Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	1NKF
Title	:	CALCIUM-BINDING PEPTIDE, NMR, 30 STRUCTURES
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Deposited on	:	1998-03-09

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:

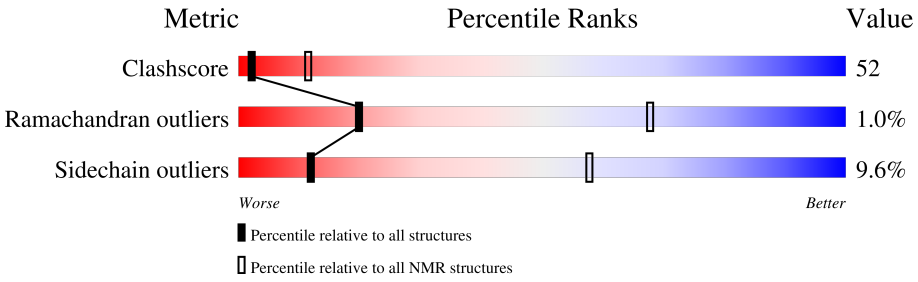
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 (#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 >=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	18	44% 44% 11%

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:1-A:16 (16)	0.20	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 4 clusters. No single-model clusters were found.

Cluster number	Models
1	3, 4, 5, 6, 7, 8, 9, 13, 16, 18, 19, 26, 28, 29
2	1, 2, 10, 12, 14, 22, 24, 30
3	11, 15, 17, 20, 21, 27
4	23, 25

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 215 atoms, of which 100 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CALCIUM-BINDING HEXADECAPEPTIDE.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	18	214	67	100	19	28	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ASP	ASN	conflict	UNP P02593

- Molecule 2 is LANTHANUM (III) ION (three-letter code: LA) (formula: La).

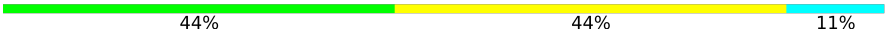
Mol	Chain	Residues	Atoms	
			Total	La
2	A	1	1	1

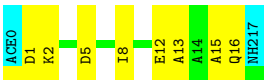
4 Residue-property plots

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: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A: 



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

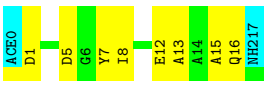
• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A: 

4.2.2 Score per residue for model 2

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

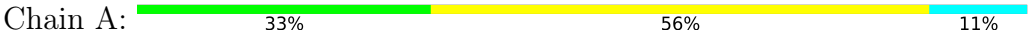
Chain A: 

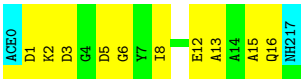


4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

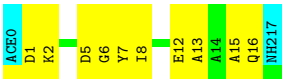




4.2.4 Score per residue for model 4

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

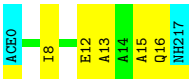
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

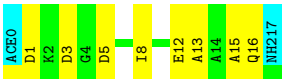
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

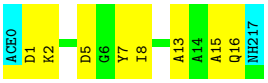
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

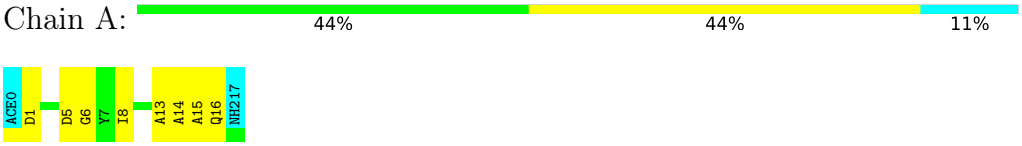
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:



4.2.9 Score per residue for model 9

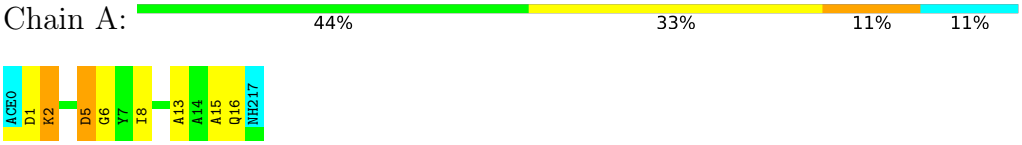
• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.10 Score per residue for model 10

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.12 Score per residue for model 12

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.13 Score per residue for model 13

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.14 Score per residue for model 14

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.15 Score per residue for model 15

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.16 Score per residue for model 16

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.17 Score per residue for model 17

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.18 Score per residue for model 18

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.19 Score per residue for model 19

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.20 Score per residue for model 20

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.21 Score per residue for model 21

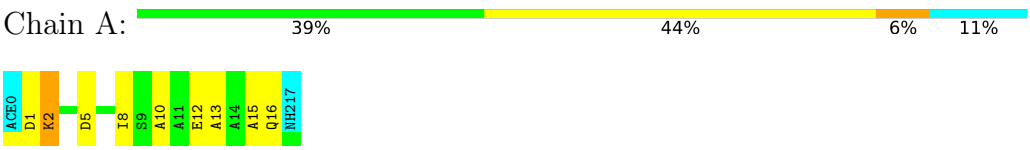
• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.22 Score per residue for model 22

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.24 Score per residue for model 24

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.25 Score per residue for model 25

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.26 Score per residue for model 26

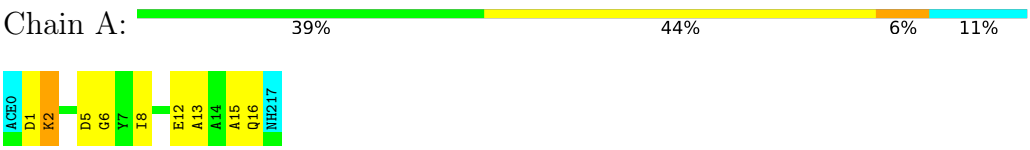
• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.27 Score per residue for model 27

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:



4.2.28 Score per residue for model 28

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.29 Score per residue for model 29

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

4.2.30 Score per residue for model 30

• Molecule 1: CALCIUM-BINDING HEXADECAPEPTIDE

Chain A:

5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING, RESTRAINED MOLECULAR DYNAMICS*.

Of the 100 calculated structures, 30 were deposited, based on the following criterion: *ENERGY, AGREEMENT WITH EXPERIMENTAL DATA*.

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

Software name	Classification	Version
X-PLOR	refinement	
NDEE	structure solution	
X-PLOR	structure solution	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

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

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	110	95	95	11±2
All	All	3330	2850	2850	322

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 52.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ALA:HB3	1:A:16:GLN:NE2	0.83	1.88	25	30
1:A:8:ILE:CG2	1:A:13:ALA:CA	0.60	2.80	1	27
1:A:8:ILE:HG21	1:A:13:ALA:HA	0.60	1.71	1	28
1:A:8:ILE:CG2	1:A:13:ALA:N	0.57	2.67	30	28
1:A:16:GLN:NE2	1:A:16:GLN:N	0.55	2.54	5	2
1:A:8:ILE:HG21	1:A:13:ALA:CA	0.55	2.32	10	18
1:A:5:ASP:OD1	1:A:6:GLY:N	0.53	2.42	20	5
1:A:1:ASP:OD2	1:A:5:ASP:N	0.52	2.43	21	10
1:A:16:GLN:N	1:A:16:GLN:CD	0.51	2.63	29	30
1:A:5:ASP:OD1	1:A:5:ASP:N	0.51	2.43	23	5
1:A:12:GLU:O	1:A:15:ALA:N	0.51	2.42	13	23
1:A:15:ALA:HB3	1:A:16:GLN:HE21	0.51	1.62	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:ASP:OD2	1:A:7:TYR:N	0.50	2.44	2	3
1:A:5:ASP:CG	1:A:7:TYR:CE1	0.50	2.85	24	1
1:A:8:ILE:HD12	1:A:8:ILE:N	0.50	2.21	20	2
1:A:8:ILE:HG23	1:A:12:GLU:HB3	0.50	1.83	20	4
1:A:9:SER:N	1:A:12:GLU:OE1	0.49	2.44	21	4
1:A:1:ASP:OD2	1:A:6:GLY:N	0.49	2.45	8	7
1:A:7:TYR:CD1	1:A:7:TYR:N	0.49	2.81	15	1
1:A:15:ALA:CB	1:A:16:GLN:NE2	0.48	2.73	27	9
1:A:5:ASP:OD1	1:A:7:TYR:N	0.47	2.47	4	3
1:A:1:ASP:OD2	1:A:5:ASP:OD1	0.47	2.32	29	16
1:A:2:LYS:HB2	1:A:16:GLN:NE2	0.47	2.25	12	12
1:A:1:ASP:OD2	1:A:5:ASP:OD2	0.47	2.33	9	2
1:A:2:LYS:CG	1:A:2:LYS:O	0.46	2.64	12	2
1:A:3:ASP:CB	1:A:5:ASP:OD2	0.45	2.65	13	1
1:A:8:ILE:CG2	1:A:13:ALA:HA	0.45	2.37	1	3
1:A:6:GLY:O	1:A:7:TYR:CD1	0.44	2.70	19	1
1:A:5:ASP:OD2	1:A:7:TYR:CZ	0.44	2.71	24	1
1:A:12:GLU:O	1:A:13:ALA:C	0.44	2.56	27	9
1:A:2:LYS:CB	1:A:16:GLN:NE2	0.43	2.81	12	1
1:A:13:ALA:O	1:A:14:ALA:C	0.43	2.57	25	6
1:A:8:ILE:HG22	1:A:13:ALA:HB2	0.43	1.90	14	1
1:A:5:ASP:OD2	1:A:7:TYR:CE1	0.43	2.72	24	1
1:A:2:LYS:O	1:A:2:LYS:HG2	0.43	2.14	1	1
1:A:1:ASP:OD2	1:A:4:GLY:CA	0.42	2.68	23	1
1:A:15:ALA:HB3	1:A:16:GLN:HE22	0.42	1.71	28	1
1:A:8:ILE:HA	1:A:12:GLU:OE1	0.42	2.15	27	11
1:A:13:ALA:O	1:A:16:GLN:O	0.42	2.37	20	1
1:A:1:ASP:OD2	1:A:7:TYR:O	0.41	2.38	14	2
1:A:8:ILE:CG1	1:A:16:GLN:HG3	0.41	2.45	28	1
1:A:6:GLY:C	1:A:7:TYR:CD1	0.41	2.94	1	1
1:A:8:ILE:CG2	1:A:13:ALA:HB2	0.41	2.45	14	1
1:A:12:GLU:O	1:A:16:GLN:HG2	0.40	2.16	14	2

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	16/18 (89%)	14±1 (87±6%)	2±1 (12±7%)	0±0 (1±2%)	20	68
All	All	480/540 (89%)	419 (87%)	56 (12%)	5 (1%)	20	68

All 2 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	10	ALA	3
1	A	4	GLY	2

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	9/9 (100%)	8±1 (90±9%)	1±1 (10±9%)	12	58
All	All	270/270 (100%)	244 (90%)	26 (10%)	12	58

All 3 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	2	LYS	12
1	A	3	ASP	9
1	A	5	ASP	5

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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided