



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 11:15 am GMT

PDB ID : 2G96  
Title : Crystal Structure of Visfatin/Pre-B Cell Colony Enhancing Factor 1/Nicotinamide Phosphoribosyltransferase In Complex with Nicotinamide Mononucleotide  
Authors : Eom, S.H.; Kim, M.-K.  
Deposited on : 2006-03-05  
Resolution : 2.90 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](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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

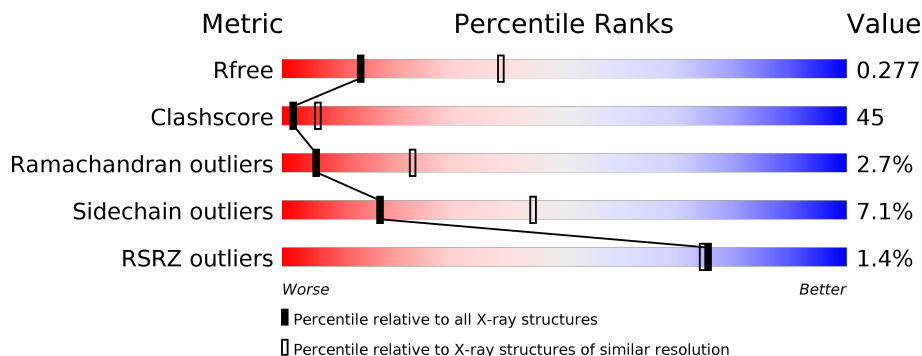
# 1 Overall quality at a glance

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	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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	491	<div> <div> <div></div> <div>31%</div> <div>56%</div> <div>6%</div> <div>6%</div> </div> <div> <div></div> <div>31%</div> <div>56%</div> <div>6%</div> <div>6%</div> </div> </div>
1	B	491	<div> <div> <div></div> <div>34%</div> <div>53%</div> <div>7%</div> <div>6%</div> </div> <div> <div></div> <div>34%</div> <div>53%</div> <div>7%</div> <div>6%</div> </div> </div>

## 2 Entry composition [i](#)

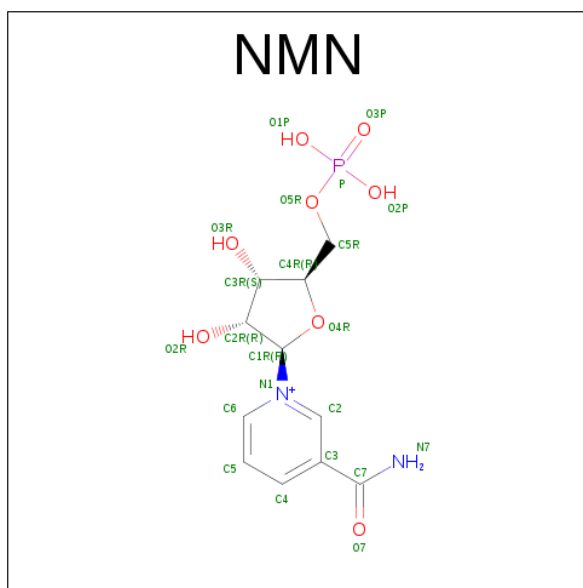
There are 3 unique types of molecules in this entry. The entry contains 7576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3700	2374	616	704	6			
1	B	463	Total	C	N	O	S	0	0	0
			3700	2374	616	704	6			

- Molecule 2 is BETA-NICOTINAMIDE RIBOSE MONOPHOSPHATE (three-letter code: NMN) (formula:  $C_{11}H_{16}N_2O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			22	11	2	8	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	82	Total 82	O 82	0	0
3	B	50	Total 50	O 50	0	0



P417	V418	A419	D420	P421	N422	K423	R424	S425	K426	K427	G428	R429	L430	S431	H433	T439	F440	V441	T442	L443	E444	E445	G446	K447	G448	D449	L450	E451	E452	L458	V461	F462	K463	K466	V467	S472	F473	D474	E475	V476	R477	Q481	L482	M483	MET	GLU	GLN	ASP	VAL	ALA	PRO	HIS			
V350	I351	G355	V356	D357	I358	N359	T360	L361	Q362	F363	I364	V365	E366	G367	N368	K369	Q370	K371	K372	W373	S374	I375	E376	N377	V378	S379	G384	A385	L386	L387	Q388	K389	L390	T391	R392	D393	L394	L395	N396	C397	K400	C401	S402	Y403	V404	V405	T406	L409	G410	V411	N412	V413	F414	K415	D416
D279	S280	Y281	D282	I283	Y284	W285	A286	C287	E288	G292	E293	D294	L295	E296	H297	L298	I299	R302	S303	T304	E305	A306	P307	L308	I309	I310	R311	P312	L318	D319	T320	K323	V324	L325	D326	I327	L328	G329	K330	K331	F332	P333	V334	N337	Y341	K342	L343	L344	P345	P346	Y347	L348	R349		
Y195	V198	S199	S200	Q201	E202	T203	A204	G205	I206	H211	N214	F215	W216	D219	T220	V221	Y230	Y231	G232	T233	K234	D235	P236	Y237	P238	G239	Y240	S241	P243	E246	T249	T250	T251	A252	W253	H257	F262	E263	H264	I265	Q268	P273	Y274	S275	V276	V277	S278								
R127	V130	L131	F132	T133	V134	E135	N136	T137	D138	P139	E140	C141	Y142	W143	L144	T145	N146	W147	I148	E149	T150	I151	L152	V153	Q154	S155	W156	Y157	P158	V161	N164	S165	Q168	K169	L172	Y175	L176	L177	E178	T179	N182	L183	D184	G185	L186	E187	Y188	K189	L190	H191	G194				

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.89Å 106.08Å 117.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 38.20 – 2.89	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.90) 81.8 (38.20-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.84 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.229 , 0.278 0.229 , 0.277	Depositor DCC
$R_{free}$ test set	1880 reflections (9.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.808	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7576	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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 58.91 % 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 1.9071e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: NMN

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	0.41	0/3788	0.66	0/5136
1	B	0.39	0/3788	0.65	0/5136
All	All	0.40	0/7576	0.65	0/10272

There are no bond length outliers.

There are no bond angle outliers.

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	3700	0	3665	365	0
1	B	3700	0	3665	344	0
2	A	22	0	14	5	0
2	B	22	0	14	3	0
3	A	82	0	0	7	0
3	B	50	0	0	2	0
All	All	7576	0	7358	666	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 45.

The worst 5 of 666 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:B:318:LEU:HD23	1:B:364:ILE:HA	1.22	1.15
1:A:435:THR:HG22	1:A:441:VAL:HG23	1.24	1.09
1:B:400:LYS:HE2	1:B:401:CYS:H	1.08	1.08
1:A:318:LEU:HD23	1:A:364:ILE:HA	1.35	1.06
1:B:365:VAL:HG22	1:B:375:ILE:HD12	1.38	1.04

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	459/491 (94%)	387 (84%)	60 (13%)	12 (3%)	6	24
1	B	459/491 (94%)	399 (87%)	47 (10%)	13 (3%)	6	22
All	All	918/982 (94%)	786 (86%)	107 (12%)	25 (3%)	6	23

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ASP
1	A	346	PRO
1	B	282	ASP
1	B	394	LEU
1	B	419	ALA

### 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	408/431 (95%)	378 (93%)	30 (7%)	16	42
1	B	408/431 (95%)	380 (93%)	28 (7%)	18	46
All	All	816/862 (95%)	758 (93%)	58 (7%)	17	44

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	392	ARG
1	B	67	ASN
1	B	386	LEU
1	A	393	ASP
1	A	451	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	412	ASN
1	B	90	HIS
1	B	370	GLN
1	B	67	ASN
1	B	97	ASN

### 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

2 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	NMN	A	1001	-	21,23,23	2.40	8 (38%)	27,34,34	1.33	5 (18%)
2	NMN	B	1002	-	21,23,23	2.58	8 (38%)	27,34,34	1.40	5 (18%)

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	NMN	A	1001	-	-	0/10/30/30	0/2/2/2
2	NMN	B	1002	-	-	0/10/30/30	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	NMN	C2R-C1R	-3.28	1.48	1.53
2	A	1001	NMN	C2R-C1R	-2.85	1.49	1.53
2	B	1002	NMN	P-O1P	-2.34	1.45	1.54
2	A	1001	NMN	P-O1P	-2.16	1.45	1.54
2	A	1001	NMN	C6-C5	2.05	1.43	1.38

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1002	NMN	O7-C7-C3	-3.12	115.97	119.62
2	A	1001	NMN	O7-C7-C3	-2.85	116.29	119.62
2	B	1002	NMN	C5-C6-N1	-2.10	117.17	120.40
2	A	1001	NMN	O2P-P-O1P	2.02	115.78	107.61
2	A	1001	NMN	O2P-P-O5R	2.32	112.90	106.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NMN	5	0
2	B	1002	NMN	3	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 [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<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	463/491 (94%)	-0.13	5 (1%) 80 79	10, 27, 45, 58	0
1	B	463/491 (94%)	-0.14	8 (1%) 70 68	11, 27, 46, 67	0
All	All	926/982 (94%)	-0.13	13 (1%) 75 74	10, 27, 45, 67	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	VAL	4.5
1	B	236	PRO	4.1
1	A	89	GLU	3.0
1	B	240	TYR	2.9
1	A	451	GLU	2.6

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NMN	B	1002	22/22	0.96	0.17	0.08	19,22,25,26	0
2	NMN	A	1001	22/22	0.96	0.18	-0.29	20,29,31,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.