



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:39 PM GMT

PDB ID : 1BW9  
Title : PHENYLALANINE DEHYDROGENASE STRUCTURE IN TERNARY COMPLEX WITH NAD<sup>+</sup> AND PHENYLPYRUVATE  
Authors : Vanhooke, J.L.; Thoden, J.B.; Brunhuber, N.M.W.; Blanchard, J.L.; Holden, H.M.  
Deposited on : 1998-10-01  
Resolution : 1.50 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

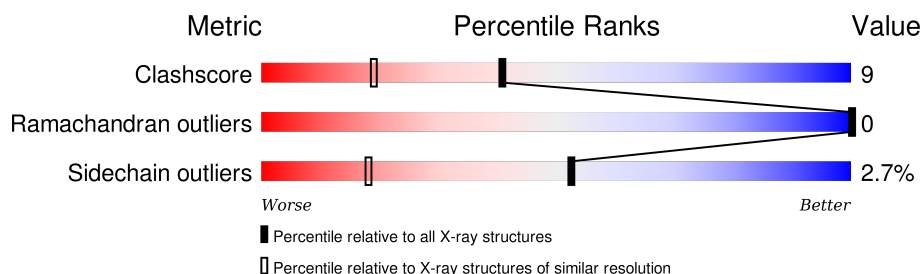
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)

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. 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	356	
2	B	356	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	EDO	B	874	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6225 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 PHENYLALANINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	9	0
			2551	1573	450	516	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	SER	ARG	SEE REMARK 999	UNP Q59771
A	20	MET	GLU	SEE REMARK 999	UNP Q59771
A	48	ASN	GLN	SEE REMARK 999	UNP Q59771

- Molecule 2 is a protein called PHENYLALANINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	347	Total	C	N	O	S	0	4	0
			2521	1558	447	505	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	419	LYS	ARG	SEE REMARK 999	UNP Q59771
B	420	MET	GLU	SEE REMARK 999	UNP Q59771

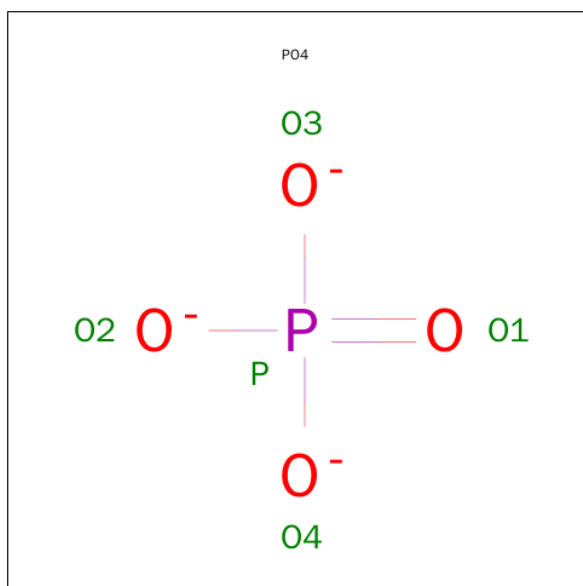
- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	K	0	0
			2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

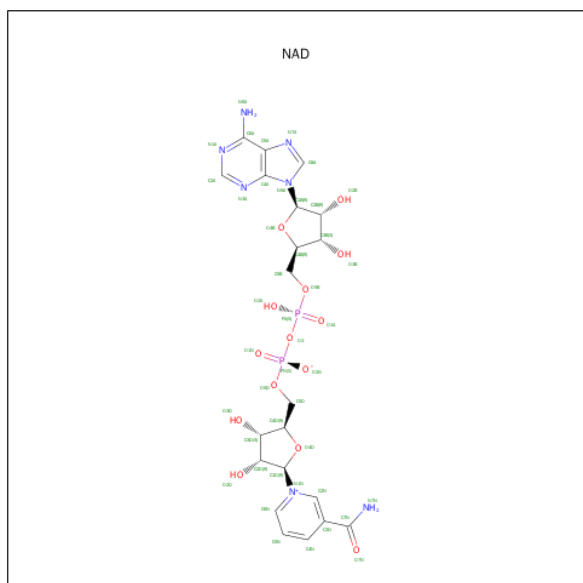
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Na	0	0
			2	2		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



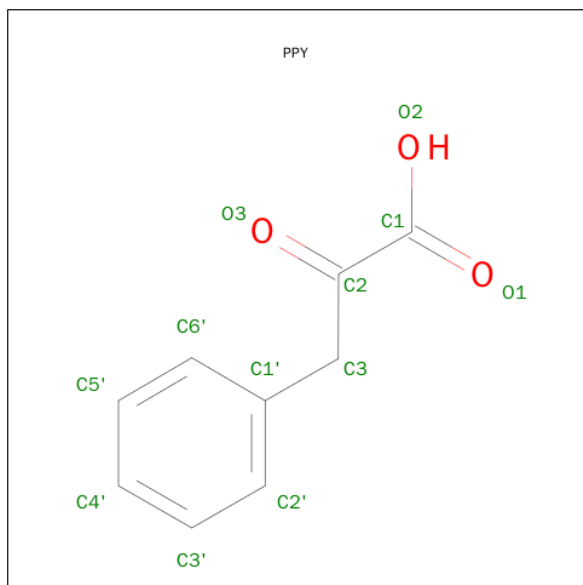
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is 3-PHENYLPYRUVIC ACID (three-letter code: PPY) (formula: C<sub>9</sub>H<sub>8</sub>O<sub>3</sub>).



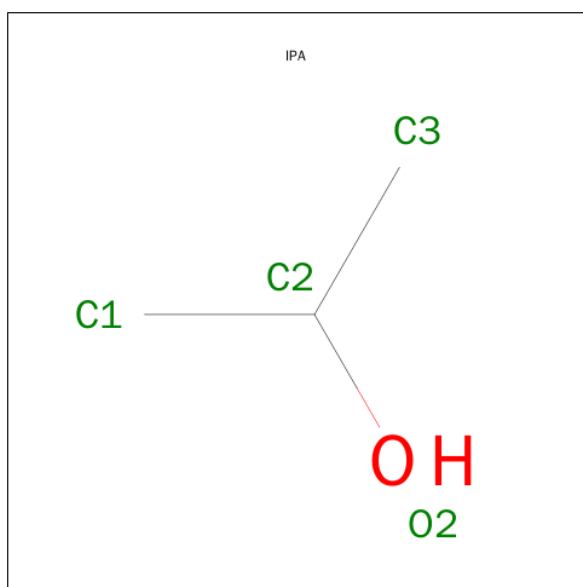
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			12	9	3		
7	B	1	Total	C	O	0	0
			12	9	3		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			4	3	1		
9	B	1	Total	C	O	0	0
			4	3	1		
9	B	1	Total	C	O	0	0
			4	3	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	519	Total	O	0	0
			519	519		
10	B	502	Total	O	0	0
			502	502		





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.30 Å   110.20 Å   113.40 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 1.50	Depositor
% Data completeness (in resolution range)	94.0 (30.00-1.50)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6225	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, NAD, NA, K, EDO, PPY, PO4

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	0.91	13/2625 (0.5%)	1.28	36/3577 (1.0%)
2	B	0.93	13/2579 (0.5%)	1.27	32/3512 (0.9%)
All	All	0.92	26/5204 (0.5%)	1.28	68/7089 (1.0%)

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	GLU	CD-OE1	7.90	1.34	1.25
1	A	104	GLU	CD-OE1	6.99	1.33	1.25
2	B	625	GLU	CD-OE1	6.83	1.33	1.25
2	B	504	GLU	CD-OE1	6.66	1.32	1.25
2	B	647	GLU	CD-OE1	6.62	1.32	1.25

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	681	TYR	CB-CG-CD2	-8.35	115.99	121.00
1	A	277	ARG	NE-CZ-NH1	8.33	124.47	120.30
2	B	525	ASP	CB-CG-OD1	-7.93	111.16	118.30
1	A	233	ASP	CB-CG-OD2	7.88	125.39	118.30
1	A	87	ARG	NE-CZ-NH1	7.35	123.98	120.30

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	2551	0	2488	49	0
2	B	2521	0	2473	31	0
3	B	2	0	0	0	0
4	B	2	0	0	0	0
5	B	5	0	0	0	0
6	A	44	0	26	11	0
6	B	27	0	12	4	0
7	A	12	0	7	3	0
7	B	12	0	7	0	0
8	B	12	0	18	6	0
9	B	16	0	31	4	0
10	A	519	0	0	6	0
10	B	502	0	0	2	0
All	All	6225	0	5062	88	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 9.

The worst 5 of 88 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)
2:B:663:ASN:HD22	9:B:862:IPA:H11	1.35	0.91
1:A:186:VAL:CG2	8:B:874:EDO:H11	2.07	0.85
1:A:186:VAL:HG21	8:B:874:EDO:H11	1.60	0.83
2:B:663:ASN:ND2	9:B:862:IPA:H11	1.99	0.77
1:A:346:ARG:O	1:A:350:THR:HG22	1.86	0.76

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	357/356 (100%)	351 (98%)	6 (2%)	0	100	100
2	B	350/356 (98%)	344 (98%)	6 (2%)	0	100	100
All	All	707/712 (99%)	695 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	266/261 (102%)	258 (97%)	8 (3%)	48	15
2	B	260/261 (100%)	252 (97%)	8 (3%)	47	14
All	All	526/522 (101%)	510 (97%)	16 (3%)	52	15

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	MET
2	B	403	ASP
2	B	542	GLU
1	A	229	SER
2	B	570	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
2	B	720	ASN
2	B	613	HIS
1	A	88	HIS
2	B	445	GLN

### 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 ⓘ

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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$
6	NAD	A	360	-	38,48,48	2.19	6 (15%)	47,73,73	2.81	13 (27%)
7	PPY	A	361	-	9,12,12	2.64	3 (33%)	10,15,15	3.66	4 (40%)
6	NAD	B	760	-	23,29,48	1.22	2 (8%)	27,45,73	1.65	5 (18%)
7	PPY	B	761	-	9,12,12	1.38	1 (11%)	10,15,15	0.95	0
9	IPA	B	860	-	3,3,3	0.26	0	3,3,3	0.42	0
9	IPA	B	861	-	3,3,3	0.49	0	3,3,3	0.52	0
9	IPA	B	862	-	3,3,3	0.69	0	3,3,3	1.15	0
9	IPA	B	863	-	3,3,3	0.17	0	3,3,3	0.43	0
8	EDO	B	871	-	3,3,3	0.34	0	2,2,2	0.52	0
8	EDO	B	873	-	3,3,3	0.44	0	2,2,2	0.30	0
8	EDO	B	874	-	3,3,3	0.41	0	2,2,2	0.43	0
5	PO4	B	880	3	4,4,4	1.01	0	6,6,6	0.30	0

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
6	NAD	A	360	-	-	0/22/62/62	0/5/5/5
7	PPY	A	361	-	-	0/4/8/8	0/1/1/1
6	NAD	B	760	-	-	0/12/32/62	0/3/3/5
7	PPY	B	761	-	-	0/4/8/8	0/1/1/1
9	IPA	B	860	-	-	0/0/0/0	0/0/0/0
9	IPA	B	861	-	-	0/0/0/0	0/0/0/0
9	IPA	B	862	-	-	0/0/0/0	0/0/0/0
9	IPA	B	863	-	-	0/0/0/0	0/0/0/0
8	EDO	B	871	-	-	0/1/1/1	0/0/0/0
8	EDO	B	873	-	-	0/1/1/1	0/0/0/0
8	EDO	B	874	-	-	0/1/1/1	0/0/0/0
5	PO4	B	880	3	-	0/0/0/0	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	360	NAD	C2N-C3N	-8.96	1.25	1.39
6	A	360	NAD	C3N-C7N	-6.64	1.40	1.50
7	A	361	PPY	C3-C2	-5.25	1.46	1.51
7	A	361	PPY	O3-C2	-4.47	1.14	1.22
7	B	761	PPY	C3-C2	-3.72	1.48	1.51

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	361	PPY	C1'-C3-C2	-9.30	92.12	114.75
6	A	360	NAD	O7N-C7N-C3N	-8.43	110.39	119.59
6	A	360	NAD	C5N-C4N-C3N	-7.30	111.15	120.33
6	A	360	NAD	C4N-C3N-C7N	-6.23	104.62	121.09
6	B	760	NAD	C1B-N9A-C4A	-4.93	119.50	126.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	360	NAD	11	0
7	A	361	PPY	3	0
6	B	760	NAD	4	0
9	B	860	IPA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	862	IPA	3	0
8	B	874	EDO	6	0

## 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.