



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 01:49 AM UTC

PDB ID : 2K0E / pdb_00002k0e
Title : A Coupled Equilibrium Shift Mechanism in Calmodulin-Mediated Signal Transduction
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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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

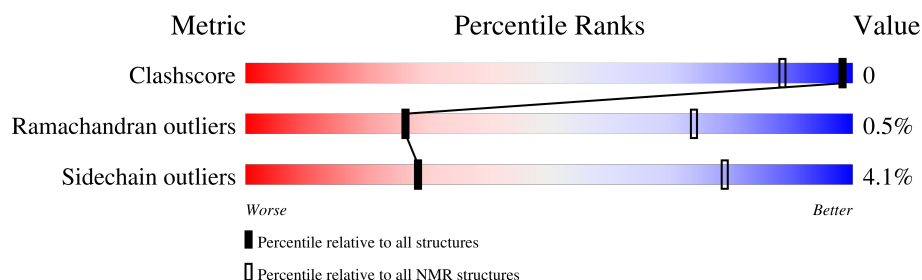
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	

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)	1.08	157
2	A:83-A:145 (63)	1.22	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 (CCD ID: CA) (formula: Ca).

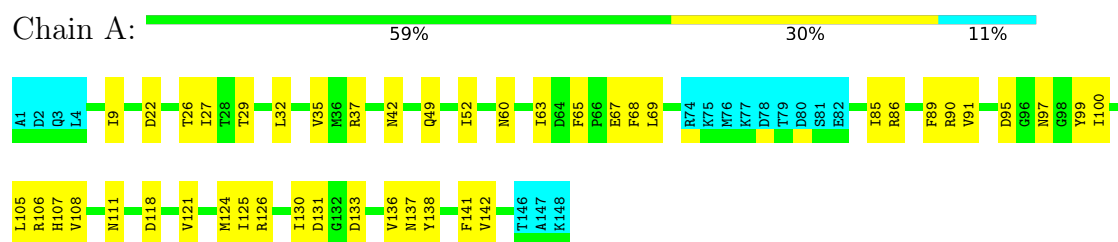
Mol	Chain	Residues	Atoms	
2	A	4	Total	Ca
			4	4

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

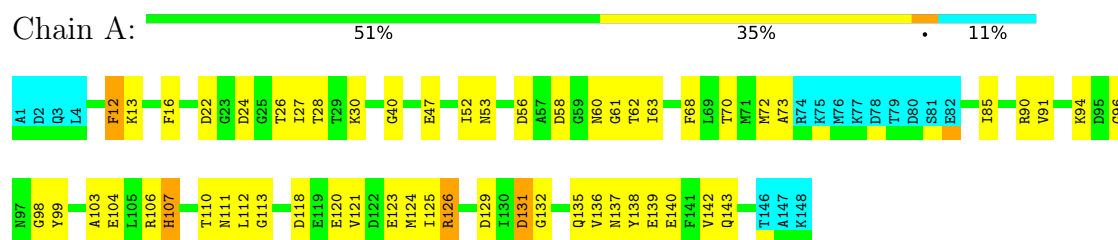


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

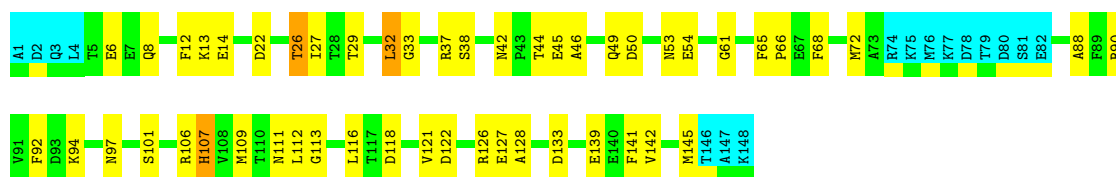
- Molecule 1: Calmodulin



4.2.2 Score per residue for model 2

- Molecule 1: Calmodulin

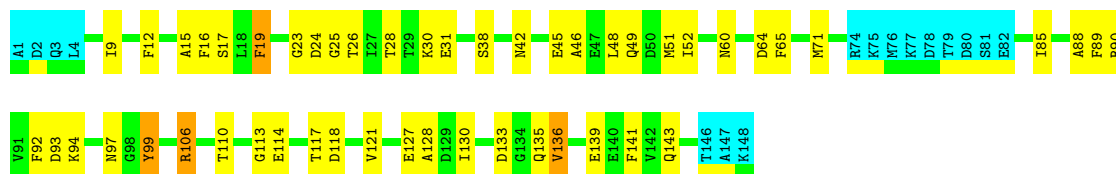




4.2.3 Score per residue for model 3

- Molecule 1: Calmodulin

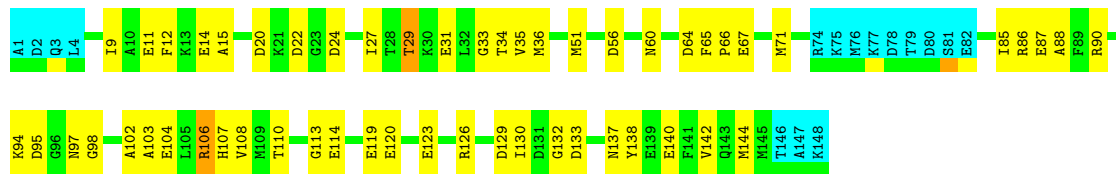
Chain A: 55% 31% 11%



4.2.4 Score per residue for model 4

- Molecule 1: Calmodulin

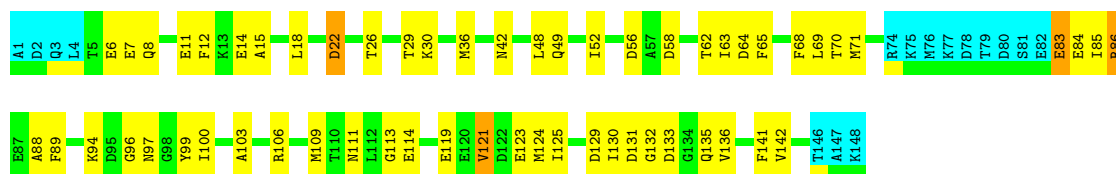
Chain A: 53% 35% 11%



4.2.5 Score per residue for model 5

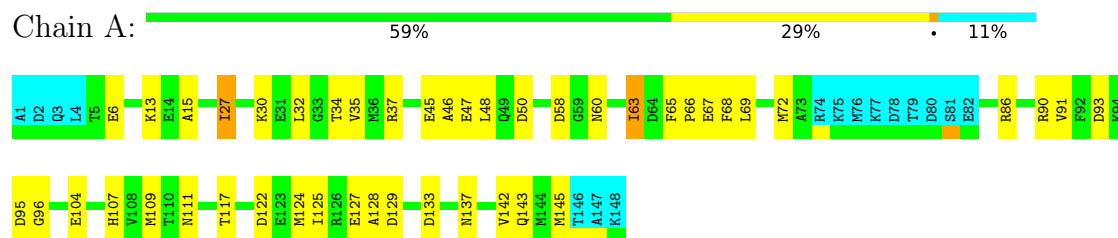
- Molecule 1: Calmodulin

Chain A: 50% 36% 11%



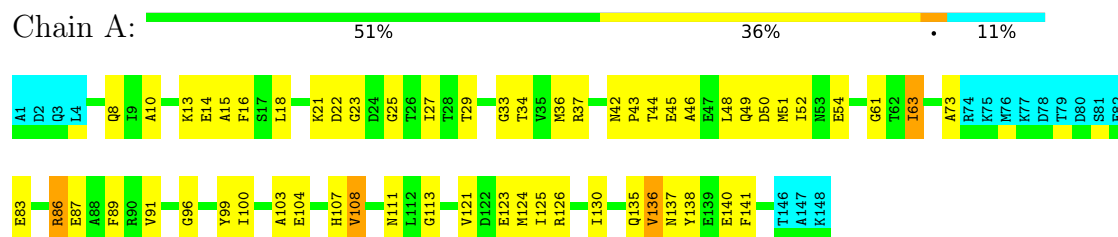
4.2.6 Score per residue for model 6

- Molecule 1: Calmodulin



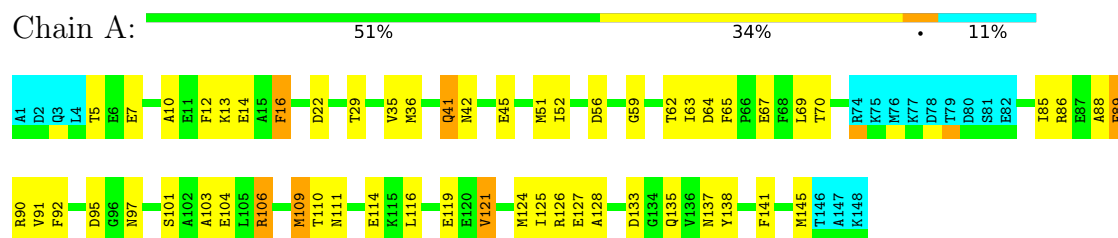
4.2.7 Score per residue for model 7

- Molecule 1: Calmodulin



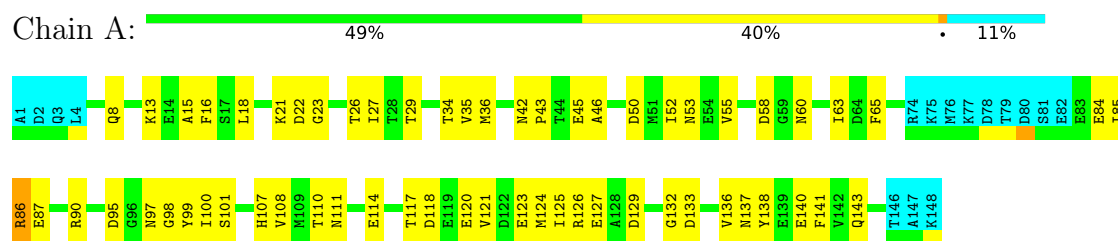
4.2.8 Score per residue for model 8

- Molecule 1: Calmodulin



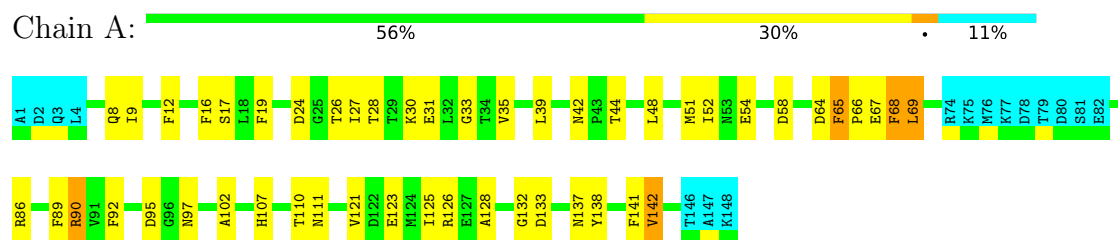
4.2.9 Score per residue for model 9

- Molecule 1: Calmodulin



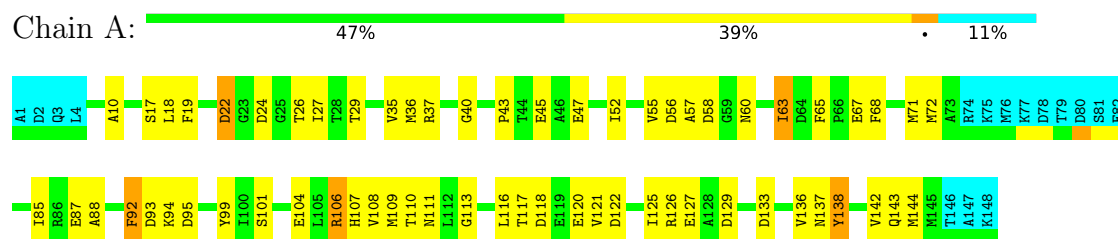
4.2.10 Score per residue for model 10

- Molecule 1: Calmodulin



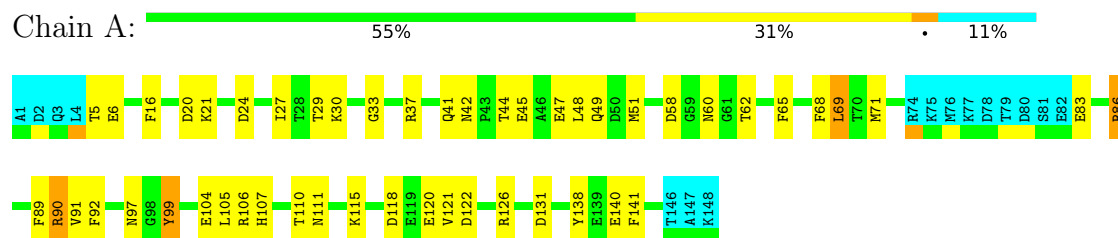
4.2.11 Score per residue for model 11

- Molecule 1: Calmodulin



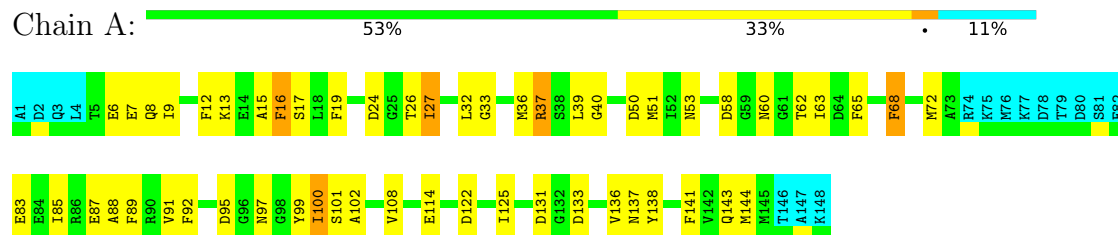
4.2.12 Score per residue for model 12

- Molecule 1: Calmodulin



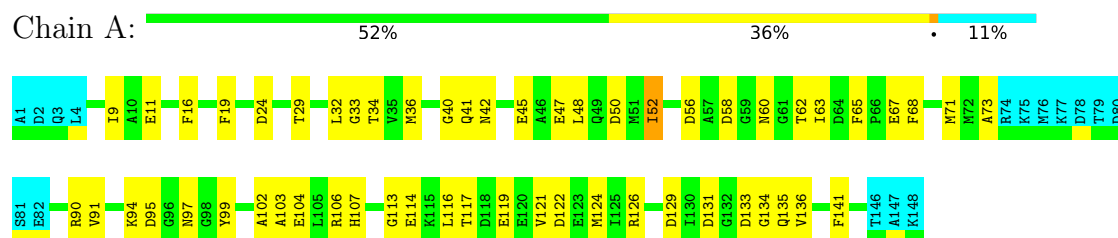
4.2.13 Score per residue for model 13

- Molecule 1: Calmodulin



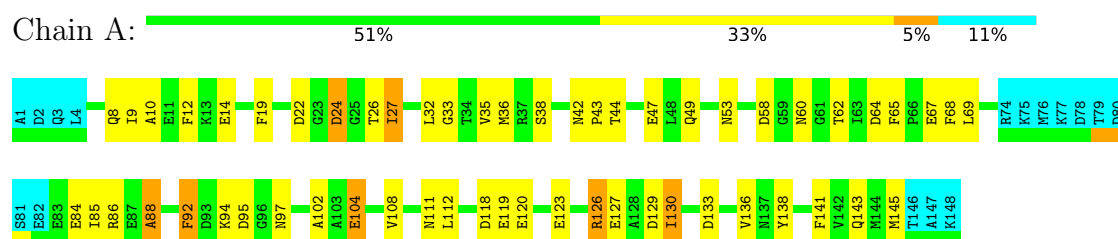
4.2.14 Score per residue for model 14

- Molecule 1: Calmodulin



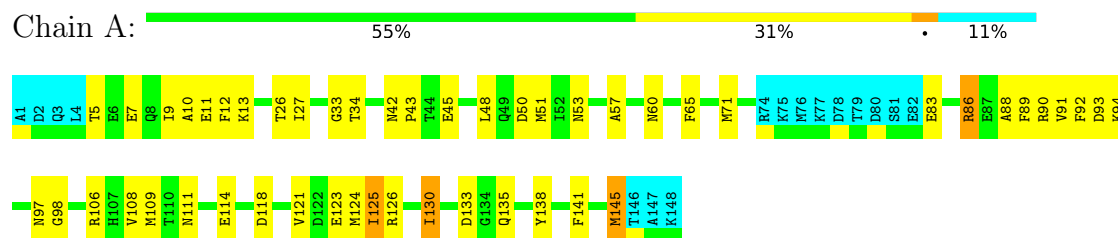
4.2.15 Score per residue for model 15

- Molecule 1: Calmodulin



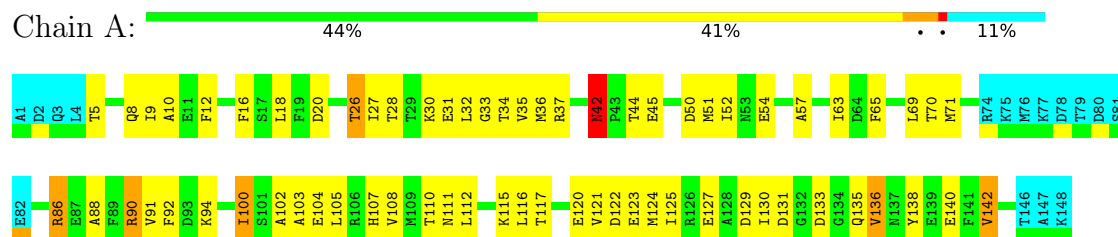
4.2.16 Score per residue for model 16

- Molecule 1: Calmodulin



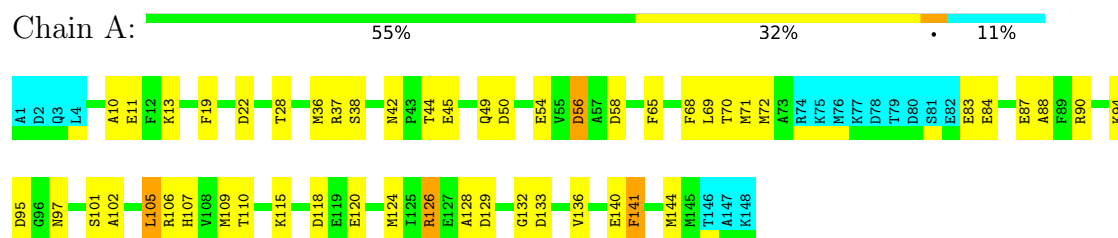
4.2.17 Score per residue for model 17

- Molecule 1: Calmodulin



4.2.18 Score per residue for model 18

- Molecule 1: Calmodulin

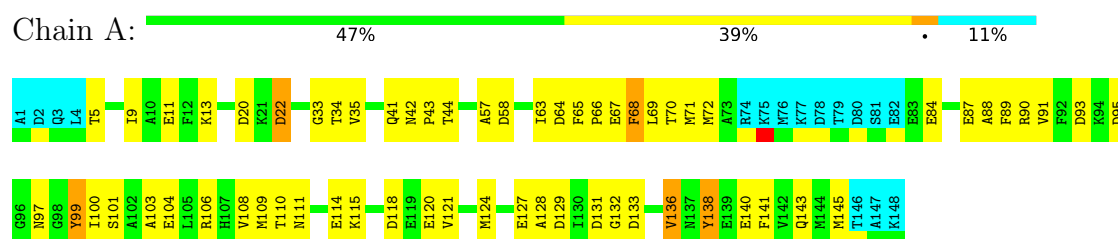


4.2.22 Score per residue for model 22

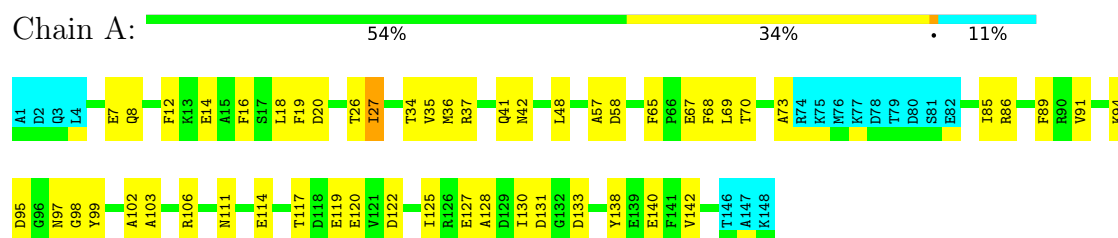
- Molecule 1: Calmodulin



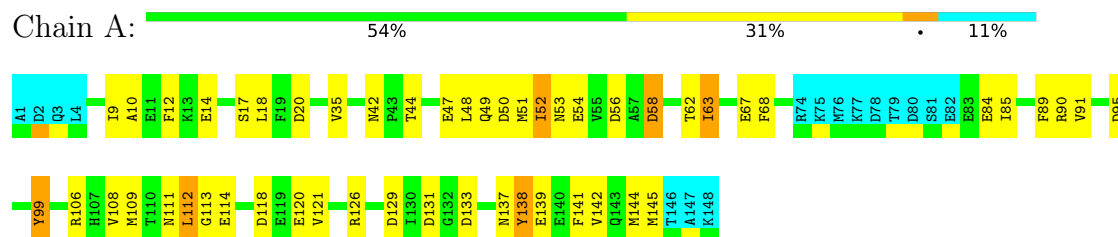
- Molecule 1: Calmodulin



- Molecule 1: Calmodulin

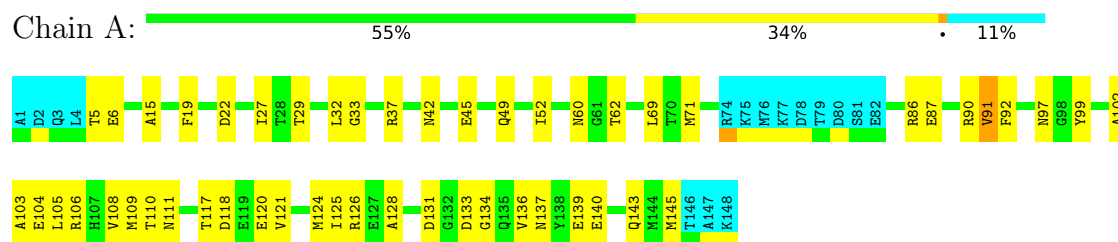


- Molecule 1: Calmodulin



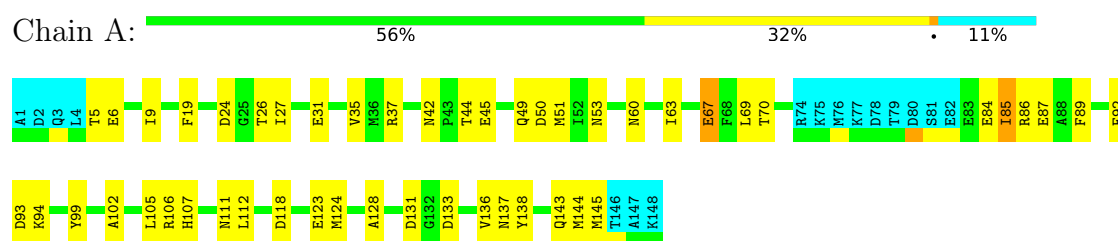
4.2.26 Score per residue for model 26

- Molecule 1: Calmodulin



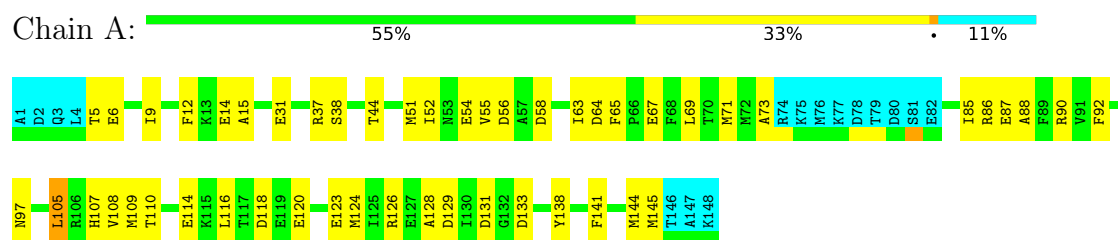
4.2.27 Score per residue for model 27

- Molecule 1: Calmodulin



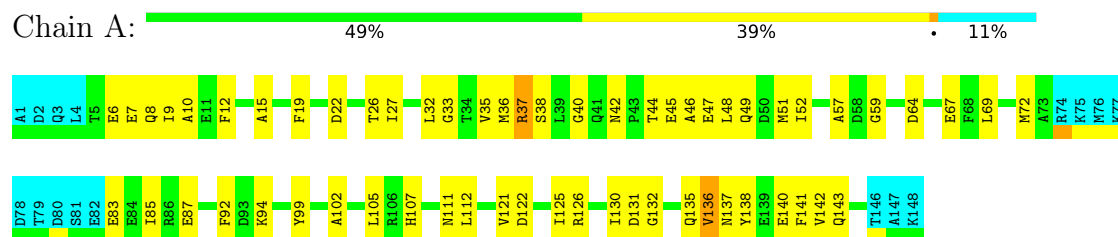
4.2.28 Score per residue for model 28

- Molecule 1: Calmodulin



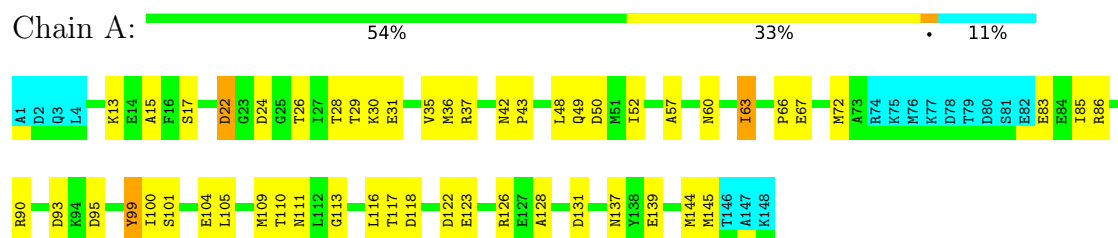
4.2.29 Score per residue for model 29

- Molecule 1: Calmodulin



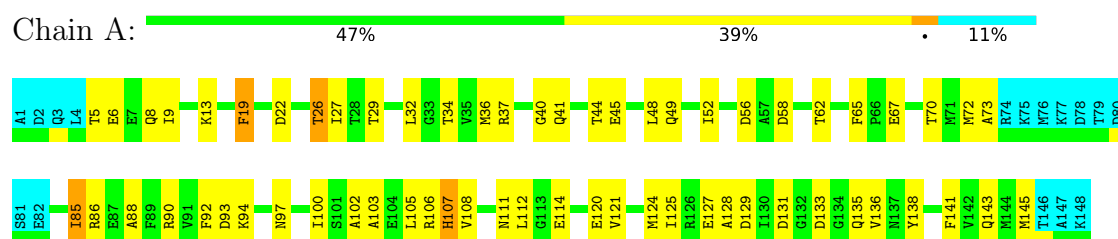
4.2.30 Score per residue for model 30

- Molecule 1: Calmodulin



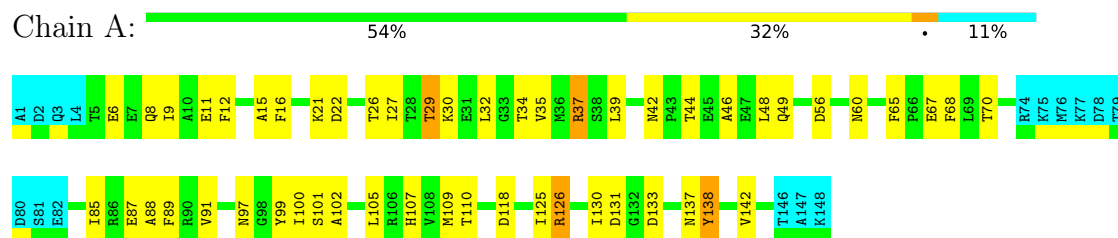
4.2.31 Score per residue for model 31

- Molecule 1: Calmodulin



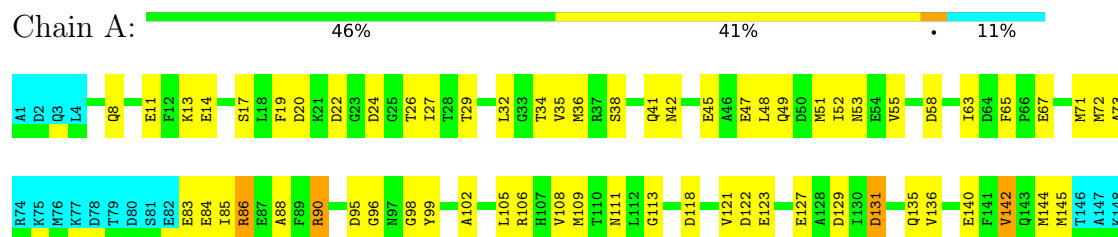
4.2.32 Score per residue for model 32

- Molecule 1: Calmodulin



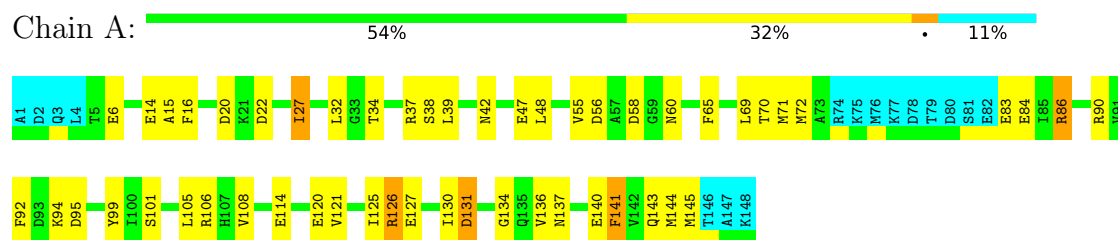
4.2.33 Score per residue for model 33

- Molecule 1: Calmodulin



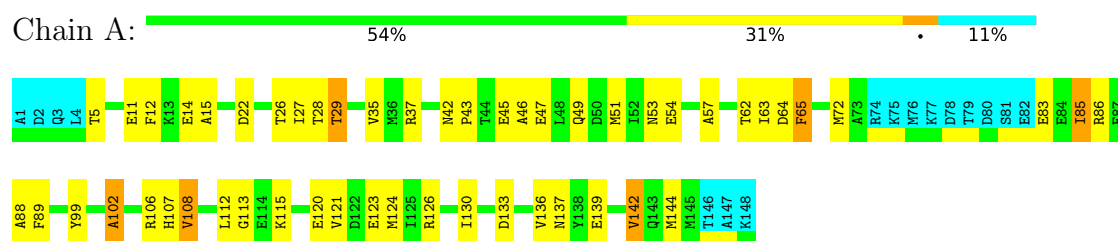
4.2.34 Score per residue for model 34

- Molecule 1: Calmodulin



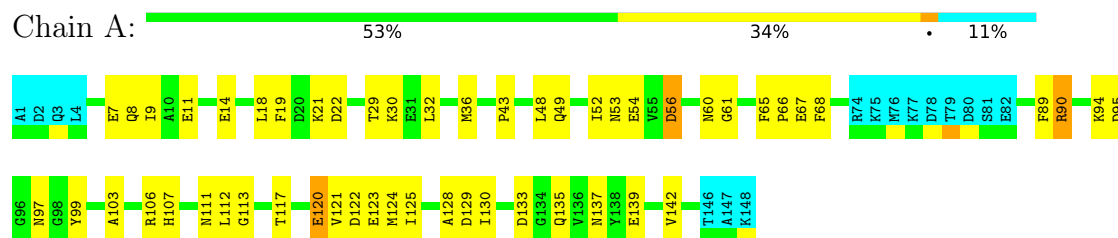
4.2.35 Score per residue for model 35

- Molecule 1: Calmodulin



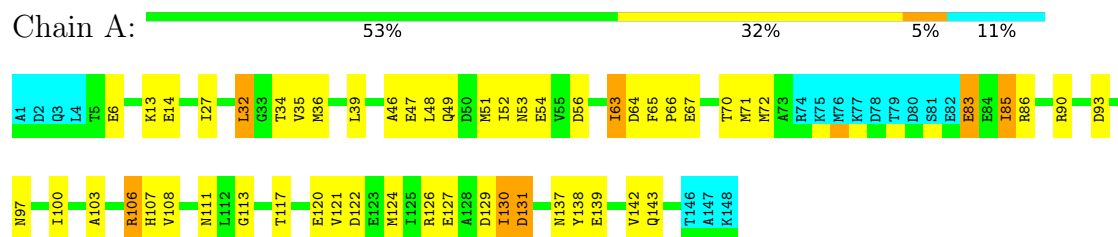
4.2.36 Score per residue for model 36

- Molecule 1: Calmodulin



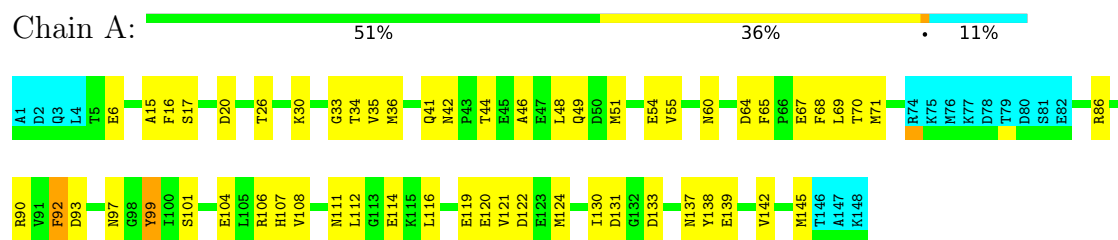
4.2.37 Score per residue for model 37

- Molecule 1: Calmodulin



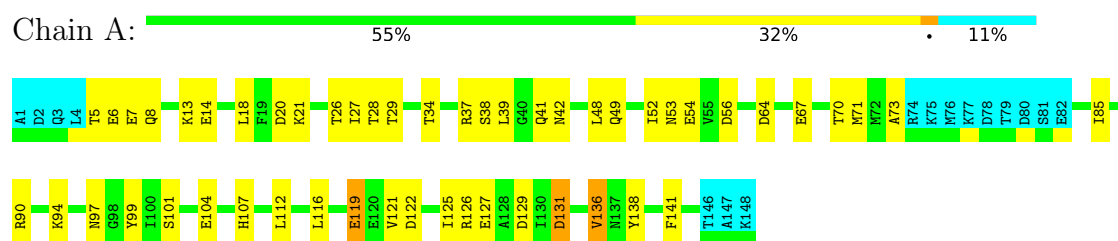
4.2.38 Score per residue for model 38

- Molecule 1: Calmodulin



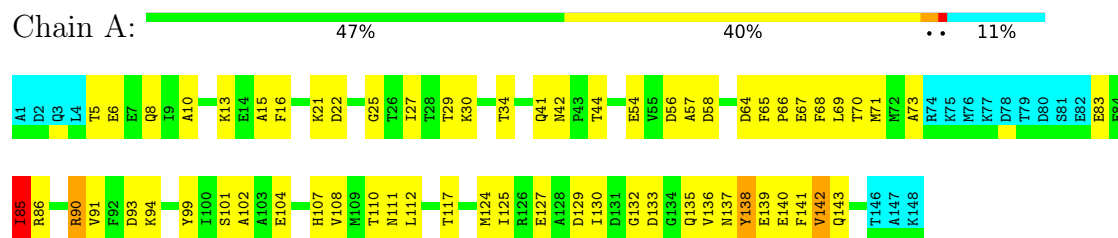
4.2.39 Score per residue for model 39

- Molecule 1: Calmodulin



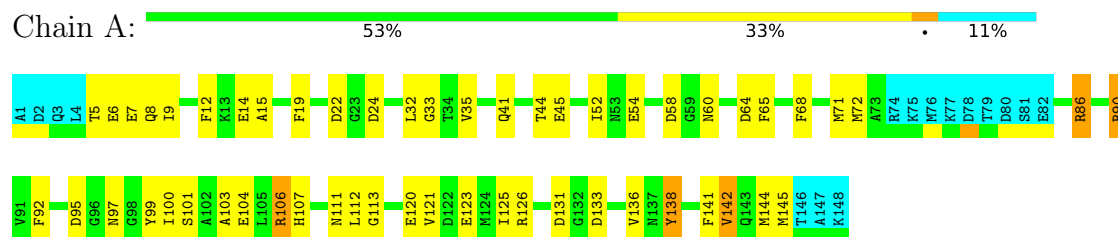
4.2.40 Score per residue for model 40

- Molecule 1: Calmodulin



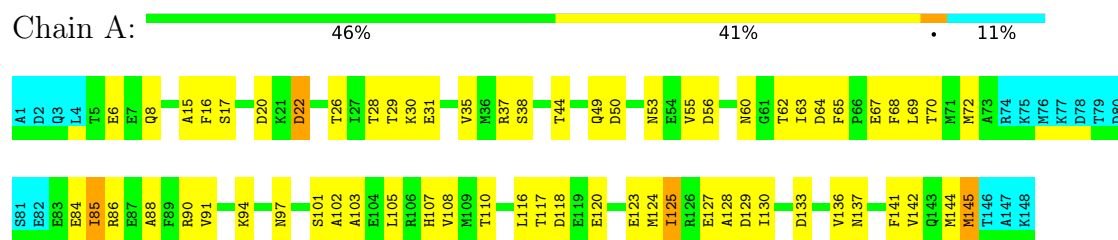
4.2.41 Score per residue for model 41

- Molecule 1: Calmodulin



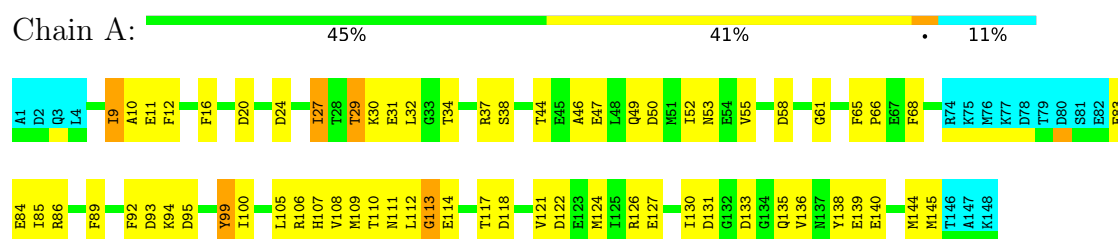
4.2.42 Score per residue for model 42

- Molecule 1: Calmodulin



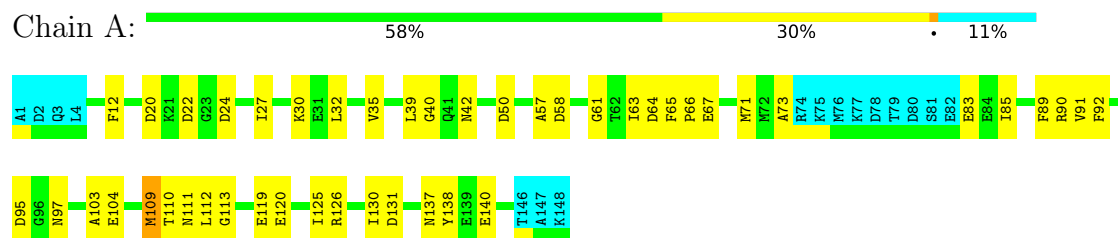
4.2.43 Score per residue for model 43

- Molecule 1: Calmodulin



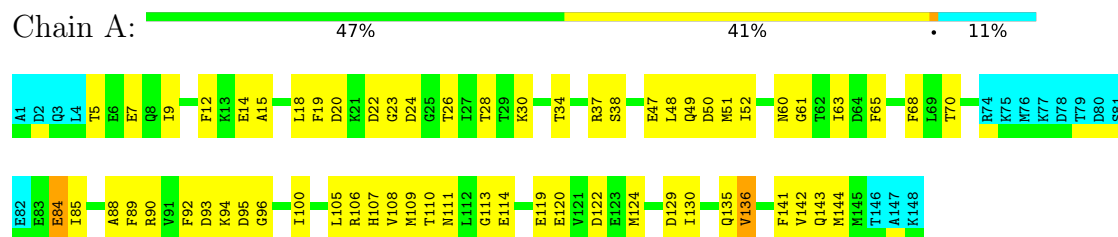
4.2.44 Score per residue for model 44

- Molecule 1: Calmodulin



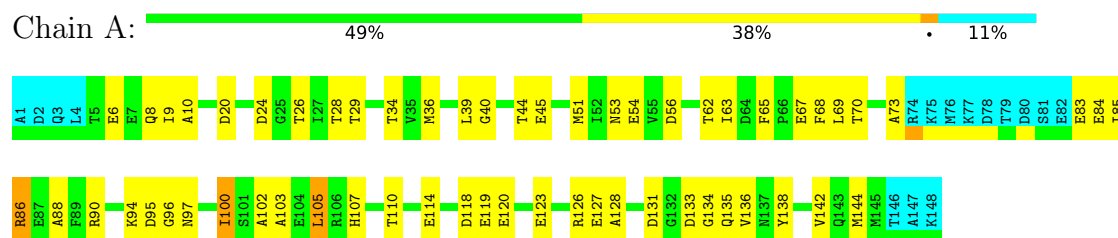
4.2.45 Score per residue for model 45

- Molecule 1: Calmodulin



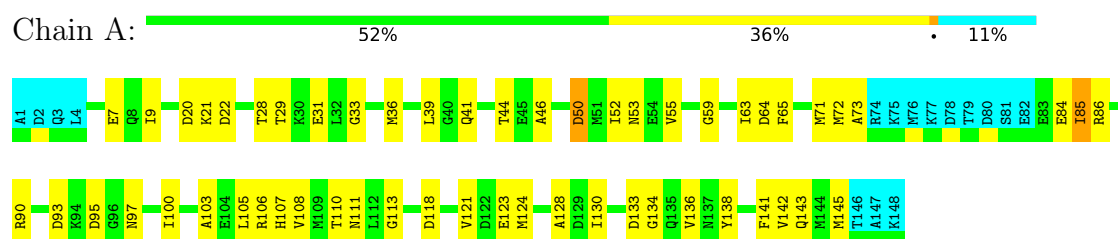
4.2.46 Score per residue for model 46

- Molecule 1: Calmodulin



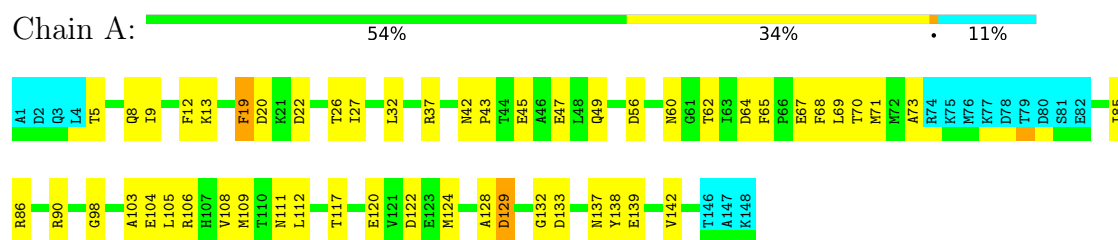
4.2.47 Score per residue for model 47

- Molecule 1: Calmodulin



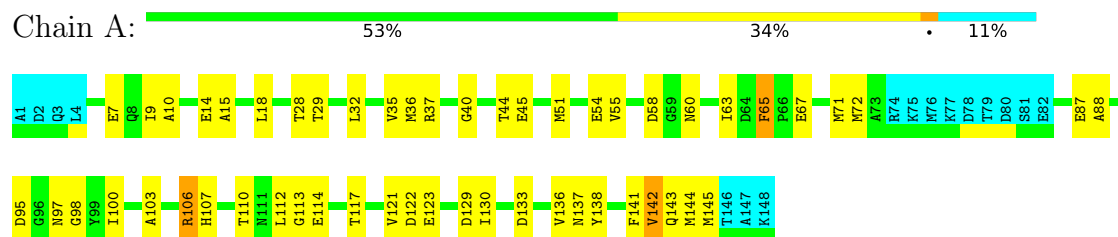
4.2.48 Score per residue for model 48

- Molecule 1: Calmodulin



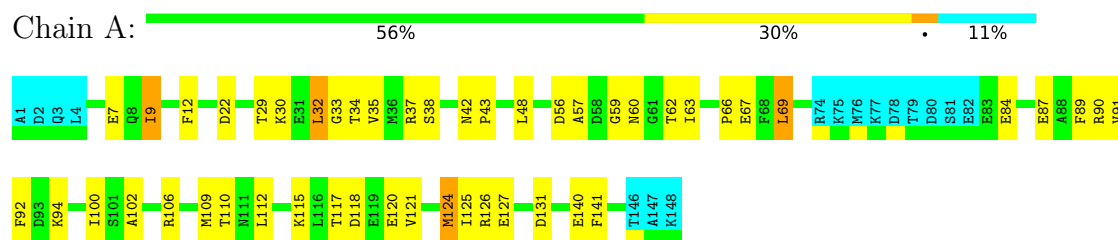
4.2.49 Score per residue for model 49

- Molecule 1: Calmodulin



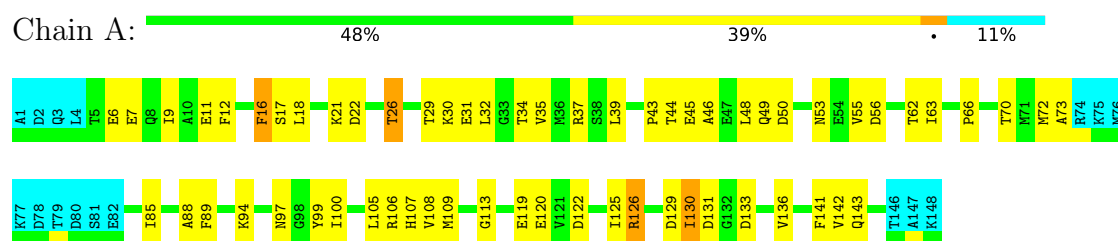
4.2.50 Score per residue for model 50

- Molecule 1: Calmodulin



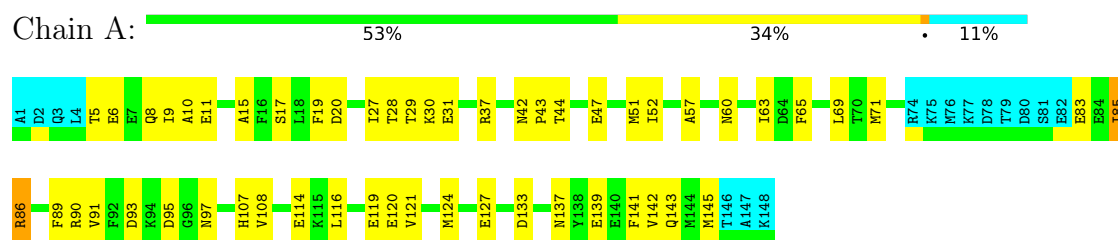
4.2.51 Score per residue for model 51

- Molecule 1: Calmodulin



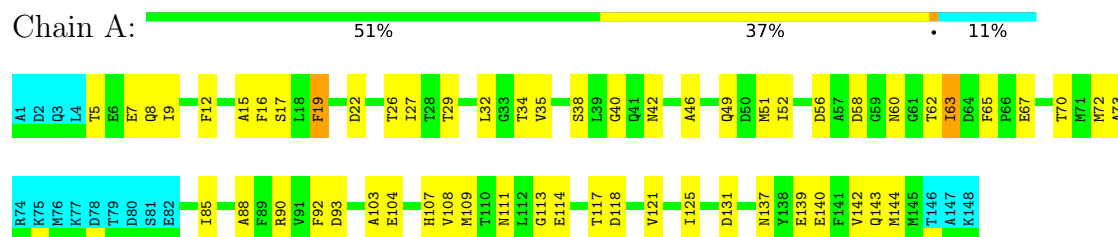
4.2.52 Score per residue for model 52

- Molecule 1: Calmodulin



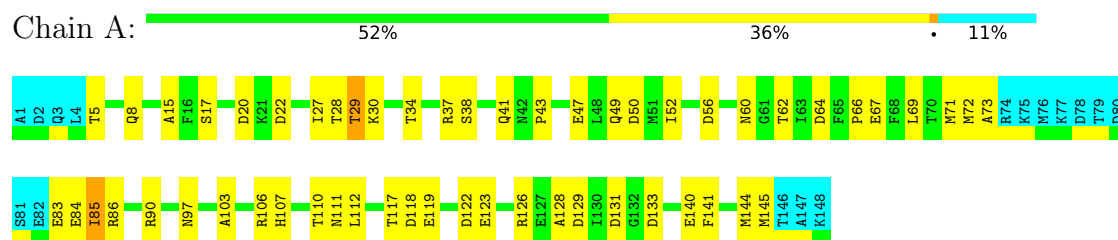
4.2.53 Score per residue for model 53

- Molecule 1: Calmodulin



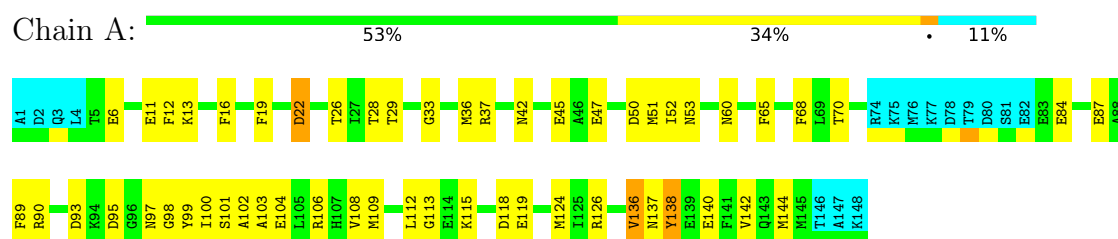
4.2.54 Score per residue for model 54

- Molecule 1: Calmodulin



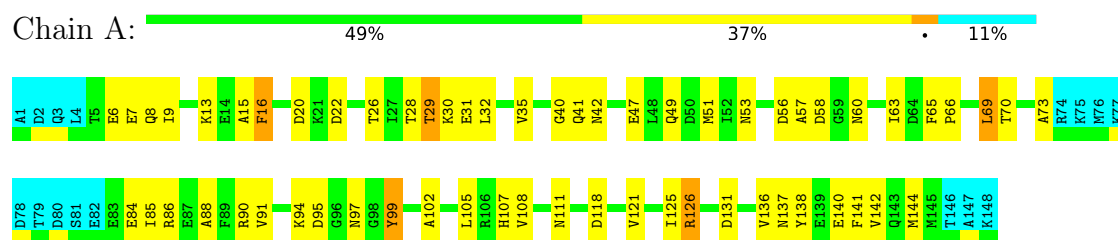
4.2.55 Score per residue for model 55

- Molecule 1: Calmodulin



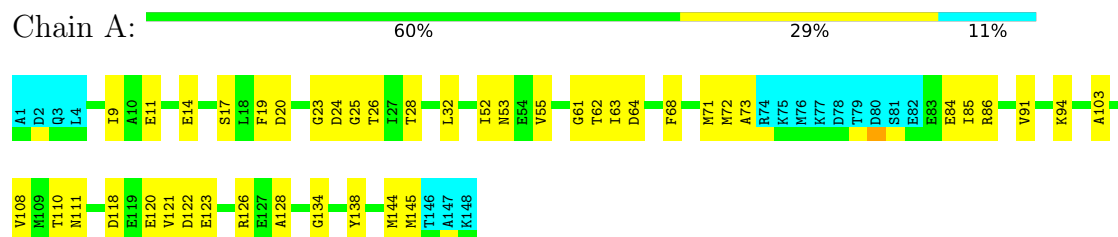
4.2.56 Score per residue for model 56

- Molecule 1: Calmodulin



4.2.57 Score per residue for model 57

- Molecule 1: Calmodulin



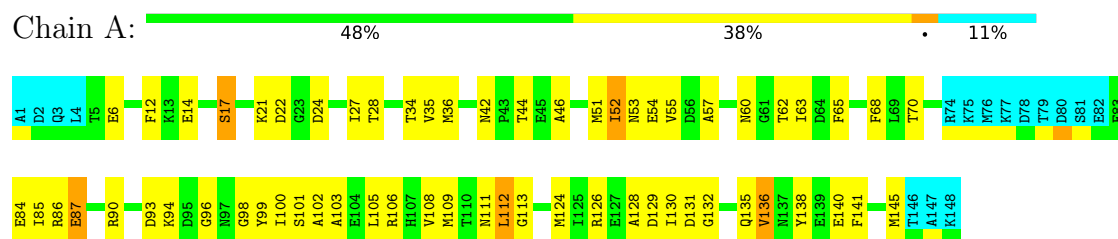
4.2.58 Score per residue for model 58

- Molecule 1: Calmodulin



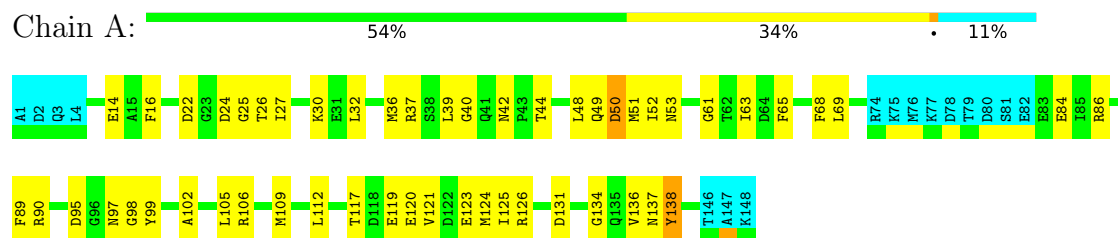
4.2.59 Score per residue for model 59

- Molecule 1: Calmodulin



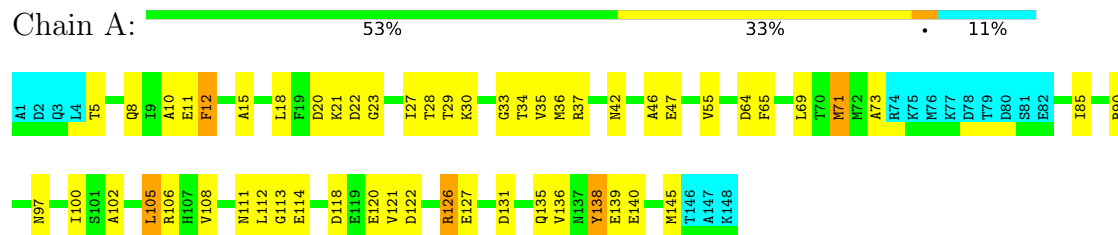
4.2.60 Score per residue for model 60

- Molecule 1: Calmodulin



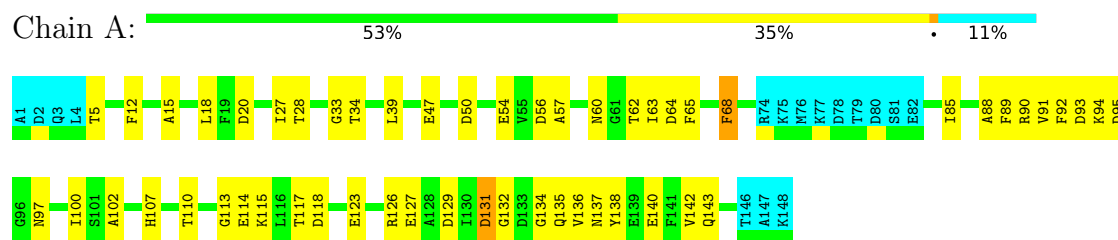
4.2.61 Score per residue for model 61

- Molecule 1: Calmodulin



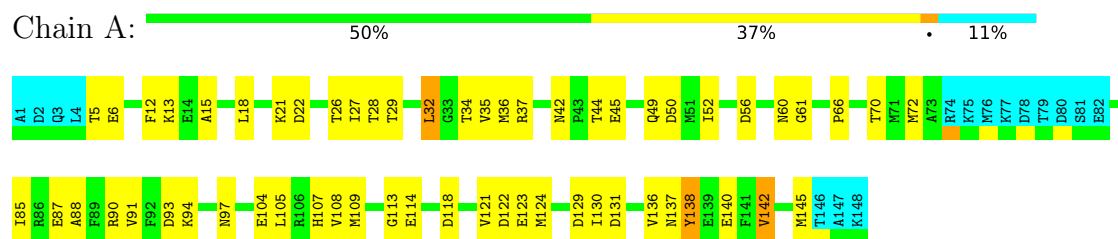
4.2.62 Score per residue for model 62

- Molecule 1: Calmodulin



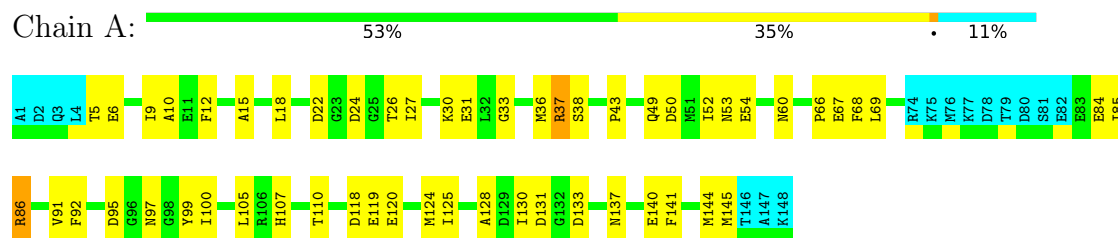
4.2.63 Score per residue for model 63

- Molecule 1: Calmodulin



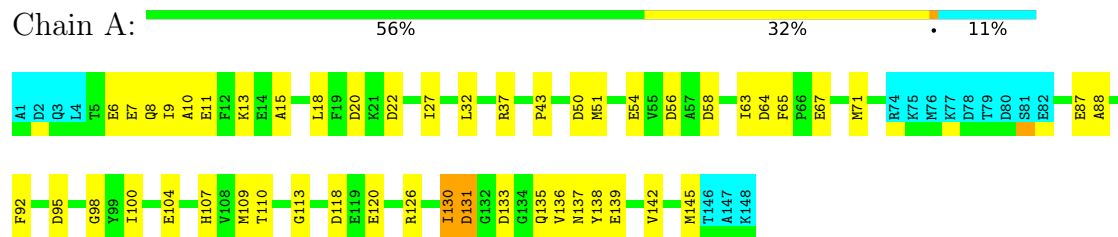
4.2.64 Score per residue for model 64

- Molecule 1: Calmodulin



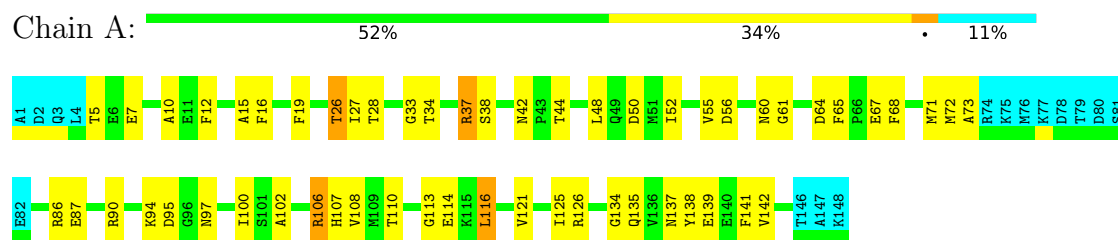
4.2.65 Score per residue for model 65

- Molecule 1: Calmodulin



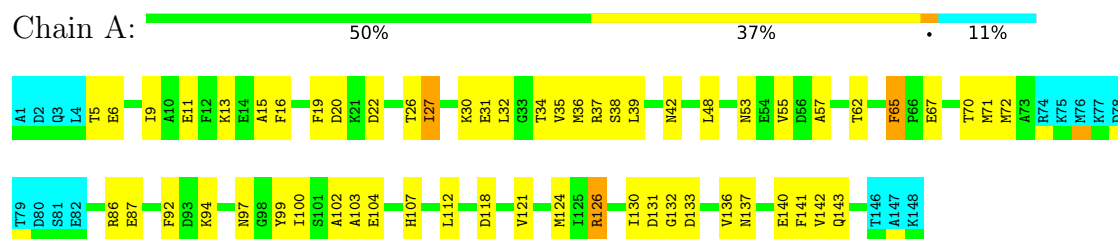
4.2.66 Score per residue for model 66

- Molecule 1: Calmodulin



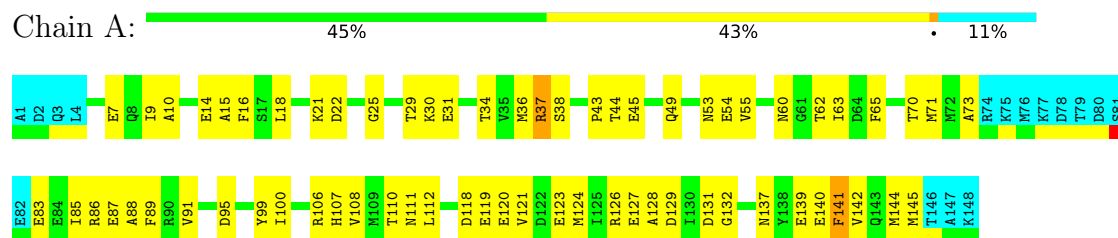
4.2.67 Score per residue for model 67

- Molecule 1: Calmodulin



4.2.68 Score per residue for model 68

- Molecule 1: Calmodulin



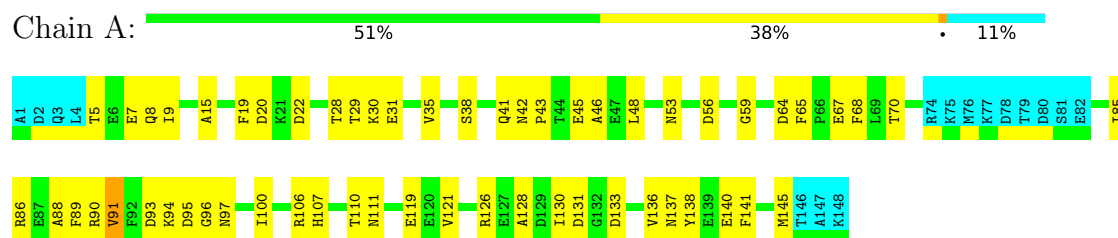
4.2.69 Score per residue for model 69

- Molecule 1: Calmodulin



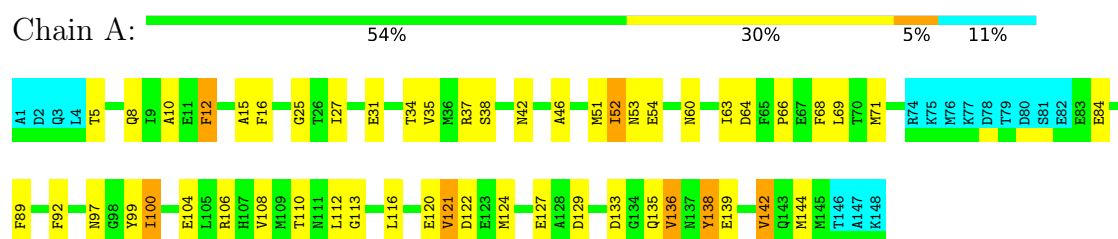
4.2.70 Score per residue for model 70

- Molecule 1: Calmodulin



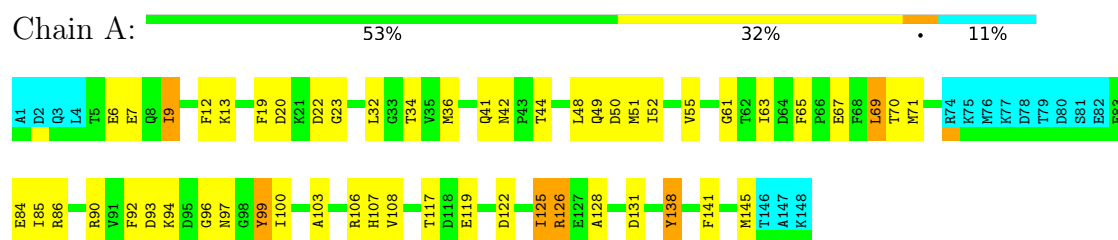
4.2.71 Score per residue for model 71

- Molecule 1: Calmodulin



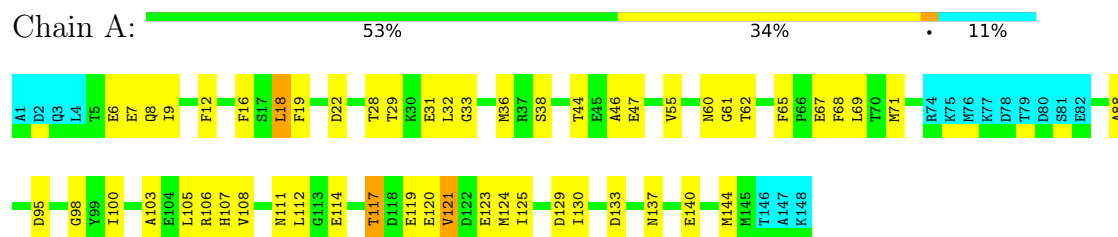
4.2.72 Score per residue for model 72

- Molecule 1: Calmodulin



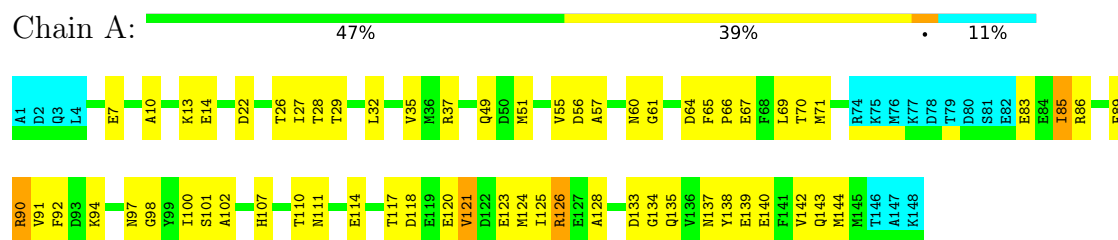
4.2.73 Score per residue for model 73

- Molecule 1: Calmodulin



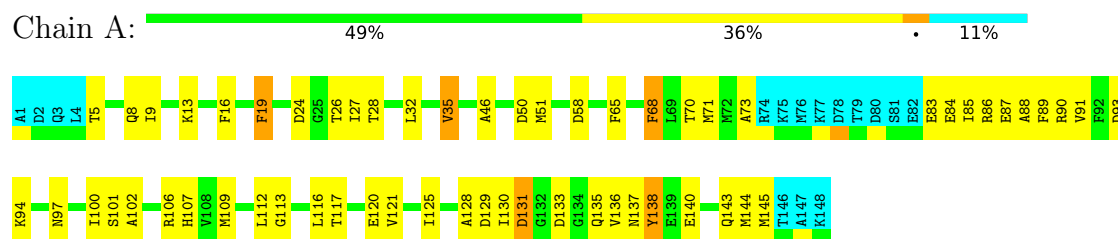
4.2.74 Score per residue for model 74

- Molecule 1: Calmodulin



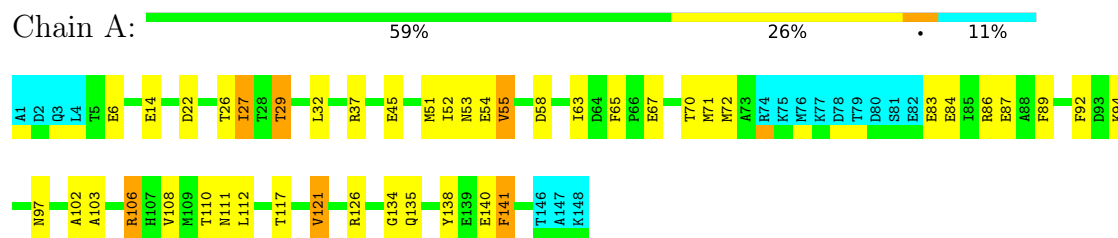
4.2.75 Score per residue for model 75

- Molecule 1: Calmodulin



4.2.76 Score per residue for model 76

- Molecule 1: Calmodulin



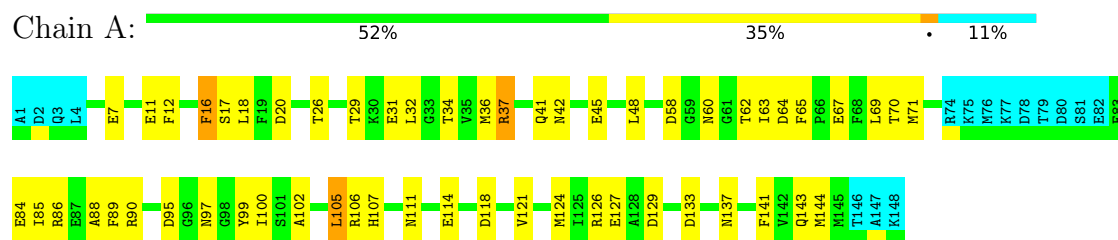
4.2.77 Score per residue for model 77

- Molecule 1: Calmodulin



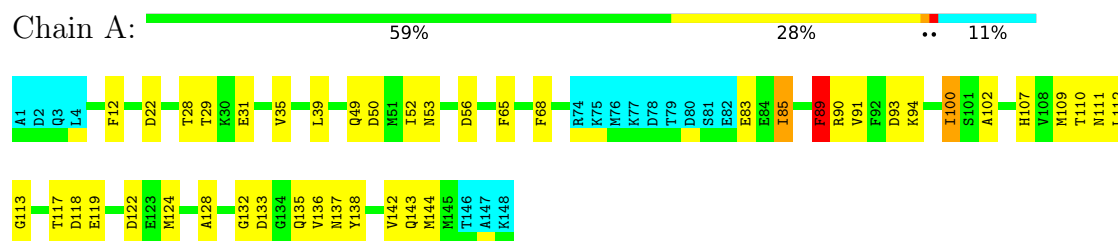
4.2.78 Score per residue for model 78

- Molecule 1: Calmodulin



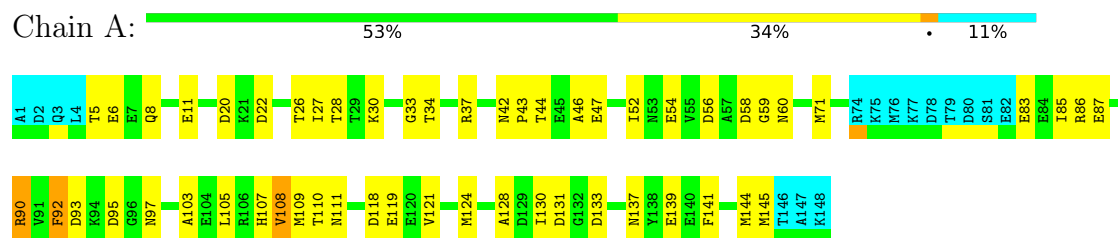
4.2.79 Score per residue for model 79

- Molecule 1: Calmodulin



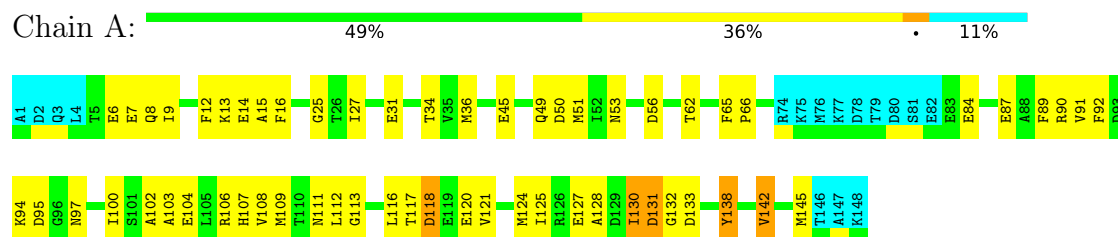
4.2.80 Score per residue for model 80

- Molecule 1: Calmodulin



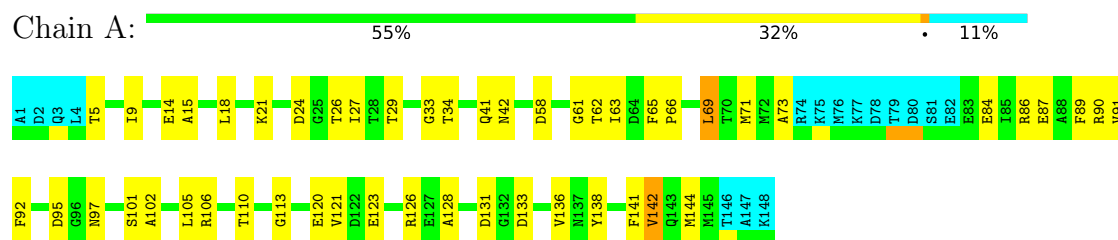
4.2.81 Score per residue for model 81

- Molecule 1: Calmodulin



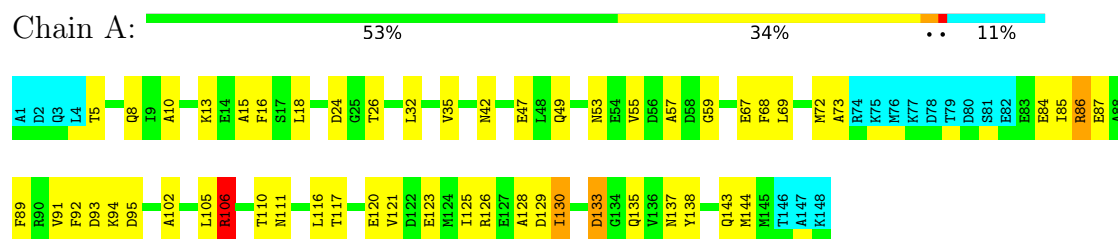
4.2.82 Score per residue for model 82

- Molecule 1: Calmodulin



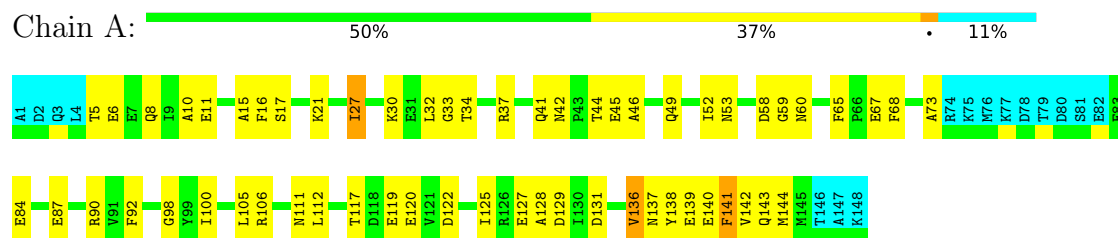
4.2.83 Score per residue for model 83

- Molecule 1: Calmodulin



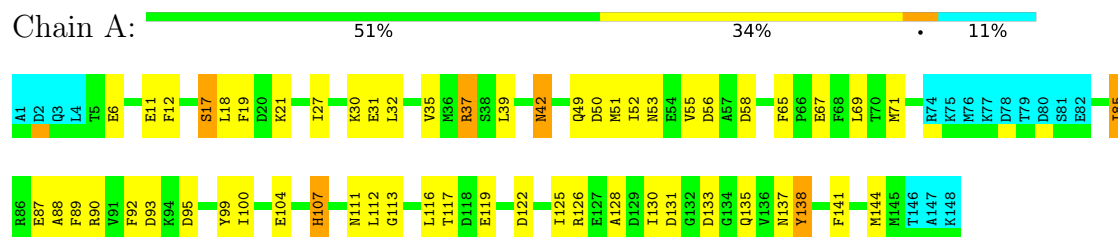
4.2.84 Score per residue for model 84

- Molecule 1: Calmodulin



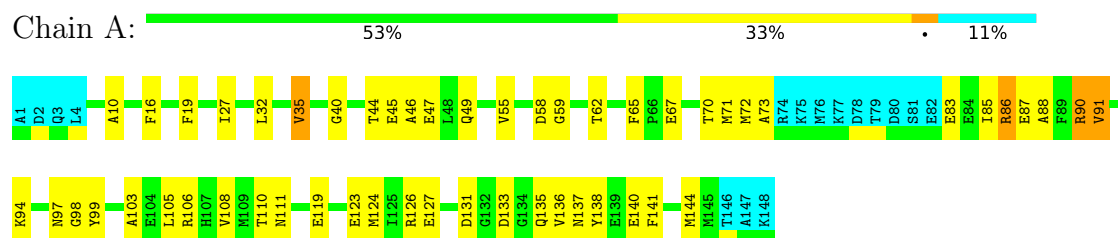
4.2.85 Score per residue for model 85

- Molecule 1: Calmodulin



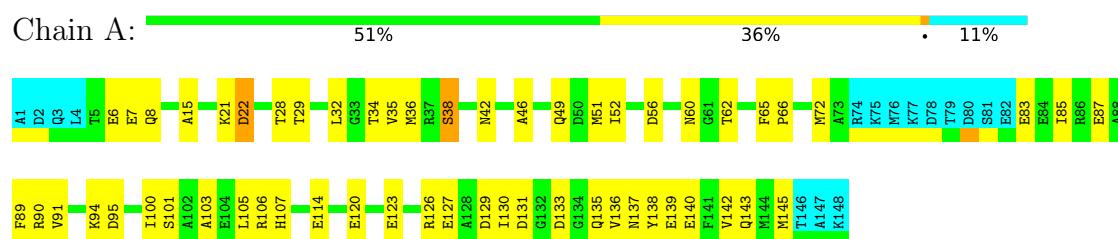
4.2.86 Score per residue for model 86

- Molecule 1: Calmodulin



4.2.87 Score per residue for model 87

- Molecule 1: Calmodulin



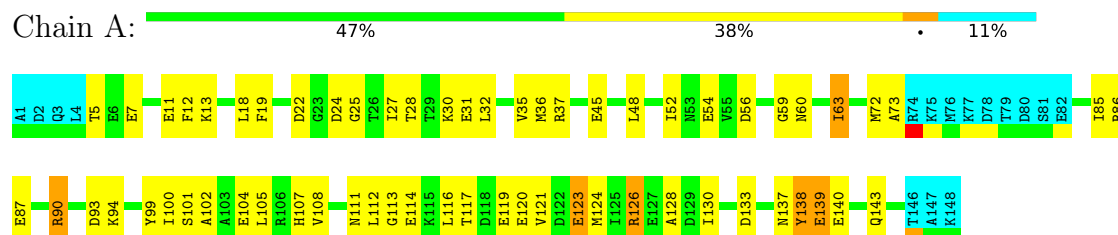
4.2.88 Score per residue for model 88

- Molecule 1: Calmodulin



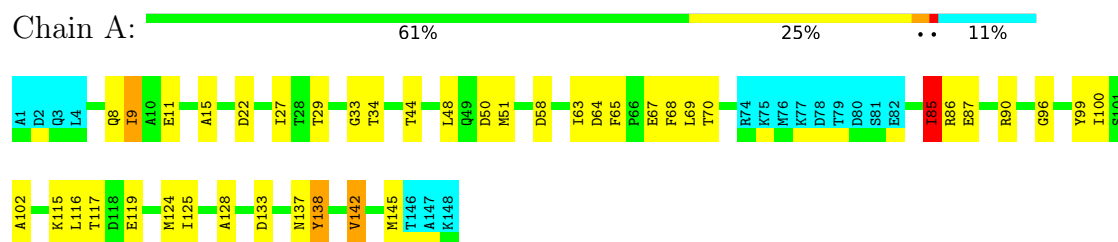
4.2.89 Score per residue for model 89

- Molecule 1: Calmodulin



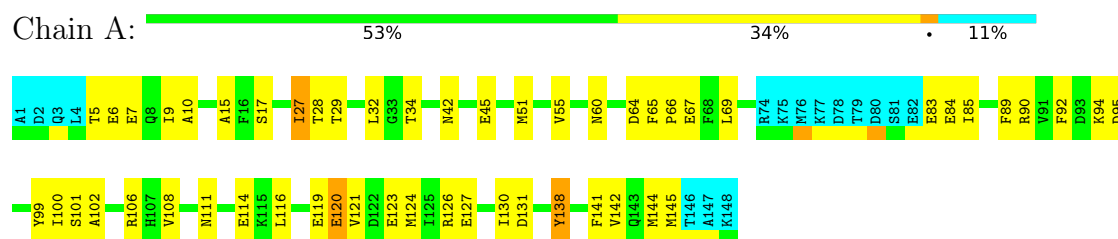
4.2.90 Score per residue for model 90

- Molecule 1: Calmodulin



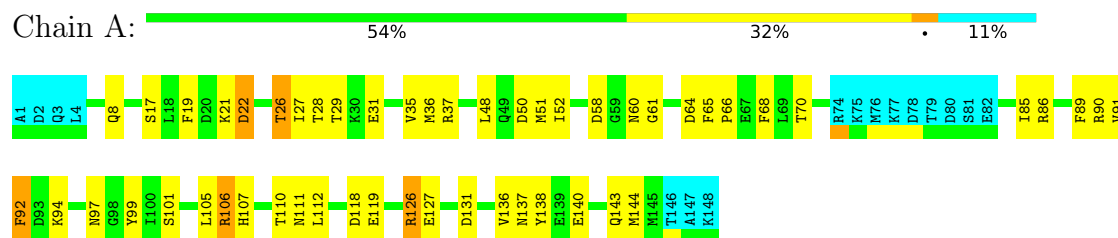
4.2.91 Score per residue for model 91

- Molecule 1: Calmodulin



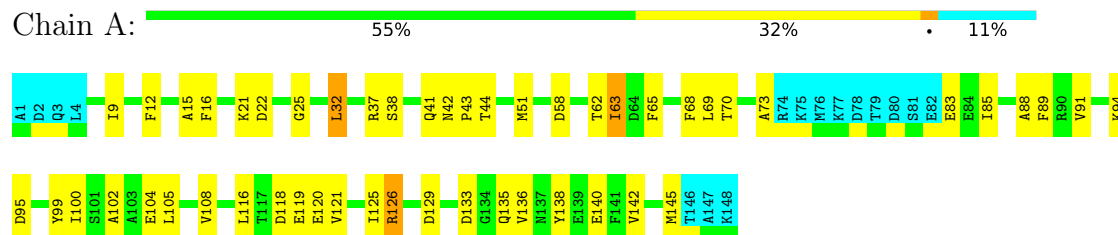
4.2.92 Score per residue for model 92

- Molecule 1: Calmodulin



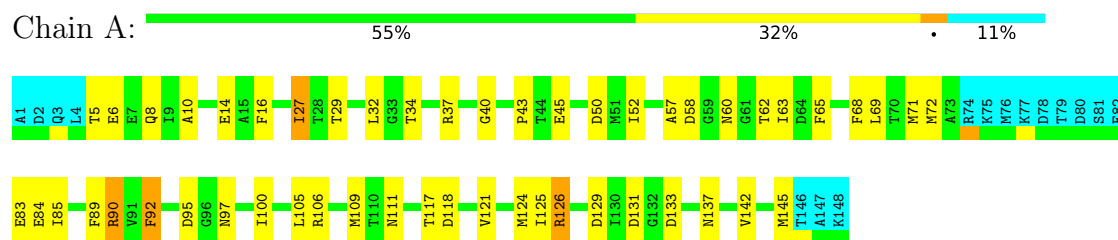
4.2.93 Score per residue for model 93

- Molecule 1: Calmodulin



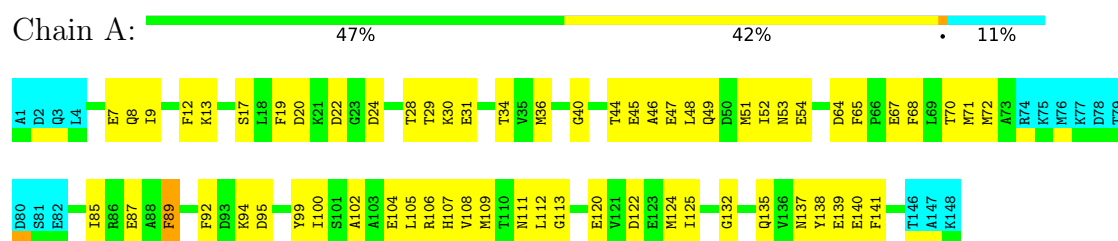
4.2.94 Score per residue for model 94

- Molecule 1: Calmodulin



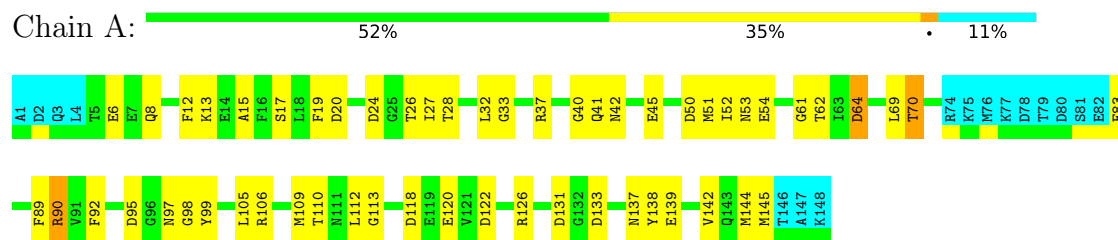
4.2.95 Score per residue for model 95

- Molecule 1: Calmodulin



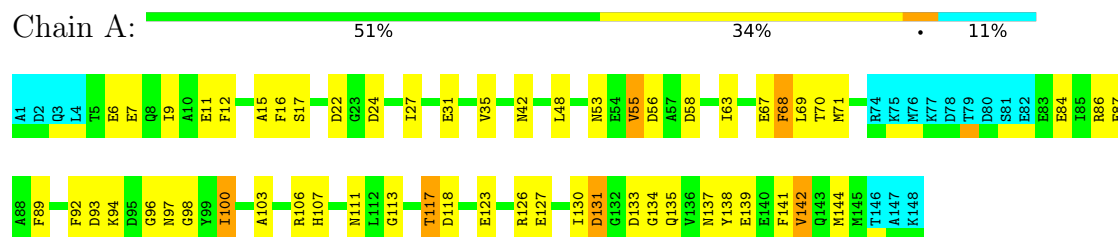
4.2.96 Score per residue for model 96

- Molecule 1: Calmodulin



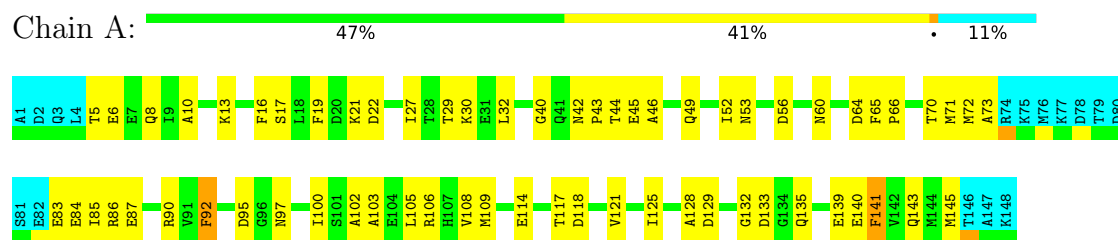
4.2.97 Score per residue for model 97

- Molecule 1: Calmodulin



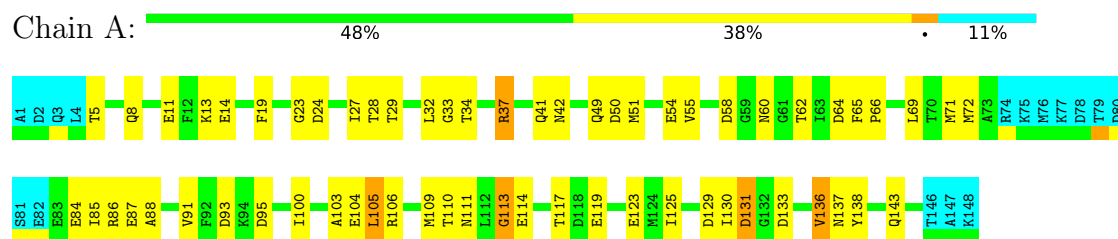
4.2.98 Score per residue for model 98

- Molecule 1: Calmodulin



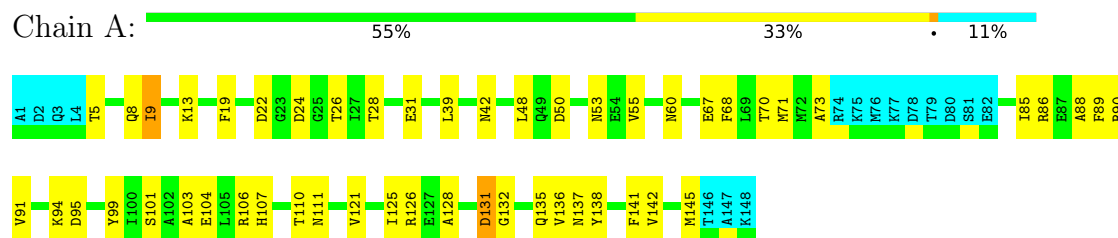
4.2.99 Score per residue for model 99

- Molecule 1: Calmodulin



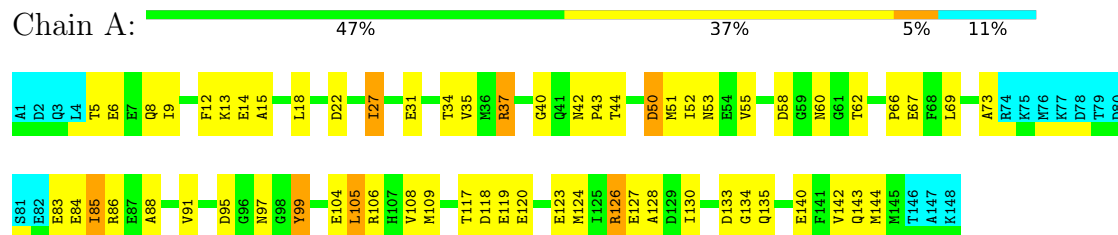
4.2.100 Score per residue for model 100

- Molecule 1: Calmodulin



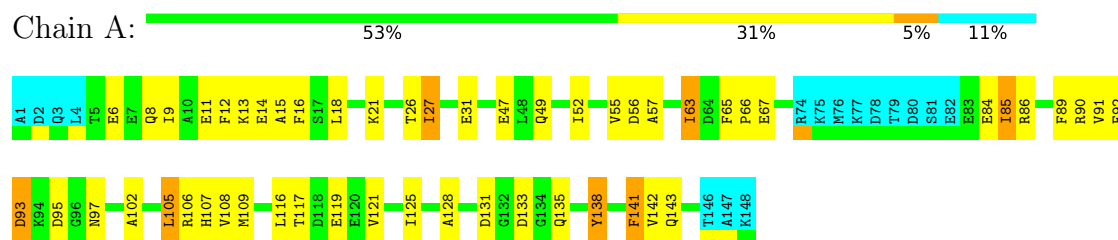
4.2.101 Score per residue for model 101

- Molecule 1: Calmodulin



4.2.102 Score per residue for model 102

- Molecule 1: Calmodulin

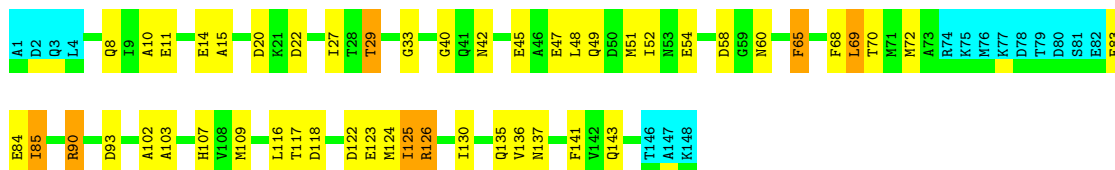




4.2.106 Score per residue for model 106

- Molecule 1: Calmodulin

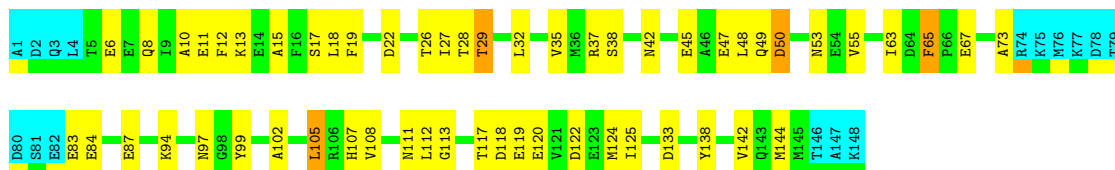
Chain A: 56% 28% 5% 11%



4.2.107 Score per residue for model 107

- Molecule 1: Calmodulin

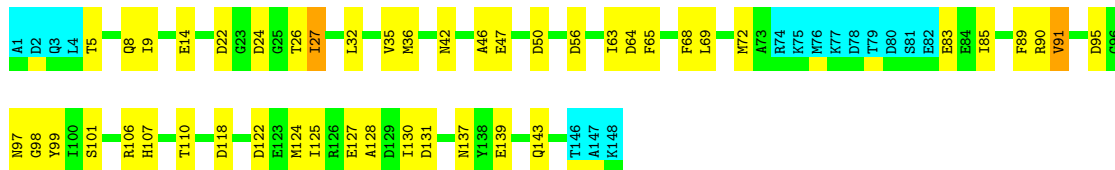
Chain A: 52% 34% 11%



4.2.108 Score per residue for model 108

- Molecule 1: Calmodulin

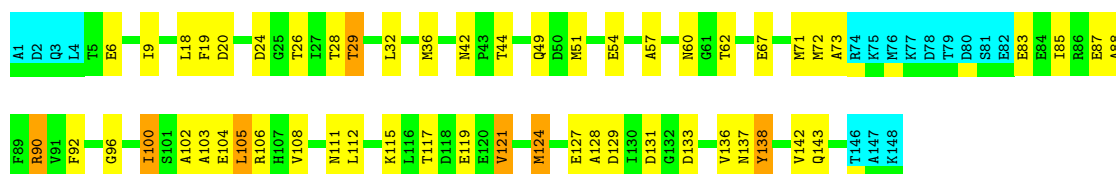
Chain A: 58% 30% 11%



4.2.109 Score per residue for model 109

- Molecule 1: Calmodulin

Chain A: 53% 32% 5% 11%



4.2.110 Score per residue for model 110

- Molecule 1: Calmodulin

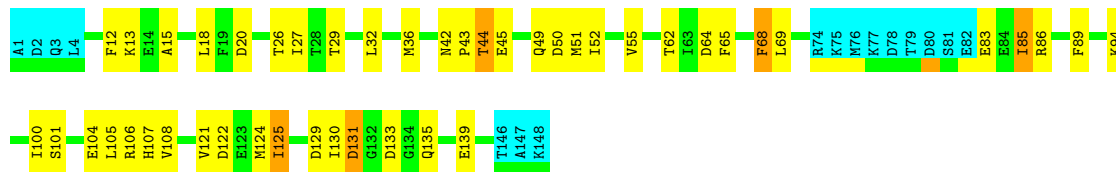
Chain A: 45% 41% 11%



4.2.111 Score per residue for model 111

- Molecule 1: Calmodulin

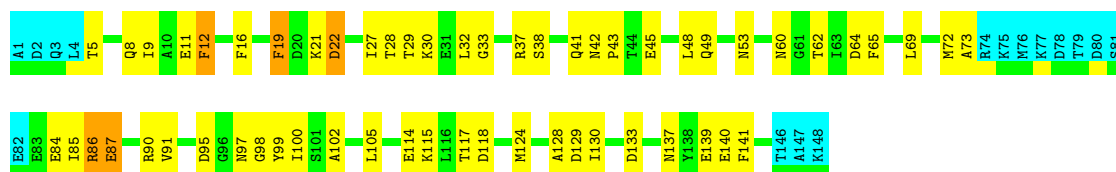
Chain A: 58% 28% 11%



4.2.112 Score per residue for model 112

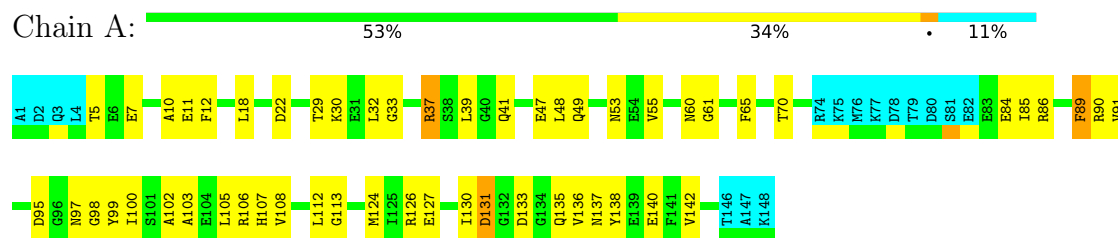
- Molecule 1: Calmodulin

Chain A: 51% 35% 11%



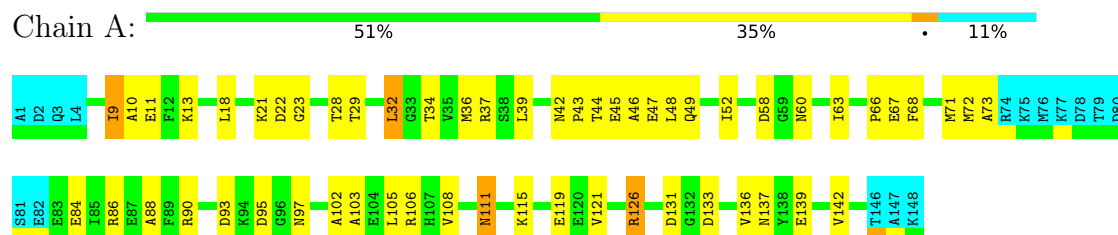
4.2.113 Score per residue for model 113

- Molecule 1: Calmodulin



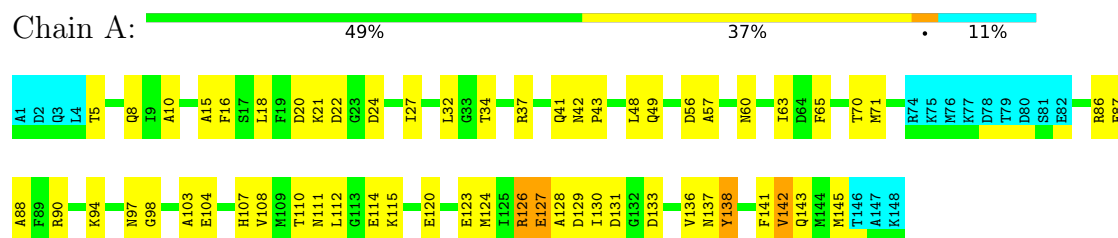
4.2.114 Score per residue for model 114

- Molecule 1: Calmodulin



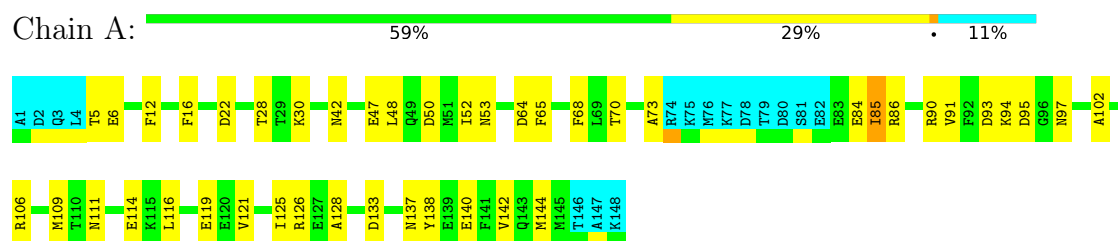
4.2.115 Score per residue for model 115

- Molecule 1: Calmodulin



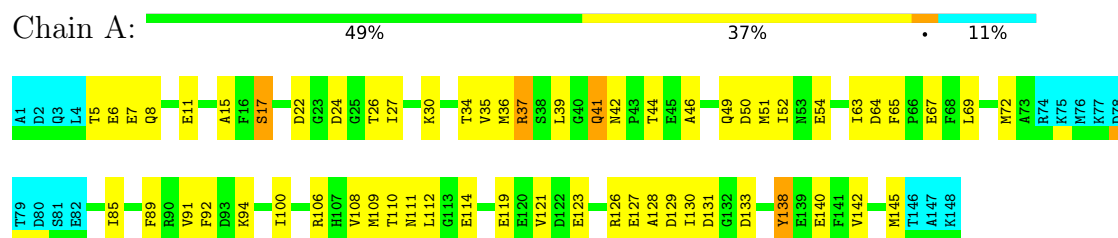
4.2.116 Score per residue for model 116

- Molecule 1: Calmodulin



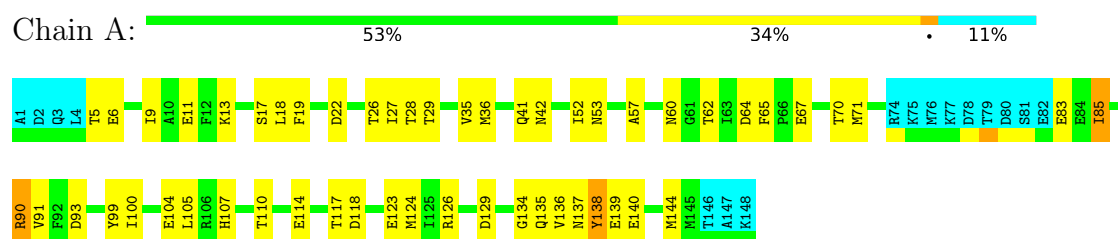
4.2.117 Score per residue for model 117

- Molecule 1: Calmodulin



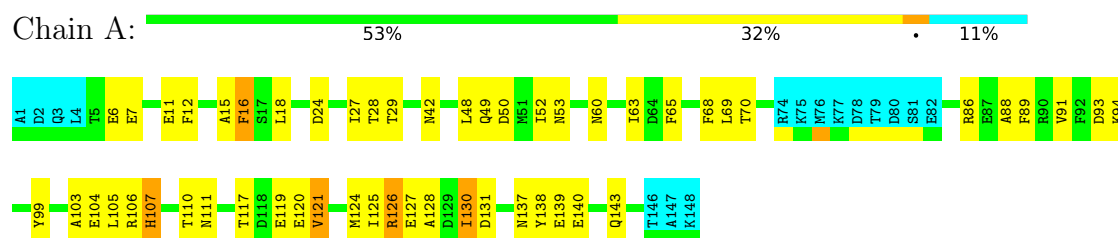
4.2.118 Score per residue for model 118

- Molecule 1: Calmodulin



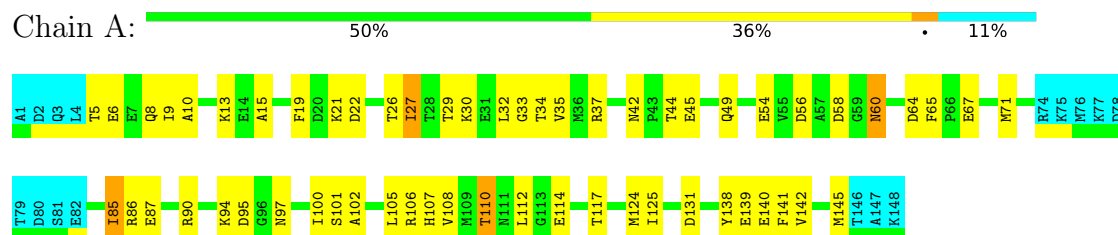
4.2.119 Score per residue for model 119

- Molecule 1: Calmodulin



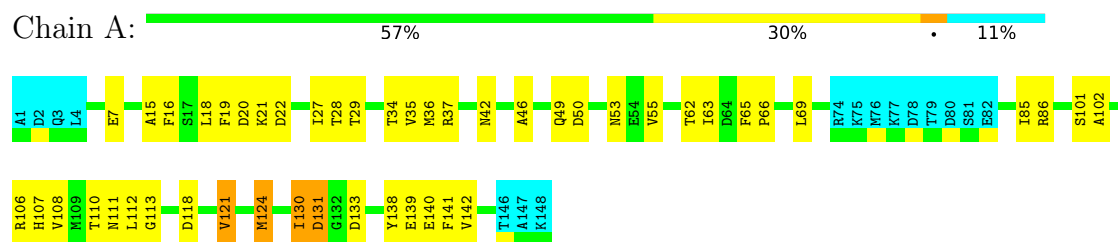
4.2.120 Score per residue for model 120

- Molecule 1: Calmodulin



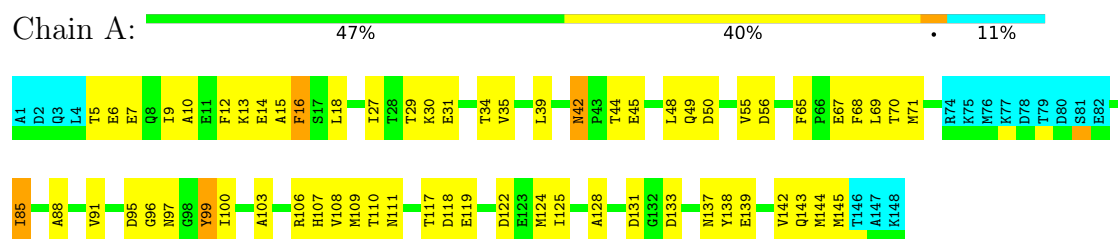
4.2.121 Score per residue for model 121

- Molecule 1: Calmodulin



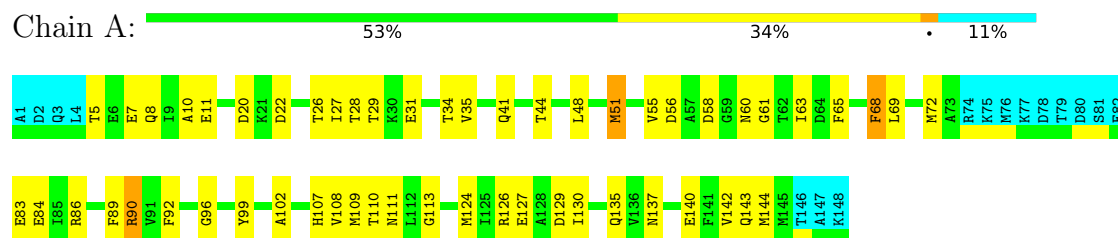
4.2.122 Score per residue for model 122

- Molecule 1: Calmodulin



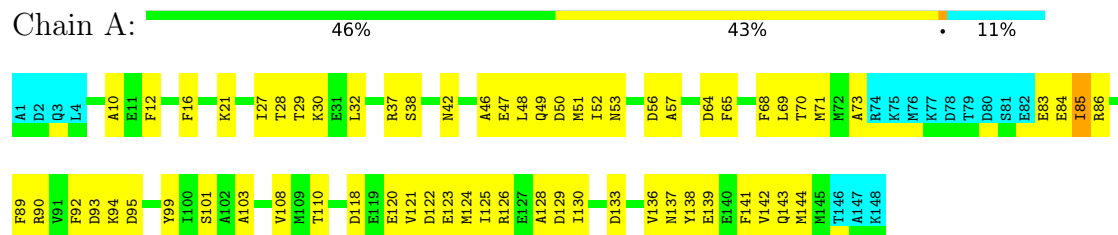
4.2.123 Score per residue for model 123

- Molecule 1: Calmodulin



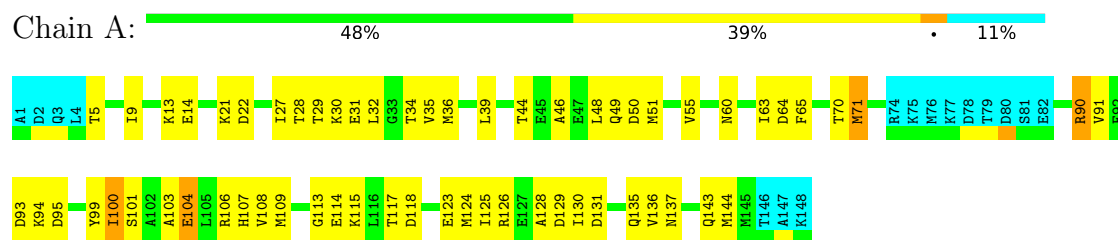
4.2.124 Score per residue for model 124

- Molecule 1: Calmodulin



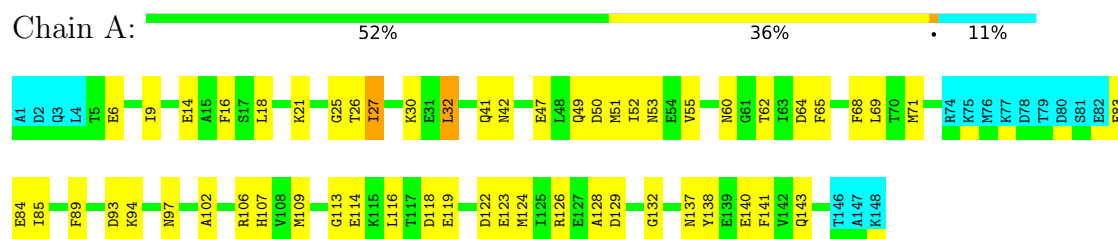
4.2.125 Score per residue for model 125

- Molecule 1: Calmodulin



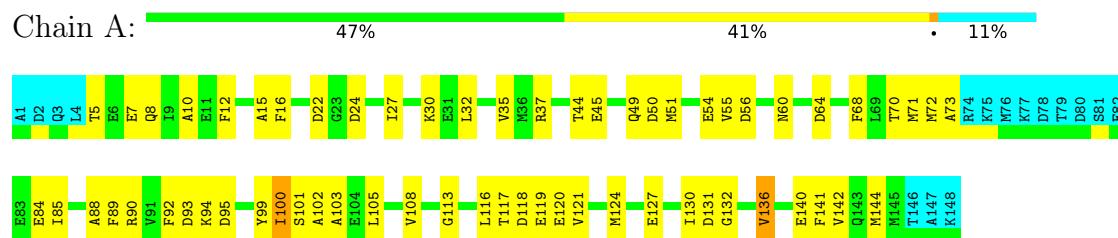
4.2.126 Score per residue for model 126

- Molecule 1: Calmodulin



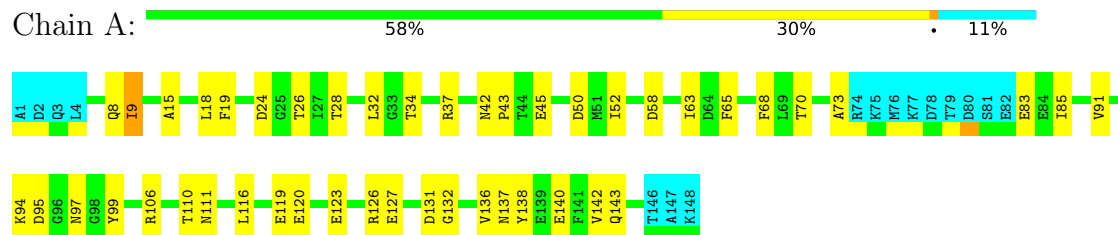
4.2.127 Score per residue for model 127

- Molecule 1: Calmodulin



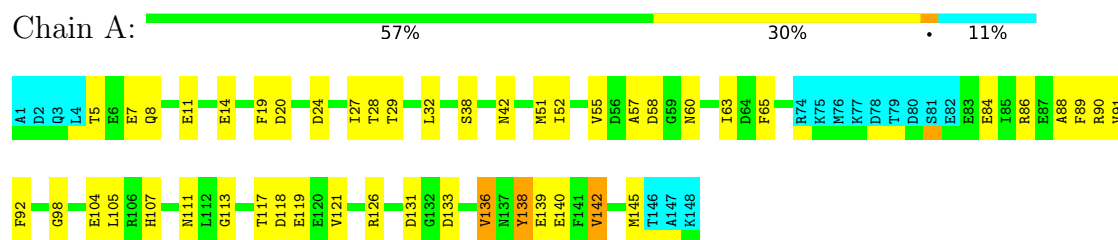
4.2.128 Score per residue for model 128

- Molecule 1: Calmodulin



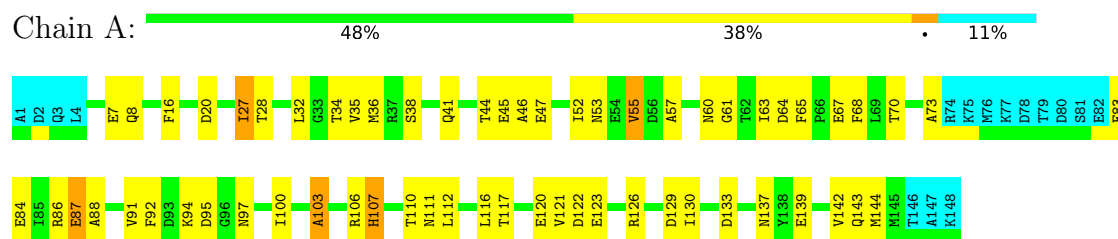
4.2.129 Score per residue for model 129

- Molecule 1: Calmodulin



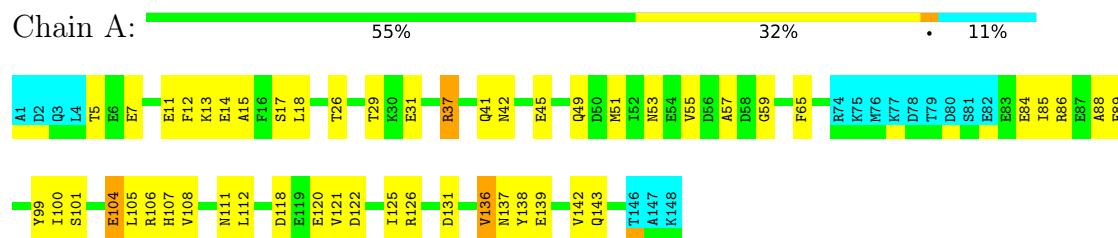
4.2.130 Score per residue for model 130

- Molecule 1: Calmodulin



4.2.131 Score per residue for model 131

- Molecule 1: Calmodulin



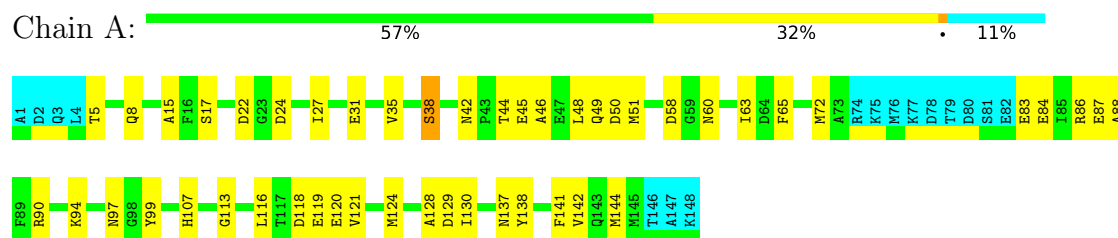
4.2.132 Score per residue for model 132

- Molecule 1: Calmodulin



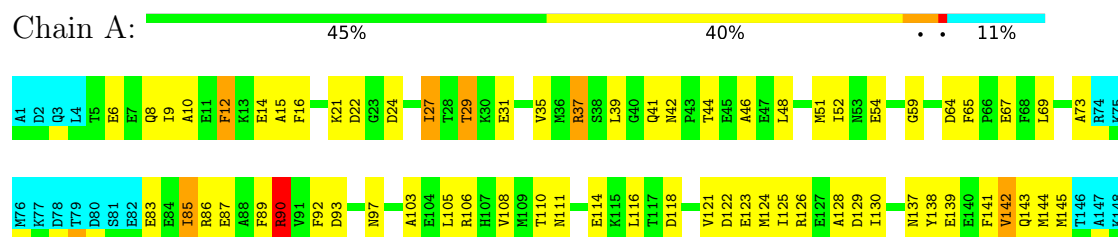
4.2.133 Score per residue for model 133

- Molecule 1: Calmodulin



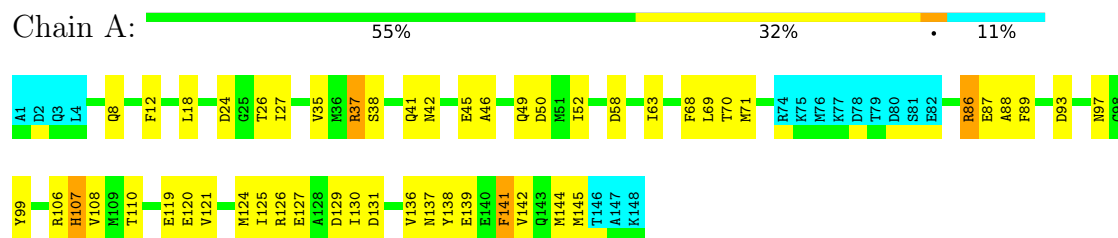
4.2.134 Score per residue for model 134

- Molecule 1: Calmodulin



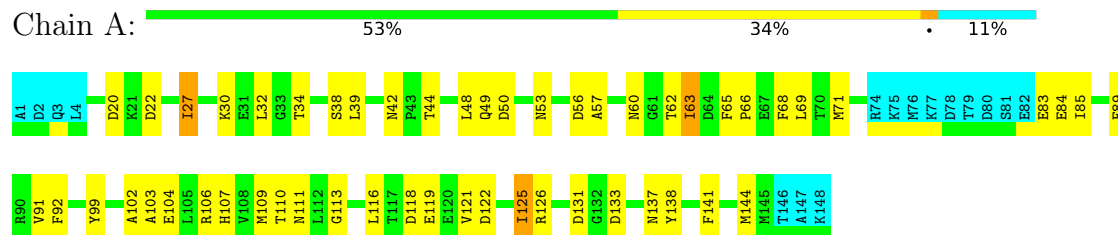
4.2.135 Score per residue for model 135

- Molecule 1: Calmodulin



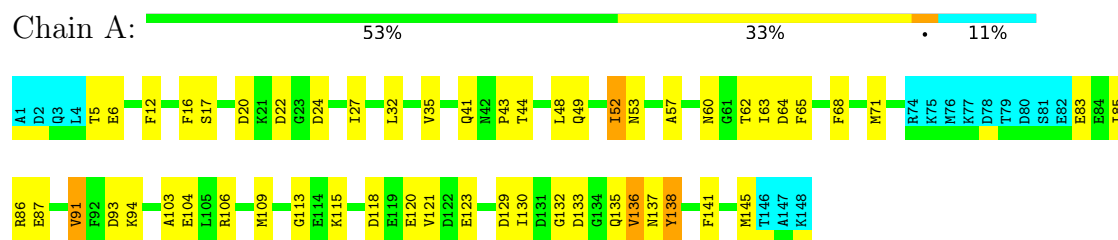
4.2.136 Score per residue for model 136

- Molecule 1: Calmodulin



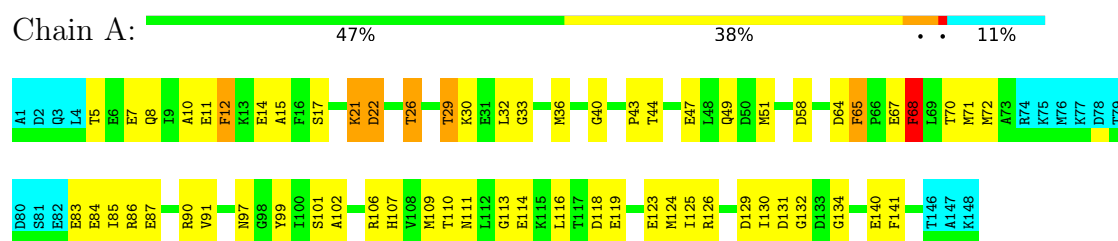
4.2.137 Score per residue for model 137

- Molecule 1: Calmodulin



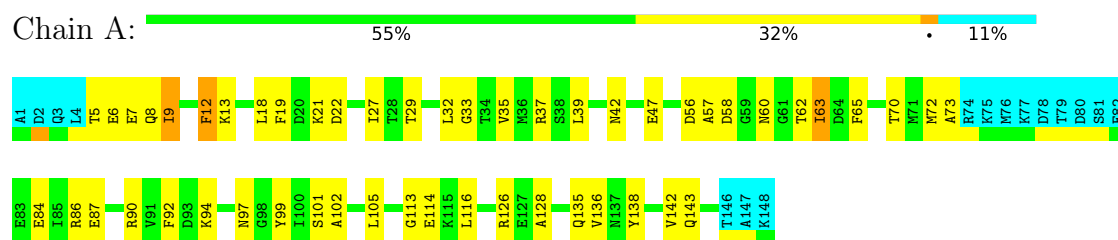
4.2.138 Score per residue for model 138

- Molecule 1: Calmodulin



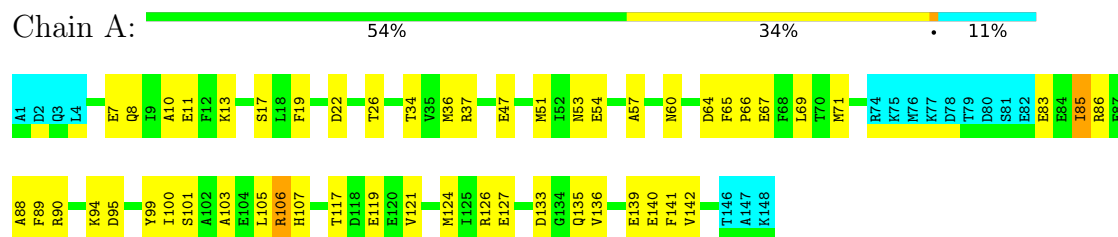
4.2.139 Score per residue for model 139

- Molecule 1: Calmodulin



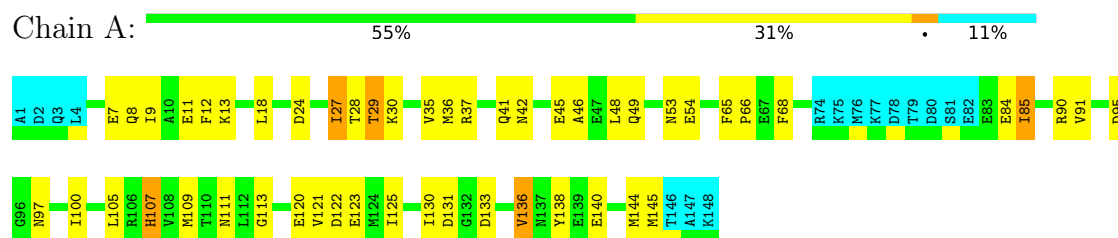
4.2.140 Score per residue for model 140

- Molecule 1: Calmodulin



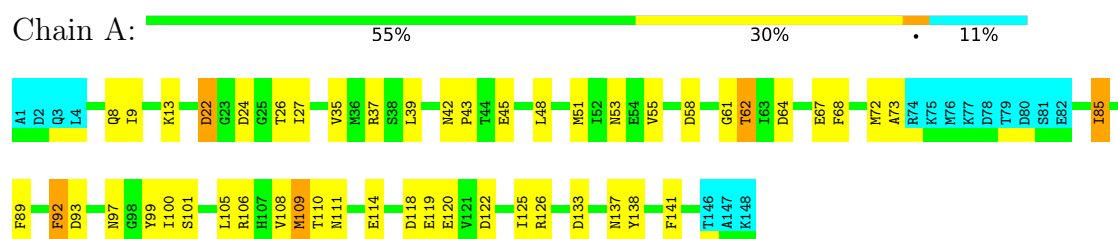
4.2.141 Score per residue for model 141

- Molecule 1: Calmodulin



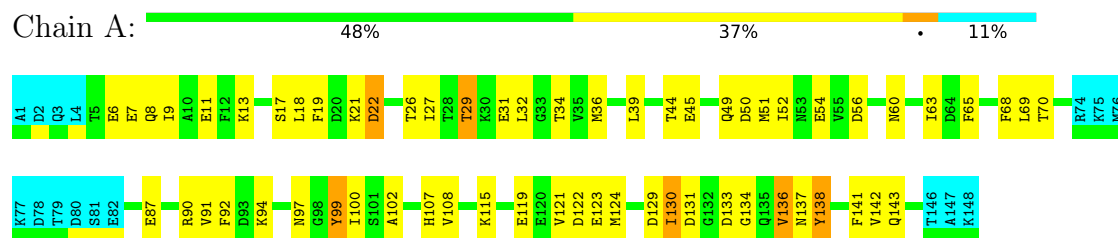
4.2.142 Score per residue for model 142

- Molecule 1: Calmodulin



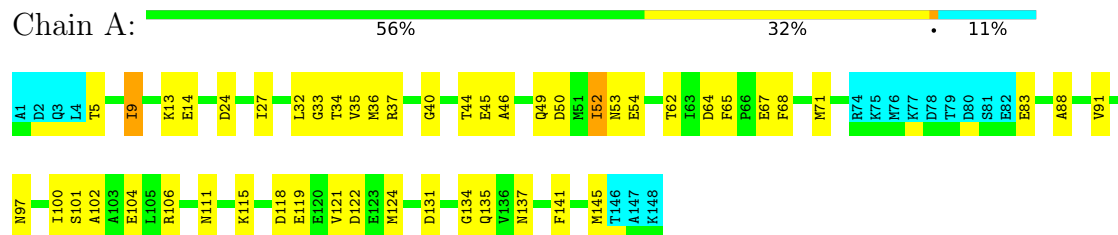
4.2.143 Score per residue for model 143

- Molecule 1: Calmodulin



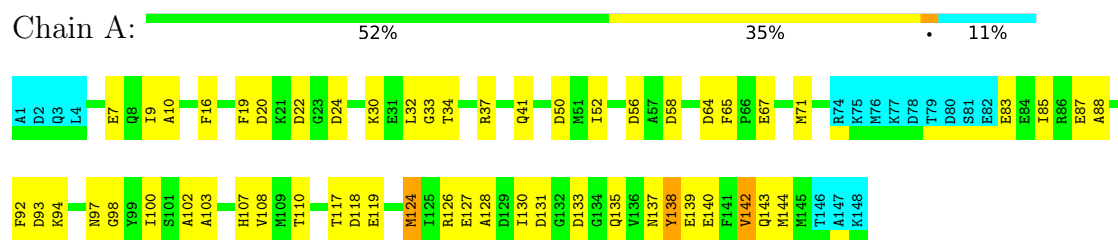
4.2.144 Score per residue for model 144

- Molecule 1: Calmodulin



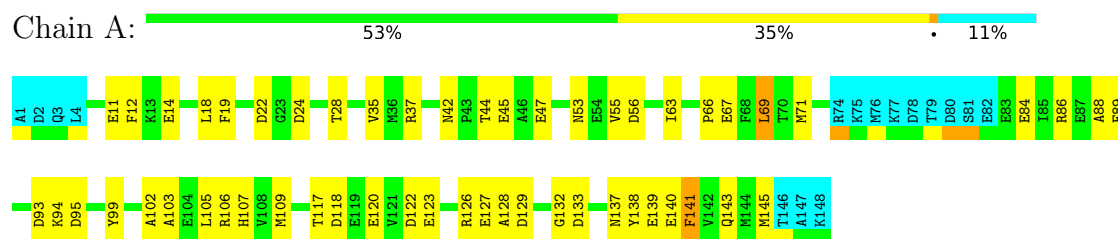
4.2.145 Score per residue for model 145

- Molecule 1: Calmodulin



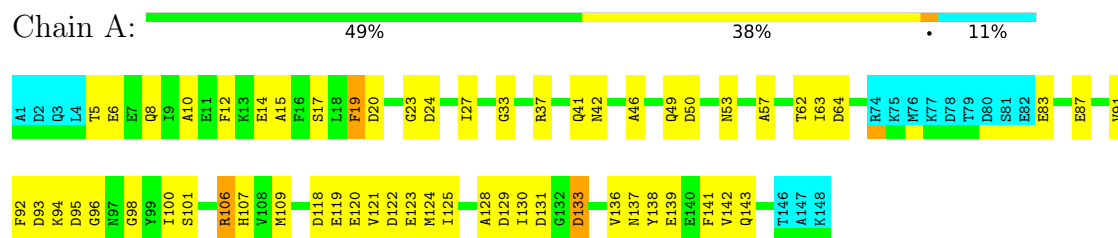
4.2.146 Score per residue for model 146

- Molecule 1: Calmodulin



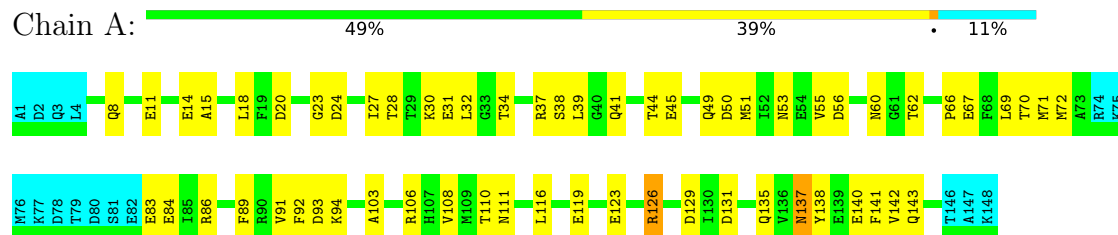
4.2.147 Score per residue for model 147

- Molecule 1: Calmodulin



4.2.148 Score per residue for model 148

- Molecule 1: Calmodulin



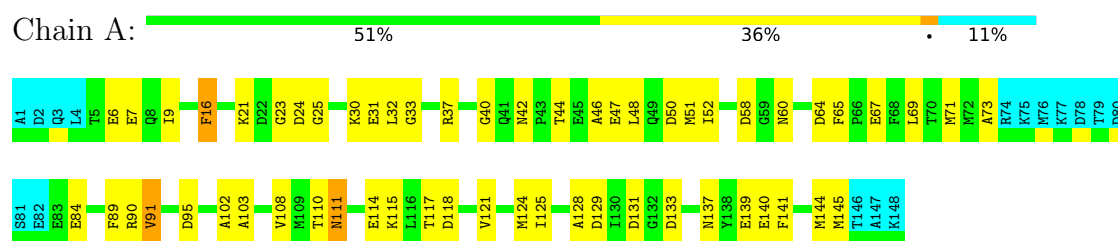
4.2.149 Score per residue for model 149

- Molecule 1: Calmodulin



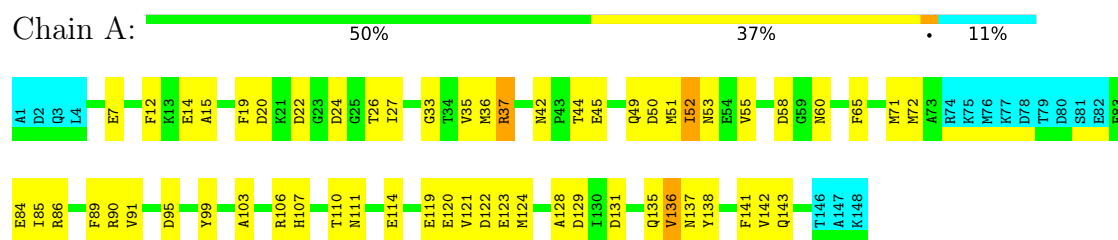
4.2.150 Score per residue for model 150

- Molecule 1: Calmodulin



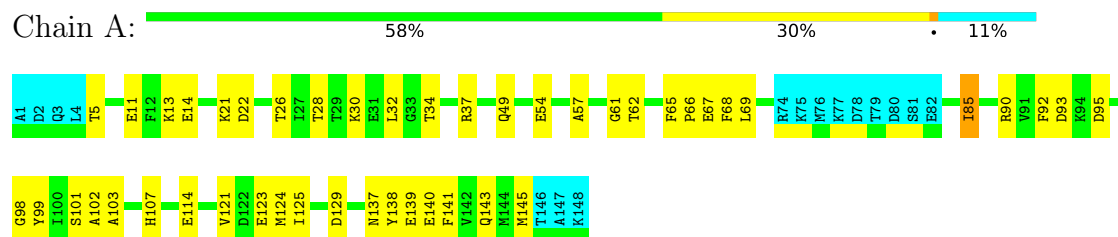
4.2.151 Score per residue for model 151

- Molecule 1: Calmodulin



4.2.152 Score per residue for model 152

- Molecule 1: Calmodulin



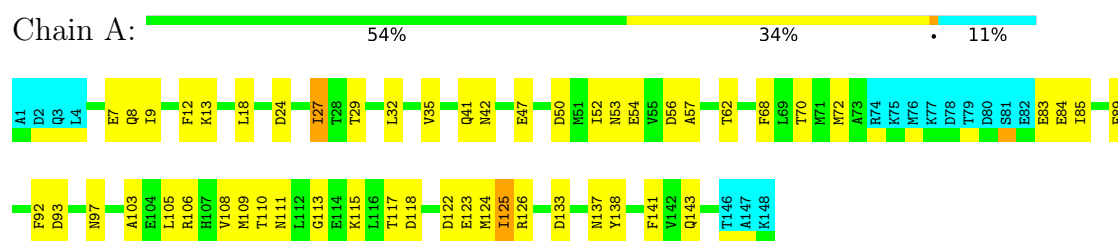
4.2.153 Score per residue for model 153

- Molecule 1: Calmodulin



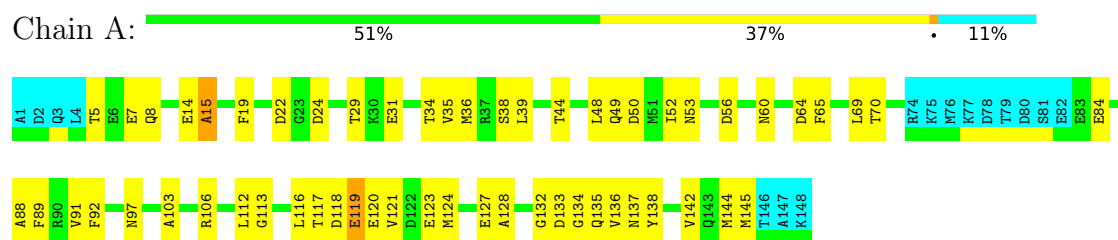
4.2.154 Score per residue for model 154

- Molecule 1: Calmodulin



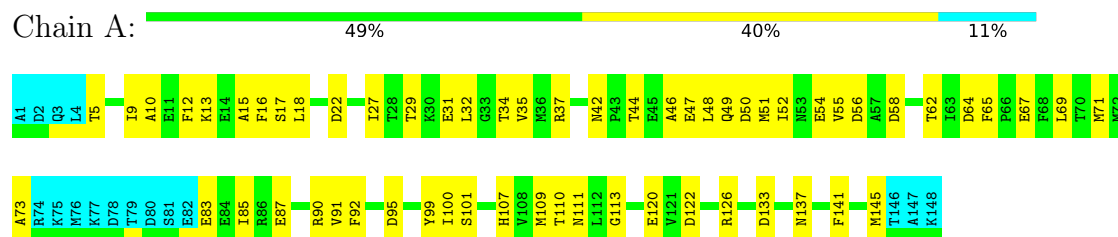
4.2.155 Score per residue for model 155

- Molecule 1: Calmodulin



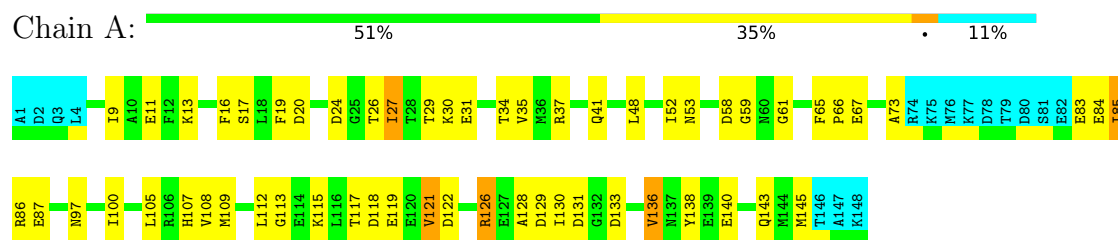
4.2.156 Score per residue for model 156

- Molecule 1: Calmodulin



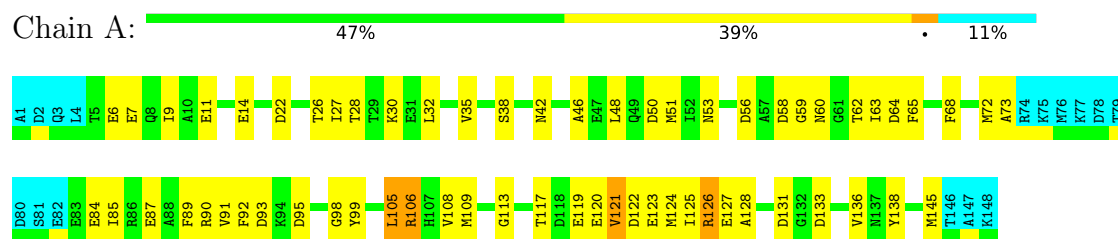
4.2.157 Score per residue for model 157 (medoid)

- Molecule 1: Calmodulin



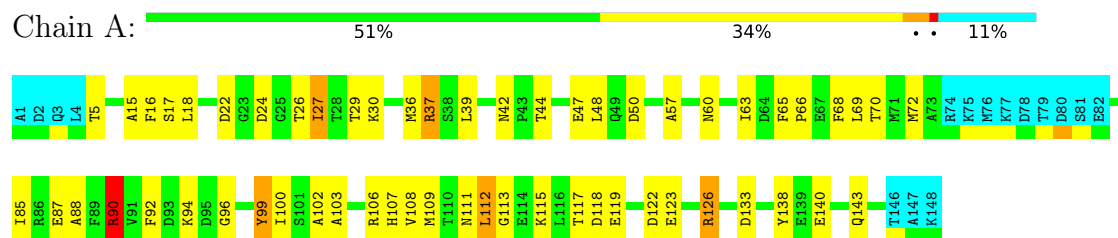
4.2.158 Score per residue for model 158

- Molecule 1: Calmodulin



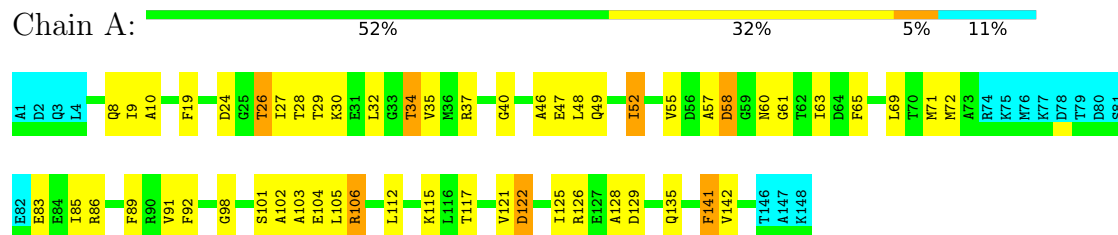
4.2.159 Score per residue for model 159

- Molecule 1: Calmodulin



4.2.160 Score per residue for model 160

- Molecule 1: Calmodulin



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	1.43±0.01	0±0/1052 (0.0± 0.0%)	2.53±0.07	78±10/1416 (5.5± 0.7%)
All	All	1.43	2/168320 (0.0%)	2.53	12559/226560 (5.5%)

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

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	130	ILE	CA-CB	-5.04	1.50	1.55	80	2

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	133	ASP	CA-CB-CG	14.79	127.39	112.60	159	68
1	A	137	ASN	CA-CB-CG	13.34	125.94	112.60	147	61
1	A	10	ALA	N-CA-C	13.07	126.79	111.11	113	19
1	A	111	ASN	CA-CB-CG	-12.88	99.72	112.60	99	33
1	A	54	GLU	N-CA-C	12.87	125.04	111.14	76	22
1	A	22	ASP	CA-CB-CG	12.71	125.31	112.60	8	33
1	A	118	ASP	N-CA-C	12.69	126.69	111.33	58	31
1	A	65	PHE	O-C-N	-12.67	110.37	120.38	58	58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	53	ASN	CA-CB-CG	-12.38	100.22	112.60	55	26
1	A	66	PRO	CA-C-N	12.36	137.25	120.44	56	21
1	A	66	PRO	C-N-CA	12.36	137.25	120.44	56	21
1	A	106	ARG	CA-C-N	12.11	136.51	120.28	154	37
1	A	106	ARG	C-N-CA	12.11	136.51	120.28	154	37
1	A	121	VAL	N-CA-C	11.99	121.93	110.42	33	32
1	A	100	ILE	N-CA-C	11.89	124.26	107.37	140	8
1	A	143	GLN	N-CA-C	11.86	124.21	111.28	1	12
1	A	111	ASN	CA-C-N	11.58	135.94	120.65	95	37
1	A	111	ASN	C-N-CA	11.58	135.94	120.65	95	37
1	A	107	HIS	CA-C-N	11.56	135.12	120.56	18	24
1	A	107	HIS	C-N-CA	11.56	135.12	120.56	18	24
1	A	65	PHE	CA-C-O	-11.47	108.08	118.63	134	46
1	A	51	MET	CA-C-N	11.45	135.22	120.56	104	45
1	A	51	MET	C-N-CA	11.45	135.22	120.56	104	45
1	A	130	ILE	N-CA-C	11.33	122.17	110.62	83	25
1	A	58	ASP	N-CA-C	11.30	124.92	111.82	34	28
1	A	29	THR	CA-C-N	11.23	135.04	120.44	58	27
1	A	29	THR	C-N-CA	11.23	135.04	120.44	58	27
1	A	92	PHE	CA-CB-CG	11.22	125.02	113.80	129	27
1	A	128	ALA	N-CA-C	11.20	124.59	111.71	157	45
1	A	97	ASN	CA-CB-CG	11.18	123.78	112.60	8	48
1	A	103	ALA	N-CA-C	11.15	123.51	111.36	7	46
1	A	100	ILE	N-CA-CB	11.08	124.89	111.60	147	30
1	A	140	GLU	CA-C-N	11.07	134.83	120.44	1	34
1	A	140	GLU	C-N-CA	11.07	134.83	120.44	1	34
1	A	125	ILE	N-CA-C	11.02	123.19	110.62	131	22
1	A	144	MET	CA-C-O	-10.96	108.79	120.63	28	10
1	A	123	GLU	CA-C-N	10.96	134.69	120.44	62	32
1	A	123	GLU	C-N-CA	10.96	134.69	120.44	62	32
1	A	131	ASP	N-CA-C	10.96	125.77	111.75	28	44
1	A	118	ASP	CA-CB-CG	-10.95	101.65	112.60	157	30
1	A	6	GLU	N-CA-C	10.94	124.29	111.71	105	26
1	A	141	PHE	N-CA-C	-10.82	99.45	111.14	98	30
1	A	131	ASP	CA-CB-CG	-10.69	101.91	112.60	46	20
1	A	107	HIS	CA-CB-CG	10.65	124.45	113.80	74	31
1	A	90	ARG	CA-C-N	10.64	134.18	120.56	134	33
1	A	90	ARG	C-N-CA	10.64	134.18	120.56	134	33
1	A	68	PHE	CA-CB-CG	-10.64	103.16	113.80	119	25
1	A	32	LEU	CA-C-N	10.63	131.74	119.94	84	52
1	A	32	LEU	C-N-CA	10.63	131.74	119.94	84	52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	117	THR	CA-C-N	10.60	134.49	120.28	158	31
1	A	117	THR	C-N-CA	10.60	134.49	120.28	158	31
1	A	42	ASN	CA-CB-CG	-10.59	102.01	112.60	84	32
1	A	69	LEU	N-CA-C	10.59	122.82	111.28	61	16
1	A	38	SER	O-C-N	-10.55	110.12	122.15	148	5
1	A	97	ASN	OD1-CG-ND2	-10.54	112.06	122.60	142	29
1	A	144	MET	N-CA-C	10.48	122.29	111.07	80	20
1	A	122	ASP	CA-CB-CG	-10.48	102.12	112.60	39	18
1	A	94	LYS	O-C-N	-10.47	111.29	122.07	137	9
1	A	30	LYS	N-CA-C	10.37	122.59	111.28	52	18
1	A	138	TYR	CA-C-O	10.37	131.71	120.82	40	6
1	A	42	ASN	O-C-N	-10.36	111.93	121.36	121	43
1	A	105	LEU	N-CA-C	10.35	122.56	111.28	109	17
1	A	110	THR	N-CA-C	10.35	123.53	111.11	145	17
1	A	27	ILE	N-CA-CB	10.32	124.91	111.90	62	65
1	A	26	THR	CA-C-N	10.28	136.77	123.10	67	10
1	A	26	THR	C-N-CA	10.28	136.77	123.10	67	10
1	A	127	GLU	N-CA-C	10.27	123.52	111.71	33	13
1	A	112	LEU	O-C-N	-10.25	111.37	122.03	109	8
1	A	106	ARG	N-CA-C	10.25	122.21	111.14	54	17
1	A	127	GLU	CA-C-N	10.25	133.76	120.44	91	20
1	A	127	GLU	C-N-CA	10.25	133.76	120.44	91	20
1	A	124	MET	N-CA-C	10.21	121.99	111.07	6	26
1	A	89	PHE	CA-C-O	10.20	131.57	120.24	94	11
1	A	53	ASN	OD1-CG-ND2	-10.19	112.41	122.60	101	13
1	A	85	ILE	CA-C-N	10.19	133.69	120.44	28	19
1	A	85	ILE	C-N-CA	10.19	133.69	120.44	28	19
1	A	83	GLU	N-CA-C	10.19	123.43	111.71	7	29
1	A	143	GLN	CA-C-N	10.18	134.28	120.54	11	37
1	A	143	GLN	C-N-CA	10.18	134.28	120.54	11	37
1	A	33	GLY	N-CA-C	10.17	125.23	112.83	150	12
1	A	137	ASN	OD1-CG-ND2	-10.14	112.46	122.60	63	16
1	A	44	THR	CA-C-N	10.14	134.03	120.65	27	30
1	A	44	THR	C-N-CA	10.14	134.03	120.65	27	30
1	A	63	ILE	N-CA-CB	10.13	123.21	111.66	115	23
1	A	73	ALA	CA-C-N	10.13	134.87	120.79	156	18
1	A	73	ALA	C-N-CA	10.13	134.87	120.79	156	18
1	A	85	ILE	N-CA-CB	10.11	122.38	110.55	158	18
1	A	102	ALA	CA-C-N	10.09	134.82	120.79	95	23
1	A	102	ALA	C-N-CA	10.09	134.82	120.79	95	23
1	A	101	SER	O-C-N	-10.09	111.76	123.06	100	17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	60	ASN	CA-CB-CG	10.09	122.69	112.60	13	31
1	A	87	GLU	N-CA-C	10.07	123.29	111.71	58	16
1	A	67	GLU	N-CA-C	10.07	121.94	110.97	100	22
1	A	86	ARG	N-CA-C	10.07	123.29	111.71	82	25
1	A	129	ASP	CA-CB-CG	-10.07	102.53	112.60	4	38
1	A	6	GLU	CA-C-N	10.05	133.51	120.44	65	30
1	A	6	GLU	C-N-CA	10.05	133.51	120.44	65	30
1	A	71	MET	CA-C-N	10.01	133.69	120.28	23	23
1	A	71	MET	C-N-CA	10.01	133.69	120.28	23	23
1	A	89	PHE	CA-CB-CG	-10.00	103.80	113.80	36	31
1	A	18	LEU	CA-C-N	9.99	134.48	120.29	119	8
1	A	18	LEU	C-N-CA	9.99	134.48	120.29	119	8
1	A	125	ILE	CA-C-N	9.98	133.66	120.28	72	35
1	A	125	ILE	C-N-CA	9.98	133.66	120.28	72	35
1	A	124	MET	CA-C-N	9.97	133.46	120.60	133	51
1	A	124	MET	C-N-CA	9.97	133.46	120.60	133	51
1	A	12	PHE	CA-CB-CG	-9.97	103.83	113.80	78	21
1	A	49	GLN	CA-C-N	9.97	133.63	120.28	18	36
1	A	49	GLN	C-N-CA	9.97	133.63	120.28	18	36
1	A	145	MET	CA-C-N	9.96	135.84	120.89	157	18
1	A	145	MET	C-N-CA	9.96	135.84	120.89	157	18
1	A	12	PHE	CA-C-N	9.93	133.59	120.28	29	33
1	A	12	PHE	C-N-CA	9.93	133.59	120.28	29	33
1	A	9	ILE	N-CA-C	-9.92	100.18	111.00	118	15
1	A	92	PHE	N-CA-C	9.92	121.69	111.07	80	19
1	A	91	VAL	N-CA-C	-9.91	102.23	111.45	1	16
1	A	36	MET	CA-C-N	9.89	133.71	120.65	143	12
1	A	36	MET	C-N-CA	9.89	133.71	120.65	143	12
1	A	11	GLU	CA-C-N	9.87	133.51	120.28	33	23
1	A	11	GLU	C-N-CA	9.87	133.51	120.28	33	23
1	A	87	GLU	O-C-N	-9.84	111.69	122.12	65	21
1	A	104	GLU	O-C-N	-9.79	110.98	122.15	38	15
1	A	56	ASP	CA-CB-CG	9.79	122.39	112.60	51	27
1	A	67	GLU	CA-C-N	9.79	133.79	120.38	140	47
1	A	67	GLU	C-N-CA	9.79	133.79	120.38	140	47
1	A	123	GLU	O-C-N	-9.78	111.00	122.15	47	10
1	A	108	VAL	N-CA-CB	9.76	125.22	110.58	35	15
1	A	42	ASN	CA-C-O	-9.74	111.36	121.29	35	13
1	A	35	VAL	O-C-N	-9.73	112.43	121.87	61	9
1	A	8	GLN	OE1-CD-NE2	-9.72	112.88	122.60	117	19
1	A	50	ASP	CA-CB-CG	-9.71	102.89	112.60	47	24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	57	ALA	CA-C-N	9.71	135.07	120.31	152	16
1	A	57	ALA	C-N-CA	9.71	135.07	120.31	152	16
1	A	144	MET	CA-C-N	9.70	133.28	120.28	74	10
1	A	144	MET	C-N-CA	9.70	133.28	120.28	74	10
1	A	8	GLN	CA-C-N	9.70	132.97	120.56	134	31
1	A	8	GLN	C-N-CA	9.70	132.97	120.56	134	31
1	A	95	ASP	N-CA-C	9.67	121.82	111.28	130	29
1	A	107	HIS	CG-CD2-NE2	9.66	116.86	107.20	111	27
1	A	70	THR	N-CA-C	9.66	121.81	111.28	75	15
1	A	29	THR	CA-C-O	9.65	131.06	120.63	46	5
1	A	95	ASP	CA-CB-CG	9.64	122.24	112.60	83	28
1	A	102	ALA	N-CA-C	9.64	124.88	112.34	90	44
1	A	32	LEU	CA-C-O	9.63	130.94	120.82	120	11
1	A	73	ALA	O-C-N	-9.62	111.92	122.12	89	13
1	A	24	ASP	CA-CB-CG	9.62	122.22	112.60	11	42
1	A	136	VAL	CB-CA-C	9.57	124.79	110.63	3	16
1	A	60	ASN	N-CA-C	9.55	125.08	113.23	153	19
1	A	64	ASP	CA-CB-CG	9.55	122.15	112.60	29	25
1	A	39	LEU	CA-C-N	9.54	136.37	120.91	85	11
1	A	39	LEU	C-N-CA	9.54	136.37	120.91	85	11
1	A	143	GLN	OE1-CD-NE2	-9.51	113.09	122.60	101	14
1	A	35	VAL	CA-C-N	9.51	133.38	120.54	10	26
1	A	35	VAL	C-N-CA	9.51	133.38	120.54	10	26
1	A	71	MET	CA-C-O	9.49	130.49	120.42	73	11
1	A	41	GLN	O-C-N	-9.47	112.45	123.06	157	13
1	A	108	VAL	N-CA-C	9.46	120.27	110.62	123	29
1	A	31	GLU	CA-C-N	9.44	132.71	120.44	56	14
1	A	31	GLU	C-N-CA	9.44	132.71	120.44	56	14
1	A	38	SER	N-CA-C	9.43	121.56	111.28	42	17
1	A	9	ILE	CA-C-N	9.43	132.70	120.44	43	33
1	A	9	ILE	C-N-CA	9.43	132.70	120.44	43	33
1	A	31	GLU	N-CA-C	9.43	122.74	111.33	150	14
1	A	45	GLU	N-CA-C	9.43	121.64	111.36	107	23
1	A	17	SER	CA-C-N	9.43	133.68	120.29	103	16
1	A	17	SER	C-N-CA	9.43	133.68	120.29	103	16
1	A	7	GLU	CA-C-N	9.43	133.26	120.44	145	12
1	A	7	GLU	C-N-CA	9.43	133.26	120.44	145	12
1	A	137	ASN	CA-C-N	9.41	133.25	120.54	37	20
1	A	137	ASN	C-N-CA	9.41	133.25	120.54	37	20
1	A	101	SER	CA-C-N	9.41	133.25	120.54	160	11
1	A	101	SER	C-N-CA	9.41	133.25	120.54	160	11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	105	LEU	CA-C-N	9.40	133.22	120.44	104	9
1	A	105	LEU	C-N-CA	9.40	133.22	120.44	104	9
1	A	122	ASP	CA-C-N	9.40	132.66	120.44	36	26
1	A	122	ASP	C-N-CA	9.40	132.66	120.44	36	26
1	A	139	GLU	N-CA-C	9.39	121.52	111.28	40	15
1	A	28	THR	CA-C-N	9.38	133.20	120.54	74	33
1	A	28	THR	C-N-CA	9.38	133.20	120.54	74	33
1	A	94	LYS	CA-C-N	9.36	133.16	120.44	24	45
1	A	94	LYS	C-N-CA	9.36	133.16	120.44	24	45
1	A	88	ALA	N-CA-C	9.35	122.33	111.11	100	17
1	A	107	HIS	CE1-NE2-CD2	-9.33	99.67	109.00	111	38
1	A	55	VAL	N-CA-C	9.30	122.03	112.83	88	17
1	A	144	MET	O-C-N	-9.27	112.29	122.12	85	16
1	A	33	GLY	CA-C-N	9.27	134.72	120.82	29	23
1	A	33	GLY	C-N-CA	9.27	134.72	120.82	29	23
1	A	90	ARG	CD-NE-CZ	-9.25	111.45	124.40	16	4
1	A	20	ASP	CA-CB-CG	9.24	121.84	112.60	56	18
1	A	47	GLU	N-CA-C	9.24	120.95	111.07	140	10
1	A	37	ARG	NE-CZ-NH1	9.23	130.74	121.50	84	16
1	A	139	GLU	CA-C-N	9.23	133.03	120.38	124	25
1	A	139	GLU	C-N-CA	9.23	133.03	120.38	124	25
1	A	145	MET	N-CA-C	-9.23	101.78	113.23	120	13
1	A	128	ALA	N-CA-CB	-9.22	96.46	110.20	108	13
1	A	142	VAL	N-CA-CB	9.22	120.67	110.62	135	13
1	A	19	PHE	CA-C-O	9.22	130.40	120.90	48	7
1	A	60	ASN	OD1-CG-ND2	-9.19	113.41	122.60	50	20
1	A	50	ASP	CA-C-N	9.19	132.59	120.28	90	32
1	A	50	ASP	C-N-CA	9.19	132.59	120.28	90	32
1	A	69	LEU	CA-C-N	9.19	132.38	120.44	136	29
1	A	69	LEU	C-N-CA	9.19	132.38	120.44	136	29
1	A	102	ALA	O-C-N	-9.17	111.74	122.20	29	10
1	A	91	VAL	CA-C-N	9.15	132.54	120.28	63	16
1	A	91	VAL	C-N-CA	9.15	132.54	120.28	63	16
1	A	22	ASP	CA-C-N	9.15	136.56	121.00	47	13
1	A	22	ASP	C-N-CA	9.15	136.56	121.00	47	13
1	A	58	ASP	CA-CB-CG	-9.14	103.46	112.60	85	19
1	A	116	LEU	O-C-N	-9.14	112.70	122.94	93	17
1	A	30	LYS	CA-C-N	9.11	132.49	120.28	44	24
1	A	30	LYS	C-N-CA	9.11	132.49	120.28	44	24
1	A	27	ILE	O-C-N	-9.11	113.42	123.26	26	14
1	A	123	GLU	CA-C-O	9.10	130.53	119.79	10	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	86	ARG	NE-CZ-NH2	-9.09	111.02	119.20	5	14
1	A	110	THR	CA-C-N	9.09	132.65	120.65	120	16
1	A	110	THR	C-N-CA	9.09	132.65	120.65	120	16
1	A	94	LYS	N-CA-C	9.09	121.12	111.03	89	23
1	A	119	GLU	CA-C-N	9.09	132.65	120.65	90	31
1	A	119	GLU	C-N-CA	9.09	132.65	120.65	90	31
1	A	98	GLY	CA-C-O	9.07	129.20	118.86	96	17
1	A	85	ILE	CA-C-O	9.07	129.58	119.42	44	8
1	A	38	SER	N-CA-CB	9.07	124.33	110.28	43	10
1	A	120	GLU	N-CA-C	9.06	121.98	111.11	51	18
1	A	86	ARG	NE-CZ-NH1	9.05	130.56	121.50	102	14
1	A	13	LYS	N-CA-C	9.02	120.72	111.07	30	18
1	A	136	VAL	CA-CB-CG2	-9.00	95.10	110.40	26	7
1	A	37	ARG	NE-CZ-NH2	-9.00	111.10	119.20	34	16
1	A	52	ILE	N-CA-CB	8.99	121.07	110.55	8	16
1	A	65	PHE	CA-CB-CG	-8.98	104.82	113.80	76	17
1	A	92	PHE	N-CA-CB	8.96	123.39	110.13	98	8
1	A	112	LEU	N-CA-C	8.95	121.03	111.28	41	26
1	A	60	ASN	CA-C-N	8.94	134.08	123.44	41	13
1	A	60	ASN	C-N-CA	8.94	134.08	123.44	41	13
1	A	59	GLY	CA-C-N	8.91	132.94	120.29	84	6
1	A	59	GLY	C-N-CA	8.91	132.94	120.29	84	6
1	A	88	ALA	O-C-N	-8.89	111.33	122.27	56	13
1	A	136	VAL	O-C-N	-8.89	113.78	123.20	67	20
1	A	15	ALA	O-C-N	-8.87	112.72	122.12	9	10
1	A	46	ALA	N-CA-C	8.86	121.89	111.71	47	21
1	A	19	PHE	CA-CB-CG	-8.85	104.95	113.80	92	25
1	A	13	LYS	O-C-N	-8.84	112.96	122.07	58	14
1	A	48	LEU	CA-C-N	8.83	132.11	120.28	95	22
1	A	48	LEU	C-N-CA	8.83	132.11	120.28	95	22
1	A	55	VAL	O-C-N	-8.83	111.53	122.57	110	9
1	A	107	HIS	CA-C-O	8.82	129.90	120.55	54	11
1	A	50	ASP	O-C-N	-8.81	112.78	122.12	122	12
1	A	126	ARG	O-C-N	-8.80	112.79	122.12	41	10
1	A	138	TYR	CA-C-N	8.80	132.07	120.28	60	10
1	A	138	TYR	C-N-CA	8.80	132.07	120.28	60	10
1	A	142	VAL	N-CA-C	-8.79	102.27	110.53	5	18
1	A	42	ASN	OD1-CG-ND2	-8.79	113.81	122.60	158	21
1	A	49	GLN	N-CA-C	8.77	121.80	111.71	141	27
1	A	130	ILE	CA-C-O	8.77	129.94	120.47	157	8
1	A	142	VAL	CA-C-N	8.76	131.83	120.44	29	16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	142	VAL	C-N-CA	8.76	131.83	120.44	29	16
1	A	21	LYS	O-C-N	-8.76	112.63	122.09	40	4
1	A	97	ASN	N-CA-C	8.75	123.52	113.02	21	23
1	A	20	ASP	N-CA-C	8.74	121.74	109.15	111	5
1	A	84	GLU	CA-C-N	8.74	132.83	120.42	34	26
1	A	84	GLU	C-N-CA	8.74	132.83	120.42	34	26
1	A	110	THR	O-C-N	-8.73	112.87	122.12	83	8
1	A	109	MET	O-C-N	-8.72	112.87	122.12	8	9
1	A	63	ILE	O-C-N	-8.72	113.35	123.03	160	11
1	A	111	ASN	OD1-CG-ND2	-8.70	113.90	122.60	24	17
1	A	126	ARG	N-CA-C	8.69	120.75	111.28	134	16
1	A	27	ILE	N-CA-C	8.68	120.27	108.11	130	3
1	A	55	VAL	CA-C-O	8.68	128.47	119.35	111	11
1	A	35	VAL	CB-CA-C	-8.67	100.88	111.97	71	19
1	A	65	PHE	N-CA-C	8.66	125.48	113.45	153	26
1	A	20	ASP	O-C-N	-8.66	112.05	122.96	151	14
1	A	129	ASP	O-C-N	-8.64	112.77	123.05	1	6
1	A	106	ARG	NE-CZ-NH1	8.64	130.14	121.50	128	16
1	A	64	ASP	O-C-N	-8.64	110.32	122.76	96	23
1	A	16	PHE	CA-CB-CG	8.63	122.43	113.80	60	22
1	A	13	LYS	CA-C-N	8.63	131.84	120.28	154	24
1	A	13	LYS	C-N-CA	8.63	131.84	120.28	154	24
1	A	16	PHE	O-C-N	-8.61	112.80	122.09	126	14
1	A	72	MET	CA-C-O	-8.60	111.84	120.70	34	7
1	A	123	GLU	N-CA-C	8.59	121.59	111.71	9	23
1	A	88	ALA	CA-C-N	8.58	131.59	120.44	35	24
1	A	88	ALA	C-N-CA	8.58	131.59	120.44	35	24
1	A	29	THR	N-CA-C	8.57	121.70	111.33	98	16
1	A	99	TYR	CA-C-O	8.57	130.52	120.66	107	12
1	A	120	GLU	CA-C-N	8.57	132.59	120.42	135	37
1	A	120	GLU	C-N-CA	8.57	132.59	120.42	135	37
1	A	138	TYR	N-CA-C	8.57	121.76	111.82	128	10
1	A	121	VAL	CA-C-N	8.55	131.73	120.28	133	35
1	A	121	VAL	C-N-CA	8.55	131.73	120.28	133	35
1	A	72	MET	O-C-N	-8.54	112.41	122.15	77	12
1	A	121	VAL	CA-C-O	8.54	129.83	120.95	132	9
1	A	55	VAL	CB-CA-C	-8.53	101.58	110.88	42	4
1	A	57	ALA	N-CA-C	8.53	121.81	111.40	23	9
1	A	106	ARG	NE-CZ-NH2	-8.52	111.53	119.20	82	21
1	A	98	GLY	N-CA-C	-8.50	103.22	115.64	58	1
1	A	119	GLU	N-CA-C	8.49	120.23	110.97	114	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	144	MET	CG-SD-CE	-8.48	82.25	100.90	85	13
1	A	129	ASP	CA-C-N	8.48	131.24	120.56	5	20
1	A	129	ASP	C-N-CA	8.48	131.24	120.56	5	20
1	A	141	PHE	O-C-N	-8.46	112.95	122.09	134	14
1	A	36	MET	O-C-N	-8.46	113.35	122.07	38	14
1	A	22	ASP	N-CA-C	8.46	120.58	111.36	104	6
1	A	100	ILE	CB-CA-C	-8.46	100.51	111.25	7	13
1	A	20	ASP	CA-C-N	8.43	131.91	120.44	157	10
1	A	20	ASP	C-N-CA	8.43	131.91	120.44	157	10
1	A	90	ARG	N-CA-C	8.43	120.55	111.36	82	13
1	A	33	GLY	O-C-N	-8.41	114.01	122.17	14	9
1	A	103	ALA	CA-C-N	8.39	131.85	120.44	69	11
1	A	103	ALA	C-N-CA	8.39	131.85	120.44	69	11
1	A	115	LYS	CA-C-O	8.39	130.02	120.54	109	12
1	A	93	ASP	CA-CB-CG	8.38	120.98	112.60	52	17
1	A	73	ALA	N-CA-C	8.38	121.47	111.33	31	15
1	A	85	ILE	N-CA-C	8.37	118.40	110.53	98	14
1	A	106	ARG	CA-C-O	8.37	129.29	120.42	73	12
1	A	9	ILE	N-CA-CB	8.36	120.33	110.55	141	10
1	A	120	GLU	O-C-N	-8.34	112.64	122.15	1	12
1	A	135	GLN	OE1-CD-NE2	-8.34	114.26	122.60	106	18
1	A	128	ALA	O-C-N	-8.34	115.11	123.62	57	6
1	A	126	ARG	CA-C-N	8.33	132.12	120.29	28	9
1	A	126	ARG	C-N-CA	8.33	132.12	120.29	28	9
1	A	45	GLU	O-C-N	-8.33	112.66	122.15	131	8
1	A	100	ILE	CA-CB-CG2	-8.32	96.36	110.50	87	12
1	A	93	ASP	CA-C-O	8.31	130.51	120.62	83	9
1	A	114	GLU	O-C-N	-8.31	113.57	122.96	116	28
1	A	68	PHE	N-CA-C	-8.30	102.19	111.07	11	11
1	A	65	PHE	CA-C-N	8.30	128.26	119.05	152	22
1	A	65	PHE	C-N-CA	8.30	128.26	119.05	152	22
1	A	111	ASN	N-CA-C	8.30	120.32	111.28	97	13
1	A	99	TYR	O-C-N	-8.29	113.15	123.27	107	20
1	A	34	THR	N-CA-C	8.29	120.31	111.28	101	21
1	A	87	GLU	CB-CG-CD	8.28	126.68	112.60	81	2
1	A	34	THR	CA-C-N	8.27	131.27	120.60	157	31
1	A	34	THR	C-N-CA	8.27	131.27	120.60	157	31
1	A	40	GLY	CA-C-O	8.26	128.37	119.04	49	9
1	A	51	MET	CG-SD-CE	-8.26	82.74	100.90	75	6
1	A	53	ASN	CA-C-N	8.26	131.67	120.44	144	15
1	A	53	ASN	C-N-CA	8.26	131.67	120.44	144	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	10	ALA	CB-CA-C	8.25	123.67	110.96	49	4
1	A	25	GLY	O-C-N	-8.25	112.48	122.30	3	6
1	A	44	THR	O-C-N	-8.24	113.04	122.68	43	7
1	A	51	MET	O-C-N	-8.23	111.69	122.39	55	10
1	A	14	GLU	CA-C-O	8.23	129.44	119.97	122	10
1	A	104	GLU	N-CA-C	8.22	120.24	111.28	26	7
1	A	48	LEU	O-C-N	-8.20	113.43	122.12	58	19
1	A	63	ILE	CA-C-O	8.19	129.52	120.59	60	9
1	A	28	THR	CA-CB-OG1	8.17	121.85	109.60	112	11
1	A	49	GLN	OE1-CD-NE2	-8.17	114.43	122.60	22	13
1	A	124	MET	CG-SD-CE	-8.16	82.94	100.90	38	11
1	A	37	ARG	N-CA-C	8.16	120.17	111.28	52	11
1	A	61	GLY	CA-C-O	8.15	128.07	119.02	92	15
1	A	43	PRO	CA-C-O	-8.15	112.51	121.23	48	7
1	A	88	ALA	CA-C-O	-8.14	112.27	120.82	3	10
1	A	93	ASP	O-C-N	-8.13	113.73	123.16	127	15
1	A	92	PHE	O-C-N	-8.13	113.38	122.08	147	9
1	A	14	GLU	N-CA-C	8.13	120.22	111.36	108	19
1	A	110	THR	N-CA-CB	8.12	121.79	110.01	136	20
1	A	15	ALA	CA-C-N	8.12	131.49	120.44	133	47
1	A	15	ALA	C-N-CA	8.12	131.49	120.44	133	47
1	A	35	VAL	N-CA-C	8.12	118.89	110.36	125	16
1	A	61	GLY	O-C-N	-8.12	112.95	122.45	74	6
1	A	62	THR	N-CA-CB	8.12	122.63	110.29	132	8
1	A	97	ASN	CA-C-N	8.11	135.20	122.30	71	6
1	A	97	ASN	C-N-CA	8.11	135.20	122.30	71	6
1	A	10	ALA	O-C-N	-8.11	113.72	122.07	66	9
1	A	106	ARG	O-C-N	-8.10	113.53	122.12	99	8
1	A	109	MET	CA-C-O	-8.10	110.66	119.97	95	8
1	A	68	PHE	CA-C-N	8.08	131.45	120.54	108	24
1	A	68	PHE	C-N-CA	8.08	131.45	120.54	108	24
1	A	11	GLU	O-C-N	-8.08	113.75	122.07	4	11
1	A	113	GLY	CA-C-O	8.08	129.05	119.19	82	9
1	A	107	HIS	O-C-N	-8.07	111.51	122.33	18	22
1	A	34	THR	CB-CA-C	-8.07	97.13	110.85	155	4
1	A	140	GLU	CA-C-O	-8.05	112.37	120.82	63	18
1	A	114	GLU	CA-C-O	-8.04	111.42	120.43	98	6
1	A	42	ASN	N-CA-CB	-8.02	100.36	110.79	159	4
1	A	52	ILE	CA-C-N	8.02	132.09	120.38	45	34
1	A	52	ILE	C-N-CA	8.02	132.09	120.38	45	34
1	A	53	ASN	N-CA-CB	8.02	122.57	110.22	43	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	64	ASP	CA-C-N	8.01	131.00	120.26	98	14
1	A	64	ASP	C-N-CA	8.01	131.00	120.26	98	14
1	A	72	MET	CG-SD-CE	-8.01	83.28	100.90	23	13
1	A	100	ILE	O-C-N	-8.00	113.83	122.95	46	29
1	A	124	MET	O-C-N	8.00	130.31	122.07	138	10
1	A	142	VAL	O-C-N	-7.98	113.61	121.83	74	16
1	A	130	ILE	O-C-N	-7.97	114.10	121.91	5	6
1	A	70	THR	O-C-N	-7.97	113.67	122.12	32	14
1	A	120	GLU	N-CA-CB	7.96	121.61	110.07	91	4
1	A	29	THR	O-C-N	-7.96	113.69	122.12	95	8
1	A	139	GLU	CA-C-O	7.95	129.08	120.10	129	7
1	A	135	GLN	O-C-N	-7.95	114.16	123.22	85	14
1	A	47	GLU	CA-C-N	7.94	131.24	120.44	83	20
1	A	47	GLU	C-N-CA	7.94	131.24	120.44	83	20
1	A	121	VAL	O-C-N	-7.94	114.17	121.87	117	14
1	A	21	LYS	CA-C-N	7.93	130.76	120.44	138	20
1	A	21	LYS	C-N-CA	7.93	130.76	120.44	138	20
1	A	12	PHE	N-CA-C	7.92	120.00	111.36	29	16
1	A	26	THR	CA-CB-OG1	7.92	121.48	109.60	42	23
1	A	110	THR	CA-C-O	7.91	129.17	120.63	83	11
1	A	18	LEU	CA-C-O	7.91	129.12	119.31	78	5
1	A	14	GLU	CA-C-N	7.89	130.85	120.28	102	25
1	A	14	GLU	C-N-CA	7.89	130.85	120.28	102	25
1	A	43	PRO	CB-CA-C	-7.88	99.09	110.75	94	12
1	A	140	GLU	O-C-N	-7.85	113.80	122.12	149	12
1	A	125	ILE	O-C-N	-7.84	113.74	121.90	6	9
1	A	91	VAL	O-C-N	-7.84	114.26	121.87	118	5
1	A	89	PHE	N-CA-C	7.84	119.46	111.07	102	17
1	A	90	ARG	CA-C-O	7.83	129.13	119.11	89	15
1	A	134	GLY	CA-C-O	7.83	126.37	119.56	47	11
1	A	139	GLU	O-C-N	-7.82	113.83	122.12	146	10
1	A	84	GLU	N-CA-C	7.82	122.66	113.20	131	25
1	A	122	ASP	N-CA-C	7.82	120.79	111.33	49	15
1	A	15	ALA	N-CA-CB	7.82	121.61	110.12	19	3
1	A	16	PHE	CA-C-N	7.82	132.19	120.31	110	14
1	A	16	PHE	C-N-CA	7.82	132.19	120.31	110	14
1	A	141	PHE	CA-CB-CG	7.81	121.61	113.80	132	15
1	A	97	ASN	O-C-N	-7.80	111.97	122.43	55	4
1	A	7	GLU	CA-CB-CG	7.80	129.70	114.10	138	2
1	A	35	VAL	CA-CB-CG2	-7.80	97.14	110.40	50	3
1	A	70	THR	CA-C-N	7.80	131.36	120.29	78	25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	70	THR	C-N-CA	7.80	131.36	120.29	78	25
1	A	46	ALA	CA-C-O	-7.79	112.57	120.90	141	10
1	A	48	LEU	CA-C-O	7.78	129.17	121.00	116	7
1	A	128	ALA	CA-C-O	7.78	127.94	120.09	57	4
1	A	42	ASN	CA-C-N	7.77	127.92	120.31	111	21
1	A	42	ASN	C-N-CA	7.77	127.92	120.31	111	21
1	A	52	ILE	O-C-N	-7.77	114.30	121.91	60	15
1	A	105	LEU	CA-C-O	-7.76	112.32	120.55	131	13
1	A	15	ALA	N-CA-C	7.76	119.74	111.28	40	26
1	A	108	VAL	O-C-N	-7.75	113.04	122.18	66	12
1	A	140	GLU	CB-CG-CD	7.75	125.77	112.60	7	3
1	A	32	LEU	N-CA-CB	7.74	122.22	110.30	14	13
1	A	7	GLU	O-C-N	-7.73	114.05	122.09	8	8
1	A	16	PHE	N-CA-C	7.73	119.34	111.07	56	10
1	A	12	PHE	O-C-N	-7.73	113.93	122.12	58	5
1	A	24	ASP	CA-C-O	7.73	128.83	120.10	148	6
1	A	45	GLU	CA-C-O	7.73	128.74	120.55	41	10
1	A	131	ASP	CB-CA-C	-7.73	97.96	110.79	59	4
1	A	23	GLY	CA-C-N	7.72	131.26	120.29	147	6
1	A	23	GLY	C-N-CA	7.72	131.26	120.29	147	6
1	A	126	ARG	CA-C-O	-7.72	112.29	120.63	7	10
1	A	69	LEU	CB-CA-C	7.72	123.60	110.79	146	4
1	A	32	LEU	O-C-N	-7.71	112.79	122.27	107	14
1	A	93	ASP	CA-C-N	7.70	131.11	120.63	47	17
1	A	93	ASP	C-N-CA	7.70	131.11	120.63	47	17
1	A	107	HIS	N-CA-C	7.70	120.65	111.33	73	16
1	A	18	LEU	N-CA-C	7.70	119.67	111.28	139	14
1	A	66	PRO	N-CA-C	-7.69	103.50	114.18	6	8
1	A	36	MET	N-CA-C	7.69	121.59	111.75	8	16
1	A	126	ARG	N-CA-CB	7.68	122.31	109.78	119	5
1	A	45	GLU	CB-CG-CD	7.68	125.66	112.60	122	4
1	A	28	THR	N-CA-C	7.68	120.94	110.35	100	8
1	A	97	ASN	CB-CA-C	7.68	122.23	109.56	101	3
1	A	46	ALA	O-C-N	-7.67	113.40	122.15	88	10
1	A	23	GLY	CA-C-O	7.67	128.51	119.46	3	3
1	A	84	GLU	CA-C-O	7.67	128.68	120.55	69	15
1	A	143	GLN	CA-C-O	-7.67	112.29	120.42	109	5
1	A	73	ALA	CA-C-O	-7.67	112.29	120.42	84	9
1	A	22	ASP	N-CA-CB	7.66	121.50	110.16	63	6
1	A	27	ILE	CB-CA-C	-7.66	100.49	110.98	105	8
1	A	83	GLU	CA-C-N	7.66	131.95	120.31	140	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	83	GLU	C-N-CA	7.66	131.95	120.31	140	20
1	A	115	LYS	O-C-N	-7.65	114.33	123.13	157	6
1	A	119	GLU	CA-C-O	7.64	128.74	120.10	122	10
1	A	68	PHE	CA-C-O	7.64	128.76	119.97	73	13
1	A	60	ASN	O-C-N	-7.64	113.44	122.15	68	4
1	A	44	THR	CA-CB-OG1	7.63	121.05	109.60	28	9
1	A	67	GLU	CB-CG-CD	-7.63	99.63	112.60	40	15
1	A	114	GLU	N-CA-C	7.63	121.41	109.96	25	10
1	A	62	THR	CA-CB-OG1	7.63	121.04	109.60	82	17
1	A	131	ASP	O-C-N	-7.62	112.97	122.35	14	11
1	A	46	ALA	CA-C-N	7.61	130.79	120.44	133	10
1	A	46	ALA	C-N-CA	7.61	130.79	120.44	133	10
1	A	44	THR	N-CA-CB	7.61	124.79	111.55	134	26
1	A	83	GLU	O-C-N	7.60	131.62	122.27	35	7
1	A	72	MET	N-CA-C	7.60	120.63	111.82	54	19
1	A	126	ARG	CD-NE-CZ	7.59	135.03	124.40	103	5
1	A	94	LYS	CA-C-O	7.59	128.72	120.90	147	9
1	A	34	THR	N-CA-CB	7.58	121.06	110.07	4	11
1	A	145	MET	CG-SD-CE	-7.58	84.23	100.90	72	17
1	A	109	MET	N-CA-CB	7.57	122.02	110.28	95	5
1	A	51	MET	N-CA-C	7.57	120.42	111.71	8	16
1	A	141	PHE	CA-C-N	7.57	130.10	120.56	2	26
1	A	141	PHE	C-N-CA	7.57	130.10	120.56	2	26
1	A	71	MET	N-CA-C	7.57	119.17	111.07	66	15
1	A	107	HIS	ND1-CE1-NE2	7.57	115.97	108.40	58	28
1	A	13	LYS	CA-C-O	7.56	128.76	120.82	58	9
1	A	10	ALA	N-CA-CB	-7.56	98.57	110.28	71	5
1	A	56	ASP	CA-C-O	7.55	129.61	120.62	28	8
1	A	103	ALA	N-CA-CB	-7.55	99.02	110.12	115	5
1	A	11	GLU	N-CA-C	7.55	119.59	111.36	84	12
1	A	109	MET	CA-C-N	7.55	131.01	120.29	44	16
1	A	109	MET	C-N-CA	7.55	131.01	120.29	44	16
1	A	40	GLY	N-CA-C	7.55	126.70	115.08	144	3
1	A	101	SER	CA-C-O	-7.54	113.39	121.99	55	6
1	A	105	LEU	O-C-N	-7.54	112.99	122.27	47	12
1	A	112	LEU	CA-C-O	7.54	128.67	120.90	25	13
1	A	132	GLY	CA-C-O	-7.54	110.52	119.72	23	10
1	A	118	ASP	CA-C-N	7.54	130.99	120.29	78	18
1	A	118	ASP	C-N-CA	7.54	130.99	120.29	78	18
1	A	109	MET	CG-SD-CE	-7.54	84.32	100.90	149	18
1	A	87	GLU	CA-C-O	-7.54	112.91	120.82	13	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	26	THR	N-CA-C	-7.52	97.57	109.23	3	7
1	A	57	ALA	N-CA-CB	-7.52	99.32	110.53	50	7
1	A	121	VAL	N-CA-CB	7.52	118.85	110.51	153	12
1	A	5	THR	O-C-N	-7.51	114.44	123.16	80	18
1	A	57	ALA	CA-C-O	7.51	128.58	120.55	23	13
1	A	126	ARG	NE-CZ-NH1	7.50	129.00	121.50	97	15
1	A	39	LEU	O-C-N	-7.50	112.97	122.34	85	4
1	A	71	MET	N-CA-CB	7.49	120.85	109.91	68	15
1	A	59	GLY	CA-C-O	7.49	127.67	119.06	104	3
1	A	136	VAL	CA-CB-CG1	7.49	123.13	110.40	143	11
1	A	138	TYR	O-C-N	-7.49	114.18	122.12	148	20
1	A	45	GLU	CA-C-N	7.48	131.69	120.31	91	21
1	A	45	GLU	C-N-CA	7.48	131.69	120.31	91	21
1	A	85	ILE	CA-CB-CG1	7.48	123.12	110.40	90	25
1	A	18	LEU	N-CA-CB	7.48	120.85	110.01	135	6
1	A	140	GLU	N-CA-C	7.47	119.06	111.07	141	19
1	A	102	ALA	N-CA-CB	-7.47	97.62	110.32	26	2
1	A	92	PHE	CA-C-O	-7.46	111.39	119.97	41	10
1	A	84	GLU	N-CA-CB	7.46	120.82	110.01	124	9
1	A	5	THR	CA-C-O	7.45	130.04	121.47	156	7
1	A	130	ILE	CA-C-N	7.45	130.76	120.63	149	16
1	A	130	ILE	C-N-CA	7.45	130.76	120.63	149	16
1	A	11	GLU	CB-CA-C	-7.44	98.20	110.85	23	3
1	A	103	ALA	CA-C-O	7.44	128.36	120.70	127	16
1	A	109	MET	N-CA-C	7.43	120.44	111.82	69	14
1	A	5	THR	CA-C-N	7.43	130.56	120.38	122	22
1	A	5	THR	C-N-CA	7.43	130.56	120.38	122	22
1	A	5	THR	CA-CB-OG1	7.42	120.74	109.60	98	16
1	A	115	LYS	N-CA-CB	-7.42	102.04	110.35	144	2
1	A	96	GLY	O-C-N	-7.41	113.78	122.45	59	8
1	A	37	ARG	N-CA-CB	7.41	121.01	110.12	29	5
1	A	111	ASN	N-CA-CB	7.41	121.01	110.12	88	9
1	A	137	ASN	N-CA-CB	7.41	121.94	110.46	35	6
1	A	68	PHE	O-C-N	-7.41	114.27	122.12	97	12
1	A	24	ASP	CA-C-N	7.40	131.77	121.26	88	5
1	A	24	ASP	C-N-CA	7.40	131.77	121.26	88	5
1	A	112	LEU	CA-C-N	7.39	131.98	122.00	120	5
1	A	112	LEU	C-N-CA	7.39	131.98	122.00	120	5
1	A	101	SER	N-CA-C	7.39	120.11	110.43	131	7
1	A	29	THR	CA-CB-CG2	-7.39	97.94	110.50	76	6
1	A	56	ASP	O-C-N	-7.38	112.64	122.38	50	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	62	THR	O-C-N	-7.38	114.68	123.31	48	9
1	A	51	MET	CA-C-O	7.37	128.79	120.90	17	6
1	A	71	MET	O-C-N	-7.37	113.75	122.15	28	15
1	A	41	GLN	OE1-CD-NE2	-7.37	115.23	122.60	72	13
1	A	69	LEU	O-C-N	-7.36	114.32	122.12	110	12
1	A	130	ILE	N-CA-CB	7.35	119.50	111.41	16	6
1	A	133	ASP	O-C-N	7.35	131.06	122.17	79	6
1	A	50	ASP	N-CA-C	7.35	118.93	111.07	135	17
1	A	121	VAL	CB-CA-C	7.33	121.63	112.02	131	9
1	A	126	ARG	NE-CZ-NH2	7.33	125.80	119.20	123	17
1	A	7	GLU	N-CA-CB	7.33	120.90	110.12	13	7
1	A	99	TYR	CA-C-N	7.32	132.84	123.10	12	9
1	A	99	TYR	C-N-CA	7.32	132.84	123.10	12	9
1	A	35	VAL	CA-C-O	-7.32	113.09	120.85	6	9
1	A	111	ASN	O-C-N	-7.32	113.27	122.27	123	7
1	A	7	GLU	CA-C-O	7.32	128.37	120.10	130	9
1	A	28	THR	CA-C-O	-7.32	113.61	121.88	95	4
1	A	34	THR	O-C-N	-7.32	114.37	122.12	54	9
1	A	22	ASP	O-C-N	-7.31	113.82	122.15	101	7
1	A	113	GLY	CA-C-N	7.30	131.75	121.24	30	9
1	A	113	GLY	C-N-CA	7.30	131.75	121.24	30	9
1	A	72	MET	CA-C-N	7.30	130.65	120.29	67	16
1	A	72	MET	C-N-CA	7.30	130.65	120.29	67	16
1	A	117	THR	O-C-N	-7.29	114.15	122.68	85	24
1	A	18	LEU	O-C-N	-7.29	113.84	122.15	121	6
1	A	39	LEU	CA-C-O	7.29	128.44	119.11	47	9
1	A	34	THR	CA-CB-CG2	7.28	122.88	110.50	68	3
1	A	7	GLU	N-CA-C	7.26	119.28	111.36	129	17
1	A	84	GLU	O-C-N	-7.26	113.87	122.15	34	8
1	A	61	GLY	CA-C-N	7.26	133.99	122.59	60	4
1	A	61	GLY	C-N-CA	7.26	133.99	122.59	60	4
1	A	129	ASP	N-CA-CB	7.26	121.55	109.94	75	12
1	A	31	GLU	O-C-N	-7.26	114.60	122.07	71	10
1	A	91	VAL	N-CA-CB	7.25	123.06	110.65	68	13
1	A	42	ASN	CB-CA-C	-7.25	102.93	110.33	34	4
1	A	67	GLU	O-C-N	-7.25	112.62	122.33	85	6
1	A	86	ARG	O-C-N	-7.24	112.64	122.33	151	10
1	A	8	GLN	CB-CG-CD	-7.23	100.31	112.60	9	3
1	A	99	TYR	N-CA-CB	-7.23	98.29	110.80	78	3
1	A	119	GLU	N-CA-CB	7.23	121.43	110.30	19	6
1	A	8	GLN	N-CA-C	7.22	121.00	111.75	70	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	98	GLY	CA-C-N	7.22	133.11	122.86	110	4
1	A	98	GLY	C-N-CA	7.22	133.11	122.86	110	4
1	A	66	PRO	N-CA-CB	7.21	110.44	103.51	101	6
1	A	47	GLU	N-CA-CB	7.21	120.72	110.12	104	8
1	A	123	GLU	CB-CA-C	-7.21	98.60	110.85	60	2
1	A	21	LYS	N-CA-CB	-7.20	99.53	110.33	121	8
1	A	59	GLY	O-C-N	-7.20	114.51	122.50	157	8
1	A	93	ASP	N-CA-C	7.20	120.14	108.63	52	1
1	A	133	ASP	N-CA-C	7.19	122.34	113.50	142	16
1	A	41	GLN	CA-C-O	7.18	129.98	121.36	24	3
1	A	54	GLU	CA-C-O	7.18	128.26	119.79	18	10
1	A	52	ILE	N-CA-C	7.18	117.31	110.42	88	13
1	A	40	GLY	O-C-N	-7.17	114.54	122.50	14	11
1	A	122	ASP	CA-C-O	-7.17	113.32	120.70	69	6
1	A	136	VAL	N-CA-CB	7.17	119.60	111.21	106	9
1	A	52	ILE	CA-CB-CG2	7.16	122.68	110.50	137	3
1	A	54	GLU	O-C-N	-7.16	113.99	122.15	106	8
1	A	60	ASN	CA-C-O	7.16	127.97	119.60	150	11
1	A	38	SER	CA-C-O	7.16	128.19	120.10	19	10
1	A	129	ASP	CA-C-O	7.15	129.91	120.11	63	10
1	A	47	GLU	CA-C-O	7.15	128.19	119.97	43	7
1	A	135	GLN	CA-C-N	7.14	132.04	122.90	1	9
1	A	135	GLN	C-N-CA	7.14	132.04	122.90	1	9
1	A	37	ARG	O-C-N	-7.14	114.55	122.12	74	7
1	A	91	VAL	CA-CB-CG1	7.13	122.52	110.40	82	11
1	A	103	ALA	O-C-N	-7.13	114.73	122.07	55	8
1	A	115	LYS	CB-CA-C	7.13	122.62	112.07	144	5
1	A	127	GLU	O-C-N	-7.13	113.50	122.27	104	9
1	A	135	GLN	CA-C-O	7.12	127.88	120.40	145	9
1	A	30	LYS	O-C-N	-7.12	114.74	122.07	58	13
1	A	34	THR	OG1-CB-CG2	-7.11	95.07	109.30	39	5
1	A	139	GLU	N-CA-CB	7.11	120.57	110.12	108	5
1	A	19	PHE	CB-CG-CD1	7.11	132.78	120.70	95	4
1	A	26	THR	O-C-N	-7.10	115.03	123.27	13	15
1	A	135	GLN	CB-CA-C	-7.09	99.11	110.81	17	5
1	A	43	PRO	N-CA-CB	7.09	111.24	103.23	51	8
1	A	106	ARG	NH1-CZ-NH2	-7.09	110.09	119.30	8	2
1	A	53	ASN	N-CA-C	7.08	119.00	111.28	132	10
1	A	70	THR	CA-C-O	7.08	128.06	120.55	32	13
1	A	17	SER	N-CA-C	7.08	119.85	111.71	3	16
1	A	133	ASP	CA-C-O	7.08	127.55	119.27	35	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	108	VAL	CA-CB-CG2	-7.08	98.37	110.40	42	4
1	A	31	GLU	CA-C-O	-7.07	113.41	120.70	143	11
1	A	99	TYR	N-CA-C	7.07	120.39	108.02	156	5
1	A	17	SER	O-C-N	-7.07	113.58	122.27	138	4
1	A	48	LEU	N-CA-CB	7.06	120.55	109.82	155	4
1	A	29	THR	N-CA-CB	7.06	120.24	110.01	39	21
1	A	19	PHE	CA-C-N	7.05	131.94	121.72	14	7
1	A	19	PHE	C-N-CA	7.05	131.94	121.72	14	7
1	A	122	ASP	O-C-N	-7.05	114.81	122.07	13	9
1	A	30	LYS	CA-C-O	7.05	127.89	120.42	45	17
1	A	117	THR	N-CA-CB	7.04	120.43	110.36	119	15
1	A	145	MET	N-CA-CB	-7.04	98.92	110.40	8	2
1	A	9	ILE	CA-C-O	-7.04	113.39	120.85	102	7
1	A	26	THR	N-CA-CB	7.03	122.59	111.20	107	11
1	A	36	MET	CG-SD-CE	-7.03	85.44	100.90	24	17
1	A	35	VAL	N-CA-CB	7.03	119.56	110.57	158	13
1	A	142	VAL	CA-C-O	7.02	128.25	120.95	25	8
1	A	6	GLU	CA-C-O	7.02	128.78	120.92	26	8
1	A	141	PHE	CA-C-O	7.01	128.04	119.97	15	14
1	A	95	ASP	CA-C-N	7.00	132.25	120.91	44	13
1	A	95	ASP	C-N-CA	7.00	132.25	120.91	44	13
1	A	8	GLN	O-C-N	-7.00	114.86	122.07	80	16
1	A	118	ASP	CA-C-O	6.99	127.96	120.55	133	8
1	A	9	ILE	O-C-N	-6.99	114.63	121.83	50	13
1	A	62	THR	CA-CB-CG2	-6.99	98.62	110.50	42	2
1	A	117	THR	CA-CB-OG1	6.99	120.08	109.60	90	11
1	A	104	GLU	CB-CG-CD	6.97	124.45	112.60	6	2
1	A	90	ARG	NE-CZ-NH2	6.97	125.47	119.20	12	11
1	A	25	GLY	CA-C-O	-6.97	111.41	118.86	57	6
1	A	142	VAL	CA-CB-CG1	6.96	122.24	110.40	71	7
1	A	11	GLU	CA-C-O	6.96	128.35	120.90	140	4
1	A	144	MET	CB-CA-C	-6.95	99.03	110.85	107	2
1	A	12	PHE	N-CA-CB	6.95	120.34	110.12	32	3
1	A	89	PHE	CA-C-N	6.95	130.28	120.28	16	8
1	A	89	PHE	C-N-CA	6.95	130.28	120.28	16	8
1	A	5	THR	N-CA-CB	6.95	120.29	110.36	120	12
1	A	91	VAL	CA-C-O	-6.94	113.83	121.05	128	6
1	A	47	GLU	CB-CG-CD	6.94	124.40	112.60	116	3
1	A	131	ASP	CA-C-N	6.94	131.37	122.00	39	6
1	A	131	ASP	C-N-CA	6.94	131.37	122.00	39	6
1	A	88	ALA	N-CA-CB	-6.94	98.25	110.39	32	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	56	ASP	CA-C-N	6.93	130.13	120.29	77	11
1	A	56	ASP	C-N-CA	6.93	130.13	120.29	77	11
1	A	32	LEU	CB-CA-C	-6.93	100.00	110.88	74	6
1	A	63	ILE	CB-CA-C	-6.93	101.42	110.84	137	10
1	A	55	VAL	CA-C-N	6.92	134.76	121.54	11	9
1	A	55	VAL	C-N-CA	6.92	134.76	121.54	11	9
1	A	119	GLU	O-C-N	-6.92	114.26	122.15	38	9
1	A	90	ARG	NE-CZ-NH1	6.91	128.41	121.50	40	15
1	A	100	ILE	CA-C-O	-6.91	112.32	120.75	49	7
1	A	47	GLU	CB-CA-C	-6.90	99.76	110.81	88	5
1	A	133	ASP	CA-C-N	6.90	131.31	122.00	87	4
1	A	133	ASP	C-N-CA	6.90	131.31	122.00	87	4
1	A	108	VAL	CB-CA-C	-6.90	103.00	112.24	111	10
1	A	46	ALA	N-CA-CB	6.89	120.25	110.12	19	4
1	A	21	LYS	N-CA-C	6.89	118.58	111.14	114	5
1	A	128	ALA	CA-C-N	6.88	131.21	121.02	54	12
1	A	128	ALA	C-N-CA	6.88	131.21	121.02	54	12
1	A	41	GLN	CA-C-N	6.88	130.42	122.85	31	7
1	A	41	GLN	C-N-CA	6.88	130.42	122.85	31	7
1	A	121	VAL	CA-CB-CG2	-6.88	98.70	110.40	23	7
1	A	116	LEU	CA-C-O	6.88	129.16	121.11	30	9
1	A	138	TYR	CB-CG-CD2	-6.87	110.49	120.80	1	5
1	A	115	LYS	N-CA-C	6.86	120.85	109.46	149	6
1	A	102	ALA	CA-C-O	6.86	127.70	119.61	127	11
1	A	21	LYS	CA-C-O	6.85	127.76	120.70	98	6
1	A	124	MET	CA-C-O	6.85	127.68	120.42	106	7
1	A	96	GLY	N-CA-C	6.85	123.82	114.92	1	5
1	A	145	MET	CA-C-O	6.84	127.28	119.27	23	8
1	A	119	GLU	CB-CG-CD	6.83	124.21	112.60	77	5
1	A	86	ARG	CA-C-N	6.83	129.98	120.29	80	6
1	A	86	ARG	C-N-CA	6.83	129.98	120.29	80	6
1	A	87	GLU	CA-C-N	6.83	129.72	120.44	26	21
1	A	87	GLU	C-N-CA	6.83	129.72	120.44	26	21
1	A	92	PHE	CB-CG-CD2	-6.82	109.10	120.70	53	3
1	A	53	ASN	CA-C-O	6.82	127.77	119.38	58	9
1	A	58	ASP	CA-C-N	6.81	131.96	122.29	11	7
1	A	58	ASP	C-N-CA	6.81	131.96	122.29	11	7
1	A	61	GLY	N-CA-C	-6.80	105.67	115.27	63	5
1	A	94	LYS	CG-CD-CE	6.79	126.91	111.30	97	4
1	A	85	ILE	O-C-N	-6.77	114.85	121.83	100	13
1	A	83	GLU	N-CA-CB	6.76	120.02	109.94	13	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	14	GLU	N-CA-CB	6.76	120.21	110.06	106	3
1	A	7	GLU	CB-CG-CD	6.76	124.09	112.60	117	5
1	A	31	GLU	CB-CG-CD	6.76	124.09	112.60	110	3
1	A	113	GLY	O-C-N	-6.75	114.66	122.22	62	9
1	A	10	ALA	CA-C-O	-6.75	113.40	120.55	84	10
1	A	142	VAL	CB-CA-C	6.74	120.33	111.70	24	9
1	A	132	GLY	N-CA-C	-6.74	105.54	115.72	127	11
1	A	50	ASP	N-CA-CB	-6.74	100.21	110.12	45	4
1	A	108	VAL	CA-C-N	6.74	129.31	120.28	73	8
1	A	108	VAL	C-N-CA	6.74	129.31	120.28	73	8
1	A	100	ILE	CA-CB-CG1	6.74	121.85	110.40	117	3
1	A	86	ARG	CA-C-O	-6.73	113.77	120.70	7	10
1	A	105	LEU	CB-CA-C	-6.73	99.62	110.79	157	11
1	A	9	ILE	CB-CA-C	6.73	120.49	111.88	58	2
1	A	55	VAL	CA-CB-CG2	6.73	121.84	110.40	142	3
1	A	42	ASN	N-CA-C	6.73	120.18	108.75	104	3
1	A	49	GLN	N-CA-CB	6.72	120.11	110.16	86	3
1	A	10	ALA	CA-C-N	6.71	129.16	120.44	20	12
1	A	10	ALA	C-N-CA	6.71	129.16	120.44	20	12
1	A	95	ASP	CA-C-O	6.71	127.66	120.55	20	8
1	A	106	ARG	CG-CD-NE	-6.70	97.26	112.00	160	8
1	A	134	GLY	O-C-N	-6.70	115.33	122.56	60	3
1	A	83	GLU	CA-C-O	6.69	127.61	119.38	80	7
1	A	116	LEU	CA-C-N	6.68	130.84	120.75	139	4
1	A	116	LEU	C-N-CA	6.68	130.84	120.75	139	4
1	A	104	GLU	CA-C-O	-6.68	113.34	120.42	93	7
1	A	107	HIS	N-CA-CB	6.68	119.94	110.12	36	2
1	A	96	GLY	CA-C-N	6.67	133.81	122.26	147	4
1	A	96	GLY	C-N-CA	6.67	133.81	122.26	147	4
1	A	111	ASN	CA-C-O	6.67	127.57	120.70	16	11
1	A	67	GLU	CA-C-O	6.67	127.64	119.97	23	10
1	A	33	GLY	CA-C-O	6.66	127.33	120.80	23	6
1	A	20	ASP	CA-C-O	6.66	130.04	120.51	54	8
1	A	54	GLU	CB-CG-CD	6.66	123.92	112.60	59	5
1	A	24	ASP	CB-CA-C	6.66	120.55	109.56	96	3
1	A	95	ASP	N-CA-CB	-6.65	100.06	110.30	68	6
1	A	120	GLU	CA-C-O	6.64	128.01	120.90	45	10
1	A	133	ASP	CB-CA-C	6.64	121.39	110.90	65	11
1	A	13	LYS	CB-CG-CD	6.63	126.56	111.30	144	1
1	A	136	VAL	CA-C-O	6.63	128.40	120.65	69	15
1	A	15	ALA	CA-C-O	6.62	127.77	120.82	131	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	137	ASN	O-C-N	-6.62	114.94	122.68	83	11
1	A	137	ASN	CB-CA-C	6.62	120.72	109.80	136	3
1	A	109	MET	CB-CA-C	6.61	122.09	110.85	147	5
1	A	71	MET	CB-CA-C	-6.61	99.62	110.85	137	2
1	A	51	MET	N-CA-CB	6.59	119.63	110.07	49	6
1	A	126	ARG	NH1-CZ-NH2	-6.59	110.74	119.30	54	6
1	A	19	PHE	N-CA-C	6.58	120.53	112.23	14	6
1	A	98	GLY	O-C-N	-6.56	115.47	122.56	19	9
1	A	66	PRO	CB-CA-C	-6.56	102.54	112.11	136	1
1	A	60	ASN	N-CA-CB	6.55	121.27	110.39	1	12
1	A	104	GLU	CA-C-N	6.55	129.72	120.28	85	27
1	A	104	GLU	C-N-CA	6.55	129.72	120.28	85	27
1	A	54	GLU	CA-C-N	6.55	130.97	120.82	134	8
1	A	54	GLU	C-N-CA	6.55	130.97	120.82	134	8
1	A	86	ARG	N-CA-CB	6.55	119.69	109.94	83	6
1	A	99	TYR	CA-CB-CG	-6.54	102.12	113.90	56	2
1	A	52	ILE	CB-CA-C	-6.54	103.45	112.02	143	8
1	A	32	LEU	N-CA-C	6.53	120.51	112.54	83	5
1	A	125	ILE	CB-CA-C	-6.53	103.53	111.88	75	3
1	A	51	MET	CB-CA-C	-6.53	98.55	110.63	142	3
1	A	64	ASP	CA-C-O	-6.52	113.70	121.66	23	3
1	A	62	THR	CA-C-O	-6.52	113.79	121.16	111	4
1	A	22	ASP	CB-CA-C	6.52	122.68	110.63	29	2
1	A	73	ALA	N-CA-CB	6.51	119.80	110.16	21	5
1	A	53	ASN	O-C-N	-6.51	114.60	122.22	141	4
1	A	116	LEU	CB-CA-C	-6.50	100.12	110.14	14	2
1	A	36	MET	CA-C-O	6.50	127.31	120.42	151	6
1	A	89	PHE	N-CA-CB	-6.50	100.32	110.06	27	7
1	A	52	ILE	CA-C-O	6.49	128.68	120.96	79	5
1	A	94	LYS	N-CA-CB	6.49	119.39	109.98	42	5
1	A	108	VAL	CA-C-O	6.48	128.04	121.17	154	10
1	A	91	VAL	CB-CA-C	6.47	120.91	112.24	70	6
1	A	83	GLU	CB-CG-CD	6.47	123.59	112.60	154	2
1	A	118	ASP	O-C-N	-6.46	114.66	122.22	79	5
1	A	22	ASP	CA-C-O	6.46	127.32	119.31	95	6
1	A	140	GLU	N-CA-CB	6.46	119.43	110.07	77	3
1	A	47	GLU	O-C-N	-6.44	114.80	122.15	62	12
1	A	58	ASP	CA-C-O	6.44	127.39	119.79	6	12
1	A	125	ILE	CA-C-O	6.44	127.64	120.95	21	6
1	A	11	GLU	N-CA-CB	6.43	119.31	109.91	78	5
1	A	43	PRO	N-CA-C	6.43	121.44	111.21	142	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	44	THR	N-CA-C	-6.42	99.45	109.72	111	4
1	A	38	SER	CA-C-N	6.41	132.94	121.66	129	5
1	A	38	SER	C-N-CA	6.41	132.94	121.66	129	5
1	A	95	ASP	O-C-N	-6.41	115.22	122.08	127	4
1	A	6	GLU	O-C-N	-6.40	115.33	122.12	85	8
1	A	29	THR	CB-CA-C	-6.40	96.93	110.31	51	3
1	A	111	ASN	CB-CA-C	-6.40	100.17	110.79	40	5
1	A	27	ILE	CA-C-O	6.40	127.94	120.71	159	8
1	A	131	ASP	CA-C-O	6.40	127.39	120.55	97	4
1	A	97	ASN	N-CA-CB	6.40	121.58	110.39	58	3
1	A	37	ARG	CG-CD-NE	-6.39	97.94	112.00	159	8
1	A	70	THR	CB-CA-C	6.39	121.71	110.85	68	2
1	A	105	LEU	CD1-CG-CD2	-6.38	96.77	110.80	17	1
1	A	13	LYS	N-CA-CB	-6.37	100.76	110.12	23	5
1	A	16	PHE	CA-C-O	6.37	127.51	120.82	84	10
1	A	48	LEU	N-CA-C	6.37	118.75	111.11	92	17
1	A	49	GLN	CA-C-O	6.37	127.29	119.97	121	15
1	A	89	PHE	O-C-N	-6.36	115.47	122.09	154	11
1	A	71	MET	CG-SD-CE	-6.36	86.90	100.90	37	5
1	A	52	ILE	CA-CB-CG1	6.36	121.20	110.40	71	1
1	A	110	THR	CA-CB-OG1	6.35	119.13	109.60	156	12
1	A	86	ARG	CB-CA-C	6.34	120.92	110.90	100	1
1	A	27	ILE	CA-CB-CG1	6.34	121.17	110.40	90	7
1	A	116	LEU	N-CA-CB	6.33	120.66	110.65	106	6
1	A	136	VAL	N-CA-C	6.33	117.91	108.54	27	4
1	A	39	LEU	N-CA-CB	-6.33	101.31	110.56	60	3
1	A	70	THR	CA-CB-OG1	6.33	119.10	109.60	124	2
1	A	85	ILE	CB-CA-C	6.33	120.68	112.14	91	6
1	A	25	GLY	N-CA-C	-6.32	106.31	114.85	150	4
1	A	88	ALA	CB-CA-C	-6.32	100.30	110.79	8	2
1	A	145	MET	CB-CA-C	-6.32	98.79	109.72	25	1
1	A	34	THR	CA-C-O	-6.31	113.86	120.55	6	8
1	A	69	LEU	CA-C-O	6.31	127.65	120.90	96	7
1	A	17	SER	CA-C-O	6.30	127.14	119.38	107	4
1	A	59	GLY	N-CA-C	6.30	124.02	115.32	69	2
1	A	92	PHE	CB-CG-CD1	6.29	131.40	120.70	139	3
1	A	64	ASP	CB-CA-C	6.29	121.34	110.45	8	4
1	A	58	ASP	N-CA-CB	6.29	119.57	110.20	139	5
1	A	90	ARG	CG-CD-NE	-6.29	98.16	112.00	53	4
1	A	134	GLY	CA-C-N	6.28	132.36	122.94	144	3
1	A	134	GLY	C-N-CA	6.28	132.36	122.94	144	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	143	GLN	N-CA-CB	6.28	119.12	110.01	103	3
1	A	9	ILE	CA-CB-CG1	6.28	121.07	110.40	100	1
1	A	12	PHE	CB-CG-CD2	-6.28	110.03	120.70	10	1
1	A	60	ASN	CB-CG-OD1	6.27	133.34	120.80	50	2
1	A	107	HIS	CB-CG-CD2	-6.26	123.06	131.20	126	9
1	A	17	SER	N-CA-CB	6.26	121.34	110.39	57	3
1	A	43	PRO	N-CD-CG	6.26	112.59	103.20	111	1
1	A	8	GLN	N-CA-CB	6.25	119.14	110.07	73	4
1	A	121	VAL	CG1-CB-CG2	-6.25	97.04	110.80	110	3
1	A	127	GLU	CB-CG-CD	-6.25	101.98	112.60	34	2
1	A	49	GLN	O-C-N	-6.25	114.91	122.22	27	9
1	A	8	GLN	CA-C-O	-6.24	114.26	120.82	106	9
1	A	145	MET	O-C-N	-6.24	114.59	122.27	64	10
1	A	23	GLY	O-C-N	-6.24	115.55	122.47	61	5
1	A	25	GLY	CA-C-N	6.24	132.58	122.29	3	2
1	A	25	GLY	C-N-CA	6.24	132.58	122.29	3	2
1	A	86	ARG	NH1-CZ-NH2	-6.22	111.22	119.30	8	3
1	A	29	THR	OG1-CB-CG2	-6.22	96.86	109.30	114	2
1	A	37	ARG	NH1-CZ-NH2	-6.21	111.22	119.30	84	5
1	A	90	ARG	CB-CG-CD	6.21	125.59	111.30	88	4
1	A	69	LEU	N-CA-CB	-6.20	101.01	110.12	110	6
1	A	141	PHE	N-CA-CB	-6.20	100.98	110.16	140	5
1	A	37	ARG	CA-C-O	6.19	126.98	119.49	6	2
1	A	67	GLU	N-CA-CB	6.19	120.49	110.40	107	4
1	A	39	LEU	N-CA-C	6.18	119.77	112.72	10	5
1	A	90	ARG	NH1-CZ-NH2	-6.18	111.26	119.30	9	4
1	A	139	GLU	CA-CB-CG	6.18	126.46	114.10	147	2
1	A	85	ILE	CA-CB-CG2	-6.18	100.00	110.50	118	10
1	A	143	GLN	O-C-N	6.17	129.19	122.15	109	9
1	A	56	ASP	CB-CA-C	6.17	121.48	111.05	46	3
1	A	90	ARG	O-C-N	-6.17	114.17	122.43	105	8
1	A	138	TYR	CB-CA-C	6.16	120.55	110.88	28	4
1	A	19	PHE	O-C-N	6.16	131.16	122.41	89	5
1	A	24	ASP	N-CA-C	-6.15	105.78	113.28	100	7
1	A	112	LEU	N-CA-CB	6.15	118.92	110.01	73	5
1	A	141	PHE	CB-CA-C	6.14	120.53	110.88	7	2
1	A	130	ILE	CB-CA-C	6.14	121.37	111.29	132	11
1	A	104	GLU	CB-CA-C	-6.14	100.41	110.85	109	3
1	A	126	ARG	CG-CD-NE	-6.14	98.49	112.00	22	2
1	A	66	PRO	N-CD-CG	6.14	112.41	103.20	69	1
1	A	138	TYR	CD1-CG-CD2	6.13	127.30	118.10	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	135	GLN	N-CA-CB	6.13	120.41	110.42	61	3
1	A	30	LYS	N-CA-CB	6.12	118.89	110.01	60	2
1	A	130	ILE	CA-CB-CG1	-6.11	100.02	110.40	134	4
1	A	134	GLY	N-CA-C	-6.10	107.28	115.21	26	4
1	A	6	GLU	N-CA-CB	-6.10	100.82	110.28	21	2
1	A	16	PHE	N-CA-CB	-6.10	101.17	110.01	58	3
1	A	62	THR	OG1-CB-CG2	-6.10	97.11	109.30	12	1
1	A	28	THR	N-CA-CB	6.09	119.68	110.42	17	3
1	A	114	GLU	CB-CG-CD	-6.09	102.25	112.60	62	1
1	A	21	LYS	CG-CD-CE	6.09	125.31	111.30	39	2
1	A	37	ARG	CA-C-N	6.09	129.04	120.28	17	10
1	A	37	ARG	C-N-CA	6.09	129.04	120.28	17	10
1	A	26	THR	CA-CB-CG2	-6.08	100.16	110.50	38	3
1	A	144	MET	CA-CB-CG	6.07	126.25	114.10	132	1
1	A	5	THR	N-CA-C	-6.07	101.02	110.42	64	4
1	A	143	GLN	CB-CG-CD	-6.06	102.29	112.60	15	2
1	A	84	GLU	CB-CA-C	-6.06	100.73	110.79	130	3
1	A	56	ASP	N-CA-CB	6.04	118.73	110.57	154	1
1	A	27	ILE	CA-CB-CG2	-6.04	100.24	110.50	20	4
1	A	106	ARG	CD-NE-CZ	-6.02	115.97	124.40	140	2
1	A	121	VAL	CA-CB-CG1	6.00	120.61	110.40	94	7
1	A	87	GLU	N-CA-CB	6.00	118.88	109.94	83	4
1	A	58	ASP	CB-CA-C	6.00	121.73	109.67	49	5
1	A	114	GLU	CA-C-N	6.00	131.63	123.11	16	3
1	A	114	GLU	C-N-CA	6.00	131.63	123.11	16	3
1	A	54	GLU	CB-CA-C	-6.00	101.42	110.90	80	2
1	A	66	PRO	O-C-N	6.00	130.72	122.38	6	3
1	A	124	MET	N-CA-CB	-6.00	101.28	110.16	109	3
1	A	68	PHE	CB-CA-C	5.99	121.04	110.85	75	3
1	A	7	GLU	CB-CA-C	-5.98	99.18	110.67	74	3
1	A	142	VAL	CA-CB-CG2	5.98	120.57	110.40	17	4
1	A	56	ASP	N-CA-C	5.98	119.23	108.17	70	6
1	A	63	ILE	N-CA-C	5.97	116.41	107.51	108	7
1	A	19	PHE	CB-CG-CD2	-5.97	110.55	120.70	129	4
1	A	138	TYR	N-CA-CB	-5.97	101.33	110.16	61	5
1	A	83	GLU	CA-CB-CG	5.96	126.02	114.10	40	2
1	A	97	ASN	CA-C-O	5.96	126.74	120.42	135	6
1	A	55	VAL	CA-CB-CG1	5.95	120.51	110.40	49	2
1	A	55	VAL	N-CA-CB	-5.95	105.44	112.39	121	3
1	A	110	THR	CA-CB-CG2	-5.95	100.39	110.50	120	3
1	A	116	LEU	CD1-CG-CD2	-5.94	97.72	110.80	149	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	105	LEU	N-CA-CB	5.94	118.62	110.01	26	1
1	A	95	ASP	CB-CA-C	5.94	120.95	110.85	91	6
1	A	135	GLN	N-CA-C	-5.93	98.60	108.75	100	8
1	A	45	GLU	CB-CA-C	-5.93	100.76	110.85	26	3
1	A	62	THR	N-CA-C	5.93	119.92	109.96	142	2
1	A	12	PHE	CA-C-O	5.93	127.03	120.63	58	5
1	A	117	THR	CA-C-O	-5.93	114.81	121.81	130	3
1	A	108	VAL	CA-CB-CG1	5.93	120.48	110.40	107	6
1	A	68	PHE	N-CA-CB	5.92	118.66	110.07	116	3
1	A	49	GLN	CB-CG-CD	-5.92	102.53	112.60	12	3
1	A	129	ASP	N-CA-C	5.92	118.78	109.96	98	4
1	A	41	GLN	CB-CG-CD	5.92	122.66	112.60	148	4
1	A	143	GLN	CG-CD-NE2	5.91	125.27	116.40	52	2
1	A	93	ASP	N-CA-CB	5.90	120.09	110.17	97	2
1	A	46	ALA	CB-CA-C	-5.90	100.82	110.85	144	1
1	A	20	ASP	N-CA-CB	5.90	119.20	109.88	77	3
1	A	50	ASP	CB-CA-C	5.90	120.14	110.88	85	2
1	A	45	GLU	N-CA-CB	5.89	118.78	110.12	51	2
1	A	30	LYS	CB-CA-C	-5.89	101.63	110.88	60	2
1	A	12	PHE	CB-CA-C	-5.88	100.67	110.68	138	3
1	A	119	GLU	CB-CA-C	5.88	120.11	110.88	127	3
1	A	127	GLU	N-CA-CB	5.87	118.58	110.07	8	6
1	A	6	GLU	CB-CG-CD	5.87	122.58	112.60	27	2
1	A	110	THR	CB-CA-C	-5.86	101.06	110.79	1	4
1	A	44	THR	CA-C-O	-5.86	114.45	121.89	18	4
1	A	41	GLN	CG-CD-NE2	5.86	125.18	116.40	38	2
1	A	114	GLU	N-CA-CB	-5.85	100.89	110.43	46	4
1	A	62	THR	CA-C-N	5.85	129.69	122.37	20	5
1	A	62	THR	C-N-CA	5.85	129.69	122.37	20	5
1	A	67	GLU	CA-CB-CG	5.85	125.80	114.10	28	1
1	A	90	ARG	N-CA-CB	-5.85	101.51	110.16	118	7
1	A	54	GLU	N-CA-CB	5.84	118.48	110.01	140	3
1	A	101	SER	CB-CA-C	5.84	120.21	109.46	40	2
1	A	43	PRO	O-C-N	-5.84	115.88	123.00	98	2
1	A	139	GLU	CB-CG-CD	5.83	122.52	112.60	121	2
1	A	14	GLU	O-C-N	-5.82	115.95	122.12	25	5
1	A	29	THR	CA-CB-OG1	5.82	118.33	109.60	90	4
1	A	127	GLU	CA-C-O	5.82	126.70	120.24	22	5
1	A	67	GLU	CG-CD-OE1	5.81	131.76	118.40	130	1
1	A	96	GLY	CA-C-O	5.80	125.73	119.06	59	3
1	A	37	ARG	CB-CG-CD	5.79	124.61	111.30	128	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	89	PHE	CB-CG-CD2	-5.79	110.86	120.70	13	2
1	A	106	ARG	CB-CA-C	5.78	121.77	110.67	160	1
1	A	28	THR	O-C-N	-5.77	115.93	122.68	66	7
1	A	57	ALA	CB-CA-C	-5.77	98.64	109.72	160	3
1	A	92	PHE	CA-C-N	5.76	131.51	122.17	50	5
1	A	92	PHE	C-N-CA	5.76	131.51	122.17	50	5
1	A	143	GLN	CB-CA-C	5.76	122.14	110.38	62	3
1	A	70	THR	N-CA-CB	5.76	118.52	109.94	74	6
1	A	132	GLY	O-C-N	-5.75	116.11	122.50	68	4
1	A	122	ASP	CB-CA-C	-5.75	101.25	110.79	21	3
1	A	132	GLY	CA-C-N	-5.75	112.32	122.26	98	2
1	A	132	GLY	C-N-CA	-5.75	112.32	122.26	98	2
1	A	125	ILE	CA-CB-CG1	5.74	120.16	110.40	6	2
1	A	37	ARG	CA-CB-CG	5.74	125.58	114.10	157	2
1	A	43	PRO	CA-C-N	5.74	131.85	121.06	149	2
1	A	43	PRO	C-N-CA	5.74	131.85	121.06	149	2
1	A	57	ALA	O-C-N	-5.73	115.44	122.20	29	3
1	A	63	ILE	CA-CB-CG2	-5.72	100.77	110.50	45	4
1	A	18	LEU	CB-CA-C	-5.72	101.12	110.85	148	2
1	A	86	ARG	CD-NE-CZ	-5.72	116.39	124.40	131	3
1	A	131	ASP	N-CA-CB	5.72	118.53	110.12	143	3
1	A	64	ASP	N-CA-C	5.72	117.92	109.69	142	1
1	A	115	LYS	CA-C-N	5.71	131.77	122.81	55	2
1	A	115	LYS	C-N-CA	5.71	131.77	122.81	55	2
1	A	106	ARG	N-CA-CB	-5.71	101.51	110.30	60	1
1	A	99	TYR	CG-CD1-CE1	-5.71	112.64	121.20	64	1
1	A	123	GLU	CB-CG-CD	5.71	122.30	112.60	97	3
1	A	133	ASP	N-CA-CB	5.70	118.75	110.26	36	2
1	A	14	GLU	CB-CG-CD	5.70	122.29	112.60	131	2
1	A	92	PHE	CB-CA-C	-5.69	101.91	110.90	96	5
1	A	91	VAL	CA-CB-CG2	5.69	120.07	110.40	68	3
1	A	17	SER	CB-CA-C	-5.68	100.12	110.63	54	2
1	A	66	PRO	CA-C-O	5.68	127.69	119.34	50	3
1	A	12	PHE	CB-CG-CD1	5.67	130.33	120.70	45	3
1	A	35	VAL	CA-CB-CG1	5.67	120.03	110.40	24	5
1	A	48	LEU	CB-CA-C	-5.66	101.39	110.79	50	4
1	A	84	GLU	CA-CB-CG	-5.66	102.78	114.10	91	1
1	A	120	GLU	CB-CG-CD	-5.66	102.98	112.60	158	2
1	A	37	ARG	CB-CA-C	-5.66	101.40	110.79	49	3
1	A	135	GLN	CG-CD-NE2	5.66	124.88	116.40	62	1
1	A	103	ALA	CB-CA-C	-5.64	98.52	110.31	58	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	130	ILE	CA-CB-CG2	5.63	120.07	110.50	64	4
1	A	144	MET	N-CA-CB	5.62	118.91	110.14	57	4
1	A	87	GLU	CB-CA-C	5.62	120.40	110.85	84	4
1	A	137	ASN	CA-C-O	-5.60	115.50	121.94	144	6
1	A	72	MET	CB-CA-C	5.59	120.08	110.79	23	1
1	A	49	GLN	CB-CA-C	-5.59	99.61	110.46	42	1
1	A	36	MET	N-CA-CB	5.59	118.95	110.28	138	2
1	A	130	ILE	CB-CG1-CD1	5.59	125.54	113.80	7	1
1	A	101	SER	N-CA-CB	5.58	118.49	110.06	125	6
1	A	24	ASP	O-C-N	-5.57	114.77	122.46	110	6
1	A	122	ASP	N-CA-CB	-5.57	101.94	110.12	2	3
1	A	107	HIS	CB-CG-ND1	5.57	131.05	122.70	156	4
1	A	19	PHE	N-CA-CB	5.56	118.36	110.13	157	2
1	A	120	GLU	CA-CB-CG	-5.55	103.00	114.10	84	2
1	A	99	TYR	CD1-CG-CD2	5.54	126.42	118.10	59	2
1	A	19	PHE	CB-CA-C	-5.54	99.63	110.11	67	2
1	A	26	THR	CA-C-O	5.54	126.69	120.70	102	3
1	A	31	GLU	N-CA-CB	-5.54	101.36	110.40	92	6
1	A	126	ARG	CB-CA-C	-5.54	101.59	110.79	21	2
1	A	125	ILE	CA-CB-CG2	5.54	119.91	110.50	135	4
1	A	11	GLU	CB-CG-CD	5.54	122.02	112.60	158	1
1	A	114	GLU	CB-CA-C	5.54	119.72	109.54	152	2
1	A	117	THR	N-CA-C	-5.53	103.09	110.55	79	3
1	A	125	ILE	CB-CG1-CD1	5.52	125.39	113.80	60	2
1	A	63	ILE	CA-CB-CG1	5.52	119.79	110.40	107	1
1	A	93	ASP	CB-CA-C	5.52	119.71	110.88	16	5
1	A	90	ARG	CB-CA-C	-5.51	100.43	110.63	120	2
1	A	137	ASN	N-CA-C	-5.50	101.86	110.17	36	8
1	A	37	ARG	CD-NE-CZ	-5.50	116.70	124.40	144	2
1	A	84	GLU	CB-CG-CD	-5.49	103.27	112.60	20	3
1	A	21	LYS	CB-CG-CD	5.46	123.87	111.30	36	1
1	A	137	ASN	CB-CG-ND2	5.46	124.59	116.40	75	2
1	A	128	ALA	CB-CA-C	-5.46	101.73	110.79	126	4
1	A	65	PHE	CB-CA-C	-5.45	102.63	112.76	35	1
1	A	99	TYR	CB-CG-CD1	-5.43	112.65	120.80	101	1
1	A	14	GLU	CB-CA-C	-5.43	101.78	110.79	99	1
1	A	111	ASN	CB-CG-ND2	-5.42	108.27	116.40	105	2
1	A	31	GLU	CB-CA-C	-5.40	101.67	110.85	134	1
1	A	127	GLU	CB-CA-C	5.40	119.36	110.88	105	3
1	A	50	ASP	CA-C-O	-5.40	115.14	120.70	127	1
1	A	99	TYR	CB-CA-C	-5.40	98.10	109.38	143	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	41	GLN	N-CA-C	5.39	117.79	110.35	40	3
1	A	110	THR	OG1-CB-CG2	-5.39	98.52	109.30	65	3
1	A	70	THR	OG1-CB-CG2	-5.38	98.54	109.30	76	2
1	A	135	GLN	CB-CG-CD	5.36	121.71	112.60	36	3
1	A	135	GLN	CA-CB-CG	5.35	124.80	114.10	155	2
1	A	126	ARG	CB-CG-CD	5.34	123.58	111.30	60	1
1	A	104	GLU	N-CA-CB	5.34	117.89	109.94	8	2
1	A	125	ILE	N-CA-CB	5.34	117.04	110.64	158	2
1	A	42	ASN	CB-CG-ND2	5.32	124.39	116.40	34	2
1	A	90	ARG	CA-CB-CG	5.32	124.74	114.10	56	4
1	A	41	GLN	CB-CA-C	5.32	119.65	110.45	130	2
1	A	126	ARG	CA-CB-CG	-5.31	103.48	114.10	134	1
1	A	44	THR	CA-CB-CG2	5.31	119.53	110.50	7	3
1	A	107	HIS	ND1-CG-CD2	-5.31	100.79	106.10	111	2
1	A	124	MET	CB-CA-C	5.31	119.21	110.88	55	1
1	A	129	ASP	CB-CA-C	5.31	117.44	110.06	138	1
1	A	99	TYR	CB-CG-CD2	-5.31	112.84	120.80	5	1
1	A	123	GLU	N-CA-CB	5.30	118.00	110.16	73	1
1	A	117	THR	CA-CB-CG2	-5.29	101.50	110.50	107	1
1	A	53	ASN	CB-CG-OD1	5.29	131.38	120.80	107	1
1	A	49	GLN	CG-CD-OE1	-5.29	110.22	120.80	111	1
1	A	70	THR	CA-CB-CG2	5.29	119.49	110.50	98	3
1	A	91	VAL	CG1-CB-CG2	-5.29	99.17	110.80	83	2
1	A	64	ASP	N-CA-CB	5.28	118.32	110.29	145	1
1	A	127	GLU	CA-CB-CG	5.28	124.66	114.10	68	2
1	A	102	ALA	CB-CA-C	5.28	119.25	110.81	160	2
1	A	53	ASN	CB-CA-C	-5.27	99.29	110.31	81	2
1	A	100	ILE	CA-C-N	5.27	131.60	122.64	130	2
1	A	100	ILE	C-N-CA	5.27	131.60	122.64	130	2
1	A	139	GLU	CB-CA-C	5.26	119.63	110.68	132	1
1	A	118	ASP	N-CA-CB	-5.25	102.13	110.22	74	2
1	A	106	ARG	CA-CB-CG	5.24	124.59	114.10	34	2
1	A	97	ASN	CB-CG-OD1	5.24	131.28	120.80	9	2
1	A	120	GLU	CB-CA-C	5.24	119.48	110.79	12	2
1	A	35	VAL	CG1-CB-CG2	-5.23	99.30	110.80	29	1
1	A	142	VAL	CG1-CB-CG2	-5.22	99.31	110.80	46	1
1	A	40	GLY	CA-C-N	5.22	132.24	122.74	101	1
1	A	40	GLY	C-N-CA	5.22	132.24	122.74	101	1
1	A	68	PHE	CB-CG-CD2	-5.22	111.83	120.70	106	1
1	A	58	ASP	O-C-N	-5.22	115.26	122.46	31	1
1	A	94	LYS	CB-CG-CD	5.21	123.28	111.30	127	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	94	LYS	CB-CA-C	5.20	119.65	111.39	127	2
1	A	138	TYR	CB-CG-CD1	5.15	128.52	120.80	65	1
1	A	101	SER	CA-CB-OG	5.14	121.38	111.10	138	1
1	A	60	ASN	CB-CA-C	5.13	119.31	110.79	109	2
1	A	13	LYS	CG-CD-CE	5.13	123.09	111.30	20	1
1	A	9	ILE	CA-CB-CG2	5.12	119.21	110.50	72	3
1	A	30	LYS	CG-CD-CE	5.12	123.08	111.30	85	2
1	A	6	GLU	CB-CA-C	-5.12	101.98	110.68	132	2
1	A	145	MET	CA-CB-CG	-5.12	103.86	114.10	146	1
1	A	16	PHE	CB-CG-CD2	5.12	129.40	120.70	3	1
1	A	86	ARG	CG-CD-NE	-5.11	100.76	112.00	101	2
1	A	99	TYR	CG-CD2-CE2	-5.10	113.55	121.20	104	2
1	A	107	HIS	CB-CA-C	-5.09	102.34	110.79	152	1
1	A	38	SER	CB-CA-C	-5.09	99.94	109.72	53	2
1	A	63	ILE	CA-C-N	5.08	132.29	122.07	5	1
1	A	63	ILE	C-N-CA	5.08	132.29	122.07	5	1
1	A	112	LEU	CB-CA-C	5.08	118.94	110.81	69	1
1	A	116	LEU	N-CA-C	5.06	117.00	108.96	110	1
1	A	115	LYS	CG-CD-CE	5.06	122.93	111.30	17	1
1	A	51	MET	CA-CB-CG	5.06	124.22	114.10	29	1
1	A	86	ARG	CB-CG-CD	5.05	122.92	111.30	97	1
1	A	67	GLU	CB-CA-C	5.05	119.43	110.85	22	1
1	A	5	THR	OG1-CB-CG2	-5.04	99.22	109.30	118	1
1	A	24	ASP	N-CA-CB	5.02	117.80	110.47	105	1
1	A	39	LEU	CB-CA-C	-5.01	100.58	110.11	113	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
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

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	19	PHE	Sidechain	10
1	A	89	PHE	Sidechain	9
1	A	92	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	128	ALA	Peptide	3
1	A	131	ASP	Peptide	3
1	A	32	LEU	Peptide,Mainchain	2
1	A	43	PRO	Peptide	2
1	A	15	ALA	Mainchain	1
1	A	50	ASP	Mainchain	1
1	A	67	GLU	Sidechain	1
1	A	125	ILE	Mainchain	1
1	A	135	GLN	Peptide	1
1	A	102	ALA	Mainchain	1
1	A	127	GLU	Mainchain	1
1	A	84	GLU	Mainchain	1
1	A	100	ILE	Mainchain	1
1	A	129	ASP	Sidechain	1
1	A	124	MET	Mainchain	1
1	A	108	VAL	Mainchain	1
1	A	36	MET	Mainchain	1
1	A	132	GLY	Mainchain,Peptide	1
1	A	120	GLU	Peptide	1
1	A	109	MET	Peptide	1
1	A	33	GLY	Mainchain	1
1	A	136	VAL	Mainchain	1
1	A	144	MET	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	106

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:83:GLU:CD	1:A:86:ARG:HH21	0.61	2.02	5	2
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:19:PHE:CD1	1:A:35:VAL:HG22	0.55	2.37	121	3
1:A:109:MET:HE3	1:A:124:MET:HE1	0.54	1.80	122	1
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:55:VAL:HG21	1:A:71:MET:HE3	0.52	1.81	125	2
1:A:121:VAL:HG12	1:A:125:ILE:HD12	0.50	1.84	21	1
1:A:45:GLU:CD	1:A:45:GLU:H	0.49	2.16	27	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:141:PHE:CZ	1:A:145:MET:HE2	0.47	2.44	137	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:106:ARG:HH12	1:A:118:ASP:CG	0.45	2.18	104	2
1:A:16:PHE:CE2	1:A:27:ILE:HD11	0.45	2.47	21	1
1:A:16:PHE:CD1	1:A:16:PHE:C	0.45	2.93	150	2
1:A:68:PHE:CZ	1:A:72:MET:HE3	0.45	2.46	123	2
1:A:8:GLN:O	1:A:12:PHE:CD2	0.45	2.70	139	1
1:A:109:MET:HE2	1:A:109:MET:HA	0.44	1.89	30	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:119:GLU:CD	1:A:119:GLU:H	0.44	2.19	151	1
1:A:88:ALA:O	1:A:92:PHE:CD1	0.44	2.71	15	1
1:A:85:ILE:HG22	1:A:145:MET:SD	0.44	2.53	42	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:PHE:CG	1:A:108:VAL:HG11	0.43	2.48	11	1
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:63:ILE:HD13	1:A:71:MET:HE1	0.43	1.90	11	1
1:A:32:LEU:HD11	1:A:63:ILE:HG13	0.43	1.90	50	1
1:A:58:ASP:CG	1:A:60:ASN:HD21	0.43	2.22	120	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:89:PHE:CD1	1:A:89:PHE:C	0.42	2.98	10	1
1:A:116:LEU:HD22	1:A:120:GLU:HG2	0.42	1.89	91	1
1:A:136:VAL:HG21	1:A:144:MET:HE1	0.42	1.91	41	1
1:A:131:ASP:HB2	1:A:133:ASP:H	0.42	1.74	75	1
1:A:137:ASN:CG	1:A:138:TYR:H	0.42	2.23	124	1
1:A:68:PHE:CE2	1:A:72:MET:HE3	0.42	2.50	138	1
1:A:105:LEU:CD2	1:A:121:VAL:HG13	0.42	2.44	158	1
1:A:6:GLU:HA	1:A:9:ILE:HD12	0.42	1.92	139	1
1:A:28:THR:HG22	1:A:62:THR:HG22	0.42	1.91	148	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:123:GLU:CD	1:A:126:ARG:HH12	0.41	2.22	89	1
1:A:105:LEU:O	1:A:109:MET:HG2	0.41	2.15	94	1
1:A:85:ILE:HG21	1:A:142:VAL:HG22	0.41	1.92	35	1
1:A:28:THR:O	1:A:32:LEU:HD12	0.41	2.16	114	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:137:ASN:CG	1:A:138:TYR:N	0.40	2.79	92	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:124:MET:HE3	1:A:124:MET:HB2	0.40	1.67	121	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%)	26	74
All	All	21120/23680 (89%)	20294 (96%)	730 (3%)	96 (0%)	26	74

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	42	ASN	2
1	A	95	ASP	2
1	A	20	ASP	2
1	A	55	VAL	2
1	A	33	GLY	1
1	A	102	ALA	1
1	A	142	VAL	1
1	A	129	ASP	1
1	A	40	GLY	1
1	A	121	VAL	1
1	A	35	VAL	1
1	A	125	ILE	1
1	A	84	GLU	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	112/126 (89%)	107±2 (96±2%)	5±2 (4±2%)	28	79
All	All	17920/20160 (89%)	17191 (96%)	729 (4%)	28	79

All 87 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	85	ILE	58
1	A	27	ILE	54
1	A	22	ASP	51
1	A	136	VAL	39
1	A	131	ASP	30
1	A	52	ILE	29
1	A	63	ILE	28
1	A	105	LEU	27
1	A	26	THR	26
1	A	29	THR	26
1	A	125	ILE	22
1	A	9	ILE	21
1	A	130	ILE	18
1	A	69	LEU	18
1	A	91	VAL	18
1	A	18	LEU	14
1	A	121	VAL	14
1	A	62	THR	14
1	A	142	VAL	13
1	A	109	MET	11
1	A	90	ARG	11
1	A	64	ASP	10
1	A	100	ILE	9
1	A	32	LEU	9
1	A	112	LEU	9
1	A	50	ASP	7
1	A	118	ASP	6
1	A	17	SER	6
1	A	108	VAL	5
1	A	110	THR	5
1	A	42	ASN	5
1	A	67	GLU	5
1	A	55	VAL	5
1	A	71	MET	4
1	A	95	ASP	4
1	A	122	ASP	4
1	A	133	ASP	4
1	A	38	SER	4
1	A	144	MET	3
1	A	34	THR	3
1	A	19	PHE	3
1	A	24	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	66	PRO	3
1	A	58	ASP	3
1	A	120	GLU	3
1	A	137	ASN	3
1	A	70	THR	3
1	A	6	GLU	3
1	A	116	LEU	3
1	A	124	MET	3
1	A	54	GLU	2
1	A	145	MET	2
1	A	45	GLU	2
1	A	37	ARG	2
1	A	39	LEU	2
1	A	119	GLU	2
1	A	60	ASN	2
1	A	106	ARG	2
1	A	117	THR	2
1	A	35	VAL	2
1	A	44	THR	2
1	A	111	ASN	2
1	A	139	GLU	2
1	A	36	MET	1
1	A	41	GLN	1
1	A	92	PHE	1
1	A	115	LYS	1
1	A	83	GLU	1
1	A	104	GLU	1
1	A	87	GLU	1
1	A	43	PRO	1
1	A	53	ASN	1
1	A	7	GLU	1
1	A	94	LYS	1
1	A	143	GLN	1
1	A	140	GLU	1
1	A	114	GLU	1
1	A	5	THR	1
1	A	72	MET	1
1	A	127	GLU	1
1	A	51	MET	1
1	A	129	ASP	1
1	A	107	HIS	1
1	A	48	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	21	LYS	1
1	A	47	GLU	1
1	A	56	ASP	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides 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