

Full wwPDB NMR Structure Validation Report (i)

Feb 15, 2022 – 07:13 AM EST

PDB ID	:	1K91
Title	:	Solution Structure of Calreticulin P-domain subdomain (residues 221-256)
Authors	:	Ellgaard, L.; Bettendorff, P.; Braun, D.; Herrmann, T.; Fiorito, F.; Guntert,
		P.; Helenius, A.; Wuthrich, K.
Deposited on	:	2001-10-26

This is a Full wwPDB NMR Structure Validation 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/NMRValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

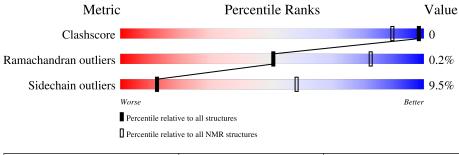
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	$egin{array}{c} { m Whole \ archive}\ (\#{ m Entries}) \end{array}$	${f NMR} \ { m archive} \ (\#{ m Entries})$
	(#Entrics)	
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	А	37	84%	•	14%



2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 18 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:222-A:253 (32)	0.32	18		

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 2 single-model clusters were found.

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



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 570 atoms, of which 267 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called CALRETICULIN.

Mol	Chain	Residues	Atoms				Trace		
1	٨	27	Total	С	Η	Ν	0	S	0
	57	570	191	267	47	64	1	0	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	220	GLY	-	cloning artifact	UNP P18418

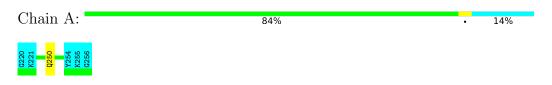


4 Residue-property plots (i)

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: CALRETICULIN



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: CALRETICULIN
Chain A: 73% 14%

4.2.2 Score per residue for model 2

• Molecule 1: CALRETICULIN

Chain A: 81% 5% 14%



14%

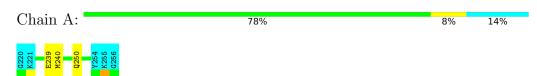
4.2.3 Score per residue for model 3

• Molecule 1: CALRETICULIN

Chain A:	81%	5%	14%
0220 1021 1022 1023 1026 1726 1726 1726 1726			

4.2.4 Score per residue for model 4

• Molecule 1: CALRETICULIN



4.2.5 Score per residue for model 5

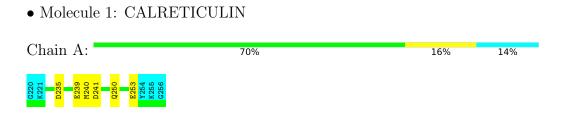
• Molecule 1: CALRETICULIN

Chain A:	84%	·	14%
6220 7254 7255 6256 6256			

4.2.6 Score per residue for model 6

Molecule 1: CALRETICULIN
Chain A: 76% 11% 14%

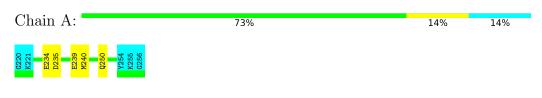
4.2.7 Score per residue for model 7





4.2.8 Score per residue for model 8

• Molecule 1: CALRETICULIN



4.2.9 Score per residue for model 9

• Molecule 1: CALRETICULIN



4.2.10 Score per residue for model 10

• Molecule 1: CALRETICULIN

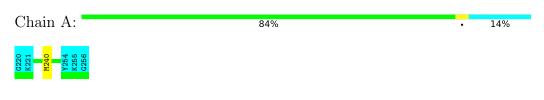
Chain A:	73%	14%	14%
6220 K221 E234 E239 M240 D241 D241 0241	Y254 G256		

4.2.11 Score per residue for model 11

Molecule 1: CALRETICULIN
Chain A:
 81%
 5%
 14%

4.2.12 Score per residue for model 12

• Molecule 1: CALRETICULIN





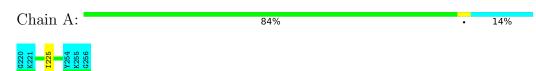
4.2.13 Score per residue for model 13

• Molecule 1: CALRETICULIN

Chain A:	78%	8%	14%
6220 K221 K221 K221 4260 K266 K266 K266 K266 K266 K266			

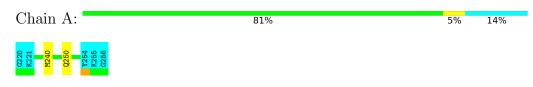
4.2.14 Score per residue for model 14

• Molecule 1: CALRETICULIN



4.2.15 Score per residue for model 15

• Molecule 1: CALRETICULIN



4.2.16 Score per residue for model 16

Molecule 1: CALRETICULIN
Chain A: 78% 8% 14%

4.2.17 Score per residue for model 17

Molecule 1: CALRETICULIN
Chain A: 76% 11%



14%

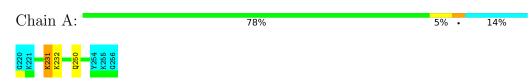
4.2.18 Score per residue for model 18 (medoid)

• Molecule 1: CALRETICULIN

Chain A:	76%	11%	14%
6220 8221 8221 8233 8233 8233 8233 8233 8235 8235 8255 825			

4.2.19 Score per residue for model 19

• Molecule 1: CALRETICULIN



4.2.20 Score per residue for model 20

• Molecule 1: CALRETICULIN

Chain A:	78%	5% •	14%
(220 (220 (231 (231 (231 (250 (256 (256 (256			



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: target function.

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

Software name	Classification	Version
DYANA	structure solution	1.82
DYANA	refinement	1.82

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

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

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	А	$0.0{\pm}0.0$	0.1 ± 0.2
All	All	0	1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	А	253	GLU	Peptide	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	А	265	226	226	0 ± 0
All	All	5300	4520	4520	2

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 0.

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

Atom-1	Atom-2	$Clash(\lambda)$	Distance(Å)	Moo	dels
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:231:LYS:HE3	1:A:232:LYS:H	0.46	1.70	19	1
1:A:231:LYS:HD2	1:A:231:LYS:H	0.40	1.77	20	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	А	32/37~(86%)	$28 \pm 1 \ (86 \pm 5\%)$	$4\pm1~(14\pm5\%)$	0±0 (0±1%)	50 82
All	All	640/740~(86%)	552 (86%)	87 (14%)	1 (0%)	50 82

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	А	253	GLU	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	30/33~(91%)	27 ± 2 (90 $\pm5\%$)	$3\pm2~(10\pm5\%)$	12	58
All	All	600/660~(91%)	543 (90%)	57~(10%)	12	58

All 16 unique residues with a non-rotameric side chain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	250	GLN	13
1	А	240	MET	8
1	А	239	GLU	7
1	А	241	ASP	6
1	А	237	ASP	4
1	А	235	ASP	4
1	А	231	LYS	3
1	А	234	GLU	3
1	А	253	GLU	2
1	А	243	GLU	1

Continued on next page...



Mol	Chain	Res	Type	Models (Total)
1	А	232	LYS	1
1	А	223	GLU	1
1	А	225	ILE	1
1	А	229	ASP	1
1	А	245	GLU	1
1	А	238	GLU	1

Continued from previous page...

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

