

# wwPDB X-ray Structure Validation Summary Report (i)

#### Oct 17, 2023 – 09:24 PM EDT

PDB ID : 2GGI

Title : The mutant E149C-A182C of Deinococcus Radiodurans N-acylamino acid

racemase

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Deposited on : 2006-03-24

Resolution : 2.20 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 (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467 Xtriage (Phenix): 1.13

EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

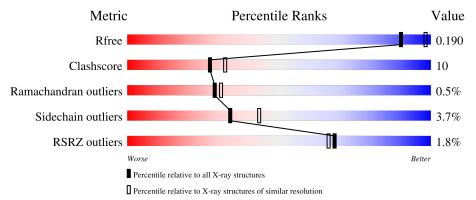
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.20 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	375	82%	13%		
1	В	375	86%	9%		<del>-</del>
1	С	375	74%	19%	•	-
1	D	375	79%	14%	•	-



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12348 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 N-acylamino acid racemase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	360	Total	С	N	Ο	S	0	0	0
1	A	300	2764	1731	507	514	12	0	U	
1	В	260	Total	С	N	О	S	0	0	0
1	Б	360	2764	1731	507	514	12	0	U	0
1	С	360	Total	С	N	О	S	0	0	0
1		300	2764	1731	507	514	12	0	U	
1	D	360	Total	С	N	О	S	0	0	0
1	ש	300	2764	1731	507	514	12	U	U	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	SER	ALA	SEE REMARK 999	UNP Q9RYA6
A	148	ASP	GLY	SEE REMARK 999	UNP Q9RYA6
A	149	CYS	GLU	engineered mutation	UNP Q9RYA6
A	158	ARG	LYS	SEE REMARK 999	UNP Q9RYA6
A	182	CYS	ALA	engineered mutation	UNP Q9RYA6
A	252	SER	ALA	SEE REMARK 999	UNP Q9RYA6
A	315	SER	PRO	SEE REMARK 999	UNP Q9RYA6
В	94	SER	ALA	SEE REMARK 999	UNP Q9RYA6
В	148	ASP	GLY	SEE REMARK 999	UNP Q9RYA6
В	149	CYS	GLU	engineered mutation	UNP Q9RYA6
В	158	ARG	LYS	SEE REMARK 999	UNP Q9RYA6
В	182	CYS	ALA	engineered mutation	UNP Q9RYA6
В	252	SER	ALA	SEE REMARK 999	UNP Q9RYA6
В	315	SER	PRO	SEE REMARK 999	UNP Q9RYA6
С	94	SER	ALA	SEE REMARK 999	UNP Q9RYA6
С	148	ASP	GLY	SEE REMARK 999	UNP Q9RYA6
С	149	CYS	GLU	engineered mutation	UNP Q9RYA6
С	158	ARG	LYS	SEE REMARK 999	UNP Q9RYA6
С	182	CYS	ALA	engineered mutation	UNP Q9RYA6
С	252	SER	ALA	SEE REMARK 999	UNP Q9RYA6
С	315	SER	PRO	SEE REMARK 999	UNP Q9RYA6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	94	SER	ALA	SEE REMARK 999	UNP Q9RYA6
D	148	ASP	GLY	SEE REMARK 999	UNP Q9RYA6
D	149	CYS	GLU	engineered mutation	UNP Q9RYA6
D	158	ARG	LYS	SEE REMARK 999	UNP Q9RYA6
D	182	CYS	ALA	engineered mutation	UNP Q9RYA6
D	252	SER	ALA	SEE REMARK 999	UNP Q9RYA6
D	315	SER	PRO	SEE REMARK 999	UNP Q9RYA6

## • Molecule 2 is water.

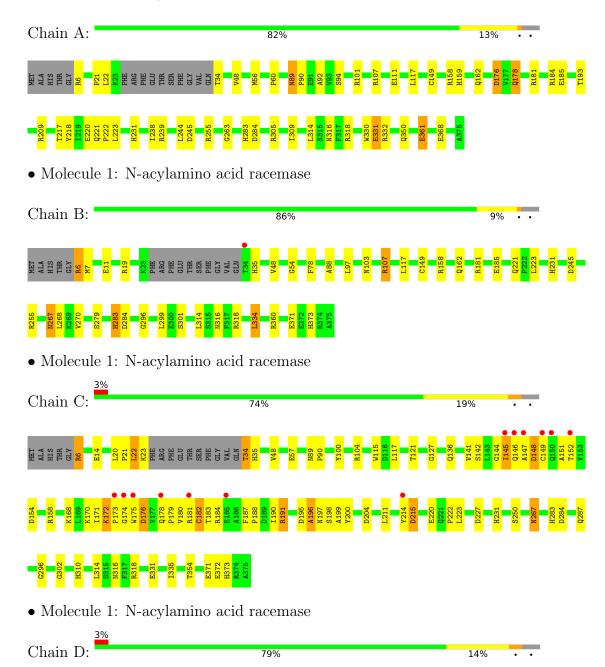
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	338	Total O 338 338	0	0
2	В	340	Total O 340 340	0	0
2	С	307	Total O 307 307	0	0
2	D	307	Total O 307 307	0	0



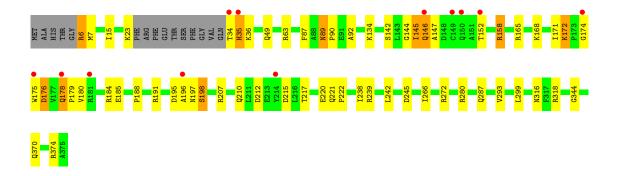
# 3 Residue-property plots (i)

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 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: N-acylamino acid racemase









# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.50Å 116.50Å 120.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 - 2.20 $29.13 - 2.20$	Depositor EDS
% Data completeness	99.1 (30.00-2.20)	Depositor
(in resolution range)	99.1 (29.13-2.20)	EDS
$R_{merge}$	(Not available)	Depositor
$\frac{R_{sym}}{\langle I/\sigma(I)\rangle^{-1}}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.79 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
D D	0.166 , 0.203	Depositor
$R, R_{free}$	0.167 , $0.190$	DCC
$R_{free}$ test set	4064 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.2	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34, 26.5	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.51, < L^2> = 0.35$	Xtriage
	0.000 for -h,-l,-k	
	0.000  for -h,l,k	
Estimated twinning fraction	0.005  for  l,-k,h	Xtriage
	0.006  for -l,-k,-h	
	0.487  for h,-k,-l	
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12348	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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		
IVIOI	Chain	RMSZ $ \# Z  > 5$		RMSZ	# Z  > 5	
1	A	0.54	0/2815	0.65	1/3819 (0.0%)	
1	В	0.54	0/2815	0.64	0/3819	
1	С	0.49	0/2815	0.65	0/3819	
1	D	0.53	0/2815	0.65	0/3819	
All	All	0.53	0/11260	0.65	$1/15276 \ (0.0\%)$	

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	В	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	101	ARG	NE-CZ-NH1	5.26	122.93	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Chain Res		Group	
1	В	97	LEU	Peptide	

## 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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2764	0	2766	51	0
1	В	2764	0	2766	35	0
1	С	2764	0	2766	81	0
1	D	2764	0	2766	58	0
2	A	338	0	0	7	0
2	В	340	0	0	5	1
2	С	307	0	0	13	0
2	D	307	0	0	18	0
All	All	12348	0	11064	223	1

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 10.

The worst 5 of 223 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:C:287:GLN:NE2	1:C:318:ARG:HH11	1.31	1.25
1:C:191:ARG:HH11	1:C:191:ARG:HG3	1.18	1.05
1:D:158:ARG:HG3	1:D:158:ARG:HH11	1.11	1.05
1:A:178:GLN:HE21	1:A:178:GLN:H	1.03	1.02
1:D:6:ARG:HG2	1:D:6:ARG:HH11	0.88	1.01

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	$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
2:B:715:HOH:O	2:B:715:HOH:O[4_555]	2.01	0.19

## 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	Perce	$\mathbf{ntiles}$
1	A	356/375~(95%)	343 (96%)	13 (4%)	0	100	100
1	В	356/375~(95%)	346 (97%)	10 (3%)	0	100	100
1	С	356/375~(95%)	337 (95%)	15 (4%)	4 (1%)	14	12
1	D	356/375~(95%)	338 (95%)	15 (4%)	3 (1%)	19	19
All	All	1424/1500 (95%)	1364 (96%)	53 (4%)	7 (0%)	29	31

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	182	CYS
1	С	198	SER
1	D	35	HIS
1	С	196	ALA
1	С	215	ASP

### 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	285/297~(96%)	275 (96%)	10 (4%)	36 46
1	В	285/297~(96%)	279 (98%)	6 (2%)	53 67
1	С	285/297 (96%)	271 (95%)	14 (5%)	25 31
1	D	285/297~(96%)	273 (96%)	12 (4%)	30 38
All	All	1140/1188 (96%)	1098 (96%)	42 (4%)	34 43

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	215	ASP
1	D	146	GLN
1	С	267	ASN
1	D	89	ASN
1	D	172	LYS



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	283	HIS
1	D	146	GLN
1	С	85	GLN
1	D	287	GLN
1	С	370	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 monosaccharides 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)

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,  $95^{th}$  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	$OWAB(Å^2)$	Q < 0.9
1	A	360/375~(96%)	-0.89	0 100 100	8, 16, 31, 55	0
1	В	360/375~(96%)	-0.89	1 (0%) 94 93	9, 16, 31, 52	0
1	С	360/375~(96%)	-0.51	13 (3%) 42 41	9, 19, 53, 68	0
1	D	360/375~(96%)	-0.50	12 (3%) 46 44	9, 19, 53, 67	0
All	All	1440/1500 (96%)	-0.70	26 (1%) 68 66	8, 17, 47, 68	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	175	TRP	8.5
1	D	175	TRP	6.5
1	С	174	GLY	3.5
1	D	174	GLY	3.5
1	D	152	THR	3.4

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.



# 6.5 Other polymers (i)

There are no such residues in this entry.

