



Full wwPDB NMR Structure Validation Report ⓘ

Mar 20, 2026 – 01:34 AM UTC

PDB ID : 2K0F / pdb_00002k0f
Title : Calmodulin complexed with calmodulin-binding peptide from smooth muscle myosin light chain kinase
Authors : Gsponer, J.; Christodoulou, J.; Cavalli, A.; Bui, J.M.; Richter, B.; Dobson, C.M.; Vendruscolo, M.
Deposited on : 2008-02-02

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

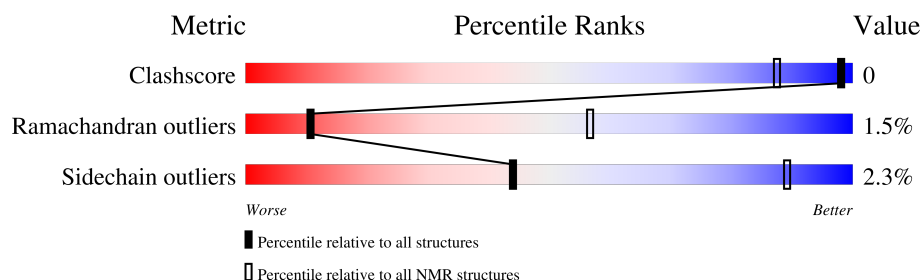
1 Overall quality at a glance

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	B	19	

2 Ensemble composition and analysis

This entry contains 160 models. Model 54 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:142, B:1-B:16 (156)	1.38	54

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 13 clusters and 7 single-model clusters were found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2494 atoms, of which 1213 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called calmodulin.

Mol	Chain	Residues	Atoms						Trace
1	A	142	Total	C	H	N	O	S	0
			2168	687	1047	180	245	9	

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

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

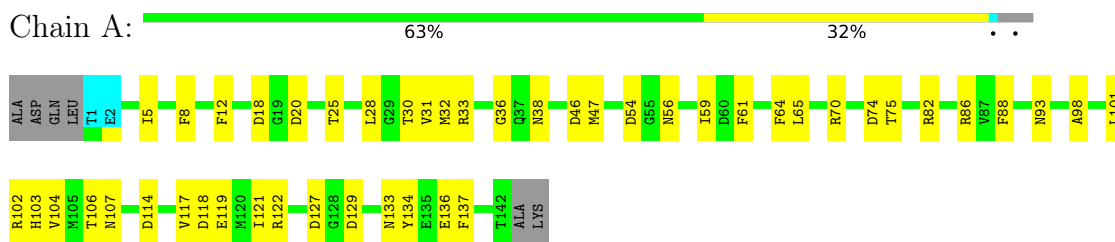
Mol	Chain	Residues	Atoms	
3	A	4	Total	Ca
			4	4

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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



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



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

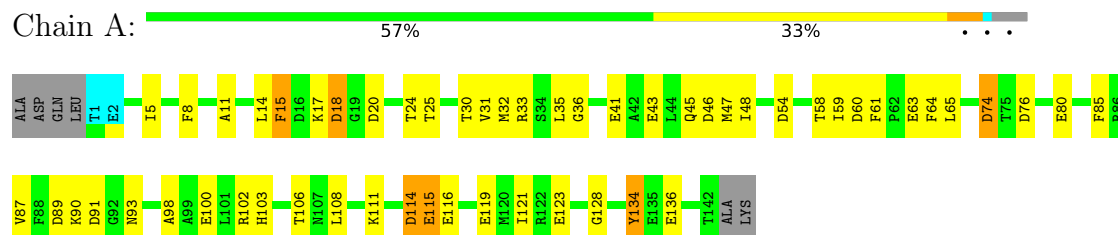


- Molecule 2: 19-mer peptide from Myosin light chain kinase

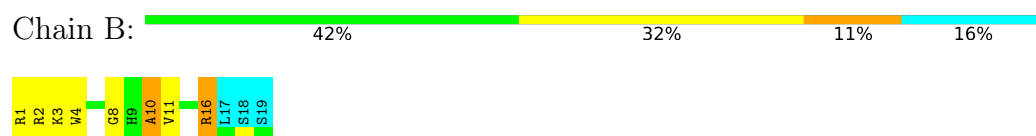


4.2.2 Score per residue for model 2

- Molecule 1: calmodulin

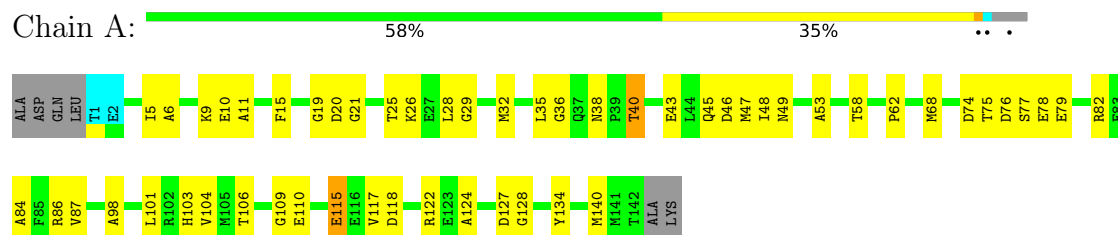


- Molecule 2: 19-mer peptide from Myosin light chain kinase

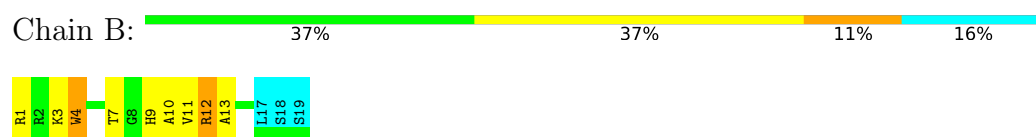


4.2.3 Score per residue for model 3

- Molecule 1: calmodulin

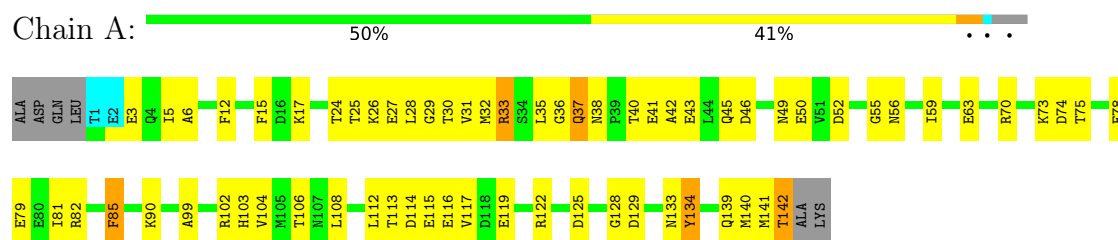


- Molecule 2: 19-mer peptide from Myosin light chain kinase

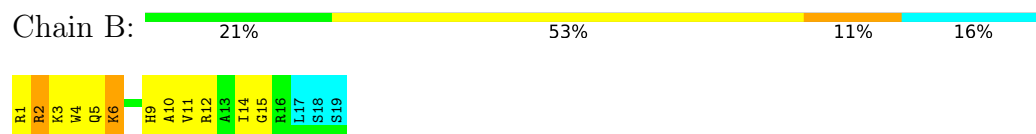


4.2.4 Score per residue for model 4

- Molecule 1: calmodulin

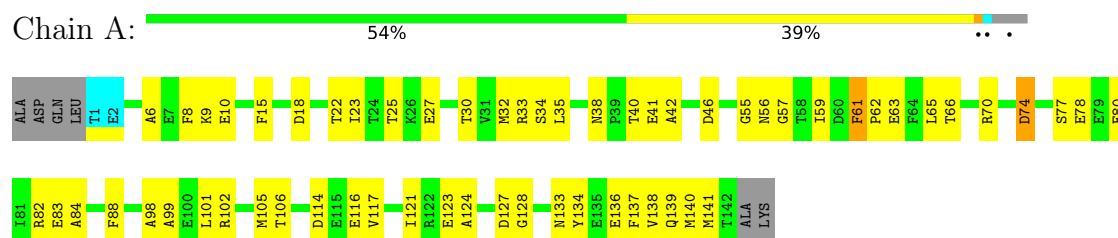


- Molecule 2: 19-mer peptide from Myosin light chain kinase

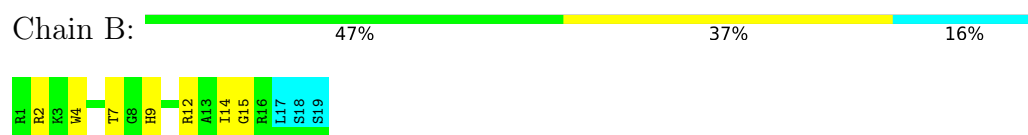


4.2.5 Score per residue for model 5

- Molecule 1: calmodulin

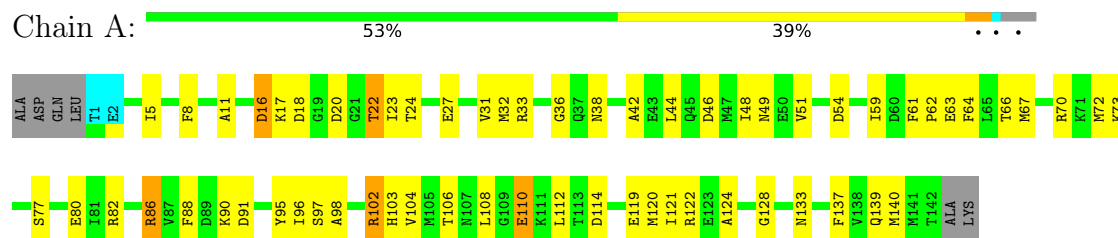


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.6 Score per residue for model 6

- Molecule 1: calmodulin



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

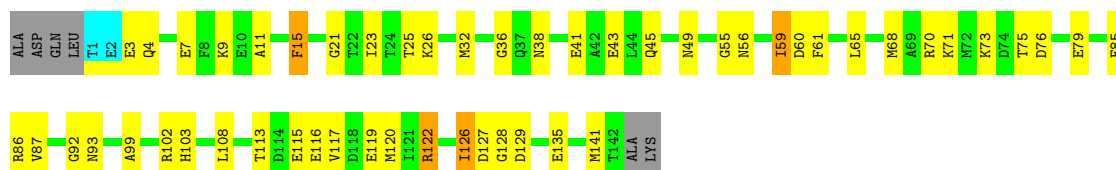




4.2.7 Score per residue for model 7

- Molecule 1: calmodulin

Chain A: 59% 32% ..



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

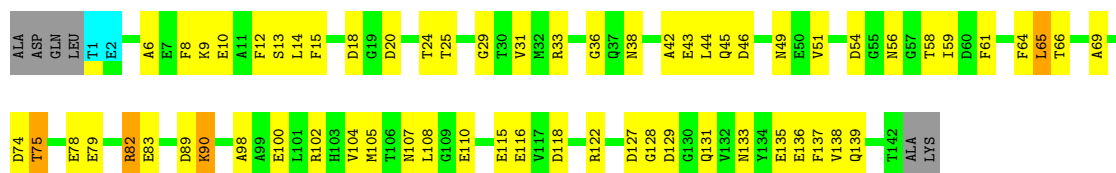
Chain B: 42% 32% 11% 16%



4.2.8 Score per residue for model 8

- Molecule 1: calmodulin

Chain A: 52% 40% ..



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

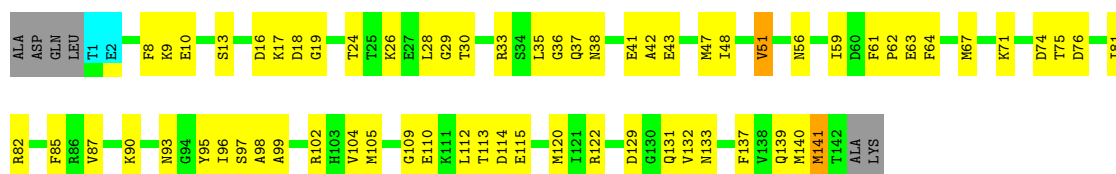
Chain B: 42% 42% 16%



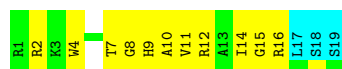
4.2.9 Score per residue for model 9

- Molecule 1: calmodulin

Chain A: 51% 43% ..

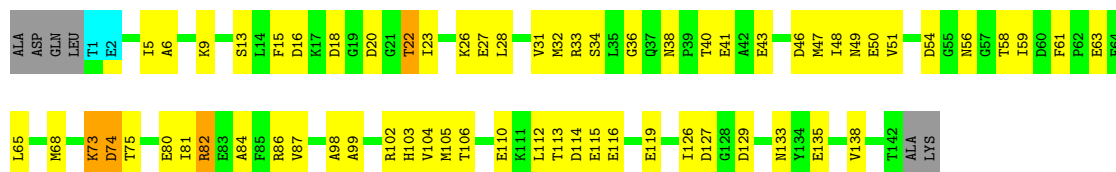


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.10 Score per residue for model 10

- Molecule 1: calmodulin

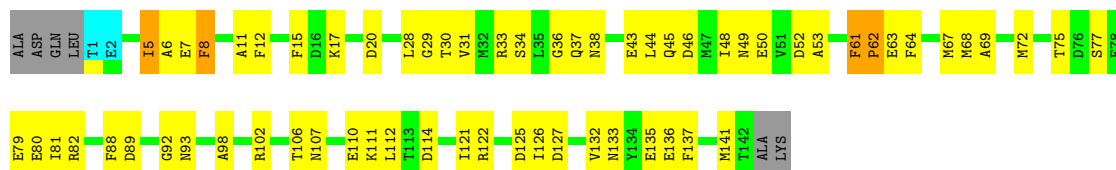


- Molecule 2: 19-mer peptide from Myosin light chain kinase



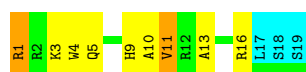
4.2.11 Score per residue for model 11

- Molecule 1: calmodulin



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

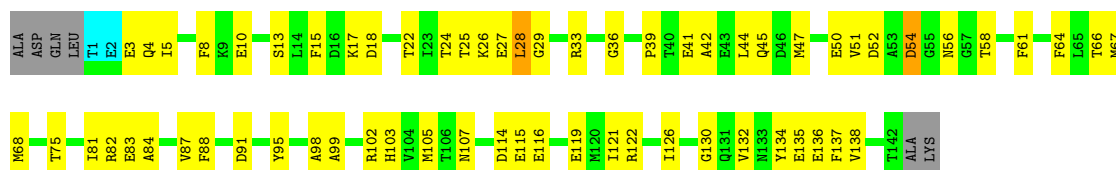




4.2.12 Score per residue for model 12

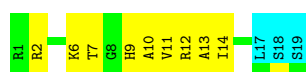
- Molecule 1: calmodulin

Chain A: 51% 42% ..



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

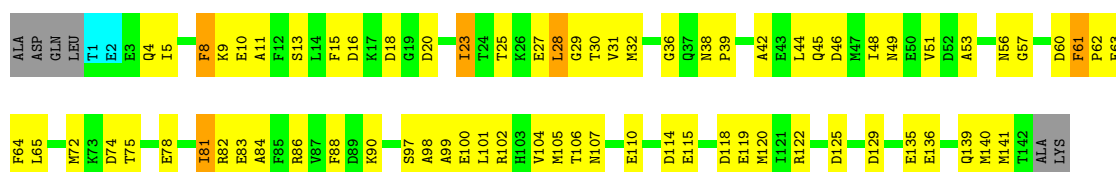
Chain B: 37% 47% 16%



4.2.13 Score per residue for model 13

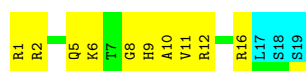
- Molecule 1: calmodulin

Chain A: 45% 46% ..



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

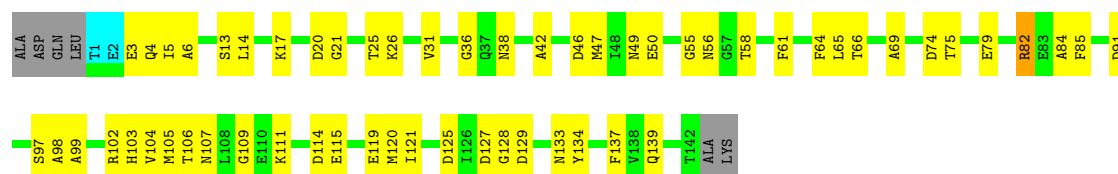
Chain B: 32% 53% 16%



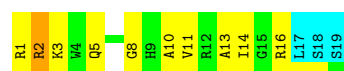
4.2.14 Score per residue for model 14

- Molecule 1: calmodulin

Chain A: 55% 39% ..

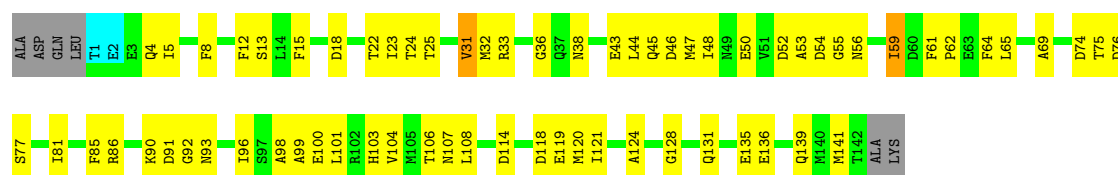


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.15 Score per residue for model 15

- Molecule 1: calmodulin

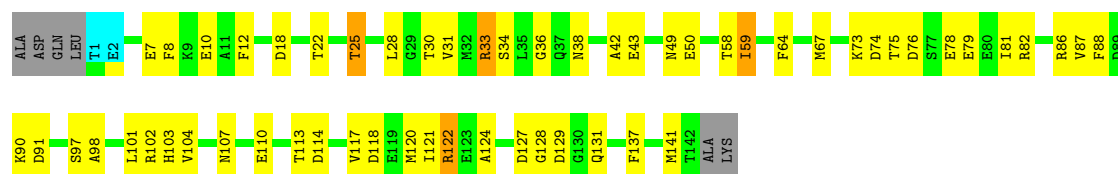


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.16 Score per residue for model 16

- Molecule 1: calmodulin



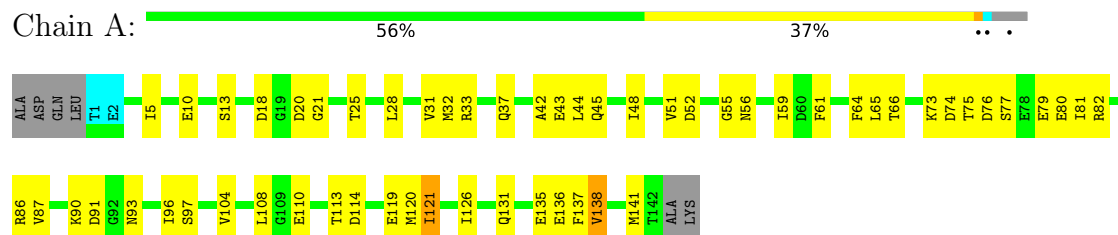
- Molecule 2: 19-mer peptide from Myosin light chain kinase





4.2.17 Score per residue for model 17

- Molecule 1: calmodulin

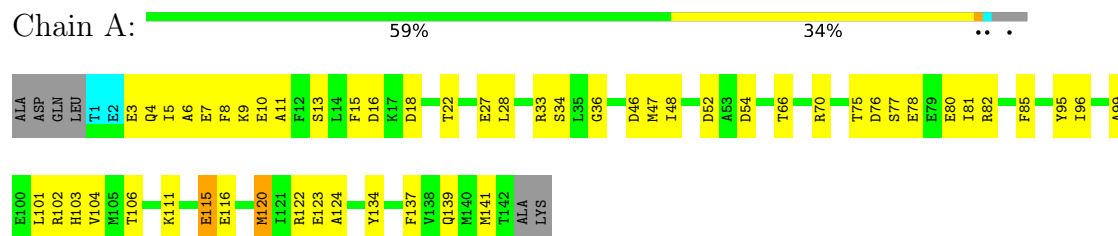


- Molecule 2: 19-mer peptide from Myosin light chain kinase

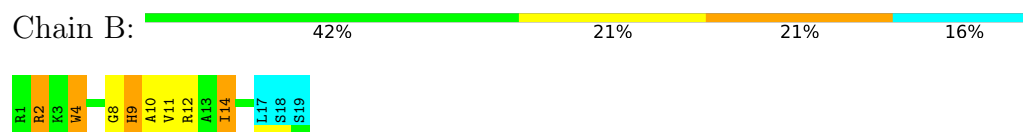


4.2.18 Score per residue for model 18

- Molecule 1: calmodulin



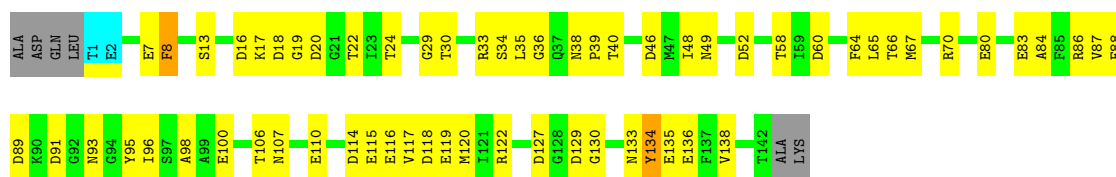
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.19 Score per residue for model 19

- Molecule 1: calmodulin



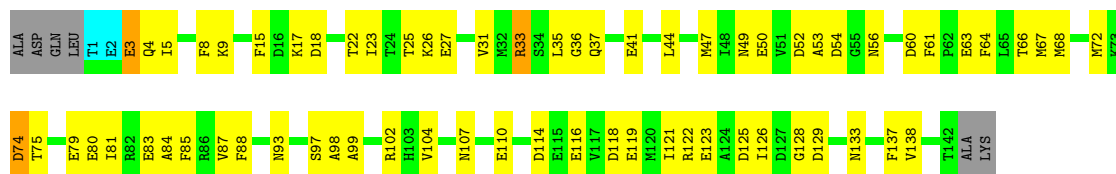


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.20 Score per residue for model 20

- Molecule 1: calmodulin

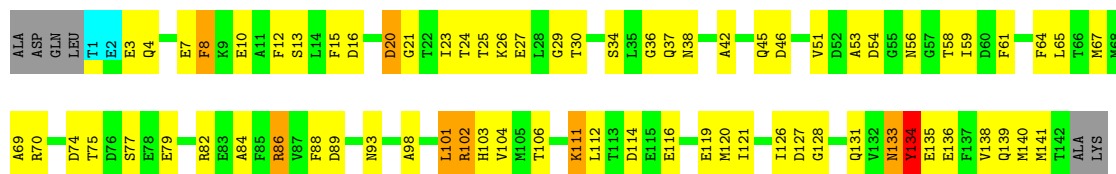


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.21 Score per residue for model 21

- Molecule 1: calmodulin



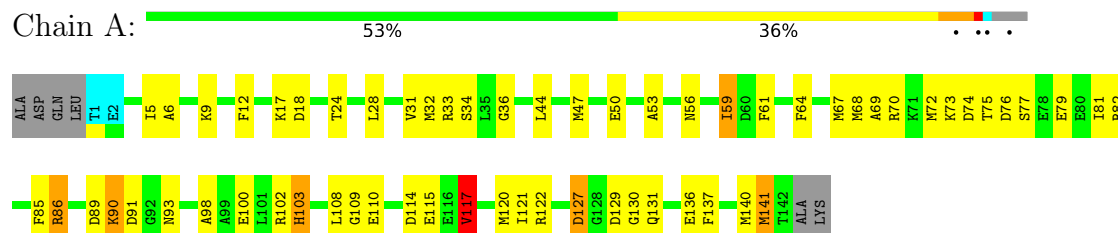
- Molecule 2: 19-mer peptide from Myosin light chain kinase





4.2.22 Score per residue for model 22

- Molecule 1: calmodulin

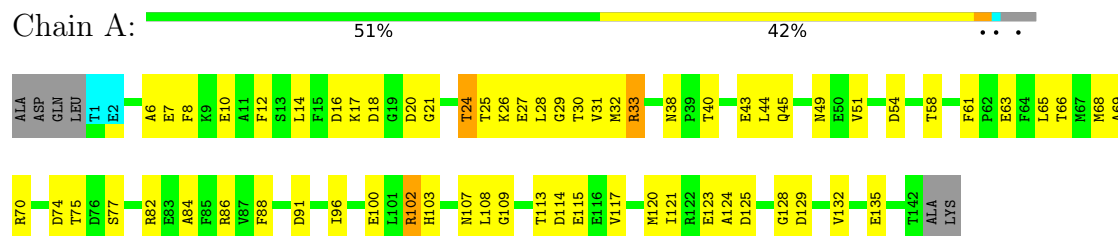


- Molecule 2: 19-mer peptide from Myosin light chain kinase

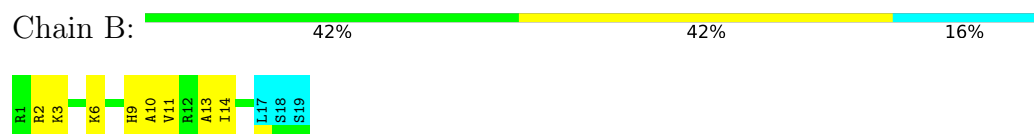


4.2.23 Score per residue for model 23

- Molecule 1: calmodulin



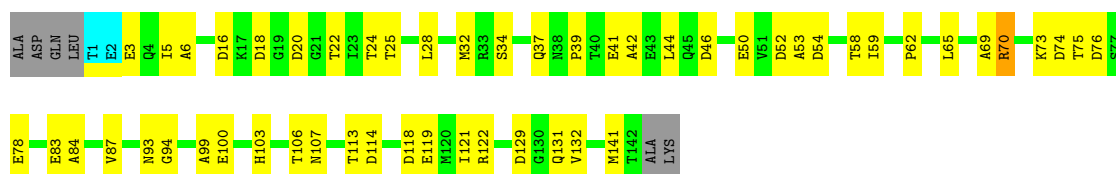
- Molecule 2: 19-mer peptide from Myosin light chain kinase



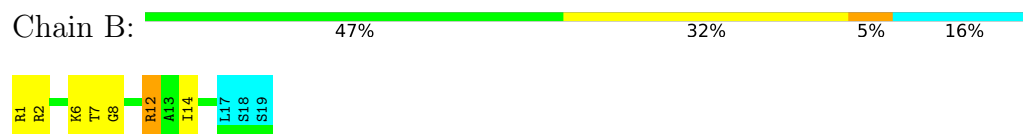
4.2.24 Score per residue for model 24

- Molecule 1: calmodulin



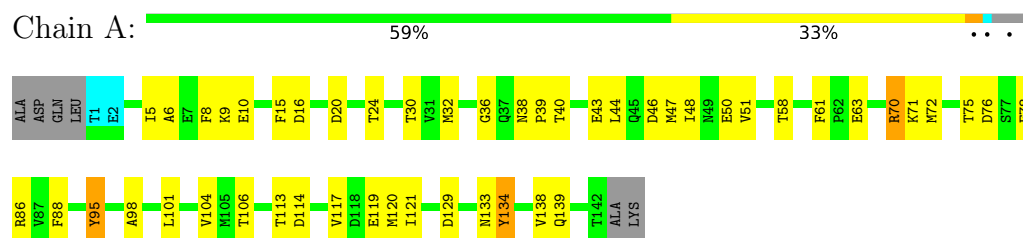


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.25 Score per residue for model 25

- Molecule 1: calmodulin

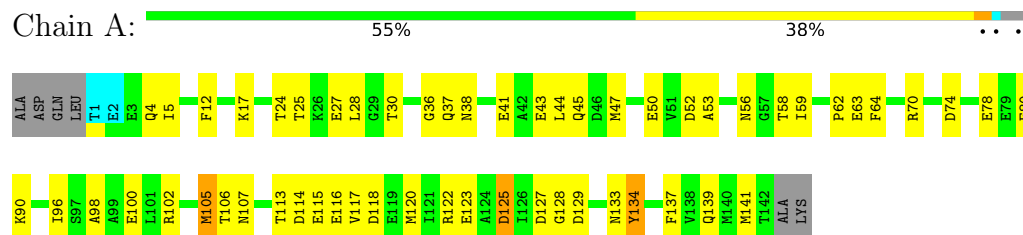


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.26 Score per residue for model 26

- Molecule 1: calmodulin



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





4.2.27 Score per residue for model 27

- Molecule 1: calmodulin

Chain A: 54% 39%



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

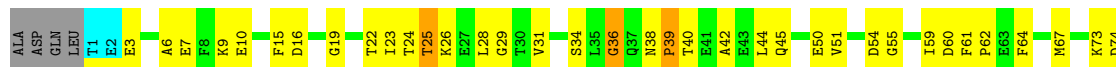
Chain B: 32% 47% 5% 16%



4.2.28 Score per residue for model 28

- Molecule 1: calmodulin

Chain A: 52% 40%



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

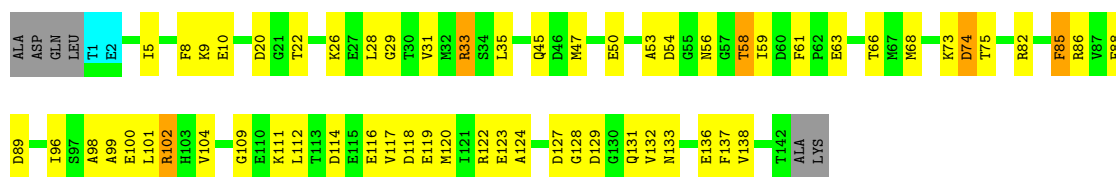
Chain B: 26% 47% 11% 16%



4.2.29 Score per residue for model 29

- Molecule 1: calmodulin

Chain A: 54% 37%



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

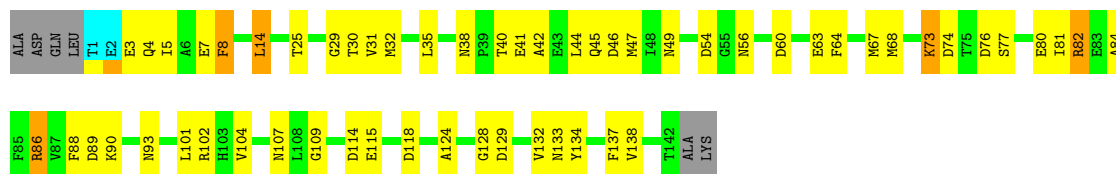
Chain B: 47% 16% 21% 16%



4.2.30 Score per residue for model 30

- Molecule 1: calmodulin

Chain A: 56% 35% ..



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

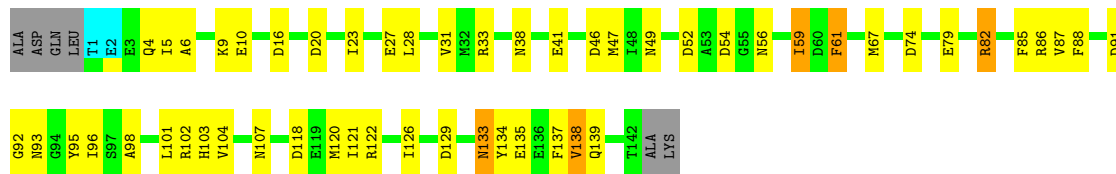
Chain B: 47% 32% 5% 16%



4.2.31 Score per residue for model 31

- Molecule 1: calmodulin

Chain A: 59% 32% ..



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

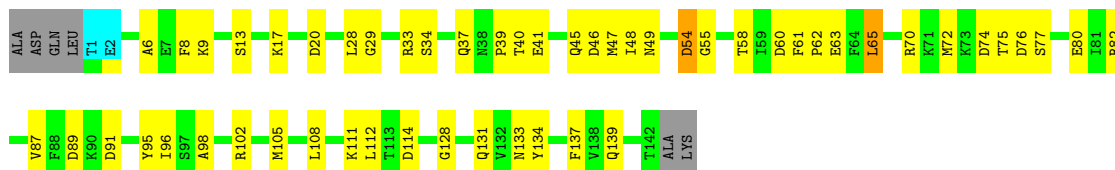
Chain B: 37% 42% 5% 16%



4.2.32 Score per residue for model 32

- Molecule 1: calmodulin

Chain A: 59% 34% ..



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

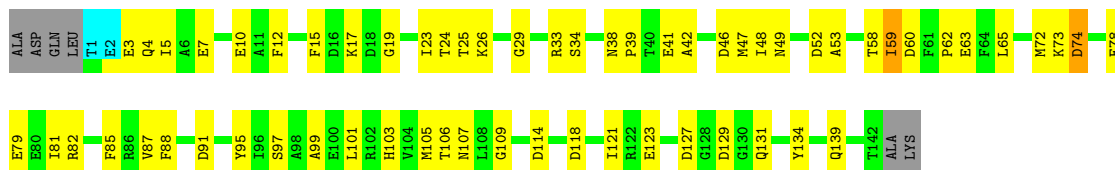
Chain B: 26% 58% 16%



4.2.33 Score per residue for model 33

- Molecule 1: calmodulin

Chain A: 53% 40% ..



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

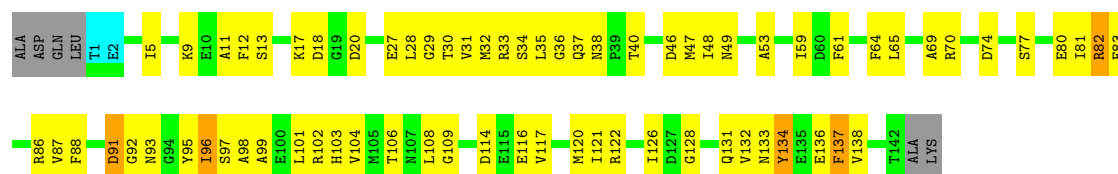
Chain B: 47% 26% 11% 16%



4.2.34 Score per residue for model 34

- Molecule 1: calmodulin

Chain A: 47% 45% ..

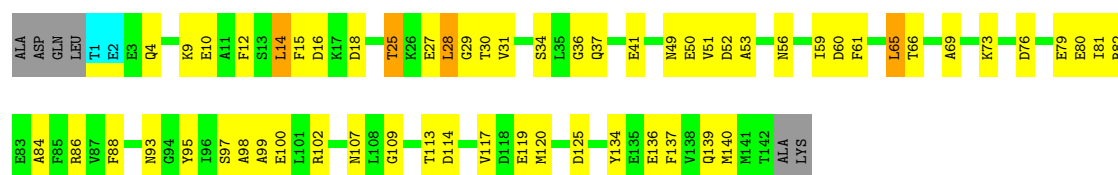


- Molecule 2: 19-mer peptide from Myosin light chain kinase

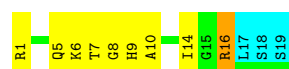


4.2.35 Score per residue for model 35

- Molecule 1: calmodulin

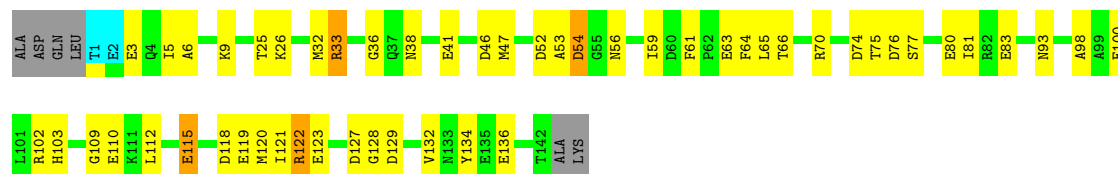


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.36 Score per residue for model 36

- Molecule 1: calmodulin



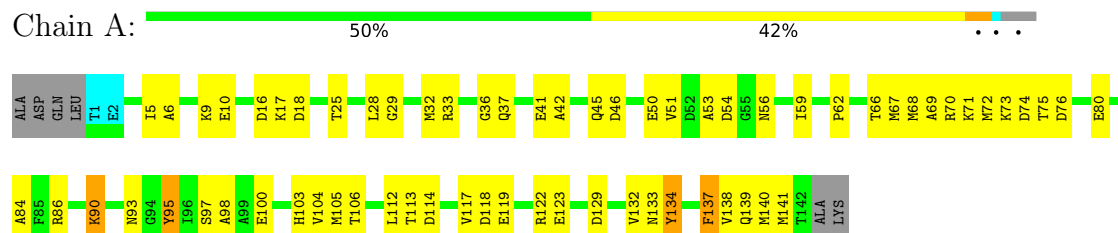
- Molecule 2: 19-mer peptide from Myosin light chain kinase



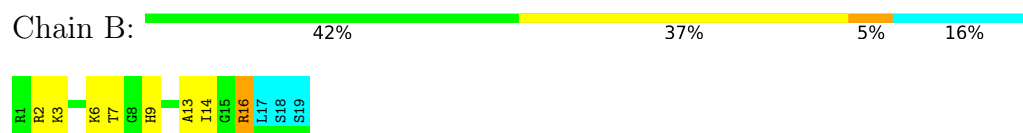


4.2.37 Score per residue for model 37

- Molecule 1: calmodulin

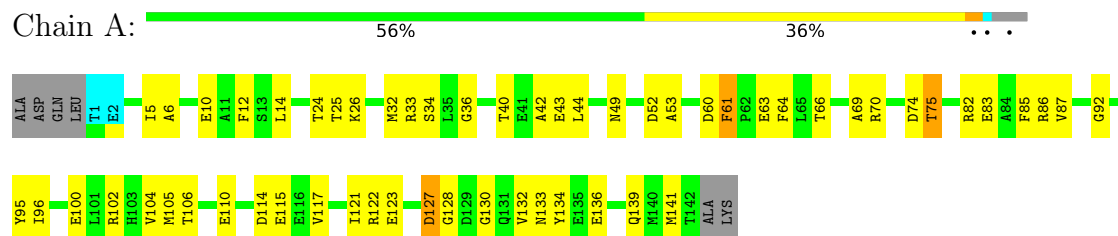


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.38 Score per residue for model 38

- Molecule 1: calmodulin



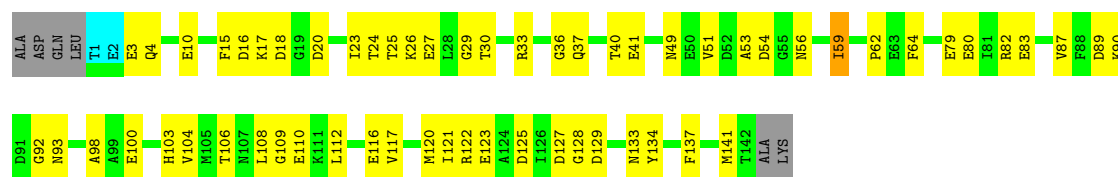
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.39 Score per residue for model 39

- Molecule 1: calmodulin



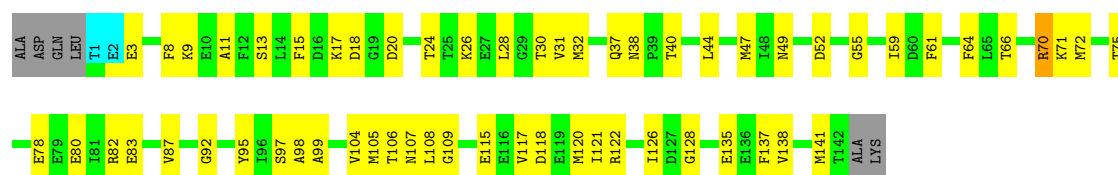


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.40 Score per residue for model 40

- Molecule 1: calmodulin

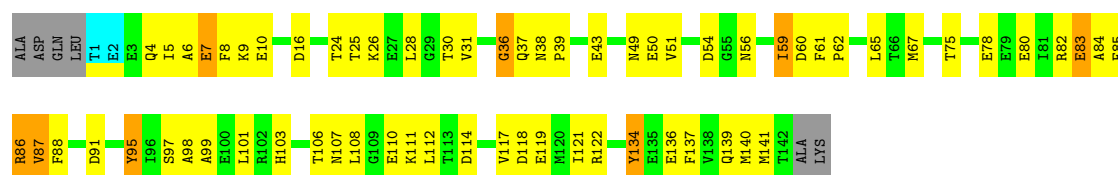


- Molecule 2: 19-mer peptide from Myosin light chain kinase



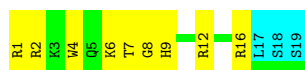
4.2.41 Score per residue for model 41

- Molecule 1: calmodulin



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





4.2.42 Score per residue for model 42

- Molecule 1: calmodulin

Chain A: 51% 40% ..



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

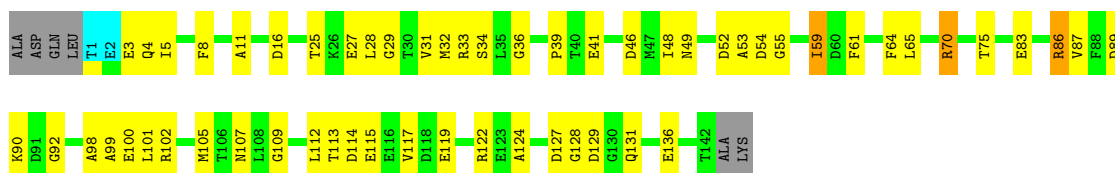
Chain B: 58% 21% 5% 16%



4.2.43 Score per residue for model 43

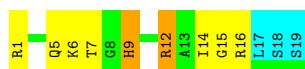
- Molecule 1: calmodulin

Chain A: 56% 36% ..



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

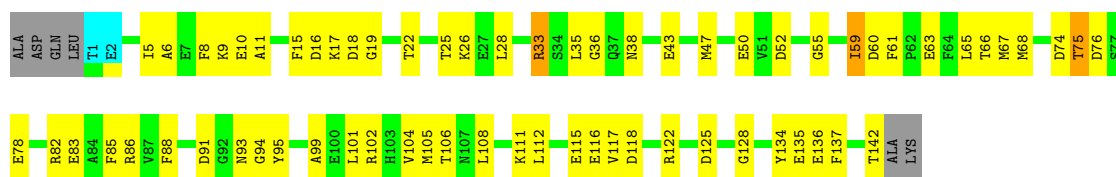
Chain B: 37% 37% 11% 16%



4.2.44 Score per residue for model 44

- Molecule 1: calmodulin

Chain A: 50% 43% ..



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



4.2.45 Score per residue for model 45

- Molecule 1: calmodulin

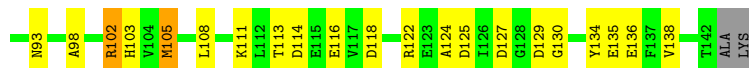


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.46 Score per residue for model 46

- Molecule 1: calmodulin



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

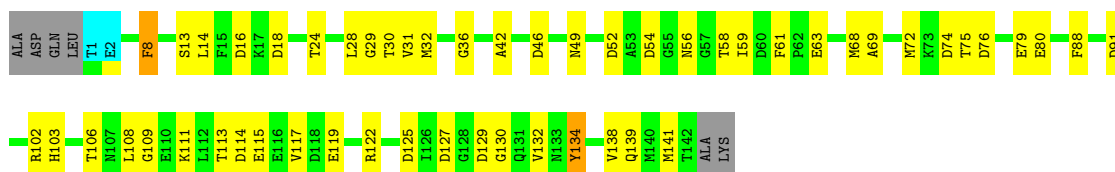




4.2.47 Score per residue for model 47

- Molecule 1: calmodulin

Chain A: 59% 34% ..



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

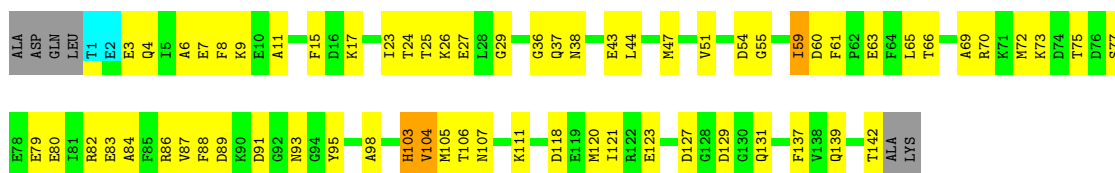
Chain B: 58% 26% 16%



4.2.48 Score per residue for model 48

- Molecule 1: calmodulin

Chain A: 51% 42% ..



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

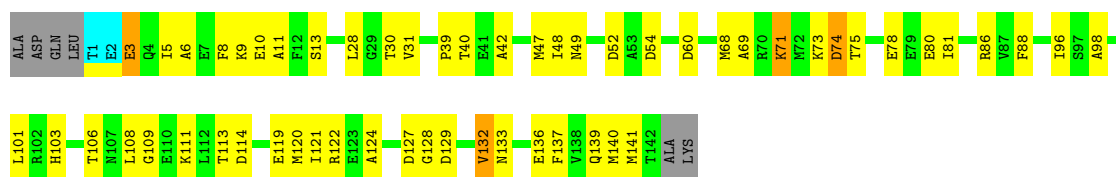
Chain B: 21% 63% 16%



4.2.49 Score per residue for model 49

- Molecule 1: calmodulin

Chain A: 57% 35% ..

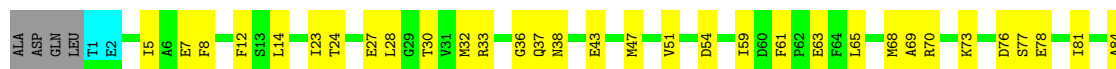


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.50 Score per residue for model 50

- Molecule 1: calmodulin

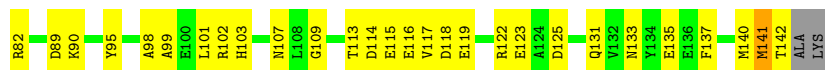
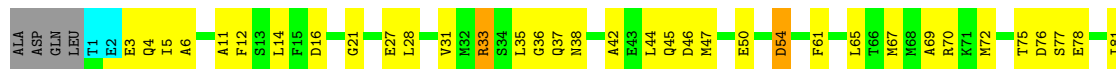


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.51 Score per residue for model 51

- Molecule 1: calmodulin



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





4.2.52 Score per residue for model 52

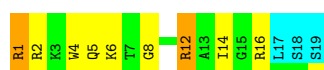
- Molecule 1: calmodulin

Chain A: 55% 37% ..



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

Chain B: 37% 37% 11% 16%



4.2.53 Score per residue for model 53

- Molecule 1: calmodulin

Chain A: 57% 34% ...



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

Chain B: 47% 32% 5% 16%



4.2.54 Score per residue for model 54 (medoid)

- Molecule 1: calmodulin

Chain A: 51% 42% ..

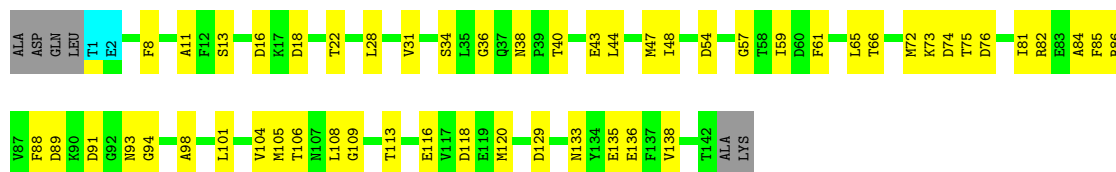


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.55 Score per residue for model 55

- Molecule 1: calmodulin

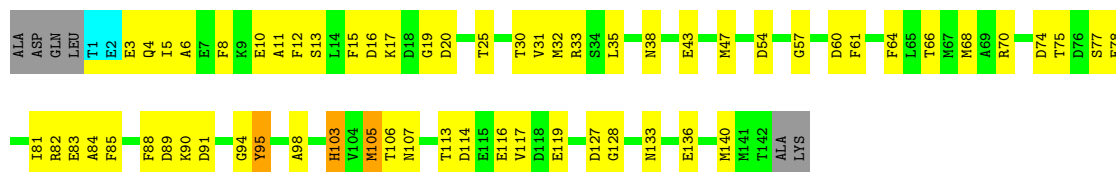


- Molecule 2: 19-mer peptide from Myosin light chain kinase



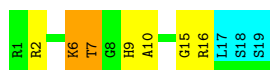
4.2.56 Score per residue for model 56

- Molecule 1: calmodulin



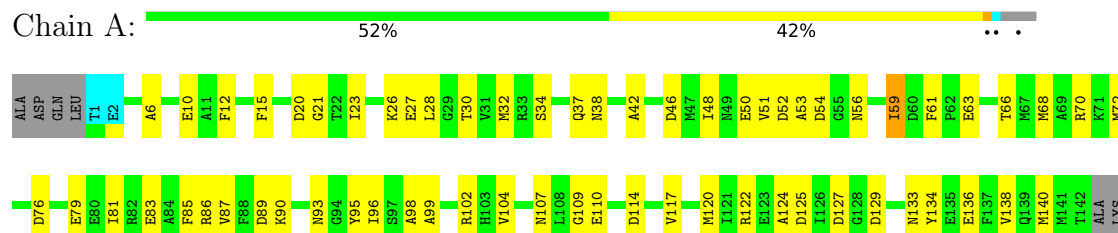
- Molecule 2: 19-mer peptide from Myosin light chain kinase



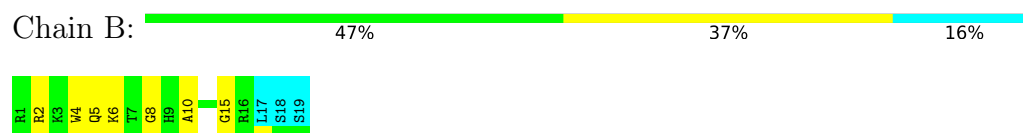


4.2.57 Score per residue for model 57

- Molecule 1: calmodulin



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

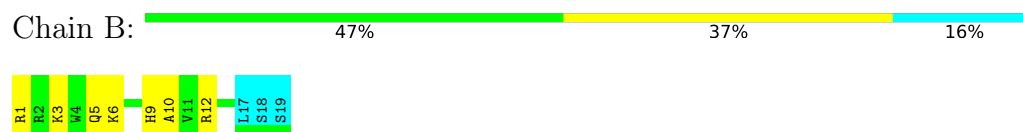


4.2.58 Score per residue for model 58

- Molecule 1: calmodulin



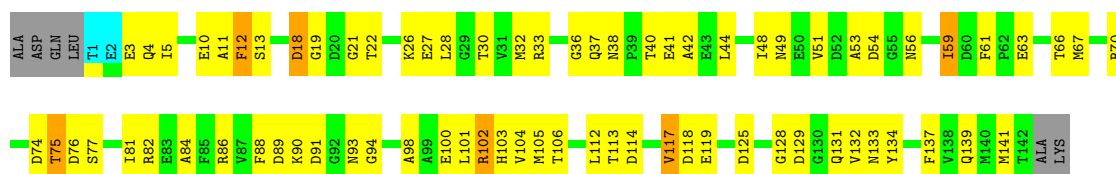
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.59 Score per residue for model 59

- Molecule 1: calmodulin



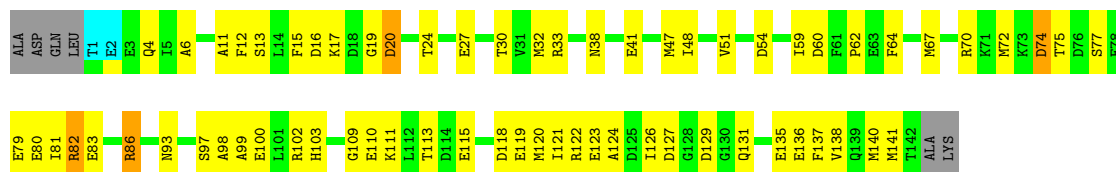


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.60 Score per residue for model 60

- Molecule 1: calmodulin

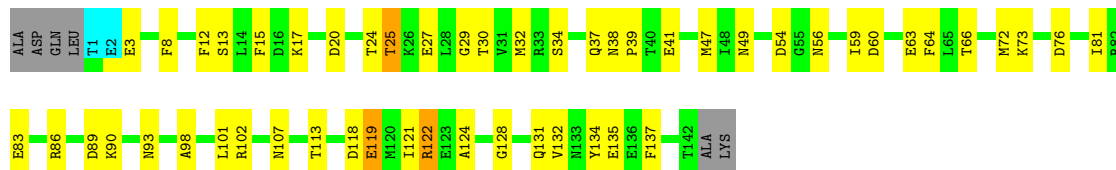


- Molecule 2: 19-mer peptide from Myosin light chain kinase



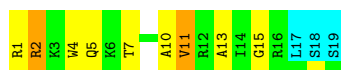
4.2.61 Score per residue for model 61

- Molecule 1: calmodulin



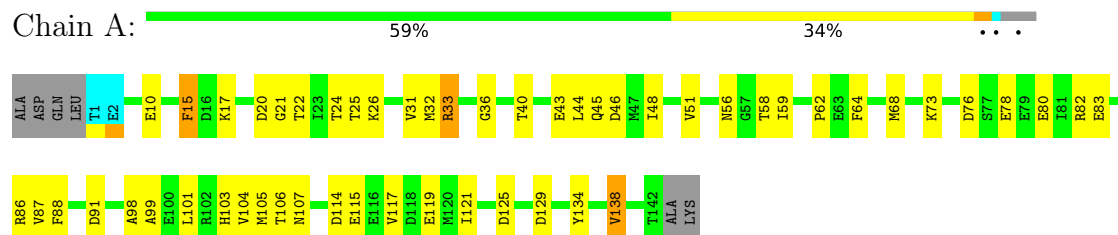
- Molecule 2: 19-mer peptide from Myosin light chain kinase



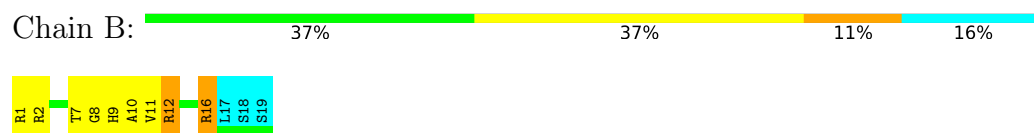


4.2.62 Score per residue for model 62

- Molecule 1: calmodulin

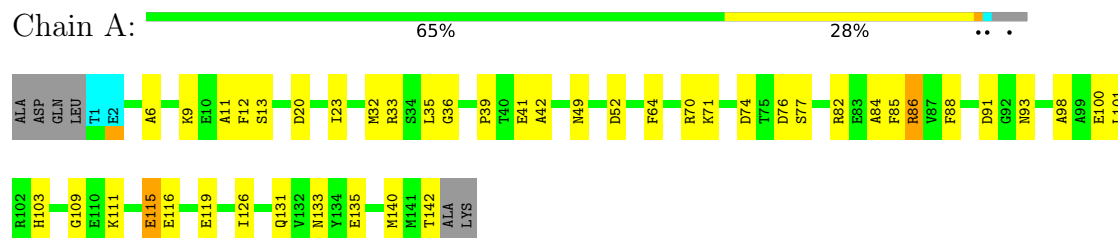


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.63 Score per residue for model 63

- Molecule 1: calmodulin



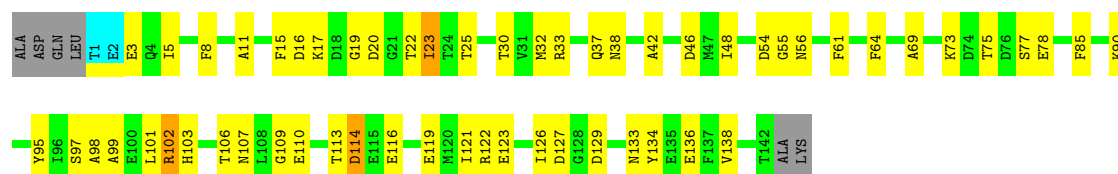
- Molecule 2: 19-mer peptide from Myosin light chain kinase



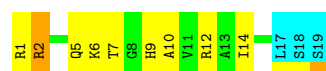
4.2.64 Score per residue for model 64

- Molecule 1: calmodulin



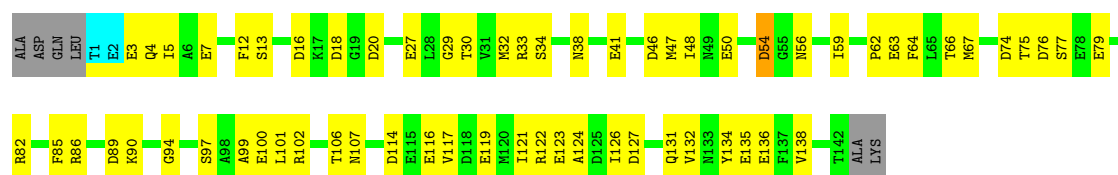


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.65 Score per residue for model 65

- Molecule 1: calmodulin

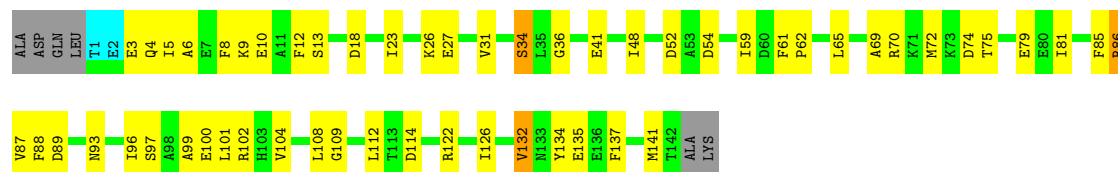


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.66 Score per residue for model 66

- Molecule 1: calmodulin



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



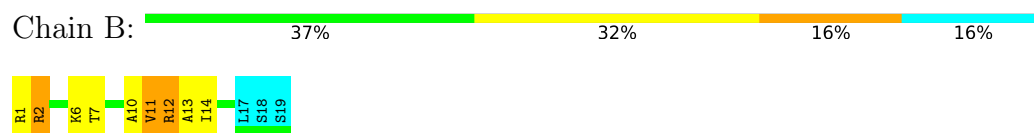


4.2.67 Score per residue for model 67

- Molecule 1: calmodulin

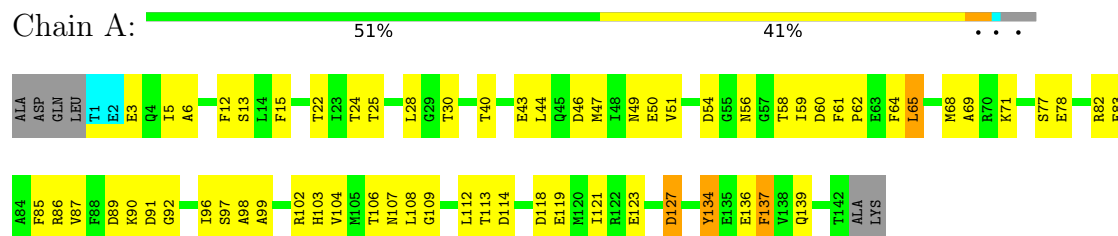


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.68 Score per residue for model 68

- Molecule 1: calmodulin



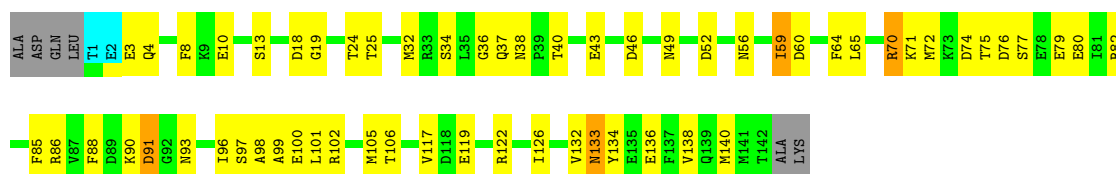
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.69 Score per residue for model 69

- Molecule 1: calmodulin



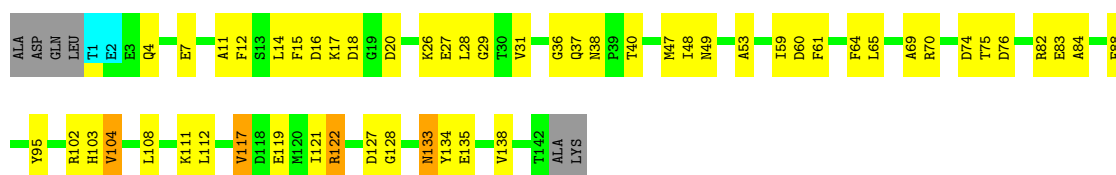


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.70 Score per residue for model 70

- Molecule 1: calmodulin

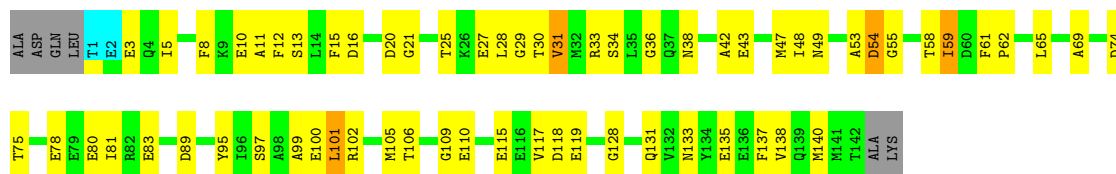


- Molecule 2: 19-mer peptide from Myosin light chain kinase



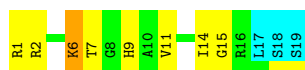
4.2.71 Score per residue for model 71

- Molecule 1: calmodulin



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





4.2.72 Score per residue for model 72

- Molecule 1: calmodulin

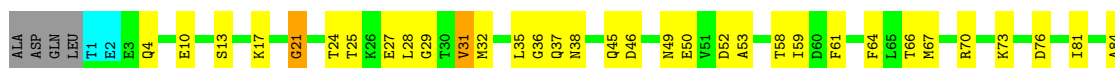


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.73 Score per residue for model 73

- Molecule 1: calmodulin



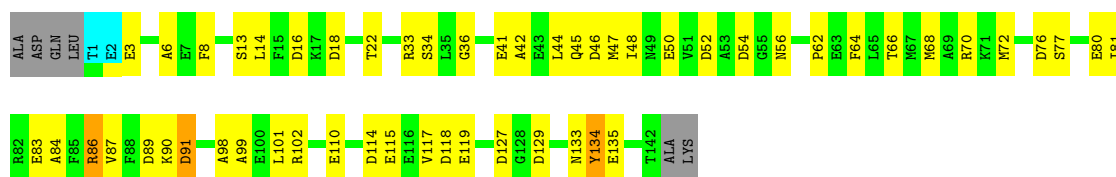
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.74 Score per residue for model 74

- Molecule 1: calmodulin



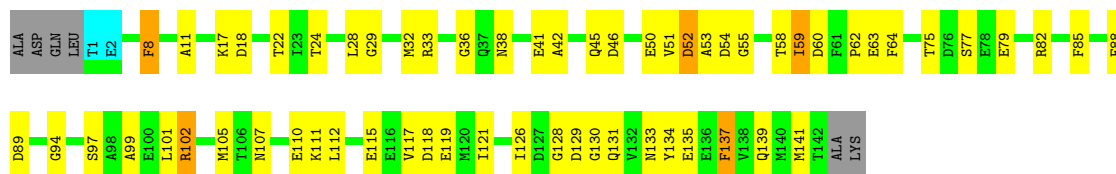


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.75 Score per residue for model 75

- Molecule 1: calmodulin

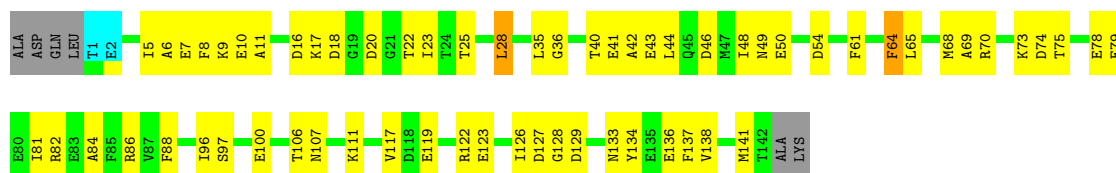


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.76 Score per residue for model 76

- Molecule 1: calmodulin



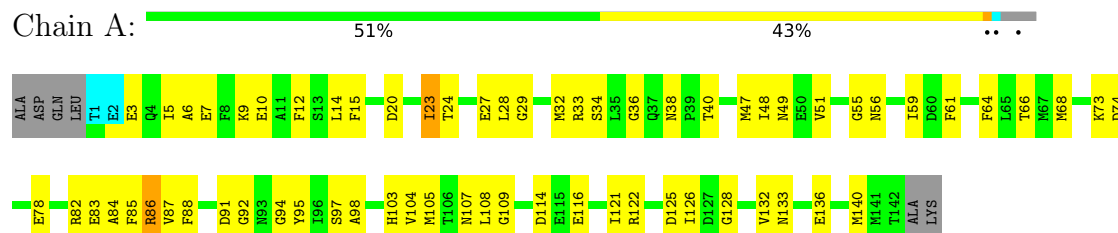
- Molecule 2: 19-mer peptide from Myosin light chain kinase





4.2.77 Score per residue for model 77

- Molecule 1: calmodulin

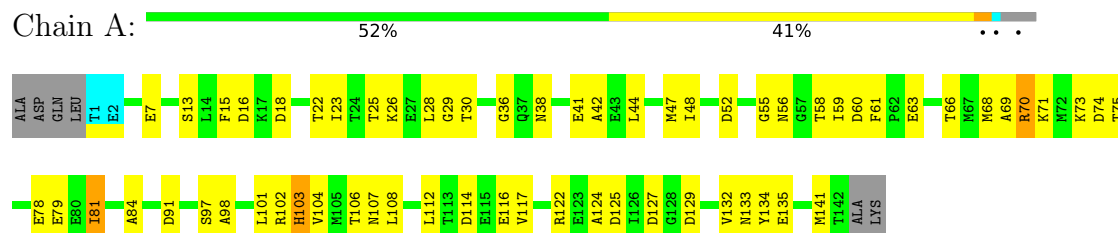


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.78 Score per residue for model 78

- Molecule 1: calmodulin



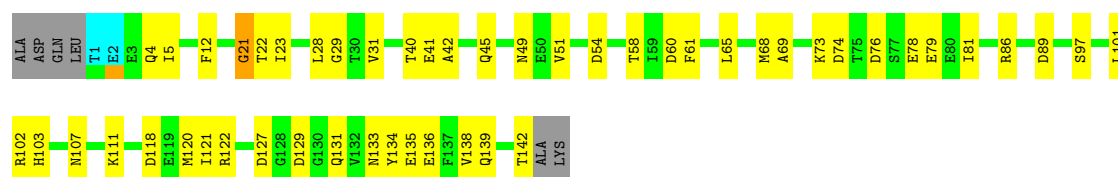
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.79 Score per residue for model 79

- Molecule 1: calmodulin



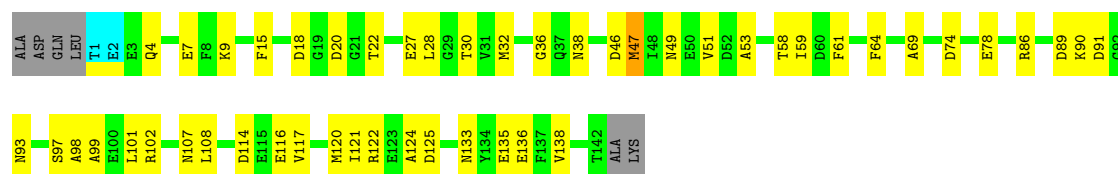


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.80 Score per residue for model 80

- Molecule 1: calmodulin

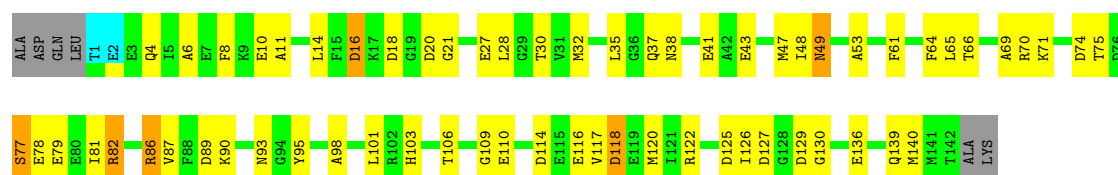


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.81 Score per residue for model 81

- Molecule 1: calmodulin



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

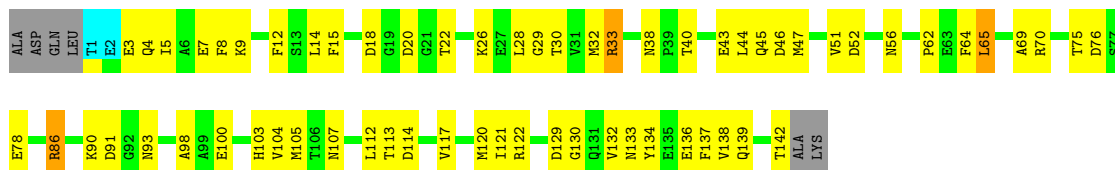




4.2.82 Score per residue for model 82

- Molecule 1: calmodulin

Chain A: 52% 41% ..



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

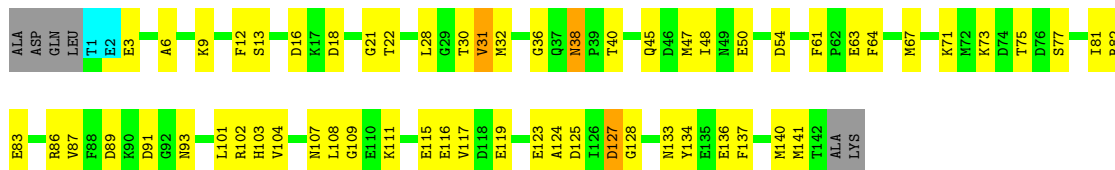
Chain B: 47% 32% 5% 16%



4.2.83 Score per residue for model 83

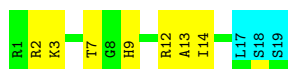
- Molecule 1: calmodulin

Chain A: 54% 39% ..



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

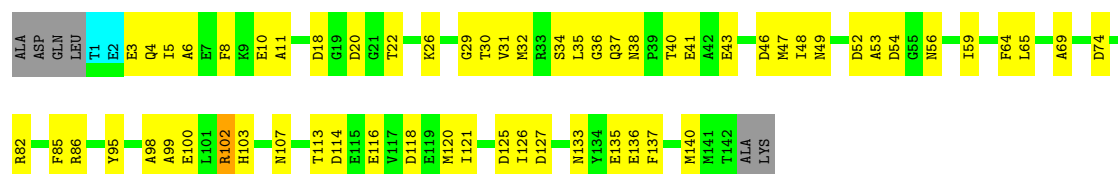
Chain B: 47% 37% 16%



4.2.84 Score per residue for model 84

- Molecule 1: calmodulin

Chain A: 54% 40% ..

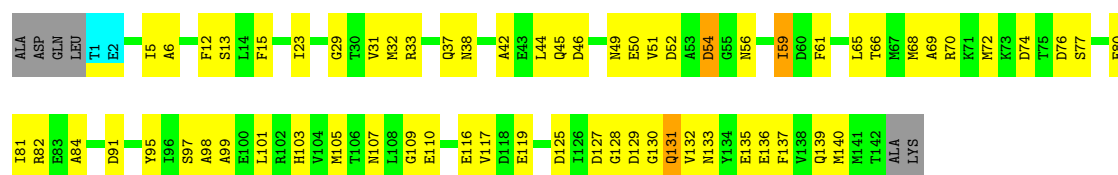


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.85 Score per residue for model 85

- Molecule 1: calmodulin

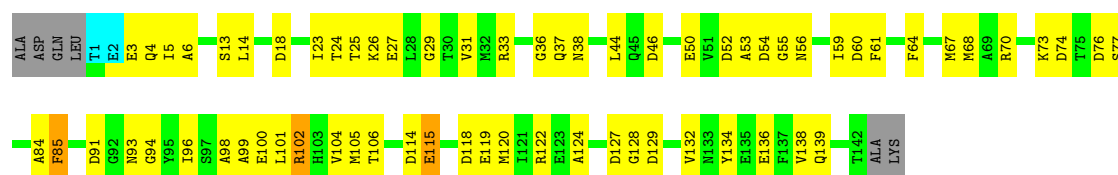


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.86 Score per residue for model 86

- Molecule 1: calmodulin



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

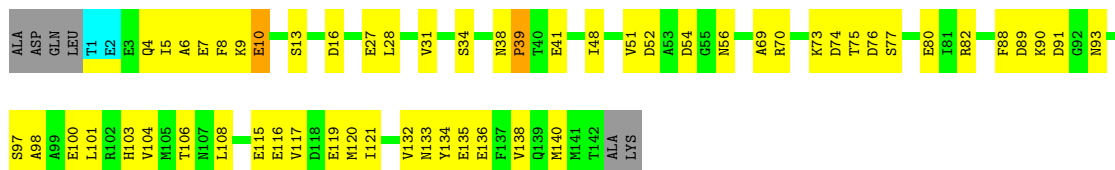




4.2.87 Score per residue for model 87

- Molecule 1: calmodulin

Chain A: 57% 36%



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

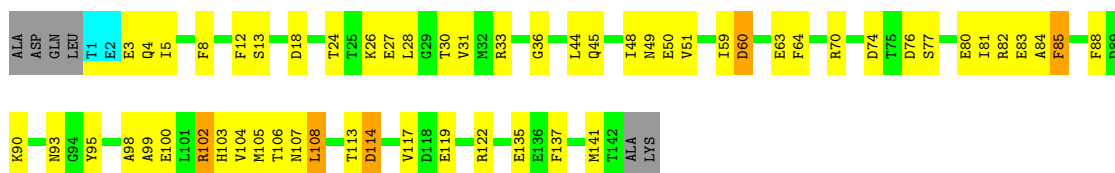
Chain B: 37% 42% 5% 16%



4.2.88 Score per residue for model 88

- Molecule 1: calmodulin

Chain A: 56% 35%



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

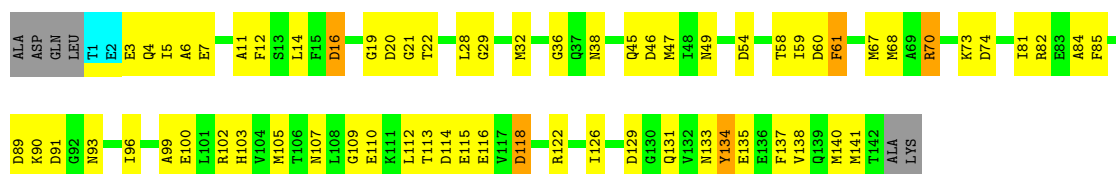
Chain B: 58% 26% 16%



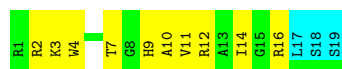
4.2.89 Score per residue for model 89

- Molecule 1: calmodulin

Chain A: 50% 41%

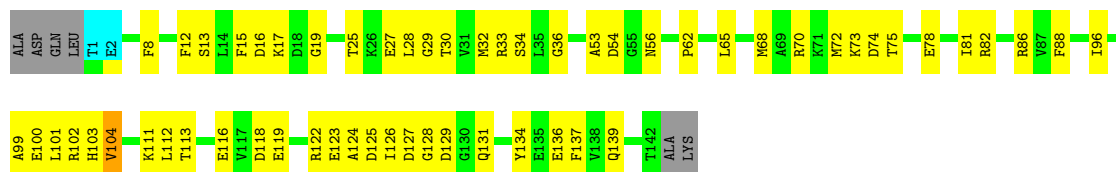


- Molecule 2: 19-mer peptide from Myosin light chain kinase

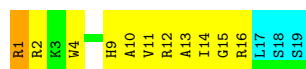


4.2.90 Score per residue for model 90

- Molecule 1: calmodulin

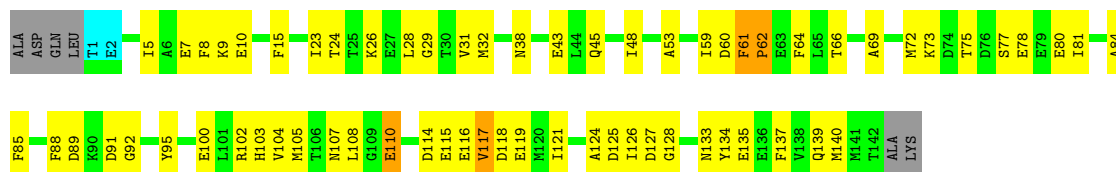


- Molecule 2: 19-mer peptide from Myosin light chain kinase



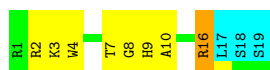
4.2.91 Score per residue for model 91

- Molecule 1: calmodulin



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

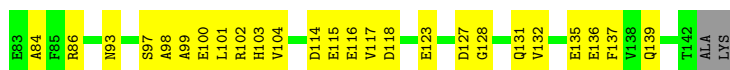




4.2.92 Score per residue for model 92

- Molecule 1: calmodulin

Chain A: 53% 40% ..



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

Chain B: 42% 42% 16%



4.2.93 Score per residue for model 93

- Molecule 1: calmodulin

Chain A: 50% 43% ..



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

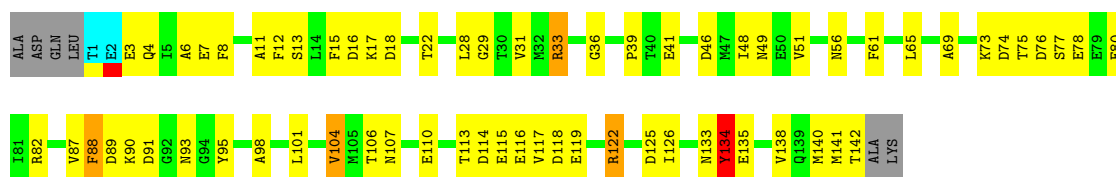
Chain B: 53% 32% 16%



4.2.94 Score per residue for model 94

- Molecule 1: calmodulin

Chain A: 50% 41% ..



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



4.2.95 Score per residue for model 95

- Molecule 1: calmodulin



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



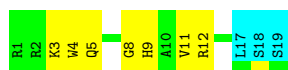
4.2.96 Score per residue for model 96

- Molecule 1: calmodulin



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

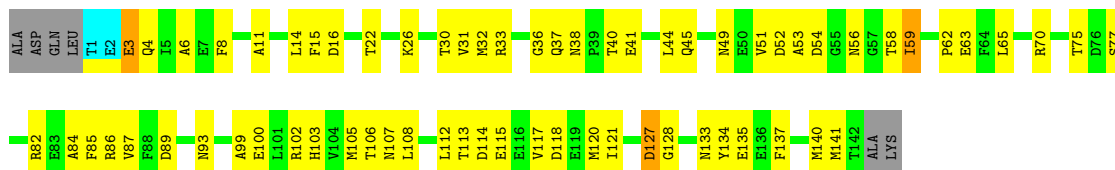




4.2.97 Score per residue for model 97

- Molecule 1: calmodulin

Chain A: 50% 43%



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

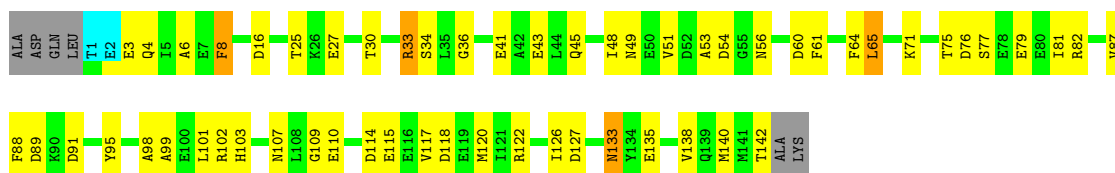
Chain B: 58% 26% 16%



4.2.98 Score per residue for model 98

- Molecule 1: calmodulin

Chain A: 56% 36%



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

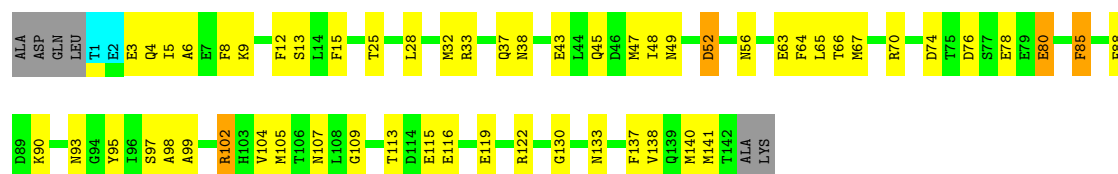
Chain B: 21% 42% 16% 5% 16%



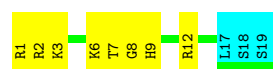
4.2.99 Score per residue for model 99

- Molecule 1: calmodulin

Chain A: 57% 35%



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



4.2.100 Score per residue for model 100

- Molecule 1: calmodulin

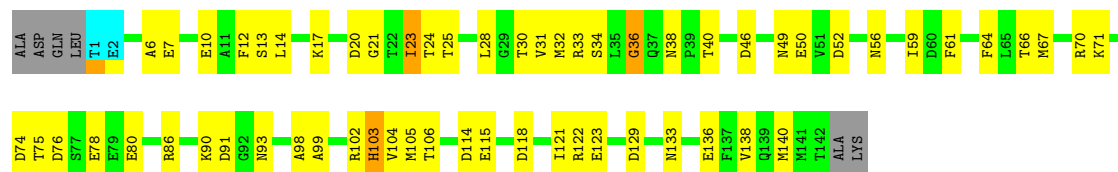


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.101 Score per residue for model 101

- Molecule 1: calmodulin



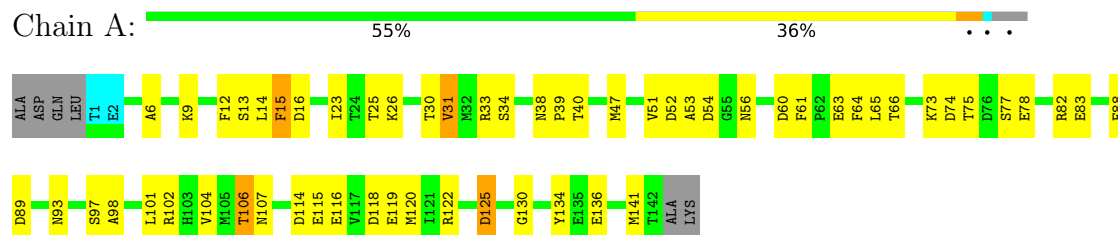
- Molecule 2: 19-mer peptide from Myosin light chain kinase



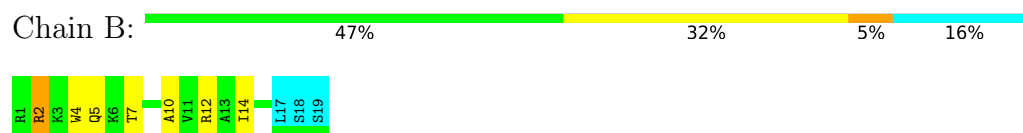


4.2.102 Score per residue for model 102

- Molecule 1: calmodulin

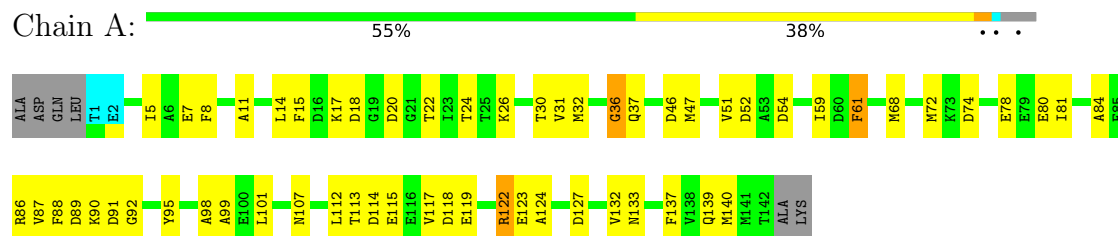


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.103 Score per residue for model 103

- Molecule 1: calmodulin



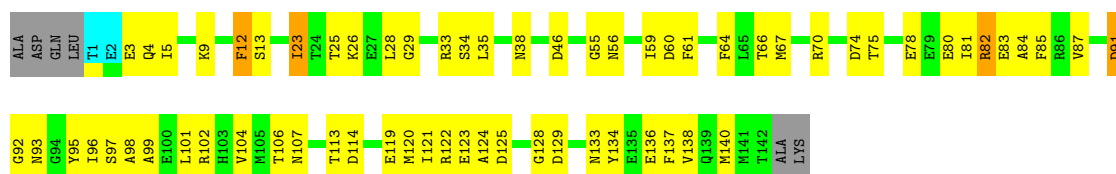
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.104 Score per residue for model 104

- Molecule 1: calmodulin





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

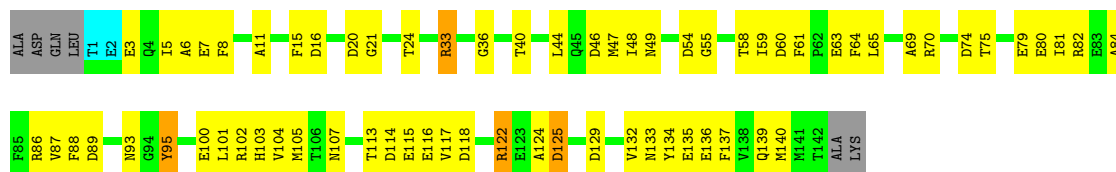
Chain B: 42% 37% 5% 16%



4.2.105 Score per residue for model 105

- Molecule 1: calmodulin

Chain A: 49% 43% ..



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

Chain B: 37% 42% 5% 16%



4.2.106 Score per residue for model 106

- Molecule 1: calmodulin

Chain A: 64% 30% ..



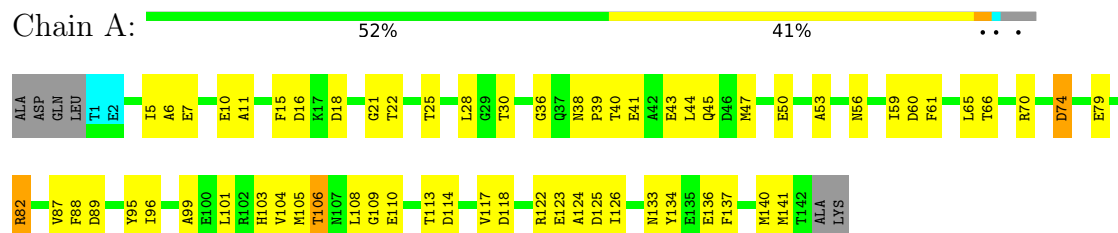
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B: 42% 37% 5% 16%

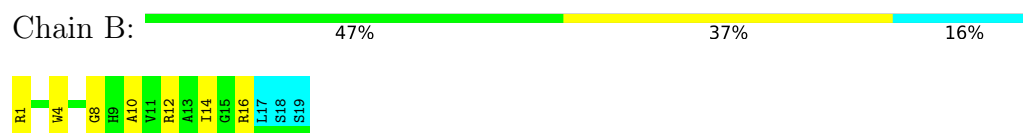


4.2.107 Score per residue for model 107

- Molecule 1: calmodulin

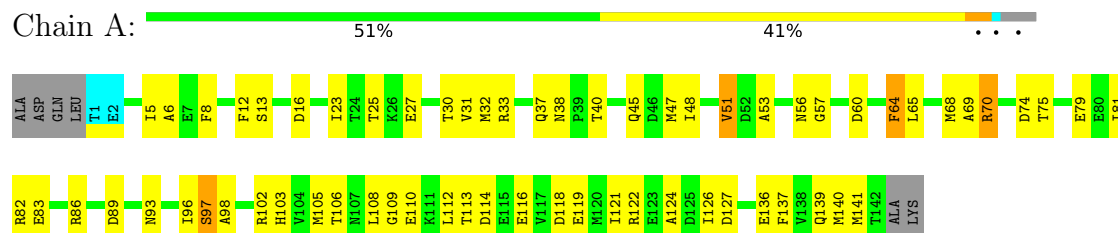


- Molecule 2: 19-mer peptide from Myosin light chain kinase

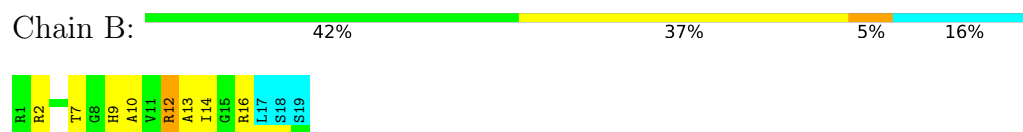


4.2.108 Score per residue for model 108

- Molecule 1: calmodulin



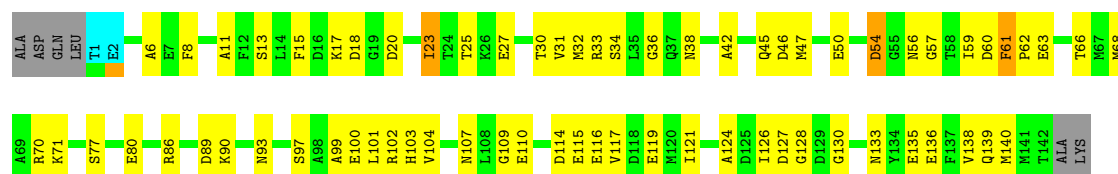
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.109 Score per residue for model 109

- Molecule 1: calmodulin



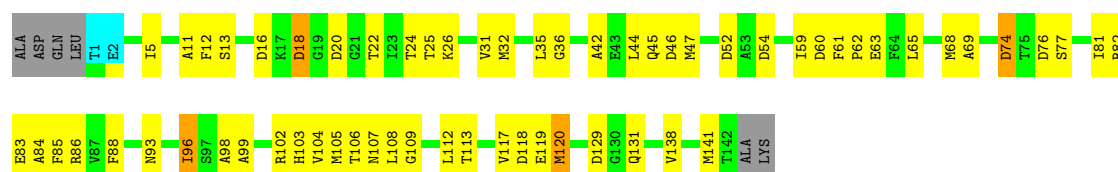


- Molecule 2: 19-mer peptide from Myosin light chain kinase

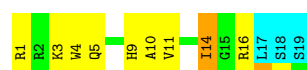


4.2.110 Score per residue for model 110

- Molecule 1: calmodulin

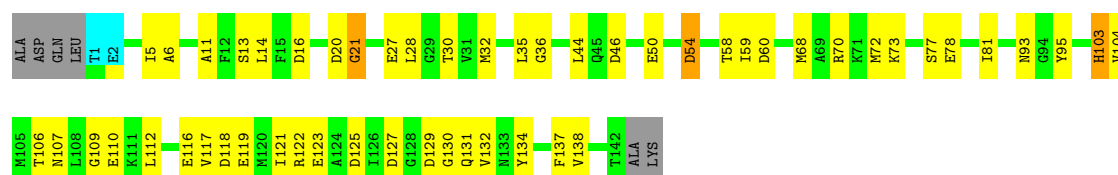


- Molecule 2: 19-mer peptide from Myosin light chain kinase



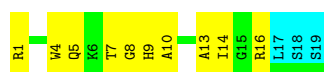
4.2.111 Score per residue for model 111

- Molecule 1: calmodulin



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





4.2.112 Score per residue for model 112

- Molecule 1: calmodulin

Chain A: 55% 36%



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

Chain B: 37% 47% 16%



4.2.113 Score per residue for model 113

- Molecule 1: calmodulin

Chain A: 57% 36%



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

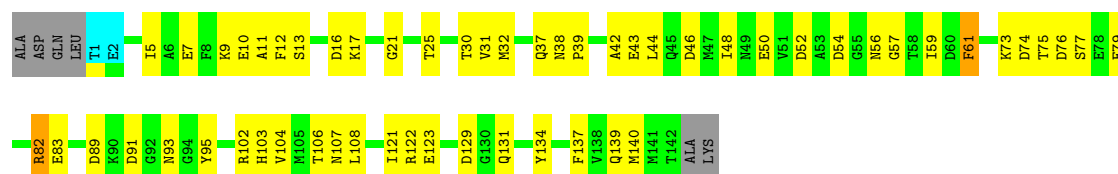
Chain B: 47% 32% 5% 16%



4.2.114 Score per residue for model 114

- Molecule 1: calmodulin

Chain A: 57% 36%

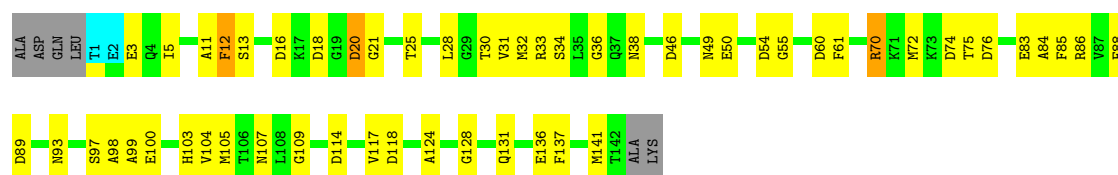


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.115 Score per residue for model 115

- Molecule 1: calmodulin

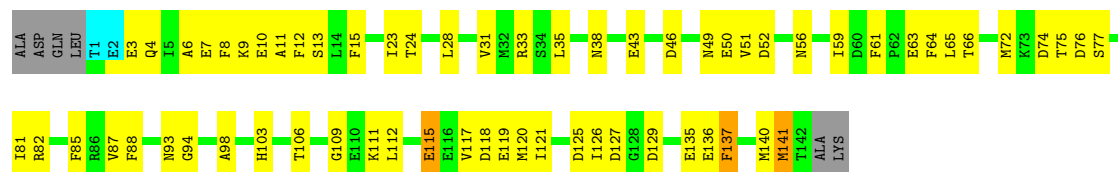


- Molecule 2: 19-mer peptide from Myosin light chain kinase

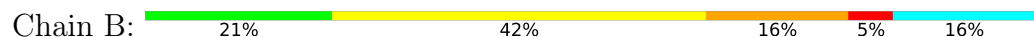


4.2.116 Score per residue for model 116

- Molecule 1: calmodulin



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

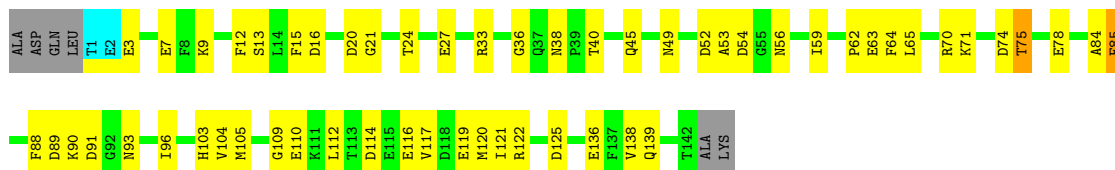




4.2.117 Score per residue for model 117

- Molecule 1: calmodulin

Chain A: 57% 36% ..



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

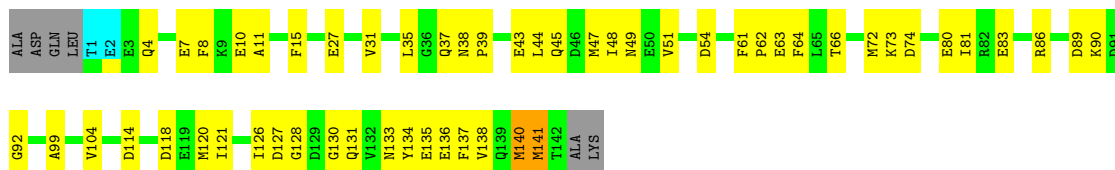
Chain B: 42% 37% 5% 16%



4.2.118 Score per residue for model 118

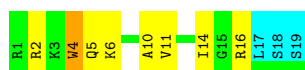
- Molecule 1: calmodulin

Chain A: 58% 35% ..



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

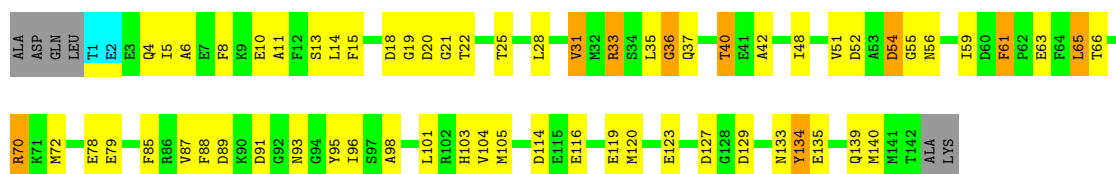
Chain B: 42% 37% 5% 16%



4.2.119 Score per residue for model 119

- Molecule 1: calmodulin

Chain A: 52% 36% 6% ..

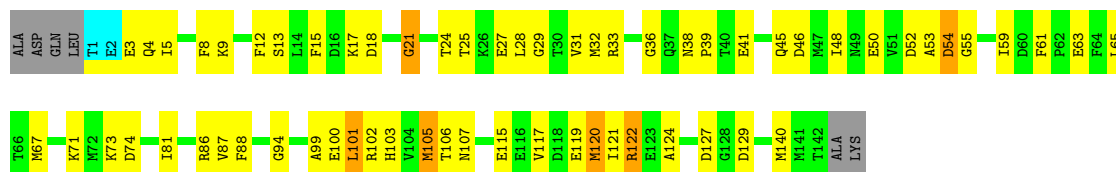


- Molecule 2: 19-mer peptide from Myosin light chain kinase

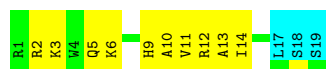


4.2.120 Score per residue for model 120

- Molecule 1: calmodulin

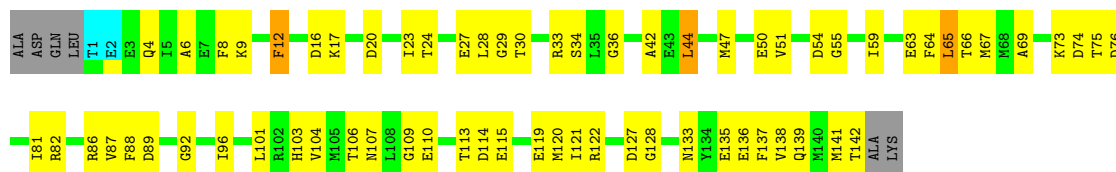


- Molecule 2: 19-mer peptide from Myosin light chain kinase



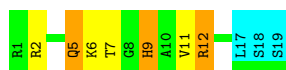
4.2.121 Score per residue for model 121

- Molecule 1: calmodulin



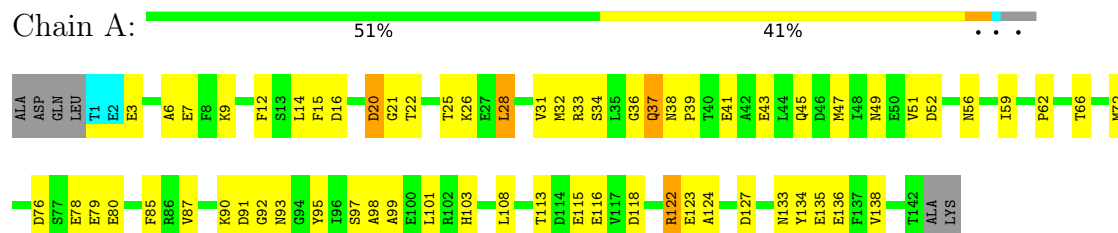
- Molecule 2: 19-mer peptide from Myosin light chain kinase



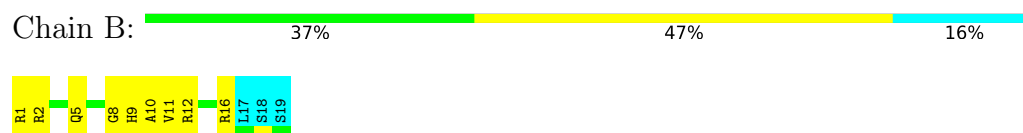


4.2.122 Score per residue for model 122

- Molecule 1: calmodulin

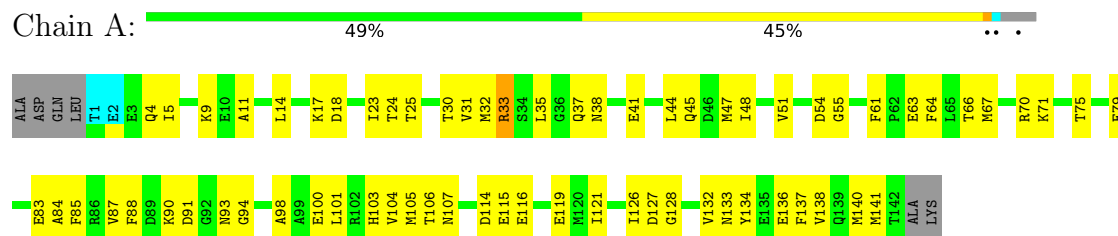


- Molecule 2: 19-mer peptide from Myosin light chain kinase

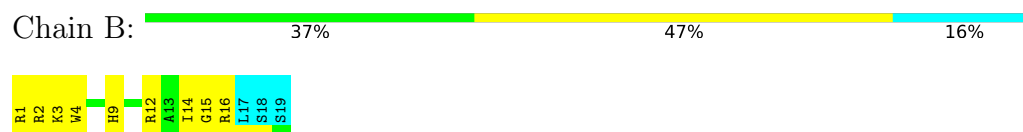


4.2.123 Score per residue for model 123

- Molecule 1: calmodulin



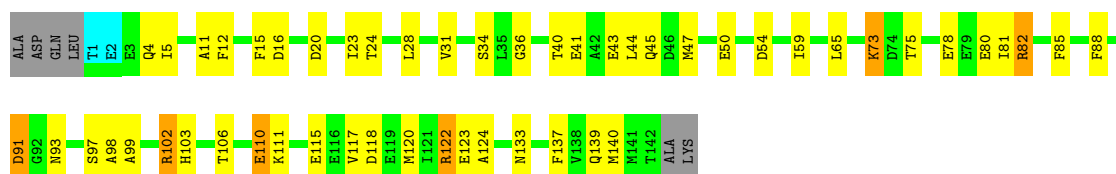
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.124 Score per residue for model 124

- Molecule 1: calmodulin



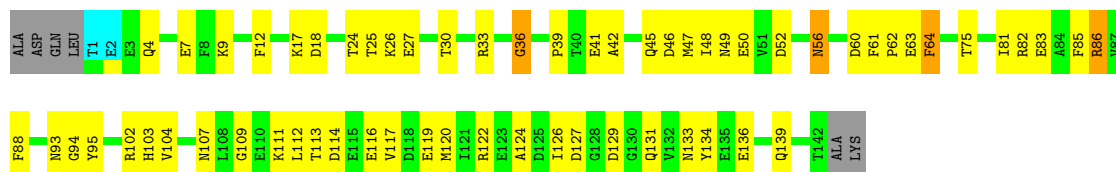


- Molecule 2: 19-mer peptide from Myosin light chain kinase

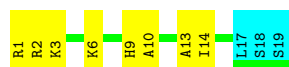


4.2.125 Score per residue for model 125

- Molecule 1: calmodulin

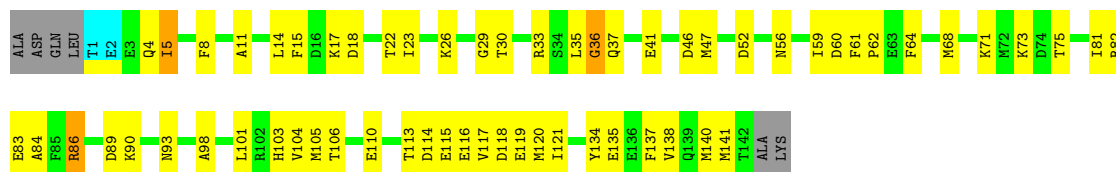


- Molecule 2: 19-mer peptide from Myosin light chain kinase



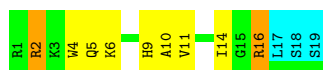
4.2.126 Score per residue for model 126

- Molecule 1: calmodulin



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

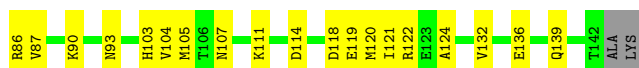




4.2.127 Score per residue for model 127

- Molecule 1: calmodulin

Chain A: 58% 36%



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

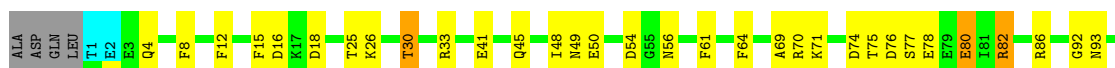
Chain B: 42% 37% 5% 16%



4.2.128 Score per residue for model 128

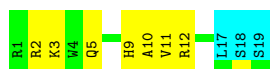
- Molecule 1: calmodulin

Chain A: 62% 30%



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

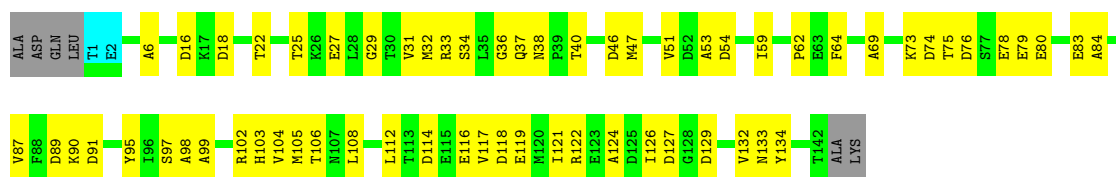
Chain B: 47% 37% 16%



4.2.129 Score per residue for model 129

- Molecule 1: calmodulin

Chain A: 53% 42%

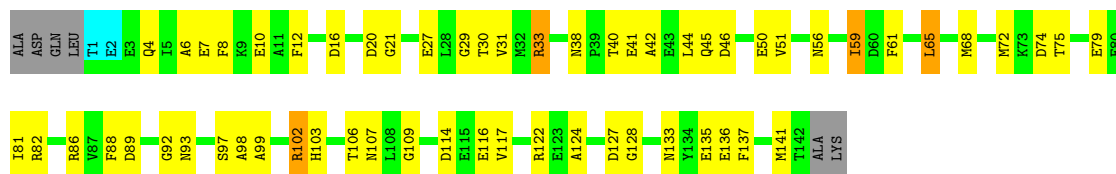


- Molecule 2: 19-mer peptide from Myosin light chain kinase

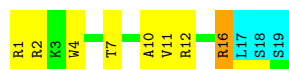


4.2.130 Score per residue for model 130

- Molecule 1: calmodulin

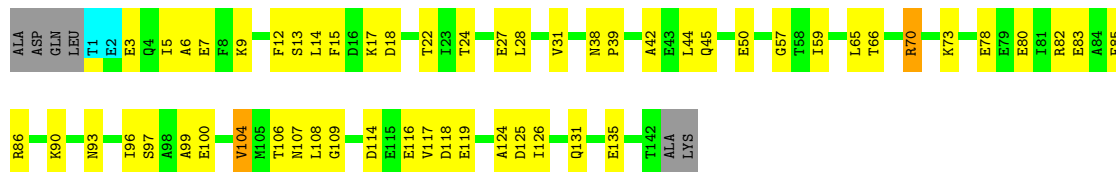


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.131 Score per residue for model 131

- Molecule 1: calmodulin



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

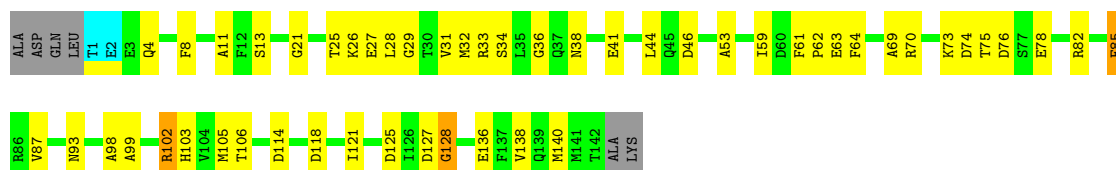




4.2.132 Score per residue for model 132

- Molecule 1: calmodulin

Chain A: 60% 32%



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

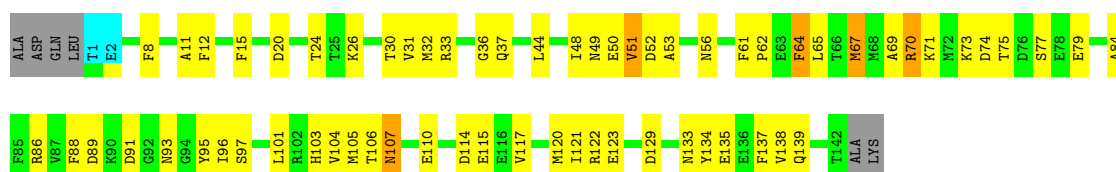
Chain B: 47% 32% 5% 16%



4.2.133 Score per residue for model 133

- Molecule 1: calmodulin

Chain A: 51% 40%



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

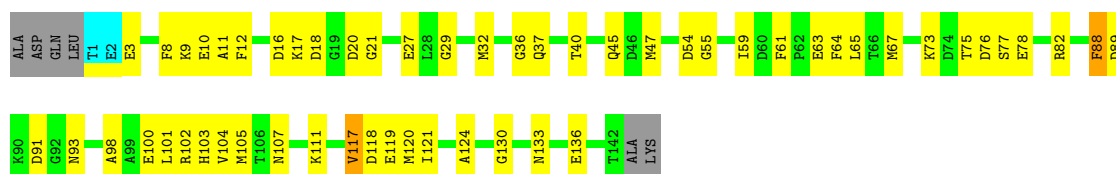
Chain B: 37% 37% 11% 16%



4.2.134 Score per residue for model 134

- Molecule 1: calmodulin

Chain A: 57% 36%

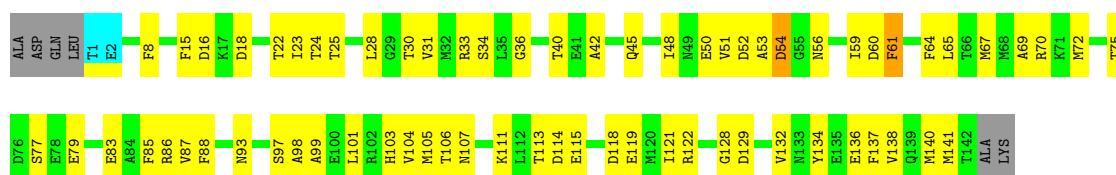


- Molecule 2: 19-mer peptide from Myosin light chain kinase

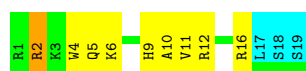


4.2.135 Score per residue for model 135

- Molecule 1: calmodulin

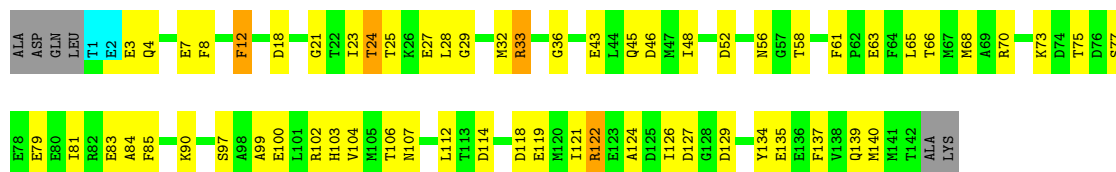


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.136 Score per residue for model 136

- Molecule 1: calmodulin



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

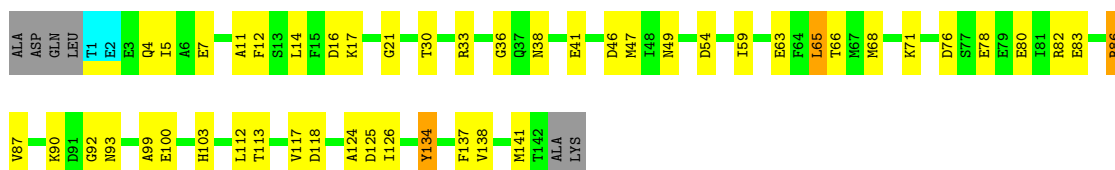




4.2.137 Score per residue for model 137

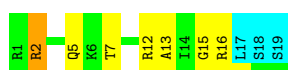
- Molecule 1: calmodulin

Chain A: 62% 30% ..



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

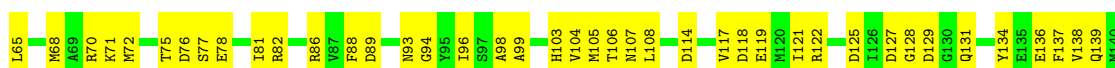
Chain B: 47% 32% 5% 16%



4.2.138 Score per residue for model 138

- Molecule 1: calmodulin

Chain A: 42% 52% ..



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

Chain B: 42% 42% 16%



4.2.139 Score per residue for model 139

- Molecule 1: calmodulin

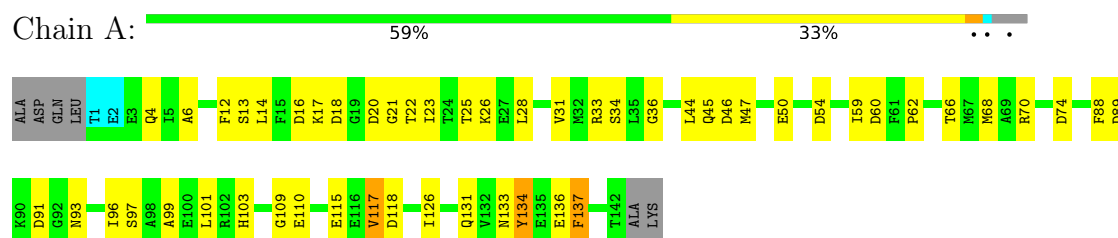


- Molecule 2: 19-mer peptide from Myosin light chain kinase

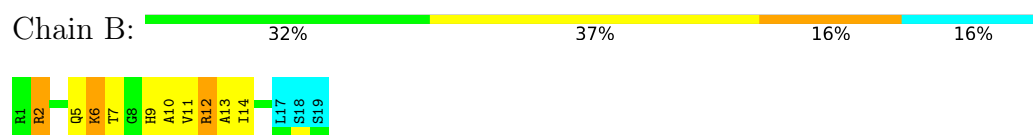


4.2.140 Score per residue for model 140

- Molecule 1: calmodulin

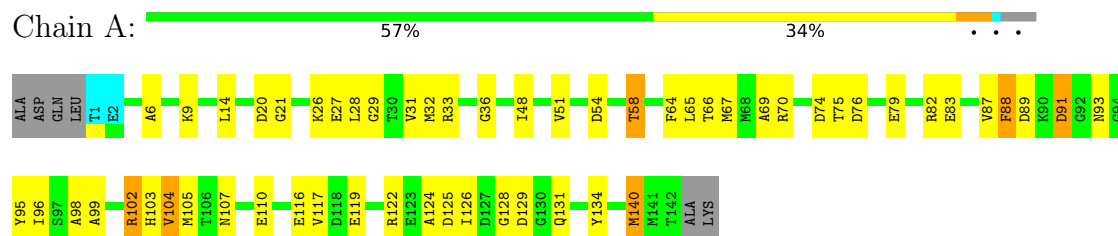


- Molecule 2: 19-mer peptide from Myosin light chain kinase



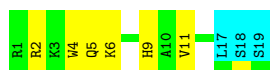
4.2.141 Score per residue for model 141

- Molecule 1: calmodulin



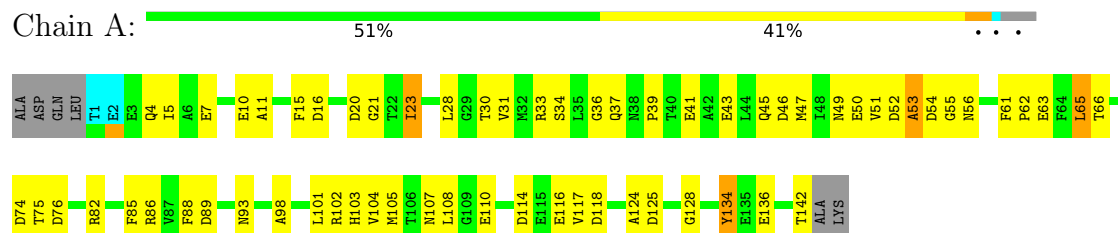
- Molecule 2: 19-mer peptide from Myosin light chain kinase





4.2.142 Score per residue for model 142

- Molecule 1: calmodulin

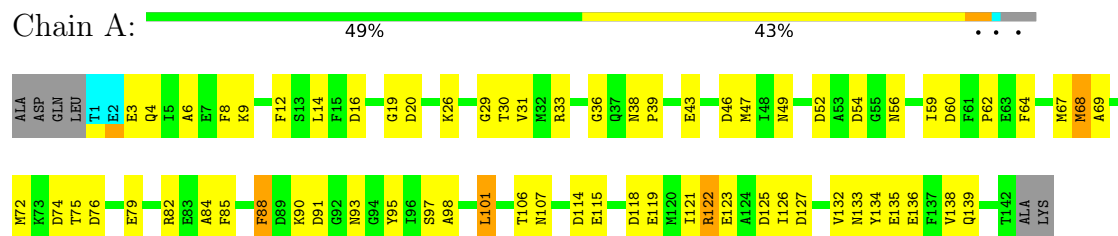


- Molecule 2: 19-mer peptide from Myosin light chain kinase

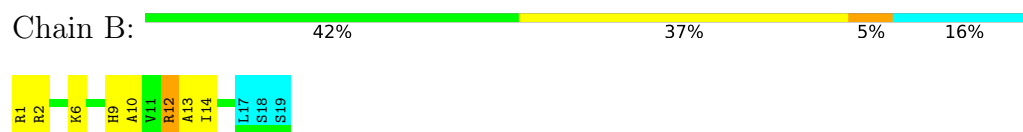


4.2.143 Score per residue for model 143

- Molecule 1: calmodulin



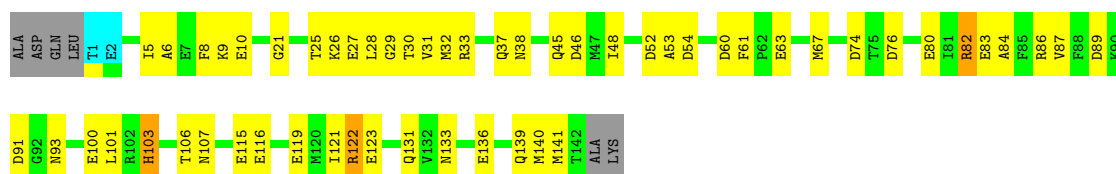
- Molecule 2: 19-mer peptide from Myosin light chain kinase



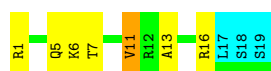
4.2.144 Score per residue for model 144

- Molecule 1: calmodulin



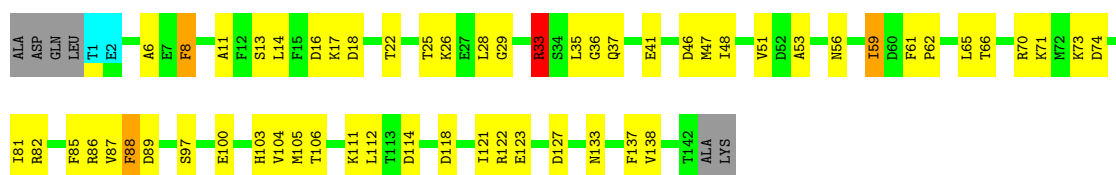


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.145 Score per residue for model 145

- Molecule 1: calmodulin

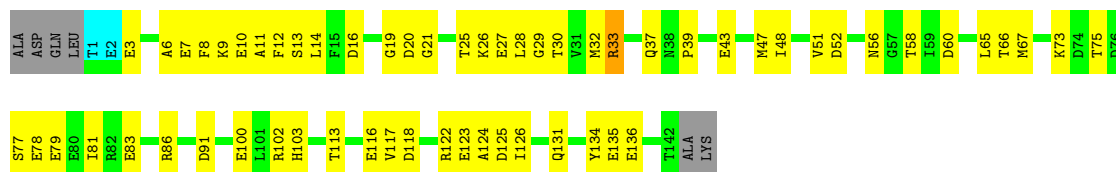


- Molecule 2: 19-mer peptide from Myosin light chain kinase



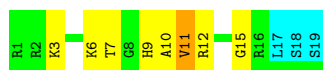
4.2.146 Score per residue for model 146

- Molecule 1: calmodulin



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





4.2.147 Score per residue for model 147

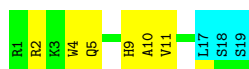
- Molecule 1: calmodulin

Chain A: 57% 36% ..



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

Chain B: 53% 32% 16%



4.2.148 Score per residue for model 148

- Molecule 1: calmodulin

Chain A: 58% 34% ..



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

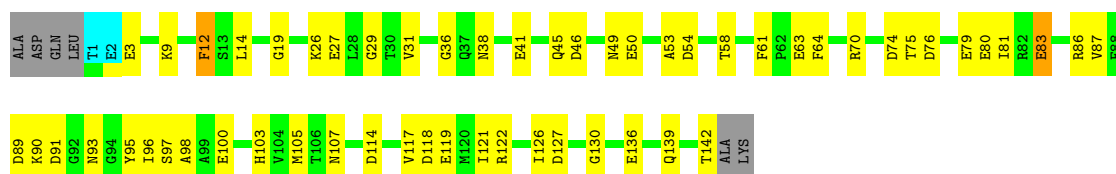
Chain B: 47% 37% 16%



4.2.149 Score per residue for model 149

- Molecule 1: calmodulin

Chain A: 57% 36% ..



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

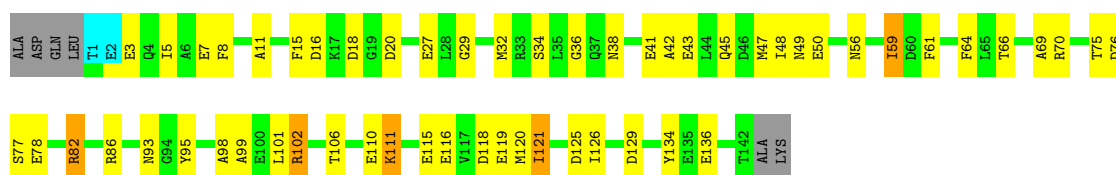
Chain B: 42% 32% 11% 16%



4.2.150 Score per residue for model 150

- Molecule 1: calmodulin

Chain A: 57% 34% ..



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

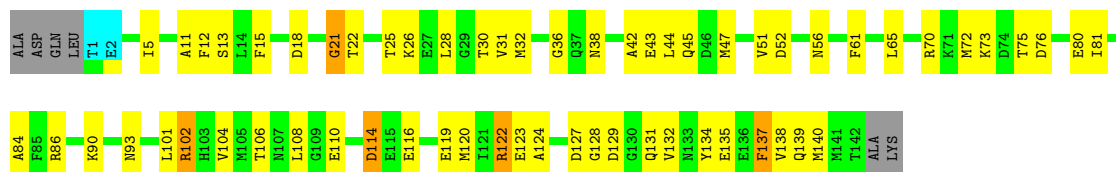
Chain B: 37% 37% 11% 16%



4.2.151 Score per residue for model 151

- Molecule 1: calmodulin

Chain A: 53% 38% ..



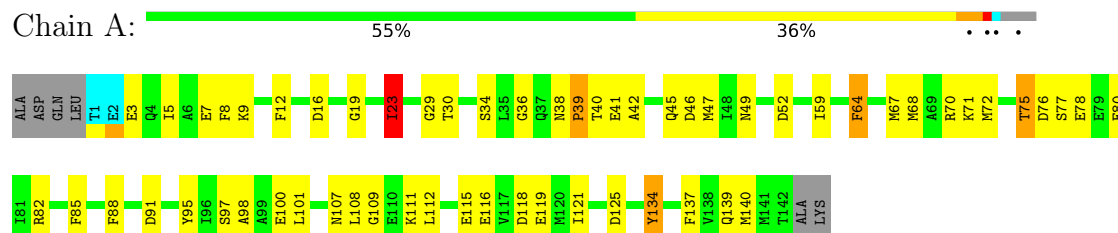
- Molecule 2: 19-mer peptide from Myosin light chain kinase

Chain B: 53% 16% 16% 16%

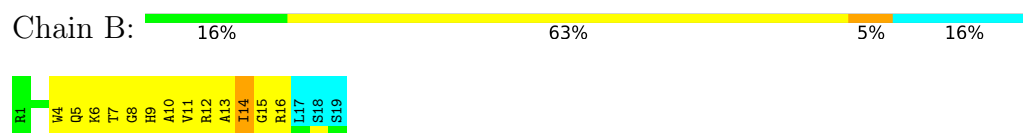


4.2.152 Score per residue for model 152

- Molecule 1: calmodulin

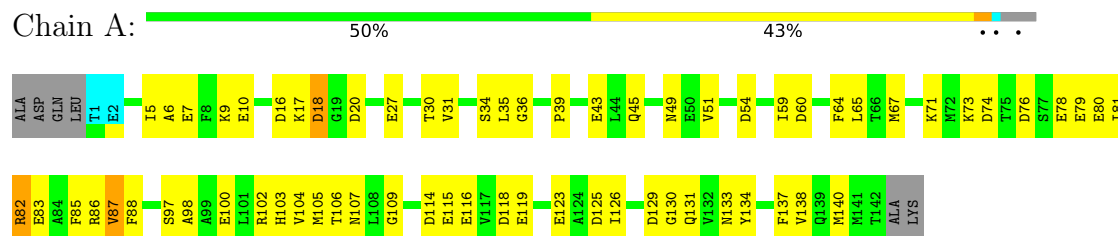


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.153 Score per residue for model 153

- Molecule 1: calmodulin



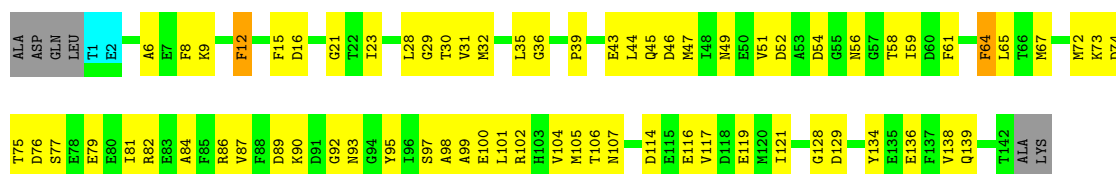
- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.154 Score per residue for model 154

- Molecule 1: calmodulin



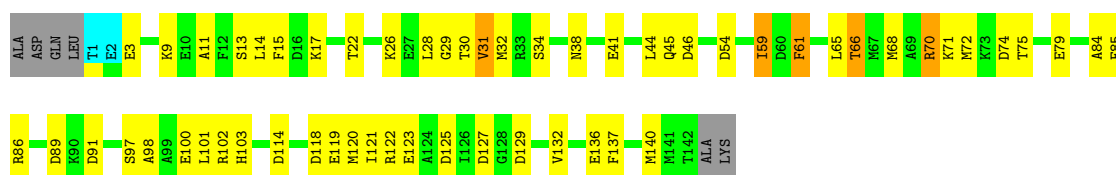


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.155 Score per residue for model 155

- Molecule 1: calmodulin

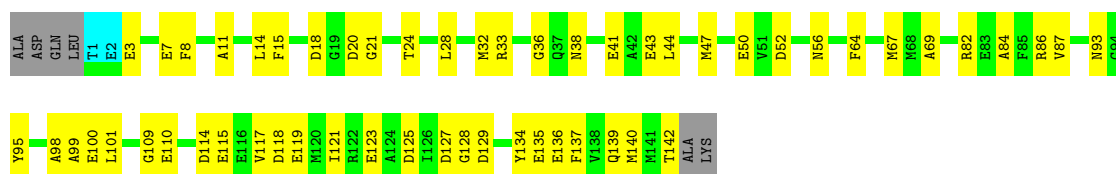


- Molecule 2: 19-mer peptide from Myosin light chain kinase



4.2.156 Score per residue for model 156

- Molecule 1: calmodulin



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

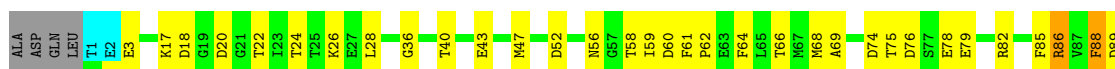




4.2.157 Score per residue for model 157

- Molecule 1: calmodulin

Chain A: 55% 39% ..



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

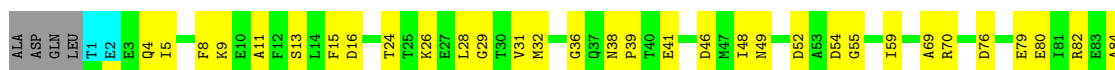
Chain B: 37% 42% 5% 16%



4.2.158 Score per residue for model 158

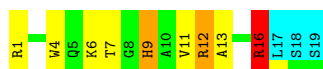
- Molecule 1: calmodulin

Chain A: 55% 39% ..



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

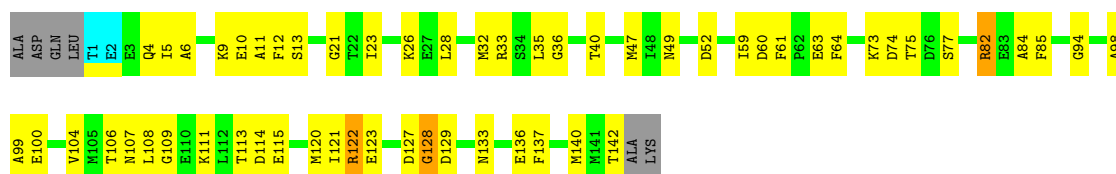
Chain B: 37% 32% 11% 5% 16%



4.2.159 Score per residue for model 159

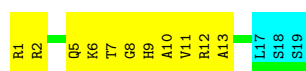
- Molecule 1: calmodulin

Chain A: 56% 36% ..



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

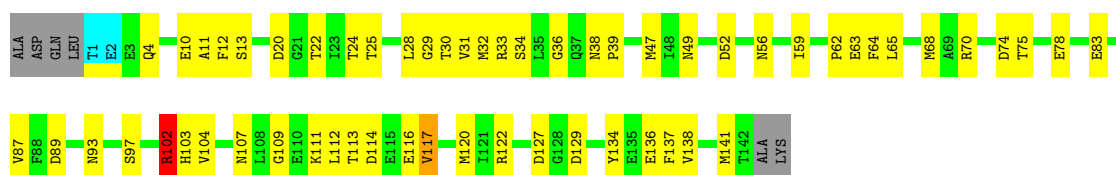
Chain B: 26% 58% 16%



4.2.160 Score per residue for model 160

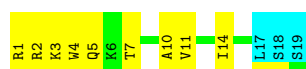
- Molecule 1: calmodulin

Chain A: 55% 38% ...



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

Chain B: 37% 47% 16%



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	1.44±0.01	0±0/1117 (0.0± 0.0%)	2.56±0.07	89±11/1499 (5.9± 0.7%)
2	B	1.66±0.02	0±0/138 (0.0± 0.0%)	2.75±0.19	13±4/183 (7.2± 2.1%)
All	All	1.46	5/200800 (0.0%)	2.59	16336/269120 (6.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.7±1.3
2	B	0.0±0.0	1.2±1.0
All	All	0	631

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	72	MET	CA-C	-7.70	1.49	1.53	37	3
1	A	93	ASN	CA-C	-7.55	1.49	1.53	115	1
1	A	74	ASP	CA-C	-6.24	1.49	1.52	17	1

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	ASN	CA-CB-CG	14.52	127.12	112.60	25	43
1	A	61	PHE	O-C-N	-14.18	109.18	120.38	105	35
2	B	11	VAL	N-CA-C	14.17	125.07	110.62	19	29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	98	ALA	CA-C-N	14.14	139.23	120.28	11	64
1	A	98	ALA	C-N-CA	14.14	139.23	120.28	11	64
1	A	70	ARG	NE-CZ-NH2	-13.33	107.20	119.20	152	16
1	A	72	MET	CA-C-O	13.21	125.60	117.94	37	10
1	A	118	ASP	CA-C-N	13.16	137.55	120.44	19	36
1	A	118	ASP	C-N-CA	13.16	137.55	120.44	19	36
2	B	14	ILE	CA-C-N	13.10	134.53	119.98	139	38
2	B	14	ILE	C-N-CA	13.10	134.53	119.98	139	38
1	A	61	PHE	CA-CB-CG	-13.08	100.72	113.80	78	25
1	A	108	LEU	N-CA-C	12.95	126.60	111.71	6	22
1	A	83	GLU	CA-C-N	12.86	137.52	120.28	41	24
1	A	83	GLU	C-N-CA	12.86	137.52	120.28	41	24
1	A	74	ASP	N-CA-C	12.82	124.78	111.07	60	27
1	A	126	ILE	N-CA-C	-12.78	101.55	111.90	148	14
1	A	129	ASP	CA-CB-CG	12.60	125.20	112.60	67	61
1	A	89	ASP	CA-C-N	12.58	137.25	120.65	121	26
1	A	89	ASP	C-N-CA	12.58	137.25	120.65	121	26
1	A	62	PRO	CA-C-N	12.44	136.61	120.44	39	18
1	A	62	PRO	C-N-CA	12.44	136.61	120.44	39	18
1	A	91	ASP	N-CA-C	12.35	124.29	111.07	63	19
2	B	2	ARG	CA-C-N	12.22	137.25	120.63	130	22
2	B	2	ARG	C-N-CA	12.22	137.25	120.63	130	22
1	A	127	ASP	N-CA-C	12.15	124.21	110.97	67	23
1	A	107	ASN	CA-CB-CG	-12.13	100.47	112.60	125	34
1	A	75	THR	CA-C-N	12.06	137.42	120.29	40	50
1	A	75	THR	C-N-CA	12.06	137.42	120.29	40	50
2	B	7	THR	CA-C-N	12.06	135.22	120.14	48	48
2	B	7	THR	C-N-CA	12.06	135.22	120.14	48	48
1	A	103	HIS	CA-CB-CG	-12.05	101.75	113.80	52	29
1	A	127	ASP	CA-CB-CG	12.05	124.65	112.60	52	18
1	A	18	ASP	CA-CB-CG	11.87	124.47	112.60	8	30
1	A	72	MET	O-C-N	-11.84	112.59	121.47	37	15
2	B	5	GLN	CA-C-N	11.75	135.72	120.44	160	30
2	B	5	GLN	C-N-CA	11.75	135.72	120.44	160	30
1	A	114	ASP	CA-C-N	11.73	135.68	120.44	9	79
1	A	114	ASP	C-N-CA	11.73	135.68	120.44	9	79
1	A	104	VAL	CA-C-N	11.68	136.32	120.44	42	25
1	A	104	VAL	C-N-CA	11.68	136.32	120.44	42	25
1	A	65	LEU	N-CA-C	11.64	123.52	111.07	24	41
2	B	8	GLY	CA-C-N	11.47	135.36	120.44	76	31
2	B	8	GLY	C-N-CA	11.47	135.36	120.44	76	31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	114	ASP	CA-CB-CG	-11.38	101.22	112.60	107	41
2	B	6	LYS	CA-C-N	11.36	135.64	120.65	148	51
2	B	6	LYS	C-N-CA	11.36	135.64	120.65	148	51
1	A	56	ASN	CA-CB-CG	11.35	123.95	112.60	95	41
2	B	9	HIS	CA-CB-CG	-11.35	102.45	113.80	128	27
1	A	63	GLU	CA-C-N	11.33	135.47	120.28	78	42
1	A	63	GLU	C-N-CA	11.33	135.47	120.28	78	42
1	A	11	ALA	N-CA-C	11.30	124.71	111.71	142	30
1	A	93	ASN	CA-CB-CG	11.30	123.90	112.60	22	58
1	A	141	MET	N-CA-C	11.27	123.25	110.97	16	34
1	A	28	LEU	CA-C-N	11.23	132.61	120.03	120	58
1	A	28	LEU	C-N-CA	11.23	132.61	120.03	120	58
1	A	66	THR	CA-C-N	11.23	135.71	120.54	140	31
1	A	66	THR	C-N-CA	11.23	135.71	120.54	140	31
1	A	118	ASP	CA-CB-CG	11.22	123.82	112.60	28	36
2	B	7	THR	O-C-N	-11.21	110.37	122.03	158	17
1	A	37	GLN	OE1-CD-NE2	-11.18	111.42	122.60	73	17
1	A	16	ASP	CA-CB-CG	11.10	123.70	112.60	39	22
2	B	2	ARG	N-CA-C	11.04	124.36	111.11	129	56
1	A	59	ILE	CB-CA-C	10.98	123.32	111.35	24	22
1	A	33	ARG	NE-CZ-NH1	10.94	132.44	121.50	88	15
1	A	122	ARG	N-CA-C	10.91	123.17	111.28	130	38
1	A	82	ARG	O-C-N	-10.90	110.32	122.09	130	19
1	A	59	ILE	N-CA-CB	10.87	122.88	110.82	22	32
1	A	46	ASP	CA-CB-CG	-10.85	101.75	112.60	125	25
1	A	4	GLN	CA-C-N	10.83	134.95	120.77	39	33
1	A	4	GLN	C-N-CA	10.83	134.95	120.77	39	33
1	A	125	ASP	CA-CB-CG	10.79	123.39	112.60	117	19
1	A	35	LEU	N-CA-C	10.76	124.02	111.11	147	18
1	A	46	ASP	CA-C-N	10.72	134.64	120.28	64	40
1	A	46	ASP	C-N-CA	10.72	134.64	120.28	64	40
1	A	134	TYR	CA-C-N	10.70	134.99	120.54	123	22
1	A	134	TYR	C-N-CA	10.70	134.99	120.54	123	22
2	B	16	ARG	CA-C-N	10.70	135.18	120.63	38	9
2	B	16	ARG	C-N-CA	10.70	135.18	120.63	38	9
1	A	9	LYS	N-CA-C	10.68	124.20	111.82	3	25
1	A	5	ILE	CA-C-N	10.67	134.57	120.28	95	45
1	A	5	ILE	C-N-CA	10.67	134.57	120.28	95	45
1	A	116	GLU	CA-C-N	10.66	134.35	120.60	141	45
1	A	116	GLU	C-N-CA	10.66	134.35	120.60	141	45
1	A	20	ASP	CA-CB-CG	10.64	123.25	112.60	29	48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	47	MET	CA-C-N	10.62	135.50	120.53	80	36
1	A	47	MET	C-N-CA	10.62	135.50	120.53	80	36
1	A	137	PHE	CA-CB-CG	10.59	124.39	113.80	140	24
1	A	137	PHE	O-C-N	-10.58	110.60	122.03	138	13
1	A	49	ASN	CA-C-N	10.57	135.00	120.63	117	30
1	A	49	ASN	C-N-CA	10.57	135.00	120.63	117	30
1	A	4	GLN	CA-C-O	-10.57	109.24	120.55	81	12
1	A	6	ALA	N-CA-C	10.56	123.79	111.11	57	40
1	A	129	ASP	N-CA-C	10.55	124.67	111.69	31	21
1	A	88	PHE	CA-CB-CG	10.55	124.35	113.80	121	32
2	B	6	LYS	CA-C-O	10.49	131.84	120.82	65	22
1	A	38	ASN	O-C-N	-10.49	111.81	121.36	82	28
1	A	34	SER	CA-C-N	10.49	134.90	120.63	19	18
1	A	34	SER	C-N-CA	10.49	134.90	120.63	19	18
1	A	121	ILE	CA-C-N	10.49	134.07	120.44	41	39
1	A	121	ILE	C-N-CA	10.49	134.07	120.44	41	39
1	A	99	ALA	CA-C-N	10.48	134.69	120.54	68	54
1	A	99	ALA	C-N-CA	10.48	134.69	120.54	68	54
1	A	20	ASP	CB-CA-C	10.45	125.54	109.34	112	9
1	A	97	SER	O-C-N	-10.44	110.73	122.84	115	15
1	A	64	PHE	CA-CB-CG	10.41	124.21	113.80	70	21
1	A	124	ALA	CA-C-N	10.37	135.47	120.95	125	19
1	A	124	ALA	C-N-CA	10.37	135.47	120.95	125	19
1	A	82	ARG	N-CA-C	10.35	122.56	111.28	77	18
1	A	117	VAL	N-CA-C	10.32	120.23	110.53	59	20
1	A	84	ALA	CA-C-N	10.30	134.08	120.28	73	41
1	A	84	ALA	C-N-CA	10.30	134.08	120.28	73	41
2	B	13	ALA	N-CA-C	10.28	122.49	111.28	77	24
1	A	95	TYR	CA-C-N	10.28	135.22	122.37	133	8
1	A	95	TYR	C-N-CA	10.28	135.22	122.37	133	8
1	A	97	SER	CA-C-N	10.27	134.04	120.28	158	32
1	A	97	SER	C-N-CA	10.27	134.04	120.28	158	32
1	A	52	ASP	CA-CB-CG	10.24	122.84	112.60	31	23
1	A	74	ASP	CA-C-O	10.23	125.60	119.77	17	14
1	A	74	ASP	CA-CB-CG	-10.23	102.37	112.60	95	31
1	A	119	GLU	N-CA-C	10.21	122.41	111.28	83	35
1	A	10	GLU	CA-C-O	-10.21	109.73	120.55	33	9
1	A	119	GLU	CA-C-N	10.17	134.27	120.44	143	51
1	A	119	GLU	C-N-CA	10.17	134.27	120.44	143	51
2	B	10	ALA	N-CA-C	10.15	122.43	111.36	10	31
1	A	88	PHE	N-CA-C	10.14	122.33	111.28	53	25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	77	SER	CA-C-N	10.12	133.60	120.44	60	32
1	A	77	SER	C-N-CA	10.12	133.60	120.44	60	32
1	A	122	ARG	CA-C-N	10.09	134.20	120.38	105	41
1	A	122	ARG	C-N-CA	10.09	134.20	120.38	105	41
1	A	56	ASN	N-CA-CB	10.09	125.09	110.16	61	7
1	A	124	ALA	N-CA-C	10.08	121.86	111.07	100	26
2	B	14	ILE	O-C-N	-10.08	110.41	121.80	16	16
1	A	104	VAL	N-CA-C	10.08	120.10	110.42	9	32
1	A	101	LEU	CA-C-N	10.08	133.54	120.44	5	37
1	A	101	LEU	C-N-CA	10.08	133.54	120.44	5	37
2	B	11	VAL	O-C-N	-10.07	110.42	121.80	61	12
2	B	12	ARG	NE-CZ-NH2	10.00	128.20	119.20	24	19
1	A	47	MET	O-C-N	-10.00	111.69	122.09	138	18
1	A	53	ALA	N-CA-C	10.00	122.26	111.36	97	15
1	A	4	GLN	OE1-CD-NE2	-9.99	112.61	122.60	65	23
1	A	15	PHE	CA-CB-CG	9.96	123.76	113.80	70	32
1	A	80	GLU	CA-C-O	-9.96	110.24	120.90	85	10
1	A	107	ASN	N-CA-C	9.96	122.21	111.36	89	20
1	A	32	MET	N-CA-C	9.92	122.10	111.28	56	31
1	A	54	ASP	N-CA-C	9.92	121.79	110.97	6	34
2	B	1	ARG	NE-CZ-NH2	-9.91	110.28	119.20	103	18
1	A	106	THR	N-CA-C	9.88	123.28	111.33	3	23
1	A	14	LEU	CA-C-N	9.85	133.84	120.44	97	10
1	A	14	LEU	C-N-CA	9.85	133.84	120.44	97	10
1	A	48	ILE	N-CA-C	9.85	120.70	110.36	150	18
1	A	12	PHE	CA-CB-CG	9.84	123.64	113.80	65	25
1	A	80	GLU	N-CA-C	9.83	121.59	111.07	6	25
1	A	117	VAL	CA-C-N	9.81	133.78	120.54	94	34
1	A	117	VAL	C-N-CA	9.81	133.78	120.54	94	34
1	A	24	THR	CA-C-N	9.80	133.80	120.38	116	35
1	A	24	THR	C-N-CA	9.80	133.80	120.38	116	35
2	B	7	THR	N-CA-C	-9.80	98.83	112.45	134	11
2	B	10	ALA	CA-C-N	9.79	132.94	120.70	86	40
2	B	10	ALA	C-N-CA	9.79	132.94	120.70	86	40
2	B	11	VAL	CA-C-O	9.79	131.04	120.47	61	13
1	A	74	ASP	CA-C-N	9.79	133.57	120.65	93	44
1	A	74	ASP	C-N-CA	9.79	133.57	120.65	93	44
1	A	51	VAL	CA-C-O	-9.77	109.70	120.25	6	9
1	A	7	GLU	CA-C-N	9.77	133.37	120.28	27	19
1	A	7	GLU	C-N-CA	9.77	133.37	120.28	27	19
1	A	68	MET	CA-C-N	9.77	133.37	120.28	85	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	68	MET	C-N-CA	9.77	133.37	120.28	85	9
1	A	33	ARG	CA-C-N	9.77	133.72	120.54	20	23
1	A	33	ARG	C-N-CA	9.77	133.72	120.54	20	23
1	A	60	ASP	CA-CB-CG	9.76	122.36	112.60	52	24
1	A	52	ASP	N-CA-C	9.75	124.66	110.42	75	11
2	B	5	GLN	N-CA-C	9.75	121.98	111.36	70	25
1	A	65	LEU	CA-C-N	9.74	133.11	120.44	19	29
1	A	65	LEU	C-N-CA	9.74	133.11	120.44	19	29
1	A	85	PHE	CA-CB-CG	-9.72	104.08	113.80	1	23
2	B	3	LYS	N-CA-C	9.72	121.56	110.97	16	27
1	A	65	LEU	O-C-N	-9.71	111.60	122.09	43	13
1	A	102	ARG	N-CA-C	9.70	123.07	111.82	129	21
1	A	48	ILE	CA-C-N	9.69	134.53	120.38	11	19
1	A	48	ILE	C-N-CA	9.69	134.53	120.38	11	19
1	A	25	THR	CA-C-N	9.68	133.80	120.63	43	38
1	A	25	THR	C-N-CA	9.68	133.80	120.63	43	38
1	A	86	ARG	N-CA-C	9.68	122.84	111.71	156	30
2	B	9	HIS	CB-CG-CD2	-9.67	118.62	131.20	120	2
1	A	117	VAL	CA-C-O	9.65	131.08	120.85	7	8
1	A	51	VAL	N-CA-C	9.65	120.46	110.62	50	18
1	A	44	LEU	O-C-N	-9.64	111.90	122.12	17	7
2	B	7	THR	CA-C-O	9.63	130.63	120.42	97	12
1	A	81	ILE	N-CA-C	9.63	120.44	110.62	55	20
1	A	75	THR	CA-C-O	9.62	130.92	120.82	64	21
1	A	117	VAL	N-CA-CB	9.57	121.75	110.55	19	14
1	A	78	GLU	O-C-N	-9.57	111.24	122.15	52	9
1	A	55	GLY	O-C-N	9.57	133.09	122.47	119	7
1	A	38	ASN	CA-CB-CG	-9.56	103.03	112.60	48	24
1	A	43	GLU	CA-C-N	9.55	133.42	120.44	124	18
1	A	43	GLU	C-N-CA	9.55	133.42	120.44	124	18
1	A	79	GLU	CA-C-N	9.54	133.42	120.54	7	44
1	A	79	GLU	C-N-CA	9.54	133.42	120.54	7	44
1	A	138	VAL	CA-C-N	9.52	133.04	120.28	80	18
1	A	138	VAL	C-N-CA	9.52	133.04	120.28	80	18
1	A	29	GLY	CA-C-N	9.51	133.02	120.28	79	44
1	A	29	GLY	C-N-CA	9.51	133.02	120.28	79	44
1	A	16	ASP	CA-C-O	9.49	130.79	120.92	47	12
1	A	6	ALA	CA-C-O	-9.49	110.74	120.90	83	10
1	A	76	ASP	CA-CB-CG	-9.48	103.12	112.60	116	27
1	A	136	GLU	CA-C-N	9.47	132.76	120.44	132	67
1	A	136	GLU	C-N-CA	9.47	132.76	120.44	132	67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	86	ARG	CA-C-N	9.47	132.54	120.70	60	18
1	A	86	ARG	C-N-CA	9.47	132.54	120.70	60	18
1	A	43	GLU	N-CA-C	9.47	122.47	111.11	38	17
1	A	42	ALA	N-CA-C	9.46	122.78	111.33	135	21
1	A	18	ASP	N-CA-C	9.46	121.68	111.36	76	14
1	A	40	THR	O-C-N	-9.45	112.07	122.85	83	18
1	A	78	GLU	CA-C-N	9.44	132.93	120.28	122	32
1	A	78	GLU	C-N-CA	9.44	132.93	120.28	122	32
1	A	90	LYS	N-CA-C	9.43	122.42	111.11	149	14
1	A	87	VAL	CA-C-N	9.41	133.24	120.44	2	19
1	A	87	VAL	C-N-CA	9.41	133.24	120.44	2	19
1	A	136	GLU	N-CA-C	9.40	122.39	111.11	139	20
1	A	114	ASP	CA-C-O	9.40	130.51	120.55	67	17
1	A	134	TYR	N-CA-C	9.39	121.52	111.28	33	31
1	A	126	ILE	CA-C-N	9.39	132.65	120.44	125	17
1	A	126	ILE	C-N-CA	9.39	132.65	120.44	125	17
1	A	119	GLU	CA-C-O	9.38	130.69	120.10	109	16
1	A	91	ASP	CA-CB-CG	9.37	121.97	112.60	2	17
2	B	5	GLN	O-C-N	-9.36	112.20	122.12	13	13
1	A	29	GLY	N-CA-C	9.34	123.94	112.64	86	17
1	A	27	GLU	CA-C-N	9.33	133.54	120.29	118	39
1	A	27	GLU	C-N-CA	9.33	133.54	120.29	118	39
1	A	76	ASP	N-CA-C	9.33	122.30	111.11	115	15
1	A	38	ASN	OD1-CG-ND2	-9.32	113.28	122.60	80	12
1	A	56	ASN	OD1-CG-ND2	-9.32	113.28	122.60	101	29
1	A	12	PHE	N-CA-CB	-9.32	96.37	110.16	85	12
1	A	5	ILE	O-C-N	-9.32	112.83	121.87	111	16
2	B	13	ALA	CA-C-N	9.30	132.07	120.72	61	26
2	B	13	ALA	C-N-CA	9.30	132.07	120.72	61	26
1	A	99	ALA	O-C-N	-9.30	111.34	122.22	85	3
1	A	31	VAL	N-CA-C	9.29	119.27	110.53	53	24
1	A	55	GLY	CA-C-O	-9.27	109.15	118.98	119	4
1	A	72	MET	CG-SD-CE	-9.27	80.51	100.90	32	10
1	A	115	GLU	N-CA-C	9.27	122.54	111.33	4	13
1	A	64	PHE	O-C-N	-9.26	112.46	122.09	84	20
2	B	9	HIS	CE1-NE2-CD2	-9.26	99.75	109.00	147	41
2	B	9	HIS	CA-C-N	9.25	132.68	120.28	26	39
2	B	9	HIS	C-N-CA	9.25	132.68	120.28	26	39
1	A	44	LEU	CA-C-N	9.25	133.05	120.38	68	23
1	A	44	LEU	C-N-CA	9.25	133.05	120.38	68	23
1	A	80	GLU	CA-C-N	9.23	133.55	120.53	147	17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	80	GLU	C-N-CA	9.23	133.55	120.53	147	17
1	A	100	GLU	CA-C-N	9.22	132.42	120.44	36	37
1	A	100	GLU	C-N-CA	9.22	132.42	120.44	36	37
1	A	49	ASN	CA-CB-CG	-9.21	103.39	112.60	1	19
1	A	64	PHE	N-CA-C	9.21	122.16	111.11	12	14
1	A	10	GLU	N-CA-C	9.20	122.29	111.71	44	18
1	A	50	GLU	N-CA-C	9.20	122.15	111.11	109	22
1	A	104	VAL	O-C-N	-9.18	112.97	121.87	153	16
2	B	12	ARG	CA-C-N	9.17	132.95	120.38	9	30
2	B	12	ARG	C-N-CA	9.17	132.95	120.38	9	30
1	A	13	SER	N-CA-CB	9.16	123.72	110.16	120	6
1	A	113	THR	CA-C-N	9.16	132.91	120.54	95	20
1	A	113	THR	C-N-CA	9.16	132.91	120.54	95	20
1	A	89	ASP	CA-CB-CG	9.15	121.75	112.60	74	25
1	A	75	THR	N-CA-C	9.15	121.25	111.28	114	20
2	B	4	TRP	N-CA-C	-9.14	101.90	113.23	113	19
1	A	140	MET	N-CA-C	9.13	121.23	111.28	57	24
1	A	98	ALA	N-CA-C	9.10	120.81	111.07	132	44
1	A	139	GLN	OE1-CD-NE2	-9.10	113.50	122.60	85	12
1	A	116	GLU	N-CA-C	9.10	121.20	111.28	28	16
1	A	120	MET	N-CA-C	9.09	122.02	111.11	104	20
1	A	11	ALA	CA-C-N	9.08	132.45	120.28	58	37
1	A	11	ALA	C-N-CA	9.08	132.45	120.28	58	37
1	A	18	ASP	CA-C-N	9.08	134.43	122.26	2	7
1	A	18	ASP	C-N-CA	9.08	134.43	122.26	2	7
1	A	103	HIS	CB-CG-CD2	-9.07	119.41	131.20	78	11
1	A	61	PHE	N-CA-C	9.07	125.08	112.75	130	13
1	A	90	LYS	CA-C-N	9.06	132.21	120.44	112	25
1	A	90	LYS	C-N-CA	9.06	132.21	120.44	112	25
1	A	31	VAL	CA-C-N	9.06	133.38	120.79	49	44
1	A	31	VAL	C-N-CA	9.06	133.38	120.79	49	44
1	A	9	LYS	CA-C-N	9.06	132.41	120.28	112	24
1	A	9	LYS	C-N-CA	9.06	132.41	120.28	112	24
2	B	4	TRP	CA-C-N	9.03	132.18	120.44	18	33
2	B	4	TRP	C-N-CA	9.03	132.18	120.44	18	33
1	A	76	ASP	CA-C-O	9.03	130.56	120.90	158	9
1	A	119	GLU	O-C-N	-9.02	111.66	122.22	109	10
1	A	54	ASP	CA-CB-CG	9.02	121.62	112.60	98	12
1	A	136	GLU	O-C-N	-9.02	111.17	122.27	108	7
1	A	20	ASP	N-CA-C	-9.02	100.69	112.68	143	14
1	A	87	VAL	N-CA-C	9.02	119.83	110.36	132	19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	43	GLU	CA-C-O	9.02	130.43	119.79	69	16
1	A	96	ILE	N-CA-CB	9.01	121.04	110.95	112	18
1	A	47	MET	CA-C-O	9.01	130.10	120.55	129	14
1	A	10	GLU	O-C-N	-8.98	112.82	122.07	31	13
2	B	14	ILE	N-CA-C	8.95	119.76	110.36	26	22
2	B	15	GLY	CA-C-N	8.95	134.31	120.89	75	22
2	B	15	GLY	C-N-CA	8.95	134.31	120.89	75	22
1	A	29	GLY	O-C-N	-8.94	112.70	122.54	89	14
1	A	76	ASP	CA-C-N	8.93	133.88	120.31	22	36
1	A	76	ASP	C-N-CA	8.93	133.88	120.31	22	36
1	A	102	ARG	NE-CZ-NH2	8.92	127.23	119.20	154	17
2	B	7	THR	N-CA-CB	8.91	123.36	110.16	62	11
1	A	104	VAL	CA-CB-CG1	8.91	125.55	110.40	158	9
1	A	103	HIS	CA-C-N	8.90	132.66	120.46	146	25
1	A	103	HIS	C-N-CA	8.90	132.66	120.46	146	25
1	A	7	GLU	N-CA-C	8.87	120.56	111.07	91	13
2	B	2	ARG	O-C-N	-8.87	112.86	122.09	129	9
1	A	47	MET	N-CA-C	8.87	121.75	111.11	65	24
1	A	63	GLU	CA-C-O	-8.86	111.07	120.55	160	6
1	A	84	ALA	CA-C-O	-8.86	111.52	120.82	76	6
1	A	139	GLN	CA-C-N	8.86	131.96	120.44	31	20
1	A	139	GLN	C-N-CA	8.86	131.96	120.44	31	20
2	B	11	VAL	CA-C-N	8.86	131.95	120.44	140	31
2	B	11	VAL	C-N-CA	8.86	131.95	120.44	140	31
1	A	44	LEU	N-CA-C	8.84	120.92	111.28	24	12
2	B	3	LYS	CA-C-O	8.82	130.08	120.82	119	11
1	A	116	GLU	CA-C-O	-8.80	111.63	120.70	122	8
1	A	69	ALA	CA-C-N	8.79	133.90	121.24	35	22
1	A	69	ALA	C-N-CA	8.79	133.90	121.24	35	22
1	A	19	GLY	CA-C-N	8.79	133.67	120.31	33	5
1	A	19	GLY	C-N-CA	8.79	133.67	120.31	33	5
1	A	133	ASN	OD1-CG-ND2	-8.79	113.81	122.60	130	22
1	A	83	GLU	O-C-N	-8.77	112.82	122.12	136	12
1	A	47	MET	N-CA-CB	8.77	123.14	109.82	118	7
1	A	137	PHE	CA-C-N	8.76	131.78	120.56	140	28
1	A	137	PHE	C-N-CA	8.76	131.78	120.56	140	28
1	A	69	ALA	O-C-N	-8.76	111.88	122.48	48	7
1	A	33	ARG	N-CA-C	8.75	121.77	111.71	42	18
1	A	86	ARG	NE-CZ-NH2	-8.74	111.33	119.20	50	15
1	A	135	GLU	N-CA-C	8.73	121.90	111.33	96	21
1	A	102	ARG	CA-C-N	8.73	132.32	120.54	104	37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	102	ARG	C-N-CA	8.73	132.32	120.54	104	37
1	A	98	ALA	CA-C-O	8.72	130.00	119.97	52	14
1	A	5	ILE	N-CA-CB	8.70	120.11	110.62	14	9
1	A	19	GLY	CA-C-O	8.70	129.73	119.46	119	4
1	A	8	PHE	CA-C-N	8.70	132.13	120.65	72	29
1	A	8	PHE	C-N-CA	8.70	132.13	120.65	72	29
1	A	79	GLU	N-CA-C	8.70	120.37	111.07	48	13
1	A	137	PHE	N-CA-C	8.69	122.38	111.69	37	12
1	A	46	ASP	N-CA-C	8.69	120.75	111.28	32	10
1	A	6	ALA	CA-C-N	8.69	133.51	120.31	22	32
1	A	6	ALA	C-N-CA	8.69	133.51	120.31	22	32
1	A	5	ILE	CA-C-O	8.68	129.98	120.95	111	11
1	A	28	LEU	CA-C-O	8.68	129.93	120.82	73	8
1	A	16	ASP	CA-C-N	8.68	132.61	120.29	35	22
1	A	16	ASP	C-N-CA	8.68	132.61	120.29	35	22
1	A	30	THR	CA-C-N	8.67	131.65	120.56	154	26
1	A	30	THR	C-N-CA	8.67	131.65	120.56	154	26
1	A	131	GLN	O-C-N	-8.66	111.89	123.15	125	14
1	A	12	PHE	CA-C-N	8.65	132.74	120.28	72	24
1	A	12	PHE	C-N-CA	8.65	132.74	120.28	72	24
1	A	105	MET	N-CA-C	8.64	121.64	111.71	100	27
1	A	129	ASP	CA-C-N	8.63	134.63	121.51	48	5
1	A	129	ASP	C-N-CA	8.63	134.63	121.51	48	5
1	A	77	SER	N-CA-C	8.63	123.06	112.54	74	14
1	A	59	ILE	CA-C-O	8.62	130.75	120.74	61	9
2	B	3	LYS	O-C-N	-8.61	113.20	122.07	119	7
1	A	94	GLY	CA-C-O	8.60	128.09	118.98	72	9
1	A	111	LYS	CA-C-N	8.56	133.66	121.42	76	9
1	A	111	LYS	C-N-CA	8.56	133.66	121.42	76	9
1	A	134	TYR	O-C-N	-8.56	112.39	122.15	111	18
2	B	9	HIS	CA-C-O	8.54	129.48	120.42	134	19
1	A	61	PHE	CA-C-N	8.54	128.67	119.28	134	13
1	A	61	PHE	C-N-CA	8.54	128.67	119.28	134	13
1	A	8	PHE	CA-C-O	-8.54	111.42	120.55	90	7
1	A	67	MET	CA-C-N	8.53	132.40	120.29	60	8
1	A	67	MET	C-N-CA	8.53	132.40	120.29	60	8
1	A	127	ASP	CA-C-N	8.52	136.33	121.07	149	2
1	A	127	ASP	C-N-CA	8.52	136.33	121.07	149	2
1	A	121	ILE	CA-C-O	-8.51	111.61	121.05	84	11
1	A	113	THR	O-C-N	-8.51	112.73	122.68	7	13
1	A	82	ARG	NE-CZ-NH2	-8.50	111.55	119.20	138	16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	85	PHE	CA-C-N	8.49	131.48	120.44	97	22
1	A	85	PHE	C-N-CA	8.49	131.48	120.44	97	22
1	A	82	ARG	CA-C-N	8.49	131.66	120.28	134	22
1	A	82	ARG	C-N-CA	8.49	131.66	120.28	134	22
1	A	49	ASN	OD1-CG-ND2	-8.49	114.11	122.60	30	18
1	A	28	LEU	N-CA-C	8.49	120.15	111.07	136	18
1	A	45	GLN	O-C-N	-8.49	113.12	122.12	73	10
1	A	13	SER	CA-C-N	8.49	132.00	120.54	110	28
1	A	13	SER	C-N-CA	8.49	132.00	120.54	110	28
1	A	120	MET	O-C-N	-8.48	113.27	122.09	124	9
1	A	8	PHE	CA-CB-CG	8.47	122.27	113.80	54	28
1	A	83	GLU	CA-C-O	-8.47	111.57	120.55	5	10
2	B	5	GLN	CA-C-O	8.47	129.53	120.55	13	5
2	B	1	ARG	CA-C-N	8.46	132.31	120.29	7	27
2	B	1	ARG	C-N-CA	8.46	132.31	120.29	7	27
1	A	26	LYS	CA-C-O	8.44	129.50	120.55	78	11
1	A	25	THR	N-CA-C	8.43	120.47	111.28	112	20
1	A	48	ILE	O-C-N	-8.43	113.14	121.90	2	18
1	A	73	LYS	O-C-N	-8.41	113.26	122.85	118	11
1	A	88	PHE	CB-CG-CD2	8.41	135.00	120.70	6	2
1	A	67	MET	CA-C-O	-8.41	112.04	120.70	12	13
1	A	85	PHE	N-CA-C	8.41	120.44	111.28	64	14
1	A	100	GLU	N-CA-C	8.40	121.19	111.11	106	20
2	B	11	VAL	CA-CB-CG1	8.40	124.67	110.40	34	6
1	A	4	GLN	N-CA-C	8.40	120.43	111.28	43	15
1	A	30	THR	N-CA-C	8.39	121.18	111.11	115	18
1	A	32	MET	CA-C-N	8.38	131.51	120.28	106	31
1	A	32	MET	C-N-CA	8.38	131.51	120.28	106	31
1	A	103	HIS	CE1-NE2-CD2	-8.38	100.61	109.00	136	42
1	A	112	LEU	O-C-N	-8.36	113.14	123.01	10	13
1	A	93	ASN	CA-C-N	8.36	134.17	122.63	123	6
1	A	93	ASN	C-N-CA	8.36	134.17	122.63	123	6
1	A	38	ASN	CA-C-N	8.36	128.39	119.78	160	22
1	A	38	ASN	C-N-CA	8.36	128.39	119.78	160	22
1	A	22	THR	N-CA-C	8.34	122.16	109.23	18	7
1	A	17	LYS	O-C-N	8.34	131.09	122.09	34	8
1	A	103	HIS	ND1-CE1-NE2	8.34	116.74	108.40	155	23
1	A	90	LYS	CA-C-O	8.34	129.29	120.70	99	11
1	A	24	THR	CA-CB-OG1	8.33	122.10	109.60	41	10
1	A	141	MET	CA-C-O	-8.33	111.59	120.42	47	8
1	A	61	PHE	CA-C-O	-8.33	110.79	118.79	92	44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	9	HIS	CG-CD2-NE2	8.32	115.52	107.20	147	25
1	A	5	ILE	N-CA-C	8.30	119.09	110.62	66	16
1	A	48	ILE	N-CA-CB	8.29	120.25	110.55	114	9
1	A	110	GLU	O-C-N	-8.28	113.78	123.06	108	15
1	A	72	MET	N-CA-CB	8.28	119.29	111.59	122	4
1	A	75	THR	N-CA-CB	8.27	122.06	110.07	129	22
1	A	103	HIS	N-CA-C	8.25	119.97	110.97	138	25
1	A	53	ALA	CA-C-N	8.24	131.53	120.65	70	30
1	A	53	ALA	C-N-CA	8.24	131.53	120.65	70	30
1	A	123	GLU	N-CA-C	8.23	119.88	111.07	37	24
1	A	97	SER	N-CA-C	8.23	120.53	110.41	17	7
1	A	89	ASP	O-C-N	-8.22	113.68	123.13	94	11
1	A	38	ASN	CA-C-O	-8.21	108.91	120.16	50	24
1	A	81	ILE	CA-C-O	-8.21	111.30	119.92	79	9
2	B	10	ALA	O-C-N	-8.20	112.59	122.11	125	15
1	A	107	ASN	CA-C-N	8.20	131.48	120.65	109	18
1	A	107	ASN	C-N-CA	8.20	131.48	120.65	109	18
1	A	81	ILE	CB-CA-C	8.19	123.20	111.65	79	5
1	A	104	VAL	CA-C-O	8.18	129.32	120.57	107	10
1	A	131	GLN	CA-C-O	8.18	129.29	120.38	111	4
1	A	93	ASN	OD1-CG-ND2	-8.18	114.42	122.60	9	23
1	A	70	ARG	NE-CZ-NH1	8.17	129.67	121.50	7	15
1	A	135	GLU	CA-C-N	8.17	132.04	120.28	156	31
1	A	135	GLU	C-N-CA	8.17	132.04	120.28	156	31
1	A	3	GLU	N-CA-C	8.17	121.10	111.71	56	13
2	B	16	ARG	CB-CA-C	8.17	124.51	110.79	135	2
1	A	17	LYS	CA-C-N	8.16	131.73	120.63	56	15
1	A	17	LYS	C-N-CA	8.16	131.73	120.63	56	15
1	A	13	SER	O-C-N	-8.16	111.20	122.46	132	7
2	B	4	TRP	CB-CG-CD2	-8.16	115.38	126.80	124	6
1	A	108	LEU	CA-C-O	8.15	130.05	120.92	27	12
1	A	106	THR	N-CA-CB	8.14	121.88	110.07	26	25
1	A	52	ASP	CA-C-N	8.14	136.72	121.81	116	25
1	A	52	ASP	C-N-CA	8.14	136.72	121.81	116	25
1	A	73	LYS	CA-C-N	8.14	131.53	120.38	136	25
1	A	73	LYS	C-N-CA	8.14	131.53	120.38	136	25
1	A	122	ARG	NE-CZ-NH2	-8.14	111.88	119.20	78	15
2	B	5	GLN	OE1-CD-NE2	-8.13	114.47	122.60	85	19
1	A	77	SER	CA-C-O	8.13	129.36	120.82	21	17
1	A	11	ALA	O-C-N	-8.13	113.31	122.09	110	11
1	A	41	GLU	N-CA-C	8.12	121.05	111.71	122	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	87	VAL	CB-CA-C	-8.11	101.37	112.24	54	8
1	A	17	LYS	CA-C-O	8.10	128.39	119.15	123	22
1	A	42	ALA	CA-C-N	8.09	131.13	120.28	79	18
1	A	42	ALA	C-N-CA	8.09	131.13	120.28	79	18
1	A	134	TYR	CA-C-O	8.09	129.13	120.55	25	12
1	A	28	LEU	N-CA-CB	8.09	121.70	109.98	17	6
1	A	39	PRO	O-C-N	-8.09	114.25	123.23	152	9
1	A	83	GLU	N-CA-C	8.07	120.08	111.28	54	17
2	B	3	LYS	CA-C-N	8.07	131.61	120.63	139	13
2	B	3	LYS	C-N-CA	8.07	131.61	120.63	139	13
1	A	26	LYS	O-C-N	-8.06	112.96	122.15	113	15
1	A	20	ASP	N-CA-CB	8.06	122.42	110.33	40	7
1	A	26	LYS	N-CA-C	8.06	120.78	111.11	40	15
1	A	42	ALA	CA-C-O	-8.06	110.70	119.97	131	8
1	A	82	ARG	NE-CZ-NH1	8.06	129.56	121.50	150	11
1	A	27	GLU	N-CA-C	8.05	119.69	111.07	86	21
1	A	46	ASP	CA-C-O	8.05	129.27	120.82	65	13
1	A	117	VAL	CB-CA-C	-8.04	101.29	112.14	98	8
1	A	81	ILE	CA-C-N	8.03	131.36	120.44	103	30
1	A	81	ILE	C-N-CA	8.03	131.36	120.44	103	30
1	A	41	GLU	CA-C-N	8.03	131.94	120.79	60	40
1	A	41	GLU	C-N-CA	8.03	131.94	120.79	60	40
1	A	40	THR	CA-C-N	8.02	131.68	120.29	10	18
1	A	40	THR	C-N-CA	8.02	131.68	120.29	10	18
1	A	10	GLU	CA-C-N	8.02	131.37	120.38	21	21
1	A	10	GLU	C-N-CA	8.02	131.37	120.38	21	21
1	A	115	GLU	O-C-N	8.02	130.33	122.07	105	15
1	A	27	GLU	N-CA-CB	8.02	121.90	110.12	51	4
1	A	62	PRO	N-CA-C	8.01	124.26	113.84	11	11
1	A	82	ARG	NH1-CZ-NH2	-8.01	108.88	119.30	150	7
1	A	113	THR	CA-C-O	-8.01	112.72	121.94	135	7
1	A	13	SER	N-CA-C	8.01	122.00	111.75	69	32
2	B	16	ARG	O-C-N	-8.01	112.48	122.17	79	7
1	A	121	ILE	N-CA-C	8.01	118.77	110.36	75	16
1	A	120	MET	CG-SD-CE	-8.00	83.31	100.90	110	16
1	A	69	ALA	CB-CA-C	-8.00	97.52	110.79	81	3
2	B	16	ARG	NE-CZ-NH1	7.99	129.49	121.50	145	14
1	A	23	ILE	N-CA-CB	7.99	120.56	111.21	92	19
1	A	73	LYS	N-CA-C	7.97	120.88	110.43	7	13
1	A	70	ARG	NH1-CZ-NH2	7.96	129.64	119.30	152	13
1	A	18	ASP	O-C-N	-7.95	113.99	123.13	129	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	26	LYS	CA-C-N	7.95	130.78	120.44	95	28
1	A	26	LYS	C-N-CA	7.95	130.78	120.44	95	28
1	A	41	GLU	O-C-N	-7.94	113.70	122.12	97	2
2	B	6	LYS	N-CA-C	7.92	119.61	110.97	34	33
1	A	77	SER	N-CA-CB	7.92	121.56	110.07	53	8
1	A	30	THR	CA-C-O	-7.91	112.55	120.70	128	14
1	A	131	GLN	CA-C-N	-7.91	112.17	122.37	114	7
1	A	131	GLN	C-N-CA	-7.91	112.17	122.37	114	7
1	A	60	ASP	CA-C-N	7.90	129.58	119.78	67	17
1	A	60	ASP	C-N-CA	7.90	129.58	119.78	67	17
1	A	96	ILE	N-CA-C	7.90	120.24	108.54	158	4
1	A	106	THR	CA-C-N	7.90	131.50	120.29	108	26
1	A	106	THR	C-N-CA	7.90	131.50	120.29	108	26
1	A	110	GLU	CA-C-N	7.89	132.92	122.42	39	7
1	A	110	GLU	C-N-CA	7.89	132.92	122.42	39	7
1	A	49	ASN	O-C-N	-7.88	110.92	122.43	149	8
1	A	3	GLU	CA-C-O	7.88	129.03	119.97	83	13
1	A	123	GLU	CA-C-O	7.88	128.91	120.55	111	7
1	A	105	MET	CA-C-N	7.87	131.15	120.44	26	21
1	A	105	MET	C-N-CA	7.87	131.15	120.44	26	21
1	A	141	MET	N-CA-CB	7.86	121.47	110.07	78	5
1	A	49	ASN	N-CA-C	7.86	121.82	111.75	143	17
1	A	138	VAL	CA-C-O	7.86	128.99	120.57	19	10
1	A	133	ASN	N-CA-CB	7.86	122.52	110.49	147	2
2	B	12	ARG	NE-CZ-NH1	7.85	129.35	121.50	129	12
1	A	51	VAL	O-C-N	-7.85	114.32	122.25	119	13
1	A	31	VAL	CB-CA-C	-7.85	101.92	111.97	73	12
1	A	136	GLU	CA-C-O	7.85	128.87	120.55	143	15
1	A	139	GLN	CB-CA-C	-7.84	98.51	110.90	6	4
1	A	61	PHE	CB-CA-C	7.83	125.60	110.17	66	3
2	B	16	ARG	N-CA-C	7.83	119.89	111.36	132	15
1	A	65	LEU	CA-C-O	-7.82	112.18	120.63	160	7
1	A	115	GLU	CA-C-O	7.82	129.68	120.92	38	5
1	A	23	ILE	O-C-N	-7.82	114.92	123.20	108	9
1	A	18	ASP	N-CA-CB	7.79	122.39	110.39	45	4
1	A	54	ASP	CA-C-O	7.79	128.68	120.42	64	9
1	A	138	VAL	N-CA-C	7.79	118.59	110.72	110	16
1	A	69	ALA	CA-C-O	7.79	128.85	119.43	24	13
1	A	139	GLN	N-CA-CB	7.78	121.56	110.12	5	5
2	B	11	VAL	CB-CA-C	7.78	124.86	112.26	55	8
2	B	10	ALA	CA-C-O	-7.77	111.03	119.97	27	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	13	ALA	CA-C-O	7.77	128.70	120.70	106	12
1	A	20	ASP	CA-C-O	7.76	128.00	119.15	70	8
1	A	140	MET	CA-C-O	7.76	128.65	120.42	132	6
2	B	1	ARG	NH1-CZ-NH2	-7.75	109.22	119.30	14	5
1	A	32	MET	O-C-N	-7.75	113.31	122.15	156	13
1	A	121	ILE	O-C-N	7.75	129.96	121.90	84	21
1	A	115	GLU	CA-C-N	7.74	130.50	120.44	92	35
1	A	115	GLU	C-N-CA	7.74	130.50	120.44	92	35
1	A	25	THR	N-CA-CB	7.74	121.47	109.94	48	15
1	A	139	GLN	N-CA-C	7.73	120.69	111.33	143	18
1	A	82	ARG	CA-C-O	7.73	128.75	120.55	142	8
1	A	45	GLN	CA-C-N	7.73	130.63	120.28	96	35
1	A	45	GLN	C-N-CA	7.73	130.63	120.28	96	35
1	A	99	ALA	N-CA-CB	-7.73	98.72	110.16	33	15
1	A	90	LYS	N-CA-CB	-7.73	98.77	109.98	136	6
1	A	113	THR	N-CA-CB	7.73	121.41	110.36	105	13
1	A	12	PHE	N-CA-C	7.72	119.48	111.14	143	15
1	A	124	ALA	O-C-N	-7.72	113.35	122.15	91	6
1	A	86	ARG	O-C-N	-7.72	113.94	122.12	153	15
1	A	14	LEU	N-CA-C	7.72	120.58	111.71	101	14
2	B	9	HIS	ND1-CE1-NE2	7.71	116.11	108.40	143	22
1	A	51	VAL	N-CA-CB	7.71	119.36	110.65	121	2
1	A	23	ILE	CA-C-O	7.71	128.82	120.57	101	5
1	A	137	PHE	N-CA-CB	-7.71	98.90	110.07	157	4
1	A	73	LYS	N-CA-CB	7.70	122.00	110.29	153	7
1	A	68	MET	N-CA-C	7.70	120.75	111.82	86	20
1	A	43	GLU	O-C-N	-7.70	113.78	122.09	91	10
1	A	105	MET	CG-SD-CE	-7.69	83.98	100.90	95	18
1	A	122	ARG	CA-C-O	7.69	128.84	119.38	47	8
1	A	35	LEU	O-C-N	-7.69	114.10	122.09	147	8
1	A	3	GLU	CA-C-N	7.68	130.43	120.44	152	21
1	A	3	GLU	C-N-CA	7.68	130.43	120.44	152	21
1	A	8	PHE	N-CA-C	-7.68	102.85	111.14	42	11
1	A	125	ASP	O-C-N	-7.67	114.47	123.22	111	11
1	A	29	GLY	CA-C-O	-7.67	112.72	121.00	47	13
1	A	21	GLY	O-C-N	-7.67	112.73	122.70	107	5
1	A	138	VAL	O-C-N	-7.67	111.54	122.12	145	9
1	A	99	ALA	N-CA-C	7.67	119.64	111.28	159	12
1	A	21	GLY	CA-C-O	7.66	125.97	118.77	101	4
1	A	71	LYS	O-C-N	-7.66	114.48	123.06	138	11
1	A	87	VAL	N-CA-CB	7.66	118.96	110.62	28	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	45	GLN	CA-C-O	7.66	128.75	120.10	153	8
1	A	64	PHE	CA-C-N	7.65	130.53	120.28	113	23
1	A	64	PHE	C-N-CA	7.65	130.53	120.28	113	23
1	A	37	GLN	O-C-N	-7.65	114.50	123.22	9	17
1	A	132	VAL	N-CA-CB	7.65	120.72	111.31	93	9
1	A	80	GLU	O-C-N	-7.64	113.91	122.08	99	8
2	B	1	ARG	NE-CZ-NH1	7.64	129.14	121.50	92	13
1	A	126	ILE	CB-CA-C	-7.64	102.77	111.55	63	7
2	B	16	ARG	NE-CZ-NH2	-7.62	112.34	119.20	145	8
1	A	114	ASP	CB-CA-C	7.62	123.00	110.81	128	2
1	A	16	ASP	N-CA-C	7.62	120.79	109.59	142	11
1	A	27	GLU	CA-C-O	7.62	128.49	120.42	108	11
1	A	114	ASP	N-CA-C	7.61	120.47	111.71	51	13
1	A	87	VAL	O-C-N	-7.61	114.18	121.87	81	11
1	A	123	GLU	CA-C-N	7.61	130.33	120.44	100	16
1	A	123	GLU	C-N-CA	7.61	130.33	120.44	100	16
1	A	38	ASN	N-CA-CB	-7.61	100.02	111.21	8	5
1	A	12	PHE	O-C-N	-7.61	114.23	122.07	21	12
1	A	102	ARG	O-C-N	-7.60	114.24	122.07	57	13
1	A	88	PHE	N-CA-CB	7.59	123.32	110.49	45	11
1	A	8	PHE	N-CA-CB	7.59	122.05	110.28	152	6
1	A	30	THR	CA-CB-OG1	7.59	120.98	109.60	54	7
1	A	101	LEU	N-CA-C	7.58	120.51	111.33	49	21
1	A	21	GLY	CA-C-N	7.58	133.83	121.86	151	11
1	A	21	GLY	C-N-CA	7.58	133.83	121.86	151	11
1	A	81	ILE	O-C-N	-7.58	114.14	121.94	76	16
1	A	103	HIS	O-C-N	-7.57	114.27	122.07	10	7
1	A	40	THR	CA-CB-OG1	7.55	120.93	109.60	32	10
1	A	38	ASN	CB-CA-C	7.55	118.03	110.33	87	12
1	A	76	ASP	O-C-N	-7.55	114.00	122.08	45	6
1	A	35	LEU	CB-CA-C	-7.55	99.03	110.88	56	2
1	A	50	GLU	CA-C-N	7.54	132.39	120.47	73	23
1	A	50	GLU	C-N-CA	7.54	132.39	120.47	73	23
1	A	121	ILE	N-CA-CB	7.54	118.88	110.51	33	9
1	A	59	ILE	CA-C-N	7.54	136.46	122.74	114	10
1	A	59	ILE	C-N-CA	7.54	136.46	122.74	114	10
1	A	132	VAL	O-C-N	-7.53	114.93	122.99	30	11
1	A	40	THR	CA-C-O	7.53	129.92	122.01	70	7
1	A	102	ARG	CD-NE-CZ	-7.52	113.88	124.40	70	6
1	A	68	MET	CG-SD-CE	-7.51	84.37	100.90	7	5
1	A	95	TYR	CB-CA-C	-7.51	97.03	109.80	156	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	106	THR	CA-CB-CG2	7.51	123.27	110.50	159	8
1	A	66	THR	O-C-N	-7.51	112.46	122.23	113	7
1	A	40	THR	N-CA-CB	7.50	121.38	110.06	28	11
1	A	8	PHE	O-C-N	7.50	131.24	122.17	90	8
1	A	8	PHE	CB-CA-C	7.50	122.74	110.90	105	9
1	A	53	ALA	CA-C-O	-7.49	111.36	119.97	117	6
1	A	77	SER	O-C-N	7.48	130.09	122.08	64	8
1	A	59	ILE	N-CA-C	7.48	118.14	108.12	5	8
1	A	126	ILE	N-CA-CB	7.48	118.97	111.57	67	7
1	A	103	HIS	CG-CD2-NE2	7.47	114.67	107.20	18	22
1	A	112	LEU	N-CA-C	7.47	121.04	110.50	37	14
1	A	138	VAL	N-CA-CB	7.47	118.76	110.62	57	7
1	A	30	THR	N-CA-CB	7.46	120.81	109.91	4	13
1	A	105	MET	O-C-N	-7.46	112.53	122.23	107	7
1	A	66	THR	N-CA-C	7.46	121.48	112.38	6	8
1	A	100	GLU	N-CA-CB	7.46	121.16	109.82	92	2
2	B	14	ILE	CA-C-O	7.45	128.52	120.47	16	11
1	A	89	ASP	CB-CA-C	7.45	118.97	109.80	55	3
1	A	122	ARG	NE-CZ-NH1	7.45	128.95	121.50	101	9
2	B	2	ARG	NE-CZ-NH2	-7.45	112.50	119.20	1	11
1	A	111	LYS	O-C-N	-7.44	112.14	122.41	147	10
1	A	117	VAL	O-C-N	-7.44	114.17	121.83	96	10
2	B	9	HIS	N-CA-C	-7.44	103.11	111.07	128	16
1	A	33	ARG	NH1-CZ-NH2	-7.43	109.64	119.30	38	3
1	A	76	ASP	N-CA-CB	7.43	121.32	110.47	86	3
1	A	71	LYS	CA-C-O	7.43	131.32	121.89	126	9
1	A	127	ASP	CA-C-O	7.43	128.80	121.00	98	1
1	A	60	ASP	O-C-N	-7.43	114.39	122.85	109	19
1	A	45	GLN	N-CA-C	7.43	119.38	111.28	130	11
1	A	51	VAL	CA-CB-CG1	-7.42	97.78	110.40	145	6
1	A	3	GLU	CB-CA-C	7.42	122.53	110.88	136	4
1	A	7	GLU	O-C-N	-7.42	114.43	122.07	27	5
1	A	104	VAL	N-CA-CB	7.42	119.23	110.55	73	9
1	A	9	LYS	CA-C-O	7.42	128.28	120.42	127	13
1	A	34	SER	N-CA-C	7.42	119.44	111.36	35	18
1	A	81	ILE	N-CA-CB	7.42	119.74	110.47	147	7
1	A	60	ASP	CA-C-O	7.41	130.56	121.89	30	5
1	A	118	ASP	N-CA-CB	-7.41	99.33	110.07	142	9
1	A	16	ASP	O-C-N	-7.41	113.16	123.01	121	16
2	B	13	ALA	O-C-N	-7.40	114.28	122.12	127	12
1	A	126	ILE	O-C-N	-7.40	114.38	122.07	116	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	109	GLY	CA-C-O	7.40	127.46	119.03	28	4
1	A	127	ASP	O-C-N	-7.40	114.28	122.12	84	8
1	A	97	SER	CA-C-O	7.39	130.53	121.81	41	7
1	A	84	ALA	O-C-N	-7.39	114.40	122.09	127	6
1	A	54	ASP	O-C-N	-7.39	112.76	122.59	41	9
1	A	100	GLU	O-C-N	-7.39	114.46	122.07	66	9
1	A	22	THR	O-C-N	-7.39	114.62	123.27	160	7
1	A	24	THR	O-C-N	-7.39	114.67	122.94	125	15
1	A	78	GLU	CB-CG-CD	7.38	125.15	112.60	50	3
1	A	100	GLU	CA-C-O	7.38	128.37	120.55	131	5
1	A	28	LEU	O-C-N	-7.37	114.48	122.07	91	12
1	A	41	GLU	CA-C-O	-7.35	112.63	120.42	63	6
2	B	16	ARG	CA-C-O	-7.34	113.29	121.00	127	6
1	A	26	LYS	CB-CA-C	7.34	123.33	110.85	82	5
1	A	98	ALA	N-CA-CB	-7.34	98.92	110.22	84	5
1	A	57	GLY	CA-C-N	7.34	134.21	123.13	138	5
1	A	57	GLY	C-N-CA	7.34	134.21	123.13	138	5
1	A	93	ASN	N-CA-CB	7.34	121.89	110.44	131	2
1	A	54	ASP	CB-CA-C	-7.33	99.36	110.88	79	10
1	A	102	ARG	NH1-CZ-NH2	-7.33	109.77	119.30	75	8
1	A	68	MET	CA-C-O	7.33	127.51	119.15	30	7
1	A	44	LEU	CA-C-O	7.33	128.25	120.70	155	12
1	A	135	GLU	O-C-N	-7.33	112.86	122.39	84	10
2	B	9	HIS	N-CA-CB	-7.33	99.32	110.16	134	5
1	A	82	ARG	N-CA-CB	-7.32	99.36	110.12	150	9
1	A	133	ASN	CA-C-N	7.32	132.83	121.19	103	31
1	A	133	ASN	C-N-CA	7.32	132.83	121.19	103	31
2	B	16	ARG	CD-NE-CZ	-7.30	114.17	124.40	1	5
1	A	5	ILE	CB-CA-C	-7.30	102.29	112.14	26	9
1	A	10	GLU	N-CA-CB	-7.29	98.73	109.82	134	2
1	A	135	GLU	CA-C-O	-7.29	113.16	120.82	130	11
1	A	99	ALA	CA-C-O	7.29	128.21	120.70	41	12
1	A	49	ASN	CA-C-O	7.29	128.36	120.20	115	8
1	A	7	GLU	CB-CG-CD	7.28	124.97	112.60	23	3
1	A	35	LEU	CA-C-O	7.28	128.13	120.42	34	7
2	B	12	ARG	N-CA-C	7.28	119.84	111.11	60	19
2	B	9	HIS	CB-CG-ND1	7.27	133.60	122.70	120	3
1	A	122	ARG	O-C-N	-7.26	114.42	122.12	133	11
1	A	58	THR	O-C-N	-7.26	114.01	123.16	25	12
2	B	15	GLY	N-CA-C	7.26	122.75	113.24	88	8
1	A	130	GLY	N-CA-C	-7.26	104.76	115.72	46	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	58	THR	N-CA-CB	7.26	122.96	111.20	26	9
1	A	125	ASP	CA-C-N	7.25	129.69	122.66	116	9
1	A	125	ASP	C-N-CA	7.25	129.69	122.66	116	9
1	A	101	LEU	CB-CA-C	-7.25	99.49	110.88	25	3
1	A	106	THR	O-C-N	-7.25	114.44	122.12	131	10
1	A	51	VAL	CA-C-N	7.25	131.42	121.05	17	22
1	A	51	VAL	C-N-CA	7.25	131.42	121.05	17	22
1	A	65	LEU	N-CA-CB	7.24	122.72	110.49	35	6
1	A	120	MET	CA-C-N	7.23	129.93	120.60	96	20
1	A	120	MET	C-N-CA	7.23	129.93	120.60	96	20
1	A	32	MET	CG-SD-CE	-7.22	85.01	100.90	115	19
2	B	12	ARG	O-C-N	-7.22	113.39	122.27	68	8
1	A	25	THR	O-C-N	-7.22	113.78	122.22	26	8
2	B	8	GLY	N-CA-C	7.22	121.64	112.83	155	10
1	A	24	THR	N-CA-C	7.22	119.84	110.53	38	4
1	A	32	MET	CA-C-O	7.21	128.07	120.42	156	9
1	A	107	ASN	OD1-CG-ND2	-7.21	115.39	122.60	15	14
1	A	96	ILE	O-C-N	-7.21	114.14	122.94	133	4
1	A	141	MET	O-C-N	-7.21	114.48	122.12	96	7
1	A	23	ILE	CA-C-N	7.21	135.14	122.67	102	3
1	A	23	ILE	C-N-CA	7.21	135.14	122.67	102	3
1	A	66	THR	CA-C-O	-7.21	113.14	121.07	61	7
1	A	118	ASP	CA-C-O	-7.21	113.25	120.82	86	10
1	A	118	ASP	N-CA-C	7.20	119.75	111.11	71	19
1	A	34	SER	O-C-N	-7.19	114.50	122.12	66	7
1	A	130	GLY	CA-C-O	7.19	126.55	118.86	128	9
1	A	46	ASP	CB-CA-C	7.19	122.72	110.79	8	6
1	A	101	LEU	CA-C-O	-7.19	113.16	121.07	147	9
1	A	69	ALA	N-CA-C	7.18	120.16	111.82	79	17
1	A	72	MET	CA-C-N	7.18	132.21	120.94	135	7
1	A	72	MET	C-N-CA	7.18	132.21	120.94	135	7
1	A	137	PHE	CA-C-O	7.18	128.29	120.90	138	6
1	A	103	HIS	CA-C-O	7.17	128.16	120.55	54	16
1	A	70	ARG	CA-C-N	7.17	131.96	122.42	140	4
1	A	70	ARG	C-N-CA	7.17	131.96	122.42	140	4
2	B	9	HIS	CB-CA-C	-7.17	96.91	110.67	27	4
1	A	114	ASP	N-CA-CB	-7.16	99.18	110.28	92	7
1	A	75	THR	O-C-N	7.16	129.54	122.09	12	11
1	A	66	THR	N-CA-CB	7.15	120.79	110.06	23	10
2	B	12	ARG	CA-C-O	7.15	128.13	120.55	62	13
2	B	8	GLY	CA-C-O	7.15	128.11	120.75	152	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	96	ILE	CA-C-O	7.14	129.02	120.74	113	5
2	B	4	TRP	CB-CA-C	-7.14	99.62	110.90	118	6
1	A	32	MET	N-CA-CB	7.13	120.56	109.94	132	8
1	A	50	GLU	N-CA-CB	7.12	120.65	109.82	75	7
1	A	89	ASP	N-CA-C	7.12	120.06	109.59	66	3
1	A	15	PHE	CA-C-N	7.12	131.68	121.50	57	11
1	A	15	PHE	C-N-CA	7.12	131.68	121.50	57	11
1	A	66	THR	CA-CB-CG2	7.12	122.60	110.50	52	7
1	A	139	GLN	CA-C-O	7.11	128.31	120.63	143	8
1	A	107	ASN	CA-C-O	-7.11	113.36	120.82	50	10
1	A	41	GLU	CB-CA-C	-7.10	98.78	110.85	36	2
1	A	139	GLN	O-C-N	-7.10	113.92	122.22	113	10
1	A	42	ALA	N-CA-CB	7.09	120.59	109.82	152	4
1	A	88	PHE	CA-C-N	7.08	133.67	122.34	13	6
1	A	88	PHE	C-N-CA	7.08	133.67	122.34	13	6
1	A	74	ASP	O-C-N	-7.07	113.94	122.22	32	10
2	B	4	TRP	N-CA-CB	7.07	120.57	109.82	130	7
1	A	131	GLN	N-CA-C	-7.07	98.89	108.86	110	4
1	A	31	VAL	O-C-N	-7.06	114.56	121.83	131	14
1	A	34	SER	CA-C-O	7.06	128.07	120.24	152	9
1	A	45	GLN	OE1-CD-NE2	-7.06	115.54	122.60	30	13
1	A	109	GLY	CA-C-N	7.06	134.88	122.67	96	9
1	A	109	GLY	C-N-CA	7.06	134.88	122.67	96	9
1	A	33	ARG	CA-C-O	7.05	128.25	120.63	1	10
1	A	46	ASP	N-CA-CB	-7.05	99.34	110.28	67	8
1	A	22	THR	CA-CB-OG1	7.05	120.18	109.60	103	20
1	A	95	TYR	O-C-N	-7.05	115.09	123.27	103	12
1	A	59	ILE	O-C-N	-7.05	114.98	122.81	105	6
1	A	12	PHE	CA-C-O	7.05	128.44	120.90	83	9
1	A	71	LYS	N-CA-C	7.05	120.95	110.52	155	9
1	A	11	ALA	N-CA-CB	7.03	120.57	110.16	114	6
1	A	53	ALA	N-CA-CB	-7.03	99.48	110.30	95	5
2	B	4	TRP	CA-C-O	7.01	127.92	120.70	156	10
1	A	128	GLY	O-C-N	-7.01	113.58	122.70	2	10
1	A	99	ALA	CB-CA-C	-7.01	99.15	110.79	107	4
1	A	58	THR	CA-C-N	7.01	131.26	122.43	92	3
1	A	58	THR	C-N-CA	7.01	131.26	122.43	92	3
1	A	88	PHE	CB-CA-C	-7.01	99.29	110.86	47	4
1	A	140	MET	CA-C-N	7.00	129.97	120.44	107	11
1	A	140	MET	C-N-CA	7.00	129.97	120.44	107	11
1	A	140	MET	O-C-N	-7.00	114.53	122.09	144	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	1	ARG	CB-CA-C	7.00	123.41	110.10	62	2
1	A	111	LYS	N-CA-CB	6.99	119.06	110.53	79	6
1	A	6	ALA	N-CA-CB	-6.99	99.82	110.16	4	2
2	B	4	TRP	CE2-CD2-CE3	6.99	125.79	118.80	48	9
1	A	70	ARG	N-CA-CB	-6.99	99.03	110.41	67	4
1	A	106	THR	OG1-CB-CG2	-6.98	95.33	109.30	76	3
1	A	102	ARG	NE-CZ-NH1	6.98	128.48	121.50	110	7
1	A	15	PHE	N-CA-C	6.98	118.89	111.28	158	19
1	A	88	PHE	CA-C-O	6.98	127.89	120.70	56	5
1	A	63	GLU	O-C-N	-6.97	113.73	122.17	25	6
1	A	70	ARG	N-CA-C	6.97	120.34	109.96	101	7
1	A	82	ARG	CB-CA-C	6.96	122.35	110.79	150	8
1	A	93	ASN	CA-C-O	6.96	127.98	119.97	59	4
1	A	86	ARG	NE-CZ-NH1	6.96	128.46	121.50	131	18
1	A	31	VAL	CA-CB-CG1	6.96	122.23	110.40	94	5
1	A	6	ALA	O-C-N	-6.96	114.86	122.09	111	16
1	A	105	MET	CA-C-O	-6.96	113.46	120.90	88	12
1	A	63	GLU	CB-CG-CD	6.96	124.43	112.60	99	4
1	A	121	ILE	CA-CB-CG2	6.95	122.32	110.50	61	4
1	A	64	PHE	CA-C-O	-6.95	113.52	120.82	64	10
1	A	67	MET	CG-SD-CE	-6.95	85.61	100.90	141	13
1	A	30	THR	O-C-N	-6.95	114.75	122.12	100	15
1	A	16	ASP	CB-CA-C	6.95	120.17	110.16	28	6
1	A	55	GLY	CA-C-N	6.95	134.53	122.09	58	6
1	A	55	GLY	C-N-CA	6.95	134.53	122.09	58	6
1	A	102	ARG	CA-C-O	-6.94	113.55	120.70	54	5
1	A	138	VAL	CB-CA-C	-6.94	102.77	112.14	65	9
1	A	70	ARG	O-C-N	-6.94	114.48	123.02	38	8
1	A	78	GLU	CA-C-O	6.93	127.94	120.24	3	15
1	A	110	GLU	N-CA-C	6.93	121.33	110.17	8	6
1	A	42	ALA	O-C-N	6.93	130.08	122.11	67	7
1	A	70	ARG	CA-C-O	6.92	129.10	121.56	59	9
1	A	3	GLU	CB-CG-CD	6.92	124.36	112.60	46	3
1	A	34	SER	N-CA-CB	6.92	120.40	110.16	71	16
1	A	64	PHE	N-CA-CB	-6.92	99.69	110.06	77	8
1	A	80	GLU	N-CA-CB	-6.92	99.56	110.28	137	4
1	A	22	THR	N-CA-CB	6.91	121.72	110.32	82	10
1	A	66	THR	CB-CA-C	-6.90	99.33	110.79	91	2
1	A	68	MET	CB-CA-C	-6.90	98.06	110.70	138	1
1	A	75	THR	CA-CB-OG1	6.90	119.95	109.60	17	9
1	A	19	GLY	N-CA-C	-6.90	104.70	115.67	28	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	67	MET	N-CA-CB	-6.90	100.07	110.07	16	6
1	A	110	GLU	CA-C-O	6.90	127.78	120.33	10	10
1	A	85	PHE	O-C-N	-6.88	114.98	122.07	72	9
1	A	15	PHE	O-C-N	-6.88	114.13	122.11	18	8
2	B	12	ARG	NH1-CZ-NH2	-6.88	110.36	119.30	24	6
1	A	125	ASP	N-CA-C	6.87	119.69	109.59	51	10
1	A	133	ASN	N-CA-C	6.87	120.50	109.79	105	5
2	B	5	GLN	CB-CA-C	-6.87	100.00	110.92	159	2
1	A	79	GLU	CA-C-O	-6.86	113.15	120.42	21	10
2	B	15	GLY	CA-C-O	6.86	127.54	119.45	98	5
1	A	41	GLU	N-CA-CB	6.86	120.31	110.16	156	5
1	A	72	MET	N-CA-C	6.85	119.81	109.95	67	6
1	A	7	GLU	N-CA-CB	-6.85	100.03	110.16	7	6
1	A	45	GLN	N-CA-CB	6.84	120.95	110.14	152	7
2	B	10	ALA	CB-CA-C	6.83	121.75	110.81	28	4
1	A	123	GLU	CB-CG-CD	6.83	124.22	112.60	113	3
1	A	62	PRO	CB-CA-C	-6.83	101.12	111.44	145	5
1	A	18	ASP	CB-CA-C	-6.83	97.29	109.24	135	6
1	A	90	LYS	O-C-N	-6.82	113.36	122.23	87	12
1	A	109	GLY	O-C-N	-6.82	113.83	122.70	93	8
1	A	48	ILE	CB-CA-C	-6.82	103.11	112.04	148	4
1	A	25	THR	CA-CB-OG1	6.82	119.82	109.60	140	6
1	A	112	LEU	CA-C-O	6.81	128.81	121.05	68	3
1	A	89	ASP	CA-C-O	6.79	128.27	120.60	109	11
2	B	8	GLY	O-C-N	6.79	128.71	122.19	136	11
1	A	123	GLU	O-C-N	-6.79	114.93	122.12	38	7
1	A	22	THR	CA-C-O	6.78	127.69	120.36	29	7
1	A	115	GLU	CB-CG-CD	6.78	124.13	112.60	103	5
2	B	10	ALA	N-CA-CB	6.78	120.12	109.82	149	9
1	A	84	ALA	N-CA-C	6.78	121.14	113.01	78	14
1	A	131	GLN	OE1-CD-NE2	-6.77	115.83	122.60	34	10
1	A	14	LEU	CB-CA-C	-6.77	97.66	110.67	23	3
1	A	85	PHE	CA-C-O	6.77	127.60	120.42	67	6
1	A	52	ASP	CB-CA-C	6.76	119.46	110.06	103	5
1	A	106	THR	CA-C-O	6.76	127.51	119.60	13	12
2	B	9	HIS	O-C-N	-6.75	114.32	122.22	94	11
2	B	14	ILE	N-CA-CB	6.75	119.71	110.54	118	9
1	A	24	THR	N-CA-CB	6.74	121.08	110.56	105	8
1	A	98	ALA	O-C-N	6.74	129.26	122.12	55	8
2	B	12	ARG	N-CA-CB	-6.74	99.84	110.28	29	4
1	A	118	ASP	O-C-N	6.73	129.26	122.12	108	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	94	GLY	O-C-N	6.73	129.51	122.51	120	7
1	A	142	THR	CA-CB-OG1	6.73	119.69	109.60	139	7
1	A	20	ASP	O-C-N	-6.72	112.89	122.03	110	4
1	A	54	ASP	CA-C-N	6.71	132.37	122.10	8	5
1	A	54	ASP	C-N-CA	6.71	132.37	122.10	8	5
2	B	15	GLY	O-C-N	-6.71	115.10	122.68	109	7
1	A	86	ARG	CA-C-O	6.71	127.60	119.49	146	6
1	A	131	GLN	N-CA-CB	6.71	122.08	110.81	32	7
1	A	82	ARG	CD-NE-CZ	6.70	133.78	124.40	126	4
1	A	9	LYS	O-C-N	-6.70	115.02	122.12	147	12
1	A	58	THR	CA-CB-OG1	6.70	119.65	109.60	54	15
1	A	31	VAL	CA-C-O	-6.70	114.07	121.17	115	7
2	B	4	TRP	CD2-CE2-CZ2	-6.69	115.71	122.40	73	6
1	A	18	ASP	CA-C-O	-6.69	111.89	119.79	131	6
1	A	22	THR	CB-CA-C	-6.69	99.05	110.16	79	4
1	A	135	GLU	CB-CA-C	-6.69	99.68	110.79	146	3
1	A	113	THR	CA-CB-OG1	6.68	119.62	109.60	108	10
1	A	89	ASP	N-CA-CB	-6.68	99.42	109.71	61	6
2	B	11	VAL	N-CA-CB	-6.67	101.47	110.54	48	5
1	A	15	PHE	CA-C-O	-6.67	113.83	120.70	78	3
1	A	26	LYS	CA-CB-CG	6.65	127.41	114.10	146	2
1	A	133	ASN	CA-C-O	6.65	130.05	121.67	145	4
1	A	113	THR	N-CA-C	-6.65	99.63	109.81	108	7
1	A	67	MET	O-C-N	-6.65	113.52	122.43	11	14
1	A	122	ARG	NH1-CZ-NH2	-6.65	110.65	119.30	105	2
1	A	48	ILE	CA-C-O	-6.63	113.06	120.96	81	5
1	A	141	MET	CB-CA-C	-6.63	100.47	110.88	115	3
1	A	39	PRO	CA-C-N	6.63	130.98	121.50	153	7
1	A	39	PRO	C-N-CA	6.63	130.98	121.50	153	7
1	A	46	ASP	O-C-N	-6.63	114.59	122.15	94	8
2	B	1	ARG	CD-NE-CZ	6.62	133.67	124.40	99	2
1	A	94	GLY	N-CA-C	-6.62	105.72	115.72	65	3
1	A	104	VAL	CB-CA-C	6.62	120.17	111.70	82	11
1	A	52	ASP	CA-C-O	6.62	128.60	121.05	146	8
1	A	130	GLY	O-C-N	6.62	129.85	122.50	149	4
1	A	52	ASP	O-C-N	-6.62	115.70	123.11	75	8
1	A	96	ILE	CB-CA-C	-6.62	104.08	111.23	31	9
2	B	6	LYS	O-C-N	6.61	128.88	122.07	135	8
2	B	2	ARG	NE-CZ-NH1	6.61	128.11	121.50	145	8
1	A	56	ASN	CB-CG-OD1	6.61	134.01	120.80	90	5
1	A	56	ASN	N-CA-C	-6.60	104.25	112.90	102	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	132	VAL	CA-CB-CG1	6.60	121.62	110.40	9	4
1	A	33	ARG	NE-CZ-NH2	-6.59	113.26	119.20	98	9
1	A	92	GLY	O-C-N	-6.59	114.13	122.70	91	6
1	A	13	SER	CB-CA-C	-6.59	99.85	110.79	63	3
1	A	11	ALA	CA-C-O	6.58	127.48	120.70	110	7
1	A	7	GLU	CA-C-O	6.58	127.56	119.79	118	6
1	A	47	MET	CG-SD-CE	-6.58	86.42	100.90	29	8
1	A	63	GLU	N-CA-C	-6.58	103.38	111.40	50	11
1	A	19	GLY	O-C-N	6.58	131.25	122.70	69	2
1	A	7	GLU	CB-CA-C	6.57	121.08	110.96	152	2
1	A	33	ARG	O-C-N	-6.57	115.16	122.12	19	9
1	A	93	ASN	N-CA-C	6.56	118.52	111.36	88	13
1	A	128	GLY	CA-C-O	6.56	124.94	118.77	138	2
1	A	39	PRO	CA-C-O	-6.56	113.44	121.31	113	1
1	A	83	GLU	CA-CB-CG	6.56	127.21	114.10	125	1
1	A	40	THR	N-CA-C	6.55	120.55	110.20	53	3
1	A	126	ILE	CA-C-O	-6.55	114.97	120.80	123	8
1	A	44	LEU	N-CA-CB	6.55	119.74	110.12	67	7
2	B	4	TRP	CB-CG-CD1	6.54	136.71	126.90	124	3
1	A	101	LEU	O-C-N	-6.54	114.53	122.11	55	14
1	A	57	GLY	CA-C-O	6.53	127.16	119.19	109	5
1	A	36	GLY	CA-C-N	6.53	132.81	122.62	103	5
1	A	36	GLY	C-N-CA	6.53	132.81	122.62	103	5
2	B	2	ARG	CB-CA-C	-6.53	99.95	110.79	24	4
1	A	71	LYS	N-CA-CB	-6.53	99.99	110.63	40	4
1	A	37	GLN	CA-C-O	-6.52	114.02	121.19	39	5
1	A	25	THR	CA-C-O	-6.52	113.93	120.90	110	7
1	A	78	GLU	N-CA-C	6.51	118.04	111.07	78	10
1	A	43	GLU	CB-CG-CD	-6.51	101.54	112.60	8	3
1	A	87	VAL	CA-CB-CG1	6.51	121.46	110.40	43	3
1	A	5	ILE	CA-CB-CG1	6.49	121.44	110.40	89	2
1	A	51	VAL	CG1-CB-CG2	-6.49	96.52	110.80	9	1
1	A	20	ASP	CA-C-N	6.49	134.13	121.41	112	2
1	A	20	ASP	C-N-CA	6.49	134.13	121.41	112	2
1	A	25	THR	OG1-CB-CG2	-6.48	96.33	109.30	86	3
1	A	120	MET	CA-C-O	-6.48	112.52	119.97	16	10
1	A	10	GLU	CB-CA-C	6.47	120.91	109.65	3	2
1	A	63	GLU	CB-CA-C	6.47	120.98	110.95	138	5
1	A	21	GLY	N-CA-C	-6.47	105.95	115.72	14	2
1	A	86	ARG	N-CA-CB	6.47	119.58	109.94	100	1
1	A	116	GLU	O-C-N	6.47	128.76	122.03	109	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	31	VAL	N-CA-CB	6.47	117.67	110.62	155	5
1	A	85	PHE	N-CA-CB	-6.46	100.60	110.16	125	5
1	A	117	VAL	CA-CB-CG1	6.46	121.39	110.40	62	6
1	A	79	GLU	N-CA-CB	-6.46	100.28	110.22	47	3
1	A	39	PRO	N-CA-CB	6.46	109.06	103.31	142	1
1	A	108	LEU	CA-C-N	6.46	131.32	121.51	129	5
1	A	108	LEU	C-N-CA	6.46	131.32	121.51	129	5
2	B	14	ILE	CB-CA-C	6.45	121.12	112.22	150	6
1	A	134	TYR	N-CA-CB	-6.44	100.67	110.01	54	3
2	B	2	ARG	CA-C-O	-6.44	114.24	121.00	69	9
1	A	137	PHE	CB-CA-C	6.44	120.87	110.96	76	3
1	A	3	GLU	O-C-N	-6.43	115.14	122.09	150	10
1	A	122	ARG	CD-NE-CZ	-6.43	115.40	124.40	43	3
1	A	91	ASP	N-CA-CB	-6.42	100.67	109.98	94	5
1	A	124	ALA	CA-C-O	6.42	127.37	120.24	78	4
1	A	78	GLU	CB-CA-C	-6.42	99.52	110.24	41	2
1	A	140	MET	N-CA-CB	-6.42	100.69	110.12	57	6
1	A	73	LYS	CB-CA-C	6.42	121.34	109.54	124	3
1	A	33	ARG	CA-CB-CG	6.42	126.93	114.10	63	1
1	A	93	ASN	CB-CG-OD1	6.41	133.61	120.80	156	3
1	A	50	GLU	CA-C-O	6.40	127.33	119.97	85	7
1	A	61	PHE	N-CA-CB	6.40	117.97	110.42	144	6
1	A	4	GLN	CA-CB-CG	6.40	126.89	114.10	124	2
1	A	58	THR	CB-CA-C	-6.40	98.57	109.51	146	1
1	A	17	LYS	N-CA-CB	6.39	120.15	110.30	12	6
1	A	136	GLU	N-CA-CB	6.39	121.00	110.39	80	3
1	A	4	GLN	O-C-N	-6.39	114.44	122.17	94	8
1	A	37	GLN	CG-CD-OE1	6.39	133.58	120.80	73	1
1	A	106	THR	CA-CB-OG1	6.39	119.18	109.60	76	7
1	A	40	THR	CA-CB-CG2	6.39	121.36	110.50	119	3
1	A	39	PRO	N-CA-C	6.38	122.43	111.77	118	3
1	A	62	PRO	O-C-N	-6.38	113.63	122.37	32	4
1	A	60	ASP	N-CA-C	-6.38	101.08	110.52	148	5
1	A	74	ASP	N-CA-CB	-6.38	100.75	110.12	155	6
1	A	35	LEU	N-CA-CB	6.38	119.59	110.16	30	5
1	A	142	THR	N-CA-CB	6.38	122.34	111.50	98	5
1	A	68	MET	N-CA-CB	-6.37	100.41	110.28	50	8
1	A	125	ASP	CA-C-O	6.37	128.13	120.81	14	7
1	A	120	MET	CB-CA-C	6.37	122.36	110.70	50	3
1	A	4	GLN	N-CA-CB	-6.36	100.51	110.44	14	5
1	A	103	HIS	CB-CA-C	-6.36	100.23	110.79	63	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	81	ILE	CA-CB-CG1	6.34	121.19	110.40	118	2
1	A	113	THR	CA-CB-CG2	-6.34	99.72	110.50	88	1
1	A	30	THR	CB-CA-C	6.33	120.94	110.81	42	7
1	A	37	GLN	N-CA-C	-6.33	98.66	109.24	57	6
1	A	68	MET	O-C-N	-6.33	114.93	122.15	160	8
1	A	43	GLU	CA-CB-CG	-6.33	101.44	114.10	55	3
1	A	53	ALA	O-C-N	6.31	130.03	122.27	117	4
1	A	17	LYS	N-CA-C	-6.31	105.71	113.41	19	12
1	A	135	GLU	N-CA-CB	6.31	119.50	110.16	55	4
1	A	123	GLU	CB-CA-C	-6.29	101.01	110.88	37	1
1	A	15	PHE	CB-CA-C	-6.29	100.35	110.79	94	7
1	A	14	LEU	O-C-N	-6.29	115.46	122.12	8	6
1	A	67	MET	N-CA-C	6.29	118.21	111.36	144	6
1	A	132	VAL	CA-C-O	6.28	127.44	120.59	45	2
1	A	56	ASN	CA-C-N	6.28	131.30	122.63	125	7
1	A	56	ASN	C-N-CA	6.28	131.30	122.63	125	7
1	A	110	GLU	N-CA-CB	-6.28	100.75	110.29	9	3
1	A	88	PHE	O-C-N	-6.28	115.25	122.03	34	10
1	A	95	TYR	N-CA-CB	6.28	121.66	110.80	129	3
1	A	58	THR	N-CA-C	-6.27	99.68	109.72	3	4
1	A	74	ASP	CB-CA-C	-6.27	101.03	110.88	154	2
1	A	111	LYS	CB-CA-C	6.27	121.58	112.05	145	1
1	A	117	VAL	CA-CB-CG2	-6.27	99.74	110.40	158	3
1	A	75	THR	CB-CA-C	-6.27	100.26	110.79	53	2
1	A	50	GLU	CB-CG-CD	6.26	123.25	112.60	14	3
1	A	111	LYS	CA-C-O	6.26	126.98	120.40	152	4
1	A	98	ALA	CB-CA-C	6.26	122.70	110.67	153	2
1	A	94	GLY	CA-C-N	6.26	131.81	122.99	116	4
1	A	94	GLY	C-N-CA	6.26	131.81	122.99	116	4
1	A	133	ASN	O-C-N	-6.26	113.55	121.74	145	5
1	A	24	THR	CA-C-O	-6.25	114.75	121.94	156	2
1	A	103	HIS	CB-CG-ND1	6.25	132.08	122.70	89	4
1	A	30	THR	CA-CB-CG2	6.25	121.12	110.50	21	3
1	A	125	ASP	N-CA-CB	-6.25	100.63	110.06	143	7
2	B	7	THR	CA-CB-OG1	-6.24	100.23	109.60	159	5
1	A	102	ARG	CG-CD-NE	-6.24	98.27	112.00	153	1
2	B	13	ALA	CB-CA-C	6.24	120.76	110.90	137	4
2	B	7	THR	CA-CB-CG2	6.24	121.11	110.50	22	1
1	A	49	ASN	CB-CG-ND2	6.23	125.74	116.40	43	1
1	A	115	GLU	N-CA-CB	6.23	119.04	110.01	51	4
1	A	14	LEU	N-CA-CB	6.22	119.47	110.20	92	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	132	VAL	CB-CA-C	-6.22	103.33	110.73	82	4
1	A	83	GLU	N-CA-CB	6.22	119.26	110.12	127	2
1	A	134	TYR	CB-CG-CD1	-6.22	111.47	120.80	76	1
1	A	91	ASP	CA-C-N	6.21	130.58	122.26	59	7
1	A	91	ASP	C-N-CA	6.21	130.58	122.26	59	7
1	A	141	MET	CG-SD-CE	-6.20	87.26	100.90	110	9
1	A	108	LEU	CB-CA-C	6.20	121.20	110.79	96	4
1	A	38	ASN	N-CA-C	6.20	120.25	108.97	6	3
1	A	101	LEU	N-CA-CB	-6.20	101.01	110.12	107	7
1	A	118	ASP	CB-CA-C	6.19	121.07	110.79	105	4
1	A	23	ILE	CB-CA-C	-6.18	102.51	110.98	123	6
1	A	57	GLY	N-CA-C	-6.18	106.72	115.43	42	3
1	A	107	ASN	O-C-N	-6.17	115.58	122.12	61	7
1	A	135	GLU	CB-CG-CD	-6.17	102.11	112.60	116	4
1	A	107	ASN	N-CA-CB	-6.16	100.16	110.39	65	6
1	A	5	ILE	CA-CB-CG2	6.16	120.97	110.50	113	3
2	B	4	TRP	O-C-N	-6.16	115.13	122.15	50	4
1	A	32	MET	CB-CA-C	-6.14	100.98	110.81	27	2
1	A	120	MET	N-CA-CB	-6.14	101.05	110.20	50	4
1	A	119	GLU	CB-CG-CD	-6.14	102.16	112.60	20	4
1	A	27	GLU	O-C-N	-6.14	114.72	122.27	92	3
1	A	134	TYR	CB-CA-C	-6.13	101.00	110.81	87	4
1	A	108	LEU	N-CA-CB	6.12	118.88	110.01	138	6
1	A	78	GLU	N-CA-CB	6.12	118.94	110.07	18	3
2	B	4	TRP	CG-CD2-CE3	-6.11	127.79	133.90	48	4
1	A	79	GLU	CB-CG-CD	6.11	122.98	112.60	130	1
2	B	11	VAL	CG1-CB-CG2	-6.11	97.37	110.80	18	3
1	A	30	THR	OG1-CB-CG2	-6.10	97.09	109.30	111	3
1	A	142	THR	OG1-CB-CG2	-6.09	97.11	109.30	159	2
1	A	26	LYS	N-CA-CB	-6.09	101.18	110.01	149	7
1	A	50	GLU	O-C-N	-6.08	115.58	122.08	142	9
1	A	33	ARG	N-CA-CB	-6.08	100.20	110.41	38	4
1	A	56	ASN	CB-CA-C	6.08	119.23	109.02	35	1
1	A	140	MET	CG-SD-CE	-6.07	87.54	100.90	6	6
1	A	86	ARG	NH1-CZ-NH2	-6.07	111.40	119.30	54	4
1	A	40	THR	CB-CA-C	6.06	120.61	109.46	108	1
1	A	90	LYS	CG-CD-CE	6.06	125.23	111.30	51	2
1	A	121	ILE	CB-CA-C	6.04	119.44	111.70	150	9
1	A	66	THR	OG1-CB-CG2	-6.04	97.23	109.30	58	2
1	A	112	LEU	N-CA-CB	6.03	118.86	110.17	90	4
1	A	79	GLU	O-C-N	-6.03	115.28	122.15	154	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	8	PHE	CB-CG-CD2	-6.03	110.45	120.70	48	2
1	A	65	LEU	CB-CA-C	-6.02	100.80	110.79	66	5
1	A	70	ARG	CG-CD-NE	-6.01	98.77	112.00	26	2
1	A	95	TYR	CB-CG-CD2	6.00	129.81	120.80	93	1
1	A	110	GLU	CB-CA-C	6.00	120.10	109.72	142	6
1	A	79	GLU	CB-CA-C	6.00	120.75	110.79	122	2
1	A	136	GLU	CB-CA-C	-6.00	97.77	110.31	80	1
1	A	142	THR	CA-CB-CG2	6.00	120.70	110.50	94	1
2	B	11	VAL	CA-CB-CG2	6.00	120.60	110.40	19	2
1	A	122	ARG	CB-CG-CD	5.99	125.06	111.30	72	1
1	A	62	PRO	N-CA-CB	5.98	108.88	103.20	82	7
1	A	140	MET	CB-CA-C	-5.97	101.50	110.88	124	3
1	A	27	GLU	CB-CG-CD	-5.97	102.45	112.60	50	4
1	A	113	THR	OG1-CB-CG2	-5.97	97.36	109.30	68	1
1	A	87	VAL	CG1-CB-CG2	5.97	123.94	110.80	135	2
1	A	92	GLY	CA-C-N	5.97	129.09	120.38	31	1
1	A	92	GLY	C-N-CA	5.97	129.09	120.38	31	1
2	B	5	GLN	CG-CD-NE2	5.97	125.35	116.40	85	5
1	A	37	GLN	CB-CG-CD	-5.97	102.46	112.60	97	3
1	A	62	PRO	CA-C-O	5.97	126.42	118.90	82	3
2	B	6	LYS	N-CA-CB	-5.96	101.20	109.91	32	4
1	A	9	LYS	CB-CA-C	-5.96	101.49	110.90	37	2
1	A	132	VAL	CA-CB-CG2	-5.96	100.27	110.40	47	2
1	A	10	GLU	CB-CG-CD	5.96	122.73	112.60	67	3
1	A	104	VAL	CA-CB-CG2	-5.95	100.28	110.40	101	2
1	A	95	TYR	CA-C-O	5.94	127.01	120.71	48	1
2	B	12	ARG	CD-NE-CZ	5.94	132.72	124.40	134	4
1	A	83	GLU	CB-CG-CD	5.94	122.69	112.60	126	2
1	A	14	LEU	CA-C-O	-5.93	114.26	120.55	77	6
2	B	14	ILE	CA-CB-CG2	-5.93	100.41	110.50	30	3
2	B	4	TRP	CZ3-CH2-CZ2	-5.93	113.79	121.50	142	2
1	A	128	GLY	CA-C-N	5.93	128.15	120.44	61	5
1	A	128	GLY	C-N-CA	5.93	128.15	120.44	61	5
1	A	116	GLU	N-CA-CB	5.92	118.56	109.91	84	5
1	A	4	GLN	CB-CG-CD	-5.92	102.53	112.60	147	7
1	A	56	ASN	CA-C-O	5.92	126.69	119.11	116	3
1	A	24	THR	CA-CB-CG2	-5.91	100.45	110.50	158	3
1	A	100	GLU	CB-CG-CD	-5.91	102.56	112.60	148	1
2	B	1	ARG	CG-CD-NE	-5.91	99.01	112.00	2	3
1	A	123	GLU	N-CA-CB	5.91	120.19	110.39	52	3
1	A	36	GLY	O-C-N	-5.90	115.03	122.70	103	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	15	PHE	CB-CG-CD1	-5.90	110.67	120.70	100	1
1	A	108	LEU	O-C-N	-5.90	115.03	122.17	114	3
1	A	93	ASN	O-C-N	-5.90	115.02	122.27	63	2
1	A	50	GLU	CB-CA-C	-5.89	101.81	110.95	11	2
1	A	84	ALA	CB-CA-C	-5.89	100.83	110.85	110	2
1	A	25	THR	CB-CA-C	-5.89	101.01	110.79	128	2
2	B	5	GLN	CB-CG-CD	-5.89	102.59	112.60	157	2
1	A	72	MET	CB-CA-C	-5.89	108.59	117.07	111	3
1	A	51	VAL	CB-CA-C	-5.87	104.80	111.55	41	2
1	A	57	GLY	O-C-N	-5.87	115.40	122.38	109	2
1	A	134	TYR	CB-CG-CD2	-5.87	112.00	120.80	86	2
1	A	73	LYS	CA-C-O	5.87	128.69	121.94	100	4
1	A	85	PHE	CB-CA-C	5.87	120.53	110.79	88	3
1	A	96	ILE	CA-CB-CG2	-5.86	100.53	110.50	157	1
1	A	6	ALA	CB-CA-C	-5.86	101.06	110.79	32	2
1	A	112	LEU	CB-CA-C	-5.86	100.69	110.29	59	3
1	A	22	THR	CA-C-N	-5.85	115.56	122.93	20	3
1	A	22	THR	C-N-CA	-5.85	115.56	122.93	20	3
1	A	33	ARG	CG-CD-NE	-5.85	99.13	112.00	116	3
1	A	58	THR	CA-C-O	5.85	127.72	121.11	92	3
1	A	58	THR	CA-CB-CG2	-5.85	100.56	110.50	29	2
1	A	111	LYS	N-CA-C	5.84	118.62	107.75	157	5
1	A	92	GLY	CA-C-O	5.83	125.16	118.98	11	1
1	A	111	LYS	CB-CG-CD	5.83	124.71	111.30	21	2
2	B	2	ARG	NH1-CZ-NH2	-5.82	111.73	119.30	145	2
1	A	107	ASN	CB-CG-ND2	5.82	125.14	116.40	139	3
1	A	64	PHE	CB-CG-CD1	5.82	130.60	120.70	75	1
1	A	128	GLY	N-CA-C	-5.82	106.46	116.01	77	1
1	A	110	GLU	CB-CG-CD	-5.82	102.70	112.60	109	1
1	A	12	PHE	CB-CA-C	5.82	120.45	110.79	137	3
2	B	16	ARG	CG-CD-NE	-5.82	99.20	112.00	7	2
1	A	124	ALA	N-CA-CB	-5.81	101.58	110.01	100	8
1	A	12	PHE	CB-CG-CD1	-5.81	110.82	120.70	72	1
1	A	131	GLN	CB-CG-CD	5.81	122.47	112.60	65	3
1	A	97	SER	N-CA-CB	-5.81	101.17	110.46	100	2
1	A	27	GLU	CB-CA-C	-5.80	100.99	110.85	132	3
1	A	69	ALA	N-CA-CB	5.80	118.39	109.98	23	5
1	A	64	PHE	CB-CA-C	5.80	120.53	110.68	9	2
1	A	87	VAL	CA-C-O	5.79	127.86	120.96	93	2
1	A	127	ASP	N-CA-CB	5.79	118.38	109.98	100	4
1	A	107	ASN	CB-CA-C	-5.79	99.92	110.63	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	5	GLN	N-CA-CB	5.79	119.22	110.30	111	3
1	A	76	ASP	CB-CA-C	-5.79	98.57	110.38	69	1
1	A	85	PHE	CB-CG-CD2	-5.79	110.86	120.70	147	1
1	A	80	GLU	CB-CG-CD	5.79	122.44	112.60	39	7
1	A	43	GLU	CB-CA-C	-5.79	101.76	110.90	143	2
1	A	54	ASP	N-CA-CB	5.78	118.91	110.47	85	5
1	A	42	ALA	CB-CA-C	-5.78	101.81	110.88	8	2
1	A	125	ASP	CB-CA-C	5.77	119.12	109.89	81	2
1	A	9	LYS	N-CA-CB	5.76	118.42	110.07	37	2
1	A	4	GLN	CG-CD-NE2	5.75	125.03	116.40	118	1
1	A	100	GLU	CA-CB-CG	-5.75	102.60	114.10	69	2
1	A	38	ASN	CB-CG-ND2	5.75	125.02	116.40	73	1
1	A	39	PRO	N-CD-CG	5.75	111.82	103.20	94	2
1	A	93	ASN	CB-CG-ND2	-5.74	107.79	116.40	39	2
1	A	59	ILE	CA-CB-CG1	5.74	120.16	110.40	69	5
1	A	37	GLN	CB-CA-C	-5.74	98.53	109.66	145	2
1	A	24	THR	CB-CA-C	-5.74	100.52	110.45	86	1
2	B	6	LYS	CB-CA-C	-5.74	101.10	110.85	13	1
1	A	124	ALA	CB-CA-C	-5.73	101.84	110.90	80	3
1	A	3	GLU	N-CA-CB	5.73	118.48	109.94	127	7
1	A	37	GLN	CG-CD-NE2	5.73	124.99	116.40	142	1
1	A	52	ASP	N-CA-CB	-5.73	99.89	109.28	49	3
1	A	119	GLU	N-CA-CB	-5.72	101.77	110.07	53	2
1	A	75	THR	CA-CB-CG2	-5.72	100.77	110.50	59	3
1	A	48	ILE	CA-CB-CG1	5.71	120.11	110.40	55	3
1	A	34	SER	CB-CA-C	-5.71	100.06	110.63	121	3
2	B	16	ARG	N-CA-CB	5.70	120.02	110.32	154	4
1	A	102	ARG	CB-CA-C	-5.70	100.98	110.68	141	2
1	A	17	LYS	CB-CA-C	5.70	121.12	109.67	103	1
1	A	91	ASP	CB-CA-C	5.68	121.10	110.70	55	4
1	A	91	ASP	CA-C-O	-5.68	113.69	120.56	123	1
1	A	22	THR	OG1-CB-CG2	-5.68	97.94	109.30	15	1
1	A	43	GLU	N-CA-CB	5.67	118.45	110.12	50	3
1	A	73	LYS	CG-CD-CE	5.67	124.34	111.30	53	2
1	A	60	ASP	N-CA-CB	-5.66	101.84	110.45	33	2
1	A	67	MET	CB-CA-C	5.65	120.38	111.39	28	2
1	A	70	ARG	CB-CA-C	-5.65	101.58	110.79	151	2
1	A	47	MET	CA-CB-CG	5.64	125.38	114.10	80	1
1	A	37	GLN	CA-CB-CG	5.62	125.34	114.10	24	1
2	B	12	ARG	CG-CD-NE	-5.62	99.64	112.00	52	6
1	A	62	PRO	N-CD-CG	5.61	111.62	103.20	142	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	86	ARG	CB-CA-C	5.61	120.10	110.79	49	1
1	A	122	ARG	N-CA-CB	-5.61	101.59	110.22	13	3
1	A	56	ASN	CB-CG-ND2	-5.61	107.99	116.40	135	2
2	B	14	ILE	CA-CB-CG1	5.60	119.93	110.40	133	5
1	A	70	ARG	CB-CG-CD	5.60	124.17	111.30	78	2
1	A	132	VAL	N-CA-C	5.59	116.79	108.23	66	1
2	B	16	ARG	CB-CG-CD	5.59	124.16	111.30	86	1
1	A	61	PHE	CB-CG-CD2	-5.59	111.20	120.70	8	1
1	A	84	ALA	N-CA-CB	5.59	118.91	110.30	123	4
1	A	33	ARG	CD-NE-CZ	-5.58	116.58	124.40	77	4
1	A	116	GLU	CB-CG-CD	-5.58	103.11	112.60	90	2
1	A	82	ARG	CG-CD-NE	-5.58	99.72	112.00	35	4
1	A	39	PRO	CB-CA-C	5.58	118.34	110.20	143	1
1	A	86	ARG	CD-NE-CZ	5.57	132.19	124.40	50	3
1	A	9	LYS	CA-CB-CG	5.56	125.22	114.10	82	1
1	A	83	GLU	CB-CA-C	-5.56	102.15	110.88	93	2
1	A	102	ARG	N-CA-CB	-5.56	101.66	109.94	83	5
1	A	96	ILE	CA-C-N	5.55	132.99	123.05	50	4
1	A	96	ILE	C-N-CA	5.55	132.99	123.05	50	4
1	A	48	ILE	CA-CB-CG2	5.54	119.93	110.50	77	3
1	A	77	SER	CB-CA-C	5.54	120.58	110.11	150	2
1	A	73	LYS	CA-CB-CG	5.53	125.16	114.10	10	1
1	A	16	ASP	N-CA-CB	-5.53	101.40	110.52	23	3
1	A	13	SER	CA-C-O	5.53	126.35	120.10	155	7
1	A	17	LYS	CB-CG-CD	5.53	124.02	111.30	60	3
1	A	127	ASP	CB-CA-C	5.53	120.25	110.85	138	3
1	A	126	ILE	CA-CB-CG1	5.52	119.79	110.40	90	1
1	A	24	THR	OG1-CB-CG2	-5.52	98.27	109.30	101	2
1	A	59	ILE	CA-CB-CG2	-5.52	101.12	110.50	73	3
1	A	109	GLY	N-CA-C	-5.52	106.96	116.01	116	1
1	A	53	ALA	CB-CA-C	5.51	120.53	110.11	29	2
1	A	58	THR	OG1-CB-CG2	-5.51	98.27	109.30	149	1
2	B	7	THR	CB-CA-C	-5.51	99.14	110.38	27	3
1	A	100	GLU	CB-CA-C	-5.51	101.48	110.85	26	3
1	A	137	PHE	CB-CG-CD2	5.51	130.06	120.70	28	1
1	A	56	ASN	O-C-N	-5.50	115.52	122.17	67	2
1	A	55	GLY	N-CA-C	-5.50	107.42	115.72	14	1
1	A	131	GLN	CG-CD-NE2	5.50	124.64	116.40	110	3
1	A	44	LEU	CB-CA-C	-5.49	101.67	110.79	24	2
1	A	66	THR	CA-CB-OG1	-5.49	101.36	109.60	52	2
1	A	115	GLU	CA-CB-CG	5.48	125.06	114.10	97	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	92	GLY	N-CA-C	-5.47	107.46	115.72	39	1
1	A	45	GLN	CB-CA-C	5.47	119.46	110.88	99	4
1	A	70	ARG	CD-NE-CZ	-5.46	116.75	124.40	119	3
1	A	122	ARG	CG-CD-NE	-5.46	99.99	112.00	65	3
1	A	129	ASP	CA-C-O	-5.45	113.22	119.60	79	6
1	A	112	LEU	CA-C-N	5.45	131.38	122.07	125	1
1	A	112	LEU	C-N-CA	5.45	131.38	122.07	125	1
1	A	107	ASN	CB-CG-OD1	5.42	131.64	120.80	20	2
1	A	91	ASP	O-C-N	-5.41	115.84	122.11	73	2
2	B	16	ARG	NH1-CZ-NH2	-5.41	112.27	119.30	37	3
1	A	95	TYR	N-CA-C	-5.40	99.64	108.76	40	3
1	A	131	GLN	CB-CA-C	-5.39	104.63	111.70	24	1
1	A	138	VAL	CA-CB-CG2	-5.39	101.23	110.40	160	3
1	A	44	LEU	CD1-CG-CD2	-5.39	98.93	110.80	124	1
1	A	141	MET	CA-C-N	5.39	131.40	121.70	49	2
1	A	141	MET	C-N-CA	5.39	131.40	121.70	49	2
2	B	7	THR	OG1-CB-CG2	-5.39	98.52	109.30	137	4
1	A	114	ASP	O-C-N	5.39	128.29	122.15	143	2
2	B	2	ARG	N-CA-CB	-5.38	101.93	110.22	149	1
1	A	32	MET	CA-CB-CG	5.38	124.87	114.10	120	1
1	A	11	ALA	CB-CA-C	-5.38	102.43	110.88	81	3
1	A	115	GLU	CB-CA-C	5.38	119.33	110.88	102	3
1	A	25	THR	CA-CB-CG2	-5.38	101.36	110.50	62	1
1	A	105	MET	N-CA-CB	-5.37	102.03	110.30	10	2
1	A	97	SER	CA-CB-OG	5.37	121.84	111.10	68	1
1	A	45	GLN	CG-CD-NE2	5.36	124.44	116.40	30	3
1	A	96	ILE	CA-CB-CG1	5.35	119.49	110.40	57	1
1	A	139	GLN	CB-CG-CD	-5.34	103.52	112.60	149	1
1	A	130	GLY	CA-C-N	5.34	130.64	122.95	102	1
1	A	130	GLY	C-N-CA	5.34	130.64	122.95	102	1
1	A	103	HIS	N-CA-CB	5.34	118.06	110.16	105	2
1	A	9	LYS	CG-CD-CE	5.34	123.57	111.30	80	1
1	A	51	VAL	CA-CB-CG2	5.31	119.43	110.40	147	3
2	B	13	ALA	N-CA-CB	5.31	118.02	110.06	149	2
1	A	41	GLU	CB-CG-CD	-5.31	103.58	112.60	31	2
1	A	31	VAL	CA-CB-CG2	5.31	119.42	110.40	71	1
1	A	129	ASP	O-C-N	-5.31	115.38	122.49	135	1
1	A	64	PHE	CB-CG-CD2	5.30	129.71	120.70	26	1
1	A	4	GLN	CB-CA-C	5.30	119.69	110.79	94	2
1	A	122	ARG	CB-CA-C	-5.30	102.56	110.88	139	1
2	B	1	ARG	N-CA-CB	-5.29	101.50	110.50	133	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	110	GLU	CA-CB-CG	5.29	124.68	114.10	94	1
1	A	7	GLU	CA-CB-CG	5.29	124.68	114.10	77	1
1	A	87	VAL	CA-CB-CG2	-5.29	101.41	110.40	120	1
1	A	105	MET	CB-CA-C	-5.29	100.85	110.63	100	1
1	A	133	ASN	CB-CG-OD1	5.28	131.36	120.80	4	2
1	A	93	ASN	CB-CA-C	5.27	117.93	109.07	1	1
1	A	47	MET	CB-CA-C	-5.27	102.05	110.79	134	4
1	A	138	VAL	CA-CB-CG1	5.26	119.35	110.40	8	3
2	B	1	ARG	O-C-N	-5.26	114.59	123.00	24	1
1	A	121	ILE	CB-CG1-CD1	5.25	124.83	113.80	61	1
1	A	63	GLU	N-CA-CB	5.25	118.09	110.26	109	2
1	A	49	ASN	CB-CA-C	-5.24	101.77	110.68	118	3
1	A	121	ILE	CA-CB-CG1	5.22	119.28	110.40	39	2
2	B	1	ARG	CA-CB-CG	5.22	124.55	114.10	86	1
1	A	35	LEU	CA-C-N	5.22	131.64	121.41	29	1
1	A	35	LEU	C-N-CA	5.22	131.64	121.41	29	1
1	A	33	ARG	CB-CG-CD	5.21	123.28	111.30	136	1
1	A	88	PHE	CB-CG-CD1	-5.21	111.85	120.70	44	1
1	A	126	ILE	CA-CB-CG2	-5.20	101.66	110.50	1	2
1	A	111	LYS	CG-CD-CE	5.19	123.25	111.30	47	1
1	A	129	ASP	N-CA-CB	5.18	118.10	110.33	116	2
1	A	64	PHE	CD1-CG-CD2	5.17	126.36	118.60	81	2
1	A	95	TYR	CA-CB-CG	-5.17	104.59	113.90	32	2
1	A	70	ARG	CA-CB-CG	5.17	124.45	114.10	109	1
1	A	63	GLU	CA-CB-CG	-5.17	103.77	114.10	42	1
1	A	75	THR	OG1-CB-CG2	-5.16	98.98	109.30	51	1
1	A	142	THR	CA-C-O	-5.16	112.03	120.80	51	1
2	B	2	ARG	CB-CG-CD	5.15	123.14	111.30	29	1
2	B	12	ARG	CA-CB-CG	5.13	124.37	114.10	150	1
1	A	46	ASP	CB-CG-OD1	5.12	130.19	118.40	21	1
2	B	2	ARG	CD-NE-CZ	-5.12	117.22	124.40	82	3
1	A	23	ILE	CA-CB-CG1	5.12	119.11	110.40	126	1
1	A	138	VAL	CG1-CB-CG2	-5.10	99.57	110.80	69	2
2	B	1	ARG	CA-C-O	-5.10	112.12	120.80	93	1
1	A	23	ILE	N-CA-C	-5.10	101.03	108.17	124	1
1	A	15	PHE	CB-CG-CD2	5.09	129.35	120.70	82	1
1	A	33	ARG	CB-CA-C	-5.09	102.20	110.85	86	2
1	A	28	LEU	CB-CA-C	-5.08	102.25	110.79	32	2
1	A	16	ASP	CB-CG-OD2	-5.08	106.71	118.40	31	1
2	B	6	LYS	CG-CD-CE	5.08	122.98	111.30	45	1
1	A	120	MET	CA-CB-CG	5.07	124.23	114.10	102	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	139	GLN	CA-CB-CG	5.07	124.23	114.10	156	1
1	A	81	ILE	CA-CB-CG2	5.07	119.11	110.50	116	2
1	A	40	THR	OG1-CB-CG2	-5.06	99.19	109.30	102	1
1	A	82	ARG	CB-CG-CD	5.05	122.91	111.30	148	1
1	A	139	GLN	CG-CD-OE1	5.04	130.88	120.80	49	1
1	A	4	GLN	CG-CD-OE1	5.04	130.88	120.80	148	1
1	A	37	GLN	CA-C-N	5.03	130.25	123.46	48	1
1	A	37	GLN	C-N-CA	5.03	130.25	123.46	48	1
1	A	37	GLN	N-CA-CB	-5.03	102.41	110.46	99	1
2	B	3	LYS	N-CA-CB	5.03	117.31	110.01	73	1
1	A	22	THR	CA-CB-CG2	5.03	119.05	110.50	119	1
1	A	133	ASN	CB-CG-ND2	-5.03	108.86	116.40	4	1
1	A	71	LYS	CA-C-N	5.02	128.46	123.04	37	2
1	A	71	LYS	C-N-CA	5.02	128.46	123.04	37	2
1	A	34	SER	CA-CB-OG	-5.02	101.07	111.10	104	1
2	B	16	ARG	CA-CB-CG	5.01	124.12	114.10	48	1
1	A	137	PHE	CB-CG-CD1	-5.01	112.19	120.70	130	1
2	B	1	ARG	CB-CG-CD	5.00	122.80	111.30	3	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
2	B	12	ARG	Sidechain	52
2	B	16	ARG	Sidechain	50
1	A	33	ARG	Sidechain	47
2	B	2	ARG	Sidechain,Peptide	47
1	A	95	TYR	Sidechain	40
1	A	102	ARG	Sidechain	39
2	B	1	ARG	Sidechain,Peptide	38
1	A	86	ARG	Sidechain	36
1	A	134	TYR	Sidechain	35
1	A	70	ARG	Sidechain	35
1	A	82	ARG	Sidechain	35
1	A	122	ARG	Sidechain	33
1	A	137	PHE	Sidechain,Mainchain	21
1	A	61	PHE	Sidechain	16
1	A	8	PHE	Sidechain	15
1	A	12	PHE	Sidechain	13
1	A	15	PHE	Sidechain	11

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

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1105	1035	1035	1±1
2	B	135	145	148	0±1
All	All	199040	188800	189279	142

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:VAL:HG21	1:A:59:ILE:HD12	0.71	1.62	39	1
1:A:8:PHE:CD2	1:A:65:LEU:HD22	0.60	2.31	139	1
1:A:28:LEU:HD23	1:A:44:LEU:HD13	0.57	1.76	13	1
1:A:68:MET:HE1	2:B:9:HIS:CD2	0.57	2.35	109	1
1:A:28:LEU:HD23	1:A:44:LEU:HD11	0.56	1.76	76	1
1:A:90:LYS:HD2	1:A:103:HIS:CD2	0.56	2.36	22	1
1:A:61:PHE:CZ	1:A:65:LEU:HD21	0.56	2.36	35	1
1:A:87:VAL:HG21	2:B:11:VAL:HG13	0.55	1.77	62	2
1:A:140:MET:HE1	2:B:4:TRP:CE3	0.55	2.37	81	1
2:B:7:THR:O	2:B:11:VAL:HG12	0.54	2.03	71	2
2:B:5:GLN:O	2:B:9:HIS:CD2	0.54	2.61	121	3
1:A:61:PHE:CE2	1:A:65:LEU:HD11	0.54	2.37	5	2
1:A:134:TYR:O	1:A:138:VAL:HG23	0.53	2.02	62	3
1:A:99:ALA:O	1:A:103:HIS:CD2	0.53	2.62	101	1
1:A:137:PHE:CZ	1:A:141:MET:HE3	0.53	2.38	116	2
1:A:14:LEU:HD23	2:B:10:ALA:CB	0.52	2.33	2	1
1:A:115:GLU:H	1:A:115:GLU:CD	0.52	2.13	122	4
1:A:67:MET:HE3	2:B:16:ARG:HG2	0.51	1.83	133	1
1:A:32:MET:HE2	2:B:14:ILE:HG23	0.50	1.83	133	1
1:A:35:LEU:HD11	1:A:108:LEU:HD21	0.50	1.83	67	1
1:A:102:ARG:HH12	1:A:114:ASP:CG	0.50	2.13	105	3
1:A:101:LEU:HD13	2:B:4:TRP:CH2	0.49	2.41	3	2
1:A:108:LEU:CD1	2:B:7:THR:HG23	0.49	2.36	88	1
1:A:61:PHE:HB3	1:A:62:PRO:HD3	0.49	1.85	11	2
1:A:108:LEU:HD12	2:B:7:THR:HG23	0.49	1.83	88	2
1:A:28:LEU:HD11	2:B:14:ILE:HD13	0.49	1.84	156	1
1:A:126:ILE:HG22	1:A:136:GLU:HG2	0.48	1.85	58	1
1:A:140:MET:HE1	2:B:4:TRP:CD2	0.48	2.44	151	3
1:A:68:MET:CE	2:B:13:ALA:HB2	0.47	2.40	3	1
2:B:5:GLN:O	2:B:9:HIS:CG	0.47	2.67	4	1
1:A:103:HIS:CE1	1:A:107:ASN:HD21	0.47	2.28	133	2
1:A:96:ILE:HD12	1:A:132:VAL:HB	0.47	1.87	34	1
1:A:102:ARG:HH21	1:A:114:ASP:CG	0.47	2.18	64	1
1:A:12:PHE:CE1	1:A:23:ILE:HD11	0.47	2.44	152	1
1:A:3:GLU:H	1:A:3:GLU:CD	0.46	2.17	24	4
1:A:101:LEU:HD13	2:B:4:TRP:CZ3	0.46	2.45	105	1
1:A:7:GLU:OE2	2:B:2:ARG:NH2	0.46	2.47	30	1
1:A:102:ARG:HH22	1:A:114:ASP:CG	0.46	2.18	151	1
1:A:105:MET:HE1	1:A:120:MET:SD	0.46	2.50	120	1
1:A:28:LEU:CD2	1:A:44:LEU:HD11	0.46	2.40	76	1
1:A:28:LEU:O	1:A:31:VAL:HG12	0.46	2.11	83	1
1:A:80:GLU:CD	2:B:12:ARG:HE	0.45	2.19	103	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:PHE:CE2	2:B:9:HIS:CE1	0.45	3.04	72	1
1:A:88:PHE:CD1	1:A:104:VAL:HG21	0.45	2.46	141	2
1:A:80:GLU:CD	2:B:16:ARG:HH22	0.45	2.19	100	1
1:A:85:PHE:CE2	1:A:134:TYR:CE1	0.45	3.05	106	1
1:A:85:PHE:CE2	1:A:96:ILE:HD11	0.45	2.45	117	1
1:A:120:MET:HE2	2:B:4:TRP:CE2	0.45	2.46	110	1
1:A:137:PHE:HA	1:A:140:MET:HE2	0.45	1.89	97	1
1:A:88:PHE:CZ	1:A:104:VAL:HG11	0.45	2.47	145	1
1:A:23:ILE:HB	1:A:59:ILE:HG23	0.45	1.88	10	3
1:A:123:GLU:CD	2:B:1:ARG:HH21	0.45	2.19	122	1
1:A:85:PHE:CD2	1:A:134:TYR:CE1	0.45	3.05	152	2
1:A:102:ARG:NH2	1:A:114:ASP:OD1	0.44	2.50	1	1
1:A:118:ASP:OD2	1:A:122:ARG:NH1	0.44	2.49	81	1
1:A:120:MET:HE2	2:B:4:TRP:CD2	0.44	2.48	18	2
1:A:88:PHE:HA	1:A:104:VAL:HG21	0.44	1.90	94	1
1:A:102:ARG:CG	1:A:117:VAL:HG11	0.44	2.43	160	1
1:A:83:GLU:O	1:A:87:VAL:HG23	0.44	2.13	137	3
1:A:20:ASP:CG	1:A:21:GLY:H	0.43	2.20	53	1
1:A:134:TYR:CE2	1:A:138:VAL:HG21	0.43	2.48	112	1
1:A:114:ASP:HA	1:A:117:VAL:HG12	0.43	1.89	22	1
1:A:54:ASP:OD1	1:A:55:GLY:N	0.43	2.50	134	2
2:B:7:THR:O	2:B:11:VAL:HG23	0.43	2.12	28	1
1:A:85:PHE:CE1	1:A:96:ILE:HD11	0.43	2.48	73	1
1:A:12:PHE:CE1	1:A:23:ILE:HG13	0.43	2.48	104	1
1:A:137:PHE:CE1	1:A:141:MET:HE3	0.42	2.49	9	1
1:A:112:LEU:H	1:A:112:LEU:HD22	0.42	1.74	129	1
1:A:8:PHE:CD2	1:A:65:LEU:CD1	0.42	3.03	8	1
1:A:79:GLU:OE1	1:A:82:ARG:NH1	0.42	2.51	14	1
1:A:23:ILE:HA	1:A:27:GLU:OE1	0.42	2.15	127	1
1:A:81:ILE:HG21	1:A:138:VAL:HG22	0.42	1.90	17	1
1:A:112:LEU:HD23	1:A:112:LEU:N	0.42	2.30	139	1
1:A:103:HIS:CD2	1:A:107:ASN:ND2	0.42	2.87	31	1
1:A:8:PHE:CE1	2:B:9:HIS:CE1	0.42	3.08	138	1
1:A:140:MET:HE3	1:A:141:MET:HE2	0.42	1.92	54	1
1:A:12:PHE:CZ	1:A:23:ILE:HG13	0.42	2.50	116	2
1:A:105:MET:HE3	2:B:7:THR:OG1	0.42	2.14	56	1
1:A:138:VAL:O	1:A:142:THR:HG23	0.42	2.14	79	1
1:A:8:PHE:CE2	1:A:65:LEU:HD13	0.42	2.50	121	1
1:A:28:LEU:HD11	1:A:32:MET:HE3	0.41	1.91	22	1
1:A:20:ASP:CG	1:A:21:GLY:N	0.41	2.78	53	1
1:A:68:MET:HG3	2:B:9:HIS:CE1	0.41	2.50	72	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:PHE:HA	2:B:9:HIS:CE1	0.41	2.50	98	1
1:A:37:GLN:O	1:A:39:PRO:HD3	0.41	2.15	122	1
1:A:119:GLU:CD	1:A:122:ARG:HH21	0.41	2.23	61	1
2:B:7:THR:O	2:B:10:ALA:HB3	0.41	2.15	146	1
1:A:15:PHE:HB2	1:A:23:ILE:HD13	0.41	1.93	13	1
1:A:116:GLU:OE1	2:B:3:LYS:NZ	0.41	2.52	129	1
1:A:124:ALA:HB1	1:A:140:MET:HE2	0.41	1.92	141	1
1:A:24:THR:HG22	1:A:58:THR:HG22	0.41	1.92	23	1
1:A:8:PHE:CD2	2:B:9:HIS:HE1	0.41	2.33	150	1
1:A:14:LEU:HD12	2:B:10:ALA:HB2	0.41	1.91	35	1
1:A:16:ASP:CG	1:A:19:GLY:H	0.41	2.24	89	1
1:A:32:MET:HE1	1:A:47:MET:SD	0.41	2.55	150	1
1:A:124:ALA:HB2	2:B:4:TRP:CE2	0.41	2.51	15	1
2:B:11:VAL:HA	2:B:14:ILE:HG22	0.41	1.93	15	1
1:A:140:MET:HE1	1:A:141:MET:HE2	0.41	1.91	22	1
1:A:80:GLU:OE2	2:B:16:ARG:NH1	0.41	2.51	124	2
1:A:28:LEU:CD2	1:A:48:ILE:HD11	0.40	2.47	141	1
1:A:7:GLU:HG2	1:A:68:MET:HE1	0.40	1.94	89	1
1:A:23:ILE:HB	1:A:59:ILE:CG2	0.40	2.46	85	1
1:A:8:PHE:CD1	2:B:9:HIS:CE1	0.40	3.10	18	1
1:A:123:GLU:OE2	2:B:1:ARG:N	0.40	2.53	29	1
1:A:118:ASP:O	1:A:122:ARG:HB2	0.40	2.16	46	1
1:A:31:VAL:O	1:A:34:SER:HB2	0.40	2.16	84	1
1:A:12:PHE:CE1	1:A:23:ILE:HD12	0.40	2.51	136	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	139/148 (94%)	128±3 (92±2%)	9±3 (6±2%)	2±2 (2±1%)	10	55
2	B	15/19 (79%)	14±1 (95±6%)	1±1 (4±5%)	0±0 (0±1%)	37	78
All	All	24640/26720 (92%)	22755 (92%)	1511 (6%)	374 (2%)	11	57

All 35 unique Ramachandran outliers are listed below. They are sorted by the frequency of

occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	36	GLY	112
1	A	128	GLY	55
1	A	109	GLY	40
1	A	21	GLY	30
1	A	127	ASP	24
1	A	55	GLY	16
1	A	92	GLY	14
1	A	74	ASP	12
1	A	54	ASP	12
1	A	19	GLY	9
1	A	91	ASP	8
2	B	2	ARG	6
1	A	52	ASP	4
1	A	73	LYS	3
1	A	16	ASP	3
1	A	35	LEU	3
1	A	39	PRO	2
1	A	77	SER	2
1	A	86	ARG	2
2	B	11	VAL	2
1	A	115	GLU	1
1	A	5	ILE	1
1	A	125	ASP	1
1	A	98	ALA	1
1	A	18	ASP	1
1	A	117	VAL	1
1	A	89	ASP	1
1	A	49	ASN	1
1	A	38	ASN	1
1	A	108	LEU	1
1	A	101	LEU	1
1	A	20	ASP	1
1	A	15	PHE	1
1	A	50	GLU	1
1	A	53	ALA	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	120/126 (95%)	117±1 (98±1%)	3±1 (2±1%)	44	89
2	B	12/15 (80%)	12±0 (98±4%)	0±0 (2±4%)	46	90
All	All	21120/22560 (94%)	20632 (98%)	488 (2%)	44	89

All 98 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	59	ILE	48
1	A	91	ASP	22
1	A	54	ASP	21
1	A	18	ASP	16
1	A	132	VAL	14
1	A	23	ILE	14
1	A	127	ASP	14
1	A	104	VAL	12
1	A	3	GLU	12
1	A	75	THR	11
2	B	11	VAL	10
1	A	39	PRO	10
1	A	20	ASP	10
2	B	14	ILE	10
1	A	117	VAL	10
2	B	6	LYS	9
1	A	110	GLU	9
1	A	101	LEU	9
1	A	74	ASP	8
1	A	133	ASN	8
1	A	112	LEU	8
1	A	25	THR	7
1	A	31	VAL	7
1	A	14	LEU	7
1	A	65	LEU	7
1	A	111	LYS	6
1	A	51	VAL	6
1	A	58	THR	6
1	A	7	GLU	6
1	A	22	THR	5
1	A	62	PRO	5
1	A	81	ILE	5
1	A	73	LYS	5
1	A	96	ILE	5

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Mol	Chain	Res	Type	Models (Total)
1	A	106	THR	5
1	A	115	GLU	4
1	A	28	LEU	4
1	A	87	VAL	4
2	B	2	ARG	4
1	A	105	MET	4
1	A	44	LEU	4
1	A	88	PHE	4
1	A	37	GLN	3
1	A	90	LYS	3
1	A	121	ILE	3
1	A	108	LEU	3
1	A	50	GLU	3
1	A	131	GLN	3
1	A	13	SER	3
1	A	125	ASP	3
1	A	56	ASN	3
2	B	16	ARG	3
1	A	40	THR	2
1	A	142	THR	2
1	A	34	SER	2
1	A	46	ASP	2
1	A	134	TYR	2
2	B	7	THR	2
1	A	77	SER	2
1	A	141	MET	2
1	A	16	ASP	2
1	A	68	MET	2
1	A	140	MET	2
1	A	48	ILE	2
1	A	139	GLN	2
1	A	118	ASP	2
1	A	32	MET	2
1	A	66	THR	2
1	A	30	THR	2
2	B	9	HIS	1
1	A	126	ILE	1
1	A	138	VAL	1
2	B	5	GLN	1
1	A	17	LYS	1
1	A	78	GLU	1
1	A	8	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	71	LYS	1
1	A	12	PHE	1
1	A	72	MET	1
1	A	52	ASP	1
1	A	10	GLU	1
1	A	60	ASP	1
1	A	9	LYS	1
1	A	122	ARG	1
1	A	97	SER	1
1	A	102	ARG	1
1	A	129	ASP	1
1	A	114	ASP	1
1	A	35	LEU	1
1	A	41	GLU	1
1	A	5	ILE	1
1	A	64	PHE	1
1	A	24	THR	1
1	A	26	LYS	1
1	A	103	HIS	1
1	A	33	ARG	1
1	A	86	ARG	1
1	A	67	MET	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