Full wwPDB NMR Structure Validation Report ⓘ

Oct 11, 2021 – 03:48 AM EDT

PDB ID	:	2K0F
Title	:	Calmodulin complexed with calmodulin-binding peptide from smooth muscle myosin light chain kinase
Authors	:	Gsponer, J.; Christodoulou, J.; Cavalli, A.; Bui, J.M.; Richter, B.; Dobson, C.M.; Vendruscolo, M.
Deposited on	:	2008-02-02

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

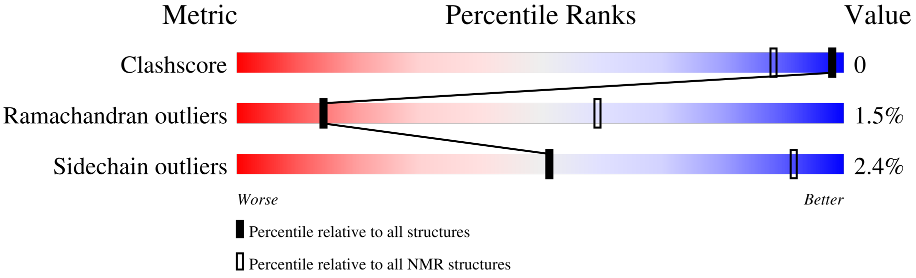
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 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	
2	B	19	

2 Ensemble composition and analysis ⓘ

This entry contains 160 models. Model 54 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:3-A:142, B:1-B:16 (156)	0.80	54

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 13 clusters and 7 single-model clusters were found.

Cluster number	Models
1	2, 4, 6, 7, 8, 11, 12, 14, 16, 18, 20, 22, 24, 28, 29, 30, 31, 32, 34, 36, 38, 40, 42, 44, 45, 46, 50, 52, 54, 56, 60, 61, 66, 70, 74, 76, 82, 86, 88, 92, 98, 102, 104, 105, 106, 108, 114, 116, 118, 120, 121, 122, 124, 126, 130, 132, 134, 135, 136, 138, 140, 142, 148, 152, 154, 156, 158, 159
2	1, 3, 9, 15, 17, 21, 23, 25, 27, 33, 37, 39, 41, 43, 53, 57, 59, 63, 69, 72, 75, 77, 79, 85, 87, 93, 95, 101, 109, 111, 117, 119, 125, 127, 133, 141, 143, 149
3	26, 62, 78, 80, 84, 96, 100, 112, 128, 144, 160
4	35, 47, 51, 67, 83, 99, 115, 131, 147
5	49, 65, 81, 97, 113, 129, 145
6	5, 13, 19, 110
7	55, 71, 103
8	58, 90, 94
9	139, 155
10	91, 107
11	137, 153
12	48, 64
13	68, 150
Single-model clusters	10; 73; 89; 123; 146; 151; 157

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2494 atoms, of which 1213 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	142	2168	687	1047	180	245	9	0

- Molecule 2 is a protein called 19-mer peptide from Myosin light chain kinase.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	19	322	95	166	37	24	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	HIS	ASN	engineered mutation	UNP Q15746

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

Mol	Chain	Residues	Atoms	
			Total	Ca
3	A	4	4	4

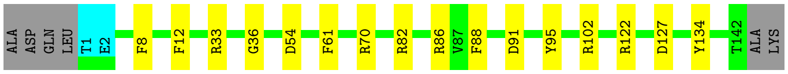
4 Residue-property plots ⓘ

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.

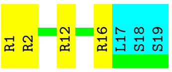
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:



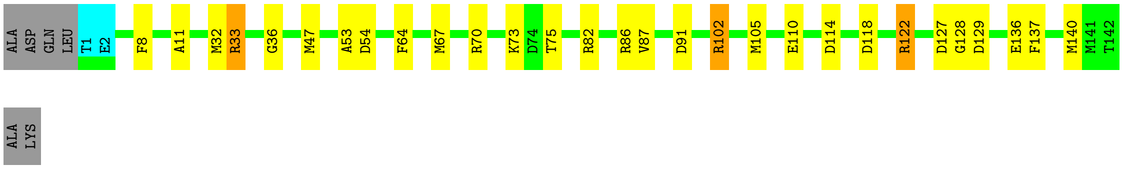
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

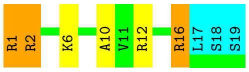
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

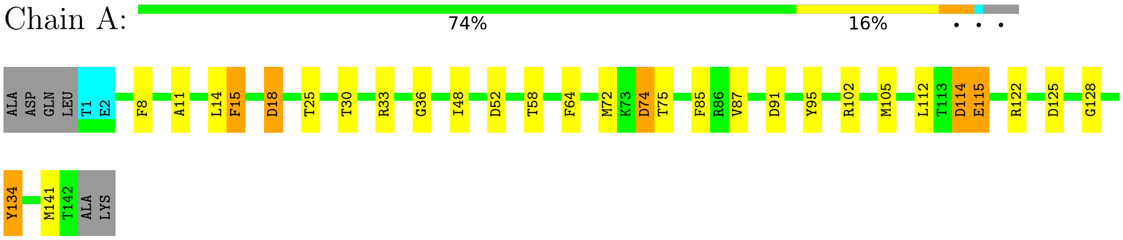
Chain B:



4.2.2 Score per residue for model 2

- Molecule 1: calmodulin

Chain A:



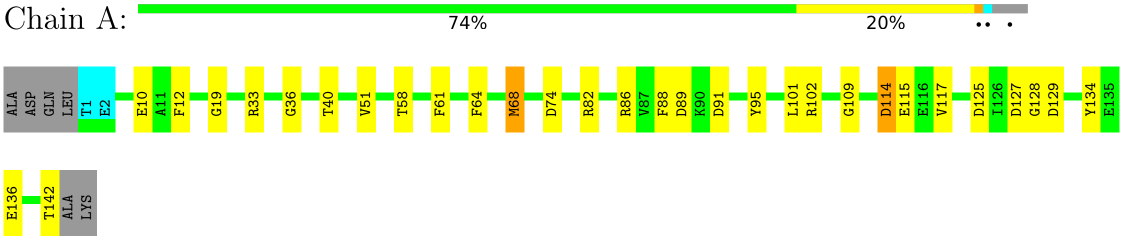
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.3 Score per residue for model 3

- Molecule 1: calmodulin

Chain A:



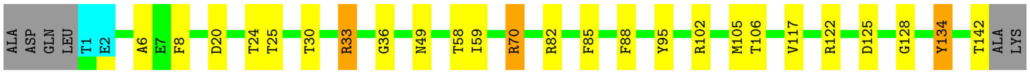
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

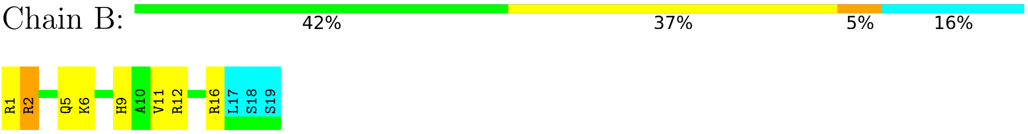
4.2.4 Score per residue for model 4

- Molecule 1: calmodulin

Chain A:

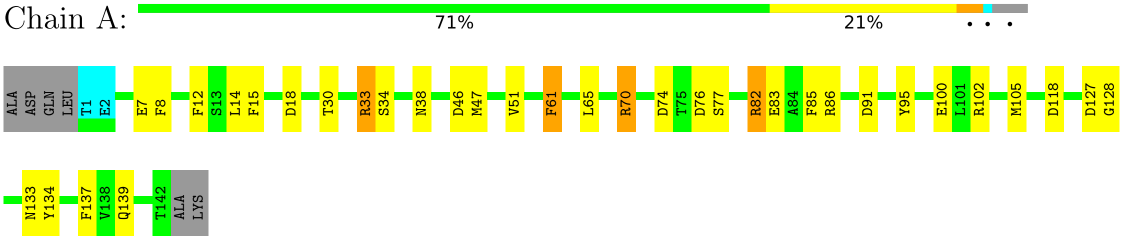


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.5 Score per residue for model 5

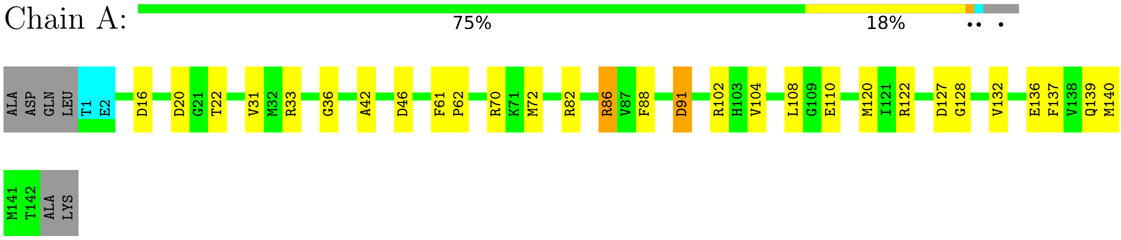
- Molecule 1: calmodulin



- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.6 Score per residue for model 6

- Molecule 1: calmodulin

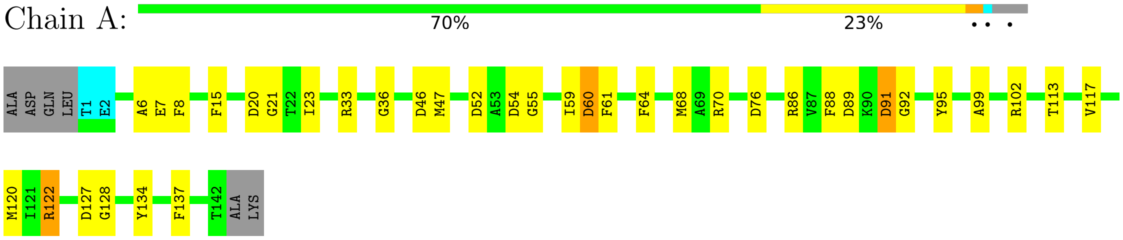


- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.7 Score per residue for model 7

- Molecule 1: calmodulin

Chain A:



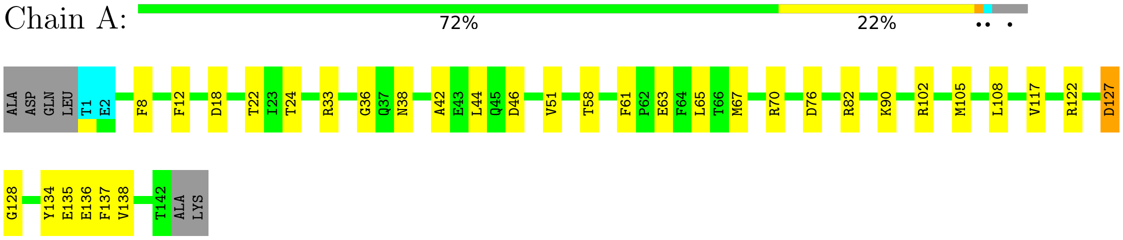
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.8 Score per residue for model 8

- Molecule 1: calmodulin

Chain A:



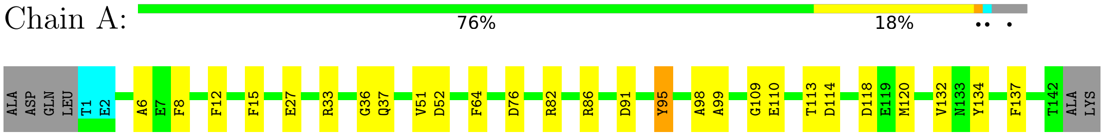
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.9 Score per residue for model 9

- Molecule 1: calmodulin

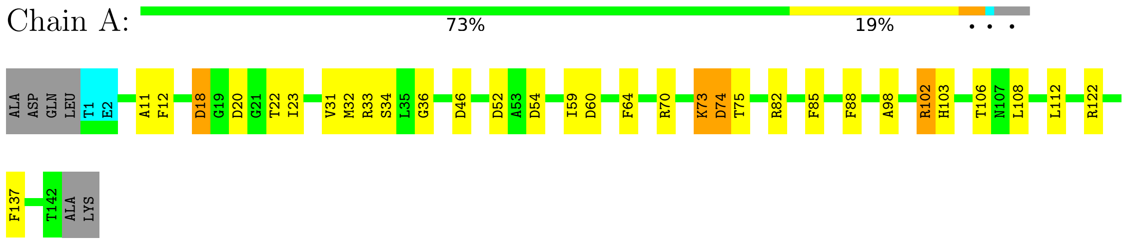
Chain A:



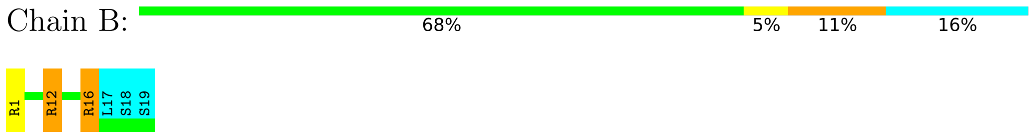
- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.10 Score per residue for model 10

- Molecule 1: calmodulin

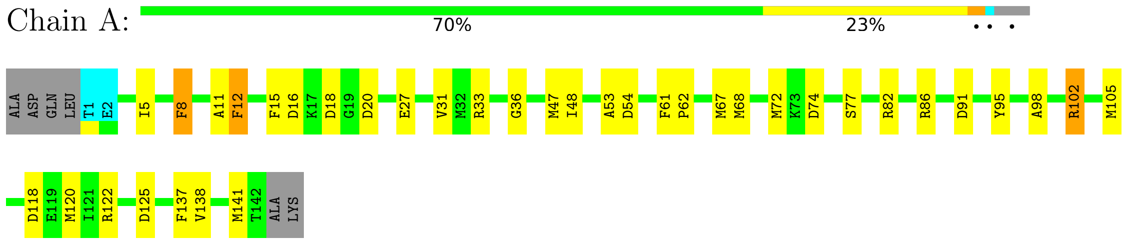


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.11 Score per residue for model 11

- Molecule 1: calmodulin

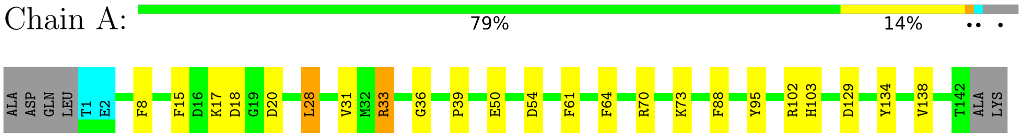


- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.12 Score per residue for model 12

- Molecule 1: calmodulin

Chain A:



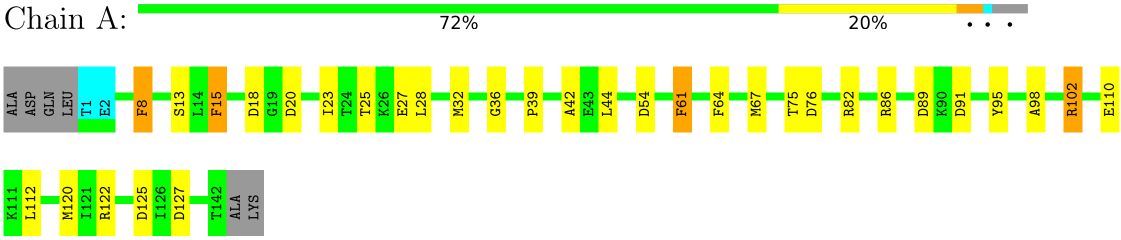
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.13 Score per residue for model 13

- Molecule 1: calmodulin

Chain A:



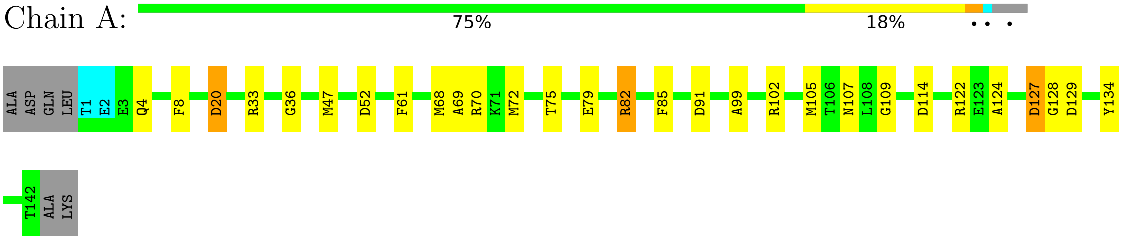
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.14 Score per residue for model 14

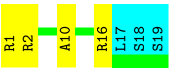
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

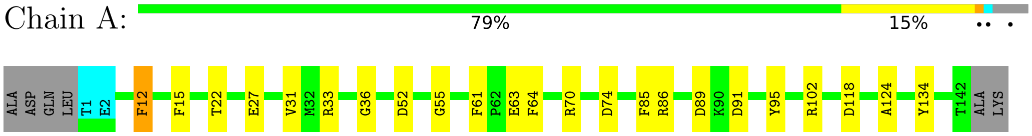
Chain B:



4.2.15 Score per residue for model 15

- Molecule 1: calmodulin

Chain A:



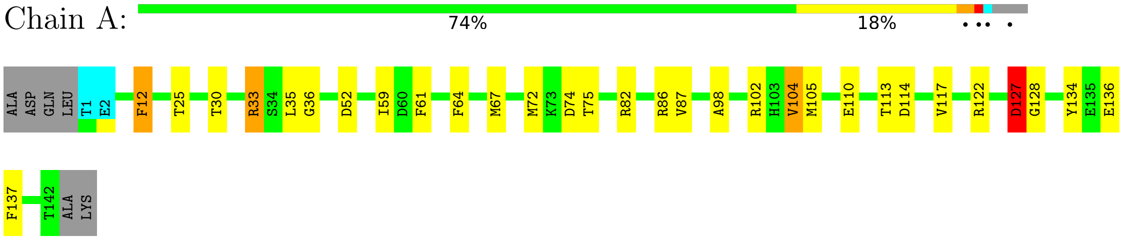
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.16 Score per residue for model 16

- Molecule 1: calmodulin

Chain A:



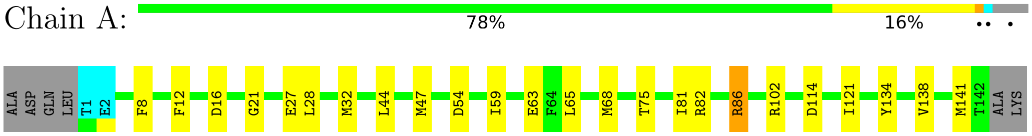
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.17 Score per residue for model 17

- Molecule 1: calmodulin

Chain A:



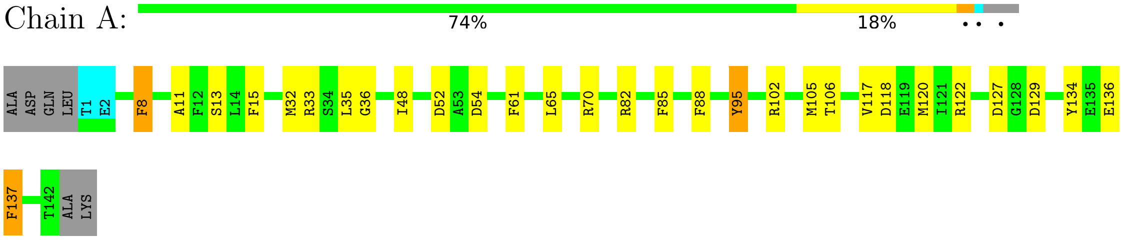
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.18 Score per residue for model 18

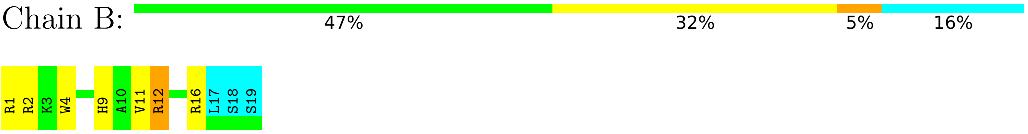
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

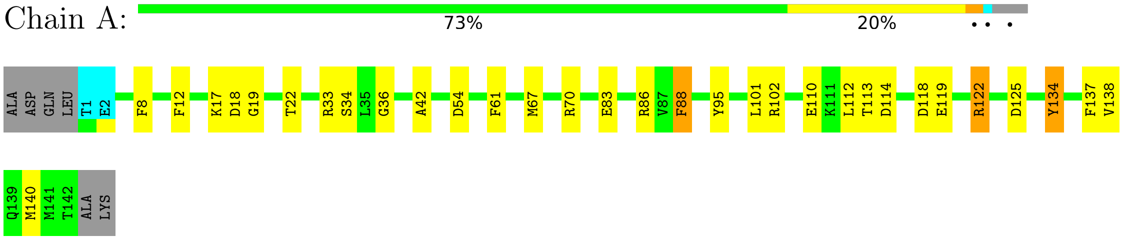
Chain B:



4.2.19 Score per residue for model 19

- Molecule 1: calmodulin

Chain A:

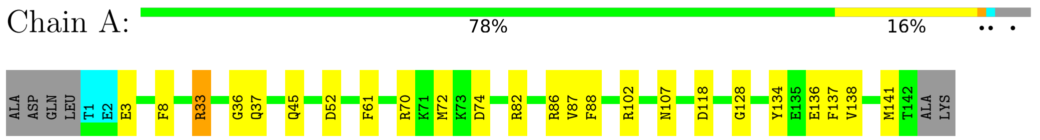


- Molecule 2: 19-mer peptide from Myosin light chain kinase

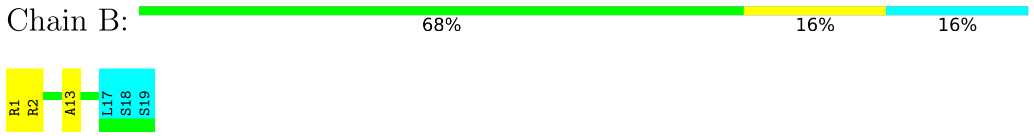
Chain B:

4.2.20 Score per residue for model 20

- Molecule 1: calmodulin

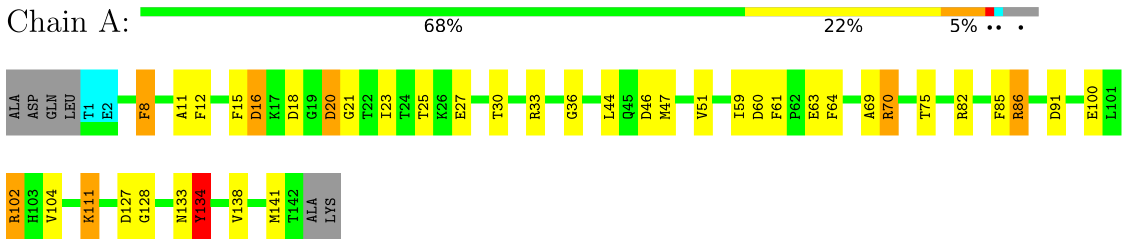


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.21 Score per residue for model 21

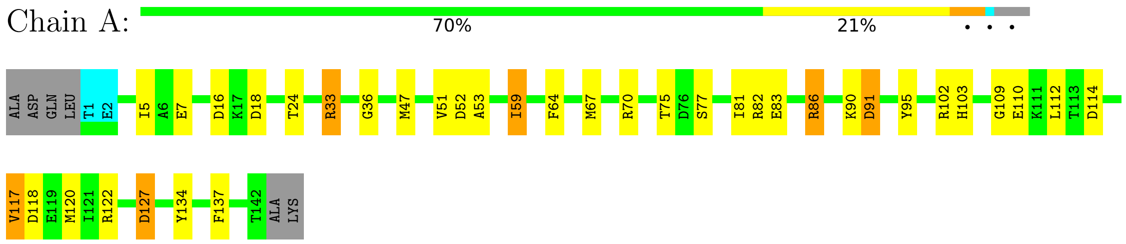
- Molecule 1: calmodulin



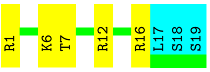
- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.22 Score per residue for model 22

- Molecule 1: calmodulin



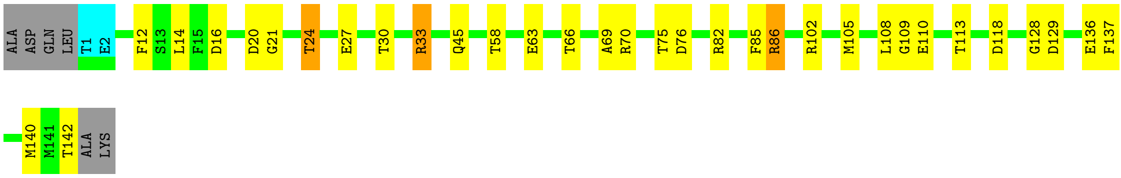
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.23 Score per residue for model 23

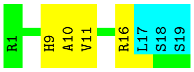
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

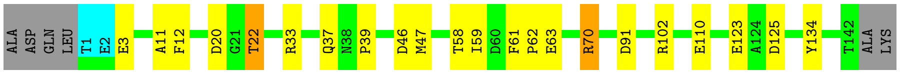
Chain B:



4.2.24 Score per residue for model 24

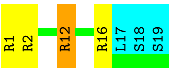
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

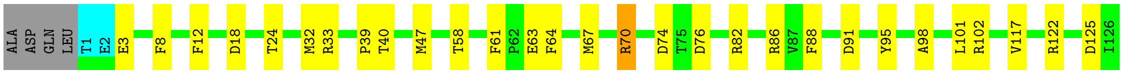
Chain B:

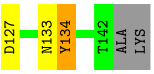


4.2.25 Score per residue for model 25

- Molecule 1: calmodulin

Chain A:

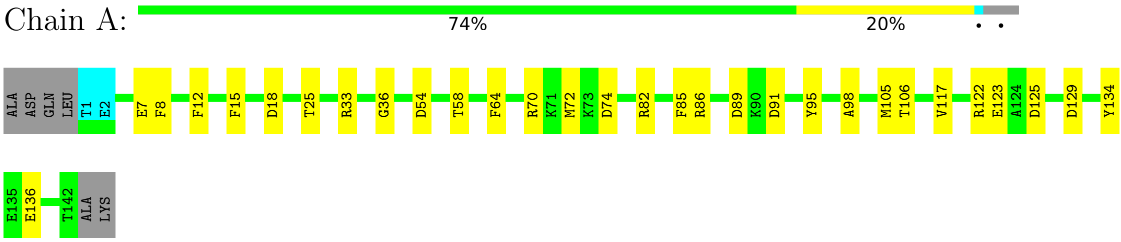




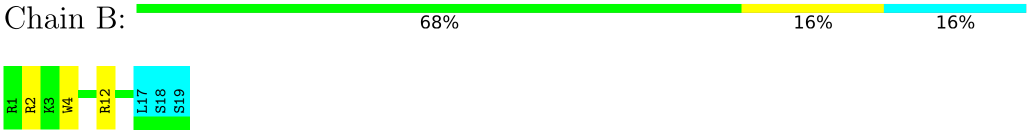
- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.26 Score per residue for model 26

- Molecule 1: calmodulin

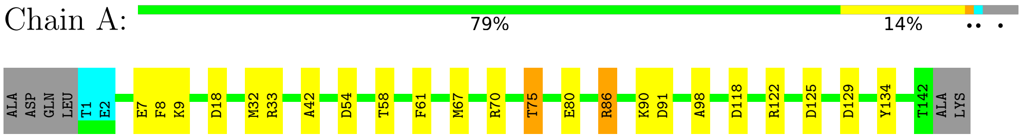


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.27 Score per residue for model 27

- Molecule 1: calmodulin

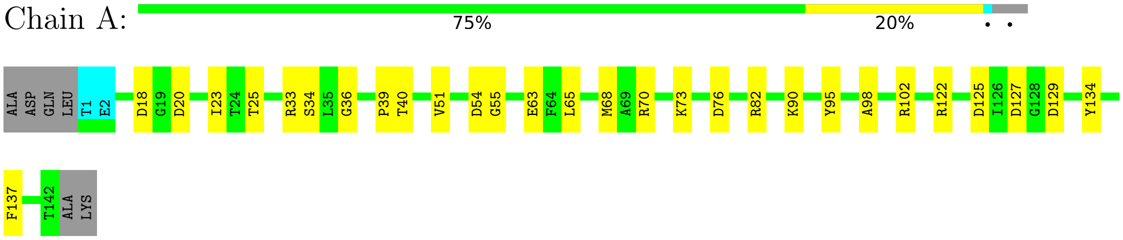


- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.28 Score per residue for model 28

- Molecule 1: calmodulin

Chain A:



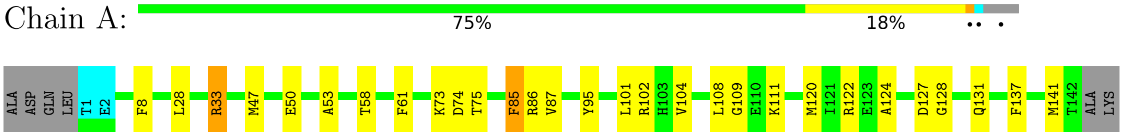
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.29 Score per residue for model 29

- Molecule 1: calmodulin

Chain A:



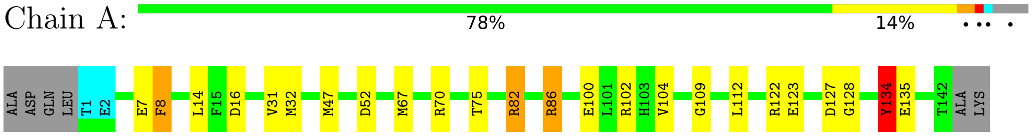
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.30 Score per residue for model 30

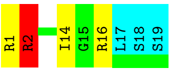
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

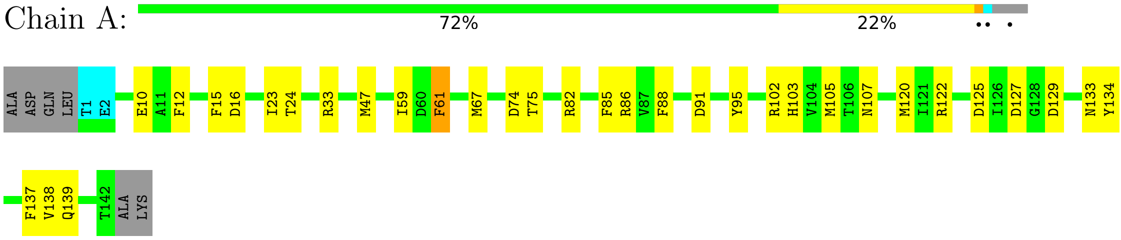
Chain B:



4.2.31 Score per residue for model 31

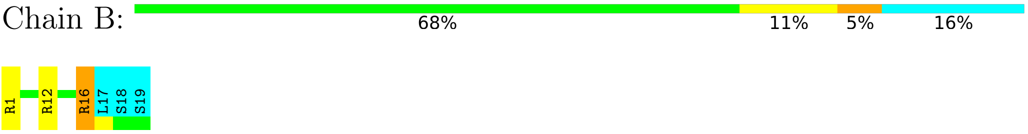
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

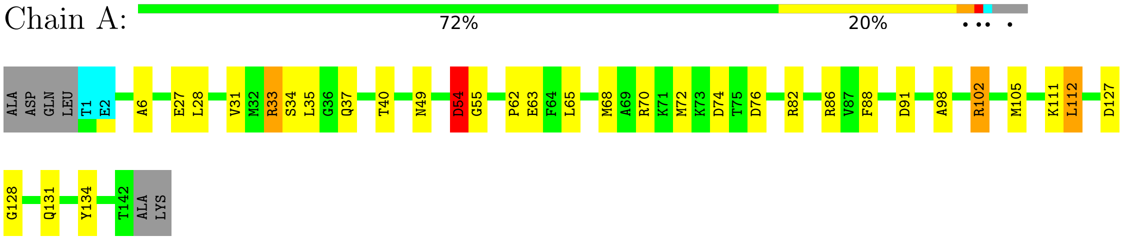
Chain B:



4.2.32 Score per residue for model 32

- Molecule 1: calmodulin

Chain A:



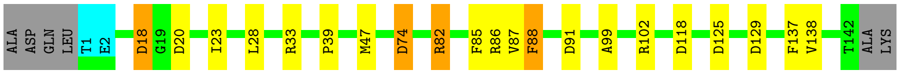
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.33 Score per residue for model 33

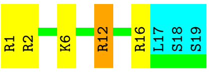
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:



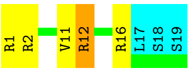
4.2.34 Score per residue for model 34

- Molecule 1: calmodulin

Chain A:

- Molecule 2: 19-mer peptide from Myosin light chain kinase

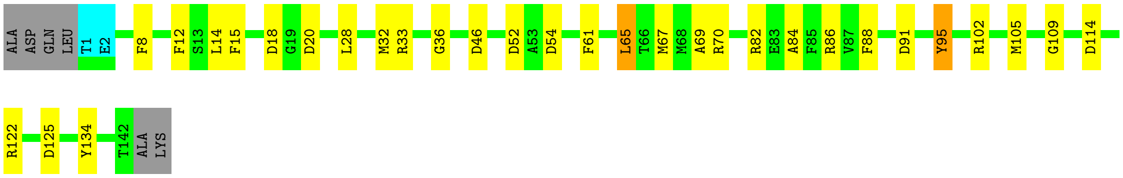
Chain B:



4.2.35 Score per residue for model 35

- Molecule 1: calmodulin

Chain A:

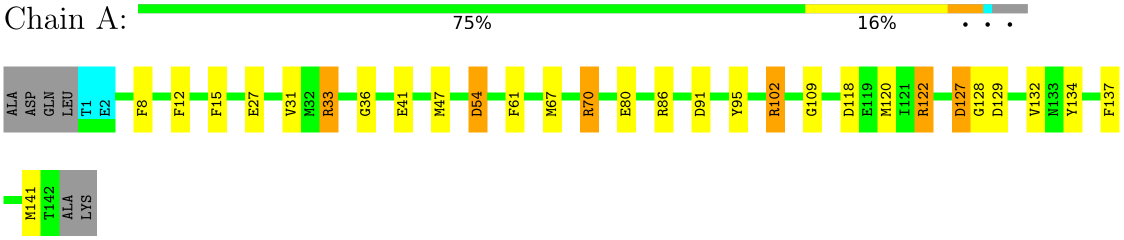


- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.36 Score per residue for model 36

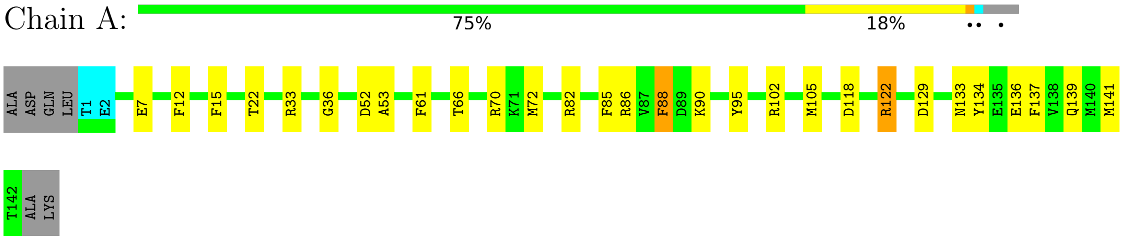
- Molecule 1: calmodulin



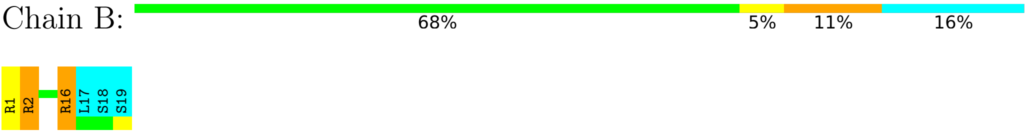
- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.37 Score per residue for model 37

- Molecule 1: calmodulin

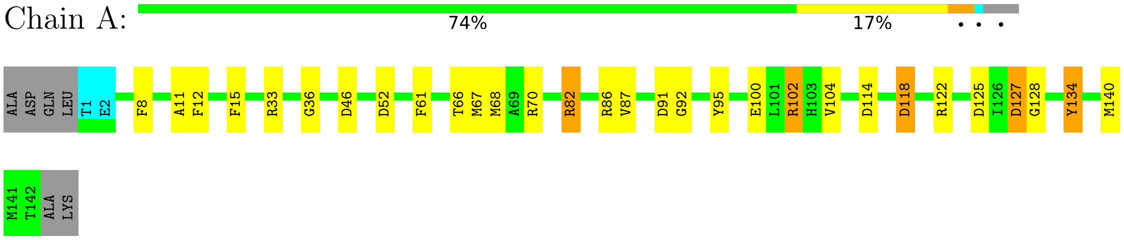


- Molecule 2: 19-mer peptide from Myosin light chain kinase

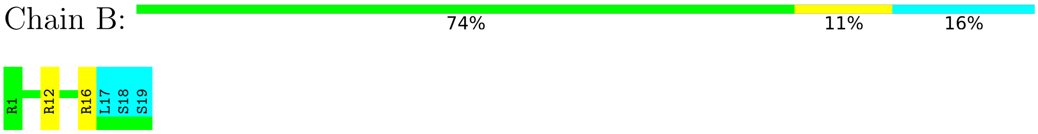


4.2.38 Score per residue for model 38

- Molecule 1: calmodulin

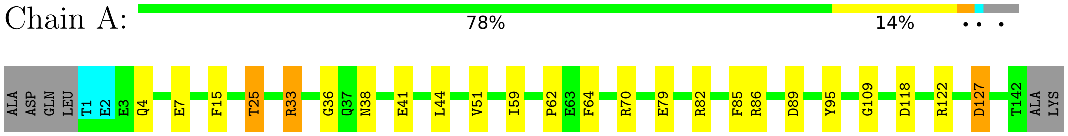


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.39 Score per residue for model 39

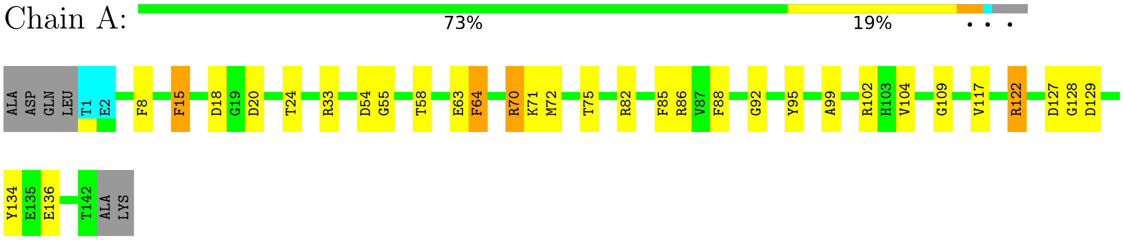
- Molecule 1: calmodulin



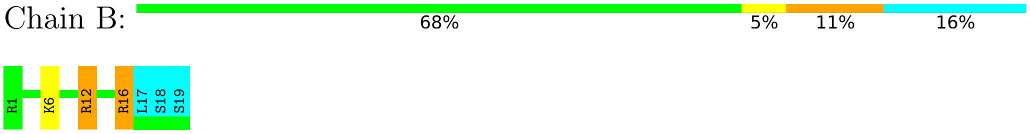
- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.40 Score per residue for model 40

- Molecule 1: calmodulin

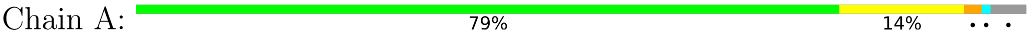


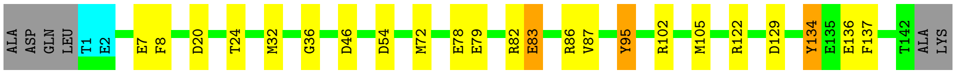
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.41 Score per residue for model 41

- Molecule 1: calmodulin

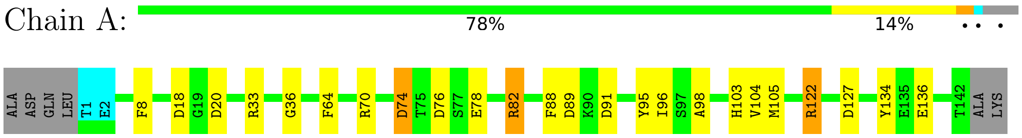




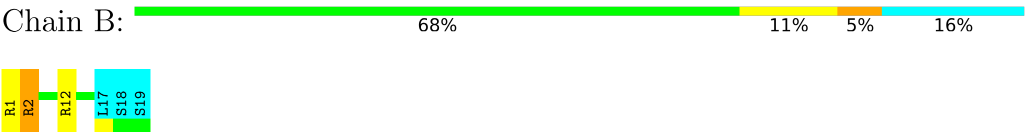
- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.42 Score per residue for model 42

- Molecule 1: calmodulin

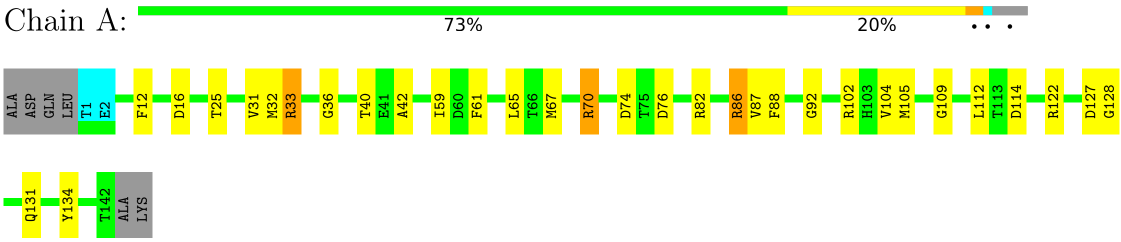


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.43 Score per residue for model 43

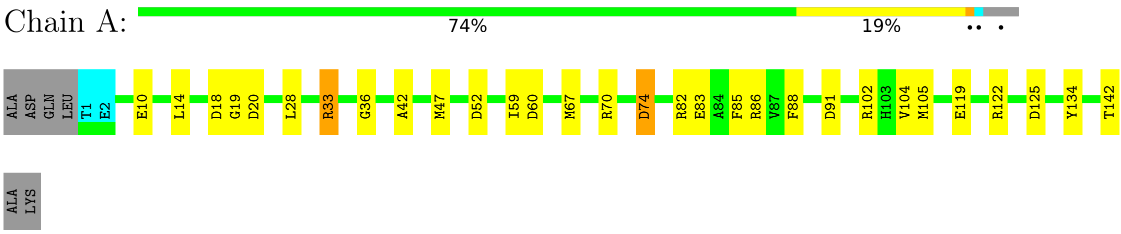
- Molecule 1: calmodulin



- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.44 Score per residue for model 44

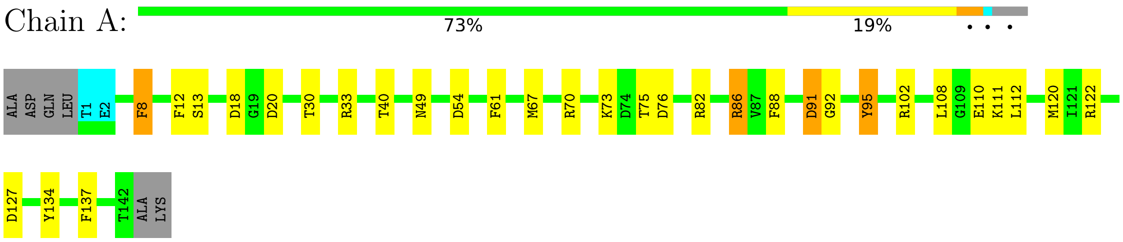
- Molecule 1: calmodulin



- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.45 Score per residue for model 45

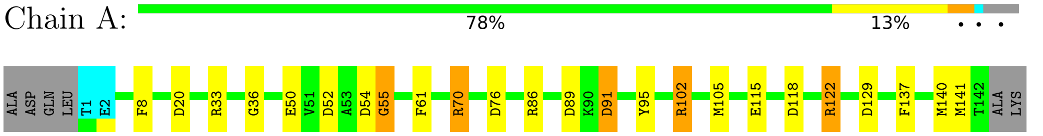
- Molecule 1: calmodulin



- Molecule 2: 19-mer peptide from Myosin light chain kinase

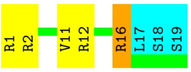
4.2.46 Score per residue for model 46

- Molecule 1: calmodulin



- Molecule 2: 19-mer peptide from Myosin light chain kinase

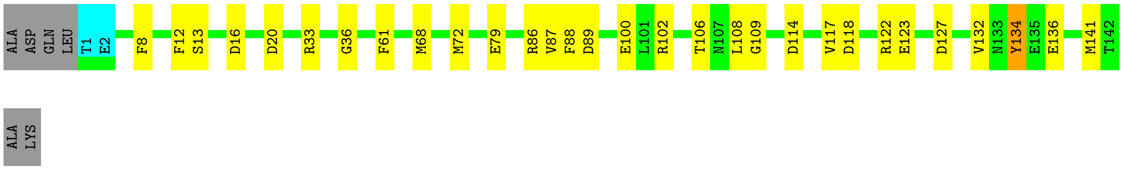
Chain B:



4.2.47 Score per residue for model 47

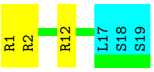
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

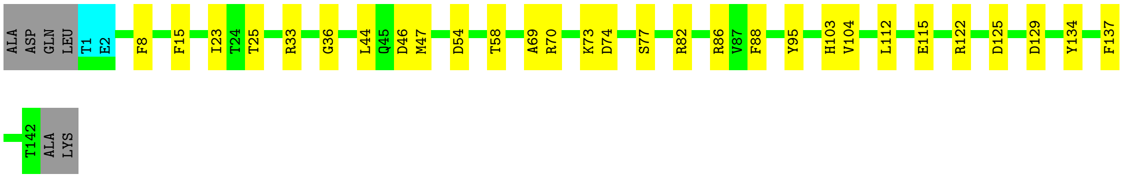
Chain B:



4.2.48 Score per residue for model 48

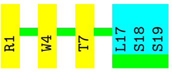
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

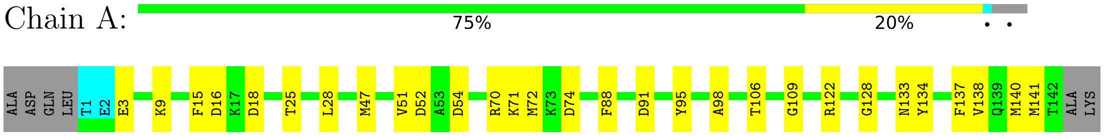
Chain B:



4.2.49 Score per residue for model 49

- Molecule 1: calmodulin

Chain A:



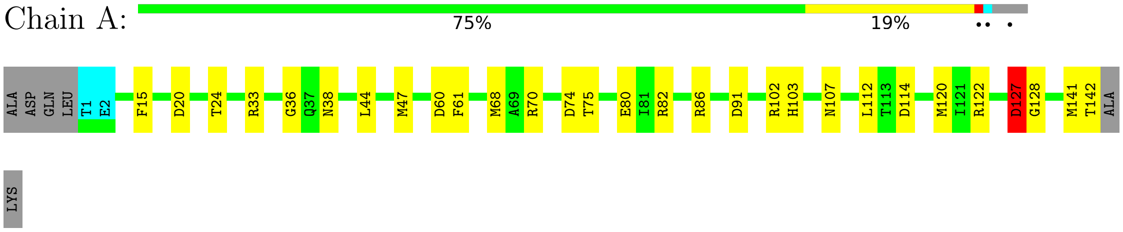
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.50 Score per residue for model 50

- Molecule 1: calmodulin

Chain A:



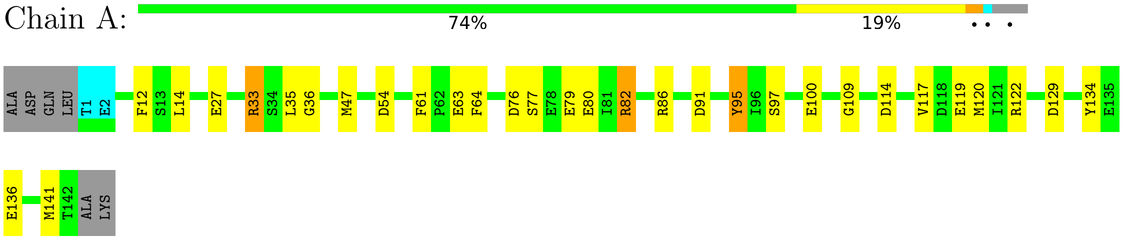
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.51 Score per residue for model 51

- Molecule 1: calmodulin

Chain A:



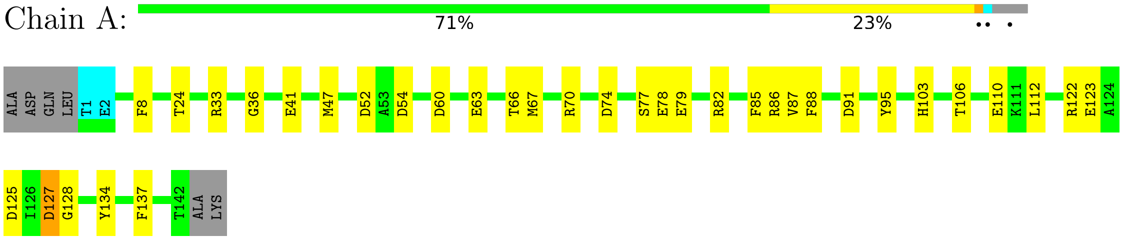
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.52 Score per residue for model 52

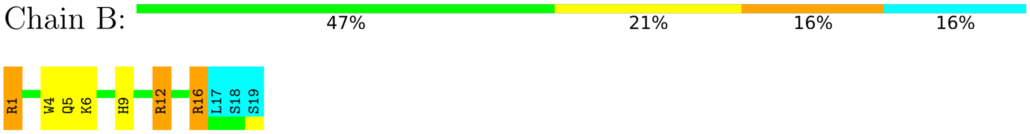
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

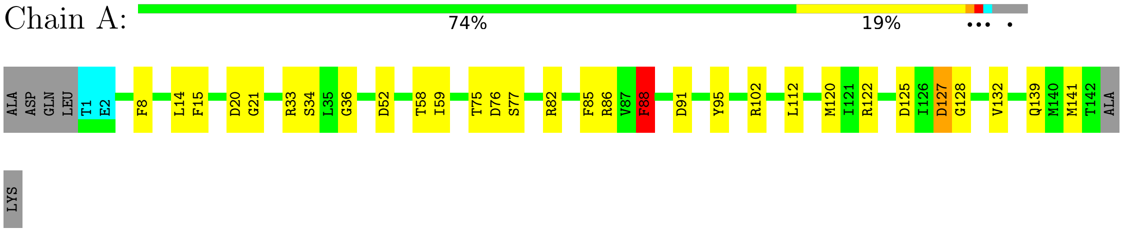
Chain B:



4.2.53 Score per residue for model 53

- Molecule 1: calmodulin

Chain A:



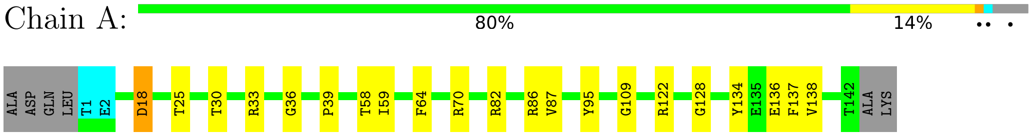
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.54 Score per residue for model 54 (medoid)

- Molecule 1: calmodulin

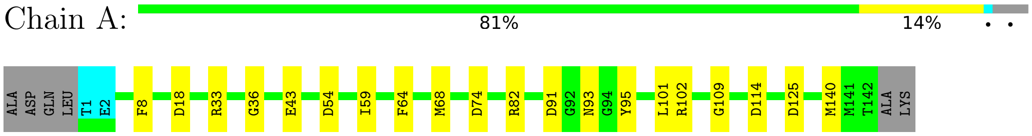
Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.55 Score per residue for model 55

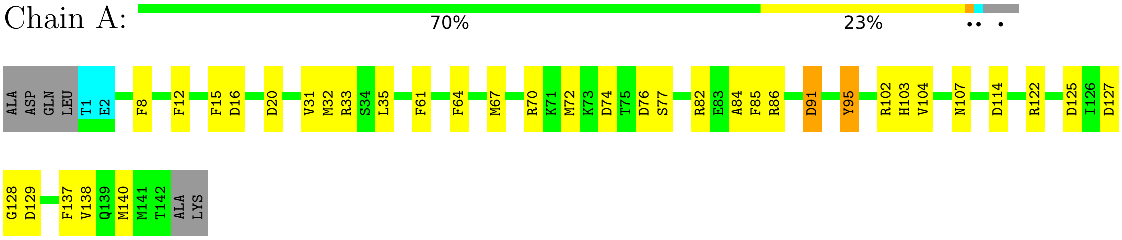
- Molecule 1: calmodulin



- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.56 Score per residue for model 56

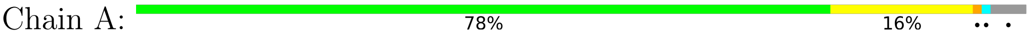
- Molecule 1: calmodulin

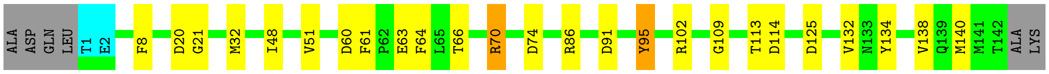


- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.57 Score per residue for model 57

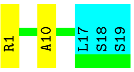
- Molecule 1: calmodulin





- Molecule 2: 19-mer peptide from Myosin light chain kinase

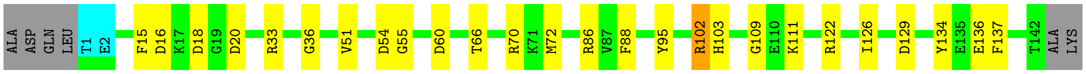
Chain B:



4.2.58 Score per residue for model 58

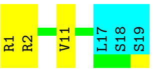
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

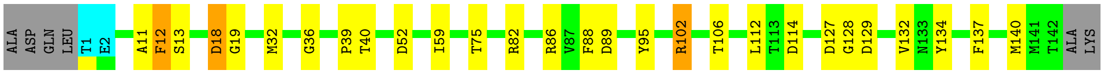
Chain B:



4.2.59 Score per residue for model 59

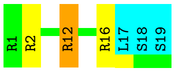
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

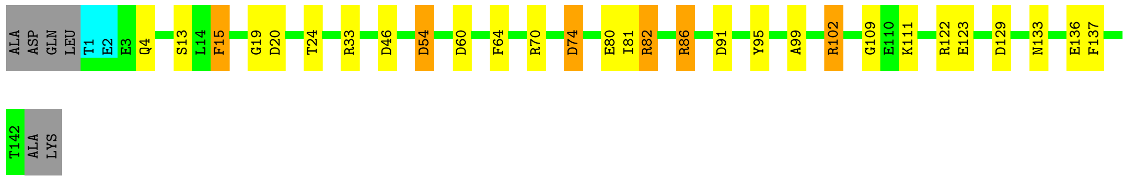
Chain B:



4.2.60 Score per residue for model 60

- Molecule 1: calmodulin

Chain A:



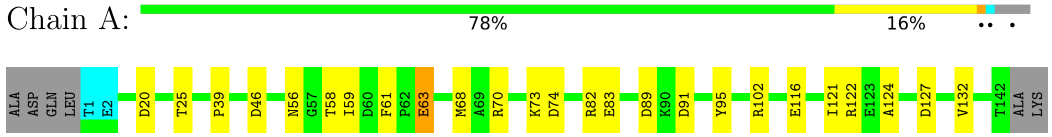
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.61 Score per residue for model 61

- Molecule 1: calmodulin

Chain A:



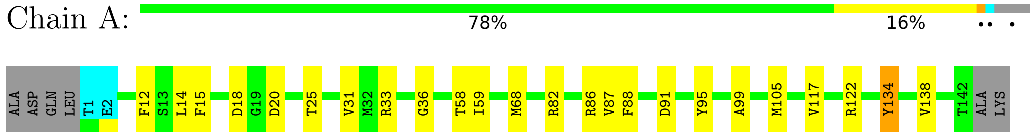
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.62 Score per residue for model 62

- Molecule 1: calmodulin

Chain A:



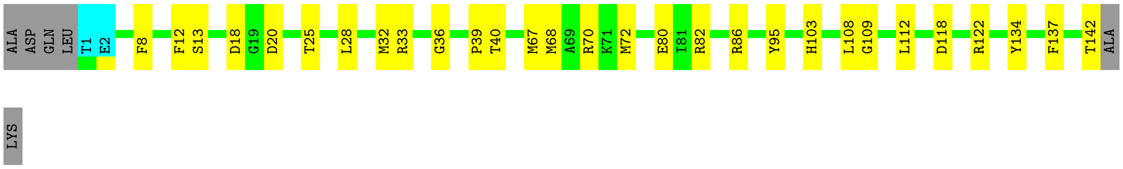
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.63 Score per residue for model 63

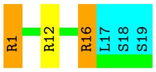
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

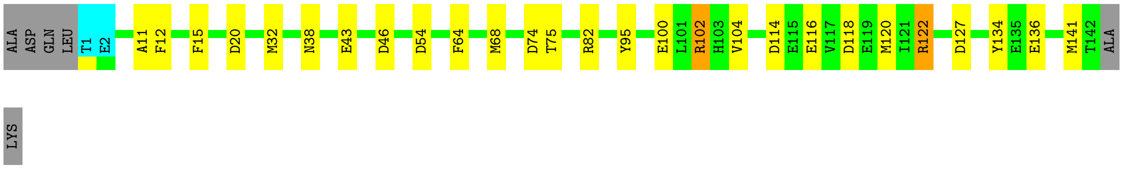
Chain B:



4.2.64 Score per residue for model 64

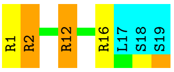
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:



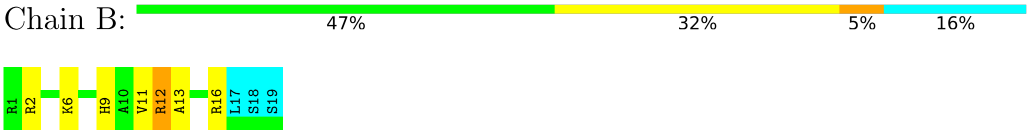
4.2.65 Score per residue for model 65

- Molecule 1: calmodulin

Chain A:

- Molecule 2: 19-mer peptide from Myosin light chain kinase

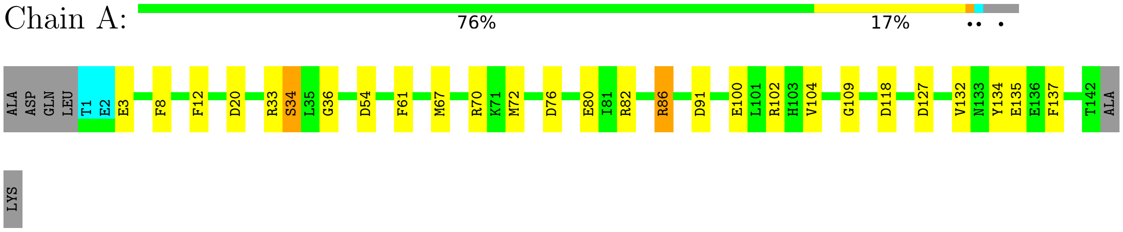
Chain B:



4.2.66 Score per residue for model 66

- Molecule 1: calmodulin

Chain A:



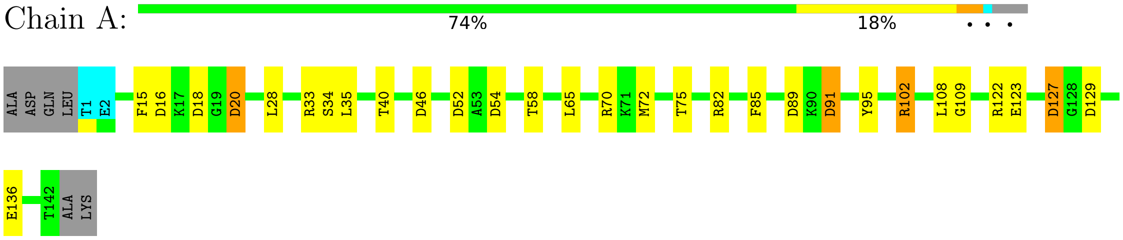
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.67 Score per residue for model 67

- Molecule 1: calmodulin

Chain A:

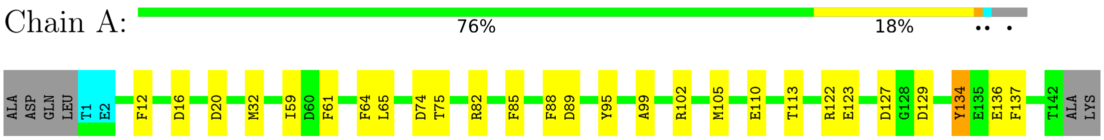


- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.68 Score per residue for model 68

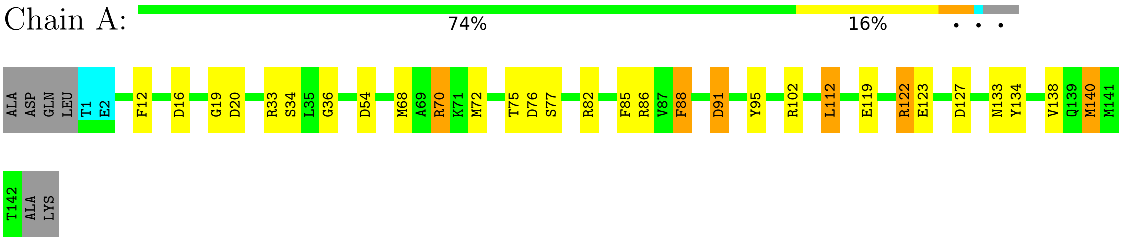
- Molecule 1: calmodulin



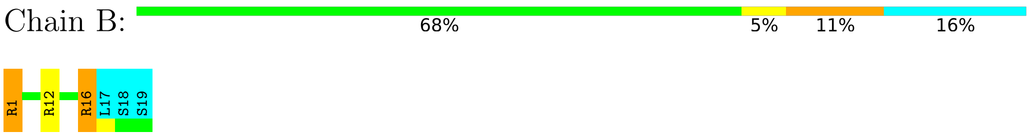
- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.69 Score per residue for model 69

- Molecule 1: calmodulin

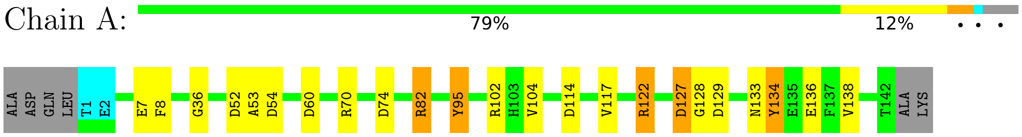


- Molecule 2: 19-mer peptide from Myosin light chain kinase

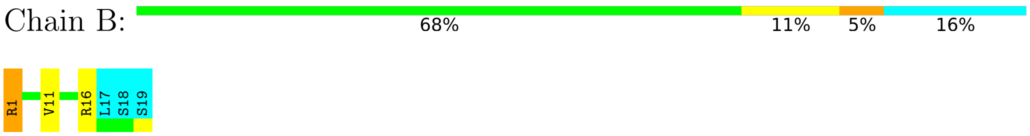


4.2.70 Score per residue for model 70

- Molecule 1: calmodulin



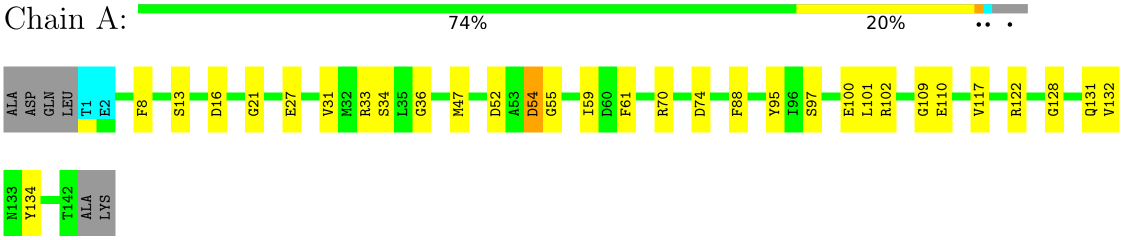
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.71 Score per residue for model 71

- Molecule 1: calmodulin

Chain A:



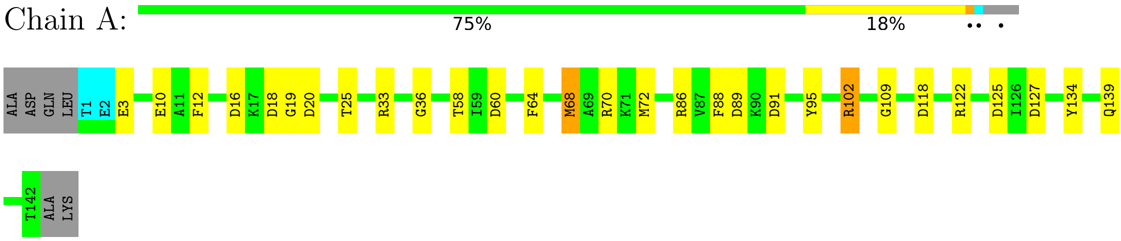
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.72 Score per residue for model 72

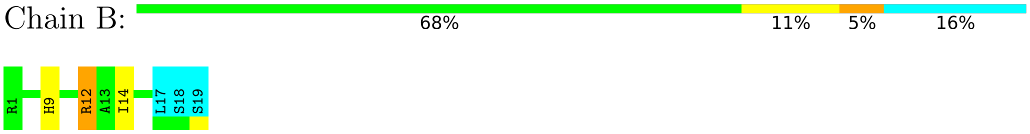
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

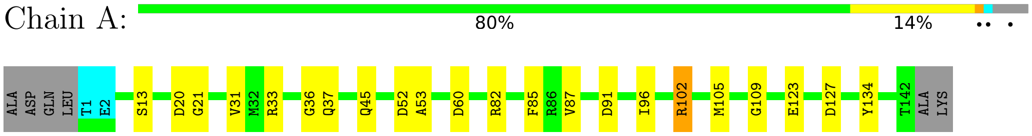
Chain B:



4.2.73 Score per residue for model 73

- Molecule 1: calmodulin

Chain A:



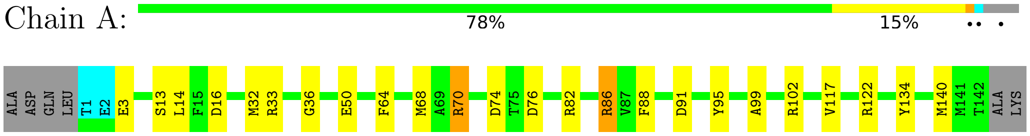
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.74 Score per residue for model 74

- Molecule 1: calmodulin

Chain A:



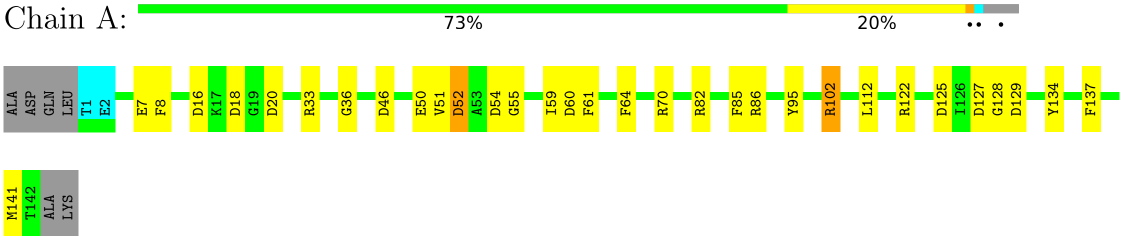
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.75 Score per residue for model 75

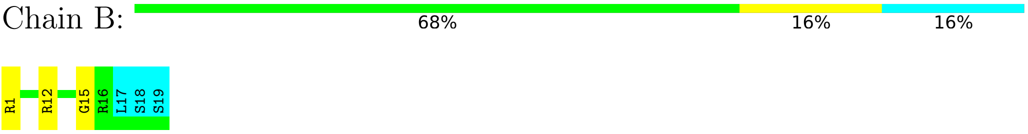
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

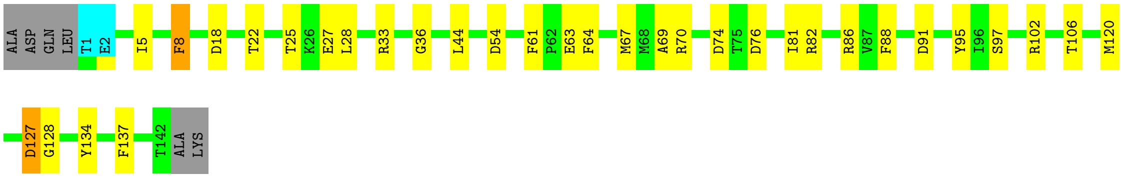
Chain B:



4.2.76 Score per residue for model 76

- Molecule 1: calmodulin

Chain A:



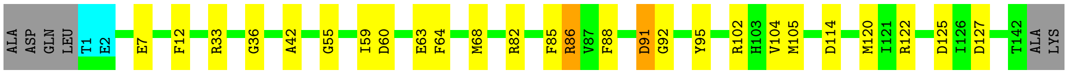
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.77 Score per residue for model 77

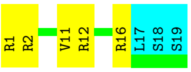
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

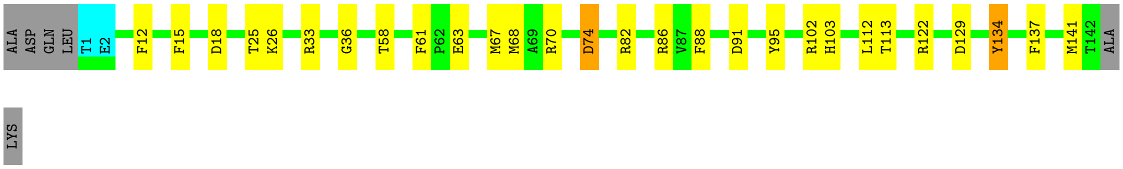
Chain B:



4.2.78 Score per residue for model 78

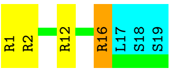
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

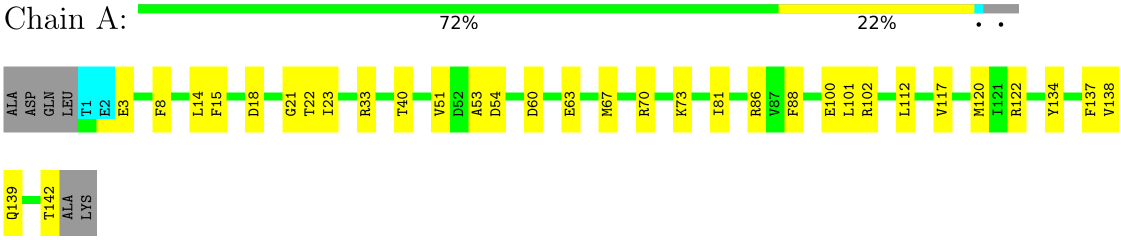
Chain B:



4.2.79 Score per residue for model 79

- Molecule 1: calmodulin

Chain A:



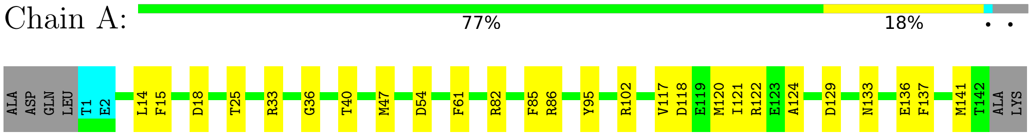
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.80 Score per residue for model 80

- Molecule 1: calmodulin

Chain A:



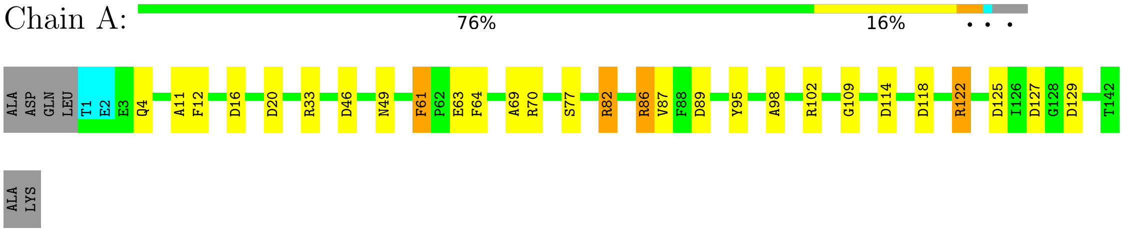
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.81 Score per residue for model 81

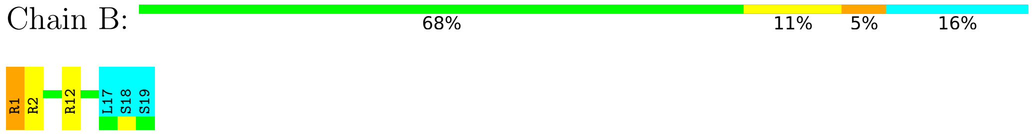
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

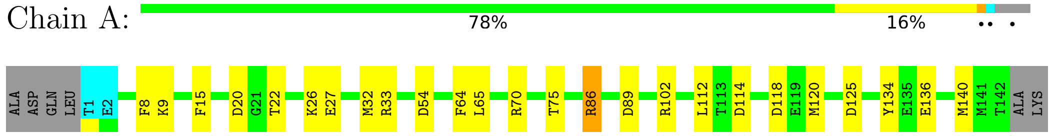
Chain B:



4.2.82 Score per residue for model 82

- Molecule 1: calmodulin

Chain A:



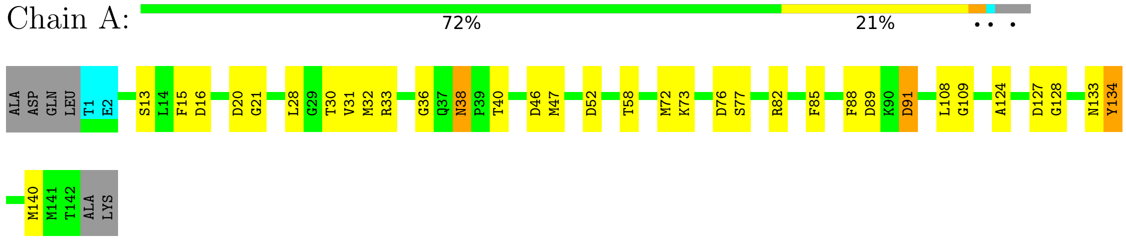
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.83 Score per residue for model 83

- Molecule 1: calmodulin

Chain A:



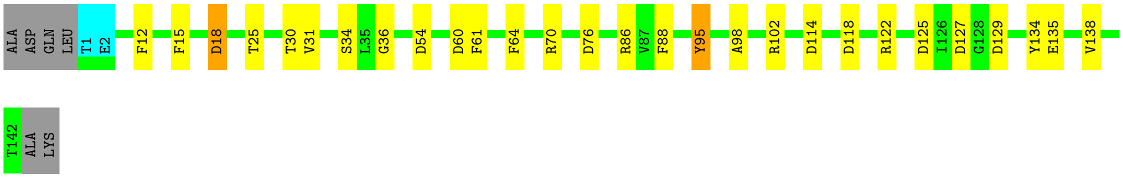
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.84 Score per residue for model 84

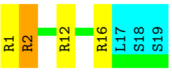
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

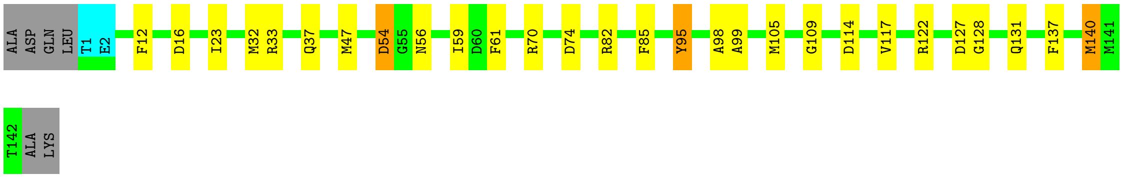
Chain B:



4.2.85 Score per residue for model 85

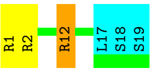
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

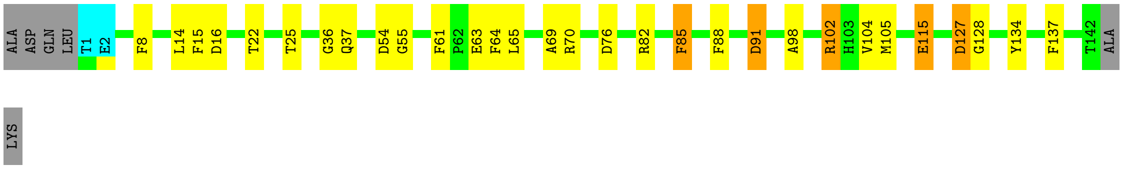
Chain B:



4.2.86 Score per residue for model 86

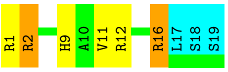
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

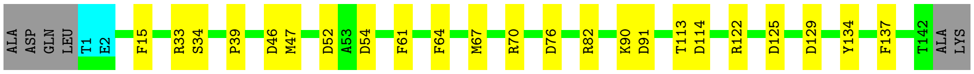
Chain B:



4.2.87 Score per residue for model 87

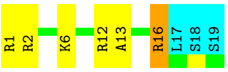
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

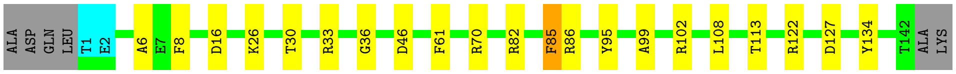
Chain B:



4.2.88 Score per residue for model 88

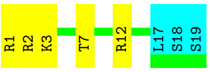
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

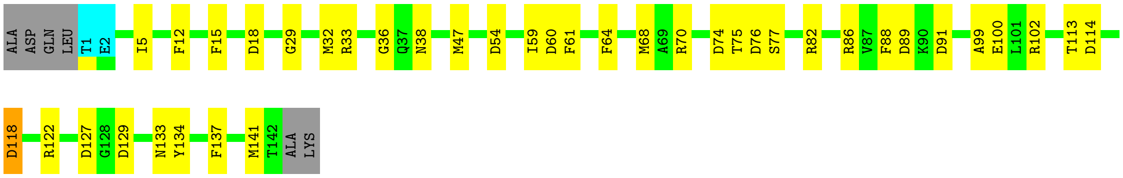
Chain B:



4.2.89 Score per residue for model 89

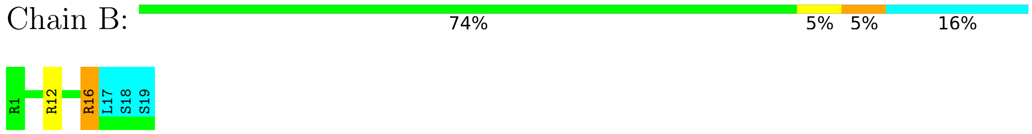
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

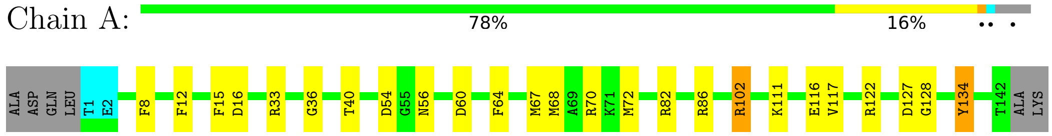
Chain B:



4.2.90 Score per residue for model 90

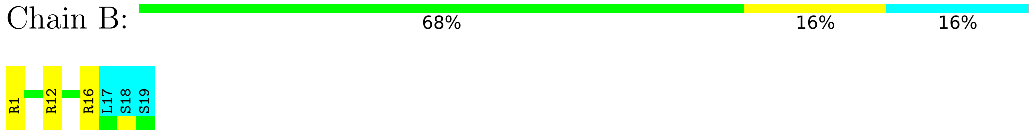
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

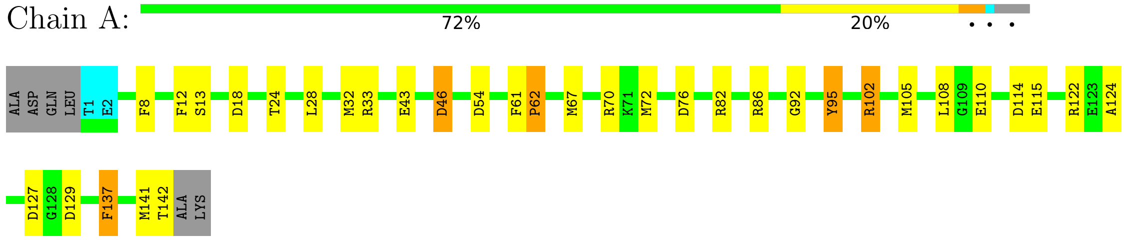
Chain B:



4.2.91 Score per residue for model 91

- Molecule 1: calmodulin

Chain A:



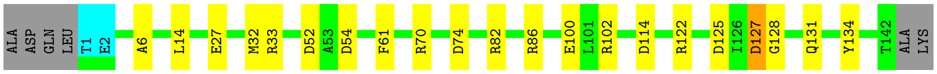
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.92 Score per residue for model 92

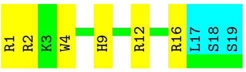
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

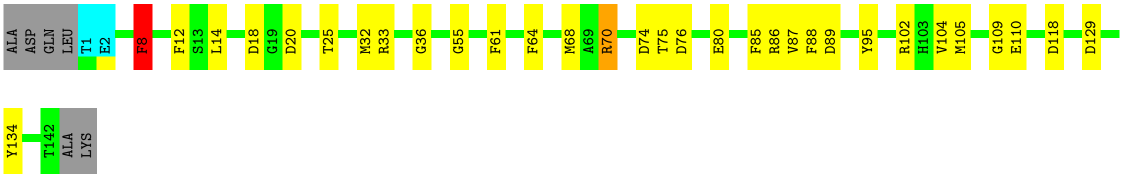
Chain B:



4.2.93 Score per residue for model 93

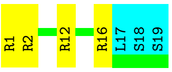
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

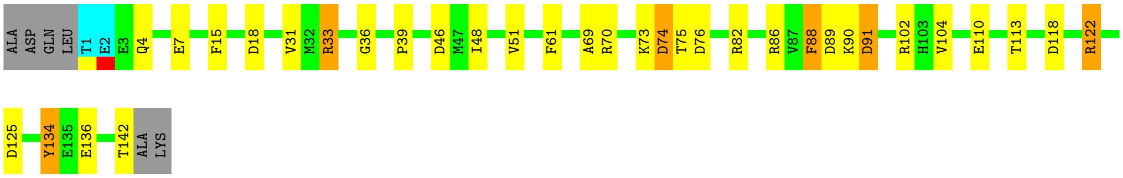
Chain B:



4.2.94 Score per residue for model 94

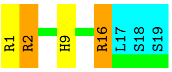
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

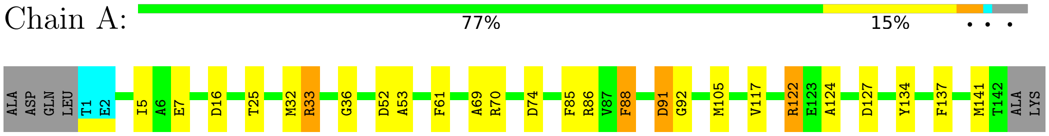
Chain B:



4.2.95 Score per residue for model 95

- Molecule 1: calmodulin

Chain A:



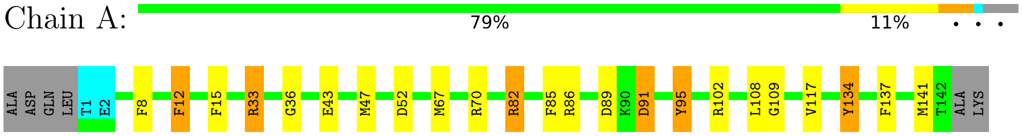
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.96 Score per residue for model 96

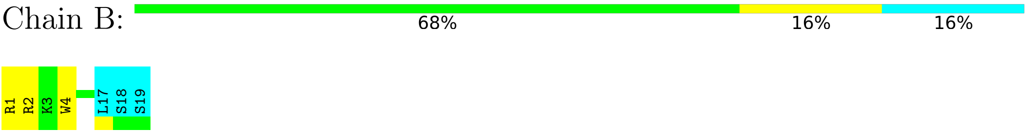
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

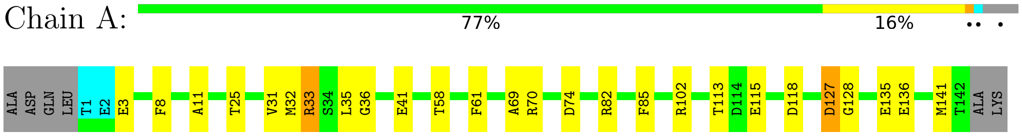
Chain B:



4.2.97 Score per residue for model 97

- Molecule 1: calmodulin

Chain A:



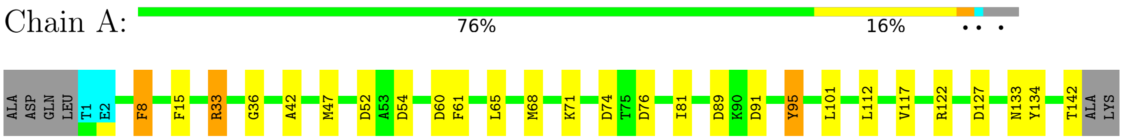
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.98 Score per residue for model 98

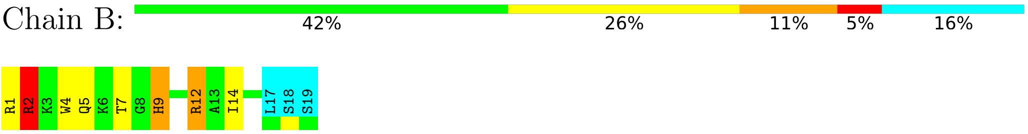
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

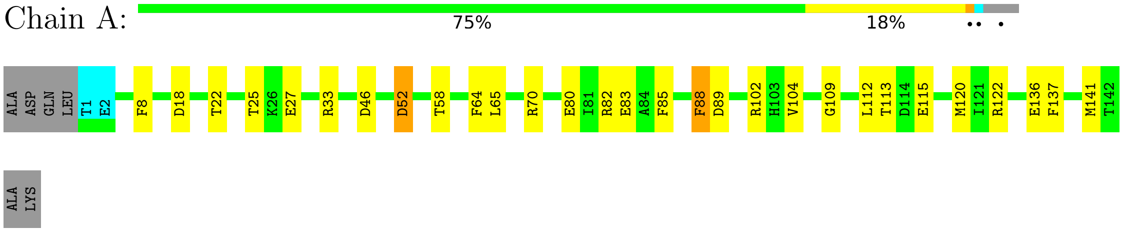
Chain B:



4.2.99 Score per residue for model 99

- Molecule 1: calmodulin

Chain A:



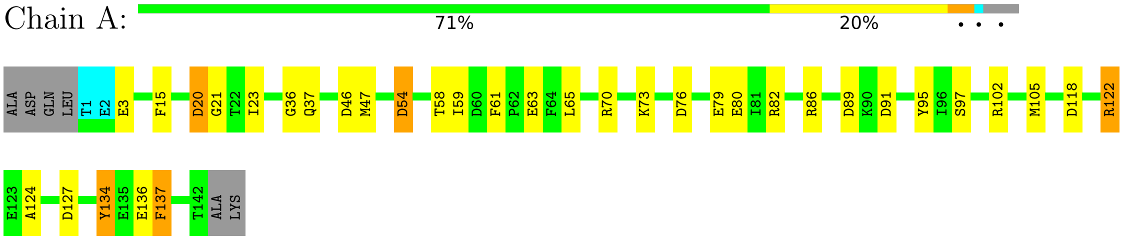
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.100 Score per residue for model 100

- Molecule 1: calmodulin

Chain A:



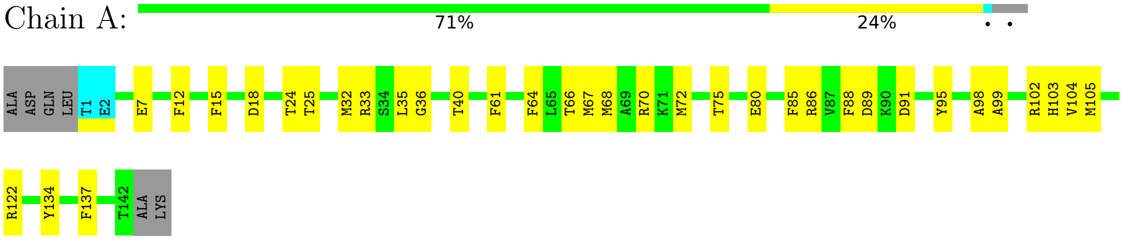
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.101 Score per residue for model 101

- Molecule 1: calmodulin

Chain A:



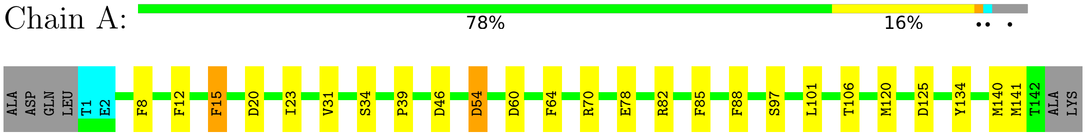
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.102 Score per residue for model 102

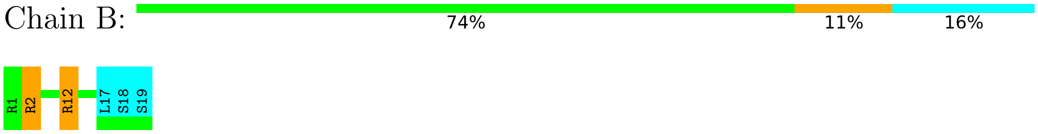
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

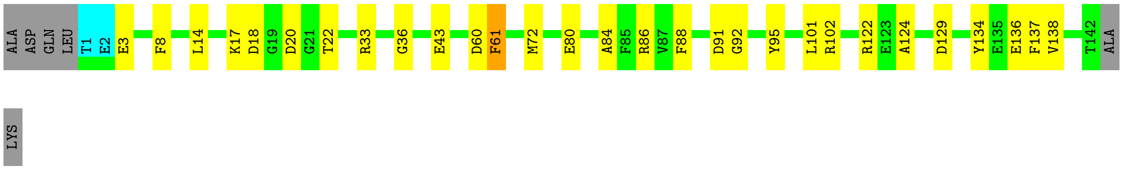
Chain B:



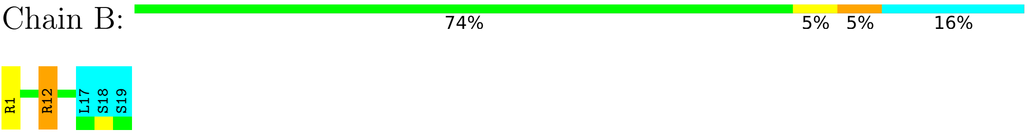
4.2.103 Score per residue for model 103

- Molecule 1: calmodulin

Chain A:

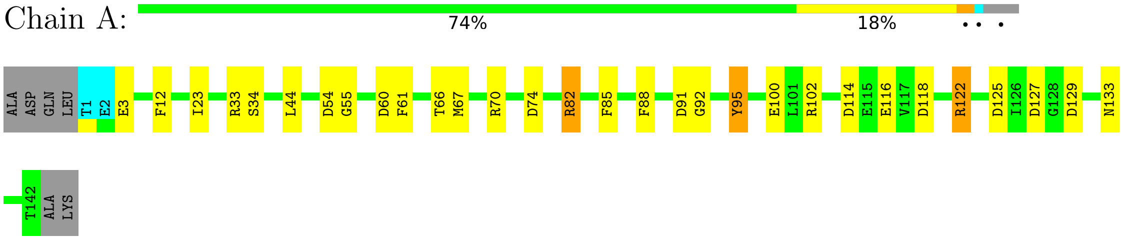


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.104 Score per residue for model 104

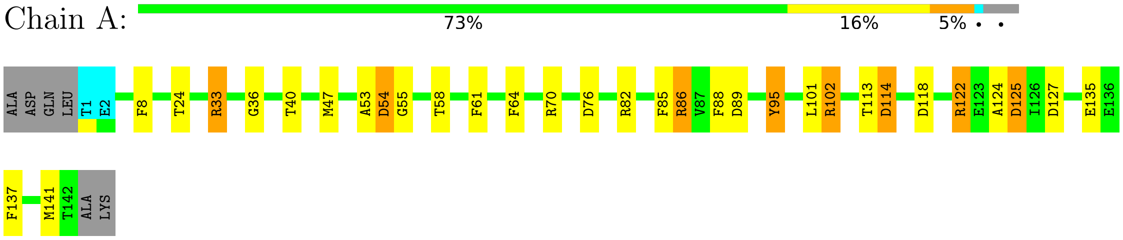
- Molecule 1: calmodulin



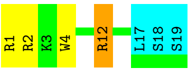
- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.105 Score per residue for model 105

- Molecule 1: calmodulin



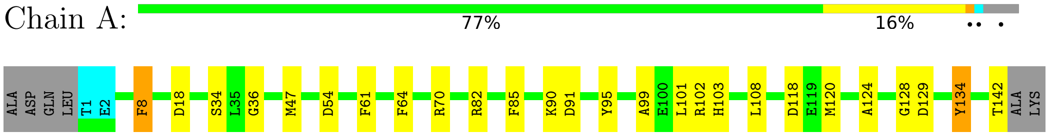
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.106 Score per residue for model 106

- Molecule 1: calmodulin

Chain A:



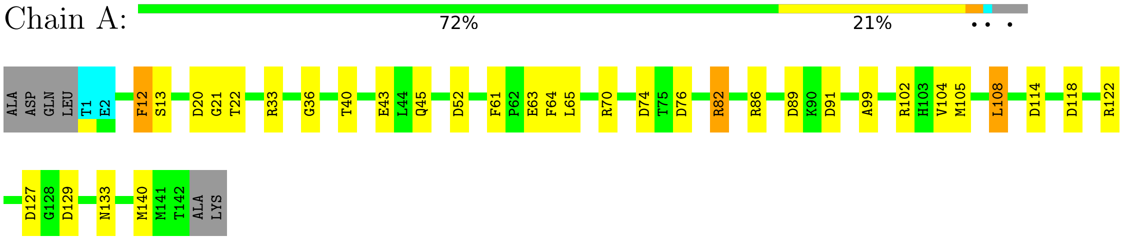
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.107 Score per residue for model 107

- Molecule 1: calmodulin

Chain A:



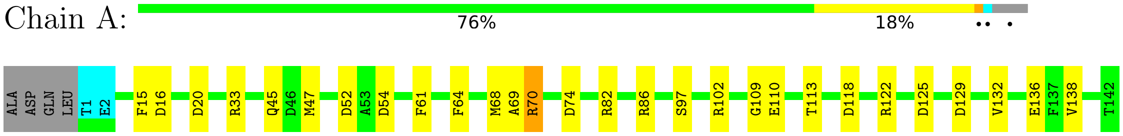
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

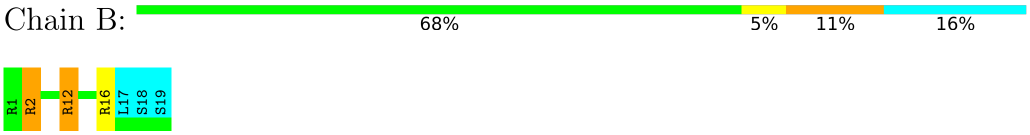
4.2.108 Score per residue for model 108

- Molecule 1: calmodulin

Chain A:

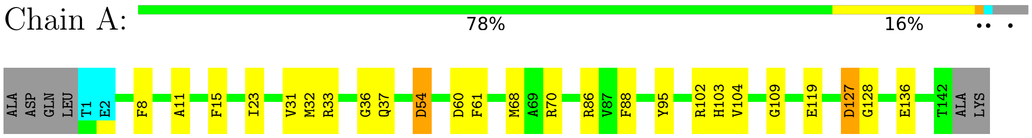


- Molecule 2: 19-mer peptide from Myosin light chain kinase

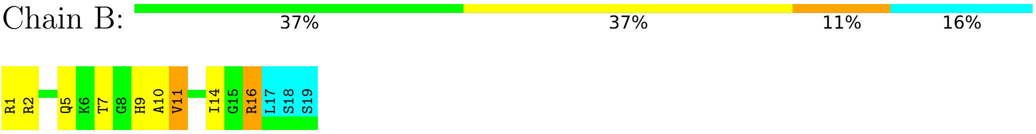


4.2.109 Score per residue for model 109

- Molecule 1: calmodulin

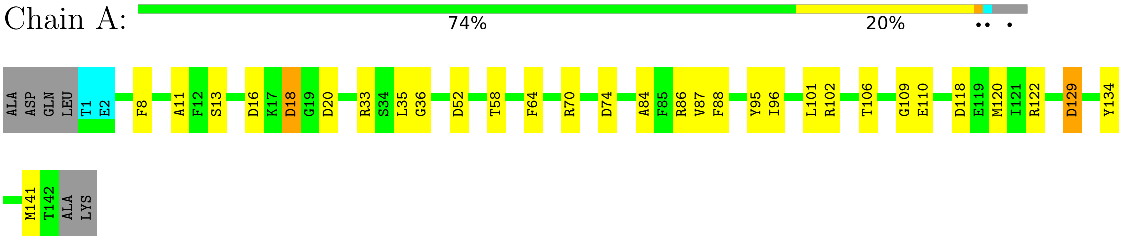


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.110 Score per residue for model 110

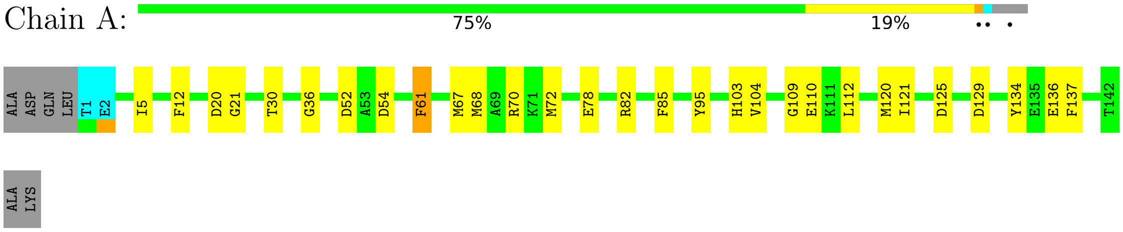
- Molecule 1: calmodulin



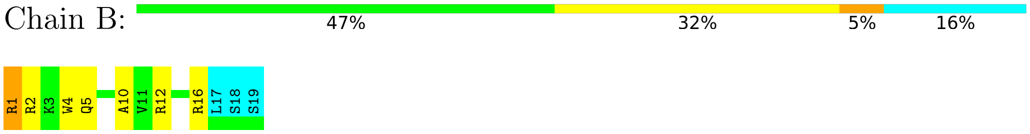
- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.111 Score per residue for model 111

- Molecule 1: calmodulin

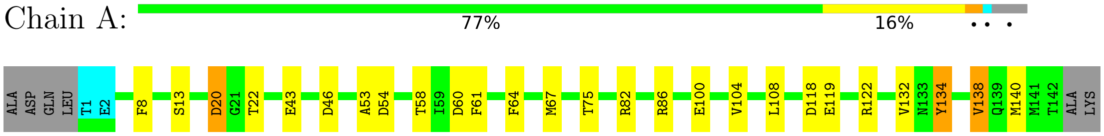


- Molecule 2: 19-mer peptide from Myosin light chain kinase

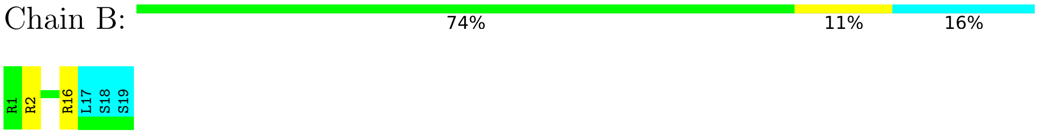


4.2.112 Score per residue for model 112

- Molecule 1: calmodulin

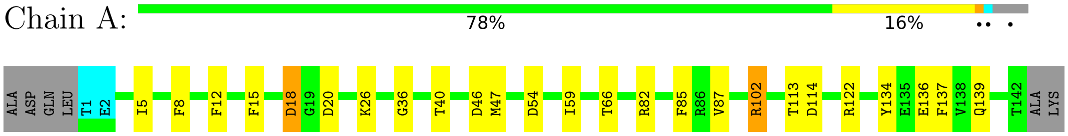


- Molecule 2: 19-mer peptide from Myosin light chain kinase

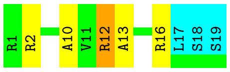


4.2.113 Score per residue for model 113

- Molecule 1: calmodulin



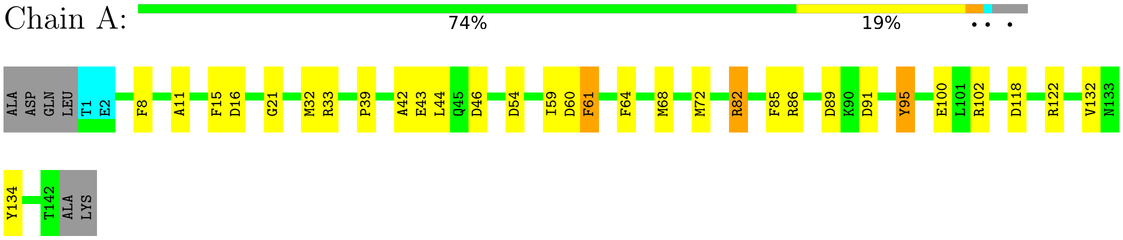
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.114 Score per residue for model 114

- Molecule 1: calmodulin

Chain A:



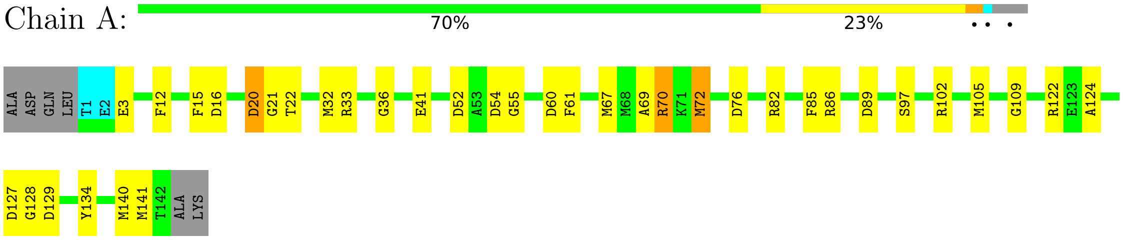
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.115 Score per residue for model 115

- Molecule 1: calmodulin

Chain A:



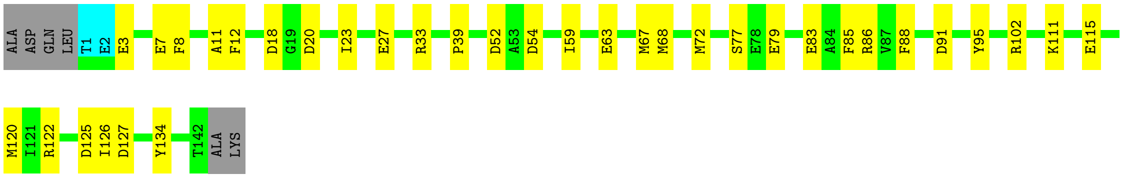
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.116 Score per residue for model 116

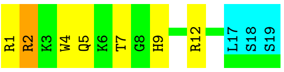
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

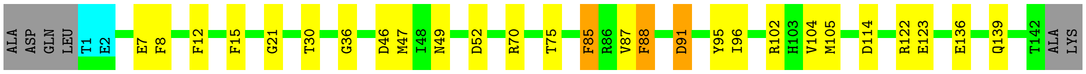
Chain B:



4.2.117 Score per residue for model 117

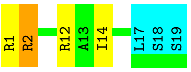
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

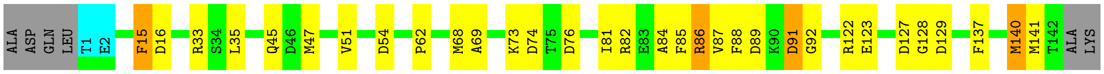
Chain B:



4.2.118 Score per residue for model 118

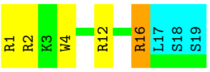
- Molecule 1: calmodulin

Chain A:



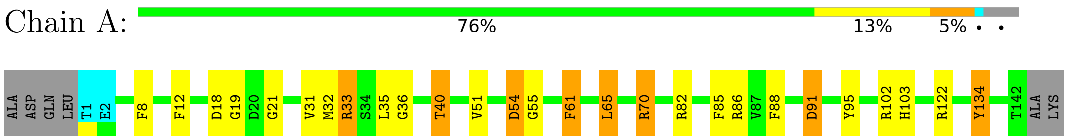
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:



4.2.119 Score per residue for model 119

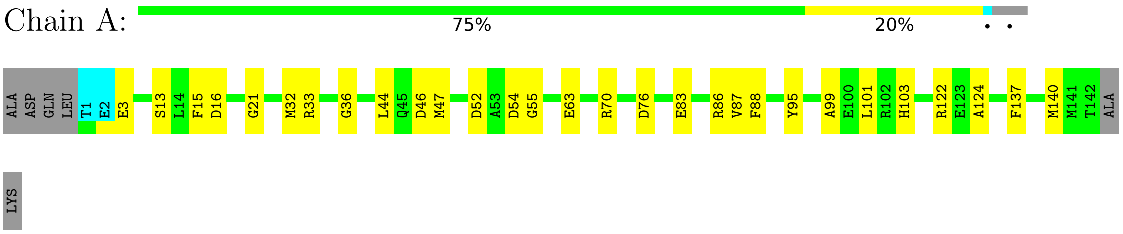
- Molecule 1: calmodulin



- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.120 Score per residue for model 120

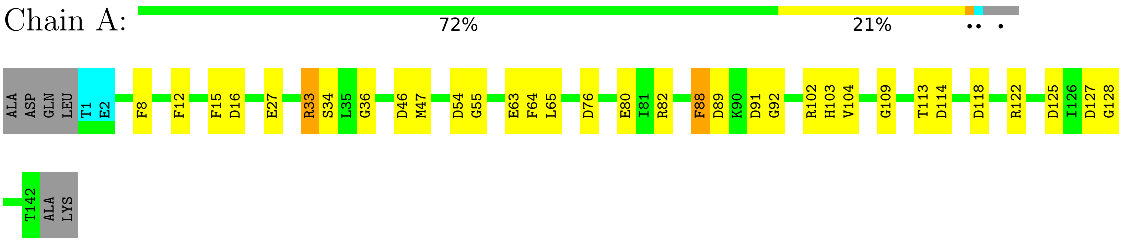
- Molecule 1: calmodulin



- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.121 Score per residue for model 121

- Molecule 1: calmodulin



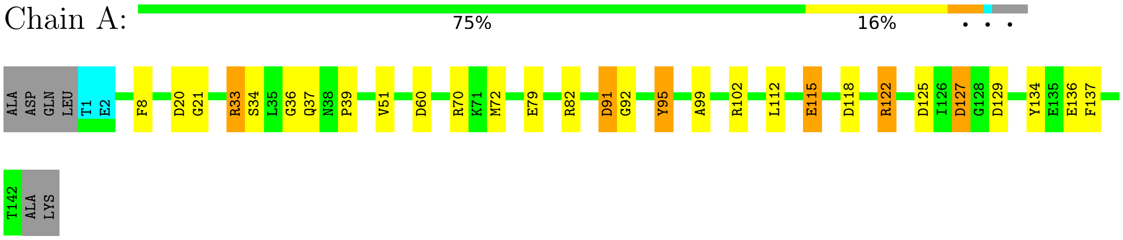
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.122 Score per residue for model 122

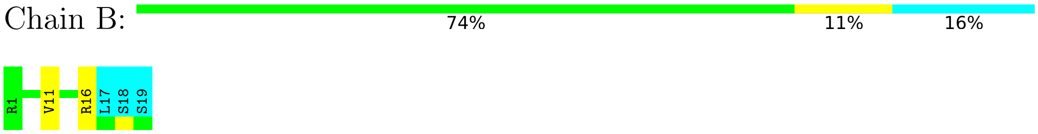
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

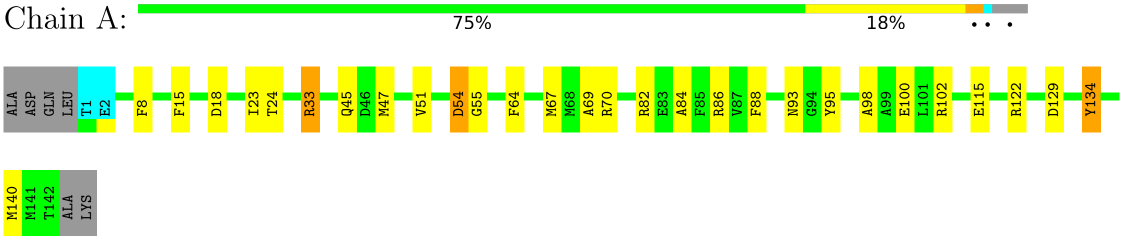
Chain B:



4.2.123 Score per residue for model 123

- Molecule 1: calmodulin

Chain A:



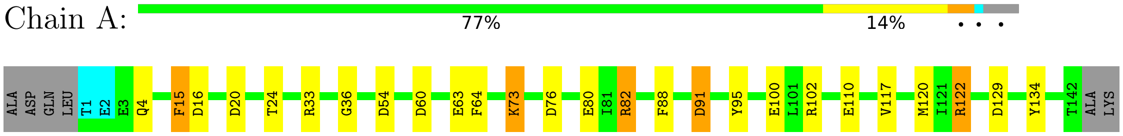
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.124 Score per residue for model 124

- Molecule 1: calmodulin

Chain A:



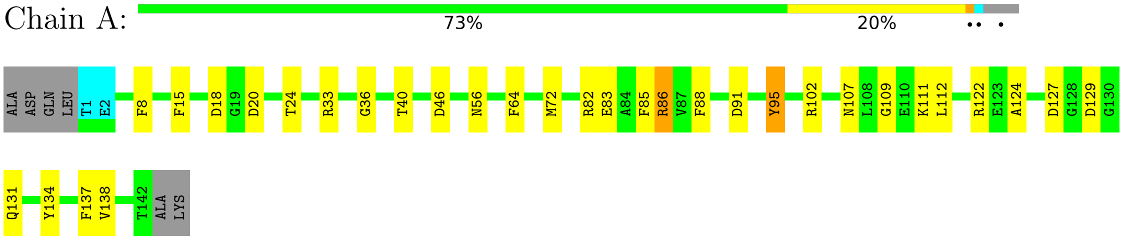
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.125 Score per residue for model 125

- Molecule 1: calmodulin

Chain A:



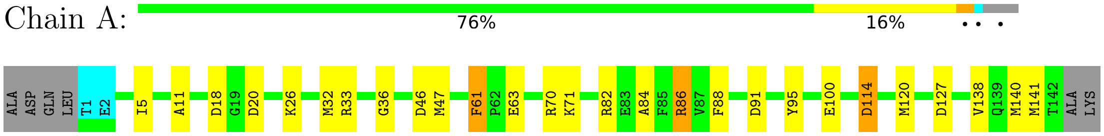
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.126 Score per residue for model 126

- Molecule 1: calmodulin

Chain A:

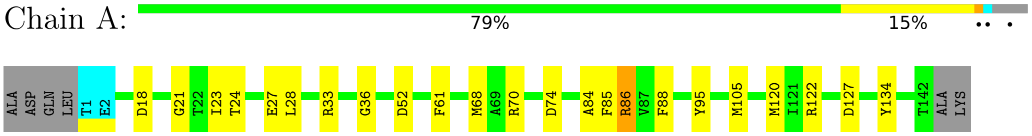


- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.127 Score per residue for model 127

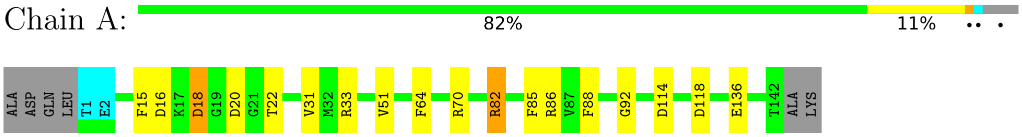
- Molecule 1: calmodulin



- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.128 Score per residue for model 128

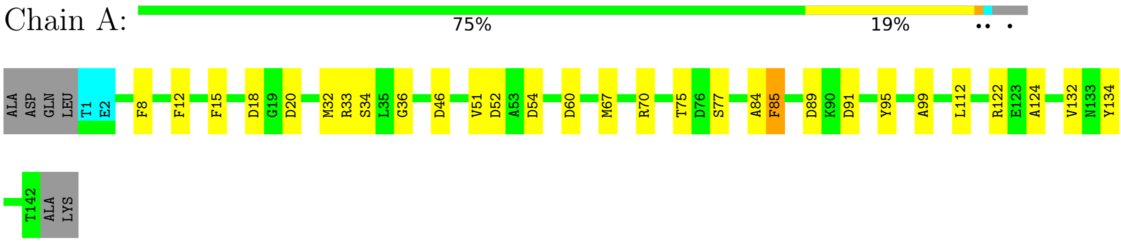
- Molecule 1: calmodulin



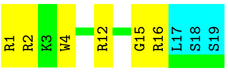
- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.129 Score per residue for model 129

- Molecule 1: calmodulin



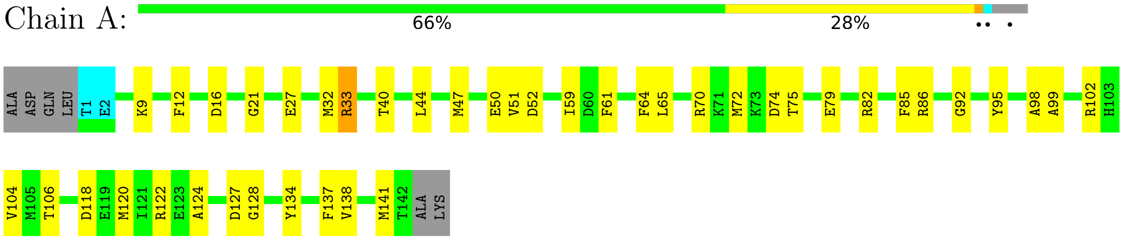
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.130 Score per residue for model 130

- Molecule 1: calmodulin

Chain A:



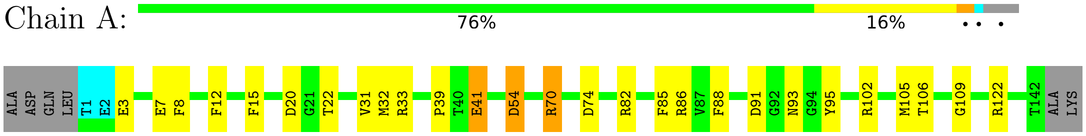
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.131 Score per residue for model 131

- Molecule 1: calmodulin

Chain A:



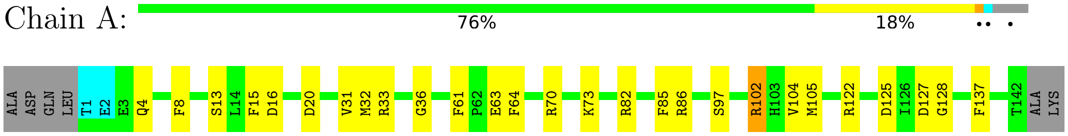
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.132 Score per residue for model 132

- Molecule 1: calmodulin

Chain A:



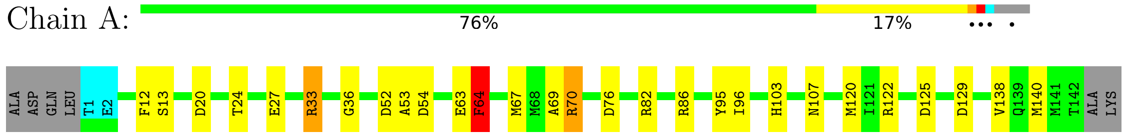
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.133 Score per residue for model 133

- Molecule 1: calmodulin

Chain A:



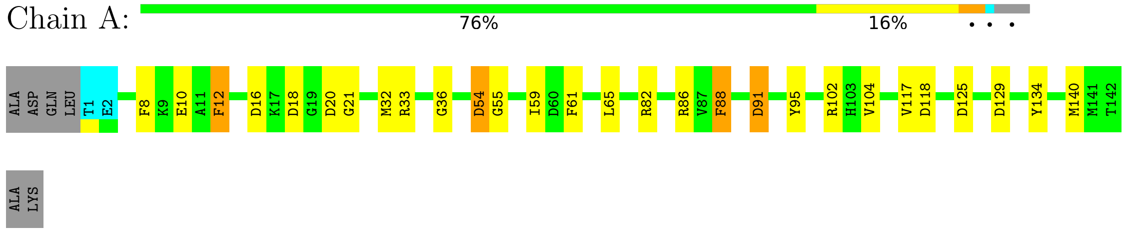
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.134 Score per residue for model 134

- Molecule 1: calmodulin

Chain A:



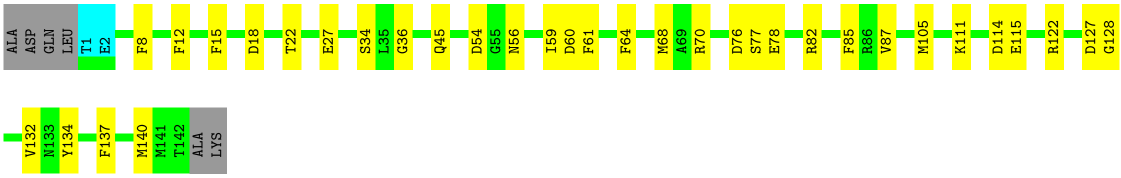
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.135 Score per residue for model 135

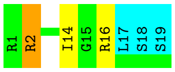
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

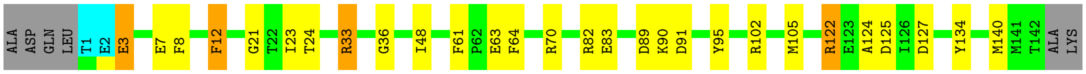
Chain B:



4.2.136 Score per residue for model 136

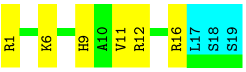
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

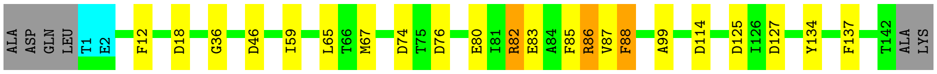
Chain B:



4.2.137 Score per residue for model 137

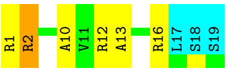
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

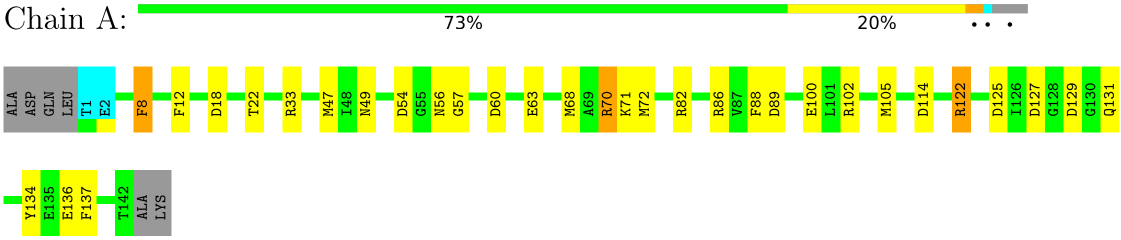
Chain B:



4.2.138 Score per residue for model 138

- Molecule 1: calmodulin

Chain A:



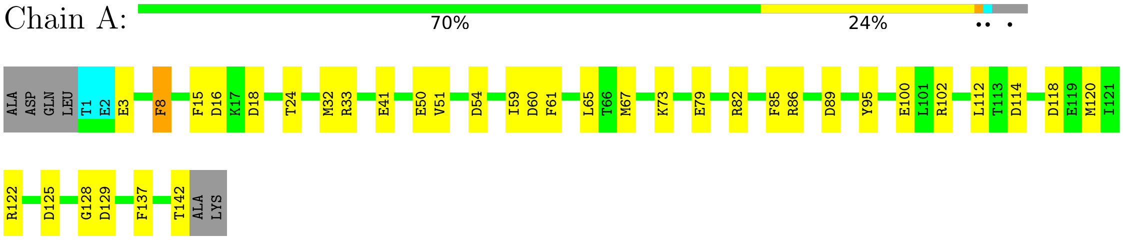
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.139 Score per residue for model 139

- Molecule 1: calmodulin

Chain A:



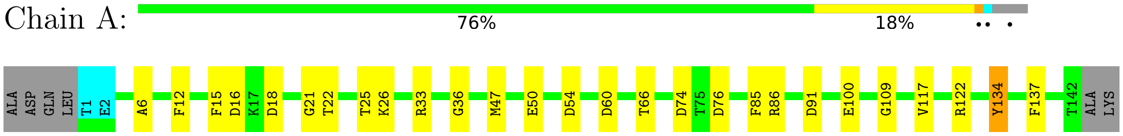
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.140 Score per residue for model 140

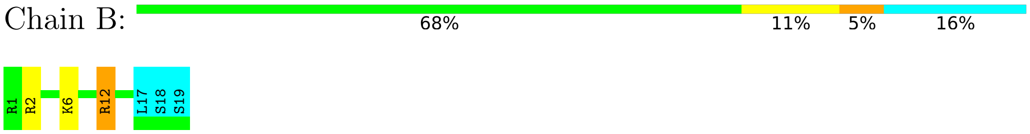
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

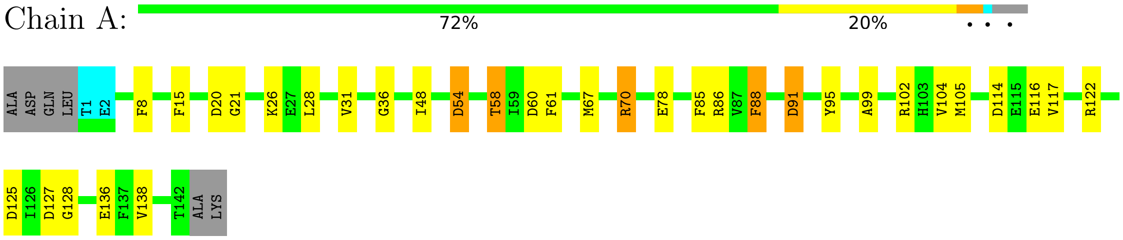
Chain B:



4.2.141 Score per residue for model 141

- Molecule 1: calmodulin

Chain A:



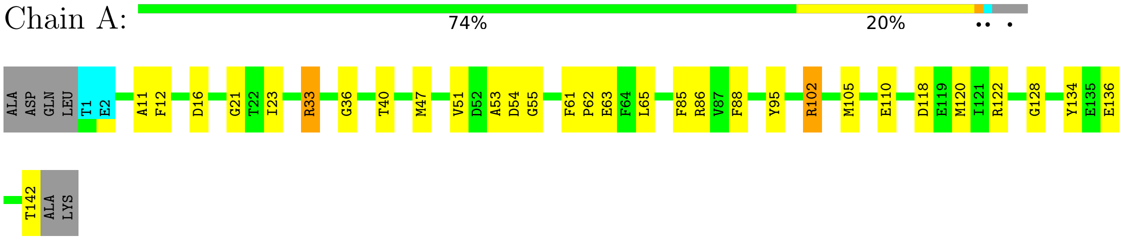
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.142 Score per residue for model 142

- Molecule 1: calmodulin

Chain A:

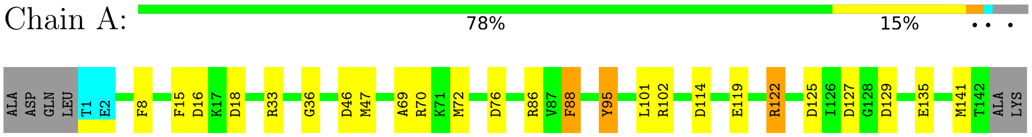


- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.143 Score per residue for model 143

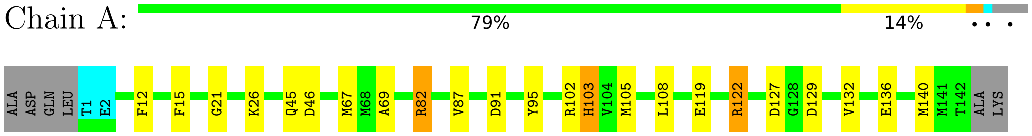
- Molecule 1: calmodulin



- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.144 Score per residue for model 144

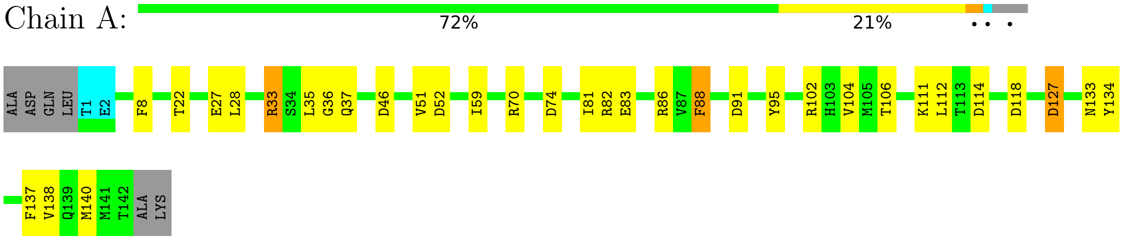
- Molecule 1: calmodulin



- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.145 Score per residue for model 145

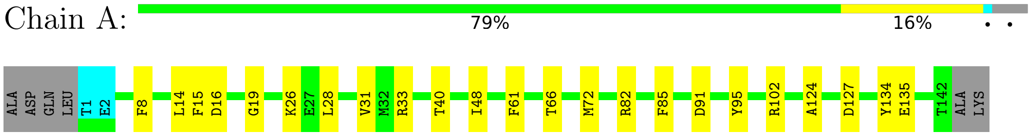
- Molecule 1: calmodulin



- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.146 Score per residue for model 146

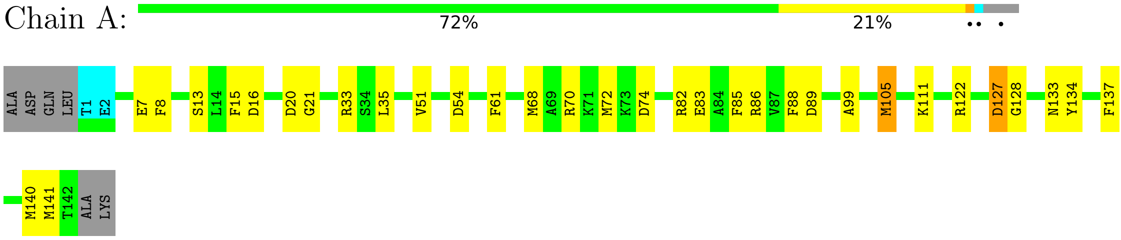
- Molecule 1: calmodulin



- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.147 Score per residue for model 147

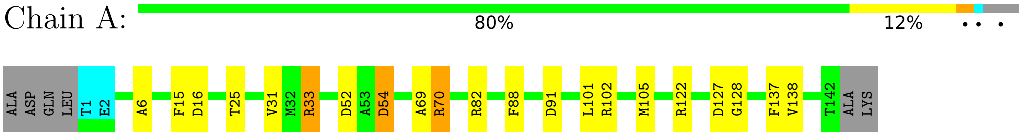
- Molecule 1: calmodulin



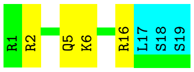
- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.148 Score per residue for model 148

- Molecule 1: calmodulin



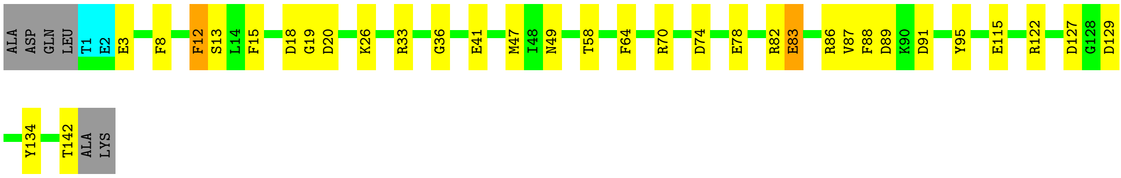
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.149 Score per residue for model 149

- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

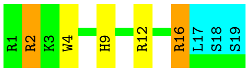
4.2.150 Score per residue for model 150

- Molecule 1: calmodulin

Chain A:

- Molecule 2: 19-mer peptide from Myosin light chain kinase

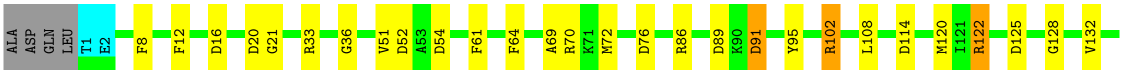
Chain B:

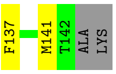


4.2.151 Score per residue for model 151

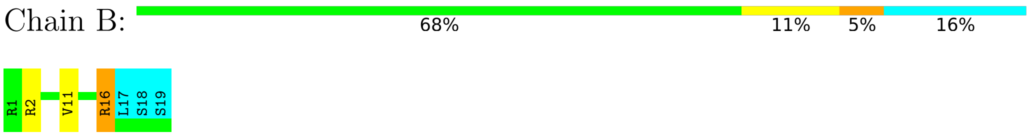
- Molecule 1: calmodulin

Chain A:



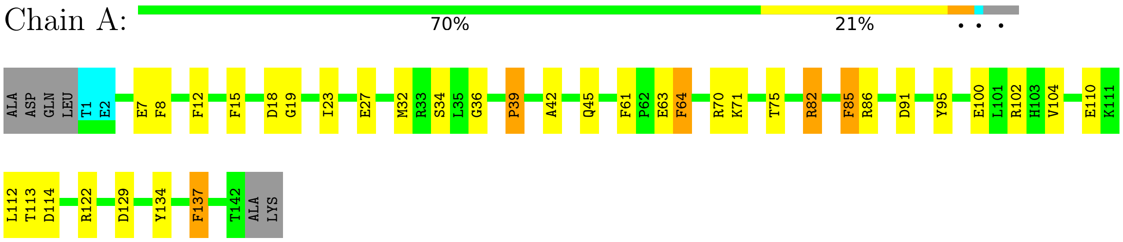


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.152 Score per residue for model 152

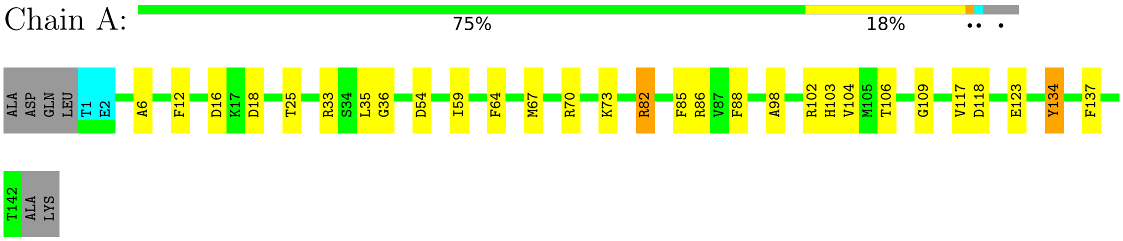
- Molecule 1: calmodulin



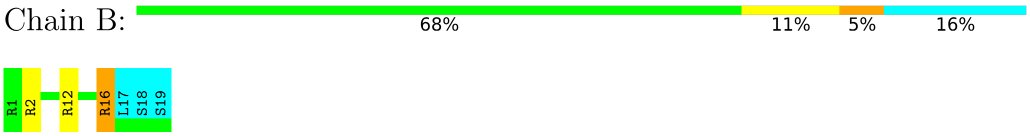
- Molecule 2: 19-mer peptide from Myosin light chain kinase

4.2.153 Score per residue for model 153

- Molecule 1: calmodulin



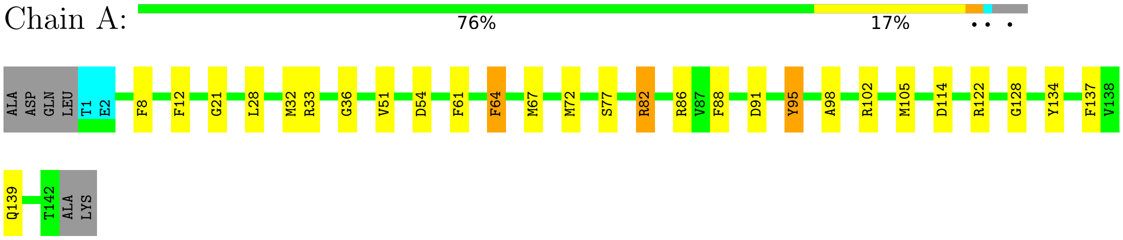
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.154 Score per residue for model 154

- Molecule 1: calmodulin

Chain A:



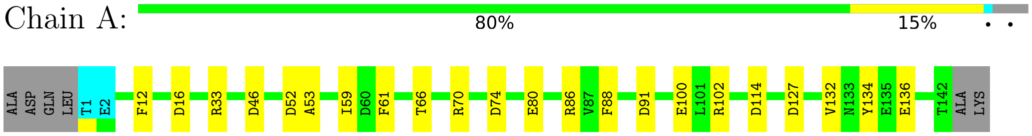
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.155 Score per residue for model 155

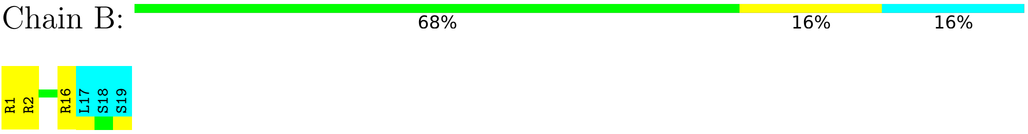
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

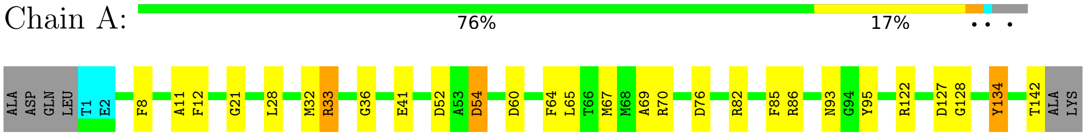
Chain B:



4.2.156 Score per residue for model 156

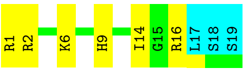
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

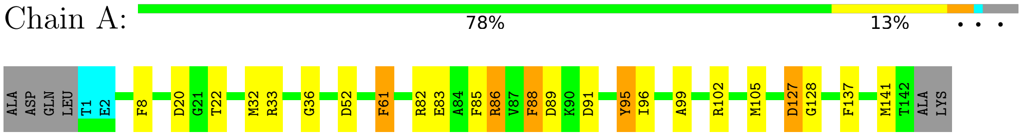
Chain B:



4.2.157 Score per residue for model 157

- Molecule 1: calmodulin

Chain A:



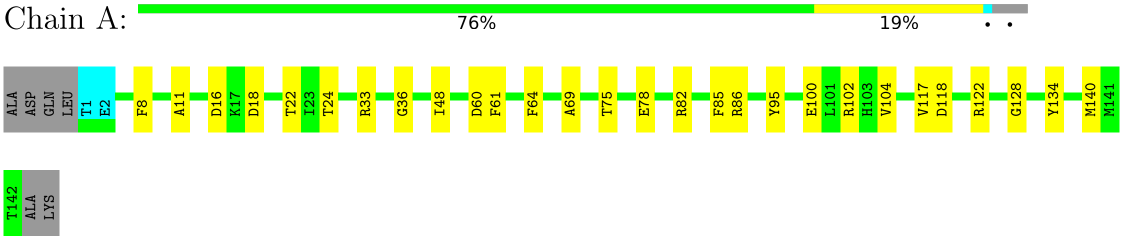
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.158 Score per residue for model 158

- Molecule 1: calmodulin

Chain A:



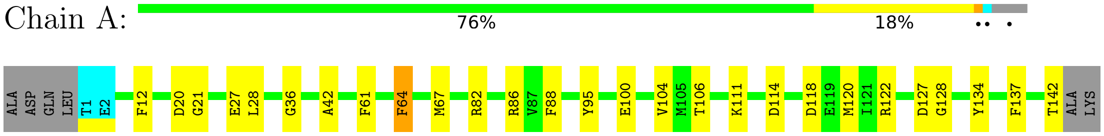
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:

4.2.159 Score per residue for model 159

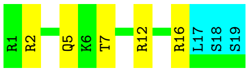
- Molecule 1: calmodulin

Chain A:



- Molecule 2: 19-mer peptide from Myosin light chain kinase

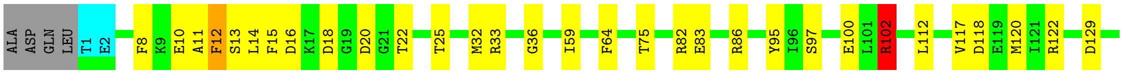
Chain B:

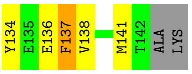


4.2.160 Score per residue for model 160

- Molecule 1: calmodulin

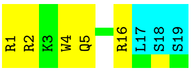
Chain A:





- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B:



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *CHARMM*.

Of the 160 calculated structures, 160 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CHARMM	refinement	C30

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

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	0.97±0.00	0±0/1117 (0.0± 0.0%)	1.97±0.07	28±5/1499 (1.9± 0.4%)
2	B	1.26±0.00	0±0/138 (0.0± 0.0%)	2.24±0.22	5±2/183 (3.0± 1.1%)
All	All	1.00	0/200800 (0.0%)	2.00	5351/269120 (2.0%)

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	2.7±1.3
2	B	0.0±0.0	1.2±1.0
All	All	0	631

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	70	ARG	NE-CZ-NH2	-26.19	107.20	120.30	152	58
1	A	33	ARG	NE-CZ-NH1	24.27	132.44	120.30	88	91
1	A	88	PHE	CB-CG-CD2	20.29	135.00	120.80	6	48
2	B	1	ARG	NE-CZ-NH2	-20.05	110.28	120.30	103	66
1	A	70	ARG	NE-CZ-NH1	18.75	129.67	120.30	7	78
1	A	82	ARG	NE-CZ-NH1	18.51	129.56	120.30	150	79
2	B	16	ARG	NE-CZ-NH1	18.38	129.49	120.30	145	78
2	B	12	ARG	NE-CZ-NH1	18.10	129.35	120.30	129	81
1	A	86	ARG	NE-CZ-NH2	-17.93	111.33	120.30	50	59
2	B	1	ARG	NE-CZ-NH1	17.68	129.14	120.30	92	86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	82	ARG	NE-CZ-NH2	-17.51	111.55	120.30	138	62
1	A	122	ARG	NE-CZ-NH1	17.30	128.95	120.30	101	81
2	B	12	ARG	NE-CZ-NH2	-17.27	111.66	120.30	139	76
1	A	122	ARG	NE-CZ-NH2	-16.85	111.88	120.30	78	72
1	A	102	ARG	NE-CZ-NH1	16.37	128.48	120.30	110	75
1	A	86	ARG	NE-CZ-NH1	16.32	128.46	120.30	131	83
2	B	16	ARG	NE-CZ-NH2	-15.93	112.34	120.30	145	67
1	A	134	TYR	CB-CG-CD1	-15.88	111.47	121.00	76	38
2	B	2	ARG	NE-CZ-NH1	15.62	128.11	120.30	145	76
2	B	2	ARG	NE-CZ-NH2	-15.61	112.50	120.30	1	70
1	A	102	ARG	NE-CZ-NH2	-15.10	112.75	120.30	153	68
1	A	134	TYR	CB-CG-CD2	-15.01	112.00	121.00	86	61
1	A	8	PHE	CB-CG-CD2	-14.78	110.45	120.80	48	56
1	A	95	TYR	CB-CG-CD2	14.68	129.81	121.00	93	54
1	A	15	PHE	CB-CG-CD1	-14.47	110.67	120.80	100	35
1	A	12	PHE	CB-CG-CD1	-14.26	110.82	120.80	72	39
1	A	85	PHE	CB-CG-CD2	-14.21	110.86	120.80	147	32
1	A	33	ARG	NE-CZ-NH2	-14.07	113.26	120.30	98	50
1	A	64	PHE	CB-CG-CD1	14.00	130.60	120.80	75	37
1	A	61	PHE	CB-CG-CD2	-13.72	111.20	120.80	8	45
1	A	137	PHE	CB-CG-CD2	13.23	130.06	120.80	28	30
1	A	46	ASP	CB-CG-OD1	13.21	130.19	118.30	21	24
1	A	16	ASP	CB-CG-OD2	-12.88	106.71	118.30	31	19
1	A	127	ASP	CB-CG-OD2	12.87	129.88	118.30	14	32
1	A	88	PHE	CB-CG-CD1	-12.78	111.85	120.80	44	48
1	A	64	PHE	CB-CG-CD2	12.73	129.71	120.80	26	29
1	A	89	ASP	CB-CG-OD1	12.56	129.61	118.30	115	18
1	A	72	MET	CG-SD-CE	-12.31	80.51	100.20	32	26
1	A	137	PHE	CB-CG-CD1	-12.30	112.19	120.80	130	33
1	A	54	ASP	CB-CG-OD1	12.22	129.30	118.30	80	19
1	A	15	PHE	CB-CG-CD2	12.21	129.35	120.80	82	48
1	A	95	TYR	CB-CG-CD1	12.04	128.23	121.00	4	44
1	A	18	ASP	CB-CG-OD2	-11.97	107.53	118.30	54	21
1	A	129	ASP	CB-CG-OD1	11.92	129.03	118.30	56	44
1	A	8	PHE	CB-CG-CD1	-11.83	112.52	120.80	152	43
1	A	85	PHE	CB-CG-CD1	11.65	128.96	120.80	147	42
1	A	46	ASP	CB-CG-OD2	-11.53	107.92	118.30	61	16
1	A	118	ASP	CB-CG-OD2	11.46	128.62	118.30	36	20
1	A	125	ASP	CB-CG-OD2	-11.41	108.03	118.30	33	22
1	A	52	ASP	CB-CG-OD1	11.25	128.42	118.30	107	25
1	A	20	ASP	CB-CG-OD1	11.14	128.32	118.30	62	38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	61	PHE	CB-CG-CD1	11.14	128.59	120.80	8	37
1	A	16	ASP	CB-CG-OD1	11.10	128.29	118.30	31	33
1	A	76	ASP	CB-CG-OD1	10.65	127.89	118.30	105	34
1	A	120	MET	CG-SD-CE	-10.56	83.31	100.20	110	34
1	A	91	ASP	CB-CG-OD1	10.48	127.73	118.30	148	32
1	A	127	ASP	CB-CG-OD1	10.39	127.65	118.30	8	22
1	A	60	ASP	CB-CG-OD1	10.31	127.58	118.30	7	17
1	A	18	ASP	CB-CG-OD1	10.26	127.54	118.30	54	25
1	A	12	PHE	CB-CG-CD2	10.22	127.96	120.80	36	33
1	A	105	MET	CG-SD-CE	-10.14	83.98	100.20	95	42
1	A	60	ASP	CB-CG-OD2	10.06	127.36	118.30	139	18
1	A	114	ASP	CB-CG-OD1	10.04	127.33	118.30	35	21
1	A	68	MET	CG-SD-CE	-9.90	84.37	100.20	7	31
1	A	20	ASP	CB-CG-OD2	-9.85	109.44	118.30	159	28
1	A	104	VAL	CA-CB-CG1	9.77	125.55	110.90	158	14
1	A	91	ASP	CB-CG-OD2	9.71	127.04	118.30	6	41
1	A	54	ASP	CB-CG-OD2	9.59	126.93	118.30	55	31
1	A	118	ASP	CB-CG-OD1	9.59	126.93	118.30	130	31
1	A	52	ASP	CB-CG-OD2	9.57	126.92	118.30	115	25
1	A	82	ARG	NH1-CZ-NH2	-9.56	108.88	119.40	150	14
1	A	32	MET	CG-SD-CE	-9.49	85.01	100.20	115	39
1	A	70	ARG	NH1-CZ-NH2	9.31	129.64	119.40	152	17
2	B	1	ARG	NH1-CZ-NH2	-9.25	109.22	119.40	14	11
1	A	114	ASP	CB-CG-OD2	-9.22	110.01	118.30	152	18
1	A	89	ASP	CB-CG-OD2	-9.19	110.03	118.30	26	20
2	B	11	VAL	CA-CB-CG1	9.18	124.67	110.90	34	11
1	A	67	MET	CG-SD-CE	-9.12	85.61	100.20	141	38
1	A	134	TYR	CG-CD1-CE1	-9.10	114.02	121.30	76	19
1	A	113	THR	CA-CB-CG2	-9.05	99.72	112.40	88	11
1	A	51	VAL	CG1-CB-CG2	-8.99	96.52	110.90	9	2
1	A	74	ASP	CB-CG-OD1	8.90	126.31	118.30	93	23
1	A	100	GLU	OE1-CD-OE2	-8.88	112.65	123.30	104	23
1	A	33	ARG	NH1-CZ-NH2	-8.88	109.64	119.40	38	7
1	A	74	ASP	CB-CG-OD2	8.85	126.26	118.30	15	17
1	A	136	GLU	OE1-CD-OE2	-8.85	112.69	123.30	20	37
1	A	13	SER	N-CA-CB	8.81	123.72	110.50	120	8
1	A	102	ARG	NH1-CZ-NH2	-8.76	109.77	119.40	75	12
1	A	51	VAL	CA-CB-CG1	-8.75	97.78	110.90	145	16
2	B	4	TRP	CB-CG-CD2	-8.63	115.38	126.60	124	9
1	A	47	MET	CG-SD-CE	-8.61	86.42	100.20	29	33
1	A	76	ASP	CB-CG-OD2	-8.60	110.56	118.30	105	23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	10	GLU	OE1-CD-OE2	-8.60	112.98	123.30	72	1
1	A	125	ASP	CB-CG-OD1	8.57	126.02	118.30	132	22
1	A	24	THR	CA-CB-CG2	-8.54	100.45	112.40	158	15
1	A	58	THR	CA-CB-CG2	-8.46	100.56	112.40	29	15
2	B	11	VAL	CG1-CB-CG2	-8.46	97.37	110.90	18	7
1	A	98	ALA	CB-CA-C	8.40	122.70	110.10	153	10
1	A	69	ALA	CB-CA-C	-8.39	97.52	110.10	81	13
1	A	75	THR	CA-CB-CG2	-8.30	100.77	112.40	59	19
1	A	66	THR	CA-CB-CG2	-8.23	100.88	112.40	104	5
2	B	12	ARG	NH1-CZ-NH2	-8.22	110.36	119.40	24	15
1	A	134	TYR	CG-CD2-CE2	-8.20	114.74	121.30	153	18
1	A	99	ALA	N-CA-CB	8.15	121.51	110.10	137	16
1	A	87	VAL	CG1-CB-CG2	8.15	123.94	110.90	135	9
1	A	63	GLU	OE1-CD-OE2	-8.09	113.59	123.30	23	30
1	A	141	MET	CG-SD-CE	-8.09	87.26	100.20	110	28
1	A	56	ASN	N-CA-CB	8.05	125.09	110.60	61	1
1	A	98	ALA	N-CA-CB	-7.98	98.92	110.10	84	9
1	A	122	ARG	NH1-CZ-NH2	-7.95	110.65	119.40	105	10
1	A	140	MET	CG-SD-CE	-7.91	87.54	100.20	6	25
1	A	12	PHE	N-CA-CB	-7.90	96.37	110.60	85	6
1	A	25	THR	CA-CB-CG2	-7.88	101.36	112.40	62	19
2	B	10	ALA	CB-CA-C	7.76	121.75	110.10	28	6
1	A	106	THR	CA-CB-CG2	7.76	123.27	112.40	159	7
1	A	82	ARG	O-C-N	-7.74	110.32	122.70	130	3
1	A	14	LEU	CB-CG-CD1	7.74	124.15	111.00	160	5
1	A	53	ALA	N-CA-CB	7.71	120.90	110.10	22	7
2	B	11	VAL	O-C-N	-7.67	110.42	122.70	61	3
1	A	61	PHE	CB-CA-C	7.60	125.60	110.40	66	7
1	A	20	ASP	CB-CA-C	7.57	125.54	110.40	112	5
1	A	137	PHE	O-C-N	-7.56	110.60	122.70	138	6
1	A	95	TYR	CG-CD1-CE1	-7.56	115.25	121.30	13	12
1	A	31	VAL	CA-CB-CG1	7.55	122.23	110.90	94	7
2	B	7	THR	O-C-N	-7.55	110.37	123.20	158	8
1	A	137	PHE	CG-CD2-CE2	-7.54	112.51	120.80	87	2
2	B	14	ILE	O-C-N	-7.53	110.41	123.20	16	6
1	A	99	ALA	CB-CA-C	7.51	121.36	110.10	7	5
1	A	42	ALA	N-CA-CB	7.49	120.59	110.10	152	7
1	A	27	GLU	OE1-CD-OE2	-7.49	114.31	123.30	145	22
1	A	97	SER	O-C-N	-7.48	110.73	122.70	115	2
1	A	11	ALA	N-CA-CB	7.48	120.57	110.10	114	10
2	B	4	TRP	CB-CG-CD1	7.47	136.71	127.00	124	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	78	GLU	O-C-N	-7.45	110.78	122.70	111	3
1	A	117	VAL	CA-CB-CG2	-7.44	99.74	110.90	158	6
1	A	14	LEU	CB-CG-CD2	-7.43	98.36	111.00	44	4
1	A	95	TYR	CZ-CE2-CD2	-7.43	113.12	119.80	84	8
1	A	77	SER	N-CA-CB	7.37	121.56	110.50	53	9
1	A	49	ASN	O-C-N	-7.36	110.92	122.70	149	4
1	A	6	ALA	N-CA-CB	-7.34	99.82	110.10	4	5
1	A	129	ASP	CB-CG-OD2	-7.33	111.71	118.30	81	23
1	A	82	ARG	CD-NE-CZ	7.27	133.78	123.60	126	3
1	A	86	ARG	NH1-CZ-NH2	-7.27	111.40	119.40	54	10
1	A	7	GLU	OE1-CD-OE2	-7.27	114.58	123.30	117	6
1	A	40	THR	CA-CB-CG2	-7.21	102.30	112.40	63	12
1	A	136	GLU	O-C-N	-7.20	111.17	122.70	108	2
1	A	123	GLU	OE1-CD-OE2	-7.20	114.67	123.30	117	12
2	B	1	ARG	CD-NE-CZ	7.19	133.67	123.60	99	2
1	A	13	SER	O-C-N	-7.19	111.20	122.70	132	3
2	B	10	ALA	N-CA-CB	7.16	120.12	110.10	149	11
1	A	135	GLU	OE1-CD-OE2	-7.16	114.71	123.30	66	5
1	A	132	VAL	CA-CB-CG1	7.14	121.62	110.90	9	7
1	A	12	PHE	CG-CD2-CE2	-7.14	112.95	120.80	43	5
1	A	47	MET	CA-CB-CG	7.11	125.38	113.30	80	4
2	B	13	ALA	CB-CA-C	7.10	120.76	110.10	137	7
1	A	99	ALA	O-C-N	-7.10	111.34	122.70	85	1
1	A	132	VAL	CA-CB-CG2	-7.09	100.27	110.90	47	4
2	B	11	VAL	CB-CA-C	7.08	124.86	111.40	55	2
1	A	138	VAL	CG1-CB-CG2	-7.08	99.57	110.90	69	12
1	A	95	TYR	CG-CD2-CE2	-7.08	115.64	121.30	61	8
1	A	104	VAL	CA-CB-CG2	-7.08	100.28	110.90	101	10
1	A	88	PHE	N-CA-CB	7.07	123.32	110.60	45	6
1	A	64	PHE	CG-CD2-CE2	-7.05	113.04	120.80	86	5
2	B	16	ARG	CB-CA-C	7.05	124.51	110.40	135	2
1	A	124	ALA	CB-CA-C	-7.05	99.53	110.10	130	5
1	A	87	VAL	CA-CB-CG1	7.04	121.46	110.90	43	5
1	A	98	ALA	C-N-CA	7.01	139.23	121.70	11	3
1	A	44	LEU	CB-CG-CD1	6.99	122.89	111.00	50	3
1	A	117	VAL	CA-CB-CG1	6.99	121.39	110.90	62	8
1	A	138	VAL	O-C-N	-6.98	111.54	122.70	145	1
2	B	2	ARG	NH1-CZ-NH2	-6.97	111.73	119.40	145	4
1	A	103	HIS	CA-CB-CG	-6.97	101.75	113.60	52	6
1	A	47	MET	N-CA-CB	6.97	123.14	110.60	118	3
1	A	53	ALA	CB-CA-C	6.96	120.53	110.10	29	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	102	ARG	CD-NE-CZ	-6.95	113.88	123.60	70	5
1	A	79	GLU	OE1-CD-OE2	-6.94	114.97	123.30	116	8
1	A	65	LEU	O-C-N	-6.94	111.60	122.70	43	3
1	A	58	THR	N-CA-CB	6.90	123.42	110.30	100	8
1	A	119	GLU	O-C-N	-6.90	111.66	122.70	109	4
1	A	47	MET	O-C-N	-6.88	111.69	122.70	138	6
2	B	7	THR	N-CA-CB	6.87	123.36	110.30	62	5
1	A	65	LEU	CB-CG-CD1	-6.84	99.37	111.00	28	1
1	A	22	THR	CA-CB-CG2	-6.83	102.84	112.40	115	6
1	A	55	GLY	O-C-N	-6.81	111.80	122.70	46	3
1	A	32	MET	CA-CB-CG	6.80	124.87	113.30	120	4
2	B	4	TRP	CG-CD2-CE3	-6.79	127.79	133.90	48	8
1	A	80	GLU	OE1-CD-OE2	-6.78	115.16	123.30	93	9
1	A	69	ALA	O-C-N	-6.76	111.88	122.70	48	1
1	A	131	GLN	O-C-N	-6.75	111.89	122.70	125	1
1	A	44	LEU	O-C-N	-6.75	111.90	122.70	17	2
2	B	9	HIS	CB-CA-C	-6.75	96.91	110.40	27	2
2	B	14	ILE	C-N-CA	6.74	136.46	122.30	72	3
2	B	16	ARG	CD-NE-CZ	-6.73	114.17	123.60	1	5
1	A	95	TYR	CB-CA-C	-6.69	97.03	110.40	156	2
1	A	78	GLU	OE1-CD-OE2	-6.68	115.28	123.30	158	4
1	A	127	ASP	C-N-CA	6.68	136.33	122.30	149	1
1	A	134	TYR	CD1-CE1-CZ	-6.67	113.79	119.80	21	3
2	B	11	VAL	CA-CB-CG2	-6.65	100.93	110.90	97	3
1	A	40	THR	O-C-N	-6.64	112.07	122.70	83	3
1	A	64	PHE	O-C-N	-6.64	112.08	122.70	132	4
1	A	134	TYR	CZ-CE2-CD2	-6.63	113.83	119.80	32	3
1	A	133	ASN	N-CA-CB	6.62	122.52	110.60	147	1
1	A	111	LYS	O-C-N	-6.60	112.14	122.70	147	4
1	A	34	SER	N-CA-CB	6.60	120.40	110.50	71	16
1	A	14	LEU	CB-CA-C	-6.60	97.66	110.20	23	2
1	A	10	GLU	N-CA-CB	-6.59	98.73	110.60	134	1
1	A	69	ALA	N-CA-CB	-6.58	100.88	110.10	76	8
1	A	22	THR	N-CA-CB	6.57	122.79	110.30	145	12
1	A	90	LYS	N-CA-CB	-6.57	98.77	110.60	136	2
2	B	7	THR	CA-CB-CG2	-6.57	103.20	112.40	106	7
1	A	20	ASP	N-CA-CB	6.57	122.42	110.60	40	3
2	B	5	GLN	O-C-N	-6.56	112.20	122.70	13	3
2	B	9	HIS	CA-CB-CG	-6.56	102.45	113.60	128	5
1	A	65	LEU	CB-CG-CD2	-6.56	99.86	111.00	156	7
1	A	18	ASP	CB-CA-C	-6.55	97.29	110.40	135	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	18	ASP	N-CA-CB	6.55	122.39	110.60	45	2
1	A	83	GLU	OE1-CD-OE2	-6.52	115.47	123.30	99	7
1	A	28	LEU	CB-CG-CD1	-6.52	99.92	111.00	12	6
2	B	12	ARG	CD-NE-CZ	6.51	132.72	123.60	134	3
2	B	4	TRP	CZ3-CH2-CZ2	-6.51	113.79	121.60	142	3
2	B	1	ARG	CB-CA-C	6.50	123.41	110.40	62	1
1	A	137	PHE	N-CA-CB	-6.50	98.90	110.60	157	3
2	B	16	ARG	NH1-CZ-NH2	-6.48	112.27	119.40	37	6
1	A	64	PHE	CD1-CE1-CZ	-6.47	112.34	120.10	40	3
1	A	26	LYS	CB-CA-C	6.46	123.33	110.40	82	1
1	A	108	LEU	CB-CG-CD2	6.46	121.98	111.00	63	4
1	A	138	VAL	CA-CB-CG2	-6.45	101.23	110.90	160	5
1	A	28	LEU	C-N-CA	6.45	135.84	122.30	145	1
1	A	86	ARG	O-C-N	-6.45	112.39	122.70	50	7
1	A	102	ARG	CG-CD-NE	-6.44	98.27	111.80	153	2
1	A	134	TYR	O-C-N	-6.44	112.39	122.70	111	5
1	A	132	VAL	CG1-CB-CG2	-6.44	100.60	110.90	71	4
1	A	120	MET	CA-CB-CG	6.43	124.23	113.30	102	2
1	A	124	ALA	N-CA-CB	6.43	119.10	110.10	146	9
1	A	70	ARG	N-CA-CB	-6.43	99.03	110.60	67	1
1	A	61	PHE	CG-CD1-CE1	6.42	127.87	120.80	27	1
1	A	95	TYR	CD1-CG-CD2	6.41	124.95	117.90	61	1
1	A	66	THR	O-C-N	-6.40	112.46	122.70	113	1
2	B	16	ARG	O-C-N	-6.39	112.48	122.70	79	3
1	A	106	THR	OG1-CB-CG2	-6.38	95.33	110.00	76	2
1	A	131	GLN	N-CA-CB	6.38	122.08	110.60	32	4
1	A	26	LYS	CA-CB-CG	6.37	127.41	113.40	146	2
1	A	110	GLU	OE1-CD-OE2	-6.36	115.67	123.30	71	8
1	A	8	PHE	N-CA-CB	6.36	122.05	110.60	152	1
1	A	122	ARG	CD-NE-CZ	6.36	132.51	123.60	11	4
1	A	55	GLY	CA-C-O	-6.36	109.15	120.60	119	1
1	A	105	MET	O-C-N	-6.36	112.53	122.70	107	1
1	A	3	GLU	OE1-CD-OE2	-6.35	115.68	123.30	79	5
1	A	114	ASP	N-CA-CB	-6.35	99.18	110.60	92	4
1	A	119	GLU	OE1-CD-OE2	-6.34	115.69	123.30	144	3
1	A	118	ASP	C-N-CA	6.34	137.55	121.70	19	2
1	A	142	THR	N-CA-CB	6.34	122.34	110.30	98	7
1	A	73	LYS	N-CA-CB	6.33	122.00	110.60	153	3
1	A	87	VAL	CA-CB-CG2	-6.33	101.41	110.90	120	4
1	A	83	GLU	C-N-CA	6.33	137.52	121.70	41	2
1	A	42	ALA	CB-CA-C	6.32	119.58	110.10	159	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	72	MET	O-C-N	-6.32	112.59	122.70	37	4
1	A	136	GLU	CB-CA-C	-6.32	97.77	110.40	80	1
2	B	10	ALA	O-C-N	-6.32	112.59	122.70	125	4
1	A	114	ASP	CB-CA-C	6.30	123.00	110.40	128	2
1	A	84	ALA	N-CA-CB	6.29	118.91	110.10	123	5
1	A	75	THR	C-N-CA	6.29	137.42	121.70	40	1
1	A	27	GLU	N-CA-CB	6.28	121.90	110.60	51	1
1	A	83	GLU	CA-CB-CG	6.28	127.21	113.40	125	1
1	A	61	PHE	O-C-N	-6.27	109.18	121.10	105	3
1	A	61	PHE	CA-C-N	6.27	134.66	117.10	139	10
1	A	93	ASN	N-CA-CB	6.27	121.89	110.60	131	1
2	B	9	HIS	N-CA-CB	-6.27	99.32	110.60	134	1
1	A	118	ASP	N-CA-CB	-6.26	99.33	110.60	142	1
1	A	46	ASP	N-CA-CB	-6.25	99.34	110.60	67	1
1	A	29	GLY	O-C-N	-6.25	112.70	122.70	89	1
1	A	82	ARG	N-CA-CB	-6.25	99.36	110.60	150	4
1	A	104	VAL	CG1-CB-CG2	-6.24	100.91	110.90	56	2
2	B	2	ARG	N-CA-C	6.24	127.85	111.00	62	2
1	A	50	GLU	N-CA-CB	-6.24	99.37	110.60	12	2
1	A	133	ASN	CA-CB-CG	6.24	127.12	113.40	25	2
1	A	24	THR	CA-CB-OG1	6.24	122.10	109.00	41	1
1	A	113	THR	O-C-N	-6.23	112.73	122.70	7	4
1	A	31	VAL	CG1-CB-CG2	-6.23	100.93	110.90	62	10
1	A	21	GLY	O-C-N	-6.23	112.73	122.70	107	1
1	A	30	THR	CA-CB-CG2	6.23	121.12	112.40	21	6
1	A	88	PHE	CG-CD1-CE1	-6.23	113.95	120.80	33	4
1	A	54	ASP	CB-CA-C	6.22	122.84	110.40	147	7
2	B	2	ARG	C-N-CA	6.22	137.25	121.70	130	1
1	A	89	ASP	C-N-CA	6.22	137.25	121.70	121	1
1	A	97	SER	N-CA-CB	-6.22	101.17	110.50	100	3
1	A	89	ASP	N-CA-CB	-6.21	99.42	110.60	61	3
1	A	56	ASN	CB-CG-OD1	6.21	134.01	121.60	90	2
1	A	70	ARG	CG-CD-NE	-6.20	98.77	111.80	26	4
1	A	64	PHE	CD1-CG-CD2	6.20	126.36	118.30	81	2
1	A	75	THR	N-CA-CB	6.19	122.06	110.30	129	5
1	A	12	PHE	CZ-CE2-CD2	6.19	127.53	120.10	43	2
1	A	84	ALA	CB-CA-C	-6.18	100.83	110.10	110	4
1	A	43	GLU	OE1-CD-OE2	-6.18	115.89	123.30	112	3
1	A	10	GLU	O-C-N	-6.17	112.82	122.70	31	3
1	A	83	GLU	O-C-N	-6.17	112.82	122.70	136	5
1	A	8	PHE	CB-CA-C	6.17	122.74	110.40	105	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	112	LEU	CB-CG-CD2	6.17	121.49	111.00	122	10
1	A	24	THR	O-C-N	-6.17	112.83	122.70	91	4
1	A	68	MET	CB-CA-C	-6.17	98.06	110.40	138	1
1	A	5	ILE	O-C-N	-6.17	112.83	122.70	111	4
1	A	46	ASP	CB-CA-C	6.16	122.72	110.40	8	3
1	A	65	LEU	N-CA-CB	6.16	122.72	110.40	35	1
1	A	140	MET	CA-CB-CG	6.16	123.77	113.30	112	2
1	A	65	LEU	CB-CA-C	-6.15	98.51	110.20	119	1
1	A	135	GLU	O-C-N	-6.15	112.86	122.70	84	2
2	B	7	THR	C-N-CA	6.15	135.22	122.30	48	3
1	A	33	ARG	CA-CB-CG	6.15	126.93	113.40	63	1
2	B	2	ARG	O-C-N	-6.15	112.86	122.70	129	5
1	A	72	MET	CA-CB-CG	6.15	123.75	113.30	116	2
1	A	95	TYR	N-CA-CB	6.14	121.66	110.60	129	2
1	A	54	ASP	O-C-N	-6.14	112.76	123.20	41	2
1	A	142	THR	CA-CB-CG2	-6.14	103.80	112.40	139	5
1	A	86	ARG	CD-NE-CZ	6.14	132.19	123.60	50	4
1	A	4	GLN	CA-CB-CG	6.13	126.89	113.40	124	2
1	A	80	GLU	N-CA-CB	-6.13	99.56	110.60	137	1
2	B	4	TRP	CH2-CZ2-CE2	6.13	123.53	117.40	96	6
1	A	115	GLU	OE1-CD-OE2	-6.11	115.97	123.30	149	5
1	A	106	THR	N-CA-CB	6.09	121.88	110.30	26	4
1	A	64	PHE	CG-CD1-CE1	-6.09	114.10	120.80	81	1
2	B	1	ARG	CG-CD-NE	-6.09	99.01	111.80	2	5
1	A	139	GLN	N-CA-CB	6.09	121.56	110.60	5	2
1	A	125	ASP	N-CA-CB	-6.09	99.65	110.60	141	5
1	A	26	LYS	O-C-N	-6.09	112.96	122.70	113	4
1	A	134	TYR	CD1-CG-CD2	6.08	124.59	117.90	112	7
1	A	104	VAL	O-C-N	-6.08	112.97	122.70	153	3
1	A	21	GLY	CA-C-O	-6.08	109.66	120.60	7	1
1	A	3	GLU	CB-CA-C	6.07	122.53	110.40	136	2
1	A	20	ASP	O-C-N	-6.07	112.89	123.20	110	1
1	A	64	PHE	N-CA-CB	-6.06	99.69	110.60	77	2
1	A	108	LEU	CB-CG-CD1	6.06	121.30	111.00	29	5
1	A	73	LYS	O-C-N	-6.06	113.00	122.70	45	4
1	A	54	ASP	OD1-CG-OD2	-6.05	111.80	123.30	102	1
1	A	95	TYR	CD1-CE1-CZ	-6.05	114.36	119.80	104	6
1	A	35	LEU	CB-CG-CD2	6.05	121.28	111.00	18	4
1	A	67	MET	CA-CB-CG	6.05	123.58	113.30	22	2
1	A	141	MET	N-CA-CB	6.04	121.47	110.60	78	3
1	A	33	ARG	CG-CD-NE	-6.04	99.13	111.80	116	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	6	ALA	CB-CA-C	-6.03	101.06	110.10	32	3
1	A	35	LEU	CB-CG-CD1	-6.01	100.77	111.00	101	1
1	A	93	ASN	CB-CG-OD1	6.01	133.61	121.60	156	2
1	A	52	ASP	C-N-CA	6.01	136.72	121.70	116	2
1	A	50	GLU	OE1-CD-OE2	-6.01	116.09	123.30	130	2
2	B	16	ARG	CG-CD-NE	-6.00	99.20	111.80	7	4
1	A	37	GLN	CG-CD-OE1	5.99	133.58	121.60	73	1
1	A	45	GLN	O-C-N	-5.99	113.12	122.70	73	4
1	A	87	VAL	O-C-N	-5.98	113.13	122.70	2	4
1	A	48	ILE	O-C-N	-5.98	113.14	122.70	2	5
2	B	12	ARG	N-CA-CB	-5.98	99.84	110.60	29	2
1	A	120	MET	CB-CA-C	5.98	122.36	110.40	50	2
1	A	82	ARG	CB-CA-C	5.98	122.35	110.40	150	2
1	A	112	LEU	O-C-N	-5.97	113.14	122.70	10	3
1	A	15	PHE	CB-CA-C	-5.97	98.47	110.40	131	3
1	A	62	PRO	C-N-CA	5.96	136.61	121.70	39	1
1	A	16	ASP	O-C-N	-5.96	113.16	122.70	121	4
1	A	7	GLU	N-CA-CB	-5.96	99.88	110.60	131	4
1	A	76	ASP	N-CA-CB	5.96	121.32	110.60	86	1
1	A	52	ASP	N-CA-CB	-5.95	99.89	110.60	49	1
1	A	139	GLN	CB-CA-C	-5.95	98.51	110.40	6	2
1	A	25	THR	OG1-CB-CG2	-5.94	96.33	110.00	86	3
2	B	3	LYS	O-C-N	-5.94	113.20	122.70	119	2
1	A	37	GLN	CB-CA-C	-5.93	98.53	110.40	145	1
1	A	76	ASP	CB-CA-C	-5.92	98.57	110.40	69	1
1	A	25	THR	N-CA-CB	5.91	121.53	110.30	99	4
2	B	4	TRP	CE2-CD2-CE3	5.91	125.79	118.70	48	6
1	A	59	ILE	C-N-CA	5.90	136.46	121.70	114	3
1	A	45	GLN	N-CA-CB	-5.90	99.98	110.60	118	2
1	A	120	MET	O-C-N	-5.89	113.27	122.70	124	2
1	A	71	LYS	N-CA-CB	-5.89	99.99	110.60	40	3
1	A	68	MET	O-C-N	-5.88	113.29	122.70	78	2
1	A	35	LEU	CB-CA-C	-5.88	99.03	110.20	56	2
1	A	38	ASN	N-CA-CB	-5.88	100.02	110.60	8	4
1	A	107	ASN	CA-CB-CG	-5.88	100.47	113.40	125	1
1	A	141	MET	CA-CB-CG	5.87	123.29	113.30	147	1
1	A	129	ASP	C-N-CA	5.87	134.63	122.30	48	2
1	A	11	ALA	O-C-N	-5.87	113.31	122.70	110	4
1	A	100	GLU	N-CA-CB	5.87	121.16	110.60	92	1
1	A	32	MET	O-C-N	-5.87	113.31	122.70	156	1
1	A	59	ILE	CB-CA-C	5.86	123.32	111.60	24	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	60	ASP	O-C-N	-5.86	113.32	122.70	104	4
1	A	11	ALA	CB-CA-C	-5.86	101.31	110.10	2	8
2	B	6	LYS	C-N-CA	5.86	136.34	121.70	1	4
1	A	116	GLU	OE1-CD-OE2	5.85	130.32	123.30	90	4
1	A	67	MET	N-CA-CB	-5.85	100.07	110.60	16	3
1	A	104	VAL	C-N-CA	5.85	136.32	121.70	42	1
1	A	113	THR	N-CA-CB	5.85	121.41	110.30	105	2
1	A	124	ALA	O-C-N	-5.84	113.35	122.70	91	2
1	A	90	LYS	O-C-N	-5.83	113.36	122.70	87	3
1	A	40	THR	N-CA-CB	5.83	121.38	110.30	28	3
2	B	12	ARG	O-C-N	-5.82	113.39	122.70	68	2
1	A	112	LEU	CB-CG-CD1	5.81	120.88	111.00	50	5
1	A	41	GLU	CB-CA-C	-5.81	98.78	110.40	36	1
1	A	107	ASN	N-CA-CB	-5.80	100.16	110.60	65	1
1	A	81	ILE	CB-CA-C	5.80	123.20	111.60	79	1
1	A	108	LEU	CB-CA-C	5.79	121.20	110.20	96	2
2	B	12	ARG	CG-CD-NE	-5.79	99.64	111.80	52	7
1	A	136	GLU	N-CA-CB	5.78	121.00	110.60	80	1
1	A	18	ASP	C-N-CA	5.78	134.43	122.30	2	5
1	A	108	LEU	N-CA-C	5.78	126.60	111.00	6	1
1	A	33	ARG	N-CA-CB	-5.78	100.20	110.60	38	1
1	A	81	ILE	O-C-N	-5.77	113.47	122.70	60	3
1	A	82	ARG	CG-CD-NE	-5.75	99.72	111.80	35	5
1	A	61	PHE	CG-CD2-CE2	5.75	127.12	120.80	104	2
1	A	39	PRO	N-CD-CG	5.75	111.82	103.20	94	2
1	A	67	MET	O-C-N	-5.74	113.52	122.70	11	1
1	A	91	ASP	OD1-CG-OD2	-5.74	112.40	123.30	7	2
1	A	28	LEU	N-CA-CB	5.74	121.87	110.40	32	3
1	A	79	GLU	N-CA-CB	-5.74	100.28	110.60	47	1
1	A	30	THR	O-C-N	-5.73	113.53	122.70	2	1
1	A	77	SER	O-C-N	-5.73	113.53	122.70	154	1
1	A	38	ASN	CA-C-N	5.72	133.13	117.10	83	1
1	A	133	ASN	O-C-N	-5.72	113.55	122.70	145	1
1	A	122	ARG	O-C-N	-5.71	113.56	122.70	47	4
1	A	121	ILE	CA-CB-CG2	5.71	122.32	110.90	61	1
1	A	66	THR	N-CA-CB	5.71	121.15	110.30	38	4
1	A	72	MET	CB-CA-C	5.71	121.82	110.40	103	2
1	A	30	THR	CA-CB-OG1	5.70	120.98	109.00	54	2
1	A	128	GLY	O-C-N	-5.70	113.58	122.70	2	1
1	A	37	GLN	O-C-N	-5.70	113.58	122.70	86	4
1	A	101	LEU	CB-CG-CD2	-5.70	101.31	111.00	102	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	31	VAL	CA-CB-CG2	-5.70	102.36	110.90	11	4
1	A	88	PHE	CB-CA-C	-5.69	99.01	110.40	138	2
1	A	51	VAL	CA-CB-CG2	5.69	119.43	110.90	147	5
1	A	40	THR	CA-CB-OG1	5.68	120.93	109.00	32	4
1	A	72	MET	N-CA-CB	-5.68	100.37	110.60	154	2
1	A	117	VAL	CG1-CB-CG2	-5.68	101.81	110.90	74	5
1	A	24	THR	N-CA-CB	5.67	121.08	110.30	105	2
1	A	62	PRO	O-C-N	-5.67	113.63	122.70	32	2
1	A	28	LEU	O-C-N	-5.67	113.57	123.20	127	4
1	A	68	MET	N-CA-CB	-5.66	100.41	110.60	50	2
1	A	137	PHE	CD1-CG-CD2	5.66	125.66	118.30	1	1
2	B	13	ALA	N-CA-CB	5.66	118.02	110.10	149	3
1	A	93	ASN	C-N-CA	5.65	134.17	122.30	123	1
1	A	74	ASP	O-C-N	-5.65	113.66	122.70	70	3
1	A	89	ASP	O-C-N	-5.64	113.68	122.70	94	2
1	A	101	LEU	CB-CA-C	-5.64	99.49	110.20	25	1
1	A	20	ASP	C-N-CA	5.63	134.13	122.30	112	1
1	A	138	VAL	CA-CB-CG1	5.63	119.35	110.90	8	6
1	A	41	GLU	O-C-N	-5.62	113.70	122.70	97	1
1	A	114	ASP	C-N-CA	5.62	135.76	121.70	16	3
1	A	122	ARG	CG-CD-NE	-5.62	99.99	111.80	65	3
1	A	137	PHE	CB-CA-C	5.61	121.62	110.40	100	2
1	A	62	PRO	N-CD-CG	5.61	111.62	103.20	142	1
1	A	30	THR	OG1-CB-CG2	-5.61	97.09	110.00	111	1
2	B	5	GLN	C-N-CA	5.61	135.72	121.70	160	2
1	A	63	GLU	O-C-N	-5.61	113.73	122.70	25	1
1	A	4	GLN	N-CA-CB	-5.60	100.51	110.60	14	1
1	A	66	THR	C-N-CA	5.60	135.71	121.70	140	1
1	A	142	THR	OG1-CB-CG2	-5.60	97.11	110.00	159	2
1	A	111	LYS	CB-CA-C	5.59	121.58	110.40	145	1
2	B	6	LYS	CA-C-O	5.59	131.84	120.10	65	2
1	A	25	THR	O-C-N	-5.58	113.78	122.70	26	1
1	A	43	GLU	O-C-N	-5.58	113.78	122.70	91	3
1	A	102	ARG	O-C-N	-5.58	113.78	122.70	136	2
1	A	110	GLU	O-C-N	-5.57	113.78	122.70	108	2
1	A	53	ALA	O-C-N	-5.57	113.78	122.70	70	2
1	A	8	PHE	CG-CD2-CE2	-5.56	114.68	120.80	112	1
1	A	77	SER	CB-CA-C	-5.56	99.54	110.10	5	2
2	B	4	TRP	NE1-CE2-CZ2	5.56	136.51	130.40	111	1
1	A	85	PHE	N-CA-CB	-5.56	100.60	110.60	125	5
1	A	66	THR	OG1-CB-CG2	-5.55	97.23	110.00	58	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	39	PRO	N-CA-CB	5.55	109.96	103.30	116	1
1	A	109	GLY	O-C-N	-5.54	113.83	122.70	93	2
2	B	4	TRP	N-CA-CB	5.54	120.57	110.60	130	3
1	A	70	ARG	O-C-N	-5.54	113.84	122.70	26	2
1	A	114	ASP	CA-CB-CG	-5.54	101.22	113.40	107	2
1	A	32	MET	N-CA-CB	5.54	120.56	110.60	132	2
1	A	30	THR	N-CA-CB	5.53	120.81	110.30	4	3
1	A	47	MET	C-N-CA	5.52	135.50	121.70	80	1
1	A	134	TYR	N-CA-CB	-5.52	100.67	110.60	54	1
1	A	91	ASP	N-CA-CB	-5.52	100.67	110.60	94	1
1	A	124	ALA	C-N-CA	5.51	135.47	121.70	125	1
1	A	140	MET	N-CA-CB	-5.51	100.69	110.60	57	2
1	A	63	GLU	C-N-CA	5.51	135.47	121.70	78	1
1	A	115	GLU	N-CA-CB	-5.50	100.70	110.60	135	2
2	B	8	GLY	O-C-N	-5.50	113.90	122.70	35	1
1	A	113	THR	OG1-CB-CG2	-5.50	97.36	110.00	68	1
1	A	80	GLU	O-C-N	-5.50	113.91	122.70	99	1
2	B	4	TRP	CD2-CE2-CZ2	-5.50	115.71	122.30	73	2
1	A	5	ILE	CA-CB-CG1	5.49	121.44	111.00	89	1
1	A	61	PHE	CA-CB-CG	-5.49	100.72	113.90	78	1
1	A	139	GLN	O-C-N	-5.49	113.92	122.70	113	1
1	A	7	GLU	CG-CD-OE2	5.48	129.26	118.30	26	1
1	A	73	LYS	C-N-CA	5.48	135.41	121.70	94	3
1	A	110	GLU	N-CA-CB	-5.47	100.75	110.60	9	1
1	A	73	LYS	CB-CA-C	5.47	121.34	110.40	124	3
1	A	74	ASP	N-CA-CB	-5.47	100.75	110.60	155	1
1	A	15	PHE	CG-CD1-CE1	-5.47	114.79	120.80	146	1
1	A	51	VAL	C-N-CA	5.46	135.36	121.70	28	1
2	B	8	GLY	C-N-CA	5.46	135.36	121.70	76	1
1	A	103	HIS	O-C-N	-5.46	113.97	122.70	119	3
1	A	136	GLU	CG-CD-OE2	5.45	129.21	118.30	99	1
1	A	133	ASN	CB-CA-C	5.44	121.28	110.40	80	3
1	A	85	PHE	CG-CD2-CE2	5.44	126.78	120.80	21	2
1	A	78	GLU	CB-CA-C	-5.44	99.52	110.40	41	1
1	A	76	ASP	O-C-N	-5.43	114.00	122.70	45	1
1	A	43	GLU	CA-CB-CG	-5.43	101.44	113.40	55	1
1	A	22	THR	O-C-N	-5.43	114.00	122.70	107	2
1	A	58	THR	O-C-N	-5.43	114.01	122.70	25	2
1	A	51	VAL	O-C-N	-5.43	114.01	122.70	142	3
1	A	37	GLN	CA-CB-CG	5.43	125.34	113.40	24	1
1	A	97	SER	C-N-CA	5.43	135.28	121.70	76	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	18	ASP	O-C-N	-5.42	113.99	123.20	129	2
1	A	15	PHE	CG-CD2-CE2	-5.41	114.85	120.80	125	3
1	A	44	LEU	CB-CG-CD2	5.41	120.19	111.00	21	3
1	A	95	TYR	C-N-CA	5.41	135.22	121.70	133	1
2	B	14	ILE	CG1-CB-CG2	-5.40	99.52	111.40	135	1
1	A	13	SER	CB-CA-C	-5.40	99.84	110.10	107	5
1	A	41	GLU	N-CA-CB	5.39	120.31	110.60	156	2
1	A	8	PHE	O-C-N	-5.39	114.07	122.70	5	4
2	B	16	ARG	C-N-CA	5.39	135.18	121.70	38	1
1	A	111	LYS	N-CA-CB	5.39	120.30	110.60	29	2
2	B	4	TRP	CB-CA-C	-5.39	99.62	110.40	118	1
1	A	23	ILE	C-N-CA	5.38	135.14	121.70	102	1
1	A	45	GLN	CB-CA-C	-5.38	99.65	110.40	108	2
2	B	15	GLY	C-N-CA	5.37	135.13	121.70	129	2
1	A	9	LYS	CA-CB-CG	5.37	125.22	113.40	82	1
1	A	129	ASP	CA-CB-CG	5.37	125.20	113.40	67	2
1	A	17	LYS	CB-CA-C	5.36	121.12	110.40	103	1
1	A	81	ILE	CA-CB-CG1	5.36	121.19	111.00	118	1
1	A	135	GLU	CB-CA-C	-5.36	99.68	110.40	146	1
1	A	15	PHE	O-C-N	-5.36	114.13	122.70	18	1
1	A	92	GLY	O-C-N	-5.36	114.13	122.70	91	2
1	A	8	PHE	CG-CD1-CE1	5.36	126.69	120.80	40	1
1	A	35	LEU	O-C-N	-5.36	114.10	123.20	147	3
1	A	91	ASP	CB-CA-C	5.35	121.10	110.40	55	2
1	A	96	ILE	O-C-N	-5.35	114.14	122.70	133	1
1	A	73	LYS	CA-CB-CG	5.35	125.16	113.40	10	1
1	A	71	LYS	CA-C-O	5.34	131.32	120.10	126	1
1	A	19	GLY	O-C-N	5.34	131.25	122.70	69	1
1	A	7	GLU	CB-CA-C	5.34	121.08	110.40	152	2
1	A	12	PHE	CD1-CE1-CZ	-5.34	113.69	120.10	151	2
1	A	118	ASP	CB-CA-C	5.34	121.07	110.40	105	2
1	A	117	VAL	O-C-N	-5.33	114.17	122.70	96	2
1	A	38	ASN	CA-C-O	-5.33	108.91	120.10	50	1
1	A	123	GLU	N-CA-CB	5.33	120.19	110.60	52	1
1	A	76	ASP	OD1-CG-OD2	-5.33	113.18	123.30	74	1
1	A	22	THR	CA-CB-OG1	5.32	120.18	109.00	103	1
1	A	49	ASN	C-N-CA	5.32	135.00	121.70	117	1
1	A	75	THR	O-C-N	-5.32	114.19	122.70	94	2
1	A	117	VAL	CB-CA-C	-5.32	101.29	111.40	98	1
1	A	61	PHE	N-CA-CB	-5.32	101.03	110.60	66	1
1	A	134	TYR	C-N-CA	5.32	134.99	121.70	123	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	110	GLU	CB-CA-C	-5.31	99.77	110.40	19	2
1	A	120	MET	N-CA-CB	-5.31	101.05	110.60	50	1
1	A	17	LYS	N-CA-CB	5.30	120.15	110.60	12	1
1	A	4	GLN	C-N-CA	5.30	134.95	121.70	39	2
1	A	115	GLU	CA-CB-CG	5.30	125.06	113.40	97	2
1	A	46	ASP	CA-CB-CG	-5.29	101.75	113.40	125	1
1	A	111	LYS	C-N-CA	5.29	134.93	121.70	32	1
1	A	12	PHE	O-C-N	-5.29	114.23	122.70	21	3
1	A	63	GLU	CB-CA-C	5.29	120.98	110.40	138	1
1	A	34	SER	CB-CA-C	-5.28	100.06	110.10	121	2
1	A	34	SER	C-N-CA	5.28	134.90	121.70	19	1
1	A	23	ILE	O-C-N	-5.28	114.25	122.70	79	3
1	A	87	VAL	CB-CA-C	-5.28	101.37	111.40	54	1
1	A	39	PRO	O-C-N	-5.28	114.25	122.70	152	1
1	A	48	ILE	CA-CB-CG1	-5.28	100.98	111.00	18	1
2	B	4	TRP	CD1-NE1-CE2	5.27	113.75	109.00	101	2
1	A	109	GLY	C-N-CA	5.27	134.88	121.70	96	1
1	A	137	PHE	CD1-CE1-CZ	-5.26	113.78	120.10	95	1
1	A	85	PHE	CG-CD1-CE1	5.26	126.59	120.80	146	2
2	B	13	ALA	O-C-N	-5.26	114.28	122.70	127	1
1	A	128	GLY	CA-C-O	-5.26	111.13	120.60	106	1
1	A	10	GLU	CB-CA-C	5.25	120.91	110.40	3	1
1	A	59	ILE	N-CA-CB	5.25	122.88	110.80	22	1
1	A	127	ASP	O-C-N	-5.25	114.28	123.20	84	2
1	A	17	LYS	O-C-N	5.25	131.09	122.70	34	2
2	B	14	ILE	CA-CB-CG2	-5.25	100.41	110.90	30	1
1	A	107	ASN	CB-CA-C	-5.24	99.92	110.40	14	1
1	A	22	THR	OG1-CB-CG2	-5.24	97.94	110.00	15	1
1	A	85	PHE	CD1-CE1-CZ	-5.24	113.81	120.10	119	1
1	A	15	PHE	CZ-CE2-CD2	-5.24	113.81	120.10	123	1
2	B	9	HIS	O-C-N	-5.24	114.32	122.70	94	2
1	A	41	GLU	OE1-CD-OE2	-5.24	117.02	123.30	39	4
1	A	26	LYS	N-CA-CB	-5.24	101.18	110.60	149	1
1	A	121	ILE	O-C-N	-5.23	114.33	122.70	34	3
2	B	16	ARG	N-CA-CB	5.23	120.02	110.60	154	1
1	A	117	VAL	CA-C-O	5.23	131.08	120.10	7	1
2	B	2	ARG	CD-NE-CZ	5.23	130.92	123.60	19	1
1	A	7	GLU	CG-CD-OE1	-5.22	107.85	118.30	26	1
2	B	2	ARG	CB-CA-C	-5.22	99.95	110.40	24	1
1	A	33	ARG	CD-NE-CZ	5.22	130.91	123.60	158	3
2	B	6	LYS	N-CA-CB	-5.22	101.20	110.60	32	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	75	THR	CA-CB-OG1	5.21	119.95	109.00	17	1
2	B	6	LYS	CA-C-N	-5.21	105.73	117.20	32	1
1	A	61	PHE	N-CA-C	5.21	125.08	111.00	130	1
2	B	11	VAL	N-CA-C	5.21	125.07	111.00	19	1
2	B	11	VAL	CA-C-O	5.21	131.04	120.10	61	1
1	A	85	PHE	C-N-CA	5.21	134.72	121.70	157	1
1	A	119	GLU	C-N-CA	5.20	134.70	121.70	51	2
1	A	126	ILE	O-C-N	-5.20	114.38	122.70	116	1
1	A	99	ALA	C-N-CA	5.20	134.69	121.70	68	1
1	A	101	LEU	CA-CB-CG	5.20	127.25	115.30	19	1
2	B	5	GLN	CB-CA-C	-5.20	100.00	110.40	159	1
1	A	65	LEU	CA-C-N	5.19	128.61	117.20	100	1
1	A	84	ALA	O-C-N	-5.19	114.40	122.70	127	1
1	A	96	ILE	CA-CB-CG2	-5.18	100.53	110.90	157	1
1	A	122	ARG	CB-CG-CD	5.18	125.06	111.60	72	1
2	B	4	TRP	NE1-CE2-CD2	5.18	112.48	107.30	141	1
1	A	46	ASP	C-N-CA	5.18	134.64	121.70	64	1
1	A	79	GLU	CB-CA-C	5.18	120.75	110.40	122	1
1	A	4	GLN	CA-C-O	-5.17	109.24	120.10	81	1
1	A	7	GLU	O-C-N	-5.17	114.43	122.70	27	1
1	A	106	THR	O-C-N	-5.17	114.44	122.70	131	2
1	A	4	GLN	O-C-N	-5.16	114.44	122.70	94	1
1	A	75	THR	CA-C-O	5.15	130.92	120.10	64	1
1	A	25	THR	CA-CB-OG1	5.15	119.82	109.00	140	1
1	A	100	GLU	O-C-N	-5.15	114.46	122.70	158	2
1	A	5	ILE	C-N-CA	5.15	134.57	121.70	95	1
1	A	20	ASP	OD1-CG-OD2	-5.15	113.52	123.30	65	2
1	A	125	ASP	O-C-N	-5.14	114.47	122.70	111	2
2	B	4	TRP	CG-CD1-NE1	5.14	115.24	110.10	11	1
1	A	141	MET	O-C-N	-5.14	114.48	122.70	96	1
2	B	4	TRP	CD2-CE3-CZ3	-5.14	112.12	118.80	147	2
1	A	71	LYS	O-C-N	-5.14	114.48	122.70	138	1
1	A	6	ALA	O-C-N	-5.13	114.48	122.70	148	1
1	A	48	ILE	C-N-CA	5.13	134.53	121.70	11	1
1	A	55	GLY	C-N-CA	5.13	134.53	121.70	58	1
1	A	7	GLU	CA-CB-CG	5.13	124.68	113.40	77	1
1	A	110	GLU	CA-CB-CG	5.13	124.68	113.40	94	1
1	A	34	SER	O-C-N	-5.13	114.50	122.70	66	1
2	B	4	TRP	CE3-CZ3-CH2	5.12	126.83	121.20	32	1
1	A	103	HIS	CB-CA-C	-5.12	100.16	110.40	42	2
1	A	42	ALA	C-N-CA	5.12	134.50	121.70	152	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	127	ASP	CA-CB-CG	5.12	124.65	113.40	52	1
1	A	100	GLU	CG-CD-OE2	5.11	128.53	118.30	21	1
1	A	16	ASP	N-CA-CB	-5.11	101.40	110.60	23	1
1	A	133	ASN	C-N-CA	5.11	134.48	121.70	49	1
1	A	101	LEU	O-C-N	-5.11	114.53	122.70	55	1
1	A	140	MET	O-C-N	-5.11	114.53	122.70	144	2
1	A	88	PHE	CD1-CG-CD2	-5.11	111.66	118.30	6	3
1	A	74	ASP	N-CA-C	5.11	124.78	111.00	60	1
1	A	137	PHE	CG-CD1-CE1	-5.10	115.19	120.80	46	1
1	A	24	THR	OG1-CB-CG2	-5.10	98.27	110.00	101	1
1	A	49	ASN	CB-CA-C	5.10	120.60	110.40	138	1
1	A	58	THR	OG1-CB-CG2	-5.10	98.27	110.00	149	1
2	B	2	ARG	CG-CD-NE	-5.09	101.10	111.80	98	1
1	A	89	ASP	CB-CA-C	5.09	120.59	110.40	67	1
1	A	16	ASP	CA-C-O	5.09	130.79	120.10	47	1
1	A	142	THR	CA-CB-OG1	5.09	119.69	109.00	139	1
1	A	86	ARG	N-CA-C	5.09	124.74	111.00	27	1
1	A	127	ASP	N-CA-CB	5.09	119.76	110.60	50	1
1	A	31	VAL	O-C-N	-5.09	114.56	122.70	131	2
1	A	108	LEU	C-N-CA	5.08	132.98	122.30	47	1
1	A	111	LYS	CD-CE-NZ	-5.08	100.01	111.70	135	1
1	A	107	ASN	O-C-N	-5.08	114.57	122.70	56	1
1	A	141	MET	CB-CA-C	-5.08	100.24	110.40	95	1
1	A	70	ARG	CD-NE-CZ	5.08	130.71	123.60	108	1
1	A	11	ALA	N-CA-C	5.08	124.71	111.00	142	1
1	A	44	LEU	CB-CA-C	5.08	119.84	110.20	50	1
2	B	1	ARG	O-C-N	-5.07	114.59	122.70	24	1
1	A	58	THR	CA-CB-OG1	5.07	119.65	109.00	54	1
1	A	19	GLY	CA-C-O	5.07	129.73	120.60	119	1
1	A	59	ILE	CA-C-O	5.07	130.75	120.10	61	1
1	A	64	PHE	CB-CA-C	5.07	120.53	110.40	9	1
2	B	1	ARG	CA-CB-CG	5.07	124.55	113.40	86	1
1	A	46	ASP	O-C-N	-5.07	114.59	122.70	94	1
1	A	16	ASP	CA-CB-CG	-5.07	102.26	113.40	140	1
1	A	85	PHE	CB-CA-C	5.06	120.53	110.40	88	1
1	A	129	ASP	N-CA-C	5.06	124.67	111.00	31	1
1	A	52	ASP	N-CA-C	5.06	124.66	111.00	75	1
1	A	113	THR	CA-CB-OG1	5.06	119.62	109.00	108	1
1	A	116	GLU	C-N-CA	5.06	134.35	121.70	141	1
2	B	1	ARG	N-CA-CB	-5.06	101.50	110.60	133	1
2	B	4	TRP	CD1-CG-CD2	-5.05	102.26	106.30	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	9	LYS	O-C-N	-5.05	114.62	122.70	49	1
1	A	63	GLU	CG-CD-OE1	5.05	128.40	118.30	124	1
1	A	119	GLU	CA-C-O	5.04	130.69	120.10	109	1
1	A	80	GLU	C-N-CA	5.04	134.31	121.70	36	1
1	A	111	LYS	CB-CG-CD	5.04	124.71	111.60	21	1
1	A	33	ARG	CB-CA-C	5.04	120.48	110.40	104	1
1	A	97	SER	CB-CA-C	5.04	119.67	110.10	132	1
1	A	113	THR	C-N-CA	5.04	134.29	121.70	23	1
1	A	5	ILE	CA-CB-CG2	5.04	120.97	110.90	113	1
1	A	5	ILE	N-CA-CB	5.04	122.38	110.80	89	1
1	A	141	MET	CA-C-N	5.03	128.27	117.20	47	1
1	A	18	ASP	CA-CB-CG	5.03	124.47	113.40	8	1
1	A	45	GLN	CA-C-N	5.03	128.27	117.20	23	1
1	A	88	PHE	CZ-CE2-CD2	-5.03	114.06	120.10	83	1
1	A	12	PHE	CB-CA-C	5.03	120.45	110.40	137	1
1	A	28	LEU	CB-CG-CD2	5.02	119.53	111.00	33	1
1	A	70	ARG	CA-CB-CG	5.02	124.45	113.40	109	1
1	A	107	ASN	CB-CG-OD1	5.02	131.64	121.60	20	1
1	A	115	GLU	O-C-N	-5.02	114.67	122.70	2	1
2	B	7	THR	CA-C-O	5.01	130.63	120.10	97	1
1	A	74	ASP	CA-CB-CG	-5.01	102.37	113.40	95	1
1	A	112	LEU	CB-CA-C	-5.01	100.69	110.20	59	1
1	A	122	ARG	N-CA-CB	-5.01	101.59	110.60	13	1
1	A	57	GLY	C-N-CA	5.00	134.21	121.70	138	1
1	A	122	ARG	C-N-CA	5.00	134.20	121.70	105	1
1	A	43	GLU	CG-CD-OE1	5.00	128.30	118.30	112	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)
2	B	12	ARG	Sidechain	52
2	B	16	ARG	Sidechain	50
1	A	33	ARG	Sidechain	47
2	B	2	ARG	Sidechain,Peptide	47
1	A	95	TYR	Sidechain	40
1	A	102	ARG	Sidechain	39
2	B	1	ARG	Sidechain,Peptide	38
1	A	86	ARG	Sidechain	36
1	A	134	TYR	Sidechain	35

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	70	ARG	Sidechain	35
1	A	82	ARG	Sidechain	35
1	A	122	ARG	Sidechain	33
1	A	137	PHE	Sidechain,Mainchain	21
1	A	61	PHE	Sidechain	16
1	A	8	PHE	Sidechain	15
1	A	12	PHE	Sidechain	13
1	A	15	PHE	Sidechain	11
1	A	64	PHE	Sidechain	11
1	A	88	PHE	Sidechain	10
1	A	85	PHE	Sidechain	8
2	B	9	HIS	Sidechain	7
1	A	103	HIS	Sidechain,Mainchain	6
1	A	63	GLU	Sidechain,Peptide	3
1	A	112	LEU	Peptide	2
1	A	73	LYS	Peptide	2
1	A	114	ASP	Peptide	1
1	A	38	ASN	Peptide	1
1	A	39	PRO	Peptide	1
2	B	6	LYS	Mainchain	1
1	A	40	THR	Peptide	1
1	A	75	THR	Peptide	1
1	A	13	SER	Peptide	1
1	A	30	THR	Mainchain	1
1	A	115	GLU	Peptide	1
2	B	3	LYS	Mainchain	1
1	A	58	THR	Peptide	1
1	A	124	ALA	Peptide	1
1	A	140	MET	Mainchain	1
1	A	141	MET	Mainchain	1
1	A	101	LEU	Mainchain	1
1	A	100	GLU	Mainchain	1
1	A	26	LYS	Mainchain	1
1	A	83	GLU	Mainchain	1

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	1105	1035	1035	1±1
2	B	135	145	148	0±0
All	All	199040	188800	189279	103

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:VAL:HG21	1:A:59:ILE:HD12	0.71	1.62	39	1
1:A:8:PHE:CD2	1:A:65:LEU:HD22	0.60	2.31	139	1
1:A:28:LEU:HD23	1:A:44:LEU:HD13	0.57	1.76	13	1
1:A:28:LEU:HD23	1:A:44:LEU:HD11	0.56	1.76	76	1
1:A:90:LYS:HD2	1:A:103:HIS:CD2	0.56	2.36	22	1
1:A:61:PHE:CZ	1:A:65:LEU:HD21	0.56	2.36	35	1
1:A:87:VAL:HG21	2:B:11:VAL:HG13	0.55	1.77	62	2
2:B:7:THR:O	2:B:11:VAL:HG12	0.54	2.03	71	2
2:B:5:GLN:O	2:B:9:HIS:CD2	0.54	2.61	121	3
1:A:61:PHE:CE2	1:A:65:LEU:HD11	0.54	2.37	5	2
1:A:134:TYR:O	1:A:138:VAL:HG23	0.53	2.02	62	3
1:A:99:ALA:O	1:A:103:HIS:CD2	0.53	2.62	101	1
1:A:14:LEU:HD23	2:B:10:ALA:CB	0.52	2.33	2	1
1:A:35:LEU:HD11	1:A:108:LEU:HD21	0.50	1.83	67	1
1:A:101:LEU:HD13	2:B:4:TRP:CH2	0.49	2.41	3	2
1:A:108:LEU:CD1	2:B:7:THR:HG23	0.49	2.36	88	1
1:A:61:PHE:HB3	1:A:62:PRO:HD3	0.49	1.85	11	2
1:A:108:LEU:HD12	2:B:7:THR:HG23	0.49	1.83	88	2
1:A:28:LEU:HD11	2:B:14:ILE:HD13	0.49	1.84	156	1
1:A:126:ILE:HG22	1:A:136:GLU:HG2	0.48	1.85	58	1
1:A:115:GLU:H	1:A:115:GLU:CD	0.47	2.13	122	1
1:A:68:MET:CE	2:B:13:ALA:HB2	0.47	2.40	3	1
2:B:5:GLN:O	2:B:9:HIS:CG	0.47	2.67	4	1
1:A:103:HIS:CE1	1:A:107:ASN:HD21	0.47	2.28	133	2
1:A:96:ILE:HD12	1:A:132:VAL:HB	0.47	1.87	34	1
1:A:12:PHE:CE1	1:A:23:ILE:HD11	0.47	2.44	152	1
1:A:101:LEU:HD13	2:B:4:TRP:CZ3	0.46	2.45	105	1
1:A:7:GLU:OE2	2:B:2:ARG:NH2	0.46	2.47	30	1
1:A:28:LEU:CD2	1:A:44:LEU:HD11	0.46	2.40	76	1
1:A:28:LEU:O	1:A:31:VAL:HG12	0.46	2.11	83	1
1:A:64:PHE:CE2	2:B:9:HIS:CE1	0.45	3.04	72	1
1:A:88:PHE:CD1	1:A:104:VAL:HG21	0.45	2.46	141	2
1:A:102:ARG:HH12	1:A:114:ASP:CG	0.45	2.13	105	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:PHE:CE2	1:A:134:TYR:CE1	0.45	3.05	106	1
1:A:85:PHE:CE2	1:A:96:ILE:HD11	0.45	2.45	117	1
1:A:88:PHE:CZ	1:A:104:VAL:HG11	0.45	2.47	145	1
1:A:23:ILE:HB	1:A:59:ILE:HG23	0.45	1.88	10	3
1:A:85:PHE:CD2	1:A:134:TYR:CE1	0.45	3.05	152	2
1:A:102:ARG:NH2	1:A:114:ASP:OD1	0.44	2.50	1	1
1:A:118:ASP:OD2	1:A:122:ARG:NH1	0.44	2.49	81	1
1:A:88:PHE:HA	1:A:104:VAL:HG21	0.44	1.90	94	1
1:A:102:ARG:CG	1:A:117:VAL:HG11	0.44	2.43	160	1
1:A:83:GLU:O	1:A:87:VAL:HG23	0.44	2.13	137	3
1:A:134:TYR:CE2	1:A:138:VAL:HG21	0.43	2.48	112	1
1:A:114:ASP:HA	1:A:117:VAL:HG12	0.43	1.89	22	1
1:A:54:ASP:OD1	1:A:55:GLY:N	0.43	2.50	134	2
2:B:7:THR:O	2:B:11:VAL:HG23	0.43	2.12	28	1
1:A:85:PHE:CE1	1:A:96:ILE:HD11	0.43	2.48	73	1
1:A:12:PHE:CE1	1:A:23:ILE:HG13	0.43	2.48	104	1
1:A:112:LEU:H	1:A:112:LEU:HD22	0.42	1.74	129	1
1:A:8:PHE:CD2	1:A:65:LEU:CD1	0.42	3.03	8	1
1:A:79:GLU:OE1	1:A:82:ARG:NH1	0.42	2.51	14	1
1:A:3:GLU:H	1:A:3:GLU:CD	0.42	2.17	24	1
1:A:23:ILE:HA	1:A:27:GLU:OE1	0.42	2.15	127	1
1:A:81:ILE:HG21	1:A:138:VAL:HG22	0.42	1.90	17	1
1:A:112:LEU:HD23	1:A:112:LEU:N	0.42	2.30	139	1
1:A:103:HIS:CD2	1:A:107:ASN:ND2	0.42	2.87	31	1
1:A:102:ARG:HH21	1:A:114:ASP:CG	0.42	2.18	64	1
1:A:8:PHE:CE1	2:B:9:HIS:CE1	0.42	3.08	138	1
1:A:12:PHE:CZ	1:A:23:ILE:HG13	0.42	2.50	116	2
1:A:138:VAL:O	1:A:142:THR:HG23	0.42	2.14	79	1
1:A:8:PHE:CE2	1:A:65:LEU:HD13	0.42	2.50	121	1
1:A:68:MET:HG3	2:B:9:HIS:CE1	0.41	2.50	72	1
1:A:8:PHE:HA	2:B:9:HIS:CE1	0.41	2.50	98	1
1:A:37:GLN:O	1:A:39:PRO:HD3	0.41	2.15	122	1
1:A:102:ARG:HH22	1:A:114:ASP:CG	0.41	2.18	151	1
2:B:7:THR:O	2:B:10:ALA:HB3	0.41	2.15	146	1
1:A:15:PHE:HB2	1:A:23:ILE:HD13	0.41	1.93	13	1
1:A:24:THR:HG22	1:A:58:THR:HG22	0.41	1.92	23	1
1:A:8:PHE:CD2	2:B:9:HIS:HE1	0.41	2.33	150	1
1:A:14:LEU:HD12	2:B:10:ALA:HB2	0.41	1.91	35	1
1:A:80:GLU:CD	2:B:16:ARG:HH22	0.41	2.19	100	1
1:A:80:GLU:CD	2:B:12:ARG:HE	0.41	2.19	103	1
1:A:115:GLU:CD	1:A:115:GLU:H	0.41	2.19	123	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:ALA:HB2	2:B:4:TRP:CE2	0.41	2.51	15	1
2:B:11:VAL:HA	2:B:14:ILE:HG22	0.41	1.93	15	1
1:A:80:GLU:OE2	2:B:16:ARG:NH1	0.41	2.51	124	2
1:A:28:LEU:CD2	1:A:48:ILE:HD11	0.40	2.47	141	1
1:A:23:ILE:HB	1:A:59:ILE:CG2	0.40	2.46	85	1
1:A:8:PHE:CD1	2:B:9:HIS:CE1	0.40	3.10	18	1
1:A:118:ASP:O	1:A:122:ARG:HB2	0.40	2.16	46	1
1:A:31:VAL:O	1:A:34:SER:HB2	0.40	2.16	84	1
1:A:12:PHE:CE1	1:A:23:ILE:HD12	0.40	2.51	136	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	139/148 (94%)	128±3 (92±2%)	9±3 (6±2%)	2±2 (2±1%)	13	57
2	B	15/19 (79%)	14±1 (95±6%)	1±1 (4±5%)	0±0 (0±1%)	44	80
All	All	24640/26720 (92%)	22755 (92%)	1511 (6%)	374 (2%)	14	59

All 35 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	36	GLY	112
1	A	128	GLY	55
1	A	109	GLY	40
1	A	21	GLY	30
1	A	127	ASP	24
1	A	55	GLY	16
1	A	92	GLY	14
1	A	74	ASP	12
1	A	54	ASP	12
1	A	19	GLY	9
1	A	91	ASP	8
2	B	2	ARG	6

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Mol	Chain	Res	Type	Models (Total)
1	A	52	ASP	4
1	A	73	LYS	3
1	A	16	ASP	3
1	A	35	LEU	3
1	A	39	PRO	2
1	A	77	SER	2
1	A	86	ARG	2
2	B	11	VAL	2
1	A	115	GLU	1
1	A	5	ILE	1
1	A	125	ASP	1
1	A	98	ALA	1
1	A	18	ASP	1
1	A	117	VAL	1
1	A	89	ASP	1
1	A	49	ASN	1
1	A	38	ASN	1
1	A	108	LEU	1
1	A	101	LEU	1
1	A	20	ASP	1
1	A	15	PHE	1
1	A	50	GLU	1
1	A	53	ALA	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	120/126 (95%)	117±2 (98±1%)	3±2 (2±1%)	50	91
2	B	12/15 (80%)	12±0 (98±4%)	0±0 (2±4%)	59	93
All	All	21120/22560 (94%)	20609 (98%)	511 (2%)	51	92

All 99 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	91	ASP	36

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Mol	Chain	Res	Type	Models (Total)
1	A	127	ASP	33
1	A	54	ASP	31
1	A	59	ILE	27
1	A	18	ASP	24
1	A	20	ASP	16
1	A	74	ASP	13
1	A	3	GLU	13
1	A	88	PHE	13
1	A	39	PRO	11
2	B	6	LYS	10
1	A	110	GLU	9
1	A	133	ASN	9
1	A	112	LEU	9
1	A	114	ASP	8
2	B	11	VAL	8
1	A	104	VAL	7
1	A	65	LEU	7
2	B	16	ARG	7
1	A	134	TYR	6
1	A	75	THR	6
1	A	8	PHE	6
1	A	117	VAL	6
1	A	105	MET	6
1	A	23	ILE	6
1	A	101	LEU	6
1	A	7	GLU	5
1	A	118	ASP	5
1	A	60	ASP	5
1	A	13	SER	5
2	B	14	ILE	5
1	A	14	LEU	5
1	A	139	GLN	5
1	A	12	PHE	5
1	A	22	THR	4
1	A	25	THR	4
1	A	16	ASP	4
1	A	111	LYS	4
1	A	125	ASP	4
1	A	15	PHE	4
1	A	64	PHE	4
1	A	62	PRO	3
1	A	90	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	28	LEU	3
1	A	33	ARG	3
1	A	31	VAL	3
1	A	61	PHE	3
1	A	108	LEU	3
1	A	46	ASP	3
1	A	50	GLU	3
2	B	2	ARG	3
1	A	37	GLN	3
1	A	131	GLN	3
1	A	44	LEU	3
1	A	77	SER	3
1	A	132	VAL	3
1	A	52	ASP	3
1	A	72	MET	3
1	A	140	MET	3
1	A	56	ASN	3
1	A	40	THR	2
1	A	115	GLU	2
1	A	34	SER	2
1	A	121	ILE	2
1	A	81	ILE	2
1	A	9	LYS	2
1	A	96	ILE	2
1	A	41	GLU	2
1	A	58	THR	2
1	A	32	MET	2
2	B	5	GLN	2
1	A	66	THR	2
1	A	97	SER	2
1	A	67	MET	2
1	A	142	THR	1
1	A	45	GLN	1
1	A	87	VAL	1
1	A	78	GLU	1
1	A	71	LYS	1
1	A	141	MET	1
2	B	9	HIS	1
1	A	43	GLU	1
1	A	76	ASP	1
1	A	68	MET	1
1	A	106	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	122	ARG	1
1	A	129	ASP	1
1	A	47	MET	1
1	A	35	LEU	1
1	A	51	VAL	1
1	A	5	ILE	1
1	A	85	PHE	1
1	A	89	ASP	1
2	B	7	THR	1
1	A	24	THR	1
1	A	26	LYS	1
1	A	103	HIS	1
1	A	86	ARG	1
1	A	48	ILE	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are 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