



# wwPDB NMR Structure Validation Summary Report ⓘ

May 28, 2020 – 10:18 pm BST

PDB ID : 2K2I  
Title : NMR Solution structure of the C-terminal domain (T94-Y172) of the human centrin 2 in complex with a repeat sequence of human Sfi1 (R641-T660)  
Authors : Martinez-Sanz, J.; Assairi, L.; Blouquit, Y.; Duchambon, P.; Mouawad, L.; Craescu, C.  
Deposited on : 2008-04-02

This is a wwPDB NMR 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

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

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:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
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 : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

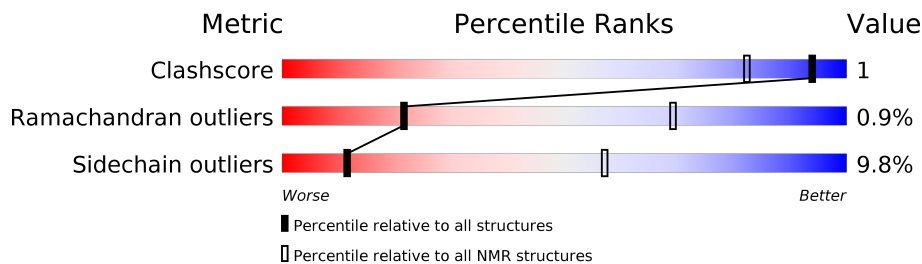
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*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	79	 75% 6% • 18%
2	B	20	 45% 5% 50%

## 2 Ensemble composition and analysis i

This entry contains 15 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:103-A:167, B:651-B:660 (75)	0.58	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 5 single-model clusters were found.

Cluster number	Models
1	2, 6, 7, 9, 15
2	3, 4, 5, 11, 14
Single-model clusters	1; 8; 10; 12; 13

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1612 atoms, of which 798 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Centrin-2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	79	1281	399	636	104	139	3	0

- Molecule 2 is a protein called SFI1 peptide.

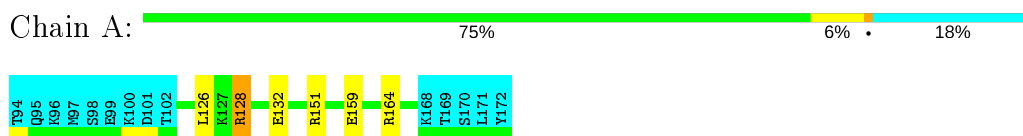
Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	20	331	105	162	37	27	0

## 4 Residue-property plots

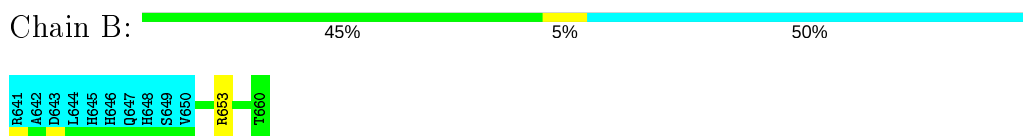
### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Centrin-2



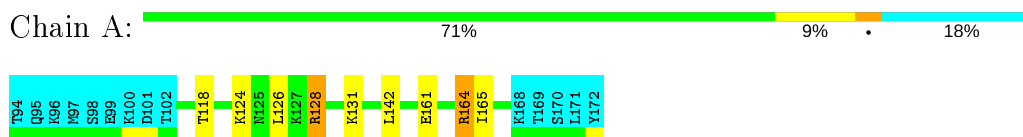
- Molecule 2: SFI1 peptide



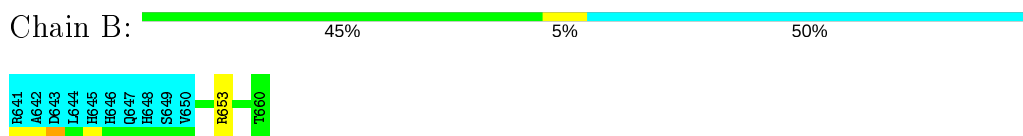
### 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 3. Colouring as in section 4.1 above.

- Molecule 1: Centrin-2



- Molecule 2: SFI1 peptide



## 5 Refinement protocol and experimental data overview (i)

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

Of the 500 calculated structures, 15 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
Discover molecular modeling system	geometry optimization	2.98
Discover molecular modeling system	refinement	2.98

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

COVALENT-GEOMETRY INFOmissingINFO

### 5.1 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 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	530	519	519	1±1
2	B	85	86	86	0±0
All	All	9225	9075	9075	22

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 1.

5 of 16 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:ARG:NH1	1:A:132:GLU:OE2	0.45	2.49	15	3
1:A:161:GLU:OE2	1:A:164:ARG:NH1	0.44	2.50	3	3
1:A:128:ARG:NH1	1:A:132:GLU:OE1	0.44	2.50	1	1
1:A:115:ASP:OD2	1:A:128:ARG:NH2	0.43	2.52	11	1
1:A:113:PHE:CD1	1:A:129:VAL:HG21	0.43	2.49	4	1

## 5.2 Torsion angles [i](#)

### 5.2.1 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	65/79 (82%)	59±2 (91±3%)	6±1 (9±2%)	0±1 (1±1%)	26	73
2	B	9/20 (45%)	8±1 (88±12%)	1±1 (10±10%)	0±0 (2±4%)	10	49
All	All	1110/1485 (75%)	1002 (90%)	98 (9%)	10 (1%)	21	69

5 of 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	653	ARG	2
1	A	136	ASN	1
2	B	659	VAL	1
1	A	150	ASP	1
1	A	116	ASP	1

### 5.2.2 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	58/72 (81%)	52±2 (90±3%)	6±2 (10±3%)	10	55
2	B	8/17 (47%)	8±0 (95±6%)	0±0 (5±6%)	28	77
All	All	990/1335 (74%)	893 (90%)	97 (10%)	11	57

5 of 38 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	126	LEU	11
1	A	159	GLU	7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	127	LYS	5
1	A	143	GLN	5
1	A	147	ASP	4

### 5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.5 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.6 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.



## 6 Chemical shift validation

No chemical shift data were provided