



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:32 pm BST

PDB ID : 2M5E
Title : Structure of the C-domain of Calcium-saturated Calmodulin bound to the IQ motif of NaV1.2
Authors : Fowler, C.A.; Feldkamp, M.D.; Yu, L.; Shea, M.A.
Deposited on : 2013-02-21

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 ⓘ symbol.

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
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 : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

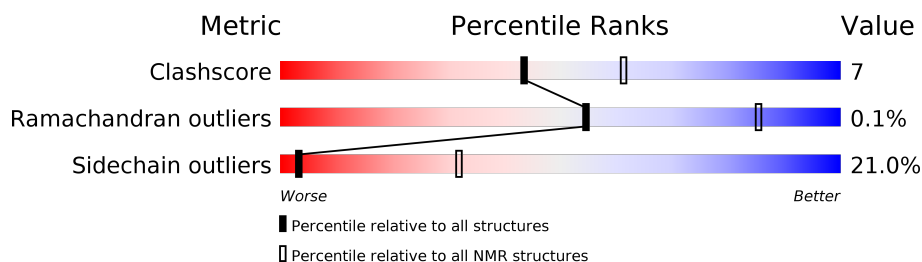
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 78%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	73	 62% 29% 10%
2	B	27	 41% 11% 48%

2 Ensemble composition and analysis

This entry contains 21 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:82-A:147, B:1907-B:1920 (80)	0.32	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 3 clusters and 3 single-model clusters were found.

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

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1643 atoms, of which 822 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms						Trace
1	A	73	Total	C	H	N	O	S	0
			1137	358	553	97	124	5	

- Molecule 2 is a protein called Sodium channel protein type 2 subunit alpha.

Mol	Chain	Residues	Atoms					Trace
2	B	27	Total	C	H	N	O	0
			504	151	269	48	36	

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

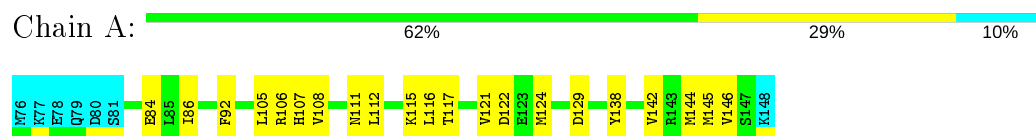
Mol	Chain	Residues	Atoms	
3	A	2	Total	Ca
			2	2

4 Residue-property plots [i](#)

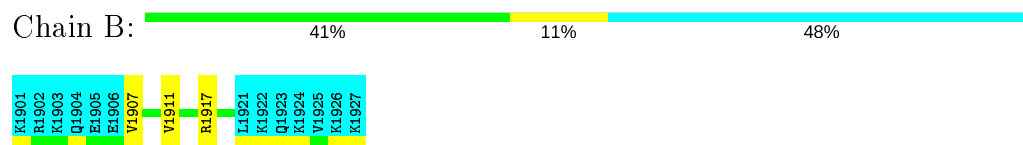
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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



- Molecule 2: Sodium channel protein type 2 subunit alpha

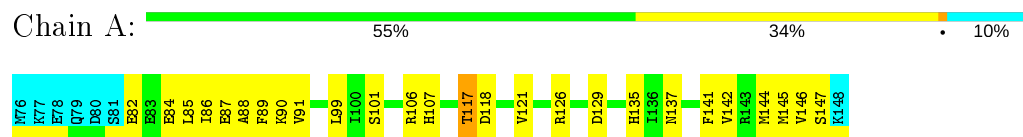


4.2 Scores per residue for each member of the ensemble

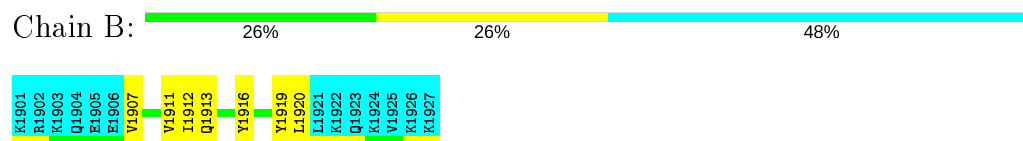
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Calmodulin

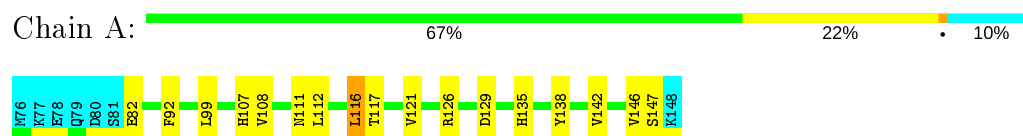


- Molecule 2: Sodium channel protein type 2 subunit alpha

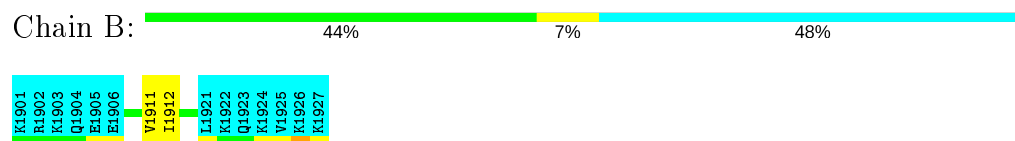


4.2.2 Score per residue for model 2

- Molecule 1: Calmodulin

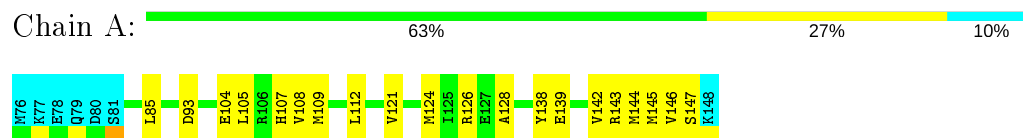


- Molecule 2: Sodium channel protein type 2 subunit alpha

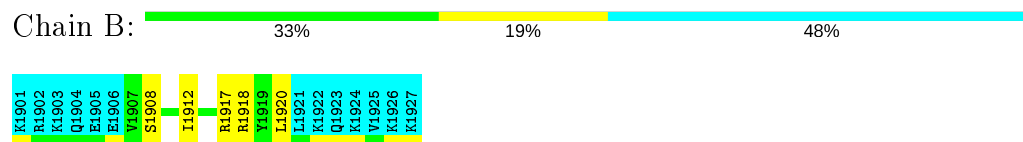


4.2.3 Score per residue for model 3

- Molecule 1: Calmodulin

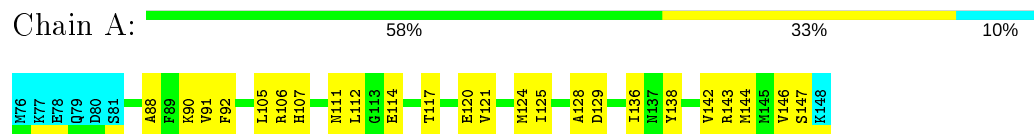


- Molecule 2: Sodium channel protein type 2 subunit alpha

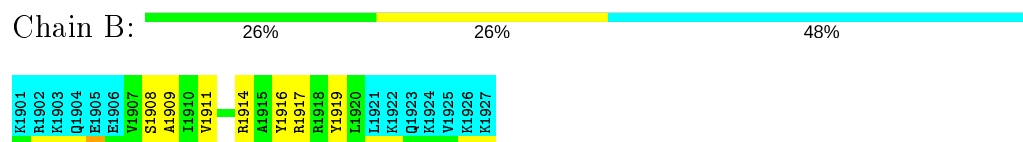


4.2.4 Score per residue for model 4

- Molecule 1: Calmodulin

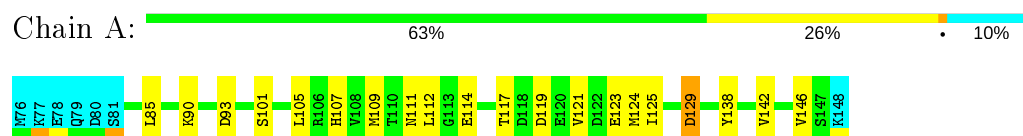


- Molecule 2: Sodium channel protein type 2 subunit alpha

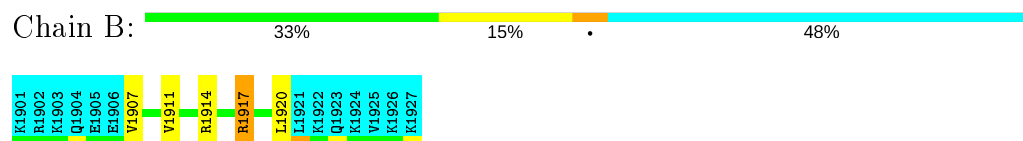


4.2.5 Score per residue for model 5

- Molecule 1: Calmodulin

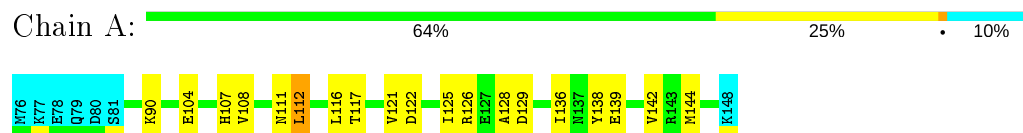


- Molecule 2: Sodium channel protein type 2 subunit alpha

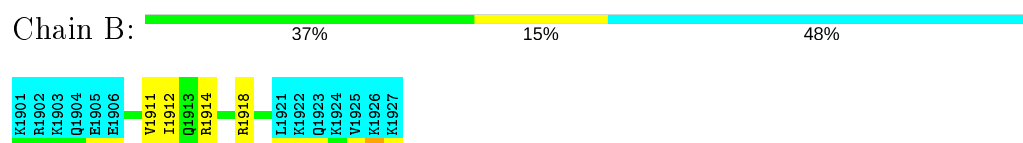


4.2.6 Score per residue for model 6

- Molecule 1: Calmodulin

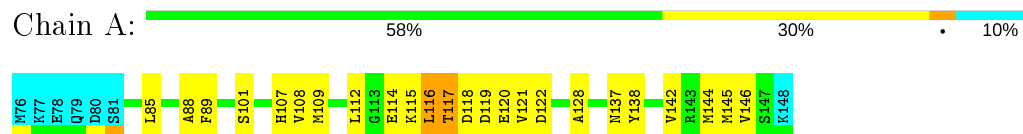


- Molecule 2: Sodium channel protein type 2 subunit alpha

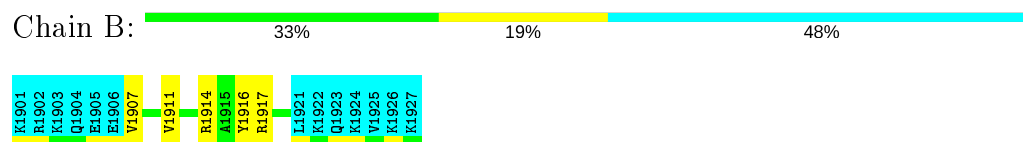


4.2.7 Score per residue for model 7

- Molecule 1: Calmodulin

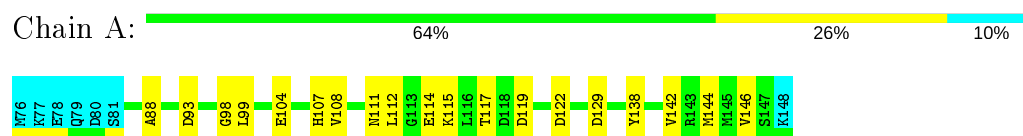


- Molecule 2: Sodium channel protein type 2 subunit alpha

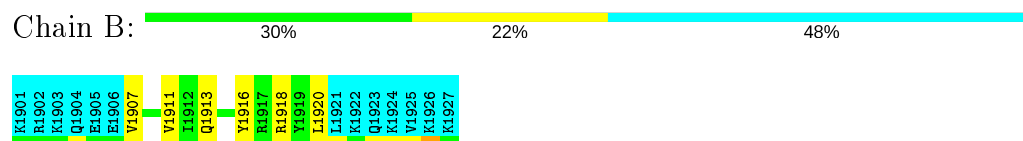


4.2.8 Score per residue for model 8

- Molecule 1: Calmodulin

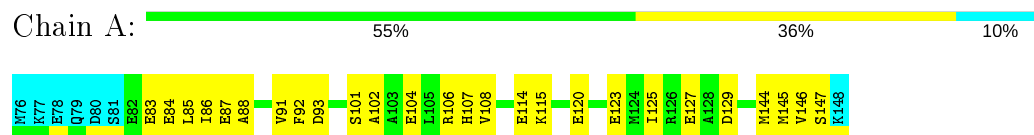


- Molecule 2: Sodium channel protein type 2 subunit alpha

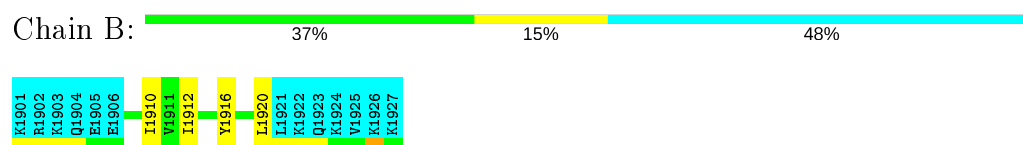


4.2.9 Score per residue for model 9

- Molecule 1: Calmodulin

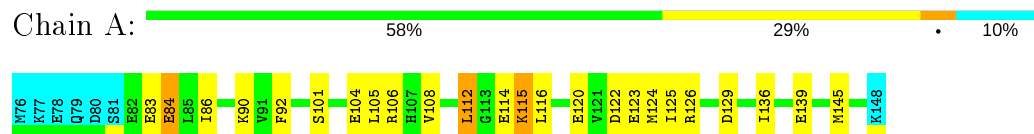


- Molecule 2: Sodium channel protein type 2 subunit alpha

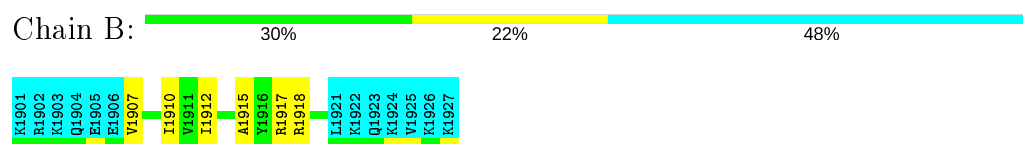


4.2.10 Score per residue for model 10

- Molecule 1: Calmodulin

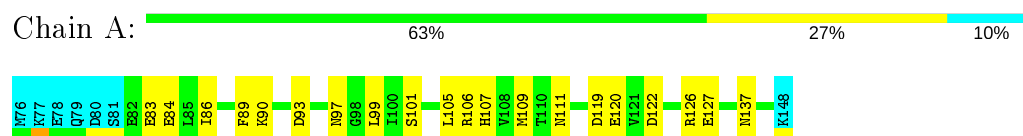


- Molecule 2: Sodium channel protein type 2 subunit alpha

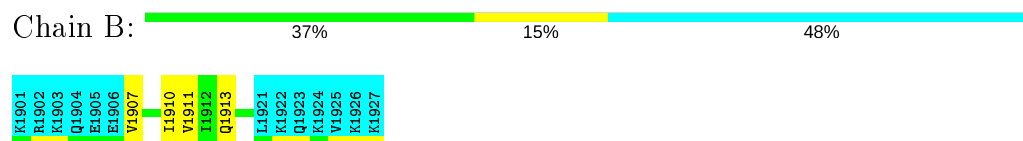


4.2.11 Score per residue for model 11

- Molecule 1: Calmodulin

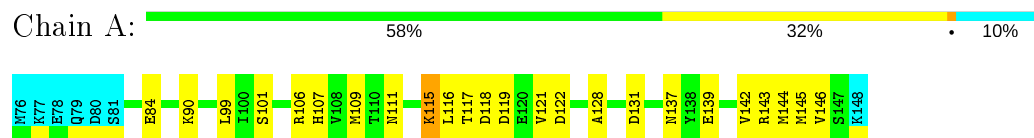


- Molecule 2: Sodium channel protein type 2 subunit alpha

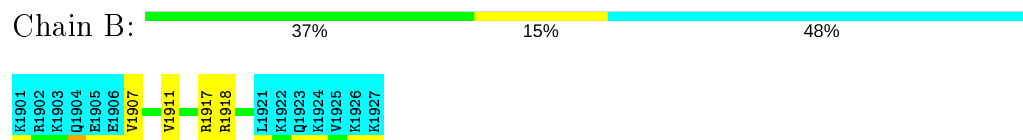


4.2.12 Score per residue for model 12

- Molecule 1: Calmodulin

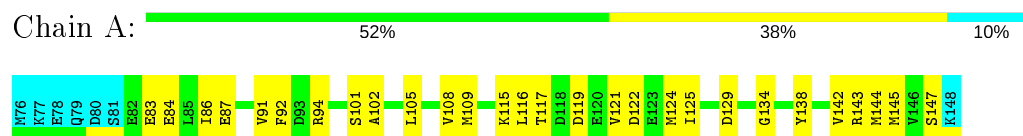


- Molecule 2: Sodium channel protein type 2 subunit alpha

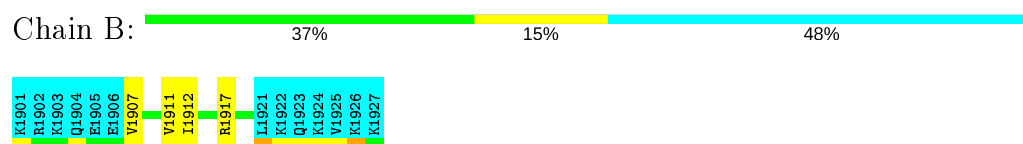


4.2.13 Score per residue for model 13

- Molecule 1: Calmodulin

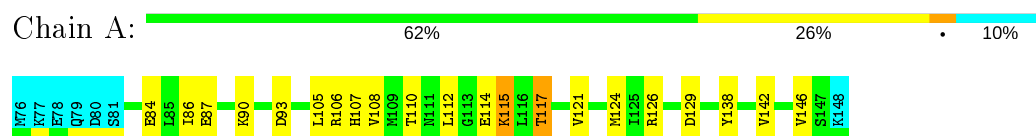


- Molecule 2: Sodium channel protein type 2 subunit alpha

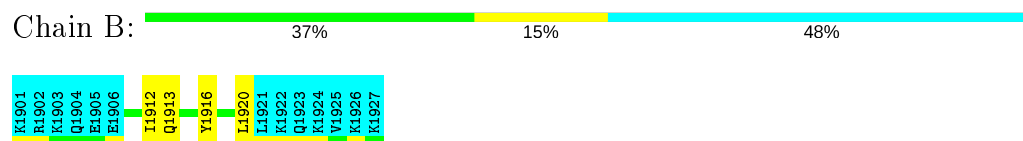


4.2.14 Score per residue for model 14

- Molecule 1: Calmodulin

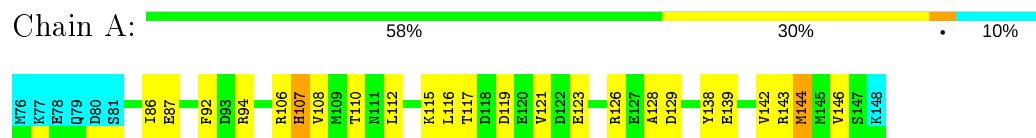


- Molecule 2: Sodium channel protein type 2 subunit alpha

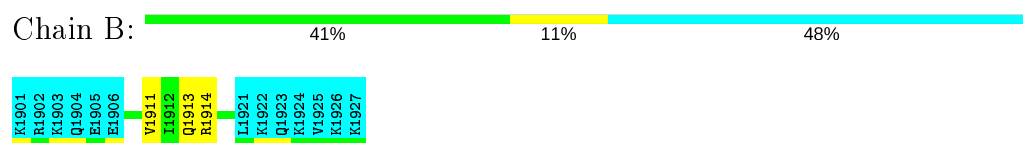


4.2.15 Score per residue for model 15

- Molecule 1: Calmodulin

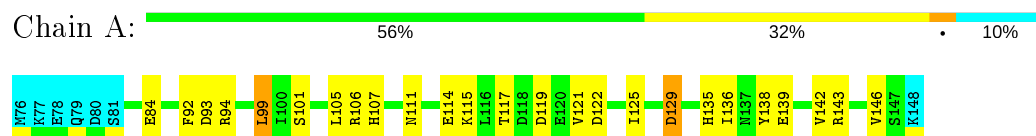


- Molecule 2: Sodium channel protein type 2 subunit alpha

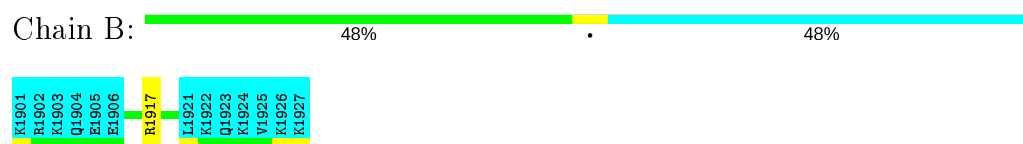


4.2.16 Score per residue for model 16

- Molecule 1: Calmodulin



- Molecule 2: Sodium channel protein type 2 subunit alpha

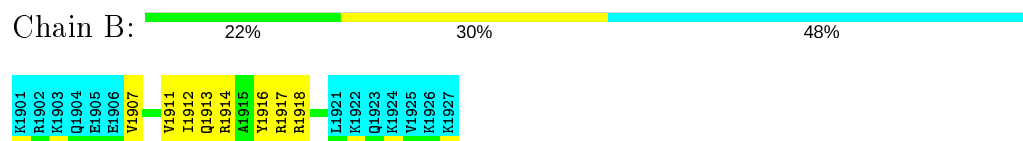


4.2.17 Score per residue for model 17

- Molecule 1: Calmodulin

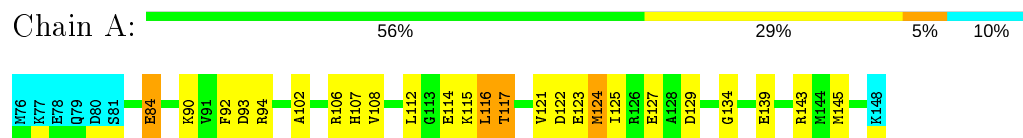


- Molecule 2: Sodium channel protein type 2 subunit alpha

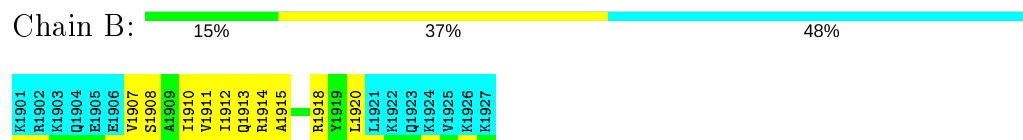


4.2.18 Score per residue for model 18

- Molecule 1: Calmodulin

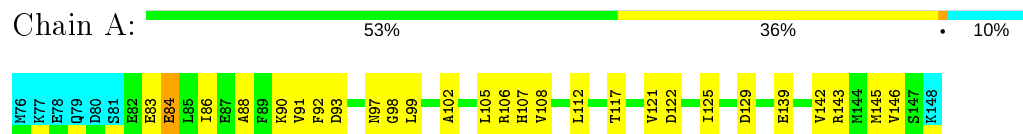


- Molecule 2: Sodium channel protein type 2 subunit alpha

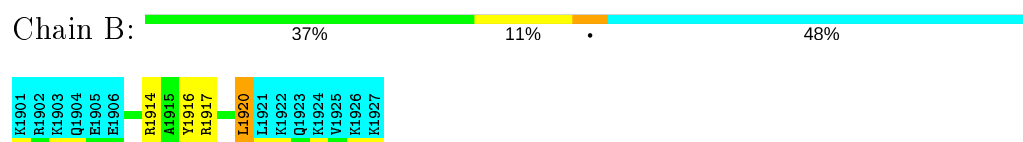


4.2.19 Score per residue for model 19

- Molecule 1: Calmodulin

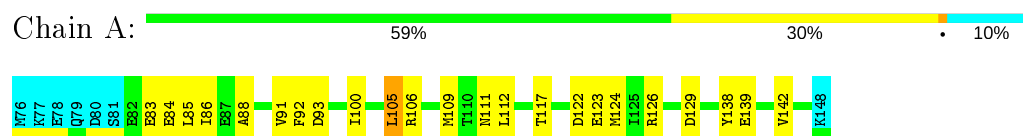


- Molecule 2: Sodium channel protein type 2 subunit alpha

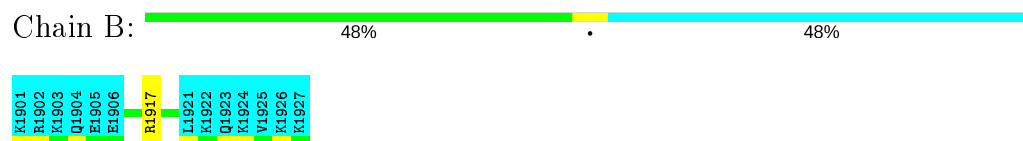


4.2.20 Score per residue for model 20

- Molecule 1: Calmodulin

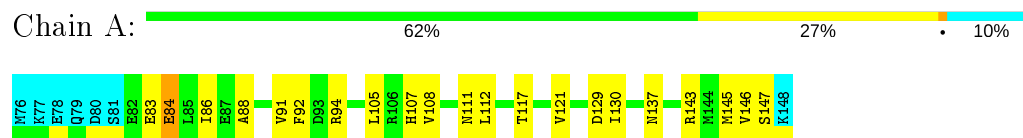


- Molecule 2: Sodium channel protein type 2 subunit alpha

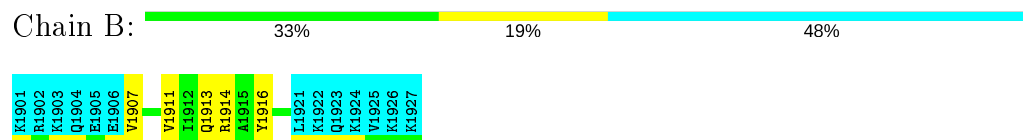


4.2.21 Score per residue for model 21

- Molecule 1: Calmodulin



- Molecule 2: Sodium channel protein type 2 subunit alpha



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 300 calculated structures, 21 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
ARIA	structure solution	2.3
CNSSOLVE	structure solution	1.21
CNSSOLVE	refinement	1.21
X-PLOR NIH	structure solution	2.23

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	2
Total number of shifts	998
Number of shifts mapped to atoms	998
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	527	496	494	8±3
2	B	120	131	131	2±1
All	All	13629	13167	13125	188

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:LEU:HD12	1:A:121:VAL:HG22	0.73	1.58	18	2
1:A:112:LEU:HD23	2:B:1915:ALA:HB1	0.73	1.59	10	1
2:B:1916:TYR:CZ	2:B:1920:LEU:HD11	0.73	2.19	14	1
1:A:138:TYR:O	1:A:142:VAL:HG23	0.72	1.84	8	13
1:A:117:THR:O	1:A:121:VAL:HG23	0.70	1.86	5	15
1:A:116:LEU:HD21	2:B:1911:VAL:HG11	0.69	1.63	15	1
1:A:142:VAL:O	1:A:146:VAL:HG23	0.69	1.88	1	1
1:A:124:MET:CG	2:B:1912:ILE:HD11	0.69	2.18	18	2
2:B:1907:VAL:O	2:B:1911:VAL:HG23	0.66	1.91	17	8
1:A:128:ALA:HB2	1:A:144:MET:SD	0.66	2.30	12	3
2:B:1907:VAL:O	2:B:1911:VAL:HG13	0.65	1.91	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:1907:VAL:HA	2:B:1910:ILE:HD12	0.64	1.70	18	3
1:A:125:ILE:HG22	1:A:129:ASP:OD2	0.64	1.92	16	3
1:A:124:MET:HG2	2:B:1912:ILE:HD11	0.64	1.69	17	2
1:A:142:VAL:O	1:A:146:VAL:HG22	0.63	1.92	4	7
1:A:125:ILE:HG21	1:A:134:GLY:O	0.63	1.93	18	2
1:A:116:LEU:CD1	1:A:121:VAL:HG22	0.62	2.24	18	3
1:A:115:LYS:C	1:A:116:LEU:HD22	0.60	2.16	12	1
1:A:108:VAL:O	1:A:112:LEU:HD13	0.60	1.95	19	3
1:A:98:GLY:O	1:A:99:LEU:HD22	0.60	1.96	19	1
1:A:125:ILE:CD1	1:A:136:ILE:HD11	0.59	2.27	4	2
1:A:124:MET:HE2	2:B:1912:ILE:HD11	0.57	1.74	10	1
1:A:108:VAL:O	1:A:112:LEU:HD23	0.57	1.98	15	1
1:A:92:PHE:CD2	1:A:100:ILE:HD13	0.57	2.34	20	1
1:A:116:LEU:N	1:A:116:LEU:HD23	0.56	2.16	7	1
1:A:105:LEU:HD22	1:A:125:ILE:CD1	0.56	2.30	5	2
1:A:83:GLU:O	1:A:86:ILE:HG22	0.56	2.01	13	7
1:A:144:MET:SD	2:B:1912:ILE:HD13	0.55	2.41	9	4
1:A:108:VAL:HG12	1:A:112:LEU:HD13	0.55	1.75	6	3
1:A:107:HIS:CD2	1:A:108:VAL:HG13	0.55	2.37	7	1
1:A:125:ILE:HD12	1:A:136:ILE:HD11	0.54	1.78	4	1
1:A:98:GLY:C	1:A:99:LEU:HD22	0.53	2.24	19	1
1:A:124:MET:CE	2:B:1912:ILE:HD11	0.53	2.33	10	1
1:A:104:GLU:O	1:A:108:VAL:HG23	0.52	2.04	9	5
1:A:91:VAL:HG21	2:B:1919:TYR:OH	0.52	2.05	1	2
1:A:102:ALA:HA	1:A:125:ILE:HD11	0.52	1.81	17	5
1:A:146:VAL:HG12	1:A:146:VAL:O	0.52	2.05	1	3
1:A:124:MET:HG3	2:B:1912:ILE:HD11	0.52	1.81	18	1
1:A:102:ALA:HB2	1:A:125:ILE:CD1	0.52	2.34	17	1
1:A:146:VAL:O	1:A:146:VAL:HG12	0.52	2.04	2	3
1:A:125:ILE:HG23	1:A:136:ILE:HD11	0.52	1.82	10	1
1:A:87:GLU:O	1:A:91:VAL:HG23	0.51	2.06	9	3
2:B:1916:TYR:CE2	2:B:1920:LEU:HD11	0.50	2.41	9	1
1:A:116:LEU:HD11	1:A:121:VAL:HG22	0.50	1.82	6	1
1:A:107:HIS:NE2	1:A:108:VAL:HG13	0.50	2.21	7	1
1:A:82:GLU:O	1:A:86:ILE:HG22	0.49	2.08	1	1
1:A:108:VAL:HG12	1:A:112:LEU:CD1	0.48	2.39	14	1
1:A:98:GLY:C	1:A:99:LEU:HD12	0.48	2.29	8	1
1:A:125:ILE:HD13	1:A:136:ILE:HD11	0.47	1.84	16	2
1:A:105:LEU:HD22	1:A:125:ILE:HD11	0.47	1.85	5	2
1:A:105:LEU:HD23	1:A:121:VAL:HG13	0.47	1.86	3	1
1:A:92:PHE:CE1	1:A:108:VAL:HG11	0.47	2.45	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:LEU:HD23	1:A:135:HIS:HB2	0.46	1.86	2	1
1:A:128:ALA:HB2	1:A:144:MET:CE	0.46	2.40	6	1
1:A:130:ILE:O	1:A:130:ILE:HG22	0.46	2.10	21	1
1:A:92:PHE:CE1	1:A:108:VAL:HG21	0.46	2.46	18	1
1:A:114:GLU:HG3	2:B:1915:ALA:HB2	0.46	1.87	18	1
1:A:105:LEU:O	1:A:105:LEU:HD13	0.46	2.11	20	1
1:A:107:HIS:CD2	1:A:108:VAL:N	0.46	2.83	19	2
1:A:107:HIS:O	1:A:110:THR:HG22	0.46	2.10	15	1
1:A:128:ALA:HB2	1:A:144:MET:HG3	0.46	1.88	7	1
1:A:85:LEU:HD23	1:A:85:LEU:N	0.46	2.25	1	1
1:A:116:LEU:HD23	1:A:116:LEU:N	0.46	2.26	2	2
1:A:98:GLY:O	1:A:99:LEU:HD12	0.46	2.11	8	1
1:A:92:PHE:CD2	1:A:108:VAL:HG11	0.45	2.46	13	1
1:A:99:LEU:HD13	1:A:135:HIS:HB3	0.45	1.88	16	1
1:A:92:PHE:CE2	1:A:108:VAL:HG21	0.45	2.47	21	1
1:A:92:PHE:HA	1:A:108:VAL:HG21	0.45	1.88	9	1
1:A:88:ALA:HB2	2:B:1916:TYR:CE1	0.44	2.47	8	7
1:A:105:LEU:HD12	1:A:136:ILE:CD1	0.44	2.43	16	1
1:A:92:PHE:HD2	1:A:100:ILE:HD13	0.44	1.72	20	1
1:A:86:ILE:HG23	1:A:87:GLU:N	0.43	2.28	15	2
1:A:92:PHE:HA	1:A:108:VAL:HG11	0.43	1.90	15	1
1:A:91:VAL:HG23	1:A:92:PHE:N	0.42	2.29	17	1
2:B:1911:VAL:HG13	2:B:1912:ILE:N	0.42	2.30	2	2
2:B:1916:TYR:CZ	2:B:1920:LEU:CD1	0.42	3.00	14	1
1:A:92:PHE:CZ	1:A:108:VAL:HG11	0.42	2.50	10	1
1:A:99:LEU:HD22	1:A:135:HIS:CB	0.42	2.45	1	1
1:A:124:MET:SD	2:B:1912:ILE:HD11	0.42	2.54	14	2
1:A:128:ALA:CB	1:A:144:MET:HE3	0.41	2.45	15	1
1:A:88:ALA:HA	1:A:91:VAL:HG12	0.41	1.92	19	3
1:A:115:LYS:C	1:A:116:LEU:HD12	0.41	2.35	10	1
2:B:1916:TYR:CE2	2:B:1920:LEU:HD13	0.41	2.50	19	1
1:A:105:LEU:HD23	1:A:109:MET:CG	0.41	2.46	11	1
1:A:102:ALA:CA	1:A:125:ILE:HD11	0.41	2.46	17	1
1:A:91:VAL:HG13	1:A:92:PHE:N	0.41	2.31	21	1
1:A:92:PHE:CD2	1:A:108:VAL:HG21	0.41	2.51	21	1
1:A:83:GLU:HA	1:A:86:ILE:HD12	0.40	1.92	17	1
2:B:1908:SER:HA	2:B:1911:VAL:HG22	0.40	1.93	4	1
1:A:109:MET:SD	1:A:116:LEU:HD13	0.40	2.56	13	1
1:A:110:THR:HG23	1:A:115:LYS:HE3	0.40	1.94	14	1

6.3 Torsion angles

6.3.1 Protein backbone

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	66/73 (90%)	63±1 (95±2%)	3±1 (5±2%)	0±0 (0±0%)	54	85
2	B	14/27 (52%)	14±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	1680/2100 (80%)	1608 (96%)	71 (4%)	1 (0%)	54	85

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	147	SER	1

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	57/64 (89%)	45±3 (78±5%)	12±3 (22±5%)	3	30
2	B	12/25 (48%)	10±1 (83±10%)	2±1 (17±10%)	4	39
All	All	1449/1869 (78%)	1145 (79%)	304 (21%)	3	32

All 44 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	129	ASP	17
1	A	107	HIS	16
1	A	106	ARG	13
1	A	122	ASP	12
1	A	115	LYS	11
1	A	111	ASN	11
1	A	145	MET	11

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Mol	Chain	Res	Type	Models (Total)
2	B	1917	ARG	11
1	A	139	GLU	10
1	A	126	ARG	10
1	A	90	LYS	10
1	A	93	ASP	10
1	A	101	SER	9
1	A	119	ASP	9
1	A	143	ARG	9
1	A	112	LEU	9
2	B	1914	ARG	9
1	A	114	GLU	9
2	B	1913	GLN	8
1	A	147	SER	7
2	B	1918	ARG	7
1	A	105	LEU	6
1	A	117	THR	6
1	A	123	GLU	6
2	B	1920	LEU	6
1	A	124	MET	5
1	A	109	MET	5
1	A	94	ARG	5
1	A	137	ASN	5
1	A	120	GLU	5
1	A	84	GLU	5
1	A	92	PHE	4
1	A	116	LEU	4
1	A	127	GLU	4
1	A	118	ASP	4
1	A	89	PHE	3
1	A	99	LEU	3
1	A	144	MET	2
1	A	97	ASN	2
2	B	1908	SER	2
2	B	1910	ILE	1
1	A	141	PHE	1
1	A	131	ASP	1
1	A	82	GLU	1

6.3.3 RNA ⓘ

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 68% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *CaM_shifts*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	862
Number of shifts mapped to atoms	862
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	72	-0.29 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	67	0.19 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	72	-0.39 ± 0.19	None needed (< 0.5 ppm)
^{15}N	71	0.13 ± 0.17	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 70%, i.e. 703 atoms were assigned a chemical shift out of a possible 1003. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	330/400 (82%)	132/160 (82%)	132/160 (82%)	66/80 (82%)
Sidechain	335/536 (62%)	196/309 (63%)	133/200 (66%)	6/27 (22%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	38/67 (57%)	21/35 (60%)	17/28 (61%)	0/4 (0%)
Overall	703/1003 (70%)	349/504 (69%)	282/388 (73%)	72/111 (65%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 59%, i.e. 768 atoms were assigned a chemical shift out of a possible 1306. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	358/500 (72%)	143/200 (72%)	144/200 (72%)	71/100 (71%)
Sidechain	372/739 (50%)	217/431 (50%)	148/267 (55%)	7/41 (17%)
Aromatic	38/67 (57%)	21/35 (60%)	17/28 (61%)	0/4 (0%)
Overall	768/1306 (59%)	381/666 (57%)	309/495 (62%)	78/145 (54%)

7.1.4 Statistically unusual chemical shifts ⓘ

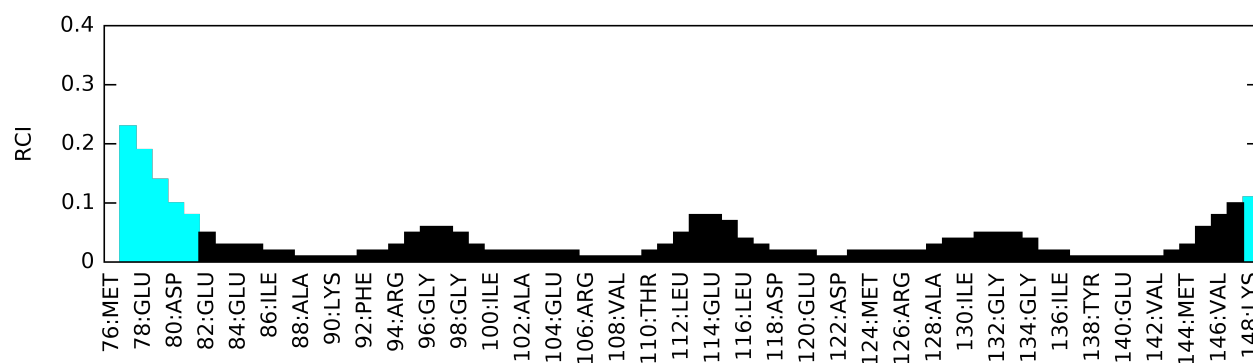
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	93	ASP	HB2	1.34	4.07 – 1.37	-5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: input_cs.cif

Chemical shift list name: *peptide_shifts*

7.2.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	136
Number of shifts mapped to atoms	136
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.2.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 8%, i.e. 83 atoms were assigned a chemical shift out of a possible 1003. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	28/400 (7%)	28/160 (18%)	0/160 (0%)	0/80 (0%)
Sidechain	47/536 (9%)	47/309 (15%)	0/200 (0%)	0/27 (0%)
Aromatic	8/67 (12%)	8/35 (23%)	0/28 (0%)	0/4 (0%)
Overall	83/1003 (8%)	83/504 (16%)	0/388 (0%)	0/111 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 9%, i.e. 114 atoms were assigned a chemical shift out of a possible 1306. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	42/500 (8%)	42/200 (21%)	0/200 (0%)	0/100 (0%)
Sidechain	64/739 (9%)	64/431 (15%)	0/267 (0%)	0/41 (0%)
Aromatic	8/67 (12%)	8/35 (23%)	0/28 (0%)	0/4 (0%)
Overall	114/1306 (9%)	114/666 (17%)	0/495 (0%)	0/145 (0%)

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain B:

