited on	:	1997-07-15
Resolution	:	2.90 Å(reported)

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 2.90 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	Percentile Ranks	Value
Rfree		0.231
Clashscore		4
Ramachandran outliers		0.8%
Sidechain outliers		8.9%
RSRZ outliers		4.0%

Worse ———————————————— *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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 <=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.

Mol	Chain	Length	Quality of chain
1	A	761	4% — 79% / 16% / ·· ·
1	B	761	4% — 79% / 16% / ·· ·
1	C	761	3% — 79% / 16% / ·· ·
2	D	20	15% — 60% / 20% / 20%
2	E	20	10% — 60% / 20% / 20%
2	F	20	5% — 60% / 20% / 20%

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Mol	Chain	Length	Quality of chain
2	P	20	5% 5% 5% 85%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 18258 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	734	Total 5844	C 3712	N 1004	O 1104	S 24	0	0	0
1	B	734	Total 5844	C 3712	N 1004	O 1104	S 24	0	0	0
1	C	734	Total 5844	C 3712	N 1004	O 1104	S 24	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	730	PHE	TYR	ENGINEERED	UNP P00452
B	730	PHE	TYR	ENGINEERED	UNP P00452
C	730	PHE	TYR	ENGINEERED	UNP P00452

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	16	Total 129	C 77	N 19	O 33	0	0	0
2	E	16	Total 129	C 77	N 19	O 33	0	0	0
2	F	16	Total 129	C 77	N 19	O 33	0	0	0
2	P	3	Total 27	C 20	N 3	O 4	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	104	Total 104	O 104	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	104	Total 104	O 104	0	0
3	C	104	Total 104	O 104	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

Chain A:

• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

Chain B:

L662 Q686 I693 N696 P705 S706 K716 K727 T728 Y731 D736 G737 ALA GLU ASP ALA GLN ASP ASP LEU VAL PRO SER ILE GLN ASP GLY CYS GLU SER GLY ALA CYS LYS ILE

• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

Chain C:

3%
79%   16%

MET ASN GLN N4 L5 K9 R10 D11 G12 S13 T14 E15 R16 I17 N18 K21 R24 I38 S39 Q40 V41 E42 S45 D51 K54 T55 S56 R72 Y79 R83 K91 Q96 F97 E98 P99 E111 H118 L119 L120 E121 D122 F128 M131

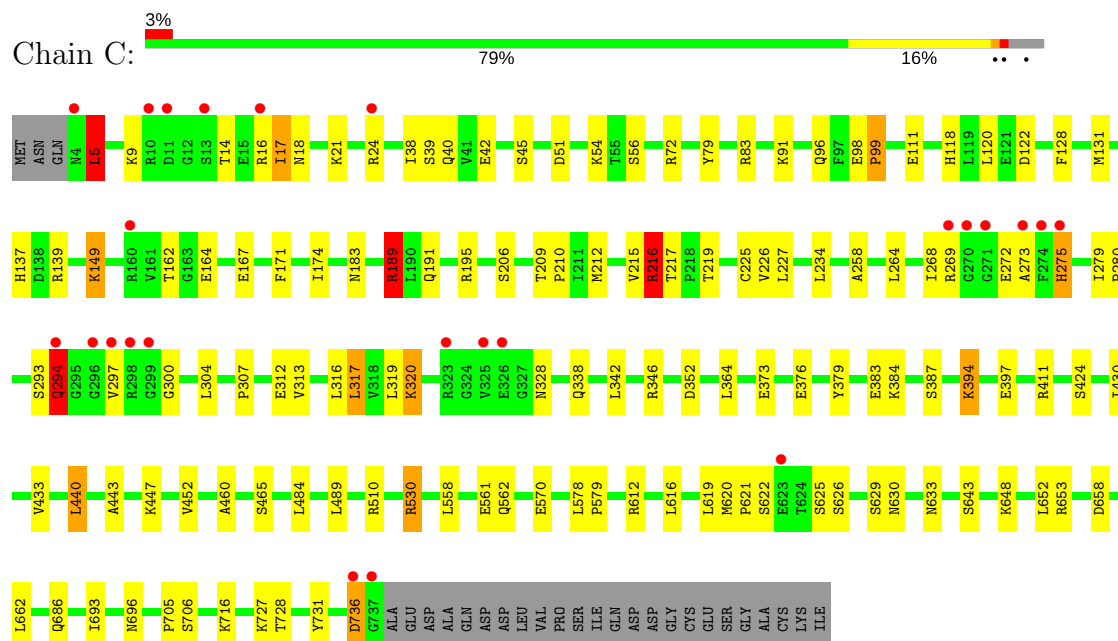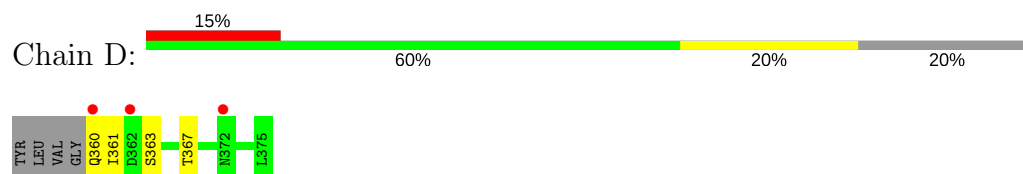H137 D138 R139 K149 R160 V161 T162 G163 E164 E167 F171 I174 N183 R189 L190 Q191 R195 S206 T209 P210 I211 M212 V215 R216 T217 P218 T219 C225 V226 L227 L234 A258 L264 I268 R269 G270 G271 E272 A273 F274 H275 I279 P280

S293 Q294 G295 G296 V297 R298 G299 G300 L304 P307 E312 V313 L316 L317 V318 L319 K320 R323 G324 V325 E326 G327 N328 Q338 L342 R346 D352 L364 E373 E376 Y379 E383 K384 S387 K394 E397 R411 S424 I430

V433 L440 A443 K447 V452 A460 S465 L484 L489 R510 R530 L558 E561 Q562 E570 L578 P579 R612 L616 L619 M620 P621 E623 T624 S625 S626 S629 N630 N633 S643 K648 L652 R653 D658

L662 Q686 I693 N696 P705 S706 K716 K727 T728 Y731 D736 G737 ALA GLU ASP ALA GLN ASP ASP LEU VAL PRO SER ILE GLN ASP GLY CYS GLU SER GLY ALA CYS LYS ILE

• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain D:

15%
60%   20%   20%

TYR LEU VAL GLY Q360 I361 D362 S363 T367 N372 L375

• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain E:

10%
60%   20%   20%

TYR LEU VAL GLY Q360 I361 D362 S363 T367 D368 L375

• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain F:

5%
60%   20%   20%

TYR LEU VAL GLY Q360 I361 D362 S363 T367 L375

• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain P:

5% 5% 5%   85%

Y1 L2 V3 GLY GLN ILE ASP SER GLU VAL ASP THR ASP ASP LEU SER ASN PHE GLN LEU

4   Data and refinement statistics   (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	227.82Å 227.82Å 343.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-2.90) 96.1 (20.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 2.88Å)	Xtriage
Refinement program	REFMAC, TNT	Depositor
R, R_{free}	0.210 , 0.245 0.216 , 0.231	Depositor DCC
R_{free} test set	2008 reflections (2.85%)	DCC
Wilson B-factor (Å^2)	46.3	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.8	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18258	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.36	0/5972	0.88	5/8088 (0.1%)
1	B	0.36	0/5972	0.88	5/8088 (0.1%)
1	C	0.36	0/5972	0.88	5/8088 (0.1%)
2	D	0.36	0/129	0.75	0/173
2	E	0.36	0/129	0.75	0/173
2	F	0.36	0/129	0.75	0/173
2	P	0.72	0/27	1.81	1/36 (2.8%)
All	All	0.36	0/18330	0.88	16/24819 (0.1%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	653	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	B	653	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	A	653	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	B	653	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	C	653	ARG	NE-CZ-NH2	-6.17	117.22	120.30

There are no chirality outliers.

There are no planarity outliers.

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	5844	0	5770	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5844	0	5770	53	0
1	C	5844	0	5770	54	0
2	D	129	0	111	0	0
2	E	129	0	111	0	0
2	F	129	0	111	0	0
2	P	27	0	31	1	0
3	A	104	0	0	0	0
3	B	104	0	0	0	0
3	C	104	0	0	0	0
All	All	18258	0	17674	160	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 160 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:394:LYS:HB3	1:A:397:GLU:HG3	1.68	0.76
1:C:215:VAL:O	1:C:216:ARG:HB3	1.85	0.76
1:B:394:LYS:HB3	1:B:397:GLU:HG3	1.68	0.75
1:C:394:LYS:HB3	1:C:397:GLU:HG3	1.68	0.75
1:A:215:VAL:O	1:A:216:ARG:HB3	1.85	0.75

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	732/761 (96%)	697 (95%)	29 (4%)	6 (1%)	22	57
1	B	732/761 (96%)	697 (95%)	29 (4%)	6 (1%)	22	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	732/761 (96%)	697 (95%)	29 (4%)	6 (1%)	22	57
2	D	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
2	E	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
2	F	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
2	P	1/20 (5%)	0	1 (100%)	0	100	100
All	All	2239/2363 (95%)	2130 (95%)	91 (4%)	18 (1%)	22	57

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	B	294	GLN
1	C	294	GLN
1	A	216	ARG
1	A	273	ALA

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	629/651 (97%)	576 (92%)	53 (8%)	13	36
1	B	629/651 (97%)	576 (92%)	53 (8%)	13	36
1	C	629/651 (97%)	576 (92%)	53 (8%)	13	36
2	D	16/19 (84%)	12 (75%)	4 (25%)	1	2
2	E	16/19 (84%)	12 (75%)	4 (25%)	1	2
2	F	16/19 (84%)	12 (75%)	4 (25%)	1	2
2	P	3/19 (16%)	2 (67%)	1 (33%)	0	0
All	All	1938/2029 (96%)	1766 (91%)	172 (9%)	11	33

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	183	ASN
1	B	447	LYS
1	C	625	SER
1	B	216	ARG
1	B	317	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	250	GLN
1	B	328	ASN
1	C	630	ASN
1	B	275	HIS
1	B	596	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	734/761 (96%)	-0.41	30 (4%)	38	32	10, 24, 77, 108	0
1	B	734/761 (96%)	-0.01	30 (4%)	38	32	10, 24, 77, 108	0
1	C	734/761 (96%)	-0.08	24 (3%)	47	40	10, 24, 77, 108	0
2	D	16/20 (80%)	0.76	3 (18%)	1	1	45, 82, 91, 97	0
2	E	16/20 (80%)	0.84	2 (12%)	4	3	45, 82, 91, 97	0
2	F	16/20 (80%)	0.91	1 (6%)	21	16	45, 82, 91, 97	0
2	P	3/20 (15%)	0.37	0	100	100	30, 30, 37, 43	0
All	All	2253/2363 (95%)	-0.15	90 (3%)	39	34	10, 25, 83, 108	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	737	GLY	6.8
1	A	297	VAL	6.6
1	A	296	GLY	6.5
1	B	294	GLN	5.8
1	C	4	ASN	5.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.