



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2KXP  
Title : Solution NMR structure of V-1 bound to capping protein (CP)  
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Deposited on : 2010-05-11

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

<http://wwpdb.org/validation/2016/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:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

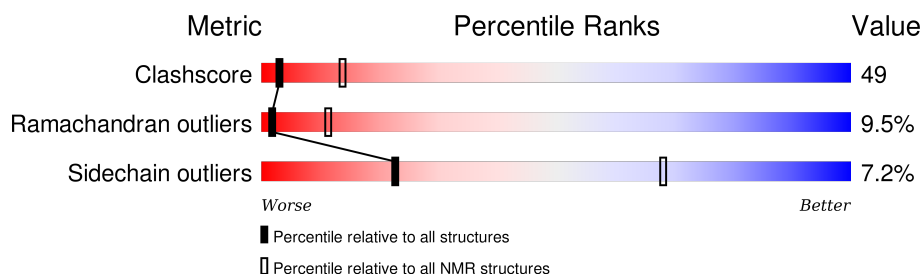
# 1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	275	
2	B	270	
3	C	118	

## 2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:7-A:281, B:302-B:571 (545)	0.00	7
2	C:601-C:718 (118)	0.00	8

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 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 6, 9
2	7, 10
3	4, 8
Single-model clusters	5

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

There are 3 unique types of molecules in this entry. The entry contains 10511 atoms, of which 5229 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called F-actin-capping protein subunit alpha-1.

Mol	Chain	Residues	Atoms						Trace
1	A	275	Total	C	H	N	O	S	0
			4416	1413	2177	392	429	5	

- Molecule 2 is a protein called F-actin-capping protein subunit beta isoforms 1 and 2.

Mol	Chain	Residues	Atoms						Trace
2	B	270	Total	C	H	N	O	S	0
			4276	1334	2135	374	423	10	

- Molecule 3 is a protein called Myotrophin.

Mol	Chain	Residues	Atoms						Trace
3	C	118	Total	C	H	N	O	S	0
			1819	570	917	152	175	5	



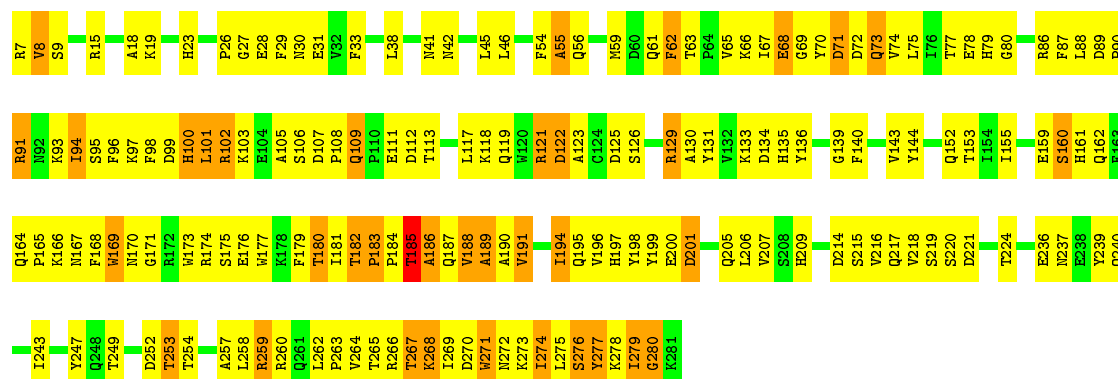


## 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 7. Colouring as in section 4.1 above.

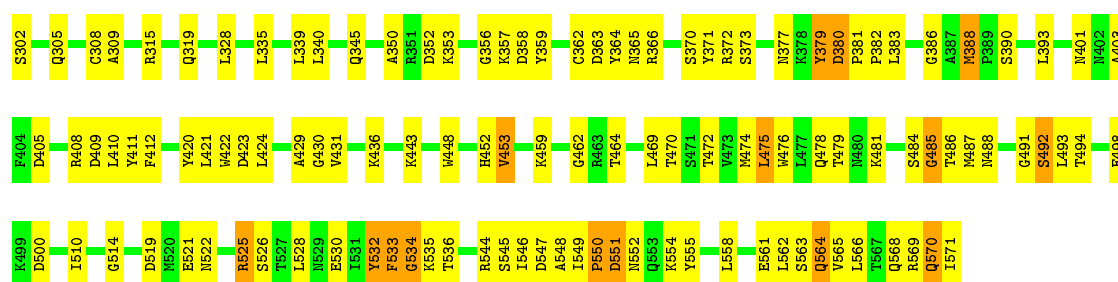
- Molecule 1: F-actin-capping protein subunit alpha-1

Chain A: 37% 49% 13%



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain B: 57% 38% 6%



- Molecule 3: Myotrophin

Chain C: 39% 42% 17%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, simulated annealing*.

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	2.23

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](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 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 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	2239	2177	2166	269±10
2	B	2141	2135	2128	148±7
3	C	902	917	909	118±8
All	All	52820	52290	52030	5123

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 49.

5 of 1661 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:276:SER:O	1:A:278:LYS:N	1.32	1.62	4	10
1:A:182:THR:OG1	1:A:184:PRO:HG3	1.25	1.30	7	1
3:C:688:LEU:HD13	3:C:689:SER:N	1.23	1.49	4	2
1:A:273:LYS:O	1:A:277:TYR:HB3	1.22	1.35	8	10
3:C:673:LEU:O	3:C:676:VAL:HG22	1.18	0.99	3	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	273/275 (99%)	194±0 (71±0%)	48±0 (17±0%)	32±0 (12±0%)	1	8
2	B	268/270 (99%)	227±0 (85±0%)	31±0 (12±0%)	10±0 (4±0%)	7	36
3	C	116/118 (98%)	62±0 (53±0%)	33±0 (28±0%)	21±0 (18±0%)	0	3
All	All	6570/6630 (99%)	4827 (73%)	1116 (17%)	627 (10%)	2	11

5 of 63 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	C	662	ASN	10
1	A	166	LYS	10
1	A	121	ARG	10
1	A	258	LEU	10
1	A	71	ASP	10

### 6.3.2 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 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	243/243 (100%)	227±1 (93±1%)	16±1 (7±1%)	25	71
2	B	241/241 (100%)	228±3 (95±1%)	13±3 (5±1%)	32	77
3	C	96/96 (100%)	83±2 (87±3%)	13±2 (13±3%)	9	50
All	All	5800/5800 (100%)	5384 (93%)	416 (7%)	23	68

5 of 145 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	175	SER	10
2	B	533	PHE	10
1	A	100	HIS	10
2	B	380	ASP	10
1	A	160	SER	10

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no carbohydrates 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](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided