



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 07:21 am BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
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) : 2.11

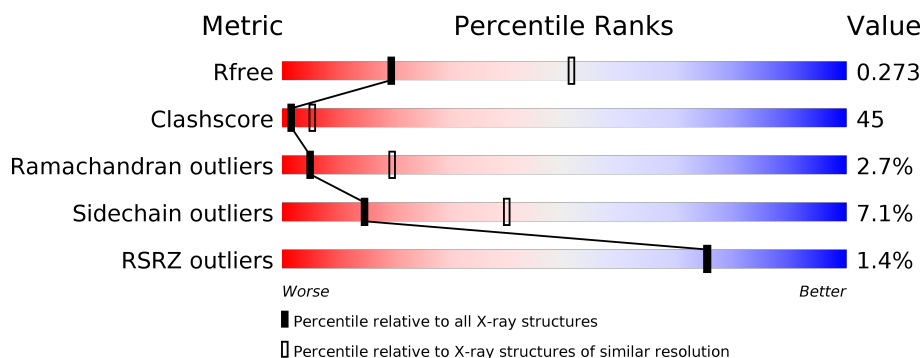
1 Overall quality at a glance

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 ≥ 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 $\leq 5\%$. 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](#)

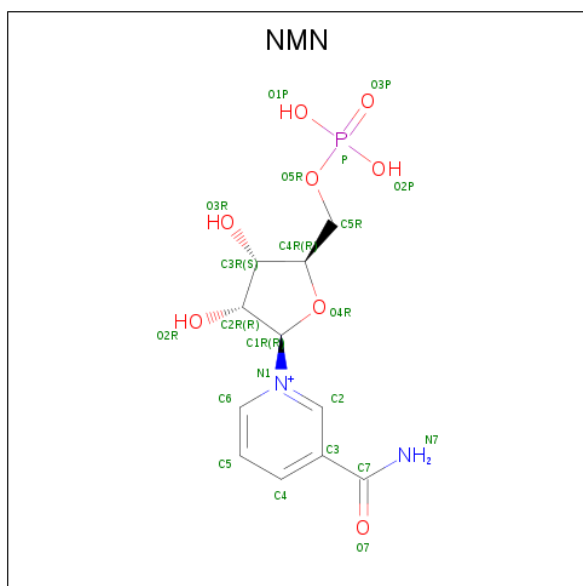
There are 3 unique types of molecules in this entry. The entry contains 7576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: C₁₁H₁₆N₂O₈P).



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		

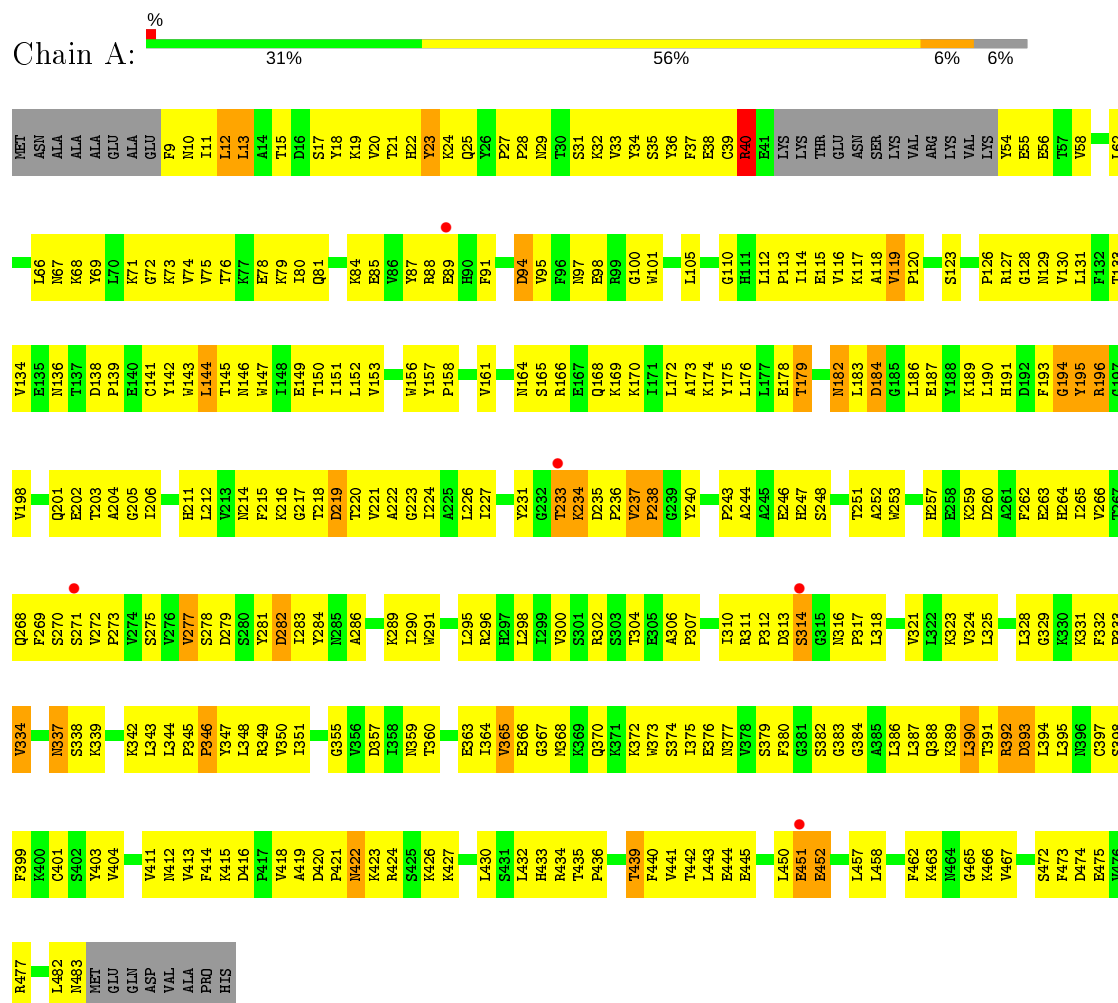
- Molecule 3 is water.

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Nicotinamide phosphoribosyltransferase



P417	V350	D279	Y195	R127	Q63
V416	I351	S280	Y198	V130	M67
A419	D420	D282	S199	L131	K68
P421	V356	I283	S200	F132	Y69
N422	D357	Y284	D201	T133	L70
K423	I358	N285	E202	V134	K71
R424	N359	I286	T203	E135	G72
S425	T360	C287	A204	N136	K73
K426	L361	E288	G205	T137	V74
K427	Q362		I206	D138	V75
G428	E363	G292	H211	P139	T76
R429	I364	E293		E140	
L430	V365	D294	N214	C141	K79
S431	E366	I295	F215	Y142	I80
L432	G367	R296	K216	W143	Q81
R433	N368	E297		L144	E82
	K369	I298		T145	A83
T439	Q370	I299	D219	N146	K84
F440	K371		T220	W147	E85
V441	K372	R302	V221	I148	V86
T442	W373	S303		E149	Y87
L443	S374	T304	Y230	T150	R88
P444	I375	E305	Y231	I151	E89
E445	E376	A306	G232	L152	H90
G446	N377	P307	T233	V153	F91
K447	V378	L308	K234	Q154	Q92
G448	S379	I309	D235	S155	D93
D449		I310	P236	W156	D94
L450	G384	R311	V237	Y157	V95
E451	A385	P312	P238	P158	F96
E452	L386		G239		I97
	L387	I318	Y240	V161	E98
L458	Q388	D319	S241	M164	R99
	K389	T320	P243	S165	G100
V461	L390	K323	E246	Q168	M102
F462	T391	V324		K169	Y103
K463	R392	I325		L172	I104
K466	L394	D326	T249		L105
V467	L395	I327	I250		E106
	N396	L328	T251		K107
S472	C397	G329	A252	Y175	Y108
F473		K330	W253	L176	D109
D474	K400	K331		L177	G110
E475	C401	F332	R257	E178	H111
V476	S402	V333		T179	L112
R477	Y403	V334	F262		P113
	V404		H263	N182	I114
D481	V405	I337	H264	L183	E115
L482	T406		I265	D184	V116
R483		Y341	Q268	G185	
MET	L409	K342		L186	V119
GLU	G410	I343		E187	P120
GLN	V411	L344	P273	Y188	E121
ASP	N412	P345	V274	K189	G122
VAL	V413	F346	S275	L190	S123
F414	K414	I347	V276	H191	V124
ALA	K415	L348	V277		I125
PRO		R349	S278	G194	P126
HIS	D416				

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	5.84 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.278 0.227 , 0.273	Depositor DCC
R_{free} test set	2030 reflections (9.81%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.808	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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%)	5	20
1	B	459/491 (94%)	399 (87%)	47 (10%)	13 (3%)	5	19
All	All	918/982 (94%)	786 (86%)	107 (12%)	25 (3%)	5	19

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%)	13	38
1	B	408/431 (95%)	380 (93%)	28 (7%)	15	41
All	All	816/862 (95%)	758 (93%)	58 (7%)	14	40

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	-	22,23,23	2.64	10 (45%)	30,34,34	1.41	7 (23%)
2	NMN	B	1002	-	22,23,23	2.97	10 (45%)	30,34,34	1.36	6 (20%)

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	-	-	1/14/30/30	0/2/2/2
2	NMN	B	1002	-	-	1/14/30/30	0/2/2/2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	NMN	C2-N1	7.16	1.43	1.35
2	B	1002	NMN	C4-C3	6.35	1.50	1.39
2	A	1001	NMN	C4-C3	6.25	1.50	1.39
2	A	1001	NMN	C2-N1	5.60	1.41	1.35
2	B	1002	NMN	C6-N1	4.90	1.47	1.35

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1002	NMN	C3-C7-N7	3.20	121.59	117.75
2	B	1002	NMN	O7-C7-C3	-3.06	115.97	119.63
2	A	1001	NMN	O7-C7-C3	-2.79	116.29	119.63
2	A	1001	NMN	C3-C7-N7	2.74	121.04	117.75
2	A	1001	NMN	C3R-C2R-C1R	2.54	104.81	100.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	NMN	O4R-C4R-C5R-O5R
2	B	1002	NMN	O4R-C4R-C5R-O5R

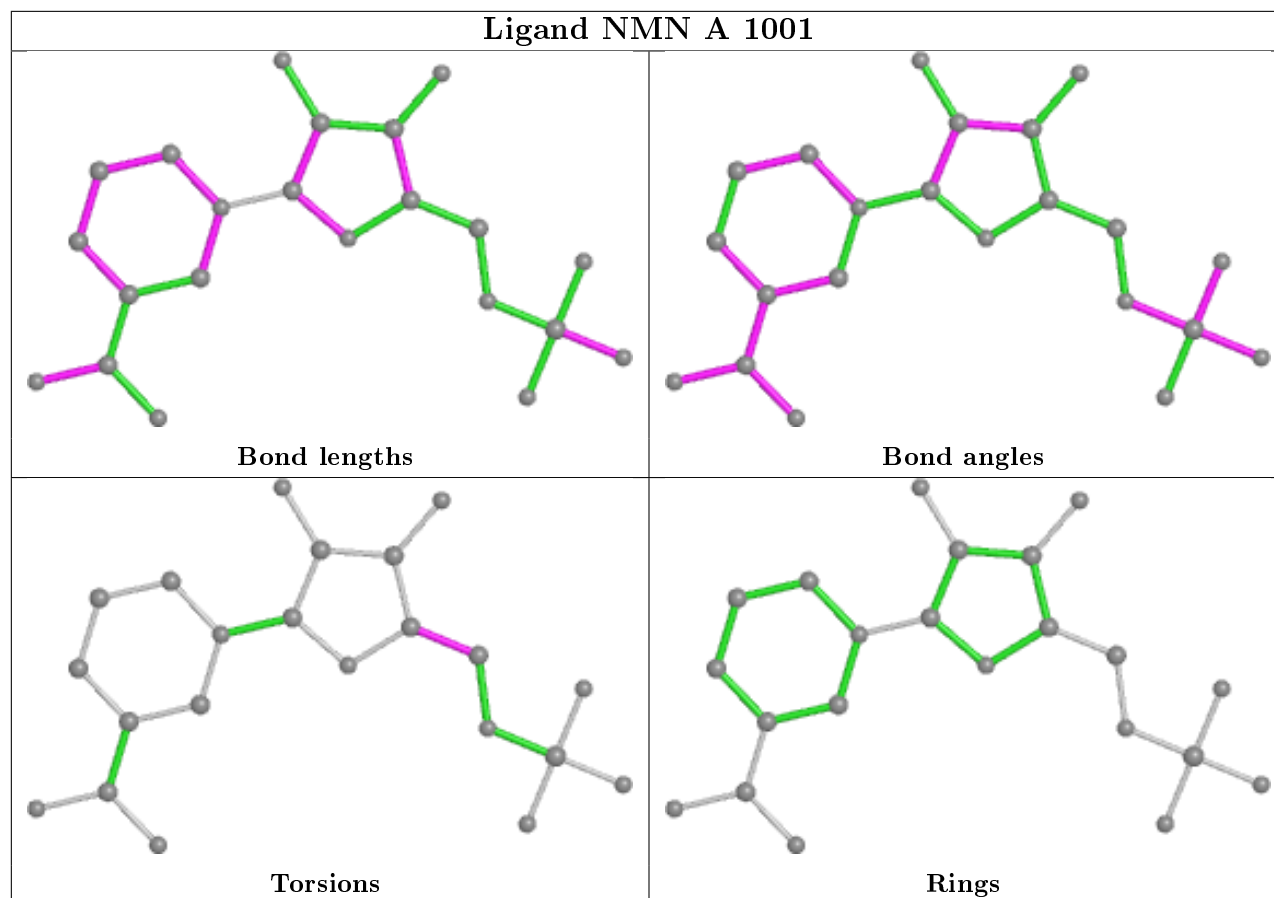
There are no ring outliers.

2 monomers are involved in 8 short contacts:

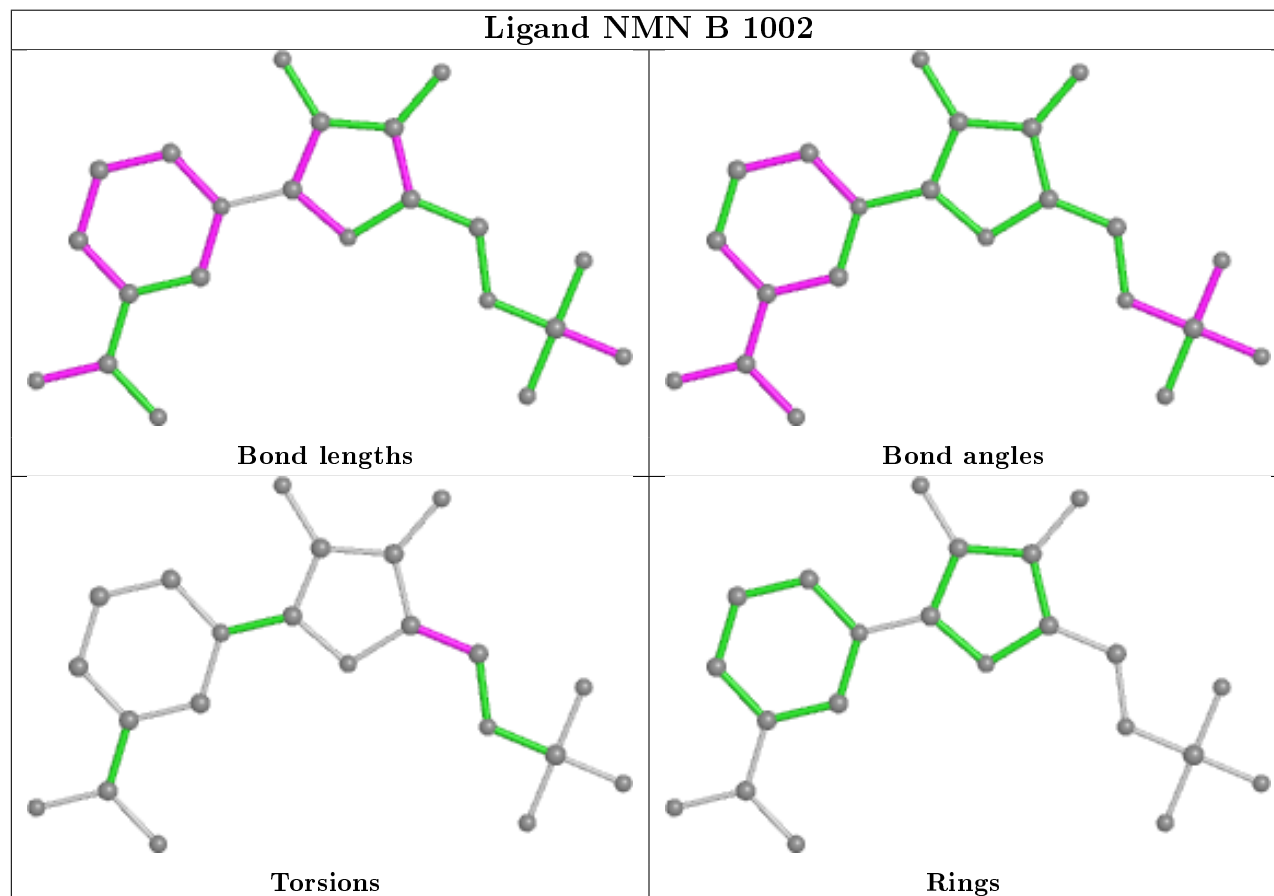
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NMN	5	0
2	B	1002	NMN	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NMN A 1001



Ligand NMN B 1002



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, 95th 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	463/491 (94%)	-0.13	5 (1%) 80 80	10, 27, 45, 58	0
1	B	463/491 (94%)	-0.14	8 (1%) 70 69	11, 27, 46, 67	0
All	All	926/982 (94%)	-0.13	13 (1%) 75 75	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](#)

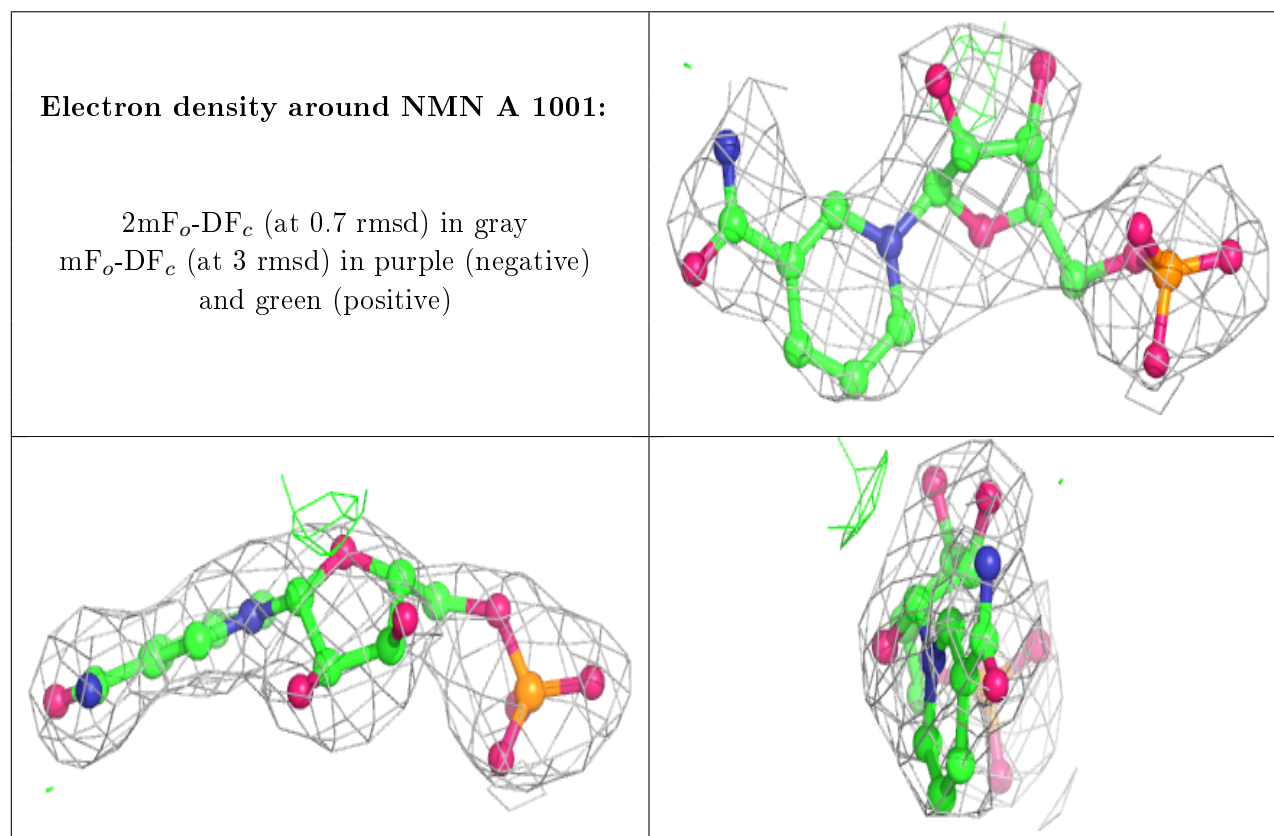
There are no carbohydrates in this entry.

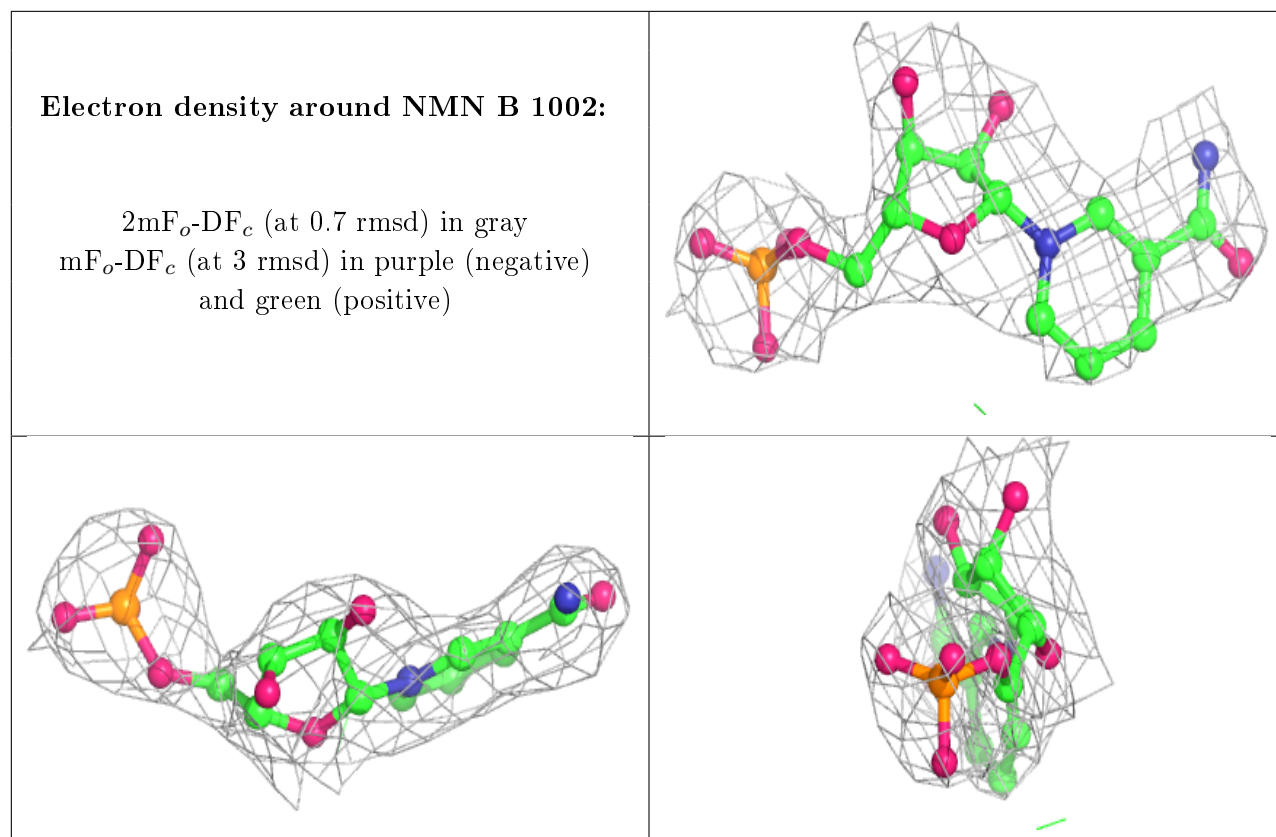
6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95th 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	B-factors(\AA^2)	Q<0.9
2	NMN	A	1001	22/22	0.96	0.18	20,29,31,32	0
2	NMN	B	1002	22/22	0.96	0.17	19,22,25,26	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.