Full wwPDB NMR Structure Validation Report (i)

Feb 8, 2022 – 05:06 PM EST

PDB ID	:	1CFC
Title	:	CALCIUM-FREE CALMODULIN
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Deposited on	:	1995-08-02

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 (i)) were used in the production of this report:

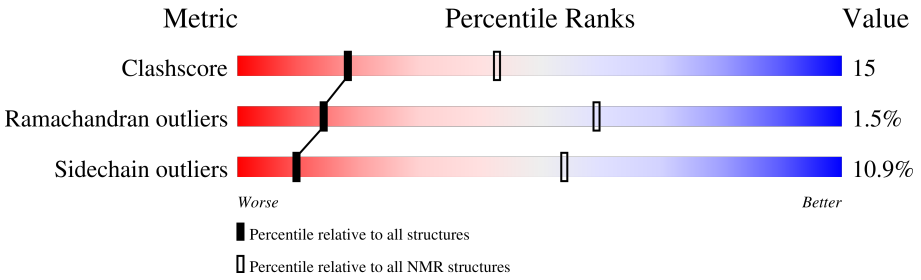
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 (#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	148	59% 14% • 24%

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 1 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 model**
1	A:8-A:50, A:61-A:73 (56)	0.14	2
2	A:82-A:93, A:99-A:130, A:134-A:146 (57)	0.23	1

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 and 3 single-model clusters were found.

Cluster number	Models
1	4, 5, 6, 11, 12, 20, 23, 25
2	2, 8, 16, 17, 19, 22, 24
3	1, 3, 9, 15, 21
4	10, 13
Single-model clusters	7; 14; 18

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2262 atoms, of which 1096 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CALMODULIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	148	2262	714	1096	188	255	9	0

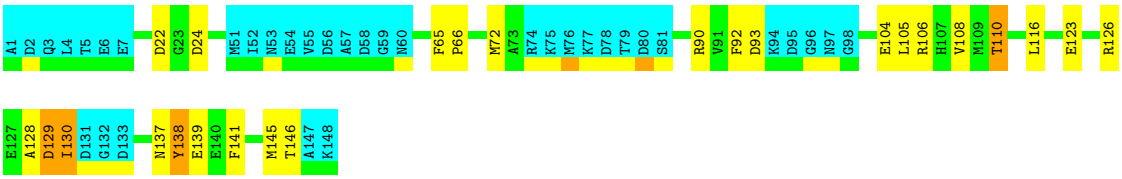
4 Residue-property plots (i)

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: CALMODULIN

Chain A: 59% 14% • 24%



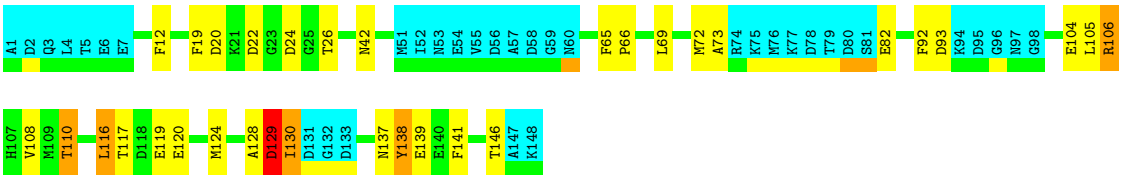
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: CALMODULIN

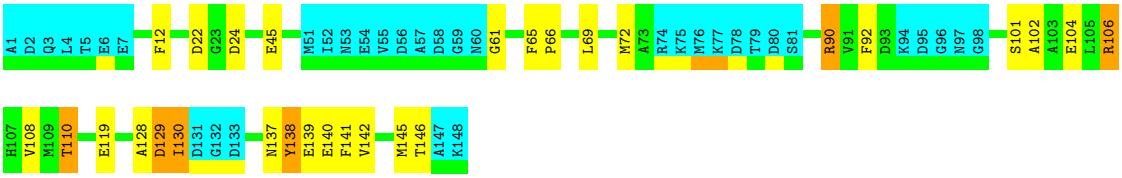
Chain A: 54% 18% • • 24%



4.2.2 Score per residue for model 2

• Molecule 1: CALMODULIN

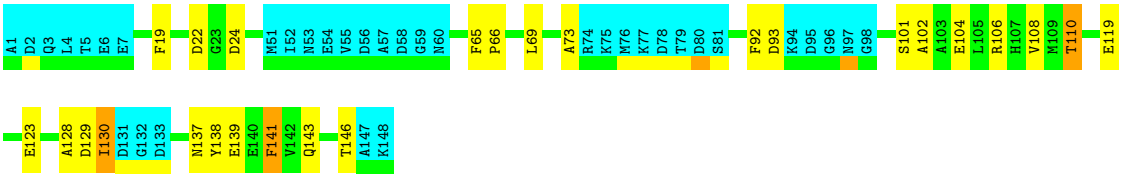
Chain A: 57% 16% • 24%



4.2.3 Score per residue for model 3

- Molecule 1: CALMODULIN

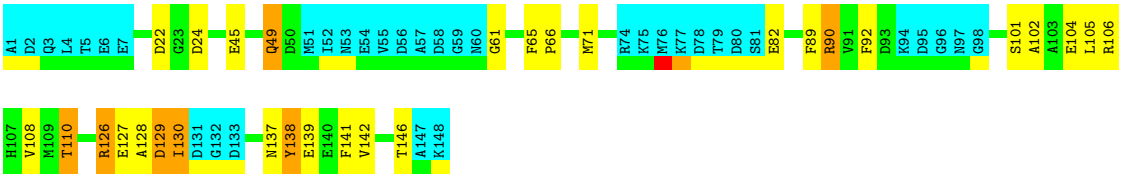
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: CALMODULIN

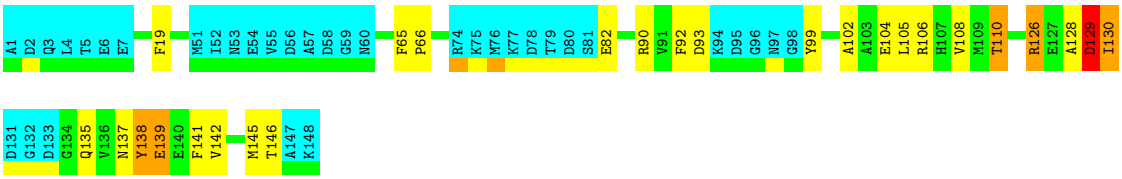
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: CALMODULIN

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: CALMODULIN

Chain A: 53% 18% 5% 24%

A1 D2 Q3 L4 T5 E6 E7 Q8 F12 D22 G23 D24 D50 M51 I52 N53 E54 V55 D56 A57 D58 G59 N60 F65 P66 M71 R74 K75 M76 K77 D78 T79 D80 S81 E82 E83 R86 E87 R90 V91 F92 D93 K94 D95 G96 N97 G98 E104 L105 R106 H107

V108 M109 T110 N111 E114 K115 E123 R126 E127 A128 D129 I130 D131 G132 D133 N137 Y138 E139 E140 F141 V142 Q143 M144 M145 T146 A147 K148

4.2.7 Score per residue for model 7

- Molecule 1: CALMODULIN

Chain A: 57% 16% • 24%

A1 D2 Q3 L4 T5 E6 E7 F12 F19 D22 G23 D24 E45 M51 I52 N53 E54 V55 D56 A57 D58 G59 N60 G61 F65 P66 R74 K75 M76 K77 D78 T79 D80 S81 R90 V91 F92 D93 K94 D95 G96 N97 G98 E104 L105 R106 H107 V108 M109 T110

E119 E123 R126 E127 A128 D129 I130 D131 G132 D133 N137 Y138 E139 E140 F141 V142 A147 K148

4.2.8 Score per residue for model 8

- Molecule 1: CALMODULIN

Chain A: 53% 21% •• 24%

A1 D2 Q3 L4 T5 E6 E7 D22 G23 D24 M51 I52 N53 E54 V55 D56 A57 D58 G59 N60 D64 F65 P66 L69 T70 M71 R74 K75 M76 K77 D78 T79 D80 S81 R86 E87 R90 V91 F92 D93 K94 D95 G96 N97 G98 S101 A102 A103 E104 L105 R106 H107

V108 M109 T110 K115 E123 R126 E127 A128 D129 I130 D131 G132 D133 G134 N137 Y138 E139 E140 F141 V142 M145 T146 A147 K148

4.2.9 Score per residue for model 9

- Molecule 1: CALMODULIN

Chain A: 55% 18% • 24%

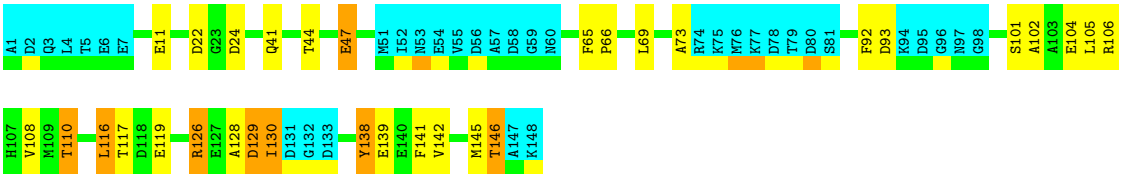
A1 D2 Q3 L4 T5 E6 E7 K13 F19 D22 G23 D24 N42 M51 I52 N53 E54 V55 D56 A57 D58 G59 N60 G61 D64 F65 P66 A73 R74 K75 M76 K77 D78 T79 D80 S81 R90 V91 F92 D93 K94 D95 G96 N97 G98 Y99 E104 L105 R106 H107 V108

M109 T110 D118 D122 E123 R126 E127 A128 D129 I130 D131 G132 D133 Y138 E139 E140 F141 V142 T146 A147 K148

4.2.10 Score per residue for model 10

- Molecule 1: CALMODULIN

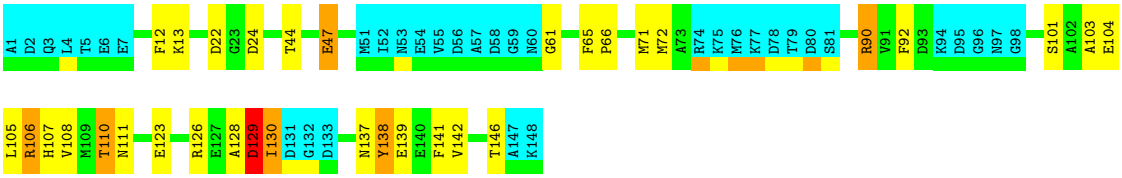
Chain A: 55% 16% 5% 24%



4.2.11 Score per residue for model 11

- Molecule 1: CALMODULIN

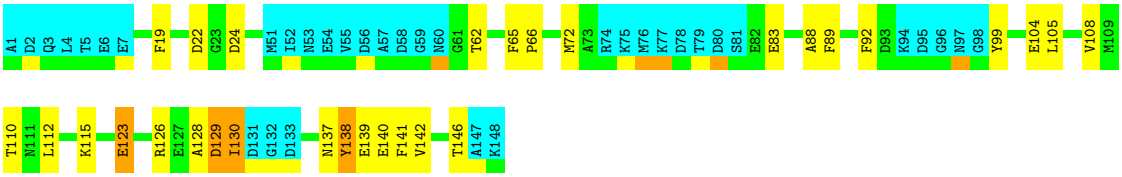
Chain A: 54% 18% • • 24%



4.2.12 Score per residue for model 12

- Molecule 1: CALMODULIN

Chain A: 56% 18% • 24%



4.2.13 Score per residue for model 13

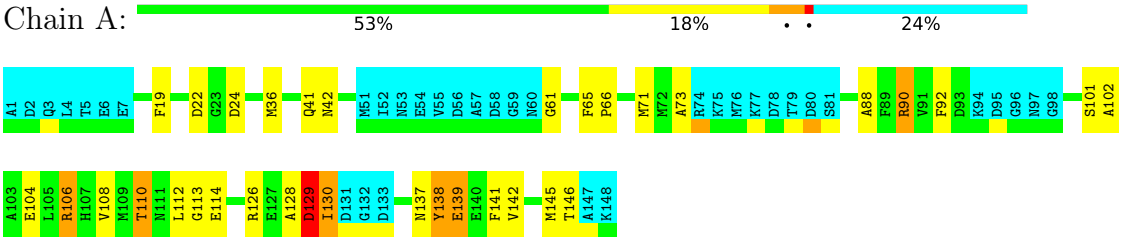
- Molecule 1: CALMODULIN

Chain A: 53% 17% 5% • 24%

4.2.14 Score per residue for model 14

- Molecule 1: CALMODULIN

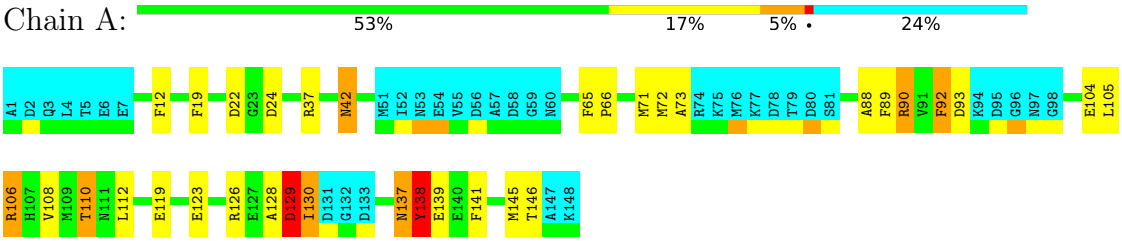
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: CALMODULIN

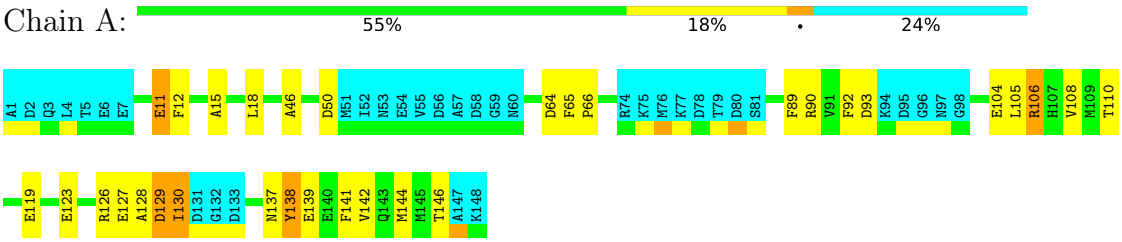
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: CALMODULIN

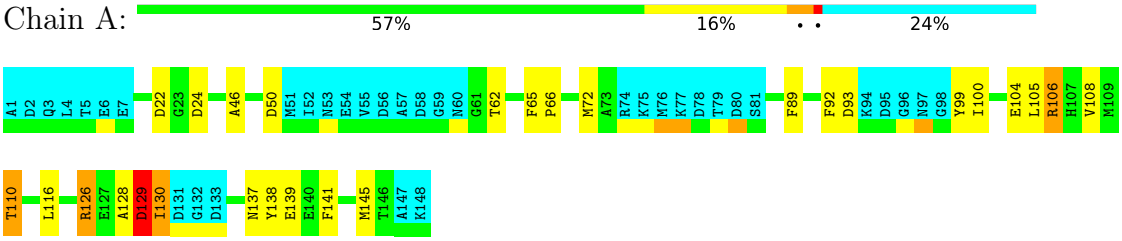
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: CALMODULIN

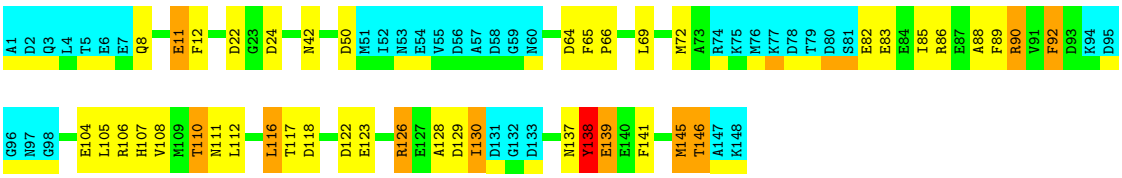
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: CALMODULIN

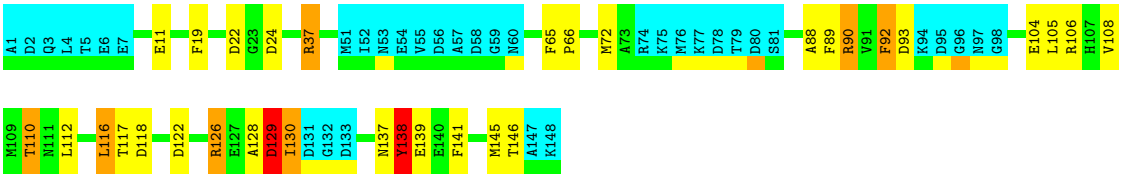
Chain A: 47% 22% 7% • 24%



4.2.19 Score per residue for model 19

- Molecule 1: CALMODULIN

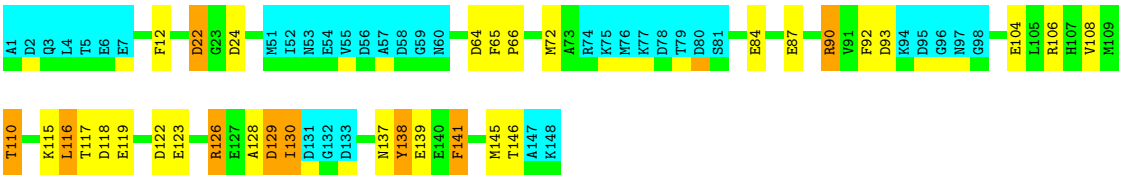
Chain A: 54% 16% 5% • 24%



4.2.20 Score per residue for model 20

- Molecule 1: CALMODULIN

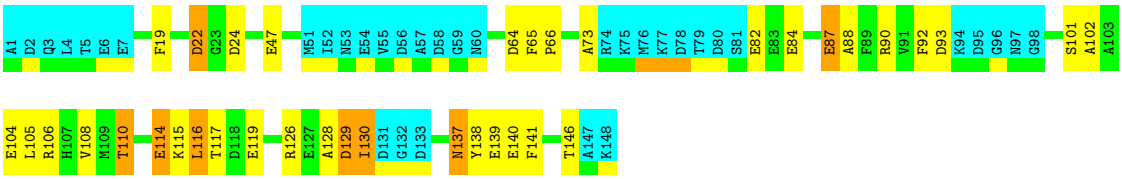
Chain A: 54% 16% 6% 24%



4.2.21 Score per residue for model 21

- Molecule 1: CALMODULIN

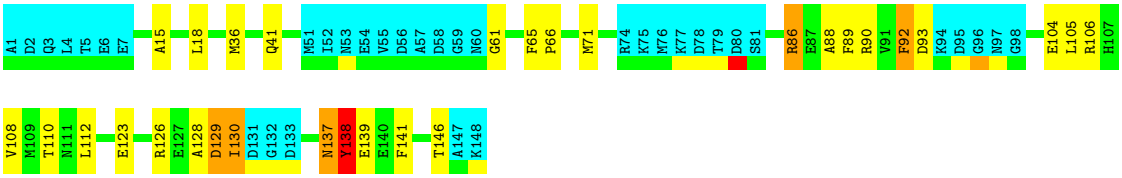
Chain A: 51% 20% 5% 24%



4.2.22 Score per residue for model 22

- Molecule 1: CALMODULIN

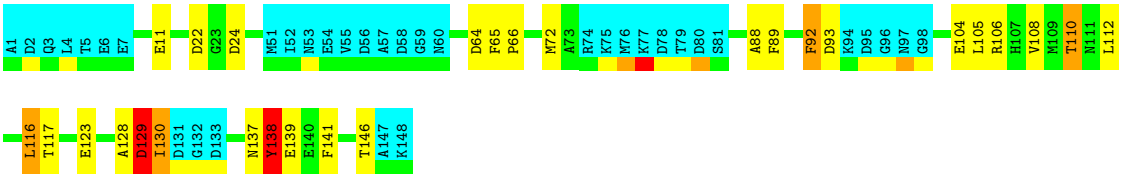
Chain A: 56% 16% • • 24%



4.2.23 Score per residue for model 23

- Molecule 1: CALMODULIN

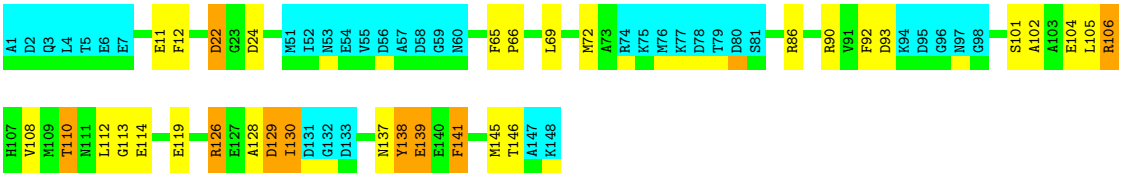
Chain A: 57% 15% • • 24%



4.2.24 Score per residue for model 24

- Molecule 1: CALMODULIN

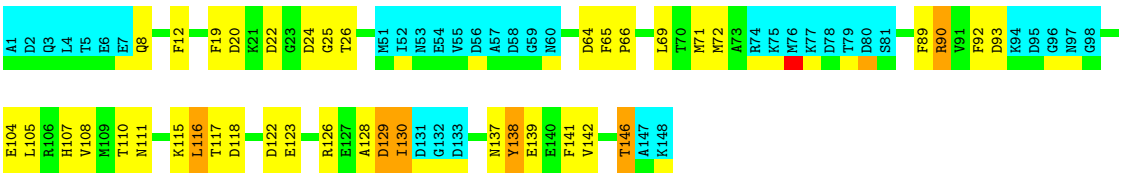
Chain A: 54% 16% 6% 24%



4.2.25 Score per residue for model 25

- Molecule 1: CALMODULIN

Chain A: 49% 23% • 24%



5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 25 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1

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	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.16±0.01	0±0/917 (0.0± 0.0%)	0.88±0.01	0±1/1235 (0.0± 0.0%)
All	All	1.16	0/22925 (0.0%)	0.88	8/30875 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	138	TYR	CB-CG-CD2	-6.05	117.37	121.00	13	2
1	A	92	PHE	CB-CG-CD1	-5.79	116.75	120.80	19	6

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	904	858	858	26±5
All	All	22600	21450	21450	647

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:PHE:CD1	1:A:108:VAL:HG22	0.86	2.05	24	18
1:A:92:PHE:CD2	1:A:108:VAL:HG22	0.85	2.06	4	7
1:A:112:LEU:O	1:A:114:GLU:N	0.77	2.18	14	2
1:A:128:ALA:O	1:A:130:ILE:N	0.74	2.21	6	25
1:A:92:PHE:CG	1:A:108:VAL:HG22	0.73	2.18	3	21
1:A:116:LEU:HD12	1:A:116:LEU:C	0.73	2.05	19	8
1:A:116:LEU:HD12	1:A:117:THR:N	0.72	2.00	21	8
1:A:104:GLU:O	1:A:108:VAL:HG23	0.72	1.84	1	25
1:A:137:ASN:ND2	1:A:137:ASN:H	0.63	1.92	21	1
1:A:137:ASN:ND2	1:A:139:GLU:H	0.60	1.93	25	1
1:A:12:PHE:CG	1:A:72:MET:SD	0.59	2.95	15	2
1:A:138:TYR:CD1	1:A:138:TYR:N	0.59	2.69	24	18
1:A:138:TYR:CD1	1:A:139:GLU:N	0.58	2.72	19	6
1:A:12:PHE:CD2	1:A:72:MET:SD	0.58	2.97	1	5
1:A:137:ASN:O	1:A:139:GLU:N	0.57	2.38	19	8
1:A:99:TYR:CE1	1:A:137:ASN:ND2	0.56	2.73	13	1
1:A:137:ASN:HD21	1:A:139:GLU:H	0.56	1.43	25	1
1:A:65:PHE:CZ	1:A:69:LEU:HD21	0.55	2.36	25	8
1:A:36:MET:SD	1:A:41:GLN:NE2	0.55	2.79	14	1
1:A:93:ASP:OD2	1:A:99:TYR:N	0.55	2.40	5	2
1:A:49:GLN:NE2	1:A:49:GLN:N	0.54	2.54	4	1
1:A:37:ARG:CZ	1:A:42:ASN:ND2	0.54	2.71	13	2
1:A:137:ASN:ND2	1:A:139:GLU:N	0.54	2.55	25	1
1:A:126:ARG:CG	1:A:126:ARG:HH11	0.54	2.16	25	20
1:A:106:ARG:NH1	1:A:106:ARG:CG	0.54	2.71	16	2
1:A:137:ASN:OD1	1:A:139:GLU:N	0.53	2.41	20	2
1:A:92:PHE:CG	1:A:108:VAL:CG2	0.53	2.92	17	25
1:A:90:ARG:NH1	1:A:90:ARG:CG	0.53	2.71	13	11
1:A:90:ARG:CG	1:A:90:ARG:HH11	0.53	2.16	18	13
1:A:126:ARG:NH1	1:A:126:ARG:CG	0.53	2.72	8	17
1:A:106:ARG:CG	1:A:106:ARG:HH11	0.53	2.16	24	4
1:A:86:ARG:NH1	1:A:86:ARG:CG	0.53	2.72	22	4
1:A:138:TYR:CD2	1:A:139:GLU:OE2	0.53	2.61	25	2
1:A:37:ARG:NH1	1:A:37:ARG:CG	0.53	2.72	13	2
1:A:90:ARG:CG	1:A:90:ARG:NH1	0.53	2.71	18	3
1:A:89:PHE:CG	1:A:108:VAL:HG11	0.53	2.39	13	6
1:A:107:HIS:NE2	1:A:111:ASN:OD1	0.53	2.41	13	3
1:A:12:PHE:CD1	1:A:72:MET:SD	0.52	3.02	1	2
1:A:126:ARG:CG	1:A:126:ARG:NH1	0.52	2.71	25	4
1:A:135:GLN:H	1:A:135:GLN:CD	0.52	2.05	5	1
1:A:137:ASN:O	1:A:137:ASN:ND2	0.52	2.42	22	1
1:A:87:GLU:OE2	1:A:88:ALA:N	0.52	2.42	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:PHE:CE2	1:A:72:MET:SD	0.52	3.02	20	4
1:A:137:ASN:ND2	1:A:138:TYR:H	0.52	2.02	17	3
1:A:107:HIS:CD2	1:A:111:ASN:OD1	0.52	2.62	11	2
1:A:106:ARG:CG	1:A:106:ARG:NH1	0.51	2.71	24	2
1:A:116:LEU:C	1:A:116:LEU:CD1	0.51	2.76	21	8
1:A:120:GLU:O	1:A:124:MET:SD	0.51	2.69	1	1
1:A:86:ARG:CG	1:A:86:ARG:HH11	0.51	2.17	22	3
1:A:138:TYR:CE2	1:A:139:GLU:OE2	0.51	2.63	16	1
1:A:129:ASP:N	1:A:129:ASP:OD1	0.51	2.42	10	4
1:A:88:ALA:HB2	1:A:112:LEU:HD21	0.51	1.82	15	7
1:A:49:GLN:N	1:A:49:GLN:CD	0.51	2.64	4	1
1:A:137:ASN:CG	1:A:138:TYR:N	0.50	2.64	25	11
1:A:20:ASP:OD2	1:A:26:THR:N	0.50	2.45	25	2
1:A:37:ARG:CG	1:A:37:ARG:HH11	0.50	2.18	13	2
1:A:36:MET:SD	1:A:41:GLN:OE1	0.50	2.70	22	1
1:A:106:ARG:O	1:A:110:THR:OG1	0.50	2.30	18	20
1:A:102:ALA:HB1	1:A:106:ARG:HH12	0.50	1.66	5	1
1:A:114:GLU:CG	1:A:115:LYS:N	0.50	2.74	21	1
1:A:89:PHE:CD1	1:A:108:VAL:HG11	0.49	2.42	13	5
1:A:139:GLU:N	1:A:139:GLU:OE1	0.49	2.45	24	1
1:A:22:ASP:O	1:A:24:ASP:N	0.49	2.46	3	15
1:A:116:LEU:CD1	1:A:145:MET:SD	0.49	3.01	17	1
1:A:115:LYS:CB	1:A:115:LYS:NZ	0.49	2.75	6	1
1:A:22:ASP:C	1:A:24:ASP:N	0.49	2.66	9	21
1:A:138:TYR:O	1:A:142:VAL:HG23	0.48	2.08	9	12
1:A:19:PHE:N	1:A:19:PHE:CD1	0.48	2.81	1	2
1:A:135:GLN:CD	1:A:135:GLN:N	0.48	2.67	5	1
1:A:11:GLU:CG	1:A:12:PHE:N	0.48	2.75	16	1
1:A:19:PHE:CD1	1:A:19:PHE:N	0.48	2.81	5	10
1:A:119:GLU:N	1:A:119:GLU:CD	0.48	2.67	13	6
1:A:129:ASP:OD1	1:A:129:ASP:N	0.48	2.46	8	1
1:A:119:GLU:N	1:A:119:GLU:OE1	0.48	2.46	16	1
1:A:139:GLU:CG	1:A:140:GLU:N	0.47	2.77	7	4
1:A:130:ILE:CG2	1:A:130:ILE:O	0.47	2.63	5	10
1:A:130:ILE:O	1:A:130:ILE:CG2	0.47	2.63	12	12
1:A:127:GLU:OE1	1:A:127:GLU:N	0.47	2.48	4	1
1:A:12:PHE:CD1	1:A:12:PHE:N	0.46	2.83	7	2
1:A:45:GLU:H	1:A:45:GLU:CD	0.46	2.13	2	2
1:A:44:THR:HG1	1:A:47:GLU:CD	0.45	2.13	11	2
1:A:89:PHE:CD1	1:A:108:VAL:HG21	0.45	2.46	16	4
1:A:107:HIS:NE2	1:A:111:ASN:CG	0.45	2.70	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:ARG:NH2	1:A:42:ASN:ND2	0.45	2.64	15	1
1:A:22:ASP:N	1:A:22:ASP:OD1	0.45	2.50	24	2
1:A:119:GLU:N	1:A:119:GLU:OE2	0.45	2.49	15	2
1:A:138:TYR:O	1:A:139:GLU:C	0.45	2.55	24	18
1:A:89:PHE:CE1	1:A:105:LEU:HD12	0.45	2.47	4	1
1:A:137:ASN:O	1:A:137:ASN:OD1	0.45	2.34	15	2
1:A:143:GLN:O	1:A:146:THR:OG1	0.45	2.34	6	2
1:A:12:PHE:CE1	1:A:72:MET:SD	0.45	3.10	1	1
1:A:128:ALA:O	1:A:129:ASP:C	0.44	2.56	8	17
1:A:101:SER:OG	1:A:104:GLU:OE1	0.44	2.34	3	1
1:A:45:GLU:O	1:A:49:GLN:OE1	0.44	2.35	4	1
1:A:89:PHE:O	1:A:93:ASP:N	0.44	2.51	23	1
1:A:49:GLN:NE2	1:A:49:GLN:CA	0.44	2.80	4	1
1:A:93:ASP:O	1:A:93:ASP:OD1	0.44	2.35	5	1
1:A:138:TYR:O	1:A:141:PHE:N	0.44	2.51	3	4
1:A:114:GLU:OE1	1:A:145:MET:CE	0.44	2.66	6	1
1:A:86:ARG:CG	1:A:87:GLU:N	0.44	2.80	8	1
1:A:118:ASP:O	1:A:122:ASP:OD1	0.44	2.36	20	5
1:A:88:ALA:CB	1:A:112:LEU:HD11	0.44	2.43	14	1
1:A:15:ALA:HA	1:A:18:LEU:HD12	0.44	1.90	22	2
1:A:90:ARG:C	1:A:92:PHE:N	0.43	2.71	21	11
1:A:137:ASN:OD1	1:A:137:ASN:N	0.43	2.45	4	1
1:A:123:GLU:OE1	1:A:123:GLU:N	0.43	2.51	12	1
1:A:84:GLU:O	1:A:87:GLU:OE2	0.43	2.35	21	2
1:A:65:PHE:N	1:A:66:PRO:HD2	0.43	2.28	8	24
1:A:111:ASN:OD1	1:A:111:ASN:O	0.43	2.36	6	1
1:A:24:ASP:O	1:A:24:ASP:OD1	0.43	2.36	12	1
1:A:44:THR:OG1	1:A:47:GLU:OE2	0.43	2.35	10	2
1:A:12:PHE:CZ	1:A:72:MET:SD	0.43	3.12	1	1
1:A:20:ASP:OD2	1:A:25:GLY:CA	0.43	2.67	25	1
1:A:8:GLN:O	1:A:12:PHE:CD2	0.43	2.72	25	2
1:A:46:ALA:O	1:A:50:ASP:OD1	0.43	2.37	17	1
1:A:93:ASP:OD2	1:A:99:TYR:O	0.42	2.37	5	1
1:A:137:ASN:C	1:A:139:GLU:N	0.42	2.72	19	3
1:A:137:ASN:OD1	1:A:138:TYR:N	0.42	2.52	20	1
1:A:20:ASP:O	1:A:20:ASP:OD1	0.42	2.36	1	2
1:A:137:ASN:CG	1:A:138:TYR:H	0.42	2.18	2	2
1:A:137:ASN:OD1	1:A:139:GLU:OE1	0.42	2.37	25	1
1:A:101:SER:O	1:A:102:ALA:C	0.42	2.58	3	8
1:A:83:GLU:OE1	1:A:83:GLU:N	0.42	2.53	12	1
1:A:128:ALA:O	1:A:130:ILE:CG1	0.41	2.68	24	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:GLU:O	1:A:139:GLU:OE1	0.41	2.38	18	1
1:A:126:ARG:CG	1:A:127:GLU:N	0.41	2.83	16	1
1:A:64:ASP:OD1	1:A:64:ASP:C	0.41	2.59	18	6
1:A:101:SER:O	1:A:103:ALA:N	0.41	2.54	8	2
1:A:128:ALA:O	1:A:130:ILE:HG13	0.41	2.16	11	1
1:A:99:TYR:CD1	1:A:137:ASN:ND2	0.41	2.89	13	1
1:A:92:PHE:O	1:A:100:ILE:CG2	0.41	2.69	17	1
1:A:139:GLU:H	1:A:139:GLU:CD	0.41	2.19	25	1
1:A:65:PHE:N	1:A:66:PRO:CD	0.41	2.83	21	3
1:A:11:GLU:O	1:A:11:GLU:OE1	0.41	2.39	18	1
1:A:137:ASN:O	1:A:137:ASN:CG	0.41	2.59	22	1
1:A:139:GLU:N	1:A:139:GLU:CD	0.41	2.74	25	1
1:A:64:ASP:C	1:A:64:ASP:OD1	0.41	2.59	13	3
1:A:118:ASP:OD1	1:A:118:ASP:N	0.40	2.54	13	1
1:A:83:GLU:O	1:A:87:GLU:OE1	0.40	2.39	6	1
1:A:46:ALA:O	1:A:50:ASP:OD2	0.40	2.39	16	1
1:A:107:HIS:CD2	1:A:111:ASN:ND2	0.40	2.89	25	1
1:A:119:GLU:CD	1:A:119:GLU:H	0.40	2.20	10	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	113/148 (76%)	104±2 (92±1%)	7±2 (6±1%)	2±1 (2±1%)	14	59
All	All	2825/3700 (76%)	2601 (92%)	181 (6%)	43 (2%)	14	59

All 5 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	129	ASP	25
1	A	138	TYR	8
1	A	61	GLY	7
1	A	113	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	A	134	GLY	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	Analysed	Rotameric	Outliers	Percentiles
1	A	98/126 (78%)	87±2 (89±2%)	11±2 (11±2%)	10 54
All	All	2450/3150 (78%)	2184 (89%)	266 (11%)	10 54

All 29 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	110	THR	25
1	A	141	PHE	25
1	A	130	ILE	24
1	A	146	THR	21
1	A	105	LEU	20
1	A	138	TYR	20
1	A	129	ASP	15
1	A	123	GLU	15
1	A	106	ARG	14
1	A	90	ARG	11
1	A	145	MET	9
1	A	126	ARG	9
1	A	116	LEU	8
1	A	71	MET	8
1	A	137	ASN	6
1	A	11	GLU	6
1	A	42	ASN	5
1	A	139	GLU	5
1	A	13	LYS	3
1	A	86	ARG	3
1	A	22	ASP	3
1	A	82	GLU	2
1	A	47	GLU	2
1	A	37	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	49	GLN	1
1	A	119	GLU	1
1	A	115	LYS	1
1	A	87	GLU	1
1	A	114	GLU	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