



# wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 01:18 AM GMT

PDB ID : 2G5C  
Title : Crystal Structure of Prephenate Dehydrogenase from Aquifex aeolicus  
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Deposited on : 2006-02-22  
Resolution : 1.90 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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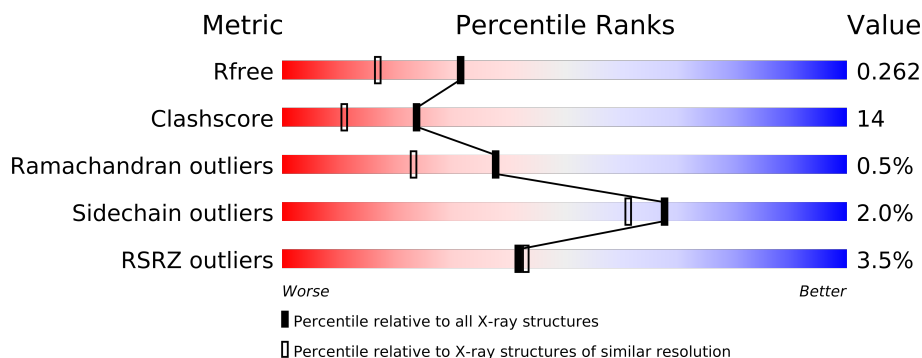
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	281	
1	B	281	
1	C	281	
1	D	281	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9487 atoms, of which 0 are hydrogen and 0 are deuterium.

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 prephenate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	Se	0	0	0
			2198	1418	360	412	8			
1	B	280	Total	C	N	O	Se	0	0	0
			2216	1429	365	415	7			
1	C	278	Total	C	N	O	Se	0	0	0
			2198	1418	363	410	7			
1	D	278	Total	C	N	O	Se	0	0	0
			2198	1418	363	410	7			

There are 32 discrepancies between the modelled and reference sequences:

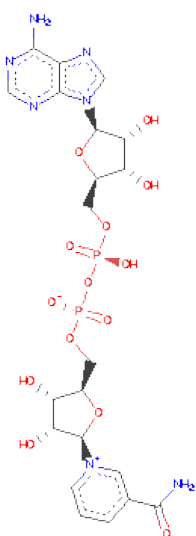
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MSE	-	INITIATING METHIONINE	UNP O67636
A	41	MSE	MET	MODIFIED RESIDUE	UNP O67636
A	96	MSE	MET	MODIFIED RESIDUE	UNP O67636
A	200	MSE	MET	MODIFIED RESIDUE	UNP O67636
A	230	MSE	MET	MODIFIED RESIDUE	UNP O67636
A	258	MSE	MET	MODIFIED RESIDUE	UNP O67636
A	271	MSE	MET	MODIFIED RESIDUE	UNP O67636
A	308	MSE	MET	MODIFIED RESIDUE	UNP O67636
B	30	MSE	-	INITIATING METHIONINE	UNP O67636
B	41	MSE	MET	MODIFIED RESIDUE	UNP O67636
B	96	MSE	MET	MODIFIED RESIDUE	UNP O67636
B	200	MSE	MET	MODIFIED RESIDUE	UNP O67636
B	230	MSE	MET	MODIFIED RESIDUE	UNP O67636
B	258	MSE	MET	MODIFIED RESIDUE	UNP O67636
B	271	MSE	MET	MODIFIED RESIDUE	UNP O67636
B	308	MSE	MET	MODIFIED RESIDUE	UNP O67636
C	30	MSE	-	INITIATING METHIONINE	UNP O67636
C	41	MSE	MET	MODIFIED RESIDUE	UNP O67636
C	96	MSE	MET	MODIFIED RESIDUE	UNP O67636
C	200	MSE	MET	MODIFIED RESIDUE	UNP O67636
C	230	MSE	MET	MODIFIED RESIDUE	UNP O67636

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Chain	Residue	Modelled	Actual	Comment	Reference
C	258	MSE	MET	MODIFIED RESIDUE	UNP O67636
C	271	MSE	MET	MODIFIED RESIDUE	UNP O67636
C	308	MSE	MET	MODIFIED RESIDUE	UNP O67636
D	30	MSE	-	INITIATING METHIONINE	UNP O67636
D	41	MSE	MET	MODIFIED RESIDUE	UNP O67636
D	96	MSE	MET	MODIFIED RESIDUE	UNP O67636
D	200	MSE	MET	MODIFIED RESIDUE	UNP O67636
D	230	MSE	MET	MODIFIED RESIDUE	UNP O67636
D	258	MSE	MET	MODIFIED RESIDUE	UNP O67636
D	271	MSE	MET	MODIFIED RESIDUE	UNP O67636
D	308	MSE	MET	MODIFIED RESIDUE	UNP O67636

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

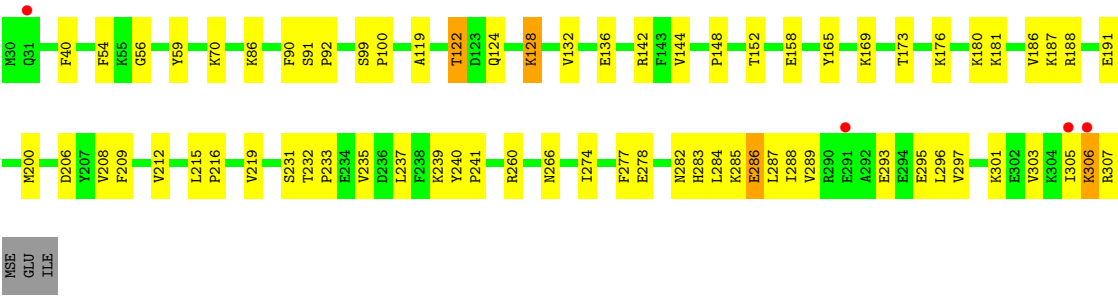
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	84	Total 84	O 84	0	0
3	B	88	Total 88	O 88	0	0
3	C	169	Total 169	O 169	0	0
3	D	160	Total 160	O 160	0	0



● Molecule 1: prephenate dehydrogenase

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.71Å 178.95Å 75.19Å 90.00° 99.15° 90.00°	Depositor
Resolution (Å)	29.93 – 1.90 34.43 – 1.89	Depositor EDS
% Data completeness (in resolution range)	88.2 (29.93-1.90) 93.4 (34.43-1.89)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.220 , 0.261 0.221 , 0.262	Depositor DCC
$R_{free}$ test set	4738 reflections (5.79%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 160792 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9487	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	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 74.78 % 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 1.4331e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD

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	0.31	0/2233	0.53	0/2990
1	B	0.31	0/2252	0.53	0/3018
1	C	0.34	0/2235	0.59	0/2998
1	D	0.34	0/2235	0.59	0/2998
All	All	0.32	0/8955	0.56	0/12004

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2198	0	2241	80	0
1	B	2216	0	2264	75	0
1	C	2198	0	2247	72	0
1	D	2198	0	2247	69	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	84	0	0	4	0
3	B	88	0	0	3	0
3	C	169	0	0	9	0
3	D	160	0	0	7	0
All	All	9487	0	9103	259	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 259 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:305:ILE:HG22	1:D:307:ARG:H	1.32	0.94
1:A:184:LYS:HB3	1:A:188:ARG:HH12	1.32	0.93
1:C:290:ARG:HD2	1:C:292:ALA:HB2	1.51	0.92
1:A:127:VAL:HG21	1:A:265:GLU:HG2	1.50	0.92
1:B:260:ARG:HD2	1:D:293:GLU:HG3	1.55	0.86

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	274/281 (98%)	254 (93%)	18 (7%)	2 (1%)	30	15
1	B	278/281 (99%)	259 (93%)	17 (6%)	2 (1%)	30	15
1	C	276/281 (98%)	264 (96%)	10 (4%)	2 (1%)	30	15
1	D	276/281 (98%)	266 (96%)	10 (4%)	0	100	100
All	All	1104/1124 (98%)	1043 (94%)	55 (5%)	6 (0%)	38	23

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	GLN

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Mol	Chain	Res	Type
1	B	151	GLY
1	C	305	ILE
1	B	152	THR
1	A	235	VAL

### 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	242/237 (102%)	237 (98%)	5 (2%)	66	59
1	B	244/237 (103%)	237 (97%)	7 (3%)	55	44
1	C	242/237 (102%)	239 (99%)	3 (1%)	82	80
1	D	242/237 (102%)	238 (98%)	4 (2%)	73	68
All	All	970/948 (102%)	951 (98%)	19 (2%)	68	61

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	223	LEU
1	B	246	LYS
1	D	122	THR
1	B	153	GLU
1	D	128	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	269	ASN
1	B	282	ASN
1	D	266	ASN
1	B	266	ASN
1	D	269	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAD	A	3686	-	48,48,48	1.46	5 (10%)	73,73,73	1.80	11 (15%)
2	NAD	B	4686	-	48,48,48	1.40	4 (8%)	73,73,73	1.78	10 (13%)
2	NAD	C	5686	-	48,48,48	1.42	4 (8%)	73,73,73	1.85	10 (13%)
2	NAD	D	6686	-	48,48,48	1.41	4 (8%)	73,73,73	1.77	9 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	3686	-	-	0/30/62/62	0/3/5/5
2	NAD	B	4686	-	-	0/30/62/62	0/3/5/5
2	NAD	C	5686	-	-	0/30/62/62	0/3/5/5
2	NAD	D	6686	-	-	0/30/62/62	0/3/5/5

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3686	NAD	O7N-C7N	5.56	1.37	1.24
2	B	4686	NAD	O7N-C7N	5.47	1.37	1.24
2	C	5686	NAD	O7N-C7N	5.42	1.36	1.24
2	D	6686	NAD	O7N-C7N	5.42	1.36	1.24
2	C	5686	NAD	C2N-N1N	3.89	1.40	1.35

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3686	NAD	N3A-C2A-N1A	-10.27	120.12	128.71
2	B	4686	NAD	N3A-C2A-N1A	-10.03	120.32	128.71
2	C	5686	NAD	N3A-C2A-N1A	-9.86	120.47	128.71
2	D	6686	NAD	N3A-C2A-N1A	-9.76	120.55	128.71
2	C	5686	NAD	C3N-C7N-N7N	5.59	124.14	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	278/281 (98%)	0.47	13 (4%) 30 30	14, 32, 50, 71	0
1	B	280/281 (99%)	0.55	15 (5%) 25 25	17, 35, 51, 68	0
1	C	278/281 (98%)	0.06	7 (2%) 54 56	13, 21, 38, 63	0
1	D	278/281 (98%)	0.06	4 (1%) 72 74	14, 22, 38, 62	0
All	All	1114/1124 (99%)	0.28	39 (3%) 42 43	13, 27, 48, 71	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	151	GLY	6.4
1	A	152	THR	6.0
1	C	306	LYS	4.8
1	B	153	GLU	4.2
1	B	113	TYR	4.2

### 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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	D	6686	44/44	0.11	-0.03	13,18,24,27	0
2	NAD	C	5686	44/44	0.11	-0.13	15,20,26,31	0
2	NAD	A	3686	44/44	0.11	-0.49	27,33,39,41	0
2	NAD	B	4686	44/44	0.12	-0.56	35,39,41,42	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.