

Full wwPDB NMR Structure Validation Report (i)

Feb 17, 2022 – 08:47 AM EST

PDB ID : 10QP

Title : STRUCTURE OF THE CA2+/C-TERMINAL DOMAIN OF CALTRACTIN

IN COMPLEX WITH THE CDC31P-BINDING DOMAIN FROM KAR1P

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Deposited on : 2003-03-10

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

The following versions of software and data (see references (i)) 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 : 2.26

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

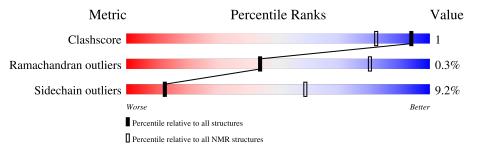
Validation Pipeline (wwPDB-VP) : 2.26

1 Overall quality at a glance (i)

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	NMR archive	
Metric	$(\# \mathrm{Entries})$	$(\# \mathrm{Entries})$	
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 >=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 <=5%

Mol	Chain	Length	Quality of chain			
1	A	77	81% 5% • 13%			
2	В	19	47%	5%	47%	



2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models).

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 n								
1	A:99-A:147, A:152-A:169,	0.25	19					
	B:244-B:253 (77)							

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 4 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 5, 6, 7, 13, 15, 17, 18, 19, 20
2	9, 14, 16
3	8, 11, 12
4	3, 10



3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1601 atoms, of which 796 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Caltractin.

Mol	Chain	Residues		Atoms					Trace
1	Λ	77	Total	С	Н	N	О	S	0
1	A	11	1233	381	605	108	137	2	U

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	GLY	-	expression tag	UNP P05434
A	94	SER	-	expression tag	UNP P05434

• Molecule 2 is a protein called Cell division control protein KAR1.

Mol	Chain	Residues	Atoms				Trace	
9	D	10	Total	С	Н	N	О	0
	D	19	368	115	191	35	27	0

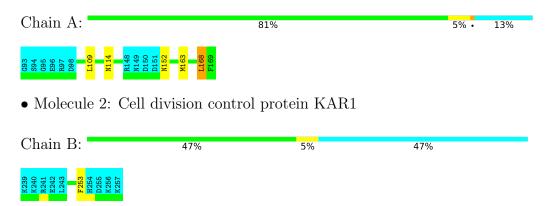


4 Residue-property plots (i)

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: Caltractin

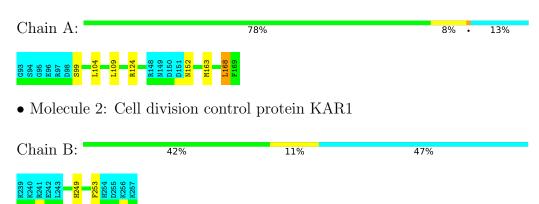


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Caltractin





4.2.2 Score per residue for model 2

• Molecule 1: Caltractin

Chain A: 73% 12% · 13%

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• Molecule 2: Cell division control protein KAR1

Chain B: 47% 5% 47%

K239 K240 R241 E242 L243 F253 H254 D255 K256

4.2.3 Score per residue for model 3

• Molecule 1: Caltractin

Chain A: 78% 8% · 13%

• Molecule 2: Cell division control protein KAR1

Chain B: 32% 21% 47%

K239
K240
K240
E242
L1243
L250
L251
L252
L255
K256
K266
K266
K266

4.2.4 Score per residue for model 4

• Molecule 1: Caltractin

Chain A: 79% 6% · 13%

C93 C93 C95 C96 C96 E96 E96 N114 N1148 N149 D150 D151 N152 E169

• Molecule 2: Cell division control protein KAR1

Chain B: 47% 5% 47%

K239 K240 R241 E242 L243 L243 F253 H254 D255 K256



4.2.5 Score per residue for model 5

• Molecule 1: Caltractin

Chain A: 81% 5% 13%

• Molecule 2: Cell division control protein KAR1

Chain B: 42% 11% 47%

K239 K240 E242 L243 H249 F263 H264 D266 K266

4.2.6 Score per residue for model 6

• Molecule 1: Caltractin

Chain A: 75% 10% · 13%

• Molecule 2: Cell division control protein KAR1

Chain B: 42% 11% 47%



4.2.7 Score per residue for model 7

• Molecule 1: Caltractin

Chain A: 81% • • 13%



• Molecule 2: Cell division control protein KAR1

Chain B: 37% 16% 47%

K239 K240 R241 E242 L243 H250 L251 L253 H254 H254 H254 H254 R256 K256



4.2.8 Score per residue for model 8

• Molecule 1: Caltractin

Chain A: 74% 12% · 13%

• Molecule 2: Cell division control protein KAR1

Chain B: 47% 5% 47%

K239 K240 R241 E242 L243 F253 H264 D265 K256

4.2.9 Score per residue for model 9

• Molecule 1: Caltractin

Chain A: 73% 13% · 13%

• Molecule 2: Cell division control protein KAR1

Chain B: 47% 5% 47%

K239 K240 R241 E242 L243 H249 H254 D255 K256

4.2.10 Score per residue for model 10

• Molecule 1: Caltractin

Chain A: 77% 9% · 13%

• Molecule 2: Cell division control protein KAR1

Chain B: 47% 5% 47%

K239 K240 R241 E242 L243 L243 F253 H254 H254 K256 K257



4.2.11 Score per residue for model 11

• Molecule 1: Caltractin

Chain A: 81% 5% · 13%

G93 S94 G96 E96 R97 D98 N14 N149 D150 D150 D155 D156 P169

• Molecule 2: Cell division control protein KAR1

Chain B: 42% 11% 47%

K239 K240 R241 E242 L243 L252 F253 H254 D255 K256

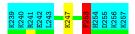
4.2.12 Score per residue for model 12

• Molecule 1: Caltractin

Chain A: 79% 6% · 13%

• Molecule 2: Cell division control protein KAR1

Chain B: 42% 5% 5% 47%



4.2.13 Score per residue for model 13

• Molecule 1: Caltractin

Chain A: 82% • • 13%

C93 C95 C95 E96 R97 N114 N114 N149 N149 D150 D150 D151

• Molecule 2: Cell division control protein KAR1

Chain B: 32% 21% 47%

K240 R240 R241 E242 L243 H249 R250 L251 L252 F253 H254 D255 K256 K256



4.2.14 Score per residue for model 14

• Molecule 1: Caltractin

Chain A: 83% ... 13%

G93 S94 G95 G95 B97 D98 N148 N148 N148 N152 N152 N152 N152

• Molecule 2: Cell division control protein KAR1

Chain B: 42% 11% 47%

K239 K240 R241 E242 L243 K247 H264 D266 K266 K257

4.2.15 Score per residue for model 15

• Molecule 1: Caltractin

Chain A: 77% 10% 13%

• Molecule 2: Cell division control protein KAR1

Chain B: 37% 16% 47%



4.2.16 Score per residue for model 16

• Molecule 1: Caltractin

Chain A: 79% 6% · 13%

• Molecule 2: Cell division control protein KAR1

Chain B: 42% 11% 47%

K239 K240 R241 L243 L243 H249 H254 D255 K257



4.2.17 Score per residue for model 17

• Molecule 1: Caltractin

Chain A: 77% 9% · 13%

• Molecule 2: Cell division control protein KAR1

Chain B: 47% 5% 47%

K239 K240 R241 E242 L243 F253 H254 D255 K256

4.2.18 Score per residue for model 18

• Molecule 1: Caltractin

Chain A: 77% 9% · 13%

• Molecule 2: Cell division control protein KAR1

Chain B: 32% 21% 47%

K239 K240 K240 K241 E242 L243 L243 L264 L261 L261 L265 K256 K266 K266 K266 K266

4.2.19 Score per residue for model 19 (medoid)

• Molecule 1: Caltractin

Chain A: 83% ... 13%

G93 S94 G95 E96 R97 D98 N114 R148 N149 D150 D150 D151

• Molecule 2: Cell division control protein KAR1

Chain B: 42% 11% 47%





4.2.20 Score per residue for model 20

• Molecule 1: Caltractin

Chain A: 79% 6% · 13%



• Molecule 2: Cell division control protein KAR1

Chain B: 37% 16% 47%





Refinement protocol and experimental data overview (i) 5



The models were refined using the following method: torsion angle dynamics.

Of the 60 calculated structures, 20 were deposited, based on the following criterion: structures with the least restraint violations, structures with the lowest energy.

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

Software name	Classification	Version
DYANA	structure solution	1.5
Amber	refinement	7.0

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

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		В	Sond lengths	Bond angles		
		RMSZ	#Z>5	RMSZ	#Z>5	
1	A	0.51 ± 0.00	$0\pm0/554~(~0.0\pm~0.0\%)$	0.83 ± 0.02	$0\pm0/738~(~0.0\pm~0.0\%)$	
2	В	0.67 ± 0.01	$0\pm0/98~(~0.0\pm~0.0\%)$	1.01 ± 0.09	$0\pm0/132~(~0.0\pm~0.2\%)$	
All	All	0.53	0/13040 (0.0%)	0.86	1/17400 (0.0%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0 ± 0.0	0.3 ± 0.5
2	В	0.0 ± 0.0	0.3 ± 0.5
All	All	0	13

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}({}^o)$	$\operatorname{Ideal}({}^{o})$	Moc Worst	
2	В	253	PHE	CB-CG-CD2	-5.53	116.93	120.80	2	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	124	ARG	Sidechain	4
2	В	249	HIS	Sidechain	4
1	A	125	ARG	Sidechain	3
2	В	250	ARG	Sidechain	1
2	В	253	PHE	Sidechain	1



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	551	542	542	2±1
2	В	94	96	96	1±0
All	All	12900	12760	12760	32

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.

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

Atom-1	Atom-2	Clash(Å)	$\operatorname{Distance}(\operatorname{\AA})$	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:168:LEU:HD23	2:B:253:PHE:CE1	0.76	2.14	10	18
1:A:166:THR:HB	1:A:168:LEU:HD12	0.60	1.73	6	3
1:A:143:ILE:HA	1:A:154:ILE:HD11	0.45	1.87	16	1
1:A:163:MET:CE	1:A:168:LEU:HD13	0.45	2.41	9	7
1:A:168:LEU:HD23	2:B:253:PHE:CZ	0.43	2.48	15	1
1:A:127:ALA:HB1	1:A:132:GLU:O	0.42	2.14	20	1
1:A:168:LEU:HD22	2:B:252:LEU:HD13	0.41	1.92	6	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	66/77~(86%)	62±2 (94±3%)	4±2 (6±3%)	0±0 (0±1%)	38	78
2	В	10/19 (53%)	9±1 (86±11%)	1±1 (14±11%)	0±0 (0±0%)	100	100
All	All	1520/1920 (79%)	1410 (93%)	105 (7%)	5 (0%)	44	80

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	132	GLU	2
1	A	152	ASN	2
1	A	99	SER	1

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	in Analysed Rotameric		Outliers	Perce	entiles
1	A	61/69 (88%)	55±2 (91±3%)	$6\pm 2 \ (9\pm 3\%)$	13	59
2	В	10/19 (53%)	9±1 (90±10%)	1±1 (10±10%)	11	56
All	All	1420/1760 (81%)	1289 (91%)	131 (9%)	13	59

All 27 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	109	LEU	20
1	A	168	LEU	18
1	A	152	ASN	12
1	A	114	ASN	12
2	В	249	HIS	6
1	A	154	ILE	6
1	A	163	MET	6
1	A	155	ASP	6
1	A	143	ILE	5
2	В	252	LEU	5
1	A	140	GLN	4
1	A	115	SER	4
1	A	99	SER	3
1	A	104	LEU	3
2	В	251	LEU	3
1	A	161	ARG	3
2	В	247	LYS	3
1	A	128	LYS	2
2	В	250	ARG	2
1	A	101	GLU	1
1	A	108	ARG	1
1	A	133	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	157	ASP	1
1	A	147	ASP	1
1	A	125	ARG	1
2	В	253	PHE	1
1	A	112	ASP	1

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 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)

There are no chain breaks in this entry.



7 Chemical shift validation (i)

No chemical shift data were provided

