



# Full wwPDB NMR Structure Validation Report ⓘ

Aug 10, 2020 – 03:30 AM BST

PDB ID : 1NXN  
Title : SOLUTION STRUCTURE OF CONTRYPHAN-VN  
Authors : Eliseo, T.; Cicero, D.O.; Polticelli, F.; Schinina, M.E.; Massilia, G.R.; Paci, M.; Ascenzi, P.  
Deposited on : 2003-02-11

This is a Full wwPDB NMR Structure Validation 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

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

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  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.13.1  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

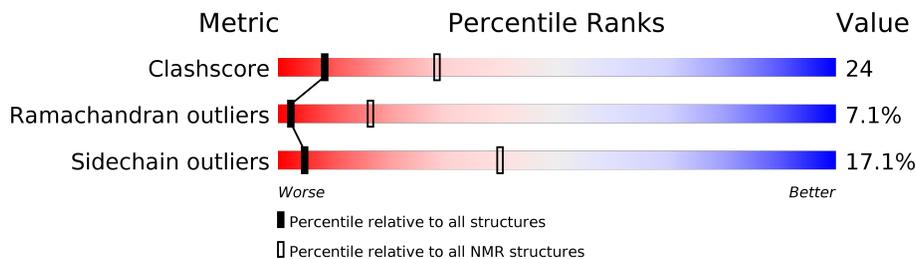
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	10	

## 2 Ensemble composition and analysis

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores.

Cyrange was unable to find well-defined residues.

Error message: The number of core atoms ( 6) was below the domain threshold value ( 8).

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 142 atoms, of which 66 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	10	142	50	66	13	11	2	1

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

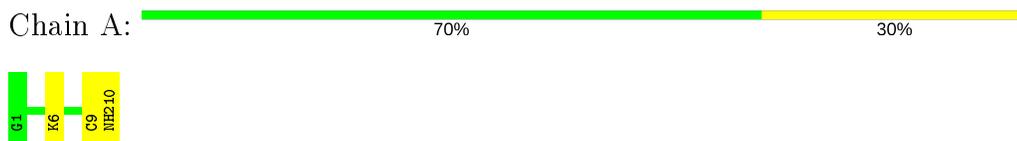
#### 4.2.1 Score per residue for model 1

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



#### 4.2.2 Score per residue for model 2

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



### 4.2.3 Score per residue for model 3

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



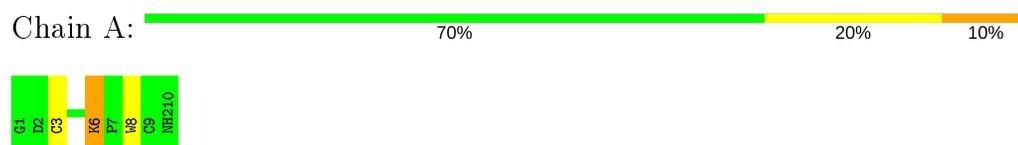
### 4.2.4 Score per residue for model 4

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



### 4.2.5 Score per residue for model 5

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



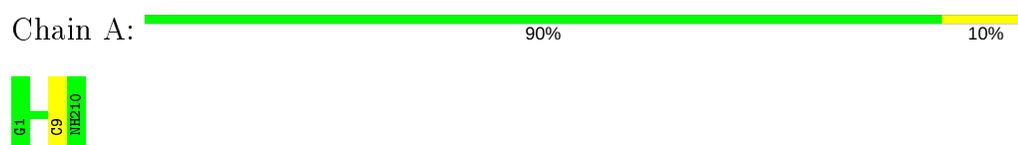
### 4.2.6 Score per residue for model 6

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



### 4.2.7 Score per residue for model 7

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



#### 4.2.8 Score per residue for model 8

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



#### 4.2.9 Score per residue for model 9

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



#### 4.2.10 Score per residue for model 10

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



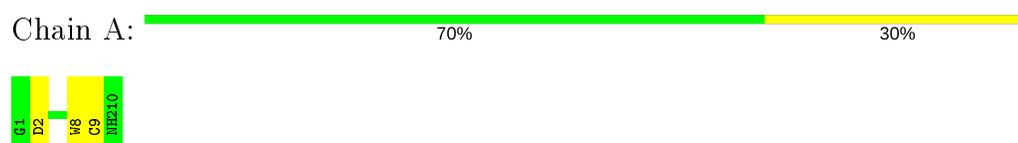
#### 4.2.11 Score per residue for model 11

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



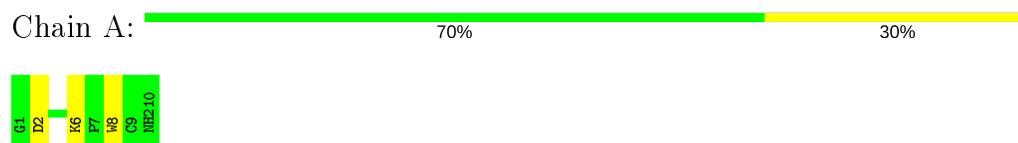
#### 4.2.12 Score per residue for model 12

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



#### 4.2.13 Score per residue for model 13

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



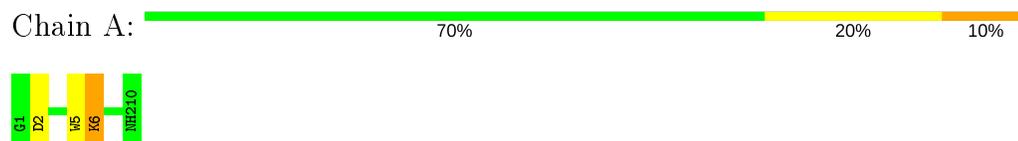
#### 4.2.14 Score per residue for model 14

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



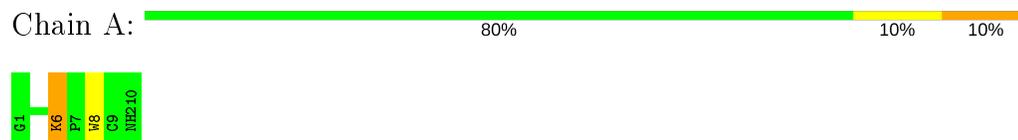
#### 4.2.15 Score per residue for model 15

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



#### 4.2.16 Score per residue for model 16

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



#### 4.2.17 Score per residue for model 17

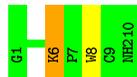
- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)



#### 4.2.18 Score per residue for model 18

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)

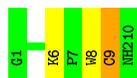
Chain A: 



#### 4.2.19 Score per residue for model 19

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)

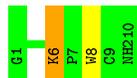
Chain A: 



#### 4.2.20 Score per residue for model 20

- Molecule 1: CONTRYPHAN-VN, MAJOR FORM (CIS CONFORMER)

Chain A: 



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *FEWEST RESTRAINTS VIOLATIONS, LOWEST ENERGY*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
XwinNMR	structure solution	
NMRPipe	structure solution	
NMRView	structure solution	
XPLOR	structure solution	1.5
XPLOR	refinement	1.5

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality i

### 6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: DTR, NH2

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 (average) 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	1.24±1.38	1±4/63 ( 1.3± 5.9%)	1.41±0.65	0±2/84 ( 0.4± 1.8%)
All	All	1.85	17/1260 ( 1.3%)	1.56	7/1680 ( 0.4%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	9	CYS	CA-CB	-24.64	0.99	1.53	1	1
1	A	2	ASP	CA-CB	-19.88	1.10	1.53	1	1
1	A	6	LYS	CE-NZ	-18.36	1.03	1.49	1	1
1	A	2	ASP	N-CA	-17.66	1.11	1.46	1	1
1	A	6	LYS	CG-CD	-17.39	0.93	1.52	1	1
1	A	9	CYS	CB-SG	-17.00	1.53	1.82	1	1
1	A	3	CYS	CB-SG	-15.33	1.56	1.82	1	1
1	A	6	LYS	CD-CE	-10.12	1.25	1.51	1	1
1	A	8	TRP	C-O	-9.33	1.05	1.23	1	1
1	A	7	PRO	N-CD	-8.36	1.36	1.47	1	1
1	A	8	TRP	C-N	-7.68	1.16	1.34	1	1
1	A	8	TRP	NE1-CE2	-6.81	1.28	1.37	1	1
1	A	1	GLY	C-N	6.17	1.48	1.34	1	1
1	A	8	TRP	CD2-CE3	-5.98	1.31	1.40	1	1
1	A	6	LYS	C-O	-5.91	1.12	1.23	1	1
1	A	8	TRP	CG-CD1	-5.71	1.28	1.36	1	1
1	A	7	PRO	CA-CB	-5.17	1.43	1.53	1	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )	Models	
								Worst	Total
1	A	6	LYS	CB-CG-CD	21.51	167.54	111.60	1	1
1	A	6	LYS	CG-CD-CE	20.97	174.81	111.90	1	1
1	A	6	LYS	CD-CE-NZ	10.88	136.73	111.70	1	1
1	A	9	CYS	N-CA-CB	10.14	128.85	110.60	1	1
1	A	9	CYS	CA-CB-SG	9.65	131.37	114.00	1	1
1	A	2	ASP	N-CA-CB	-8.35	95.57	110.60	1	1
1	A	8	TRP	O-C-N	-5.09	114.55	122.70	1	1

There are no chirality outliers.

There are no planarity outliers.

## 6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	76	65	64	3 $\pm$ 4
All	All	1520	1319	1280	68

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 24.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash( $\text{\AA}$ )	Distance( $\text{\AA}$ )	Models	
				Worst	Total
1:A:6:LYS:CG	1:A:6:LYS:CE	1.20	2.18	1	1
1:A:6:LYS:CB	1:A:6:LYS:CD	1.07	2.32	1	1
1:A:6:LYS:CG	1:A:6:LYS:CD	0.90	0.93	1	1
1:A:1:GLY:O	1:A:3:CYS:N	0.89	2.05	17	1
1:A:3:CYS:SG	1:A:9:CYS:CB	0.89	2.59	1	1
1:A:6:LYS:HG3	1:A:6:LYS:CD	0.84	1.39	1	1
1:A:6:LYS:HG2	1:A:6:LYS:CD	0.84	1.39	1	1
1:A:1:GLY:O	1:A:2:ASP:OD1	0.84	1.94	4	1
1:A:3:CYS:SG	1:A:10:NH2:N	0.83	2.51	11	1
1:A:6:LYS:CG	1:A:6:LYS:HD3	0.83	1.36	1	1
1:A:6:LYS:CG	1:A:6:LYS:HD2	0.82	1.36	1	1
1:A:2:ASP:HA	1:A:6:LYS:NZ	0.73	1.99	3	1

*Continued on next page...*

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:TRP:O	1:A:9:CYS:O	0.63	2.16	10	2
1:A:1:GLY:C	1:A:2:ASP:CG	0.62	2.57	4	1
1:A:2:ASP:CA	1:A:6:LYS:NZ	0.59	2.65	3	1
1:A:6:LYS:HD3	1:A:7:PRO:HD2	0.59	1.73	3	1
1:A:6:LYS:HD3	1:A:7:PRO:CD	0.59	2.28	3	1
1:A:6:LYS:NZ	1:A:8:TRP:CH2	0.56	2.71	13	1
1:A:1:GLY:C	1:A:3:CYS:N	0.56	2.59	17	1
1:A:1:GLY:O	1:A:2:ASP:C	0.55	2.43	17	1
1:A:2:ASP:O	1:A:6:LYS:CG	0.53	2.56	3	1
1:A:1:GLY:O	1:A:2:ASP:CG	0.53	2.47	4	2
1:A:6:LYS:NZ	1:A:8:TRP:CZ2	0.51	2.70	13	2
1:A:2:ASP:HB2	1:A:6:LYS:CE	0.51	2.35	4	1
1:A:6:LYS:HE2	1:A:8:TRP:CZ2	0.51	2.40	16	2
1:A:6:LYS:HG3	1:A:6:LYS:HD3	0.50	1.26	1	1
1:A:8:TRP:C	1:A:8:TRP:CD1	0.48	2.86	1	1
1:A:8:TRP:CD1	1:A:9:CYS:N	0.48	2.82	10	9
1:A:2:ASP:O	1:A:6:LYS:NZ	0.48	2.44	3	1
1:A:2:ASP:O	1:A:6:LYS:HG2	0.48	2.08	1	2
1:A:6:LYS:HD2	1:A:8:TRP:CZ2	0.47	2.44	3	1
1:A:6:LYS:HG2	1:A:6:LYS:HD2	0.47	1.26	1	1
1:A:2:ASP:CA	1:A:6:LYS:HZ3	0.46	2.22	3	1
1:A:2:ASP:CG	1:A:6:LYS:HE2	0.45	2.31	9	1
1:A:6:LYS:CE	1:A:8:TRP:CZ2	0.45	3.00	11	1
1:A:2:ASP:OD1	1:A:2:ASP:O	0.45	2.35	12	1
1:A:6:LYS:CG	1:A:8:TRP:CZ2	0.45	3.00	16	4
1:A:1:GLY:O	1:A:9:CYS:SG	0.44	2.76	17	1
1:A:7:PRO:HG2	1:A:8:TRP:CE3	0.43	2.49	1	1
1:A:1:GLY:C	1:A:3:CYS:H	0.43	2.15	17	1
1:A:6:LYS:CG	1:A:8:TRP:CE2	0.42	3.01	16	2
1:A:8:TRP:CG	1:A:9:CYS:N	0.42	2.87	10	1
1:A:8:TRP:C	1:A:9:CYS:O	0.41	2.59	10	1
1:A:9:CYS:SG	1:A:10:NH2:N	0.41	2.94	2	2
1:A:5:DTR:O	1:A:6:LYS:HE3	0.41	2.15	15	1
1:A:6:LYS:CD	1:A:8:TRP:CZ2	0.41	3.04	5	1
1:A:2:ASP:HB2	1:A:6:LYS:HE2	0.41	1.93	4	1
1:A:6:LYS:HG3	1:A:8:TRP:CE2	0.40	2.52	16	1
1:A:8:TRP:C	1:A:10:NH2:N	0.40	2.75	1	1
1:A:6:LYS:HG3	1:A:8:TRP:CZ2	0.40	2.52	18	1

## 6.3 Torsion angles [i](#)

### 6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	7/10 (70%)	5±1 (70±13%)	2±1 (23±8%)	1±1 (7±12%)	2	16
All	All	140/200 (70%)	98 (70%)	32 (23%)	10 (7%)	2	16

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	2	ASP	4
1	A	6	LYS	3
1	A	9	CYS	3

### 6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	7/7 (100%)	6±1 (83±10%)	1±1 (17±10%)	5	40
All	All	140/140 (100%)	116 (83%)	24 (17%)	5	40

All 4 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	6	LYS	9
1	A	3	CYS	7
1	A	9	CYS	4
1	A	2	ASP	4

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1-A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	8:TRP	C	9:CYS	N	1.16
1	A	5:DTR	C	6:LYS	N	1.06

## 7 Chemical shift validation

No chemical shift data were provided