

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

#### Aug 26, 2023 – 04:40 PM EDT

PDB ID : 3GDR

Title : Crystal structure of the D91N mutant of the orotidine 5'-monophosphate de-

carboxylase from Saccharomyces cerevisiae

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Deposited on : 2009-02-24

Resolution : 1.90 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: 2.35

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

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

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

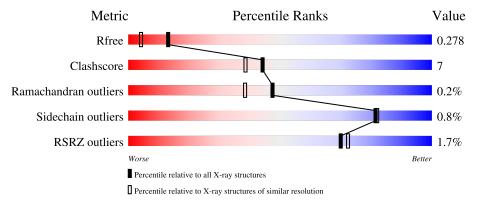
Validation Pipeline (wwPDB-VP) : 2.35

# 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 1.90 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	Whole archive $(\# \mathrm{Entries})$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	267	81%	16%	
1	В	267	84%	13%	•
1	С	267	81%	13%	• 6%
1	D	267	82%	12%	6%



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8368 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 Orotidine 5'-phosphate decarboxylase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	Λ	٨	A 260	Total	С	N	О	S	0	0	0
1	A	200	2003	1269	347	379	8	0	U		
1	В	200	Total	С	N	О	S	0	0	0	
1	Ъ	260	2003	1269	347	379	8	0	U		
1	C	252	Total	С	N	О	S	0	0	0	
1		202	1939	1228	338	364	9	0	U		
1	1 D	252	Total	С	N	О	S	0	0	0	
1		D 252	1939	1228	338	364	9	U	U	U	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ASN	ASP	engineered mutation	UNP P03962
В	91	ASN	ASP	engineered mutation	UNP P03962
С	91	ASN	ASP	engineered mutation	UNP P03962
D	91	ASN	ASP	engineered mutation	UNP P03962

• Molecule 2 is water.

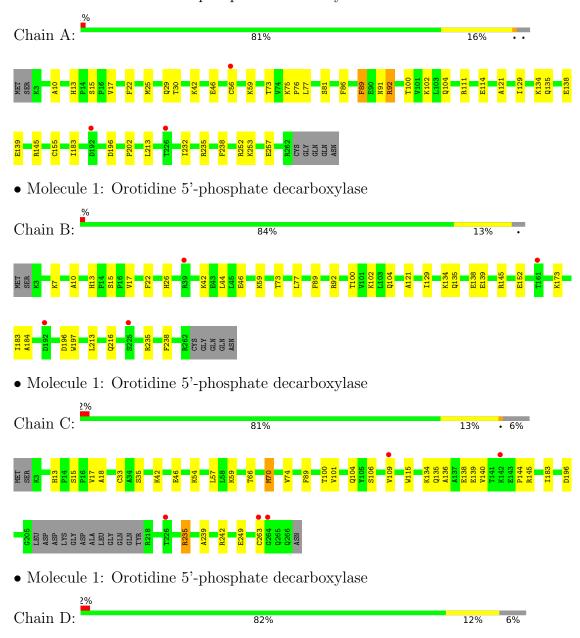
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	133	Total O 133 133	0	0
2	В	128	Total O 128 128	0	0
2	С	122	Total O 122 122	0	0
2	D	101	Total O 101 101	0	0



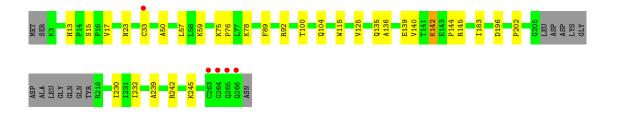
# 3 Residue-property plots (i)

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: Orotidine 5'-phosphate decarboxylase









# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	84.12Å 99.14Å 126.65Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.86 - 1.90	Depositor
rtesolution (A)	39.92 - 1.70	EDS
% Data completeness	99.3 (24.86-1.90)	Depositor
(in resolution range)	99.0 (39.92-1.70)	EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.06 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
D D.	0.252 , 0.278	Depositor
$R, R_{free}$	0.252 , $0.278$	DCC
$R_{free}$ test set	5840 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.38, 43.2	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.51, < L^2>=0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8368	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 55.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3315e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<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		
Moi   Chan	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.32	0/2036	0.59	1/2745~(0.0%)	
1	В	0.31	0/2036	0.60	1/2745~(0.0%)	
1	С	0.32	0/1970	0.60	1/2654~(0.0%)	
1	D	0.32	0/1970	0.59	1/2654~(0.0%)	
All	All	0.32	0/8012	0.59	4/10798 (0.0%)	

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$Observed(^o)$	$Ideal(^{o})$
1	D	183	ILE	N-CA-C	-6.46	93.55	111.00
1	С	183	ILE	N-CA-C	-6.40	93.71	111.00
1	В	183	ILE	N-CA-C	-6.34	93.87	111.00
1	A	183	ILE	N-CA-C	-6.11	94.51	111.00

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	2003	0	2033	29	0
1	В	2003	0	2033	24	0
1	С	1939	0	1973	29	0
1	D	1939	0	1973	25	0
2	A	133	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	128	0	0	0	0
2	С	122	0	0	3	0
2	D	101	0	0	1	0
All	All	8368	0	8012	105	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 7.

The worst 5 of 105 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
1:A:30:THR:HG23	1:A:56:CYS:SG	2.08	0.93
1:D:33:CYS:SG	1:D:57:LEU:HB3	2.11	0.91
1:B:13:HIS:HD2	1:B:15:SER:H	1.23	0.85
1:D:13:HIS:HD2	1:D:15:SER:H	1.23	0.84
1:A:13:HIS:HD2	1:A:15:SER:H	1.22	0.83

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	258/267 (97%)	247 (96%)	10 (4%)	1 (0%)	34 24
1	В	258/267 (97%)	246 (95%)	11 (4%)	1 (0%)	34 24
1	С	248/267 (93%)	238 (96%)	10 (4%)	0	100 100
1	D	248/267 (93%)	237 (96%)	11 (4%)	0	100 100
All	All	1012/1068 (95%)	968 (96%)	42 (4%)	2 (0%)	47 38

All (2) Ramachandran outliers are listed below:



Mol	Chain	$\operatorname{Res}$	Type
1	A	92	ARG
1	В	92	ARG

#### 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	$209/215 \ (97\%)$	208 (100%)	1 (0%)	88 89
1	В	$209/215 \ (97\%)$	209 (100%)	0	100 100
1	$\mathbf{C}$	$203/215 \ (94\%)$	200 (98%)	3 (2%)	65 62
1	D	203/215 (94%)	200 (98%)	3 (2%)	65 62
All	All	824/860 (96%)	817 (99%)	7 (1%)	81 82

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	235	ARG
1	D	23	ASN
1	D	142	LYS
1	D	92	ARG
1	С	101	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	$\operatorname{Res}$	$\mathbf{Type}$
1	В	135	GLN
1	С	13	HIS
1	D	61	HIS
1	С	61	HIS
1	A	135	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>	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	260/267 (97%)	-0.05	3 (1%) 79 81	15, 22, 31, 39	0
1	В	260/267~(97%)	0.06	4 (1%) 73 76	15, 22, 32, 39	0
1	С	252/267 (94%)	0.09	5 (1%) 65 68	15, 22, 33, 41	0
1	D	252/267 (94%)	0.15	5 (1%) 65 68	16, 22, 33, 43	0
All	All	1024/1068 (95%)	0.06	17 (1%) 70 72	15, 22, 32, 43	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	263	CYS	8.9
1	D	265	GLN	6.7
1	С	263	CYS	5.7
1	D	264	GLY	4.8
1	D	266	GLN	4.1

### 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.

