



Full wwPDB NMR Structure Validation Report ⓘ

Feb 17, 2018 – 11:33 pm GMT

PDB ID : 2K0E
Title : A Coupled Equilibrium Shift Mechanism in Calmodulin-Mediated Signal Transduction
Authors : Gsponer, J.; Christodoulou, J.; Cavalli, A.; Bui, J.M.; Richter, B.; Dobson, C.M.; Vendruscolo, M.
Deposited on : 2008-02-02

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

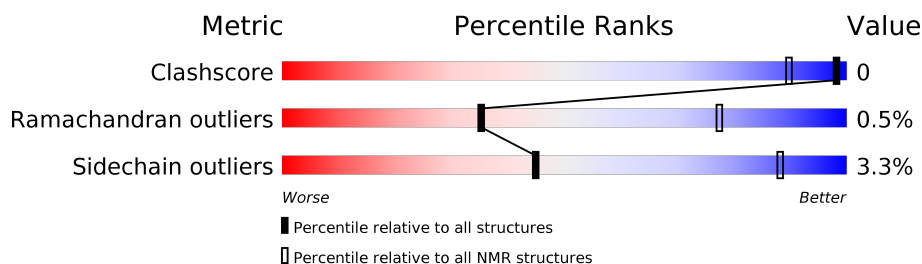
Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk30686
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	148	<div> <div></div> <div>79%</div> <div>10%</div> <div>11%</div> </div>

2 Ensemble composition and analysis

This entry contains 160 models. Model 157 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:5-A:73 (69)	0.63	157
2	A:83-A:145 (63)	0.70	2

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 24 clusters and 5 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2263 atoms, of which 1093 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms						Trace
1	A	148	Total	C	H	N	O	S	0
			2259	714	1093	188	255	9	

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

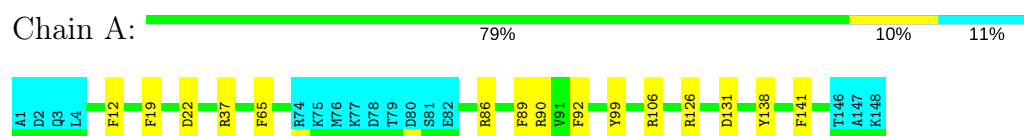
Mol	Chain	Residues	Atoms	
2	A	4	Total	Ca
			4	4

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Calmodulin

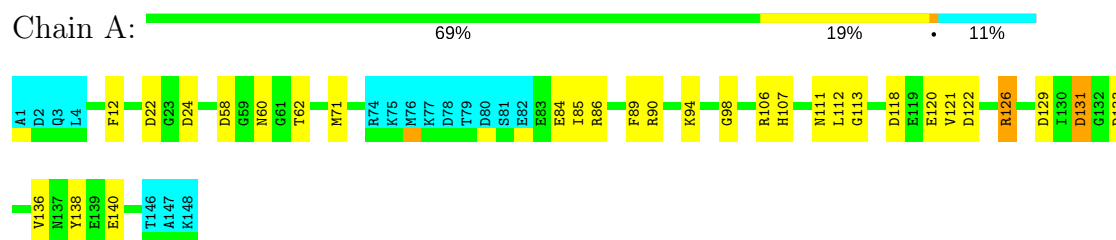


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

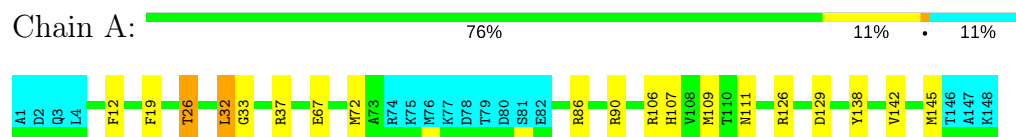
4.2.1 Score per residue for model 1

- Molecule 1: Calmodulin



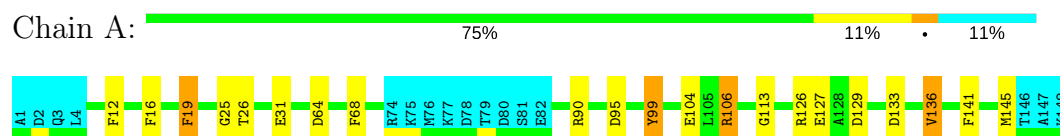
4.2.2 Score per residue for model 2

- Molecule 1: Calmodulin



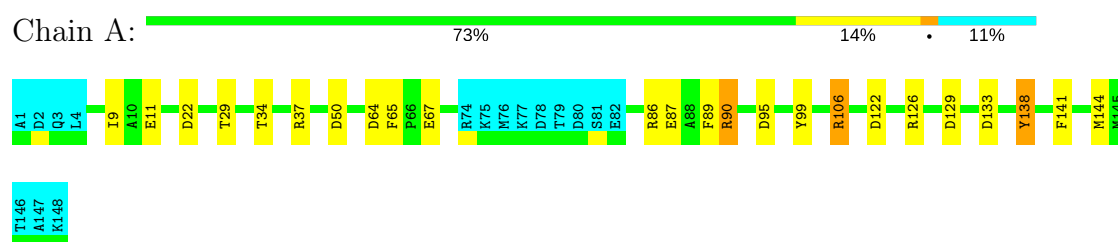
4.2.3 Score per residue for model 3

- Molecule 1: Calmodulin



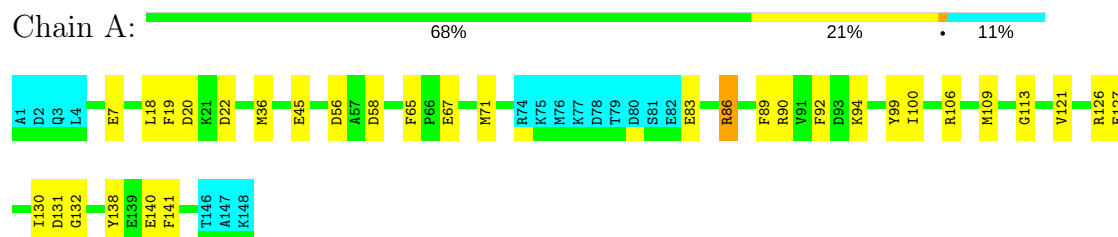
4.2.4 Score per residue for model 4

- Molecule 1: Calmodulin



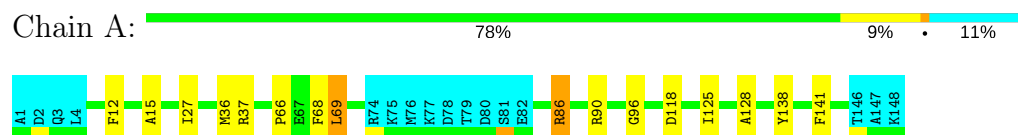
4.2.5 Score per residue for model 5

- Molecule 1: Calmodulin



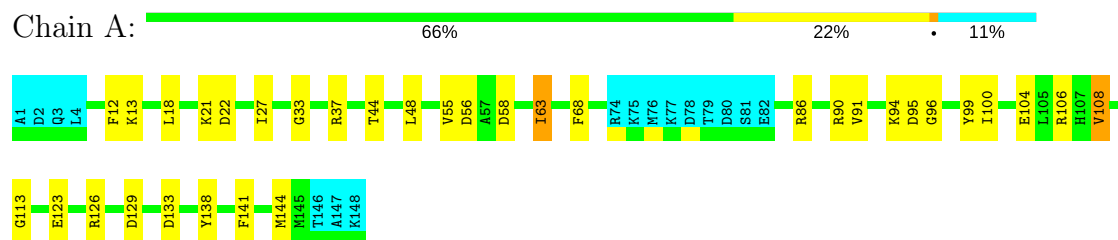
4.2.6 Score per residue for model 6

- Molecule 1: Calmodulin



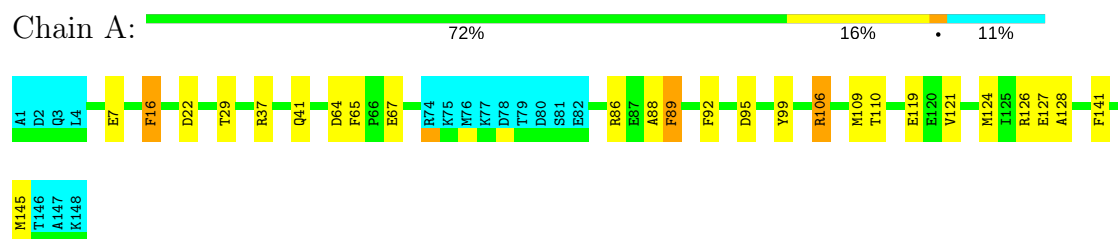
4.2.7 Score per residue for model 7

- Molecule 1: Calmodulin



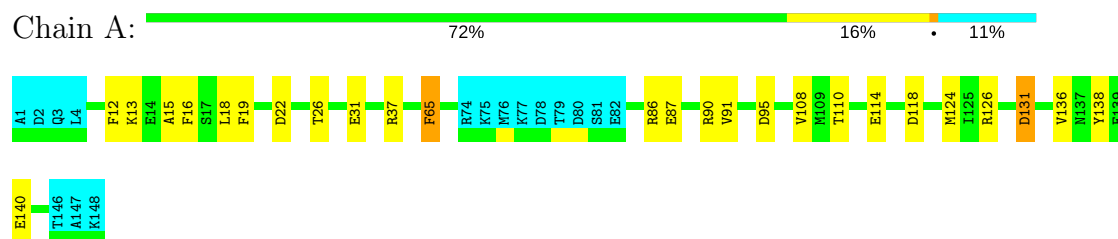
4.2.8 Score per residue for model 8

- Molecule 1: Calmodulin



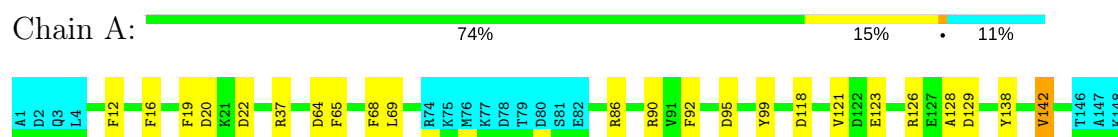
4.2.9 Score per residue for model 9

- Molecule 1: Calmodulin



4.2.10 Score per residue for model 10

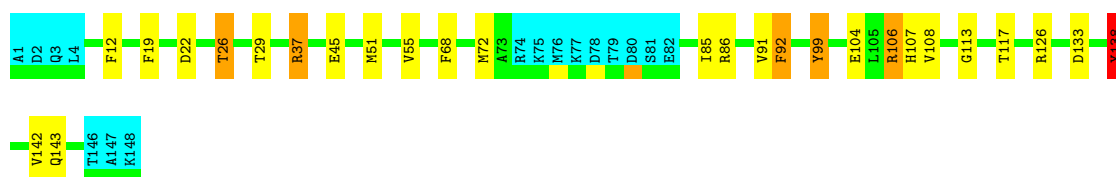
- Molecule 1: Calmodulin



4.2.11 Score per residue for model 11

- Molecule 1: Calmodulin

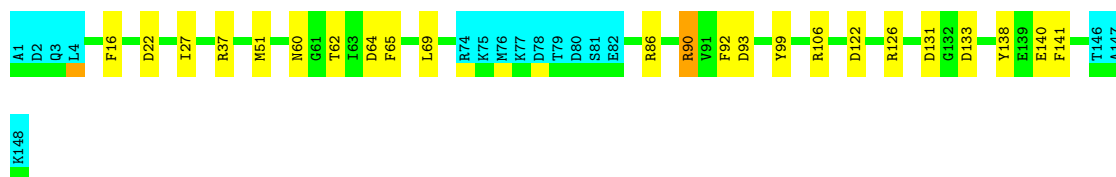




4.2.12 Score per residue for model 12

- Molecule 1: Calmodulin

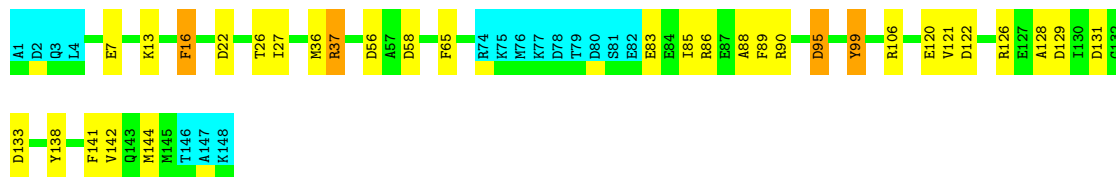
Chain A: 74% 15% 11%



4.2.13 Score per residue for model 13

- Molecule 1: Calmodulin

Chain A: 68% 19% 11%



4.2.14 Score per residue for model 14

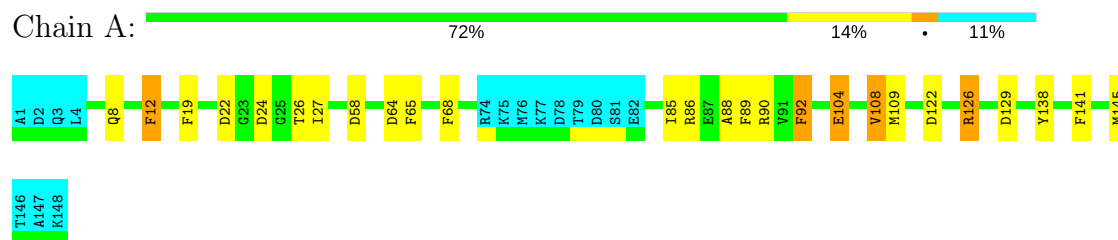
- Molecule 1: Calmodulin

Chain A: 72% 16% 11%



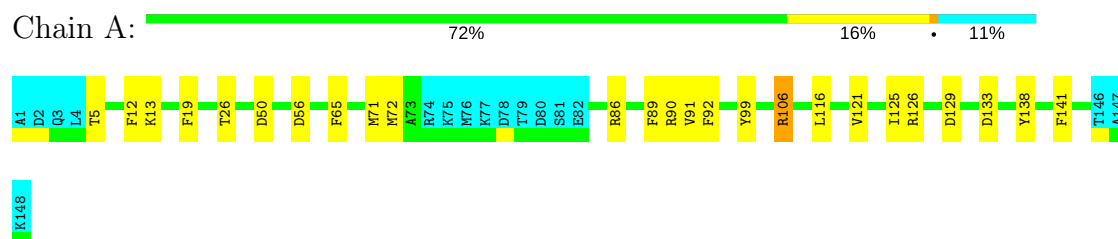
4.2.15 Score per residue for model 15

- Molecule 1: Calmodulin



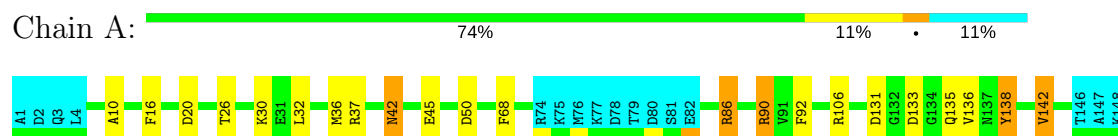
4.2.16 Score per residue for model 16

- Molecule 1: Calmodulin



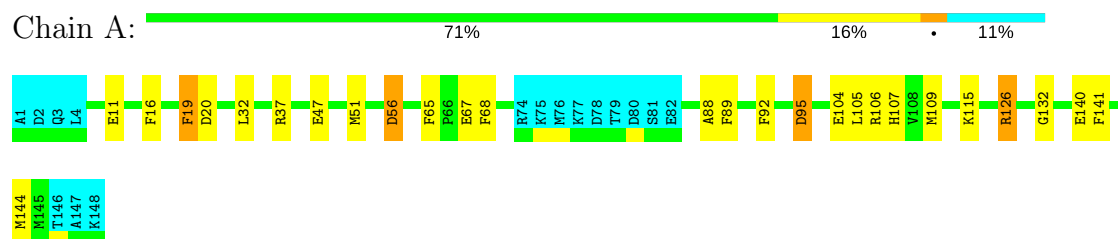
4.2.17 Score per residue for model 17

- Molecule 1: Calmodulin



4.2.18 Score per residue for model 18

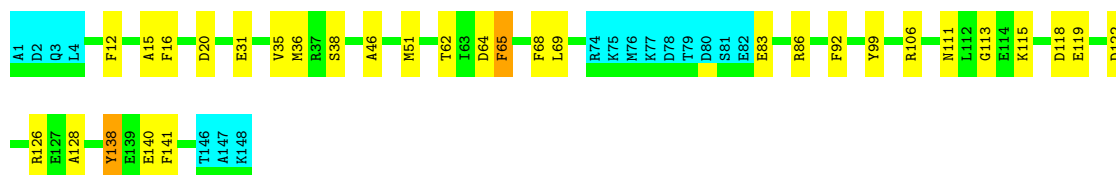
- Molecule 1: Calmodulin



4.2.19 Score per residue for model 19

- Molecule 1: Calmodulin

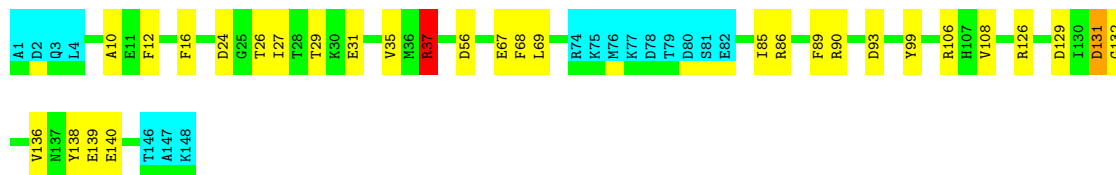




4.2.20 Score per residue for model 20

- Molecule 1: Calmodulin

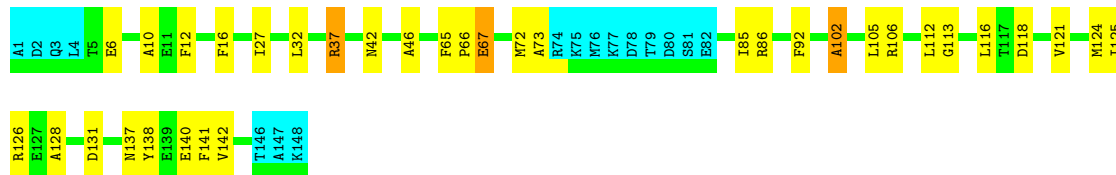
Chain A: 69% 19% 11%



4.2.21 Score per residue for model 21

- Molecule 1: Calmodulin

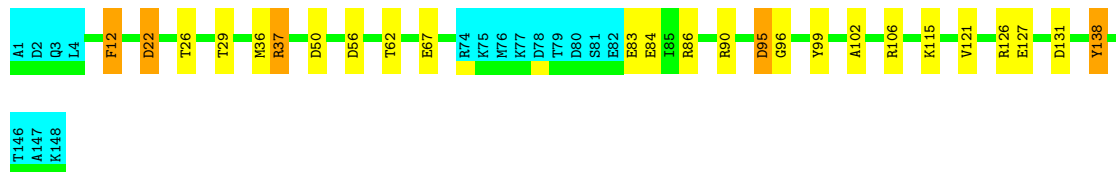
Chain A: 66% 22% 11%



4.2.22 Score per residue for model 22

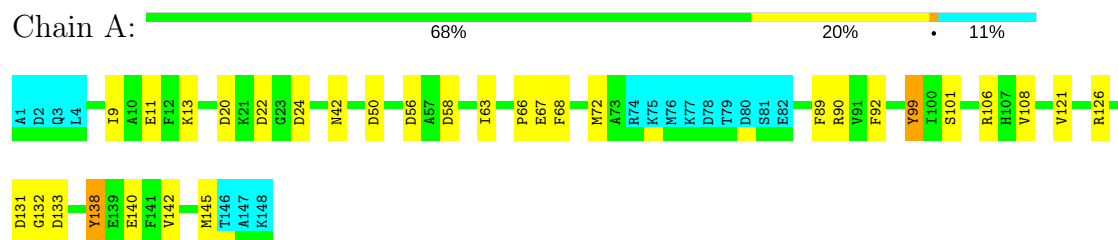
- Molecule 1: Calmodulin

Chain A: 72% 14% 11%



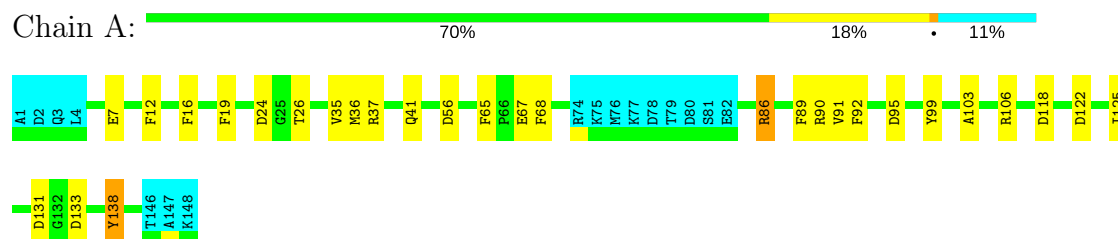
4.2.23 Score per residue for model 23

- Molecule 1: Calmodulin



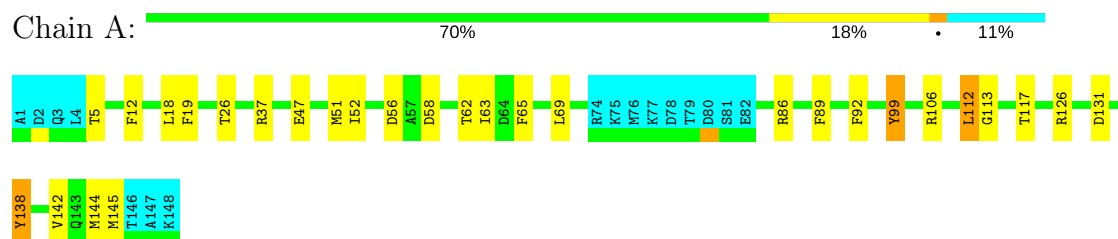
4.2.24 Score per residue for model 24

- Molecule 1: Calmodulin



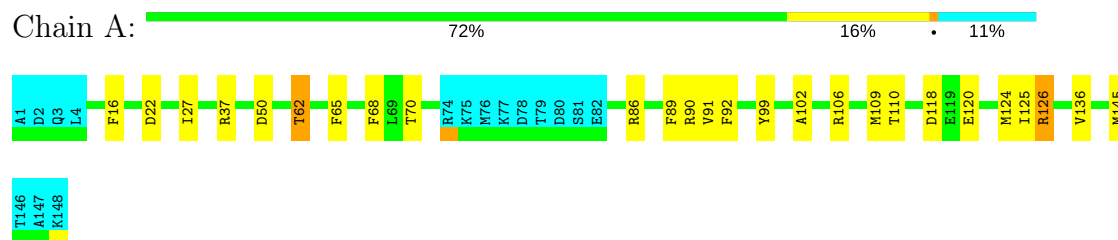
4.2.25 Score per residue for model 25

- Molecule 1: Calmodulin



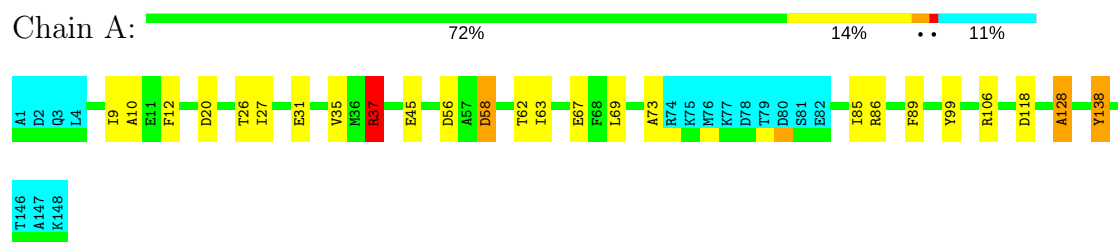
4.2.26 Score per residue for model 26

- Molecule 1: Calmodulin



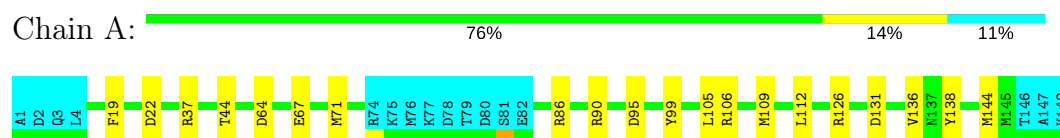
4.2.27 Score per residue for model 27

- Molecule 1: Calmodulin



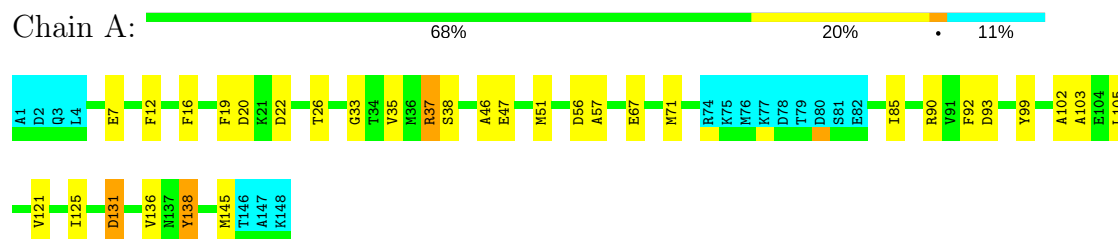
4.2.28 Score per residue for model 28

- Molecule 1: Calmodulin



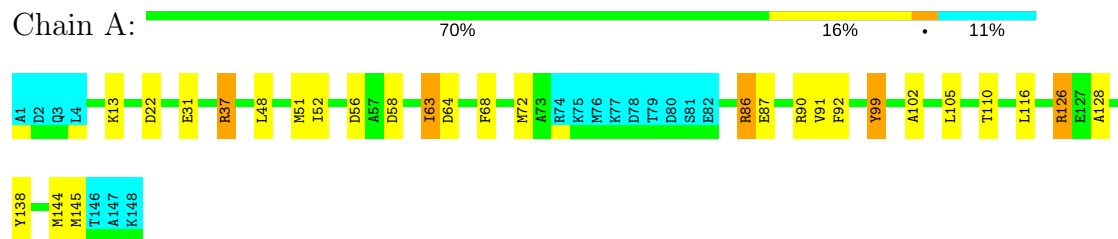
4.2.29 Score per residue for model 29

- Molecule 1: Calmodulin



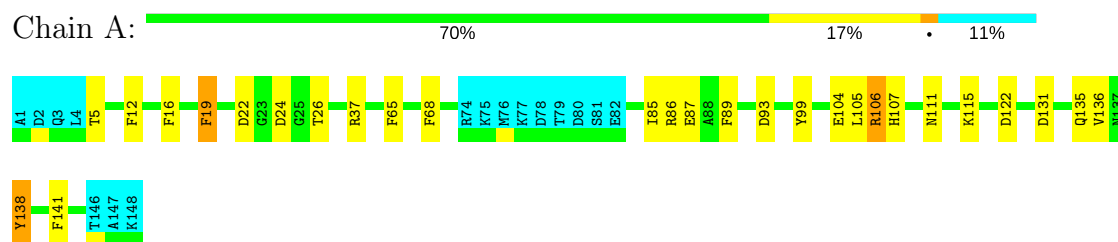
4.2.30 Score per residue for model 30

- Molecule 1: Calmodulin



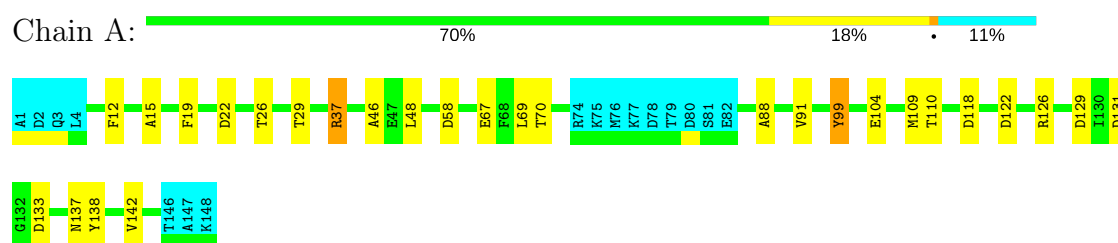
4.2.31 Score per residue for model 31

- Molecule 1: Calmodulin



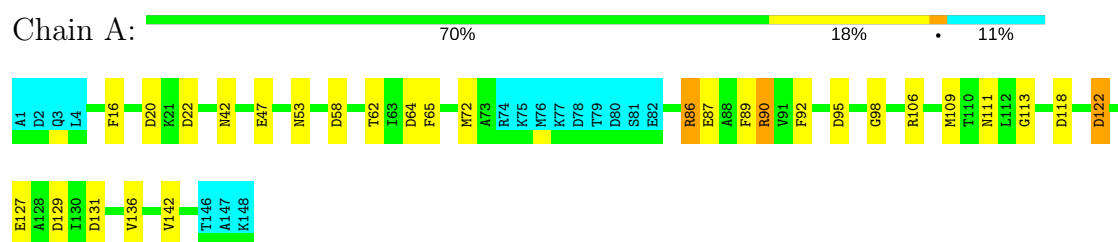
4.2.32 Score per residue for model 32

- Molecule 1: Calmodulin



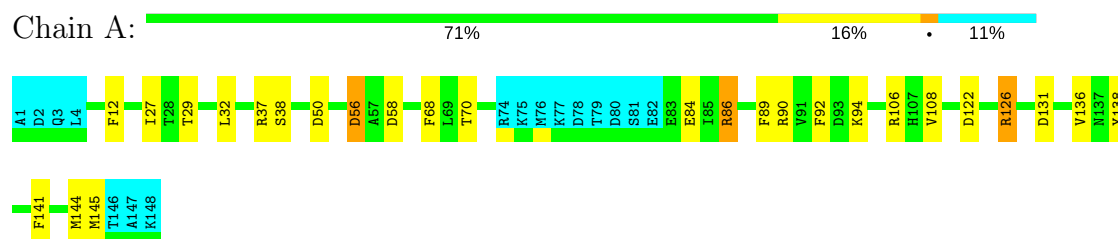
4.2.33 Score per residue for model 33

- Molecule 1: Calmodulin



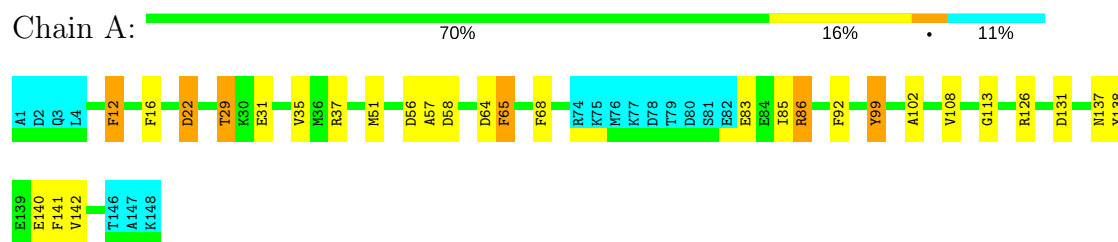
4.2.34 Score per residue for model 34

- Molecule 1: Calmodulin



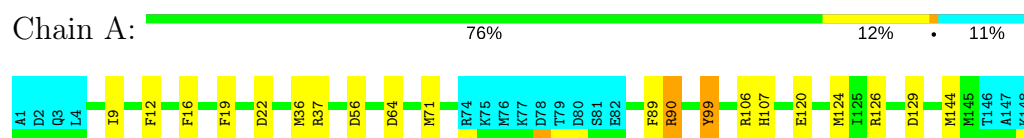
4.2.35 Score per residue for model 35

- Molecule 1: Calmodulin



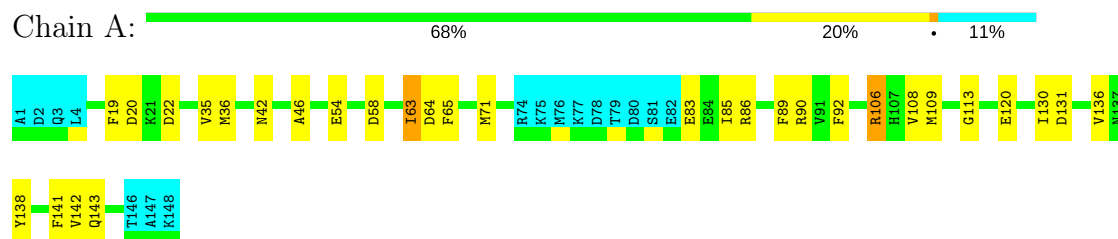
4.2.36 Score per residue for model 36

- Molecule 1: Calmodulin



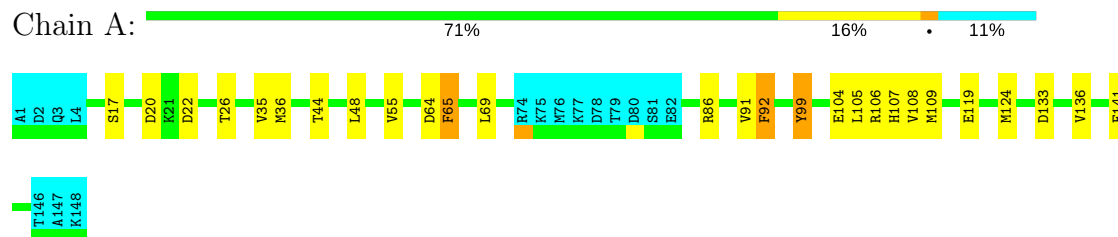
4.2.37 Score per residue for model 37

- Molecule 1: Calmodulin



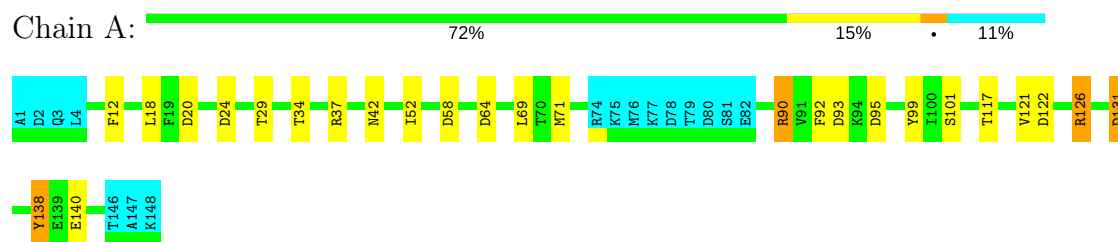
4.2.38 Score per residue for model 38

- Molecule 1: Calmodulin



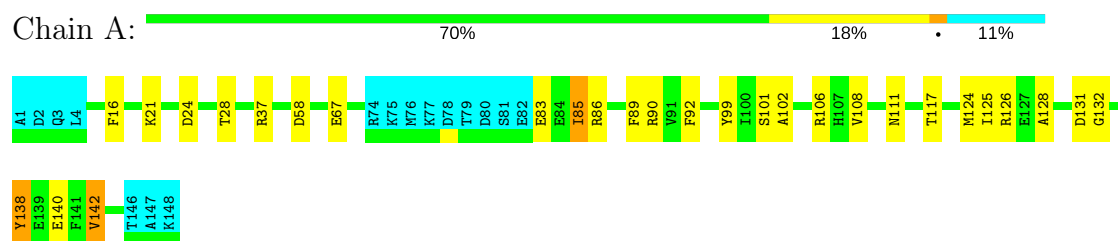
4.2.39 Score per residue for model 39

- Molecule 1: Calmodulin



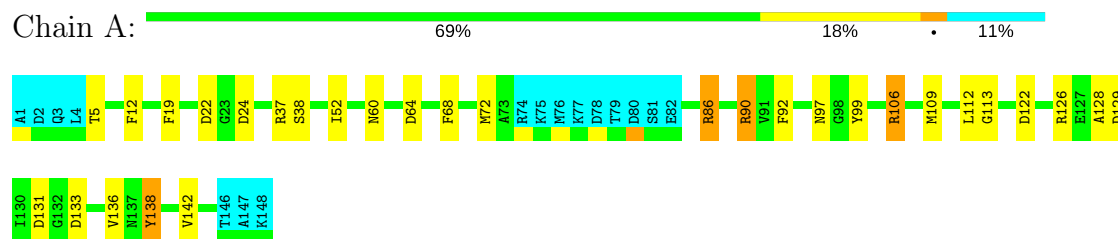
4.2.40 Score per residue for model 40

- Molecule 1: Calmodulin



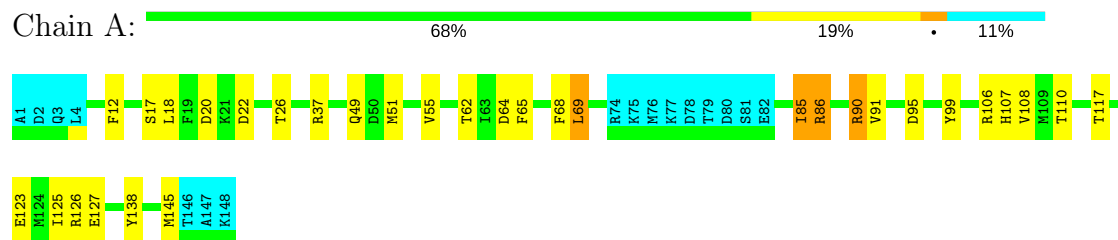
4.2.41 Score per residue for model 41

- Molecule 1: Calmodulin



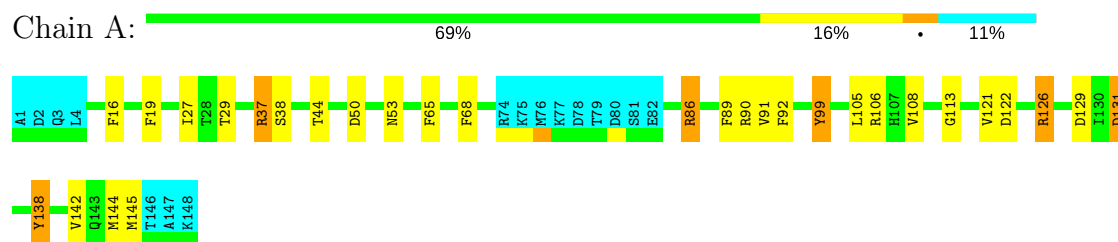
4.2.42 Score per residue for model 42

- Molecule 1: Calmodulin



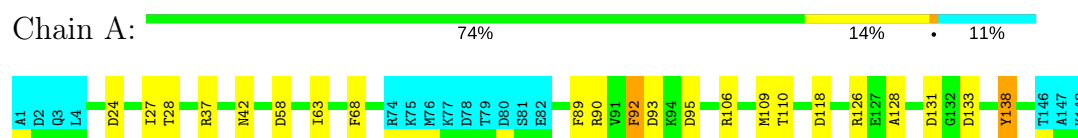
4.2.43 Score per residue for model 43

- Molecule 1: Calmodulin



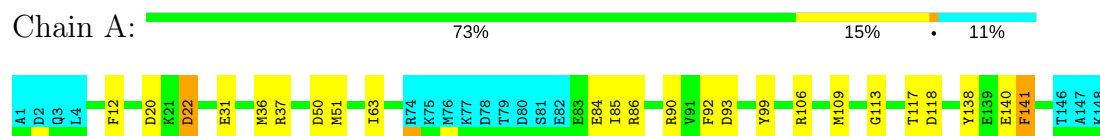
4.2.44 Score per residue for model 44

- Molecule 1: Calmodulin



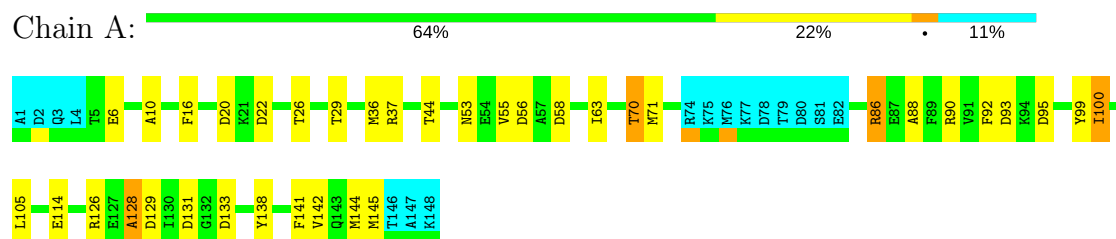
4.2.45 Score per residue for model 45

- Molecule 1: Calmodulin



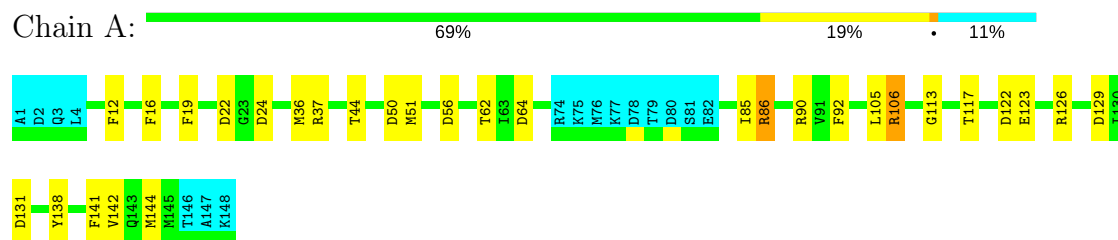
4.2.46 Score per residue for model 46

- Molecule 1: Calmodulin



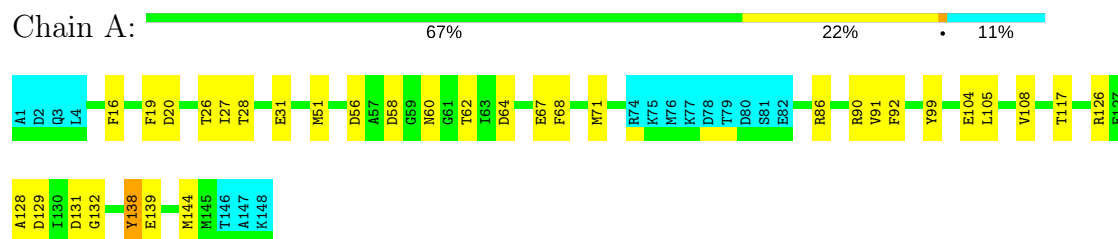
4.2.47 Score per residue for model 47

- Molecule 1: Calmodulin



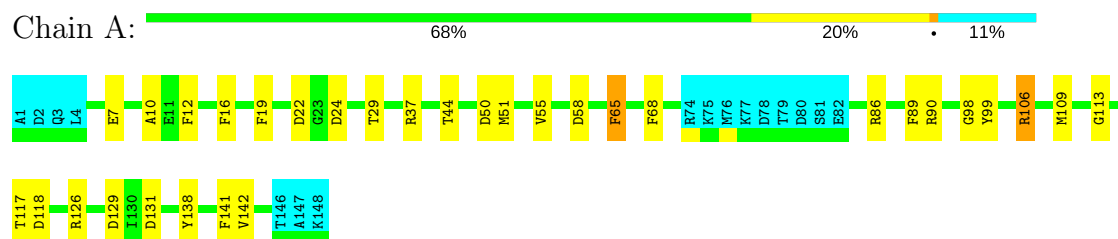
4.2.48 Score per residue for model 48

- Molecule 1: Calmodulin



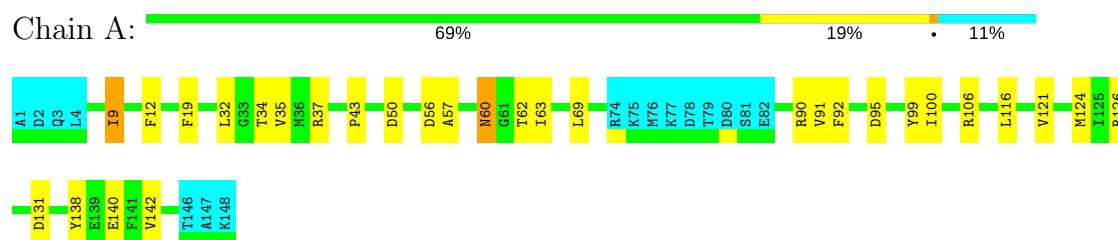
4.2.49 Score per residue for model 49

- Molecule 1: Calmodulin



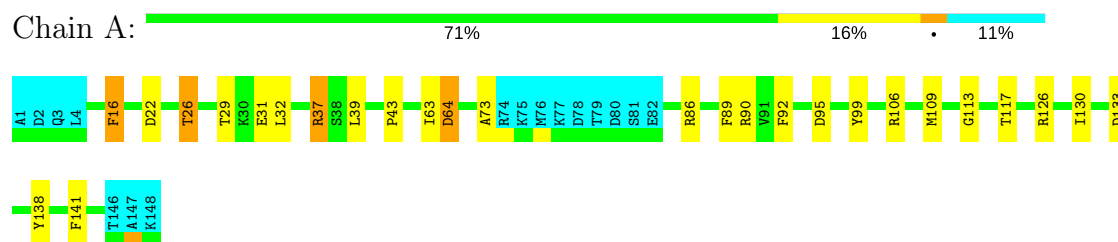
4.2.50 Score per residue for model 50

- Molecule 1: Calmodulin



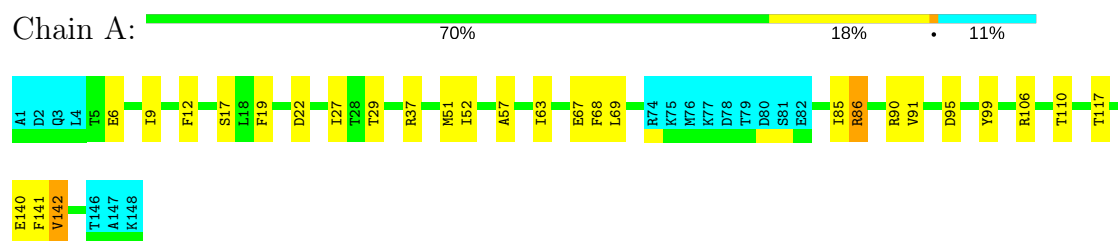
4.2.51 Score per residue for model 51

- Molecule 1: Calmodulin



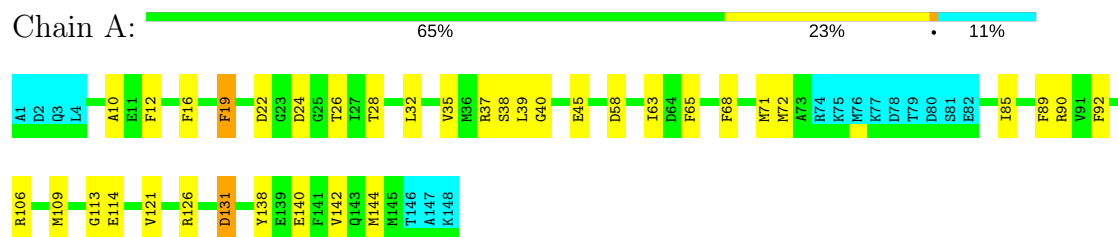
4.2.52 Score per residue for model 52

- Molecule 1: Calmodulin



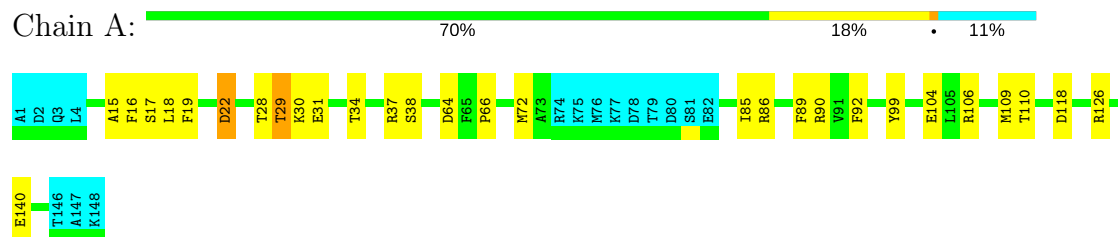
4.2.53 Score per residue for model 53

- Molecule 1: Calmodulin



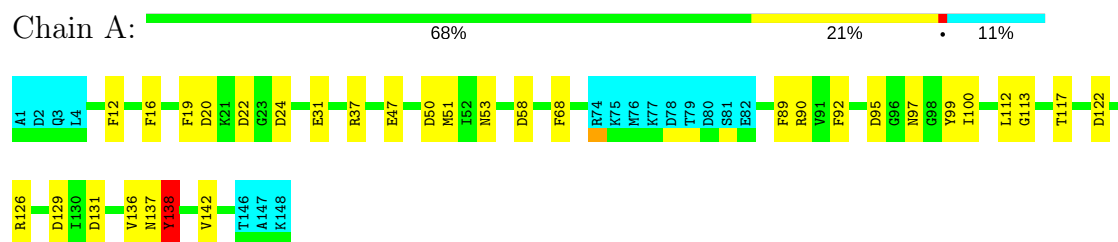
4.2.54 Score per residue for model 54

- Molecule 1: Calmodulin



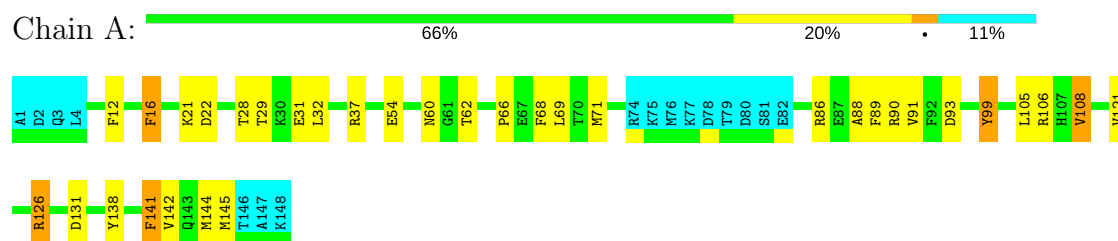
4.2.55 Score per residue for model 55

- Molecule 1: Calmodulin



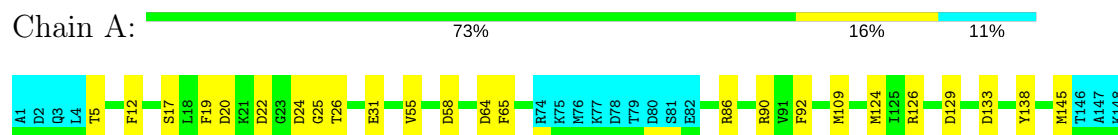
4.2.56 Score per residue for model 56

- Molecule 1: Calmodulin



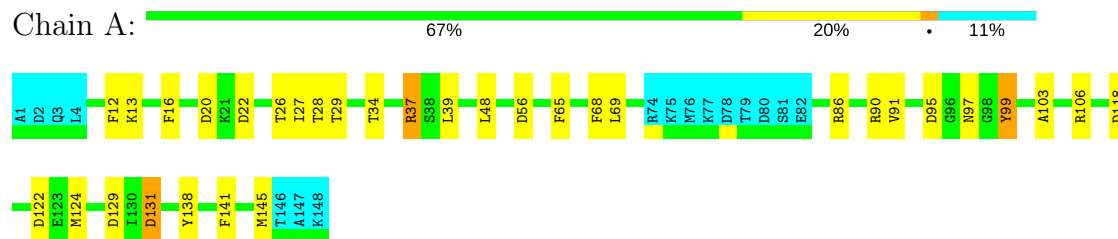
4.2.57 Score per residue for model 57

- Molecule 1: Calmodulin



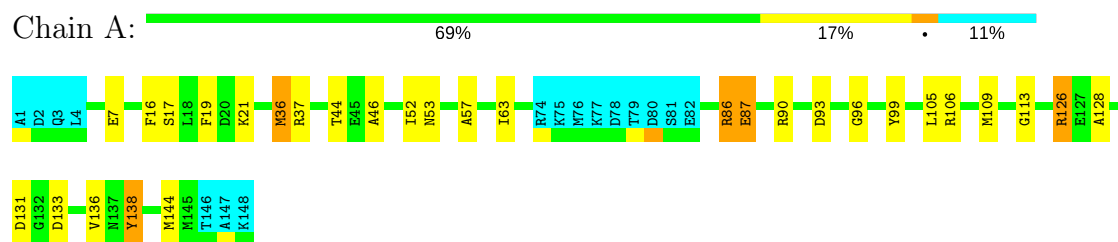
4.2.58 Score per residue for model 58

- Molecule 1: Calmodulin



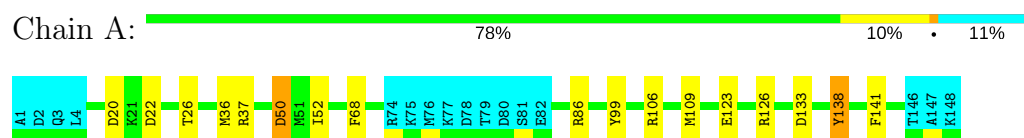
4.2.59 Score per residue for model 59

- Molecule 1: Calmodulin



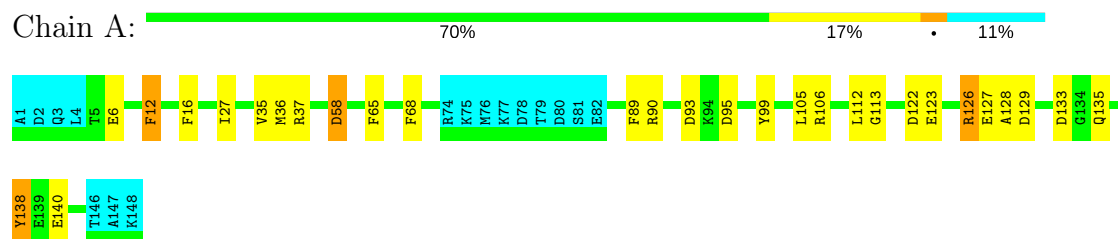
4.2.60 Score per residue for model 60

- Molecule 1: Calmodulin



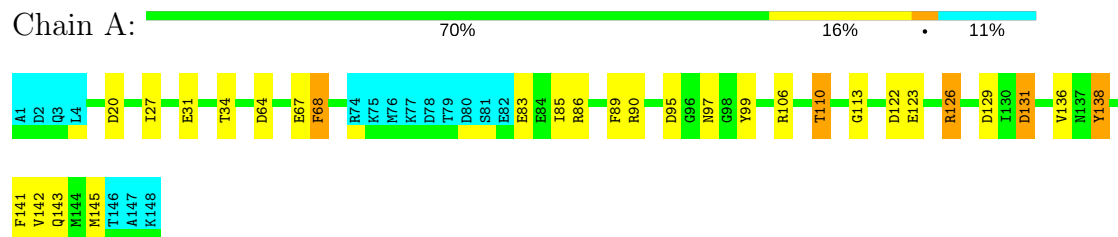
4.2.61 Score per residue for model 61

- Molecule 1: Calmodulin



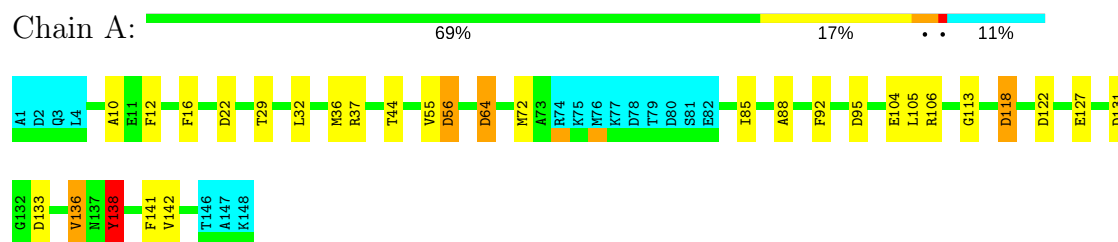
4.2.62 Score per residue for model 62

- Molecule 1: Calmodulin



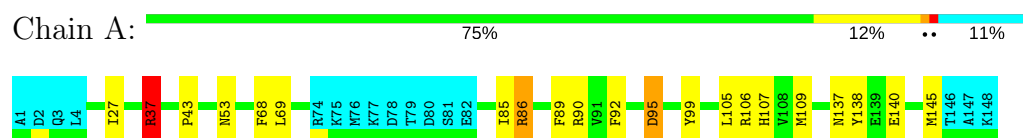
4.2.63 Score per residue for model 63

- Molecule 1: Calmodulin



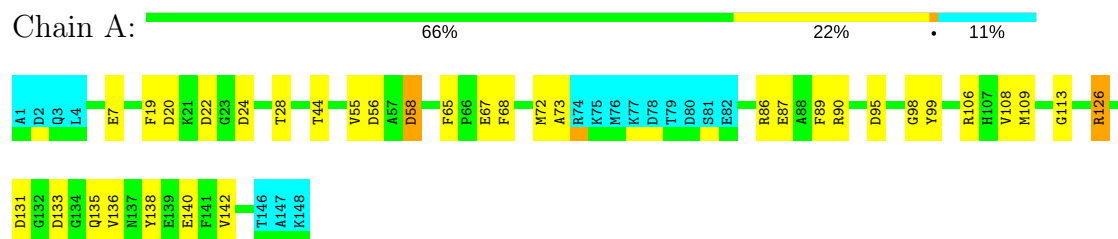
4.2.64 Score per residue for model 64

- Molecule 1: Calmodulin



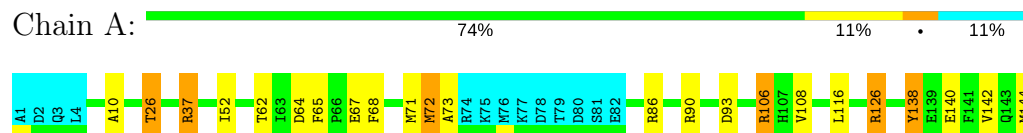
4.2.65 Score per residue for model 65

- Molecule 1: Calmodulin



4.2.66 Score per residue for model 66

- Molecule 1: Calmodulin



4.2.67 Score per residue for model 67

- Molecule 1: Calmodulin

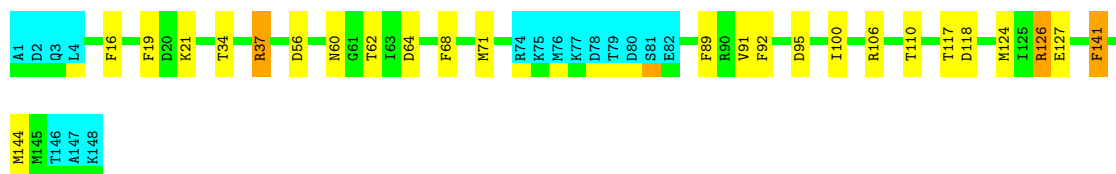
Chain A:  72% 16% 11%



4.2.68 Score per residue for model 68

- Molecule 1: Calmodulin

Chain A:  72% 15% 11%



4.2.69 Score per residue for model 69


- Molecule 1: Calmodulin

Chain A:  70% 18% 11%



4.2.70 Score per residue for model 70

- Molecule 1: Calmodulin

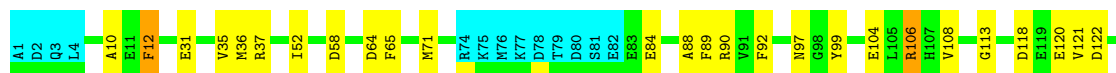
Chain A:  78% 11% 11%



4.2.71 Score per residue for model 71

- Molecule 1: Calmodulin

Chain A:  68% 18% 11%

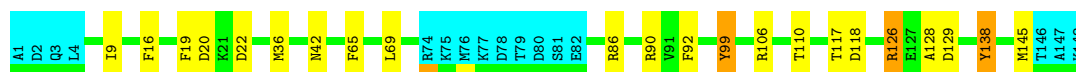




4.2.72 Score per residue for model 72

- Molecule 1: Calmodulin

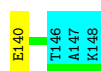
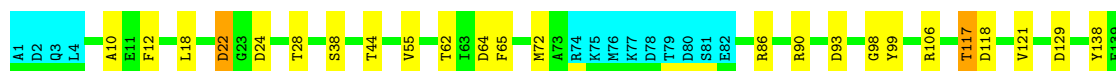
Chain A: 74% 13% 11%



4.2.73 Score per residue for model 73

- Molecule 1: Calmodulin

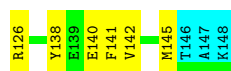
Chain A: 72% 16% 11%



4.2.74 Score per residue for model 74

- Molecule 1: Calmodulin

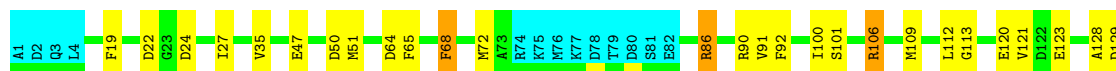
Chain A: 69% 20% 11%



4.2.75 Score per residue for model 75

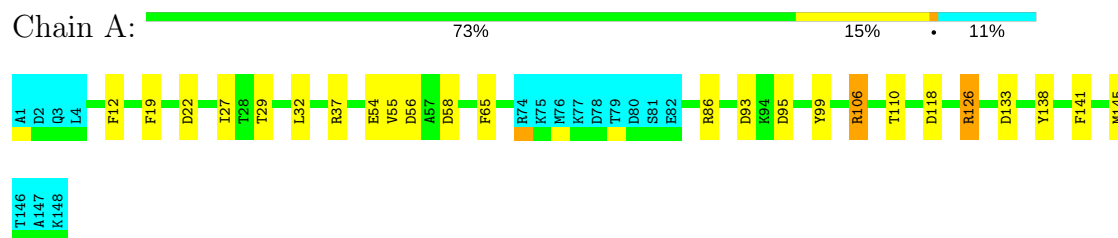
- Molecule 1: Calmodulin

Chain A: 67% 20% 11%



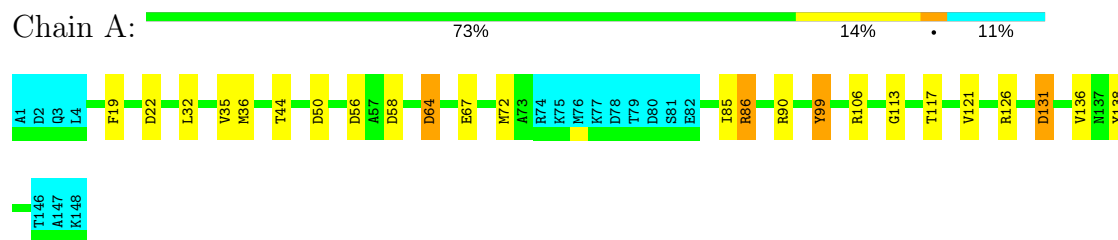
4.2.76 Score per residue for model 76

- Molecule 1: Calmodulin



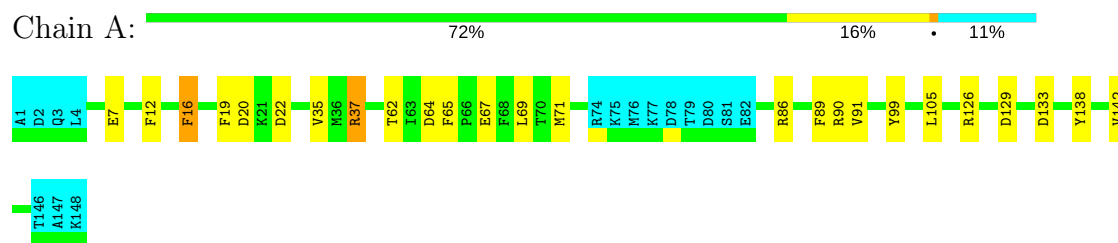
4.2.77 Score per residue for model 77

- Molecule 1: Calmodulin



4.2.78 Score per residue for model 78

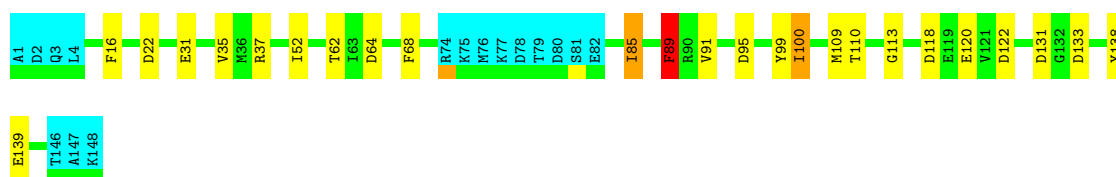
- Molecule 1: Calmodulin



4.2.79 Score per residue for model 79

- Molecule 1: Calmodulin





4.2.80 Score per residue for model 80

- Molecule 1: Calmodulin

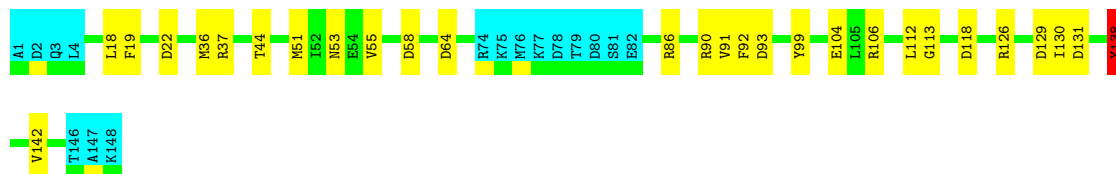
Chain A: 72% 17% 11%



4.2.81 Score per residue for model 81

- Molecule 1: Calmodulin

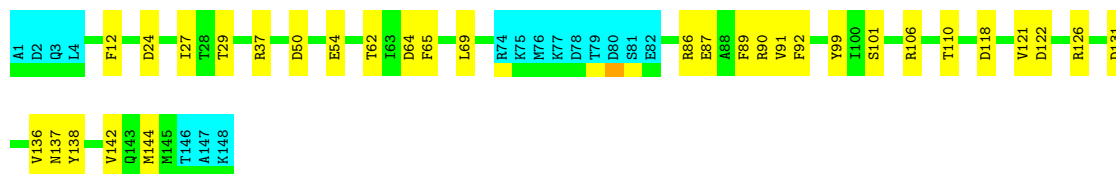
Chain A: 70% 18% 11%



4.2.82 Score per residue for model 82

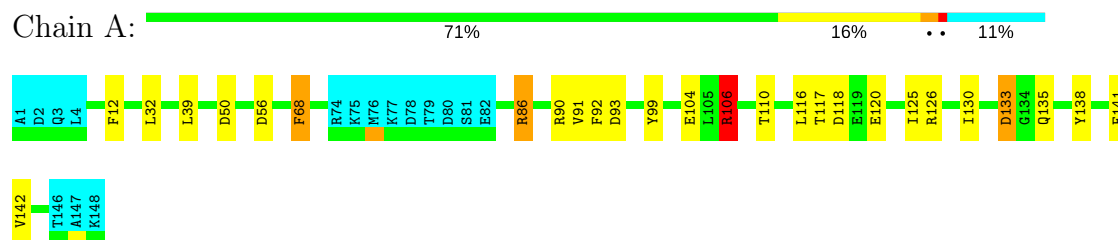
- Molecule 1: Calmodulin

Chain A: 68% 21% 11%



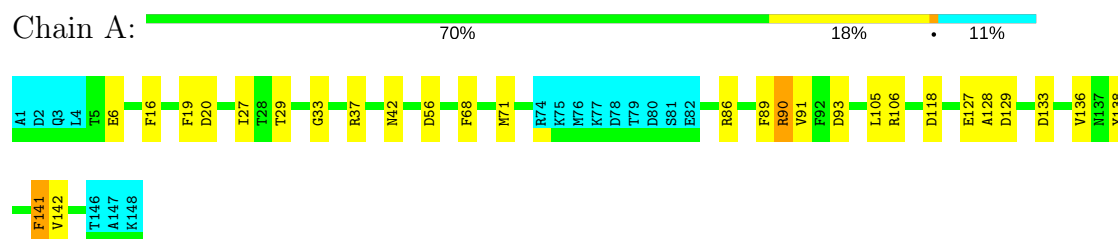
4.2.83 Score per residue for model 83

- Molecule 1: Calmodulin



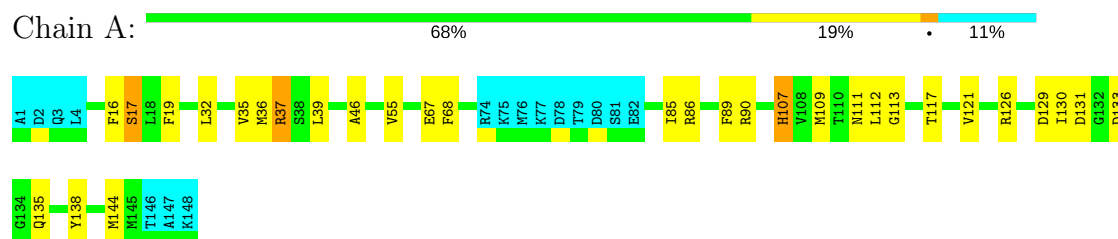
4.2.84 Score per residue for model 84

- Molecule 1: Calmodulin



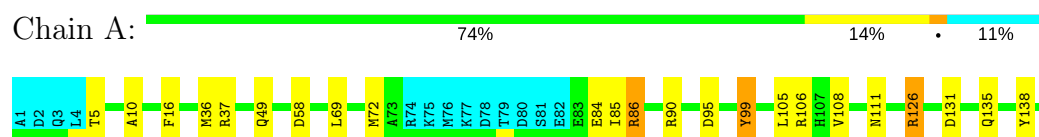
4.2.85 Score per residue for model 85

- Molecule 1: Calmodulin



4.2.86 Score per residue for model 86

- Molecule 1: Calmodulin



4.2.87 Score per residue for model 87

- Molecule 1: Calmodulin

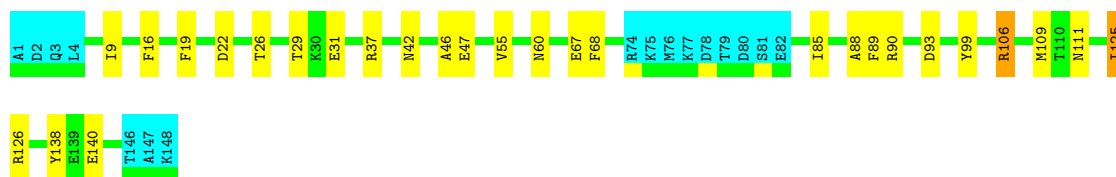




4.2.88 Score per residue for model 88

- Molecule 1: Calmodulin

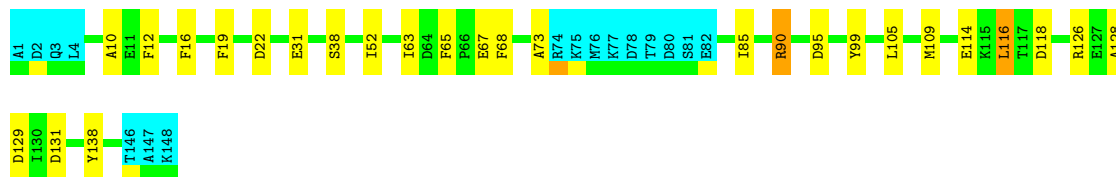
Chain A: 70% 18% 11%



4.2.89 Score per residue for model 89

- Molecule 1: Calmodulin

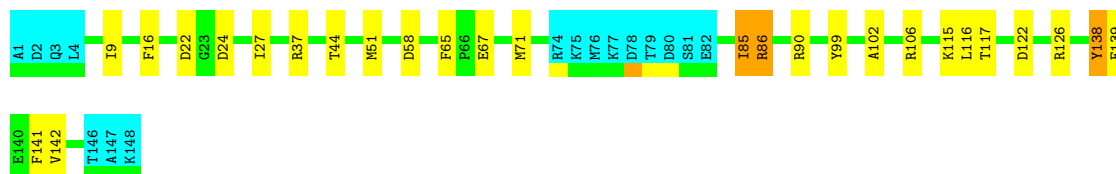
Chain A: 71% 17% 11%



4.2.90 Score per residue for model 90

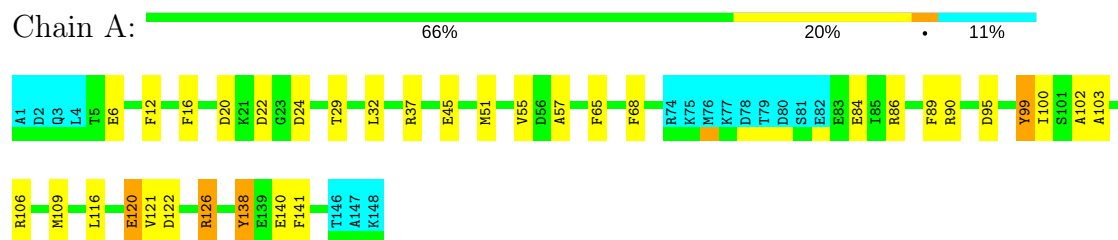
- Molecule 1: Calmodulin

Chain A: 71% 16% 11%



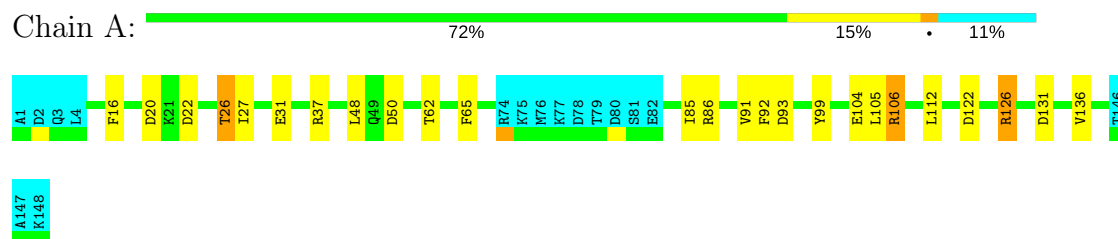
4.2.91 Score per residue for model 91

- Molecule 1: Calmodulin



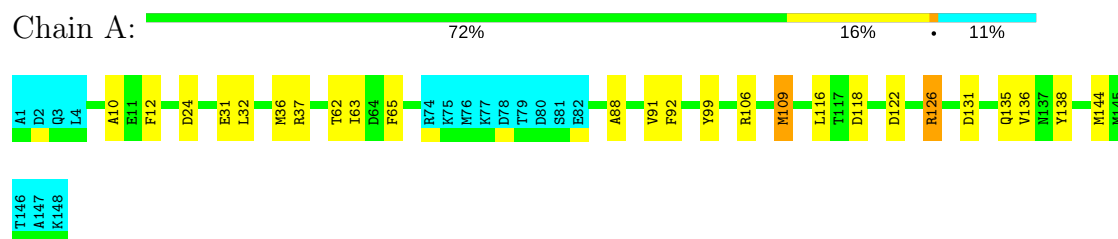
4.2.92 Score per residue for model 92

- Molecule 1: Calmodulin



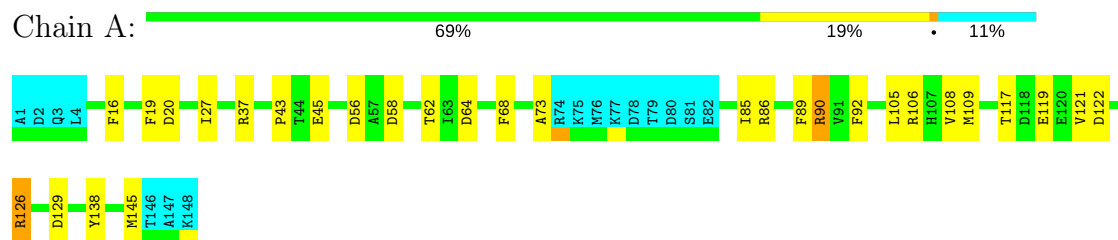
4.2.93 Score per residue for model 93

- Molecule 1: Calmodulin



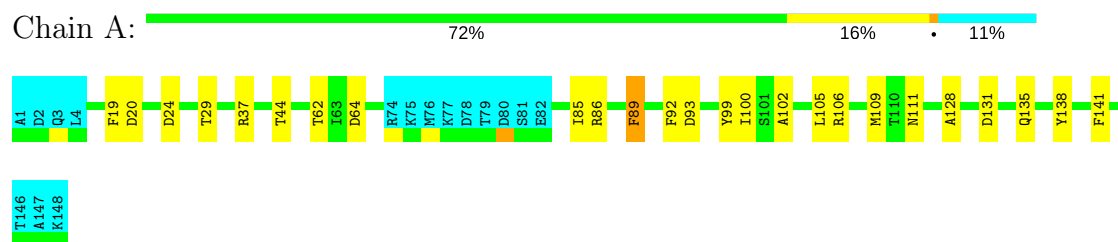
4.2.94 Score per residue for model 94

- Molecule 1: Calmodulin



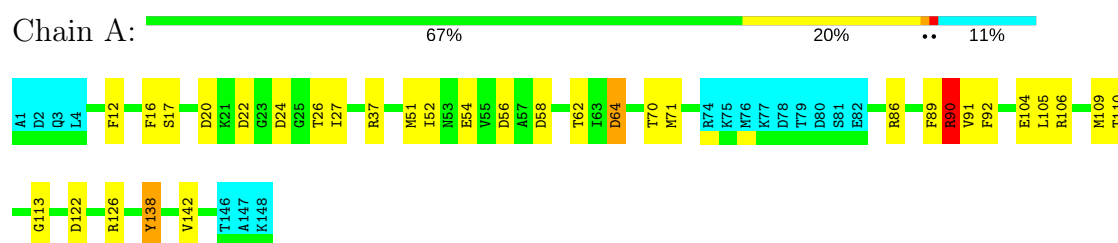
4.2.95 Score per residue for model 95

- Molecule 1: Calmodulin



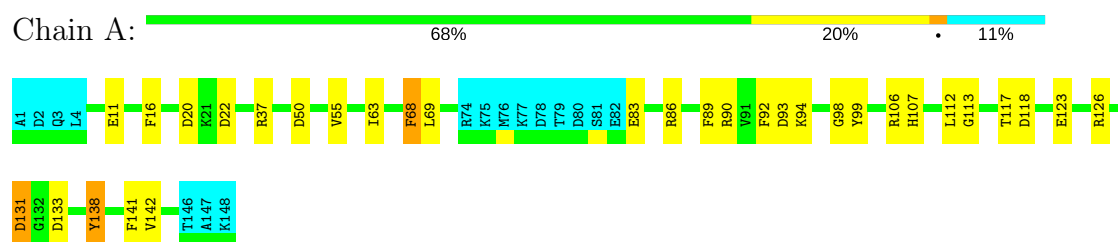
4.2.96 Score per residue for model 96

- Molecule 1: Calmodulin



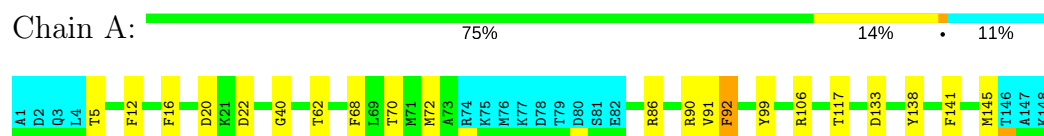
4.2.97 Score per residue for model 97

- Molecule 1: Calmodulin



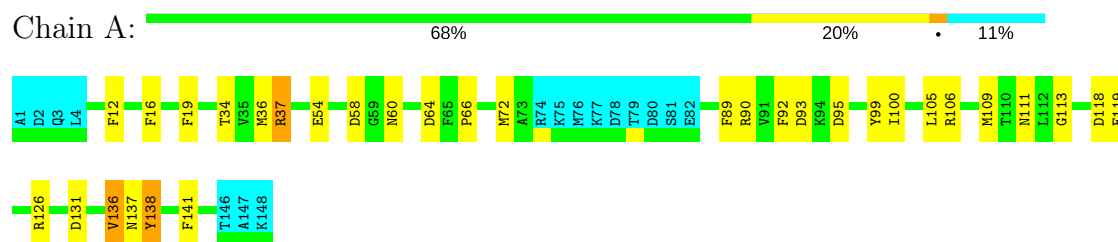
4.2.98 Score per residue for model 98

- Molecule 1: Calmodulin



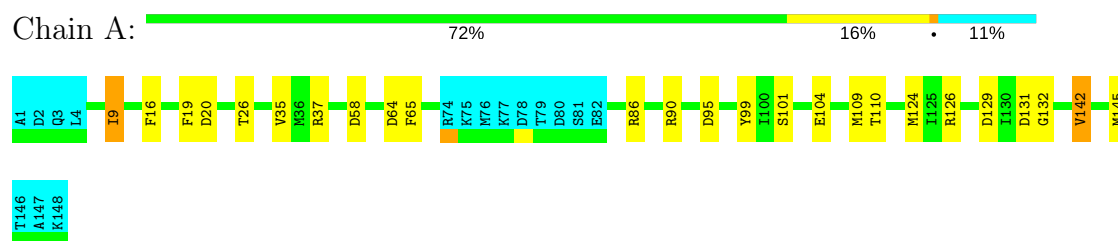
4.2.99 Score per residue for model 99

- Molecule 1: Calmodulin



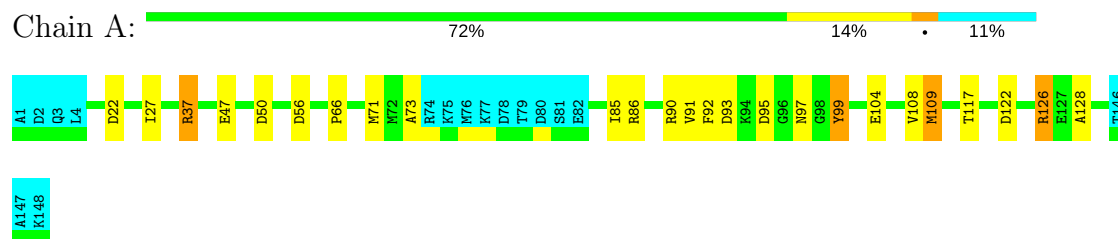
4.2.100 Score per residue for model 100

- Molecule 1: Calmodulin



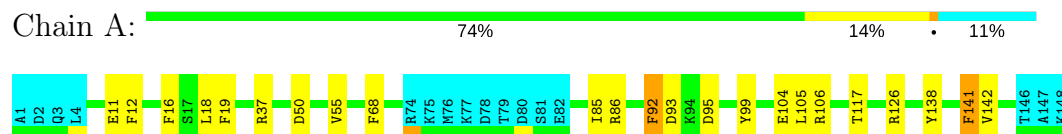
4.2.101 Score per residue for model 101

- Molecule 1: Calmodulin



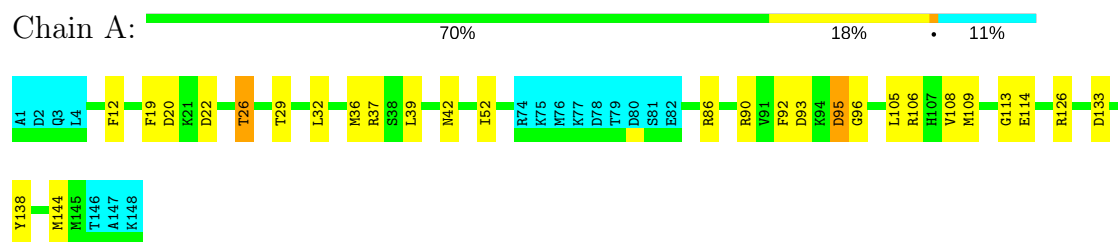
4.2.102 Score per residue for model 102

- Molecule 1: Calmodulin



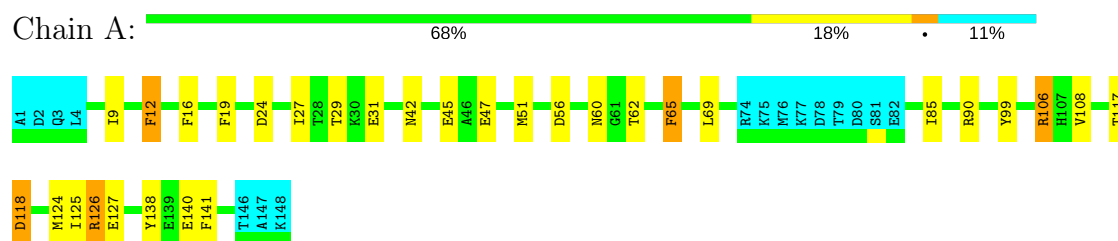
4.2.103 Score per residue for model 103

- Molecule 1: Calmodulin



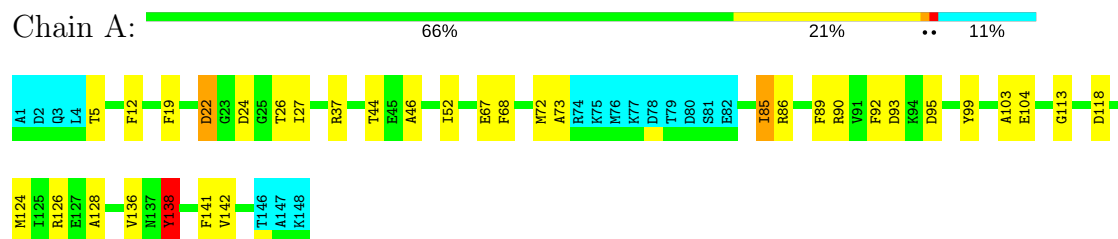
4.2.104 Score per residue for model 104

- Molecule 1: Calmodulin



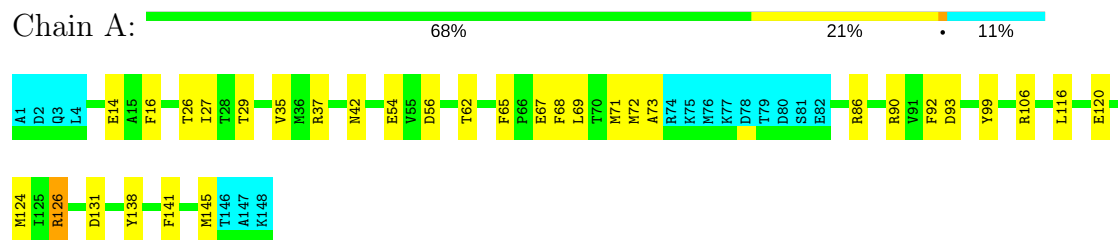
4.2.105 Score per residue for model 105

- Molecule 1: Calmodulin



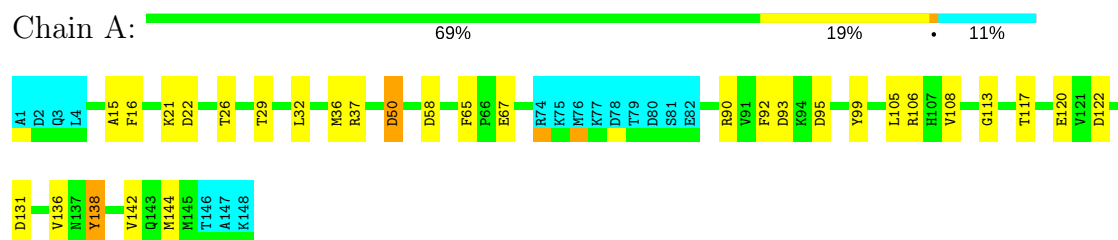
4.2.106 Score per residue for model 106

- Molecule 1: Calmodulin



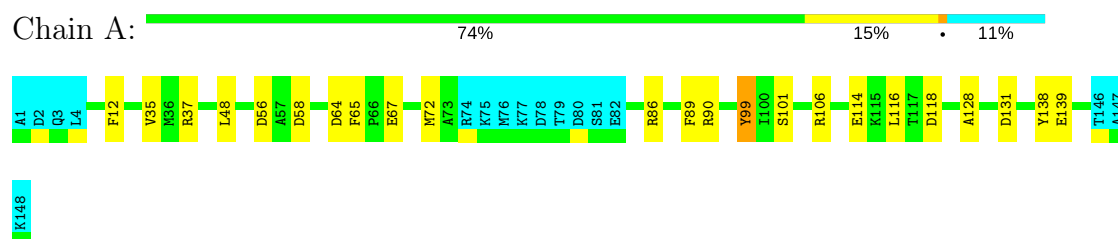
4.2.107 Score per residue for model 107

- Molecule 1: Calmodulin



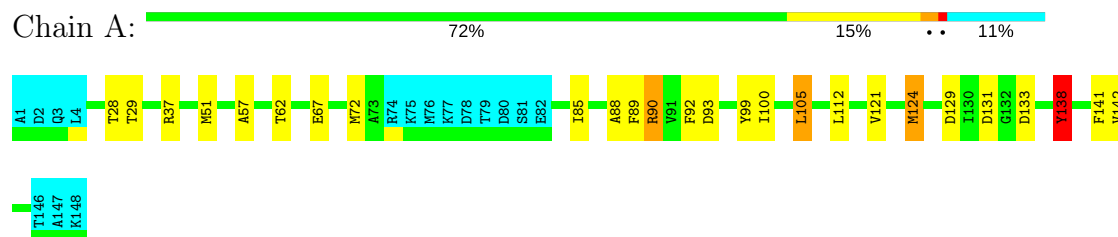
4.2.108 Score per residue for model 108

- Molecule 1: Calmodulin



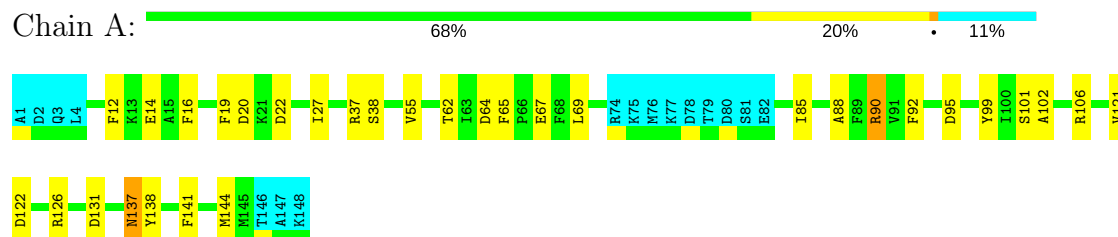
4.2.109 Score per residue for model 109

- Molecule 1: Calmodulin



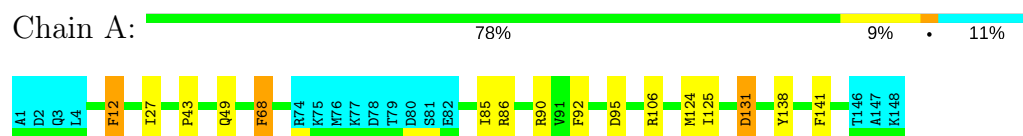
4.2.110 Score per residue for model 110

- Molecule 1: Calmodulin



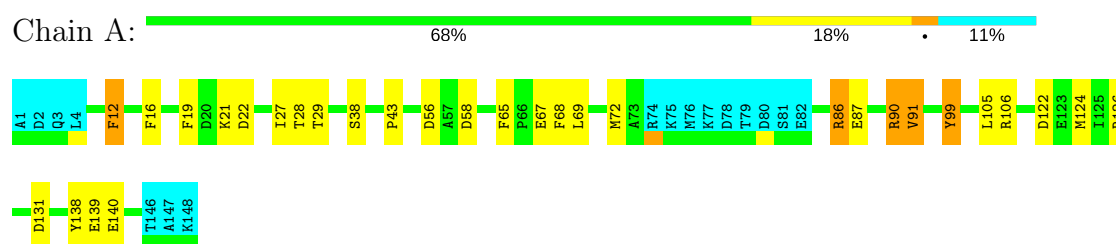
4.2.111 Score per residue for model 111

- Molecule 1: Calmodulin



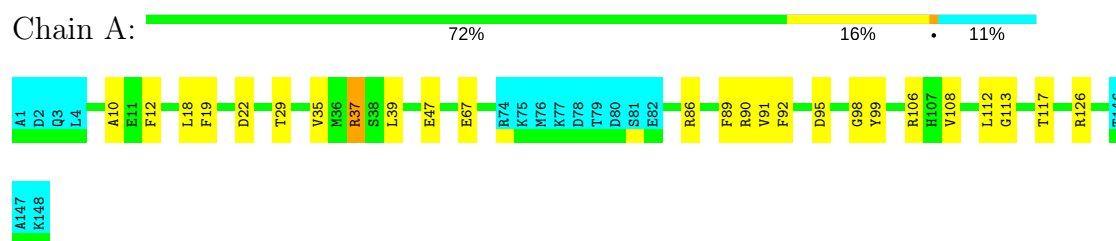
4.2.112 Score per residue for model 112

- Molecule 1: Calmodulin



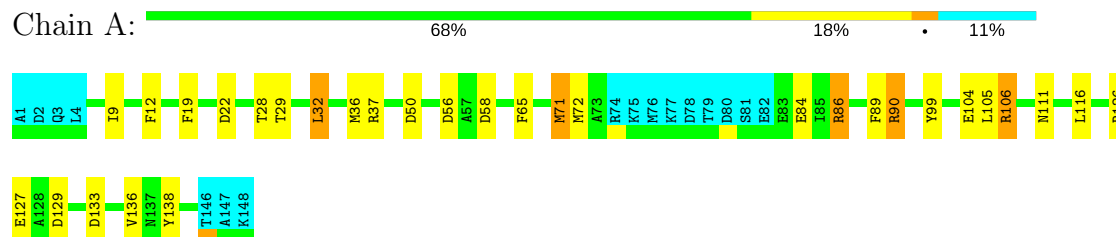
4.2.113 Score per residue for model 113

- Molecule 1: Calmodulin



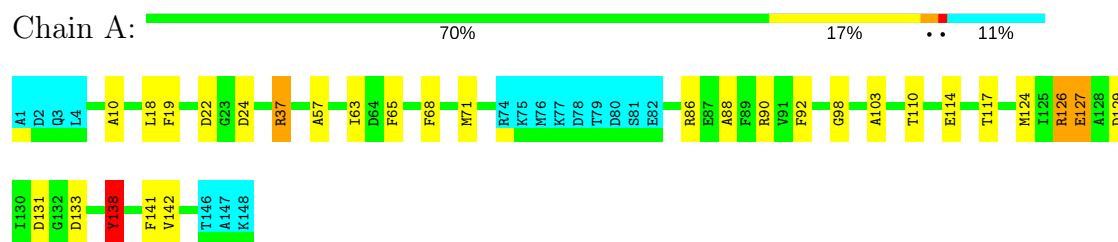
4.2.114 Score per residue for model 114

- Molecule 1: Calmodulin



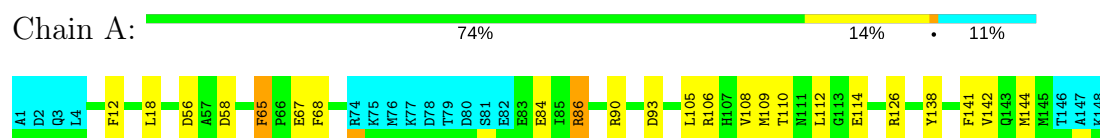
4.2.115 Score per residue for model 115

- Molecule 1: Calmodulin



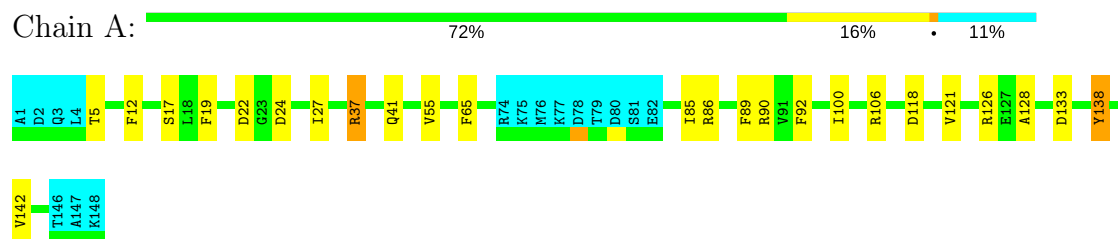
4.2.116 Score per residue for model 116

- Molecule 1: Calmodulin



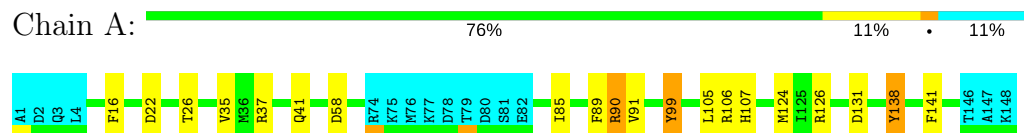
4.2.117 Score per residue for model 117

- Molecule 1: Calmodulin



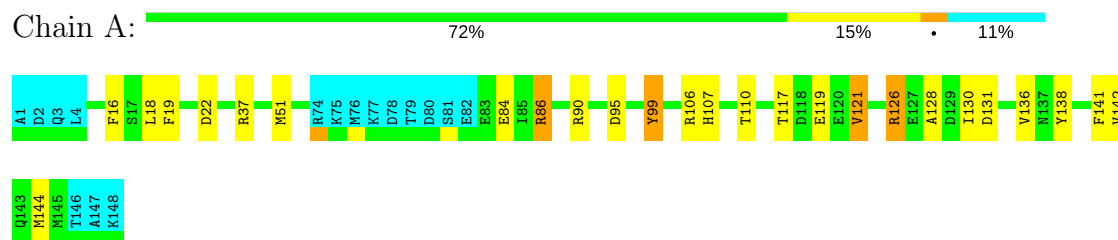
4.2.118 Score per residue for model 118

- Molecule 1: Calmodulin



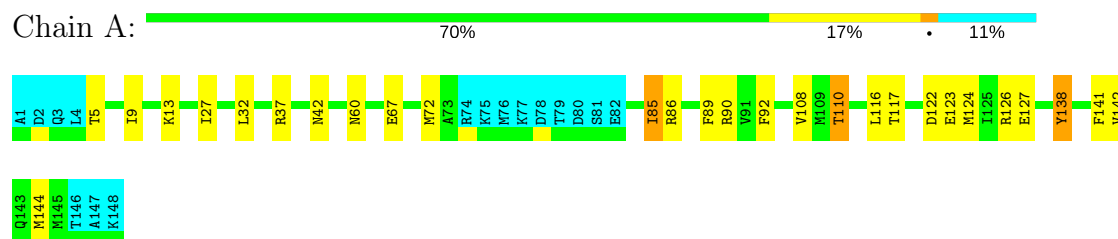
4.2.119 Score per residue for model 119

- Molecule 1: Calmodulin



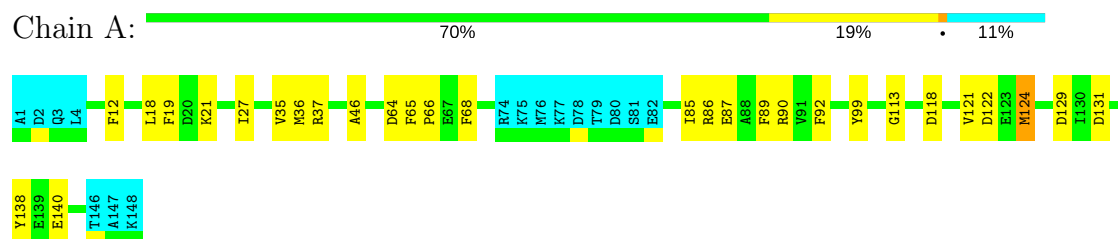
4.2.120 Score per residue for model 120

- Molecule 1: Calmodulin



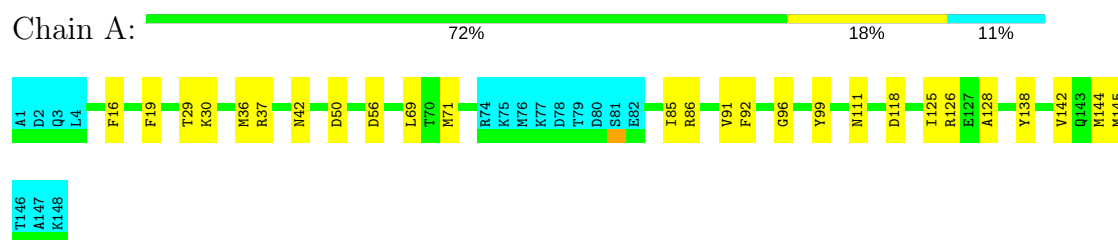
4.2.121 Score per residue for model 121

- Molecule 1: Calmodulin



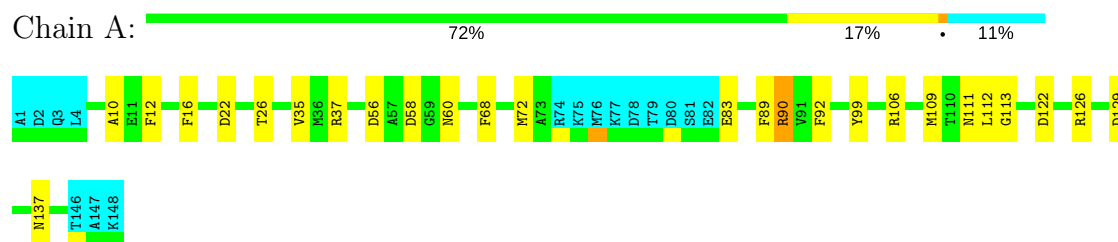
4.2.122 Score per residue for model 122

- Molecule 1: Calmodulin



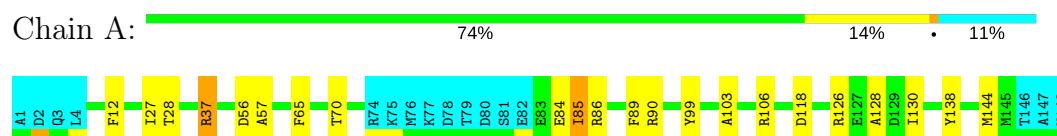
4.2.123 Score per residue for model 123

- Molecule 1: Calmodulin



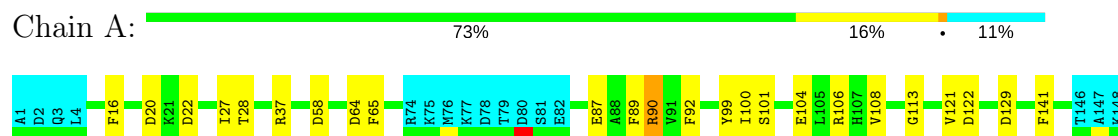
4.2.124 Score per residue for model 124

- Molecule 1: Calmodulin



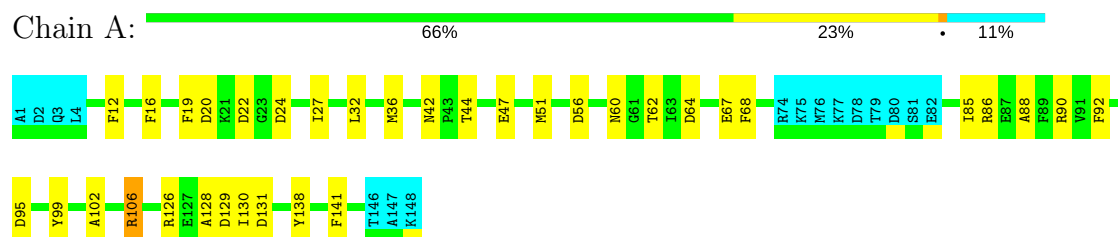
4.2.125 Score per residue for model 125

- Molecule 1: Calmodulin



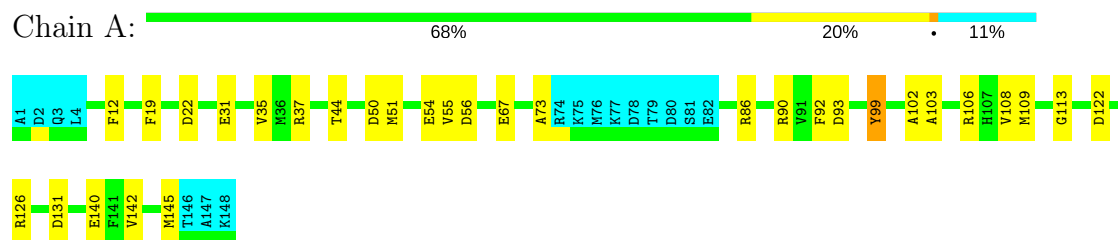
4.2.126 Score per residue for model 126

- Molecule 1: Calmodulin



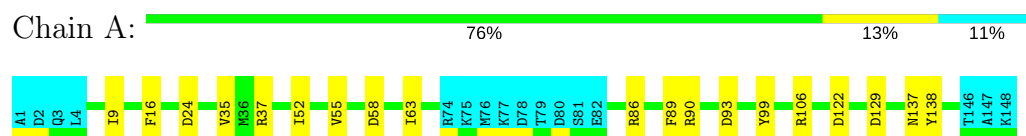
4.2.127 Score per residue for model 127

- Molecule 1: Calmodulin



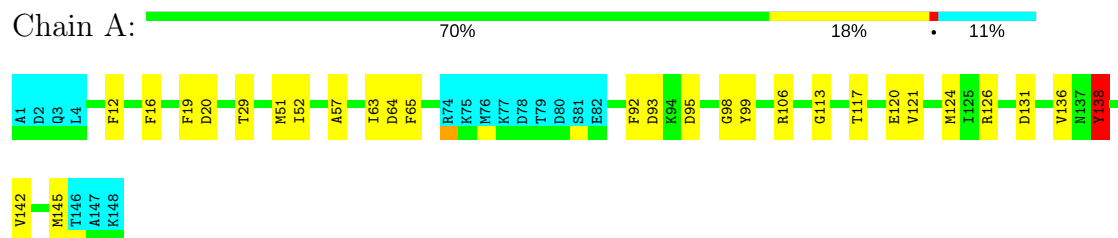
4.2.128 Score per residue for model 128

- Molecule 1: Calmodulin



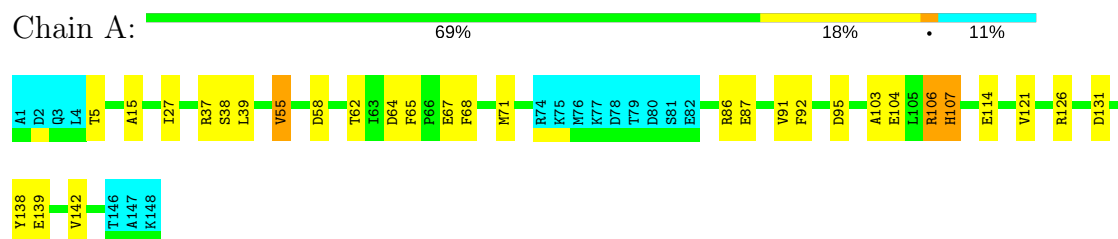
4.2.129 Score per residue for model 129

- Molecule 1: Calmodulin



4.2.130 Score per residue for model 130

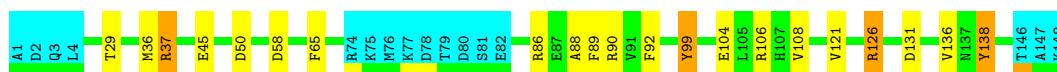
- Molecule 1: Calmodulin



4.2.131 Score per residue for model 131

- Molecule 1: Calmodulin

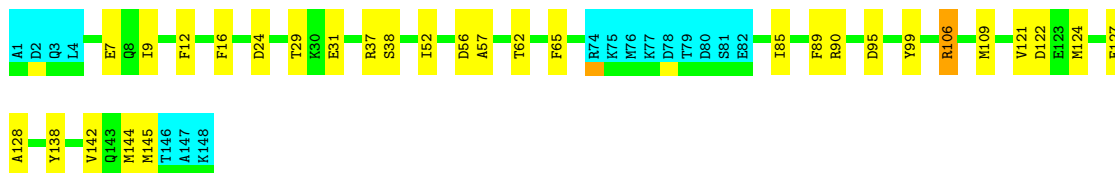




4.2.132 Score per residue for model 132

- Molecule 1: Calmodulin

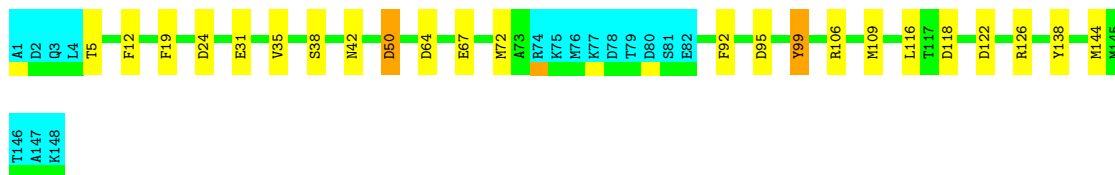
Chain A: 69% 20% 11%



4.2.133 Score per residue for model 133

- Molecule 1: Calmodulin

Chain A: 74% 14% 11%



4.2.134 Score per residue for model 134

- Molecule 1: Calmodulin

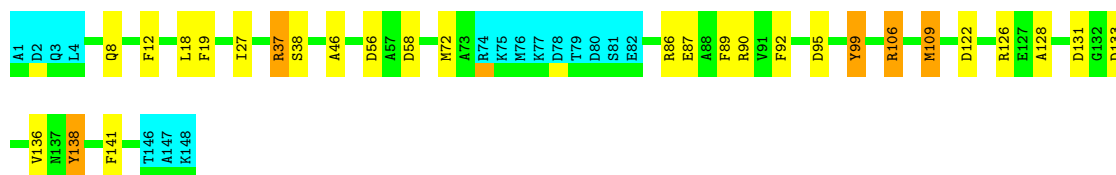
Chain A: 64% 24% 11%



4.2.135 Score per residue for model 135

- Molecule 1: Calmodulin

Chain A: 70% 16% 11%



4.2.136 Score per residue for model 136

- Molecule 1: Calmodulin

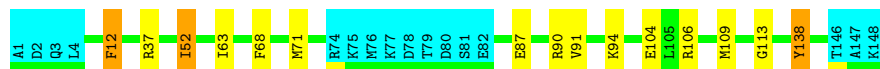
Chain A: 72% 16% 11%



4.2.137 Score per residue for model 137

- Molecule 1: Calmodulin

Chain A: 79% 8% 11%



4.2.138 Score per residue for model 138

- Molecule 1: Calmodulin

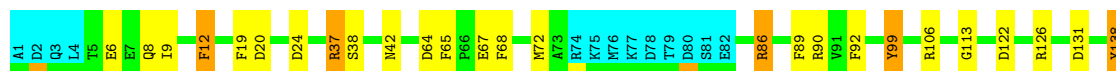
Chain A: 70% 16% 11%



4.2.139 Score per residue for model 139

- Molecule 1: Calmodulin

Chain A: 70% 16% 11%

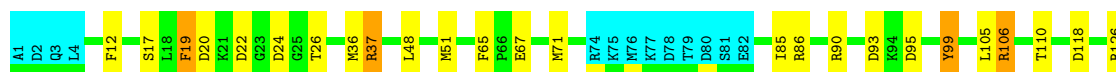




4.2.140 Score per residue for model 140

- Molecule 1: Calmodulin

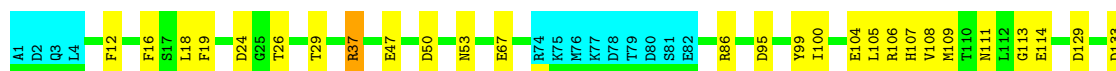
Chain A: 69% 18% 11%



4.2.141 Score per residue for model 141

- Molecule 1: Calmodulin

Chain A: 68% 20% 11%



4.2.142 Score per residue for model 142

- Molecule 1: Calmodulin

Chain A: 72% 14% 11%



4.2.143 Score per residue for model 143

- Molecule 1: Calmodulin

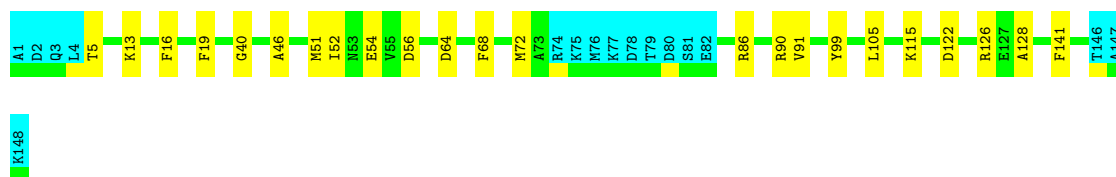
Chain A: 70% 18% 11%



4.2.144 Score per residue for model 144

- Molecule 1: Calmodulin

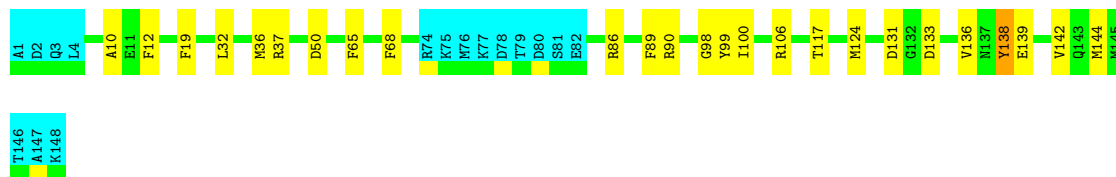
Chain A: 74% 16% 11%



4.2.145 Score per residue for model 145

- Molecule 1: Calmodulin

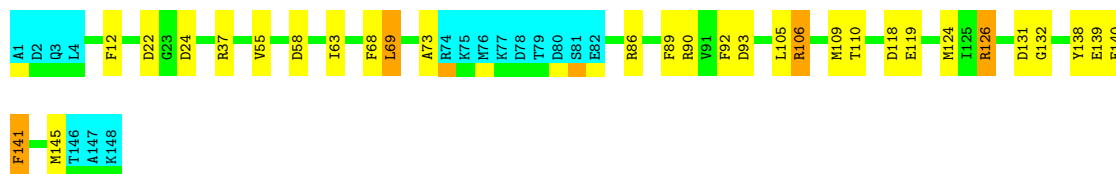
Chain A: 72% 16% 11%



4.2.146 Score per residue for model 146

- Molecule 1: Calmodulin

Chain A: 69% 18% 11%



4.2.147 Score per residue for model 147

- Molecule 1: Calmodulin

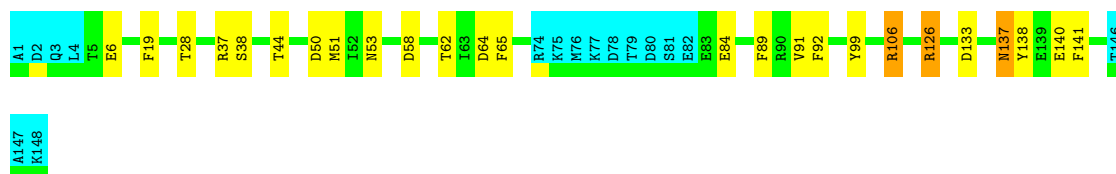
Chain A:  73% 14% 11%



4.2.148 Score per residue for model 148

- Molecule 1: Calmodulin

Chain A:  72% 15% 11%



4.2.149 Score per residue for model 149

- Molecule 1: Calmodulin

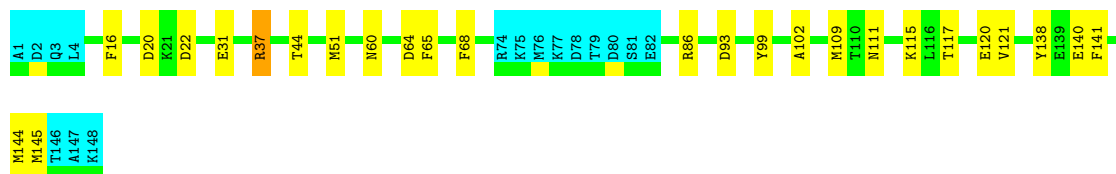
Chain A:  74% 12% 11%



4.2.150 Score per residue for model 150

- Molecule 1: Calmodulin

Chain A:  72% 17% 11%

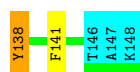


4.2.151 Score per residue for model 151

- Molecule 1: Calmodulin

Chain A:  71% 16% 11%

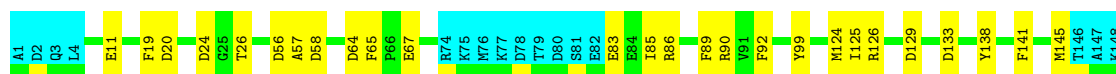




4.2.152 Score per residue for model 152

- Molecule 1: Calmodulin

Chain A: 72% 18% 11%



4.2.153 Score per residue for model 153

- Molecule 1: Calmodulin

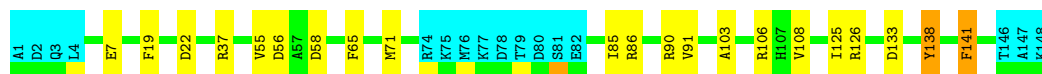
Chain A: 73% 15% 11%



4.2.154 Score per residue for model 154

- Molecule 1: Calmodulin

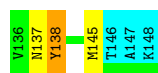
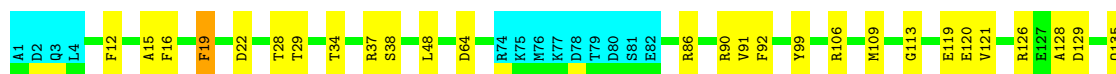
Chain A: 75% 13% 11%



4.2.155 Score per residue for model 155

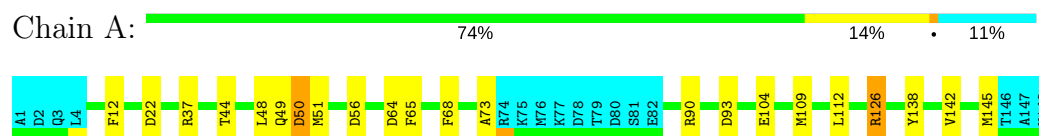
- Molecule 1: Calmodulin

Chain A: 69% 19% 11%



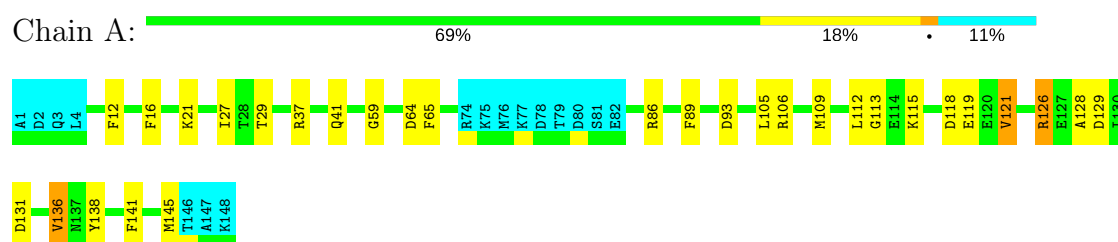
4.2.156 Score per residue for model 156

- Molecule 1: Calmodulin



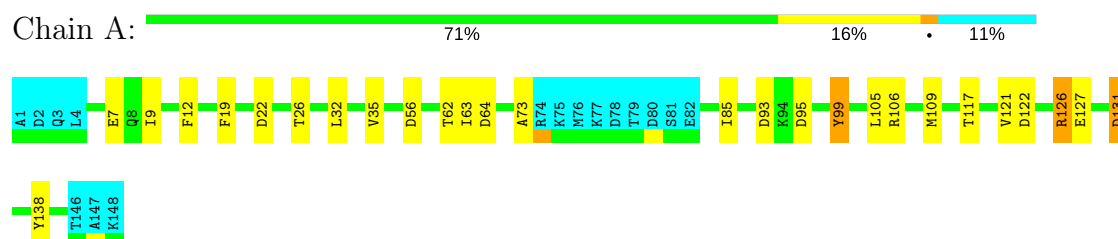
4.2.157 Score per residue for model 157 (medoid)

- Molecule 1: Calmodulin



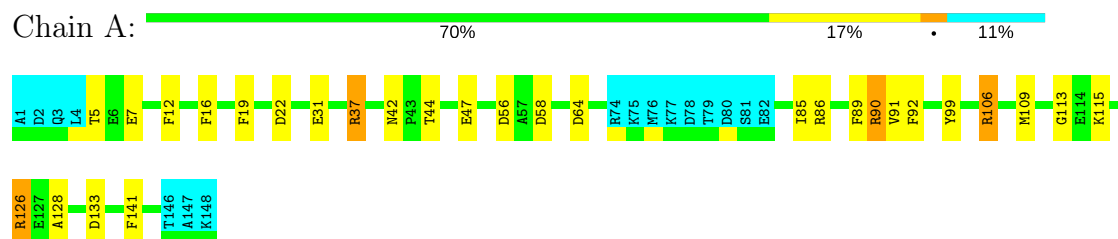
4.2.158 Score per residue for model 158

- Molecule 1: Calmodulin



4.2.159 Score per residue for model 159

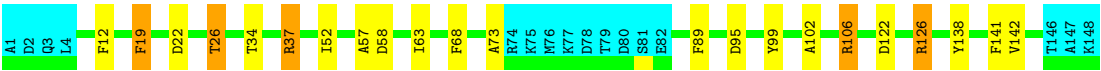
- Molecule 1: Calmodulin



4.2.160 Score per residue for model 160

● Molecule 1: Calmodulin

Chain A:  74% 11% • 11%



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

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	0.96±0.00	0±0/1052 (0.0±0.0%)	1.99±0.06	28±5/1416 (2.0±0.3%)
All	All	0.96	0/168320 (0.0%)	1.99	4451/226560 (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	2.8±1.4
All	All	0	449

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	37	ARG	NE-CZ-NH1	20.87	130.74	120.30	84	84
1	A	86	ARG	NE-CZ-NH1	20.51	130.56	120.30	102	76
1	A	106	ARG	NE-CZ-NH1	19.68	130.14	120.30	128	87
1	A	86	ARG	NE-CZ-NH2	-18.57	111.02	120.30	5	67
1	A	37	ARG	NE-CZ-NH2	-18.40	111.10	120.30	34	73
1	A	106	ARG	NE-CZ-NH2	-17.53	111.53	120.30	82	66
1	A	138	TYR	CB-CG-CD2	-17.51	110.49	121.00	1	63
1	A	126	ARG	NE-CZ-NH1	17.39	129.00	120.30	97	77
1	A	19	PHE	CB-CG-CD1	17.11	132.78	120.80	95	46
1	A	92	PHE	CB-CG-CD2	-16.71	109.10	120.80	53	64
1	A	90	ARG	NE-CZ-NH1	16.22	128.41	120.30	40	81
1	A	12	PHE	CB-CG-CD2	-15.38	110.03	120.80	10	65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	92	PHE	CB-CG-CD1	15.14	131.40	120.80	139	58
1	A	126	ARG	NE-CZ-NH2	-14.88	112.86	120.30	56	57
1	A	19	PHE	CB-CG-CD2	-14.64	110.55	120.80	129	53
1	A	89	PHE	CB-CG-CD2	-14.20	110.86	120.80	13	46
1	A	99	TYR	CB-CG-CD1	-13.92	112.65	121.00	101	59
1	A	90	ARG	NE-CZ-NH2	-13.77	113.42	120.30	17	71
1	A	12	PHE	CB-CG-CD1	13.62	130.33	120.80	45	56
1	A	99	TYR	CB-CG-CD2	-13.60	112.84	121.00	5	63
1	A	24	ASP	CB-CG-OD1	12.84	129.86	118.30	133	28
1	A	68	PHE	CB-CG-CD2	-12.82	111.83	120.80	106	38
1	A	138	TYR	CB-CG-CD1	12.54	128.52	121.00	65	61
1	A	58	ASP	CB-CG-OD1	12.48	129.53	118.30	37	30
1	A	16	PHE	CB-CG-CD2	12.29	129.40	120.80	3	37
1	A	50	ASP	CB-CG-OD1	-12.26	107.26	118.30	142	15
1	A	133	ASP	CB-CG-OD1	12.21	129.29	118.30	63	31
1	A	65	PHE	CB-CG-CD1	-12.16	112.29	120.80	70	35
1	A	118	ASP	CB-CG-OD1	12.15	129.24	118.30	72	24
1	A	141	PHE	CB-CG-CD1	11.94	129.16	120.80	69	36
1	A	16	PHE	CB-CG-CD1	11.83	129.08	120.80	144	41
1	A	65	PHE	CB-CG-CD2	-11.74	112.58	120.80	21	42
1	A	95	ASP	CB-CG-OD1	11.65	128.78	118.30	63	25
1	A	68	PHE	CB-CG-CD1	11.57	128.90	120.80	106	32
1	A	144	MET	CG-SD-CE	-11.22	82.25	100.20	85	28
1	A	89	PHE	CB-CG-CD1	11.13	128.59	120.80	13	46
1	A	129	ASP	CB-CG-OD1	11.07	128.26	118.30	81	32
1	A	51	MET	CG-SD-CE	-10.91	82.74	100.20	75	21
1	A	131	ASP	CB-CG-OD1	10.85	128.06	118.30	40	25
1	A	99	TYR	CG-CD1-CE1	-10.83	112.64	121.30	64	21
1	A	124	MET	CG-SD-CE	-10.79	82.94	100.20	38	22
1	A	122	ASP	CB-CG-OD1	10.78	128.00	118.30	55	26
1	A	50	ASP	CB-CG-OD2	10.71	127.93	118.30	142	18
1	A	72	MET	CG-SD-CE	-10.57	83.28	100.20	23	27
1	A	122	ASP	CB-CG-OD2	-10.56	108.80	118.30	110	24
1	A	133	ASP	CB-CG-OD2	-10.55	108.81	118.30	16	18
1	A	136	VAL	CA-CB-CG2	-10.53	95.10	110.90	26	19
1	A	118	ASP	CB-CG-OD2	-10.41	108.93	118.30	97	25
1	A	22	ASP	CB-CG-OD2	-10.38	108.96	118.30	12	22
1	A	22	ASP	CB-CG-OD1	10.34	127.61	118.30	77	28
1	A	29	THR	CA-CB-CG2	-10.33	97.94	112.40	76	11
1	A	20	ASP	CB-CG-OD1	10.21	127.49	118.30	142	26
1	A	145	MET	CG-SD-CE	-9.98	84.23	100.20	72	34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	141	PHE	CB-CG-CD2	-9.96	113.83	120.80	21	41
1	A	109	MET	CG-SD-CE	-9.92	84.32	100.20	149	41
1	A	20	ASP	CB-CG-OD2	9.91	127.22	118.30	136	27
1	A	62	THR	CA-CB-CG2	-9.85	98.62	112.40	42	21
1	A	93	ASP	CB-CG-OD2	9.82	127.14	118.30	92	28
1	A	128	ALA	N-CA-CB	-9.74	96.46	110.10	108	23
1	A	99	TYR	CG-CD2-CE2	-9.69	113.55	121.30	104	15
1	A	58	ASP	CB-CG-OD2	9.62	126.96	118.30	40	25
1	A	56	ASP	CB-CG-OD2	-9.62	109.64	118.30	48	22
1	A	64	ASP	CB-CG-OD2	9.56	126.91	118.30	96	22
1	A	95	ASP	CB-CG-OD2	-9.44	109.80	118.30	86	35
1	A	67	GLU	OE1-CD-OE2	-9.26	112.19	123.30	40	37
1	A	36	MET	CG-SD-CE	-9.23	85.44	100.20	24	34
1	A	38	SER	N-CA-CB	9.22	124.33	110.50	43	12
1	A	93	ASP	CB-CG-OD1	9.20	126.58	118.30	143	15
1	A	35	VAL	CA-CB-CG2	-9.17	97.14	110.90	50	9
1	A	138	TYR	CZ-CE2-CD2	9.13	128.02	119.80	90	8
1	A	10	ALA	CB-CA-C	9.05	123.67	110.10	49	10
1	A	131	ASP	CB-CG-OD2	8.99	126.39	118.30	86	28
1	A	140	GLU	OE1-CD-OE2	-8.98	112.53	123.30	66	32
1	A	102	ALA	N-CA-CB	-8.91	97.62	110.10	26	7
1	A	26	THR	CA-CB-CG2	-8.74	100.16	112.40	38	10
1	A	56	ASP	CB-CG-OD1	8.70	126.13	118.30	123	28
1	A	90	ARG	CD-NE-CZ	-8.68	111.45	123.60	16	3
1	A	64	ASP	CB-CG-OD1	8.68	126.11	118.30	63	28
1	A	121	VAL	CG1-CB-CG2	-8.66	97.04	110.90	110	7
1	A	104	GLU	OE1-CD-OE2	-8.59	113.00	123.30	54	23
1	A	99	TYR	CD1-CE1-CZ	-8.58	112.08	119.80	134	15
1	A	110	THR	CA-CB-CG2	-8.58	100.39	112.40	120	16
1	A	138	TYR	CD1-CG-CD2	8.54	127.30	117.90	12	8
1	A	24	ASP	CB-CG-OD2	-8.47	110.68	118.30	133	12
1	A	88	ALA	N-CA-CB	-8.47	98.25	110.10	32	9
1	A	106	ARG	NH1-CZ-NH2	-8.47	110.09	119.40	8	10
1	A	138	TYR	CG-CD1-CE1	-8.39	114.58	121.30	12	23
1	A	108	VAL	CA-CB-CG2	-8.35	98.37	110.90	42	6
1	A	31	GLU	OE1-CD-OE2	-8.34	113.29	123.30	57	25
1	A	71	MET	CG-SD-CE	-8.31	86.90	100.20	37	17
1	A	10	ALA	N-CA-CB	-8.24	98.57	110.10	71	8
1	A	15	ALA	N-CA-CB	8.22	121.61	110.10	19	5
1	A	126	ARG	CD-NE-CZ	8.16	135.03	123.60	103	5
1	A	136	VAL	CA-CB-CG1	8.15	123.13	110.90	143	16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	121	VAL	CA-CB-CG2	-8.13	98.70	110.90	23	11
1	A	129	ASP	CB-CG-OD2	8.05	125.55	118.30	85	27
1	A	138	TYR	CG-CD2-CE2	-7.99	114.91	121.30	108	18
1	A	103	ALA	N-CA-CB	-7.92	99.02	110.10	115	6
1	A	126	ARG	NH1-CZ-NH2	-7.88	110.74	119.40	54	18
1	A	38	SER	O-C-N	-7.86	110.12	122.70	148	4
1	A	99	TYR	CZ-CE2-CD2	7.80	126.82	119.80	92	10
1	A	117	THR	CA-CB-CG2	-7.79	101.50	112.40	107	26
1	A	91	VAL	CA-CB-CG1	7.75	122.52	110.90	82	14
1	A	99	TYR	CD1-CG-CD2	7.74	126.42	117.90	59	6
1	A	64	ASP	O-C-N	-7.74	110.32	122.70	96	6
1	A	103	ALA	CB-CA-C	-7.72	98.52	110.10	58	3
1	A	57	ALA	N-CA-CB	-7.70	99.32	110.10	50	9
1	A	142	VAL	CA-CB-CG1	-7.70	99.36	110.90	67	7
1	A	44	THR	CA-CB-CG2	-7.65	101.69	112.40	95	12
1	A	57	ALA	CB-CA-C	-7.64	98.64	110.10	160	8
1	A	44	THR	N-CA-CB	7.62	124.79	110.30	134	10
1	A	144	MET	CA-CB-CG	7.62	126.25	113.30	132	5
1	A	69	LEU	CB-CG-CD2	7.60	123.91	111.00	32	6
1	A	14	GLU	OE1-CD-OE2	-7.57	114.22	123.30	136	2
1	A	138	TYR	CD1-CE1-CZ	-7.56	112.99	119.80	151	6
1	A	34	THR	CA-CB-CG2	7.49	122.88	112.40	68	3
1	A	86	ARG	NH1-CZ-NH2	-7.44	111.22	119.40	8	10
1	A	37	ARG	NH1-CZ-NH2	-7.43	111.22	119.40	84	9
1	A	7	GLU	CA-CB-CG	7.41	129.70	113.40	138	2
1	A	90	ARG	NH1-CZ-NH2	-7.40	111.26	119.40	9	12
1	A	131	ASP	O-C-N	-7.39	110.64	123.20	58	5
1	A	46	ALA	N-CA-CB	-7.39	99.75	110.10	32	5
1	A	112	LEU	O-C-N	-7.38	110.66	123.20	157	4
1	A	123	GLU	O-C-N	-7.36	110.93	122.70	10	4
1	A	45	GLU	OE1-CD-OE2	-7.33	114.50	123.30	147	5
1	A	91	VAL	CG1-CB-CG2	-7.33	99.17	110.90	83	18
1	A	104	GLU	O-C-N	-7.32	110.98	122.70	38	5
1	A	55	VAL	CA-CB-CG2	7.29	121.84	110.90	142	5
1	A	100	ILE	CA-CB-CG2	-7.27	96.36	110.90	87	4
1	A	35	VAL	CG1-CB-CG2	-7.25	99.30	110.90	29	6
1	A	127	GLU	OE1-CD-OE2	-7.25	114.61	123.30	114	8
1	A	142	VAL	CG1-CB-CG2	-7.24	99.31	110.90	46	15
1	A	7	GLU	OE1-CD-OE2	7.24	131.99	123.30	29	5
1	A	17	SER	N-CA-CB	7.23	121.34	110.50	57	2
1	A	28	THR	CA-CB-CG2	-7.16	102.38	112.40	124	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	94	LYS	O-C-N	-7.13	111.29	122.70	137	3
1	A	123	GLU	OE1-CD-OE2	-7.12	114.75	123.30	138	6
1	A	88	ALA	O-C-N	-7.11	111.33	122.70	56	4
1	A	92	PHE	N-CA-CB	7.11	123.39	110.60	98	2
1	A	112	LEU	CB-CG-CD1	7.06	123.00	111.00	41	8
1	A	69	LEU	CB-CA-C	7.05	123.60	110.20	146	3
1	A	136	VAL	CB-CA-C	7.05	124.79	111.40	3	3
1	A	70	THR	CA-CB-CG2	-7.04	102.55	112.40	124	4
1	A	107	HIS	O-C-N	-6.99	111.51	122.70	18	4
1	A	55	VAL	O-C-N	-6.98	111.53	122.70	110	3
1	A	5	THR	CA-CB-CG2	-6.93	102.69	112.40	130	9
1	A	26	THR	N-CA-CB	6.93	123.47	110.30	20	14
1	A	73	ALA	N-CA-CB	6.93	119.80	110.10	21	8
1	A	106	ARG	CG-CD-NE	-6.92	97.26	111.80	160	9
1	A	137	ASN	CB-CA-C	6.92	124.23	110.40	64	4
1	A	51	MET	O-C-N	-6.88	111.69	122.70	55	4
1	A	87	GLU	O-C-N	-6.88	111.69	122.70	65	6
1	A	102	ALA	O-C-N	-6.85	111.74	122.70	29	2
1	A	101	SER	O-C-N	-6.84	111.76	122.70	100	4
1	A	99	TYR	N-CA-CB	-6.84	98.29	110.60	78	3
1	A	110	THR	O-C-N	-6.81	111.80	122.70	115	4
1	A	22	ASP	C-N-CA	6.79	136.56	122.30	47	2
1	A	73	ALA	O-C-N	-6.74	111.92	122.70	89	3
1	A	67	GLU	CG-CD-OE1	6.73	131.76	118.30	130	2
1	A	39	LEU	C-N-CA	6.70	136.37	122.30	85	2
1	A	48	LEU	CB-CG-CD2	6.70	122.38	111.00	32	2
1	A	55	VAL	CG1-CB-CG2	-6.69	100.20	110.90	88	5
1	A	11	GLU	O-C-N	-6.68	112.02	122.70	97	3
1	A	141	PHE	O-C-N	-6.67	112.02	122.70	15	5
1	A	102	ALA	CB-CA-C	-6.67	100.10	110.10	127	4
1	A	20	ASP	O-C-N	-6.66	112.05	122.70	151	3
1	A	53	ASN	N-CA-CB	6.65	122.57	110.60	43	3
1	A	84	GLU	OE1-CD-OE2	-6.63	115.34	123.30	119	5
1	A	43	PRO	N-CA-CB	6.62	111.24	103.30	51	2
1	A	116	LEU	CB-CG-CD2	6.60	122.23	111.00	16	4
1	A	97	ASN	O-C-N	-6.60	111.97	123.20	55	2
1	A	142	VAL	CA-CB-CG2	-6.60	101.00	110.90	122	13
1	A	37	ARG	CG-CD-NE	-6.60	97.94	111.80	159	8
1	A	60	ASN	C-N-CA	6.59	136.14	122.30	48	3
1	A	119	GLU	OE1-CD-OE2	-6.59	115.39	123.30	119	3
1	A	141	PHE	CZ-CE2-CD2	-6.58	112.20	120.10	125	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	88	ALA	CB-CA-C	-6.54	100.30	110.10	8	3
1	A	109	MET	O-C-N	-6.53	112.25	122.70	132	5
1	A	83	GLU	OE1-CD-OE2	-6.51	115.48	123.30	138	6
1	A	144	MET	O-C-N	-6.51	112.29	122.70	85	2
1	A	6	GLU	OE1-CD-OE2	-6.51	115.49	123.30	61	4
1	A	126	ARG	N-CA-CB	6.50	122.31	110.60	119	2
1	A	90	ARG	CG-CD-NE	-6.50	98.16	111.80	53	5
1	A	34	THR	OG1-CB-CG2	-6.49	95.07	110.00	39	3
1	A	62	THR	N-CA-CB	6.49	122.63	110.30	132	5
1	A	145	MET	N-CA-CB	-6.49	98.92	110.60	8	1
1	A	114	GLU	OE1-CD-OE2	6.48	131.08	123.30	130	4
1	A	83	GLU	N-CA-CB	6.48	122.26	110.60	22	2
1	A	128	ALA	CB-CA-C	6.47	119.81	110.10	101	8
1	A	121	VAL	CA-CB-CG1	6.47	120.61	110.90	94	12
1	A	72	MET	O-C-N	-6.43	112.41	122.70	77	5
1	A	51	MET	CA-CB-CG	6.42	124.22	113.30	29	7
1	A	35	VAL	O-C-N	-6.42	112.43	122.70	61	2
1	A	65	PHE	CA-C-N	6.41	135.06	117.10	115	20
1	A	108	VAL	CG1-CB-CG2	-6.41	100.64	110.90	67	7
1	A	41	GLN	O-C-N	-6.41	112.45	122.70	157	3
1	A	55	VAL	CA-CB-CG1	6.40	120.51	110.90	49	7
1	A	132	GLY	N-CA-C	6.39	129.07	113.10	40	1
1	A	25	GLY	O-C-N	-6.39	112.48	122.70	3	1
1	A	108	VAL	CA-CB-CG1	6.38	120.48	110.90	107	10
1	A	107	HIS	CA-CB-CG	6.38	124.45	113.60	74	3
1	A	85	ILE	CA-CB-CG1	6.38	123.12	111.00	90	9
1	A	133	ASP	CA-CB-CG	6.36	127.39	113.40	159	2
1	A	109	MET	N-CA-CB	6.34	122.02	110.60	95	2
1	A	19	PHE	CZ-CE2-CD2	-6.34	112.49	120.10	110	1
1	A	126	ARG	CG-CD-NE	-6.34	98.49	111.80	22	3
1	A	16	PHE	CG-CD2-CE2	-6.31	113.86	120.80	110	1
1	A	137	ASN	N-CA-CB	6.30	121.94	110.60	35	2
1	A	67	GLU	O-C-N	-6.30	112.62	122.70	85	1
1	A	21	LYS	O-C-N	-6.29	112.63	122.70	40	2
1	A	86	ARG	O-C-N	-6.29	112.64	122.70	151	2
1	A	56	ASP	O-C-N	-6.29	112.64	122.70	50	2
1	A	120	GLU	O-C-N	-6.29	112.64	122.70	1	3
1	A	32	LEU	O-C-N	-6.28	112.52	123.20	83	5
1	A	89	PHE	CG-CD1-CE1	-6.28	113.89	120.80	96	2
1	A	139	GLU	OE1-CD-OE2	-6.28	115.76	123.30	90	3
1	A	45	GLU	O-C-N	-6.28	112.66	122.70	131	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	105	LEU	O-C-N	-6.28	112.66	122.70	84	5
1	A	64	ASP	CB-CA-C	6.26	122.92	110.40	4	6
1	A	43	PRO	N-CD-CG	6.26	112.59	103.20	111	1
1	A	136	VAL	CG1-CB-CG2	-6.25	100.89	110.90	119	1
1	A	116	LEU	O-C-N	-6.25	112.70	122.70	93	4
1	A	15	ALA	O-C-N	-6.24	112.72	122.70	9	2
1	A	108	VAL	N-CA-CB	6.24	125.22	111.50	35	1
1	A	133	ASP	O-C-N	-6.23	112.61	123.20	24	2
1	A	66	PRO	C-N-CA	6.22	137.25	121.70	56	1
1	A	131	ASP	CB-CA-C	-6.22	97.96	110.40	59	2
1	A	111	ASN	CA-CB-CG	-6.22	99.72	113.40	99	1
1	A	129	ASP	O-C-N	-6.21	112.77	122.70	1	1
1	A	50	ASP	O-C-N	-6.20	112.78	122.70	122	2
1	A	73	ALA	CB-CA-C	6.20	119.39	110.10	160	5
1	A	126	ARG	O-C-N	-6.19	112.79	122.70	41	3
1	A	89	PHE	CG-CD2-CE2	6.19	127.61	120.80	34	3
1	A	46	ALA	CB-CA-C	-6.19	100.82	110.10	144	5
1	A	16	PHE	O-C-N	-6.19	112.80	122.70	126	2
1	A	54	GLU	OE1-CD-OE2	-6.19	115.87	123.30	37	6
1	A	71	MET	CA-CB-CG	6.19	123.82	113.30	90	5
1	A	12	PHE	CD1-CE1-CZ	-6.19	112.68	120.10	42	1
1	A	68	PHE	CG-CD2-CE2	-6.18	114.00	120.80	31	1
1	A	68	PHE	CG-CD1-CE1	-6.16	114.02	120.80	144	4
1	A	100	ILE	O-C-N	-6.15	112.85	122.70	5	5
1	A	99	TYR	CB-CA-C	-6.15	98.10	110.40	143	2
1	A	21	LYS	N-CA-CB	-6.15	99.53	110.60	121	3
1	A	22	ASP	CB-CA-C	6.14	122.68	110.40	29	2
1	A	97	ASN	C-N-CA	6.14	135.20	122.30	71	1
1	A	136	VAL	O-C-N	-6.14	112.88	122.70	14	3
1	A	66	PRO	N-CD-CG	6.14	112.41	103.20	69	1
1	A	18	LEU	CB-CG-CD1	-6.13	100.57	111.00	42	4
1	A	112	LEU	CB-CG-CD2	6.13	121.43	111.00	67	3
1	A	27	ILE	N-CA-CB	6.13	124.91	110.80	62	4
1	A	100	ILE	N-CA-CB	6.13	124.89	110.80	147	1
1	A	28	THR	CA-CB-OG1	6.12	121.85	109.00	112	3
1	A	91	VAL	CA-CB-CG2	6.12	120.07	110.90	68	9
1	A	120	GLU	N-CA-CB	6.12	121.61	110.60	91	2
1	A	65	PHE	CG-CD1-CE1	-6.11	114.08	120.80	24	2
1	A	115	LYS	CB-CA-C	6.11	122.62	110.40	144	3
1	A	15	ALA	CB-CA-C	6.10	119.26	110.10	32	2
1	A	97	ASN	N-CA-CB	6.10	121.58	110.60	58	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	11	GLU	CB-CA-C	-6.10	98.20	110.40	23	1
1	A	19	PHE	CG-CD1-CE1	-6.09	114.10	120.80	78	3
1	A	61	GLY	O-C-N	-6.09	112.95	122.70	74	1
1	A	13	LYS	O-C-N	-6.09	112.96	122.70	58	3
1	A	35	VAL	CA-CB-CG1	6.09	120.03	110.90	24	6
1	A	129	ASP	N-CA-CB	6.08	121.55	110.60	75	3
1	A	10	ALA	O-C-N	-6.07	112.98	122.70	115	3
1	A	120	GLU	OE1-CD-OE2	-6.07	116.02	123.30	155	7
1	A	18	LEU	CB-CG-CD2	-6.06	100.70	111.00	5	2
1	A	22	ASP	N-CA-CB	6.05	121.50	110.60	63	2
1	A	110	THR	N-CA-CB	6.05	121.79	110.30	136	4
1	A	108	VAL	O-C-N	-6.04	113.04	122.70	66	2
1	A	44	THR	O-C-N	-6.04	113.04	122.70	43	1
1	A	26	THR	C-N-CA	6.03	136.77	121.70	67	1
1	A	58	ASP	OD1-CG-OD2	-6.02	111.86	123.30	130	2
1	A	119	GLU	N-CA-CB	6.02	121.43	110.60	19	4
1	A	39	LEU	O-C-N	-6.02	112.97	123.20	85	1
1	A	53	ASN	CA-CB-CG	-5.99	100.22	113.40	55	2
1	A	95	ASP	N-CA-CB	-5.99	99.83	110.60	9	6
1	A	106	ARG	CD-NE-CZ	5.98	131.97	123.60	103	2
1	A	105	LEU	CB-CG-CD2	-5.97	100.85	111.00	63	1
1	A	99	TYR	O-C-N	-5.97	113.15	122.70	107	4
1	A	105	LEU	CB-CA-C	5.95	121.51	110.20	112	9
1	A	66	PRO	N-CA-CB	5.95	110.44	103.30	101	2
1	A	26	THR	CA-CB-OG1	5.94	121.48	109.00	42	6
1	A	99	TYR	CA-CB-CG	-5.94	102.12	113.40	56	1
1	A	139	GLU	CA-CB-CG	5.93	126.46	113.40	147	2
1	A	60	ASN	N-CA-CB	5.93	121.27	110.60	1	3
1	A	85	ILE	N-CA-CB	5.92	124.43	110.80	42	2
1	A	106	ARG	C-N-CA	5.92	136.51	121.70	154	1
1	A	51	MET	CB-CA-C	-5.92	98.55	110.40	142	2
1	A	68	PHE	CD1-CE1-CZ	5.91	127.19	120.10	41	2
1	A	97	ASN	CB-CA-C	5.91	122.23	110.40	101	2
1	A	32	LEU	N-CA-CB	5.91	122.22	110.40	14	3
1	A	117	THR	O-C-N	-5.91	113.25	122.70	145	5
1	A	19	PHE	CD1-CG-CD2	5.91	125.98	118.30	78	2
1	A	65	PHE	CZ-CE2-CD2	-5.91	113.01	120.10	35	5
1	A	123	GLU	CB-CA-C	-5.90	98.60	110.40	60	1
1	A	111	ASN	O-C-N	-5.90	113.27	122.70	123	2
1	A	141	PHE	CD1-CE1-CZ	-5.90	113.03	120.10	5	2
1	A	52	ILE	CA-CB-CG2	5.89	122.68	110.90	137	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	5	THR	N-CA-CB	5.88	121.47	110.30	31	2
1	A	60	ASN	CB-CG-OD1	5.87	133.34	121.60	50	2
1	A	143	GLN	CB-CA-C	5.87	122.14	110.40	62	1
1	A	140	GLU	O-C-N	-5.86	113.32	122.70	73	5
1	A	7	GLU	N-CA-CB	-5.86	100.05	110.60	49	3
1	A	130	ILE	O-C-N	-5.86	113.33	122.70	126	2
1	A	32	LEU	CB-CA-C	5.85	121.31	110.20	91	4
1	A	10	ALA	N-CA-C	5.85	126.79	111.00	113	1
1	A	109	MET	CB-CA-C	5.85	122.09	110.40	147	3
1	A	63	ILE	O-C-N	-5.84	113.35	122.70	160	3
1	A	36	MET	O-C-N	-5.84	113.35	122.70	38	2
1	A	92	PHE	O-C-N	-5.83	113.38	122.70	147	3
1	A	17	SER	CB-CA-C	-5.82	99.04	110.10	42	2
1	A	12	PHE	CG-CD1-CE1	-5.82	114.40	120.80	35	3
1	A	93	ASP	O-C-N	-5.82	113.39	122.70	146	4
1	A	46	ALA	O-C-N	-5.81	113.40	122.70	88	2
1	A	118	ASP	N-CA-C	5.81	126.69	111.00	58	2
1	A	145	MET	CB-CA-C	-5.81	98.79	110.40	25	1
1	A	29	THR	C-N-CA	5.81	136.22	121.70	91	2
1	A	47	GLU	OE1-CD-OE2	-5.80	116.33	123.30	141	4
1	A	27	ILE	O-C-N	-5.80	113.42	122.70	26	3
1	A	48	LEU	O-C-N	-5.79	113.43	122.70	58	4
1	A	106	ARG	O-C-N	-5.79	113.44	122.70	119	2
1	A	37	ARG	N-CA-CB	5.79	121.01	110.60	29	1
1	A	111	ASN	N-CA-CB	5.78	121.01	110.60	88	4
1	A	130	ILE	CA-CB-CG1	-5.78	100.02	111.00	134	2
1	A	92	PHE	CG-CD1-CE1	-5.78	114.44	120.80	23	1
1	A	87	GLU	OE1-CD-OE2	-5.77	116.38	123.30	30	6
1	A	50	ASP	N-CA-CB	-5.77	100.21	110.60	45	1
1	A	52	ILE	CG1-CB-CG2	-5.76	98.73	111.40	66	1
1	A	13	LYS	CB-CG-CD	5.75	126.56	111.60	144	1
1	A	127	GLU	O-C-N	-5.75	113.50	122.70	104	3
1	A	60	ASN	O-C-N	-5.74	113.44	123.20	68	3
1	A	44	THR	CA-CB-OG1	5.74	121.05	109.00	28	1
1	A	83	GLU	CA-CB-CG	5.74	126.02	113.40	40	1
1	A	62	THR	CA-CB-OG1	5.73	121.04	109.00	82	2
1	A	65	PHE	CA-C-O	-5.72	108.08	120.10	134	4
1	A	141	PHE	CG-CD1-CE1	5.72	127.09	120.80	116	3
1	A	89	PHE	N-CA-CB	-5.71	100.32	110.60	27	3
1	A	141	PHE	CG-CD2-CE2	-5.71	114.52	120.80	68	3
1	A	100	ILE	CA-CB-CG1	5.71	121.85	111.00	117	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	29	THR	OG1-CB-CG2	-5.71	96.86	110.00	114	2
1	A	69	LEU	O-C-N	-5.71	113.56	122.70	112	3
1	A	114	GLU	O-C-N	-5.71	113.57	122.70	116	4
1	A	133	ASP	CB-CA-C	5.70	121.81	110.40	11	7
1	A	17	SER	O-C-N	-5.70	113.58	122.70	138	3
1	A	137	ASN	CA-CB-CG	5.70	125.94	113.40	147	4
1	A	111	ASN	C-N-CA	5.70	135.94	121.70	95	1
1	A	31	GLU	O-C-N	-5.69	113.59	122.70	30	2
1	A	71	MET	N-CA-CB	5.69	120.85	110.60	68	3
1	A	49	GLN	CG-CD-OE1	-5.69	110.22	121.60	111	1
1	A	42	ASN	N-CA-CB	-5.69	100.36	110.60	159	3
1	A	144	MET	CB-CA-C	-5.68	99.03	110.40	107	1
1	A	106	ARG	CB-CA-C	5.68	121.77	110.40	160	1
1	A	142	VAL	O-C-N	-5.68	113.61	122.70	74	2
1	A	84	GLU	N-CA-CB	5.68	120.82	110.60	124	1
1	A	32	LEU	CB-CG-CD1	-5.68	101.35	111.00	18	4
1	A	92	PHE	CD1-CG-CD2	5.68	125.68	118.30	38	1
1	A	84	GLU	CG-CD-OE1	5.67	129.65	118.30	116	1
1	A	58	ASP	CB-CA-C	5.67	121.73	110.40	49	1
1	A	34	THR	N-CA-CB	5.66	121.06	110.30	4	1
1	A	145	MET	C-N-CA	5.66	135.84	121.70	157	1
1	A	135	GLN	CB-CA-C	-5.65	99.11	110.40	17	4
1	A	111	ASN	CB-CA-C	-5.65	99.10	110.40	33	2
1	A	65	PHE	O-C-N	-5.65	110.37	121.10	58	6
1	A	70	THR	O-C-N	-5.64	113.67	122.70	32	2
1	A	143	GLN	N-CA-CB	-5.64	100.45	110.60	37	1
1	A	39	LEU	CA-CB-CG	-5.64	102.33	115.30	53	1
1	A	67	GLU	CA-CB-CG	5.63	125.80	113.40	28	1
1	A	29	THR	O-C-N	-5.63	113.69	122.70	95	3
1	A	8	GLN	O-C-N	-5.63	113.69	122.70	15	1
1	A	123	GLU	CG-CD-OE1	5.63	129.55	118.30	138	1
1	A	16	PHE	CD1-CG-CD2	5.62	125.61	118.30	157	2
1	A	47	GLU	N-CA-CB	5.62	120.72	110.60	104	4
1	A	7	GLU	CB-CA-C	-5.61	99.18	110.40	74	1
1	A	62	THR	OG1-CB-CG2	-5.61	97.11	110.00	12	1
1	A	40	GLY	O-C-N	-5.61	113.73	122.70	98	2
1	A	125	ILE	O-C-N	-5.60	113.74	122.70	6	2
1	A	132	GLY	CA-C-O	-5.60	110.52	120.60	23	1
1	A	114	GLU	CG-CD-OE1	5.60	129.50	118.30	89	1
1	A	7	GLU	O-C-N	-5.59	113.75	122.70	158	4
1	A	71	MET	O-C-N	-5.59	113.75	122.70	28	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	5	THR	CA-CB-OG1	5.59	120.74	109.00	98	3
1	A	24	ASP	CB-CA-C	5.59	121.57	110.40	1	3
1	A	96	GLY	CA-C-N	5.58	129.48	117.20	122	1
1	A	101	SER	N-CA-CB	-5.58	102.13	110.50	108	5
1	A	116	LEU	CB-CG-CD1	5.58	120.48	111.00	120	5
1	A	96	GLY	O-C-N	-5.58	113.78	122.70	59	3
1	A	83	GLU	O-C-N	5.57	131.62	122.70	35	1
1	A	26	THR	O-C-N	-5.57	113.78	122.70	67	2
1	A	140	GLU	CG-CD-OE1	5.56	129.42	118.30	61	1
1	A	27	ILE	CB-CA-C	-5.56	100.49	111.60	105	3
1	A	53	ASN	CB-CA-C	-5.55	99.29	110.40	81	2
1	A	145	MET	CA-CB-CG	-5.55	103.86	113.30	146	3
1	A	100	ILE	CB-CA-C	-5.54	100.51	111.60	7	2
1	A	139	GLU	O-C-N	-5.54	113.83	122.70	146	1
1	A	124	MET	O-C-N	-5.54	113.83	122.70	106	2
1	A	56	ASP	CB-CA-C	5.54	121.48	110.40	46	1
1	A	35	VAL	CB-CA-C	-5.54	100.88	111.40	71	4
1	A	18	LEU	O-C-N	-5.54	113.84	122.70	121	2
1	A	139	GLU	N-CA-CB	5.54	120.57	110.60	108	1
1	A	92	PHE	CD1-CE1-CZ	-5.54	113.46	120.10	143	2
1	A	37	ARG	CA-CB-CG	5.54	125.58	113.40	157	1
1	A	138	TYR	CA-C-O	5.53	131.71	120.10	40	1
1	A	19	PHE	CG-CD2-CE2	-5.52	114.72	120.80	16	1
1	A	131	ASP	C-N-CA	5.52	133.90	122.30	56	1
1	A	54	GLU	O-C-N	-5.52	113.87	122.70	96	2
1	A	84	GLU	O-C-N	-5.52	113.87	122.70	34	2
1	A	22	ASP	O-C-N	-5.52	113.82	123.20	101	1
1	A	91	VAL	O-C-N	-5.52	113.88	122.70	52	2
1	A	67	GLU	N-CA-CB	5.50	120.49	110.60	107	1
1	A	11	GLU	OE1-CD-OE2	-5.49	116.71	123.30	152	2
1	A	12	PHE	O-C-N	-5.48	113.93	122.70	58	1
1	A	128	ALA	O-C-N	-5.47	113.94	122.70	75	1
1	A	139	GLU	CG-CD-OE1	5.47	129.25	118.30	79	1
1	A	98	GLY	CA-C-O	5.47	130.45	120.60	115	1
1	A	131	ASP	N-CA-C	5.47	125.77	111.00	28	2
1	A	13	LYS	N-CA-CB	-5.47	100.76	110.60	23	3
1	A	89	PHE	CA-C-O	5.46	131.57	120.10	94	1
1	A	119	GLU	O-C-N	-5.45	113.97	122.70	8	2
1	A	85	ILE	CA-CB-CG2	-5.45	100.00	110.90	118	5
1	A	138	TYR	O-C-N	-5.45	113.98	122.70	93	3
1	A	135	GLN	N-CA-CB	5.45	120.41	110.60	61	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	69	LEU	CB-CG-CD1	-5.44	101.75	111.00	78	3
1	A	48	LEU	CB-CG-CD1	5.44	120.25	111.00	92	2
1	A	40	GLY	N-CA-C	5.44	126.70	113.10	144	1
1	A	29	THR	CB-CA-C	-5.43	96.93	111.60	51	1
1	A	33	GLY	O-C-N	-5.43	114.01	122.70	14	2
1	A	6	GLU	N-CA-CB	-5.43	100.82	110.60	21	1
1	A	137	ASN	O-C-N	-5.43	114.02	122.70	21	2
1	A	86	ARG	CD-NE-CZ	5.43	131.20	123.60	111	4
1	A	68	PHE	CD1-CG-CD2	5.42	125.35	118.30	31	1
1	A	22	ASP	CA-CB-CG	5.42	125.31	113.40	8	1
1	A	39	LEU	CB-CG-CD2	5.42	120.21	111.00	83	1
1	A	127	GLU	CG-CD-OE2	5.41	129.12	118.30	5	1
1	A	12	PHE	N-CA-CB	5.41	120.34	110.60	32	1
1	A	68	PHE	CZ-CE2-CD2	5.41	126.59	120.10	58	1
1	A	51	MET	C-N-CA	5.41	135.22	121.70	104	1
1	A	30	LYS	O-C-N	-5.41	114.05	122.70	122	3
1	A	67	GLU	CB-CG-CD	-5.40	99.63	114.20	40	4
1	A	49	GLN	CB-CA-C	-5.40	99.61	110.40	42	1
1	A	114	GLU	N-CA-CB	-5.40	100.89	110.60	46	1
1	A	63	ILE	N-CA-CB	5.39	123.21	110.80	115	4
1	A	71	MET	CB-CA-C	-5.39	99.62	110.40	137	1
1	A	144	MET	CA-C-O	-5.39	108.79	120.10	28	1
1	A	19	PHE	CB-CA-C	-5.38	99.63	110.40	67	1
1	A	121	VAL	CB-CA-C	5.38	121.63	111.40	131	1
1	A	90	ARG	CB-CG-CD	5.38	125.59	111.60	88	2
1	A	47	GLU	CB-CA-C	-5.38	99.65	110.40	55	3
1	A	36	MET	CA-CB-CG	-5.37	104.17	113.30	59	2
1	A	52	ILE	CA-CB-CG1	5.37	121.20	111.00	71	1
1	A	107	HIS	C-N-CA	5.37	135.12	121.70	18	1
1	A	65	PHE	N-CA-C	5.36	125.48	111.00	153	1
1	A	34	THR	CB-CA-C	-5.36	97.13	111.60	155	1
1	A	27	ILE	CA-CB-CG1	5.36	121.17	111.00	90	2
1	A	57	ALA	C-N-CA	5.35	135.07	121.70	152	1
1	A	38	SER	CB-CA-C	-5.35	99.94	110.10	53	1
1	A	141	PHE	N-CA-CB	-5.34	100.98	110.60	140	2
1	A	118	ASP	CA-CB-CG	-5.34	101.65	113.40	157	2
1	A	135	GLN	O-C-N	-5.34	114.16	122.70	85	2
1	A	14	GLU	N-CA-CB	5.34	120.21	110.60	106	1
1	A	90	ARG	O-C-N	-5.33	114.17	122.70	105	3
1	A	27	ILE	CA-CB-CG2	-5.33	100.24	110.90	20	1
1	A	117	THR	N-CA-CB	5.33	120.43	110.30	119	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	121	VAL	O-C-N	-5.33	114.17	122.70	117	1
1	A	69	LEU	CA-CB-CG	5.32	127.54	115.30	39	1
1	A	101	SER	CB-CA-C	5.32	120.21	110.10	40	2
1	A	104	GLU	CG-CD-OE2	5.32	128.94	118.30	130	1
1	A	68	PHE	CB-CA-C	5.32	121.04	110.40	75	1
1	A	115	LYS	O-C-N	-5.31	114.21	122.70	150	3
1	A	116	LEU	CB-CA-C	-5.30	100.12	110.20	14	1
1	A	29	THR	N-CA-CB	5.30	120.38	110.30	52	5
1	A	9	ILE	CA-CB-CG1	5.30	121.07	111.00	100	1
1	A	16	PHE	CD1-CE1-CZ	-5.30	113.74	120.10	159	1
1	A	31	GLU	CG-CD-OE1	5.30	128.90	118.30	159	1
1	A	91	VAL	N-CA-CB	5.28	123.12	111.50	52	2
1	A	19	PHE	O-C-N	5.28	131.16	122.70	89	1
1	A	49	GLN	N-CA-CB	5.28	120.11	110.60	86	1
1	A	117	THR	CA-CB-OG1	5.28	120.08	109.00	90	2
1	A	95	ASP	CB-CA-C	5.28	120.95	110.40	91	1
1	A	42	ASN	CB-CG-OD1	-5.27	111.05	121.60	23	1
1	A	90	ARG	CB-CA-C	5.27	120.95	110.40	28	1
1	A	52	ILE	O-C-N	-5.27	114.27	122.70	79	2
1	A	93	ASP	N-CA-CB	5.27	120.09	110.60	97	1
1	A	68	PHE	O-C-N	-5.27	114.27	122.70	97	3
1	A	73	ALA	C-N-CA	5.27	134.87	121.70	156	1
1	A	86	ARG	CB-CA-C	5.26	120.92	110.40	100	1
1	A	86	ARG	CG-CD-NE	-5.26	100.76	111.80	101	2
1	A	140	GLU	C-N-CA	5.25	134.83	121.70	1	1
1	A	140	GLU	CG-CD-OE2	-5.25	107.80	118.30	61	3
1	A	102	ALA	C-N-CA	5.25	134.82	121.70	95	1
1	A	72	MET	CA-CB-CG	5.24	122.22	113.30	153	2
1	A	16	PHE	N-CA-CB	-5.24	101.17	110.60	58	1
1	A	39	LEU	CB-CG-CD1	-5.24	102.10	111.00	130	2
1	A	127	GLU	CB-CA-C	5.23	120.86	110.40	61	1
1	A	18	LEU	N-CA-CB	5.23	120.85	110.40	135	1
1	A	55	VAL	C-N-CA	5.22	134.76	121.70	11	1
1	A	131	ASP	CA-CB-CG	-5.22	101.91	113.40	46	1
1	A	133	ASP	OD1-CG-OD2	-5.22	113.39	123.30	142	1
1	A	29	THR	CA-C-O	5.22	131.06	120.10	46	1
1	A	60	ASN	N-CA-C	5.21	125.08	111.00	153	1
1	A	33	GLY	C-N-CA	5.21	134.72	121.70	29	1
1	A	34	THR	O-C-N	-5.21	114.37	122.70	54	1
1	A	49	GLN	O-C-N	-5.20	114.38	122.70	156	1
1	A	87	GLU	CA-C-N	5.20	128.64	117.20	67	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	54	GLU	N-CA-C	5.20	125.04	111.00	76	1
1	A	11	GLU	CG-CD-OE2	5.19	128.69	118.30	18	1
1	A	123	GLU	C-N-CA	5.19	134.69	121.70	62	1
1	A	65	PHE	CD1-CG-CD2	5.19	125.05	118.30	70	1
1	A	12	PHE	CG-CD2-CE2	-5.19	115.09	120.80	116	1
1	A	107	HIS	N-CA-CB	5.19	119.94	110.60	36	2
1	A	135	GLN	CA-CB-CG	5.18	124.80	113.40	155	2
1	A	42	ASN	CA-CB-CG	-5.17	102.01	113.40	84	1
1	A	124	MET	N-CA-CB	-5.17	101.28	110.60	109	1
1	A	55	VAL	CB-CA-C	-5.17	101.58	111.40	42	1
1	A	43	PRO	CB-CA-C	-5.16	99.09	112.00	94	1
1	A	5	THR	O-C-N	-5.16	114.44	122.70	80	2
1	A	32	LEU	CA-C-O	5.16	130.94	120.10	120	1
1	A	58	ASP	N-CA-C	5.16	124.92	111.00	34	1
1	A	90	ARG	CA-CB-CG	5.16	124.74	113.40	56	1
1	A	138	TYR	N-CA-CB	-5.15	101.33	110.60	61	1
1	A	102	ALA	N-CA-C	5.15	124.90	111.00	21	2
1	A	32	LEU	CB-CG-CD2	5.15	119.75	111.00	80	1
1	A	94	LYS	CD-CE-NZ	-5.13	99.89	111.70	5	1
1	A	66	PRO	O-C-N	-5.13	114.48	122.70	121	2
1	A	144	MET	N-CA-CB	-5.13	101.36	110.60	68	1
1	A	31	GLU	N-CA-CB	-5.13	101.36	110.60	92	1
1	A	16	PHE	N-CA-C	5.13	124.86	111.00	104	1
1	A	116	LEU	N-CA-CB	5.13	120.66	110.40	106	2
1	A	122	ASP	CA-CB-CG	-5.13	102.12	113.40	39	1
1	A	24	ASP	O-C-N	-5.12	114.50	123.20	95	1
1	A	127	GLU	CA-CB-CG	5.12	124.66	113.40	68	2
1	A	59	GLY	O-C-N	-5.12	114.51	122.70	157	1
1	A	117	THR	C-N-CA	5.12	134.49	121.70	158	1
1	A	18	LEU	C-N-CA	5.11	134.48	121.70	119	1
1	A	50	ASP	OD1-CG-OD2	-5.11	113.59	123.30	156	1
1	A	89	PHE	CD1-CG-CD2	5.11	124.94	118.30	96	1
1	A	25	GLY	CA-C-O	-5.11	111.41	120.60	57	1
1	A	138	TYR	CB-CA-C	5.10	120.61	110.40	16	2
1	A	32	LEU	C-N-CA	5.10	133.01	122.30	34	1
1	A	37	ARG	O-C-N	-5.09	114.55	122.70	74	2
1	A	42	ASN	CA-C-N	5.09	131.35	117.10	103	1
1	A	63	ILE	CB-CA-C	-5.09	101.42	111.60	137	1
1	A	106	ARG	CA-CB-CG	5.09	124.59	113.40	34	2
1	A	65	PHE	CG-CD2-CE2	5.08	126.39	120.80	131	2
1	A	113	GLY	O-C-N	-5.08	114.57	122.70	96	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	47	GLU	O-C-N	-5.08	114.58	122.70	159	1
1	A	48	LEU	N-CA-CB	5.08	120.55	110.40	155	1
1	A	37	ARG	CB-CA-C	-5.07	100.25	110.40	148	1
1	A	95	ASP	OD1-CG-OD2	-5.07	113.67	123.30	28	3
1	A	48	LEU	CB-CA-C	-5.07	100.57	110.20	30	1
1	A	145	MET	O-C-N	-5.07	114.59	122.70	64	1
1	A	63	ILE	CA-CB-CG2	-5.07	100.77	110.90	45	1
1	A	95	ASP	C-N-CA	5.07	132.94	122.30	99	1
1	A	141	PHE	CB-CA-C	5.06	120.53	110.40	7	1
1	A	39	LEU	CB-CA-C	-5.06	100.58	110.20	113	1
1	A	53	ASN	O-C-N	-5.06	114.60	122.70	141	1
1	A	106	ARG	N-CA-CB	-5.05	101.51	110.60	60	1
1	A	86	ARG	N-CA-CB	5.05	119.69	110.60	83	1
1	A	90	ARG	N-CA-CB	-5.05	101.51	110.60	118	1
1	A	105	LEU	CB-CG-CD1	-5.05	102.42	111.00	109	1
1	A	9	ILE	O-C-N	-5.04	114.63	122.70	50	1
1	A	21	LYS	CD-CE-NZ	-5.04	100.10	111.70	56	1
1	A	65	PHE	CB-CA-C	5.04	120.48	110.40	93	1
1	A	143	GLN	C-N-CA	5.03	134.28	121.70	11	1
1	A	128	ALA	N-CA-C	5.03	124.59	111.00	157	1
1	A	118	ASP	O-C-N	-5.03	114.66	122.70	79	1
1	A	109	MET	CA-CB-CG	5.02	121.84	113.30	93	1
1	A	51	MET	N-CA-CB	5.02	119.63	110.60	49	1
1	A	9	ILE	CG1-CB-CG2	-5.01	100.38	111.40	23	1
1	A	62	THR	O-C-N	-5.01	114.68	122.70	48	1
1	A	42	ASN	O-C-N	-5.01	111.58	121.10	126	1
1	A	140	GLU	N-CA-CB	-5.01	101.59	110.60	64	1
1	A	94	LYS	CG-CD-CE	5.00	126.91	111.90	97	1
1	A	37	ARG	CB-CG-CD	5.00	124.61	111.60	128	1
1	A	67	GLU	CG-CD-OE2	5.00	128.31	118.30	140	1
1	A	91	VAL	CB-CA-C	5.00	120.91	111.40	70	1
1	A	124	MET	CA-CB-CG	5.00	121.80	113.30	111	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)
1	A	138	TYR	Sidechain	75
1	A	126	ARG	Sidechain	53
1	A	37	ARG	Sidechain	45

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	99	TYR	Sidechain,Mainchain	44
1	A	106	ARG	Sidechain	38
1	A	86	ARG	Sidechain	37
1	A	90	ARG	Sidechain	28
1	A	141	PHE	Sidechain	18
1	A	68	PHE	Sidechain	14
1	A	12	PHE	Sidechain	13
1	A	19	PHE	Sidechain	10
1	A	92	PHE	Sidechain	9
1	A	89	PHE	Sidechain	9
1	A	65	PHE	Sidechain	9
1	A	16	PHE	Sidechain	7
1	A	42	ASN	Peptide	5
1	A	107	HIS	Sidechain	4
1	A	131	ASP	Peptide	3
1	A	128	ALA	Peptide	3
1	A	43	PRO	Peptide	2
1	A	32	LEU	Peptide,Mainchain	2
1	A	129	ASP	Sidechain	1
1	A	100	ILE	Mainchain	1
1	A	124	MET	Mainchain	1
1	A	36	MET	Mainchain	1
1	A	33	GLY	Mainchain	1
1	A	15	ALA	Mainchain	1
1	A	132	GLY	Mainchain,Peptide	1
1	A	125	ILE	Mainchain	1
1	A	120	GLU	Peptide	1
1	A	144	MET	Mainchain	1
1	A	67	GLU	Sidechain	1
1	A	136	VAL	Mainchain	1
1	A	109	MET	Peptide	1
1	A	108	VAL	Mainchain	1
1	A	135	GLN	Peptide	1
1	A	84	GLU	Mainchain	1
1	A	50	ASP	Mainchain	1
1	A	102	ALA	Mainchain	1
1	A	127	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	1039	967	967	1±1
All	All	166880	154720	154720	87

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:92:PHE:HA	1:A:108:VAL:HG21	0.70	1.63	38	2
1:A:85:ILE:HD12	1:A:142:VAL:HG13	0.62	1.68	40	1
1:A:104:GLU:O	1:A:108:VAL:HG23	0.61	1.95	131	4
1:A:138:TYR:O	1:A:142:VAL:HG23	0.59	1.98	41	13
1:A:83:GLU:CD	1:A:86:ARG:HH21	0.57	2.02	5	2
1:A:19:PHE:CD1	1:A:35:VAL:HG22	0.55	2.37	121	3
1:A:103:ALA:O	1:A:107:HIS:CD2	0.54	2.61	130	1
1:A:104:GLU:O	1:A:108:VAL:HG22	0.53	2.04	7	1
1:A:92:PHE:CD1	1:A:108:VAL:HG11	0.53	2.39	71	1
1:A:107:HIS:CE1	1:A:111:ASN:HD21	0.52	2.23	1	5
1:A:121:VAL:HG12	1:A:125:ILE:HD12	0.50	1.84	21	1
1:A:85:ILE:HD12	1:A:142:VAL:HG22	0.49	1.83	52	3
1:A:52:ILE:HG12	1:A:63:ILE:HD11	0.49	1.83	129	1
1:A:92:PHE:CE1	1:A:105:LEU:HD12	0.48	2.43	102	1
1:A:121:VAL:O	1:A:124:MET:HB3	0.47	2.09	121	1
1:A:138:TYR:CZ	1:A:142:VAL:HG21	0.47	2.45	134	1
1:A:106:ARG:HA	1:A:116:LEU:HD12	0.47	1.87	83	1
1:A:122:ASP:HA	1:A:125:ILE:HD12	0.46	1.85	147	1
1:A:65:PHE:CZ	1:A:69:LEU:HD21	0.46	2.46	10	2
1:A:128:ALA:HB2	1:A:144:MET:SD	0.46	2.51	30	3
1:A:87:GLU:O	1:A:91:VAL:HG23	0.46	2.11	137	3
1:A:68:PHE:CE2	1:A:72:MET:HG3	0.45	2.47	66	1
1:A:16:PHE:CE2	1:A:27:ILE:HD11	0.45	2.47	21	1
1:A:8:GLN:O	1:A:12:PHE:CD2	0.45	2.70	139	1
1:A:45:GLU:H	1:A:45:GLU:CD	0.45	2.16	27	1
1:A:99:TYR:CE2	1:A:137:ASN:HB3	0.44	2.47	123	1
1:A:31:GLU:O	1:A:35:VAL:HG23	0.44	2.13	19	1
1:A:8:GLN:HB3	1:A:12:PHE:CE2	0.44	2.48	135	1
1:A:85:ILE:HG22	1:A:145:MET:SD	0.44	2.53	42	1
1:A:88:ALA:O	1:A:92:PHE:CD1	0.44	2.71	15	1
1:A:92:PHE:CG	1:A:108:VAL:HG11	0.43	2.48	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:PHE:CE1	1:A:100:ILE:HG13	0.43	2.48	79	1
1:A:52:ILE:HG23	1:A:63:ILE:HD11	0.43	1.89	52	1
1:A:92:PHE:CD1	1:A:105:LEU:HD12	0.43	2.48	142	1
1:A:32:LEU:HD11	1:A:63:ILE:HG13	0.43	1.90	50	1
1:A:32:LEU:HD11	1:A:63:ILE:HD12	0.43	1.90	136	2
1:A:16:PHE:CD2	1:A:27:ILE:HD11	0.43	2.48	21	1
1:A:87:GLU:OE2	1:A:90:ARG:NH2	0.43	2.52	4	1
1:A:12:PHE:CE1	1:A:72:MET:HB3	0.42	2.48	112	1
1:A:116:LEU:HD22	1:A:120:GLU:HG2	0.42	1.89	91	1
1:A:105:LEU:CD2	1:A:121:VAL:HG13	0.42	2.44	158	1
1:A:131:ASP:HB2	1:A:133:ASP:H	0.42	1.74	75	1
1:A:28:THR:HG22	1:A:62:THR:HG22	0.42	1.91	148	1
1:A:6:GLU:HA	1:A:9:ILE:HD12	0.42	1.92	139	1
1:A:117:THR:O	1:A:121:VAL:HG23	0.41	2.15	73	1
1:A:37:ARG:HA	1:A:41:GLN:O	0.41	2.15	117	1
1:A:105:LEU:O	1:A:109:MET:HG2	0.41	2.15	94	1
1:A:106:ARG:HH12	1:A:118:ASP:CG	0.41	2.18	104	1
1:A:28:THR:O	1:A:32:LEU:HD12	0.41	2.16	114	1
1:A:85:ILE:HG21	1:A:142:VAL:HG22	0.41	1.92	35	1
1:A:138:TYR:CE2	1:A:142:VAL:HG21	0.41	2.50	56	1
1:A:13:LYS:HA	1:A:65:PHE:CE1	0.41	2.51	9	1
1:A:16:PHE:CD1	1:A:16:PHE:C	0.40	2.93	150	1
1:A:15:ALA:O	1:A:19:PHE:CD2	0.40	2.74	155	1
1:A:120:GLU:O	1:A:124:MET:HG3	0.40	2.17	36	1
1:A:138:TYR:CZ	1:A:142:VAL:CG2	0.40	3.05	117	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	132/148 (89%)	127±2 (96±2%)	5±2 (3±2%)	1±1 (0±1%)	35	77
All	All	21120/23680 (89%)	20294 (96%)	730 (3%)	96 (0%)	35	77

All 20 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	113	GLY	47
1	A	98	GLY	9
1	A	56	ASP	7
1	A	132	GLY	6
1	A	131	ASP	4
1	A	96	GLY	3
1	A	93	ASP	3
1	A	55	VAL	2
1	A	42	ASN	2
1	A	95	ASP	2
1	A	20	ASP	2
1	A	129	ASP	1
1	A	33	GLY	1
1	A	84	GLU	1
1	A	121	VAL	1
1	A	40	GLY	1
1	A	102	ALA	1
1	A	35	VAL	1
1	A	142	VAL	1
1	A	125	ILE	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	112/126 (89%)	108±2 (97±2%)	4±2 (3±2%)	45	88
All	All	17920/20160 (89%)	17337 (97%)	583 (3%)	45	88

All 82 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	22	ASP	53
1	A	85	ILE	46
1	A	131	ASP	33
1	A	27	ILE	31
1	A	26	THR	24
1	A	105	LEU	22

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Mol	Chain	Res	Type	Models (Total)
1	A	64	ASP	22
1	A	29	THR	21
1	A	9	ILE	18
1	A	63	ILE	16
1	A	52	ILE	16
1	A	69	LEU	14
1	A	109	MET	12
1	A	125	ILE	12
1	A	136	VAL	11
1	A	58	ASP	10
1	A	142	VAL	10
1	A	121	VAL	9
1	A	62	THR	9
1	A	130	ILE	8
1	A	18	LEU	8
1	A	37	ARG	7
1	A	32	LEU	7
1	A	50	ASP	7
1	A	118	ASP	7
1	A	133	ASP	6
1	A	42	ASN	6
1	A	112	LEU	6
1	A	90	ARG	6
1	A	95	ASP	6
1	A	17	SER	6
1	A	55	VAL	5
1	A	19	PHE	5
1	A	21	LYS	4
1	A	122	ASP	4
1	A	106	ARG	4
1	A	137	ASN	4
1	A	100	ILE	4
1	A	108	VAL	4
1	A	71	MET	4
1	A	60	ASN	4
1	A	38	SER	3
1	A	67	GLU	3
1	A	24	ASP	3
1	A	115	LYS	3
1	A	66	PRO	3
1	A	129	ASP	3
1	A	139	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	124	MET	3
1	A	110	THR	3
1	A	56	ASP	3
1	A	94	LYS	2
1	A	70	THR	2
1	A	7	GLU	2
1	A	45	GLU	2
1	A	116	LEU	2
1	A	114	GLU	2
1	A	144	MET	2
1	A	34	THR	2
1	A	111	ASN	2
1	A	6	GLU	2
1	A	91	VAL	2
1	A	84	GLU	1
1	A	47	GLU	1
1	A	13	LYS	1
1	A	104	GLU	1
1	A	39	LEU	1
1	A	107	HIS	1
1	A	54	GLU	1
1	A	5	THR	1
1	A	36	MET	1
1	A	83	GLU	1
1	A	20	ASP	1
1	A	41	GLN	1
1	A	120	GLU	1
1	A	53	ASN	1
1	A	117	THR	1
1	A	127	GLU	1
1	A	72	MET	1
1	A	43	PRO	1
1	A	87	GLU	1
1	A	44	THR	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 [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided