



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 09:15 PM UTC

PDB ID : 2LJ5 / pdb_00002lj5
BMRB ID : 17919
Title : Description of the Structural fluctuations of proteins from structure-based calculations of Residual dipolar couplings
Authors : De Simone, A.; Montalvao, R.; Vendruscolo, M.
Deposited on : 2011-09-06

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

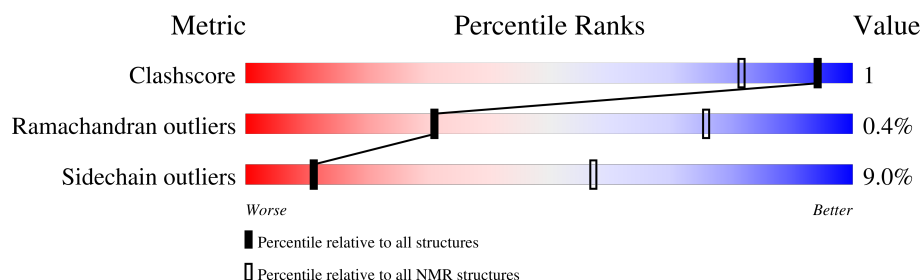
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 42%.

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	76	32% 62% 7%

2 Ensemble composition and analysis

This entry contains 301 models. Model 210 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:1-A:71 (71)	0.61	210

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 5 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 52, 53, 54, 55, 56, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160, 161, 162, 164, 165, 166, 167, 168, 169, 170, 171, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 190, 191, 192, 193, 194, 195, 196, 197, 198, 199, 200, 201, 203, 204, 205, 206, 207, 208, 209, 210, 211, 212, 213, 214, 215, 216, 217, 218, 219, 220, 221, 222, 223, 224, 225, 226, 227, 228, 229, 230, 232, 233, 234, 235, 236, 237, 238, 239, 240, 241, 242, 243, 244, 245, 246, 247, 249, 250, 251, 252, 253, 254, 255, 256, 257, 258, 259, 260, 261, 262, 263, 264, 265, 266, 267, 268, 269, 270, 271, 272, 273, 274, 275, 276, 277, 278, 279, 280, 281, 282, 283, 284, 285, 286, 287, 288, 289, 290, 291, 292, 293, 294, 295, 296, 297, 298, 299, 300, 301
2	51, 88, 231
3	5, 163

4	57, 202
5	104, 248

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1231 atoms, of which 629 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin.

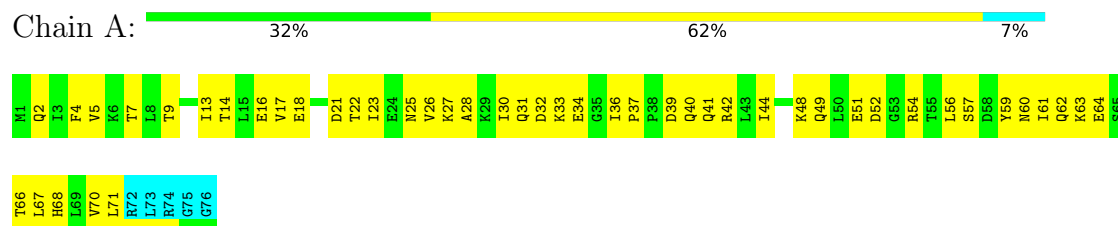
Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1231	378	629	105	118	1	

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: Ubiquitin

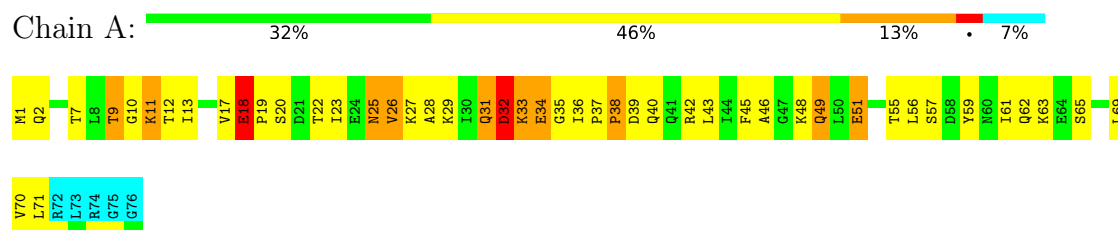


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

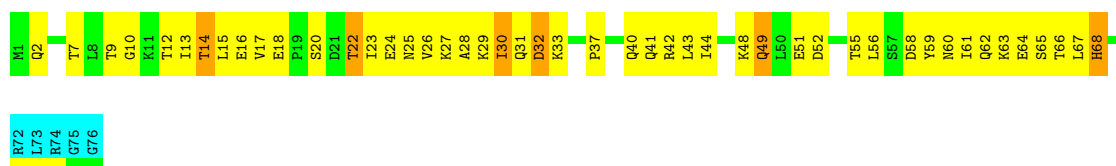
- Molecule 1: Ubiquitin



4.2.2 Score per residue for model 2

- Molecule 1: Ubiquitin

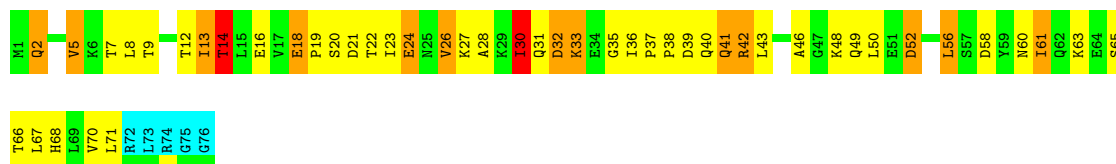




4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin

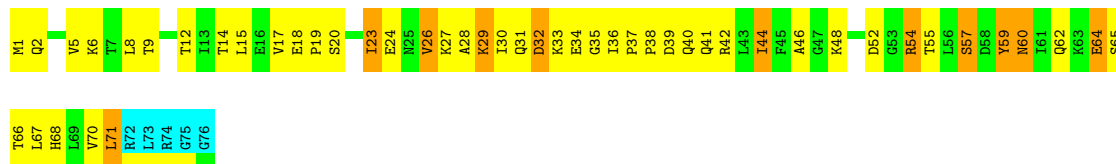
Chain A: 30% 43% 17% 7%



4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin

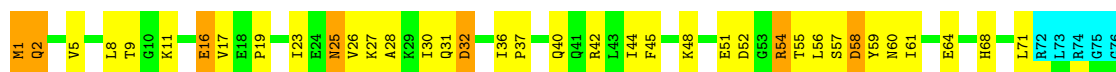
Chain A: 29% 50% 14% 7%



4.2.5 Score per residue for model 5

- Molecule 1: Ubiquitin

Chain A: 45% 39% 9% 7%



4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin

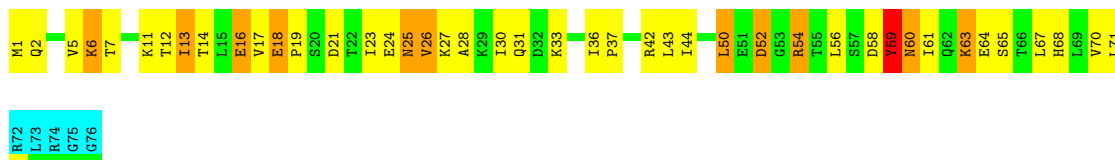
Chain A: 42% 37% 12% 7%



4.2.7 Score per residue for model 7

- Molecule 1: Ubiquitin

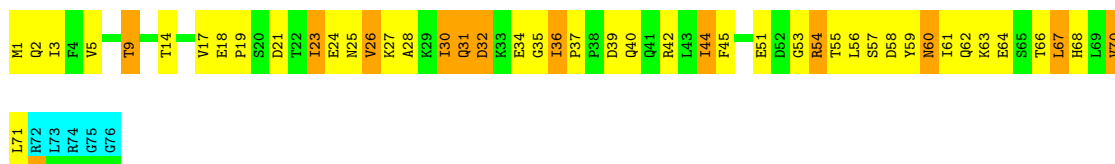
Chain A: 37% 41% 14% 7%



4.2.8 Score per residue for model 8

- Molecule 1: Ubiquitin

Chain A: 33% 45% 16% 7%



4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin

Chain A: 38% 45% 11% 7%



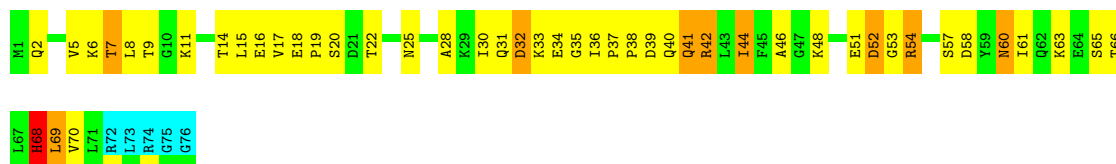
4.2.10 Score per residue for model 10

- Molecule 1: Ubiquitin

Chain A: 34% 42% 17% 7%

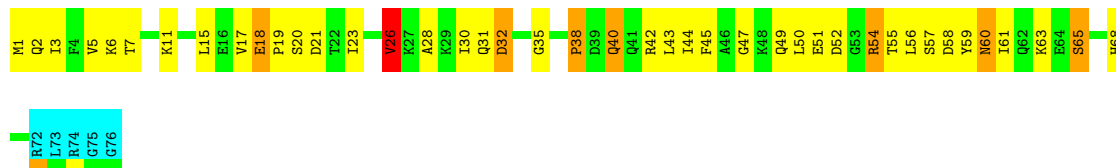
4.2.11 Score per residue for model 11

- Molecule 1: Ubiquitin



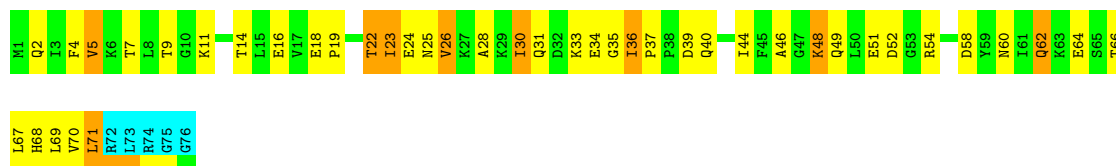
4.2.12 Score per residue for model 12

- Molecule 1: Ubiquitin



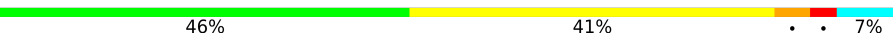
4.2.13 Score per residue for model 13

- Molecule 1: Ubiquitin



4.2.14 Score per residue for model 14

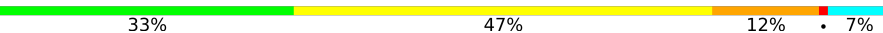
- Molecule 1: Ubiquitin

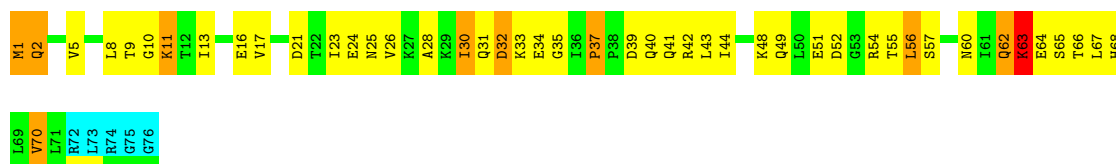
Chain A:  46% 41% 7%



4.2.15 Score per residue for model 15

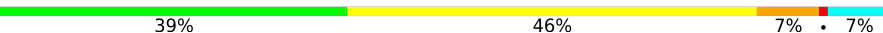
- Molecule 1: Ubiquitin

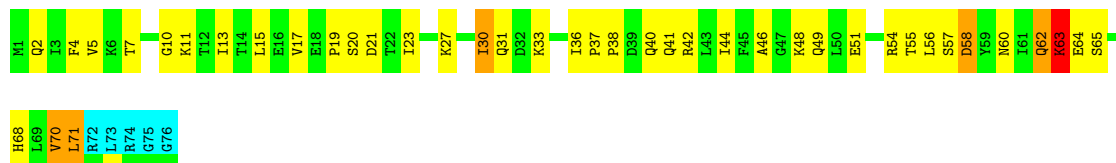
Chain A:  33% 47% 12% 7%



4.2.16 Score per residue for model 16

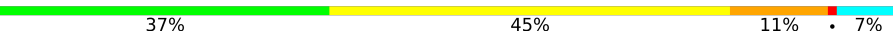
- Molecule 1: Ubiquitin

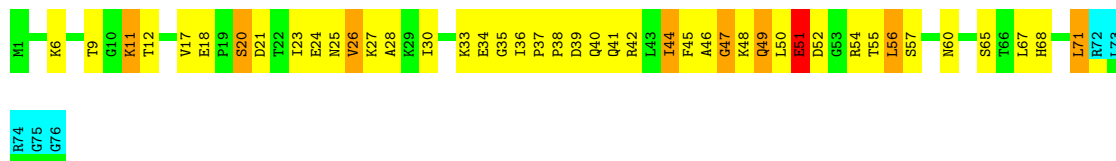
Chain A:  39% 46% 7% 7%



4.2.17 Score per residue for model 17

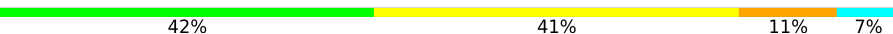
- Molecule 1: Ubiquitin

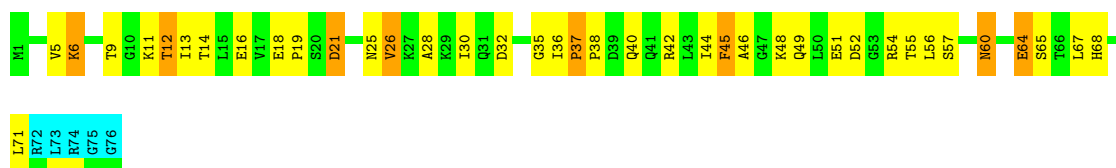
Chain A:  37% 45% 11% 7%



4.2.18 Score per residue for model 18

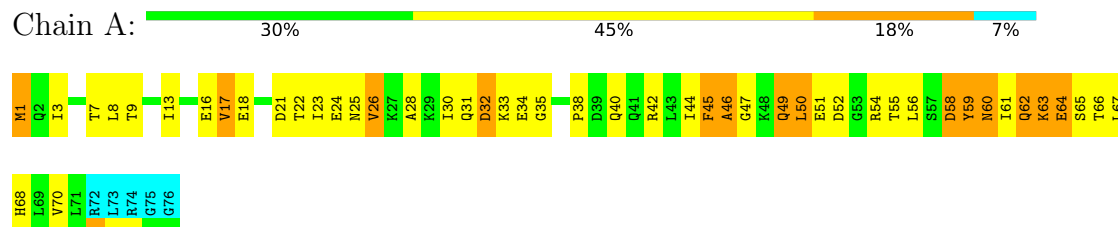
- Molecule 1: Ubiquitin

Chain A:  42% 41% 11% 7%



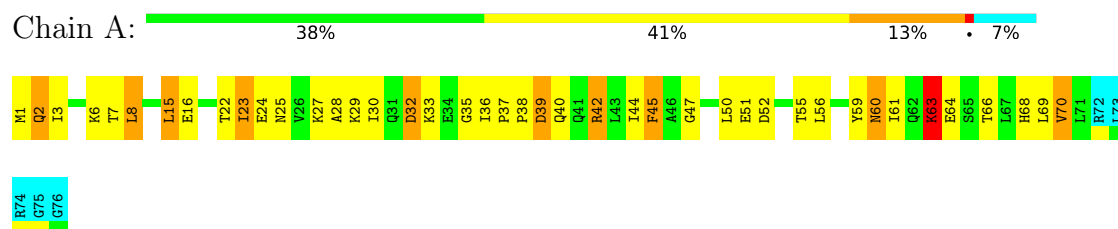
4.2.19 Score per residue for model 19

- Molecule 1: Ubiquitin



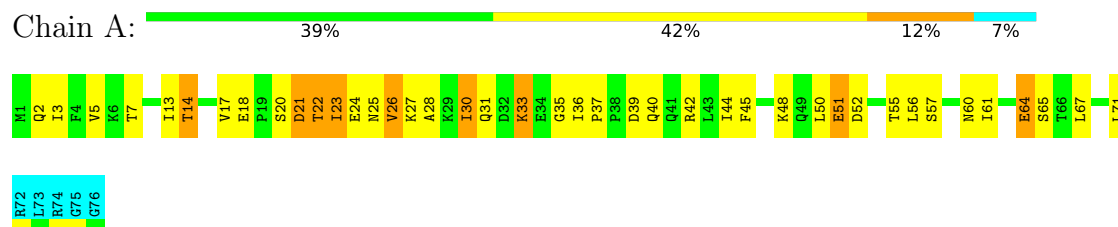
4.2.20 Score per residue for model 20

- Molecule 1: Ubiquitin



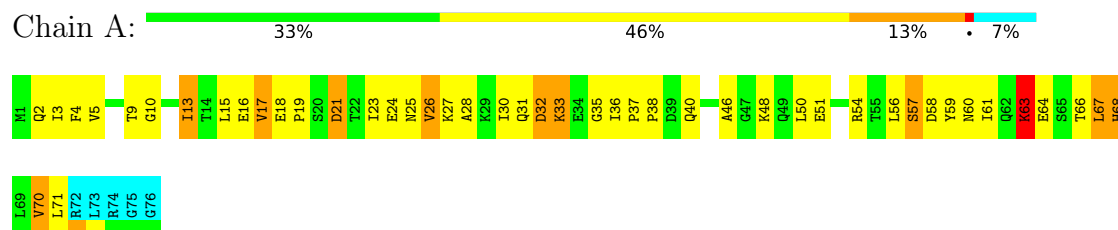
4.2.21 Score per residue for model 21

- Molecule 1: Ubiquitin



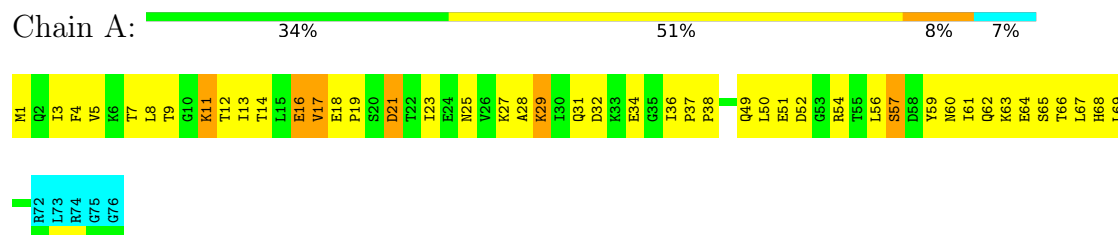
4.2.22 Score per residue for model 22

- Molecule 1: Ubiquitin



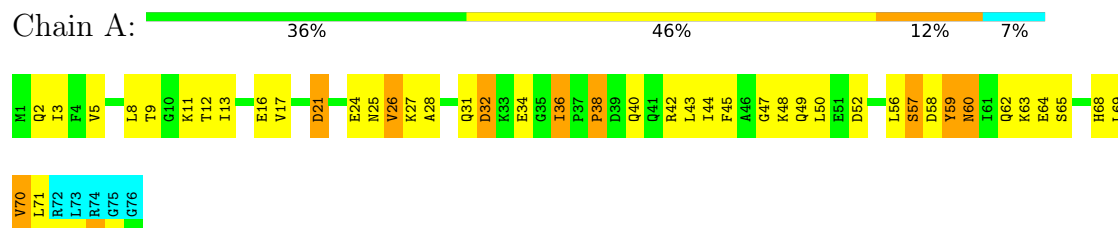
4.2.23 Score per residue for model 23

- Molecule 1: Ubiquitin



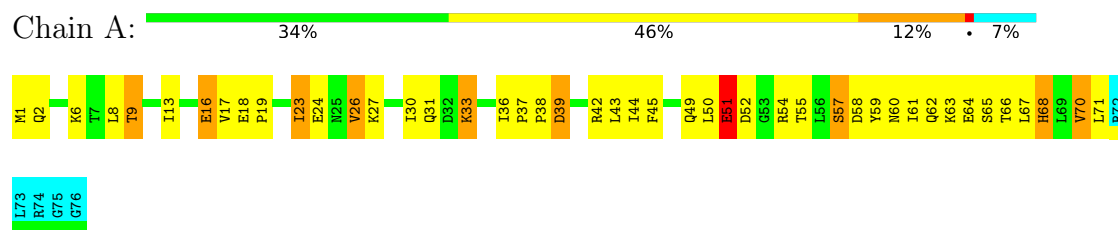
4.2.24 Score per residue for model 24

- Molecule 1: Ubiquitin



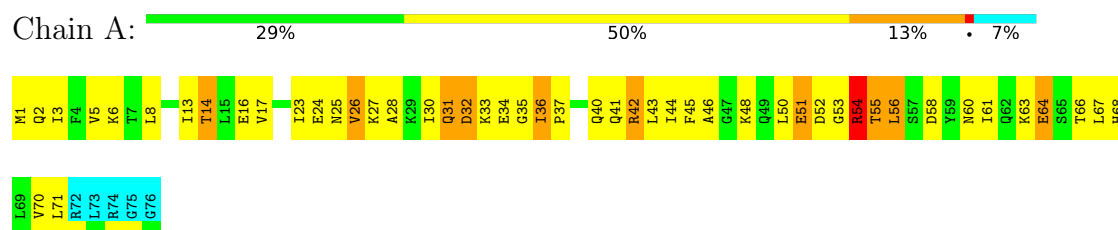
4.2.25 Score per residue for model 25

- Molecule 1: Ubiquitin



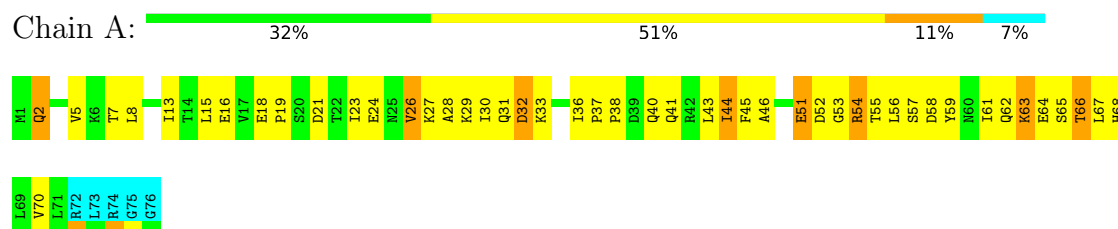
4.2.26 Score per residue for model 26

- Molecule 1: Ubiquitin



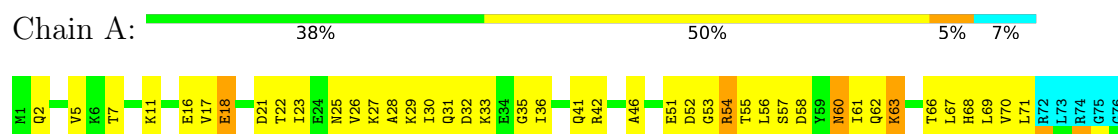
4.2.27 Score per residue for model 27

- Molecule 1: Ubiquitin



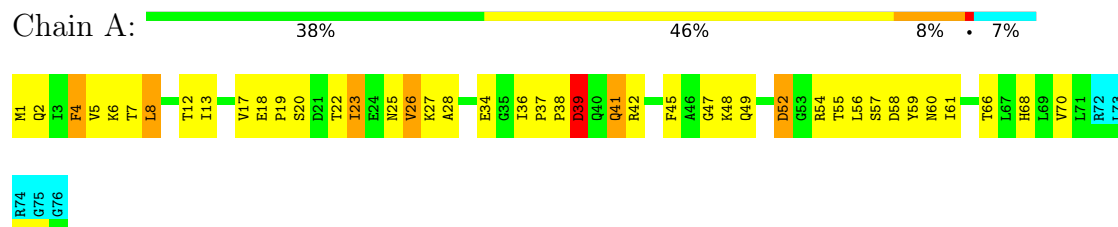
4.2.28 Score per residue for model 28

- Molecule 1: Ubiquitin



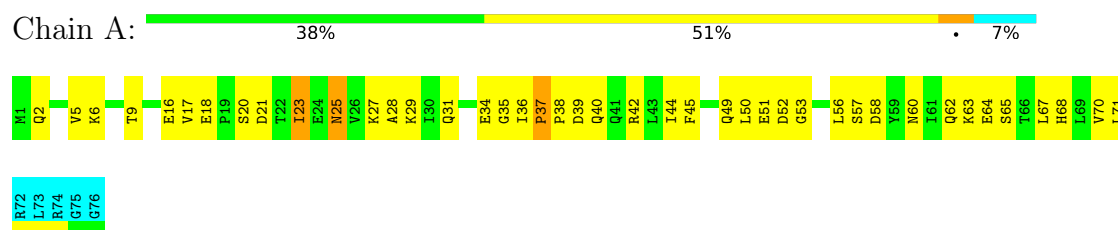
4.2.29 Score per residue for model 29

- Molecule 1: Ubiquitin



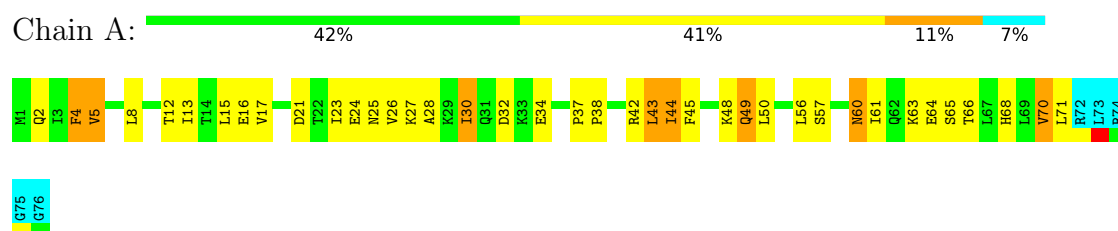
4.2.30 Score per residue for model 30

- Molecule 1: Ubiquitin



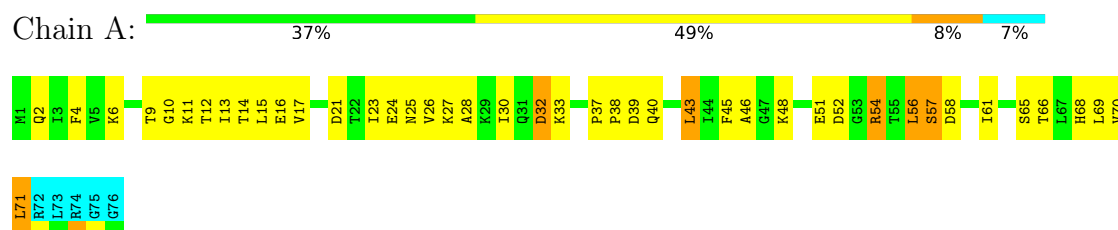
4.2.31 Score per residue for model 31

- Molecule 1: Ubiquitin



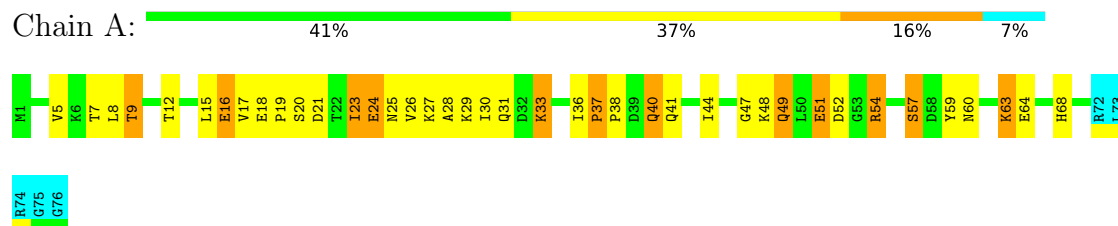
4.2.32 Score per residue for model 32

- Molecule 1: Ubiquitin



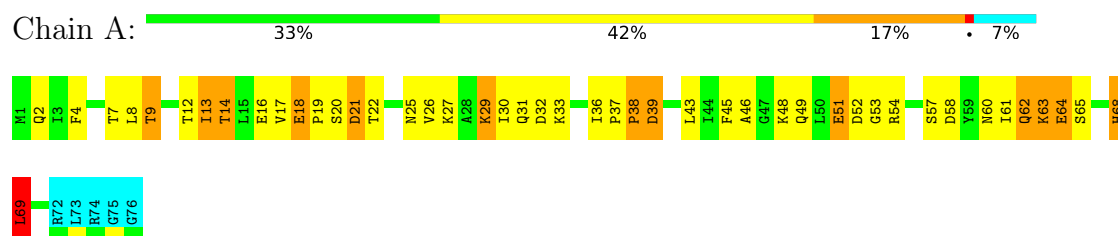
4.2.33 Score per residue for model 33

- Molecule 1: Ubiquitin



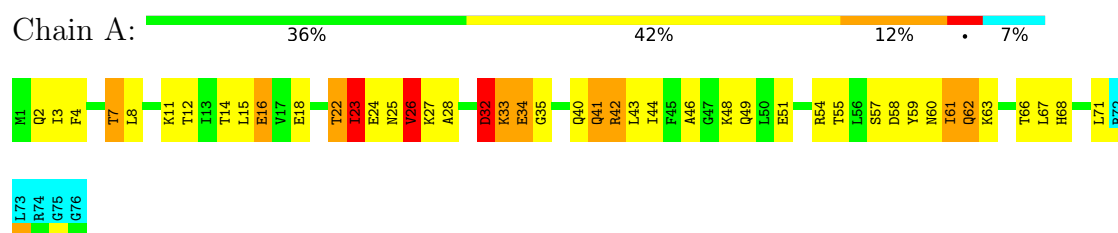
4.2.34 Score per residue for model 34

- Molecule 1: Ubiquitin



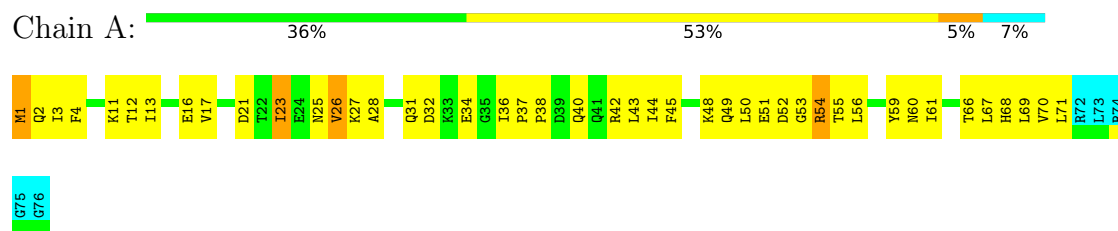
4.2.35 Score per residue for model 35

- Molecule 1: Ubiquitin



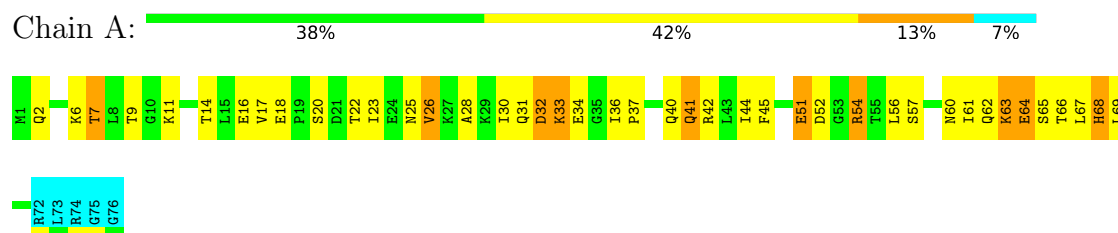
4.2.36 Score per residue for model 36

- Molecule 1: Ubiquitin



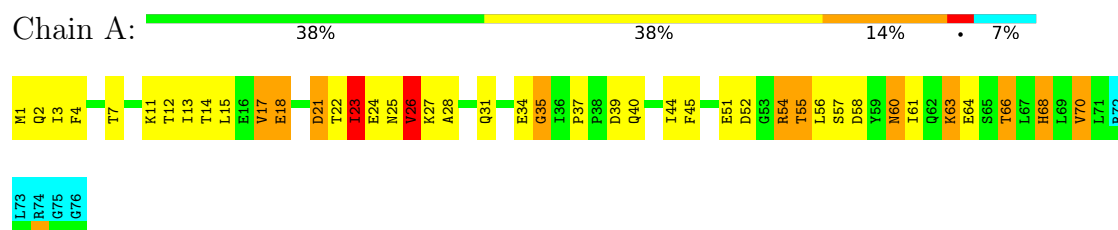
4.2.37 Score per residue for model 37

- Molecule 1: Ubiquitin



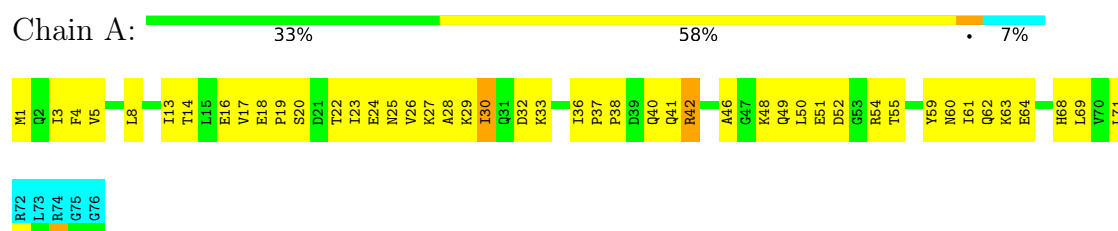
4.2.38 Score per residue for model 38

- Molecule 1: Ubiquitin



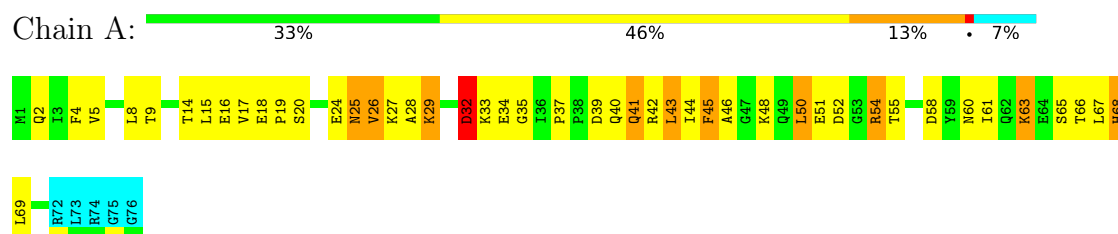
4.2.39 Score per residue for model 39

- Molecule 1: Ubiquitin



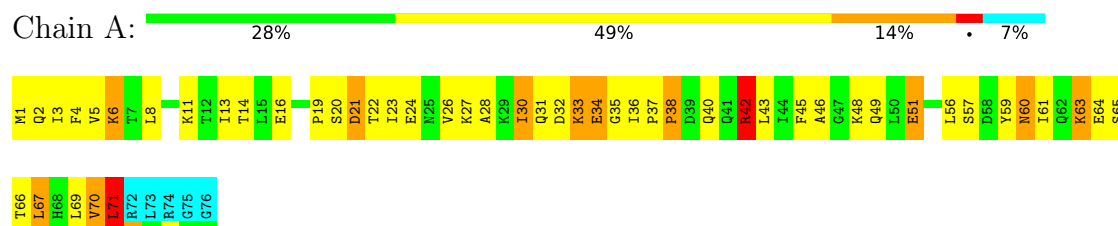
4.2.40 Score per residue for model 40

- Molecule 1: Ubiquitin



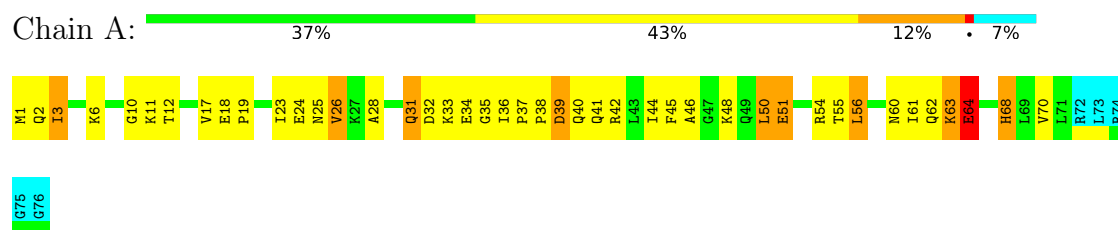
4.2.41 Score per residue for model 41

- Molecule 1: Ubiquitin



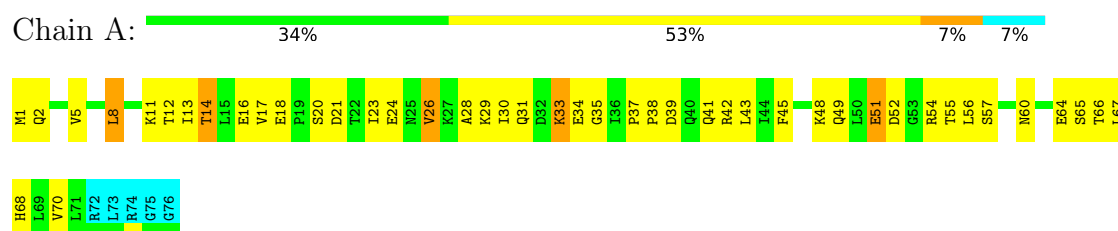
4.2.46 Score per residue for model 46

- Molecule 1: Ubiquitin



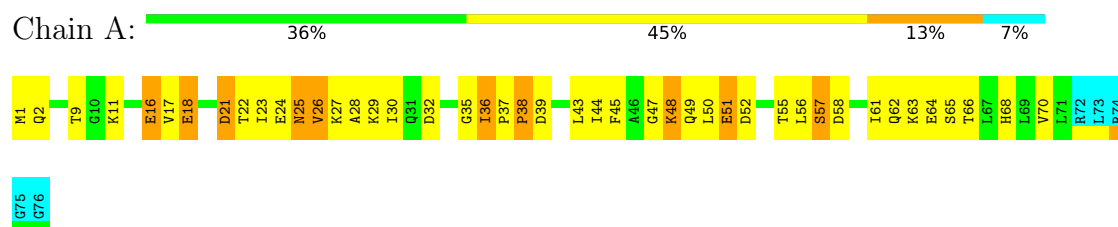
4.2.47 Score per residue for model 47

- Molecule 1: Ubiquitin



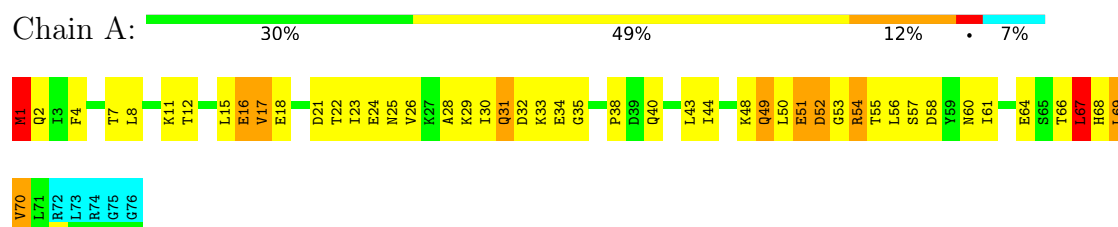
4.2.48 Score per residue for model 48

- Molecule 1: Ubiquitin



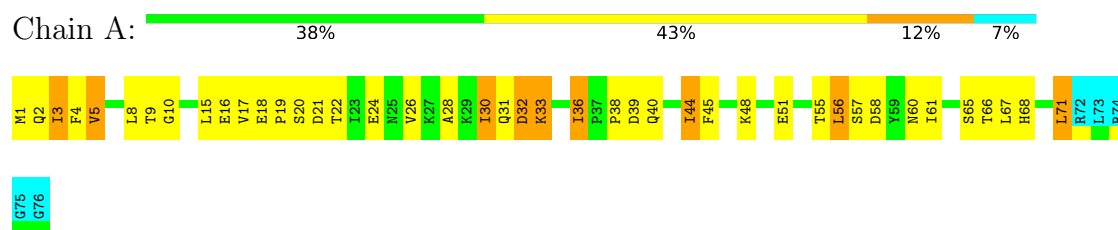
4.2.49 Score per residue for model 49

- Molecule 1: Ubiquitin



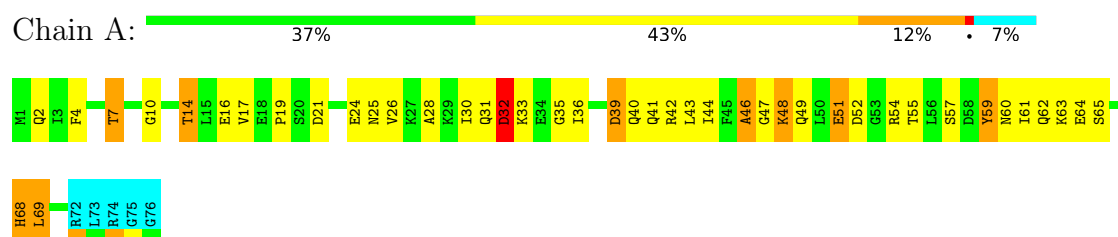
4.2.50 Score per residue for model 50

- Molecule 1: Ubiquitin



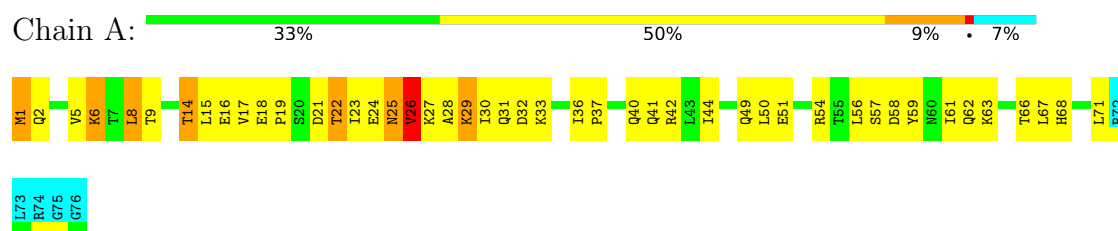
4.2.51 Score per residue for model 51

- Molecule 1: Ubiquitin



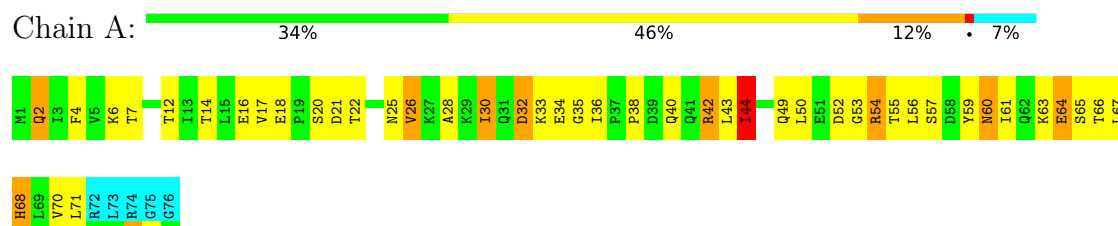
4.2.52 Score per residue for model 52

- Molecule 1: Ubiquitin



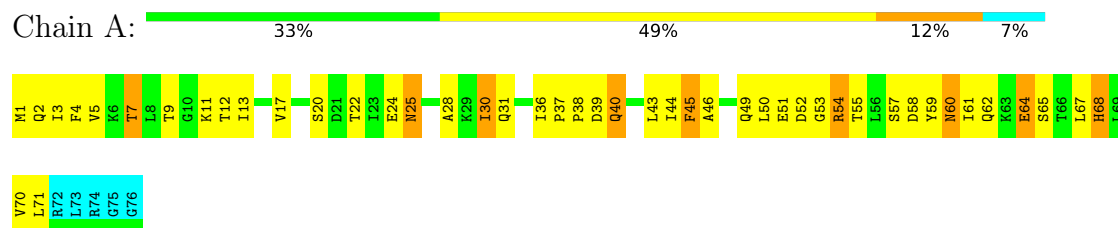
4.2.53 Score per residue for model 53

- Molecule 1: Ubiquitin



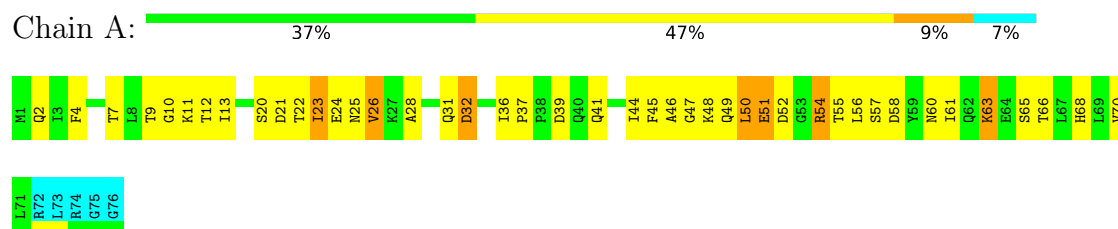
4.2.54 Score per residue for model 54

- Molecule 1: Ubiquitin



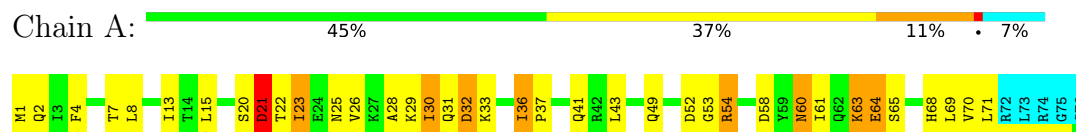
4.2.55 Score per residue for model 55

- Molecule 1: Ubiquitin



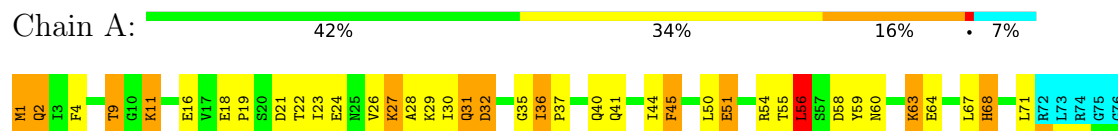
4.2.56 Score per residue for model 56

- Molecule 1: Ubiquitin



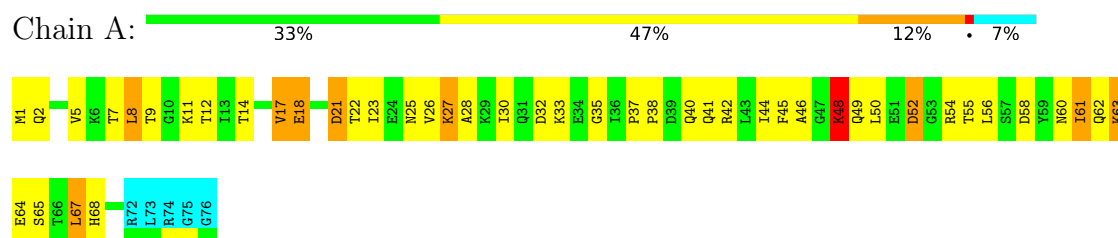
4.2.57 Score per residue for model 57

- Molecule 1: Ubiquitin



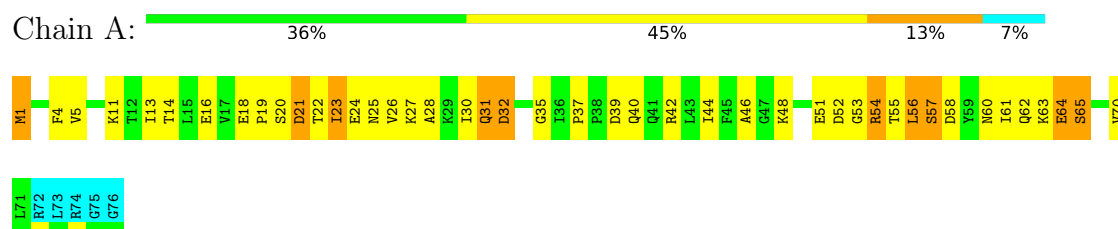
4.2.58 Score per residue for model 58

- Molecule 1: Ubiquitin



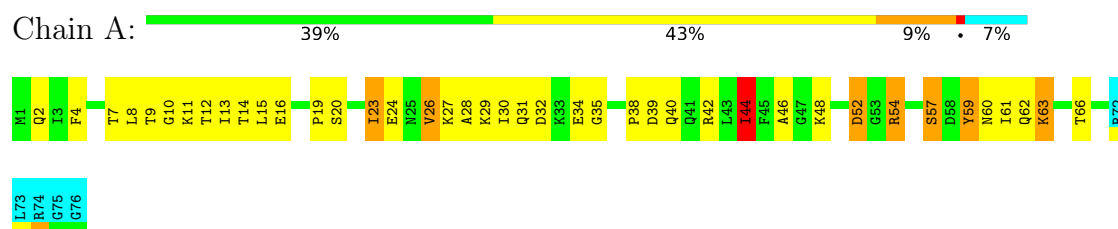
4.2.59 Score per residue for model 59

- Molecule 1: Ubiquitin



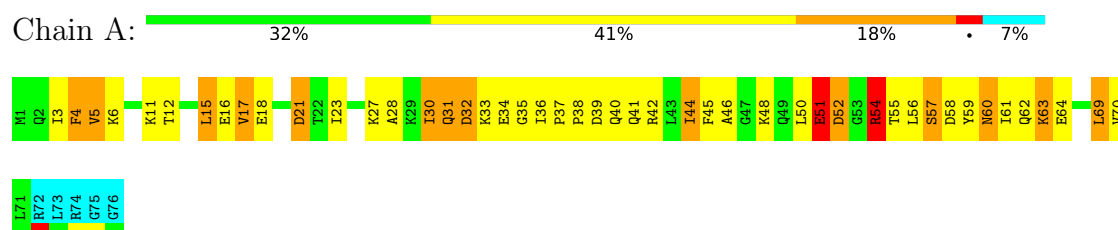
4.2.60 Score per residue for model 60

- Molecule 1: Ubiquitin



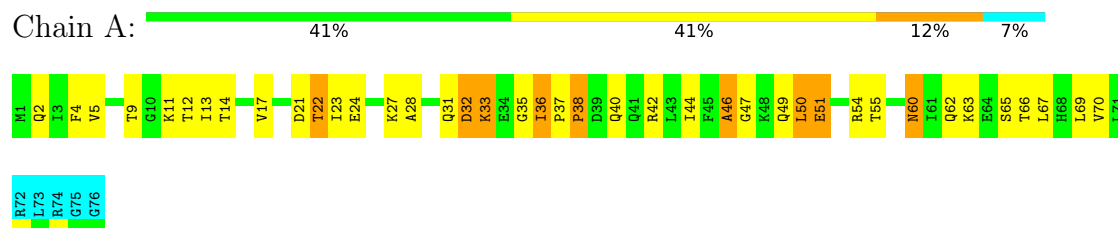
4.2.61 Score per residue for model 61

- Molecule 1: Ubiquitin



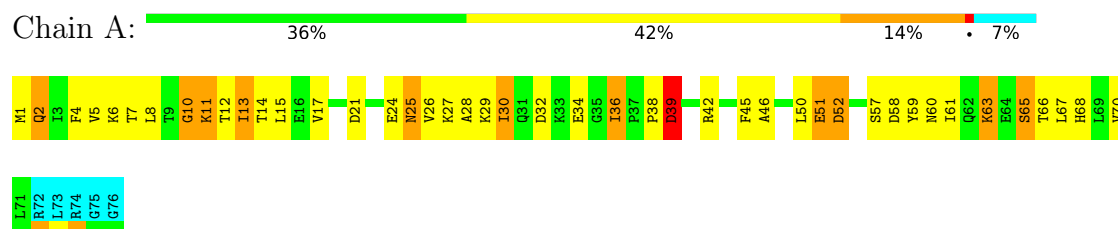
4.2.62 Score per residue for model 62

- Molecule 1: Ubiquitin



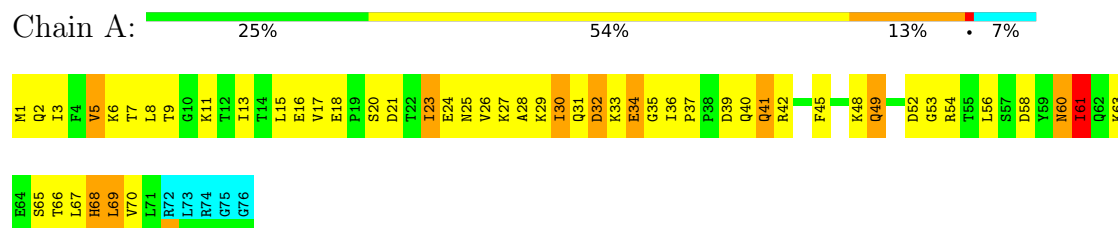
4.2.63 Score per residue for model 63

- Molecule 1: Ubiquitin



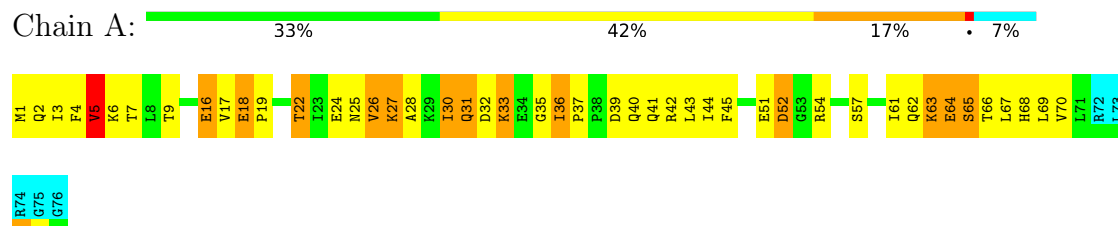
4.2.64 Score per residue for model 64

- Molecule 1: Ubiquitin



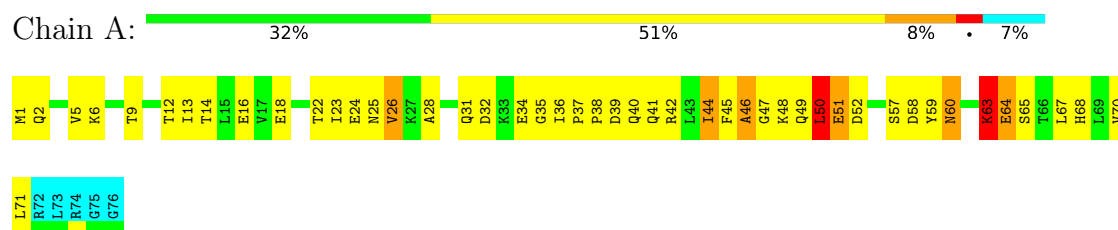
4.2.65 Score per residue for model 65

- Molecule 1: Ubiquitin



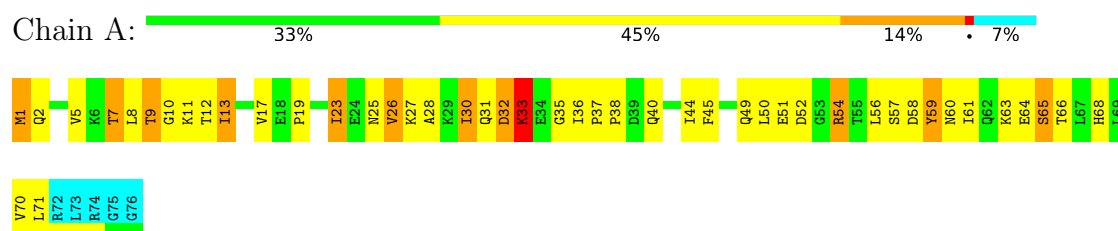
4.2.66 Score per residue for model 66

- Molecule 1: Ubiquitin



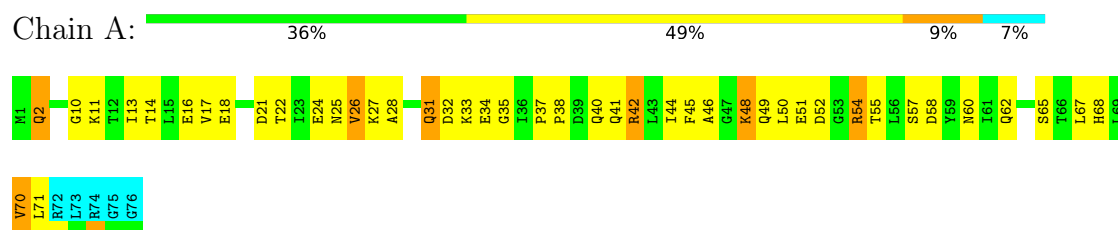
4.2.67 Score per residue for model 67

- Molecule 1: Ubiquitin



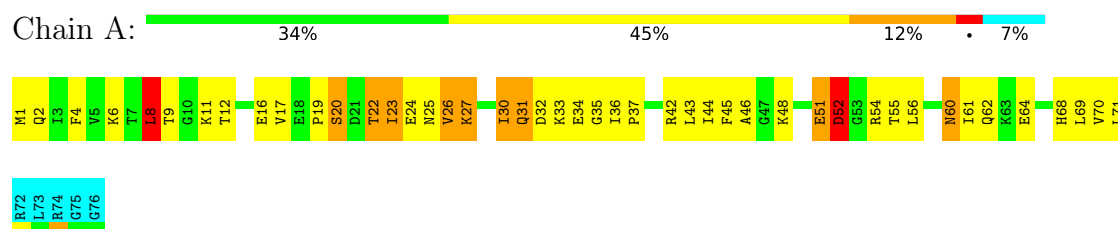
4.2.68 Score per residue for model 68

- Molecule 1: Ubiquitin



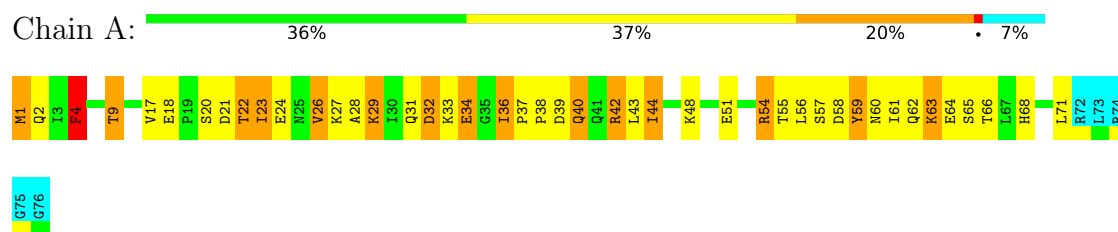
4.2.69 Score per residue for model 69

- Molecule 1: Ubiquitin



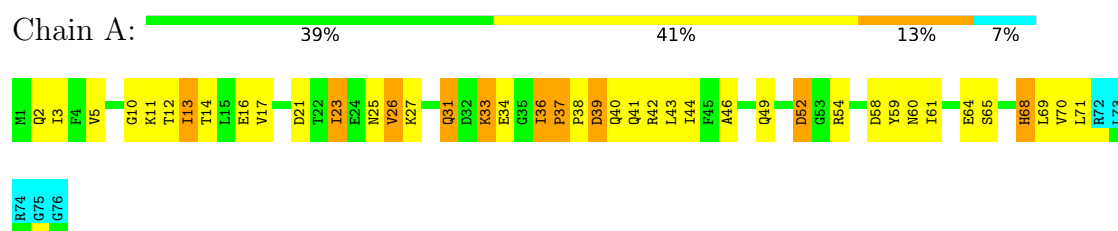
4.2.70 Score per residue for model 70

- Molecule 1: Ubiquitin



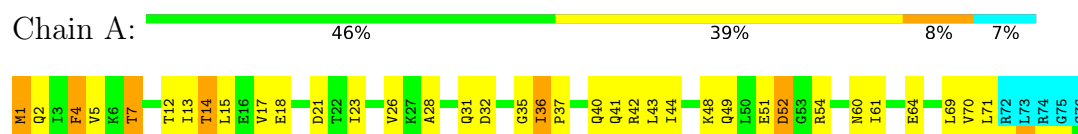
4.2.71 Score per residue for model 71

- Molecule 1: Ubiquitin



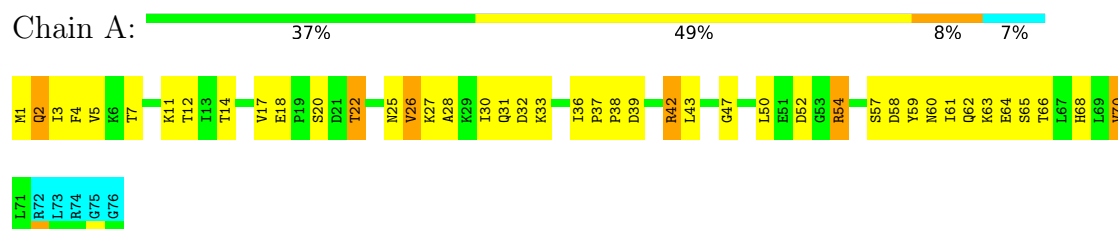
4.2.72 Score per residue for model 72

- Molecule 1: Ubiquitin



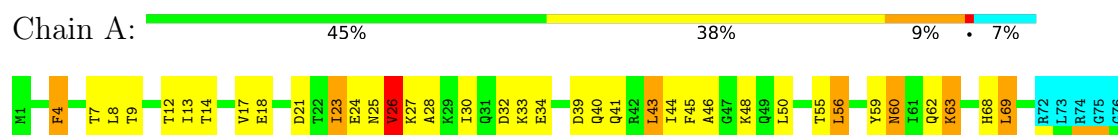
4.2.73 Score per residue for model 73

- Molecule 1: Ubiquitin



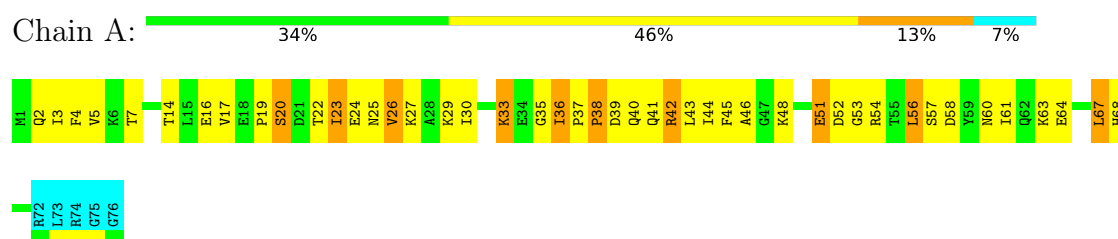
4.2.74 Score per residue for model 74

- Molecule 1: Ubiquitin



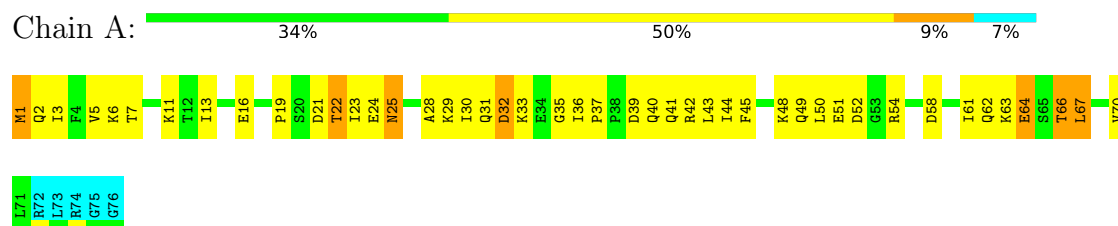
4.2.75 Score per residue for model 75

- Molecule 1: Ubiquitin



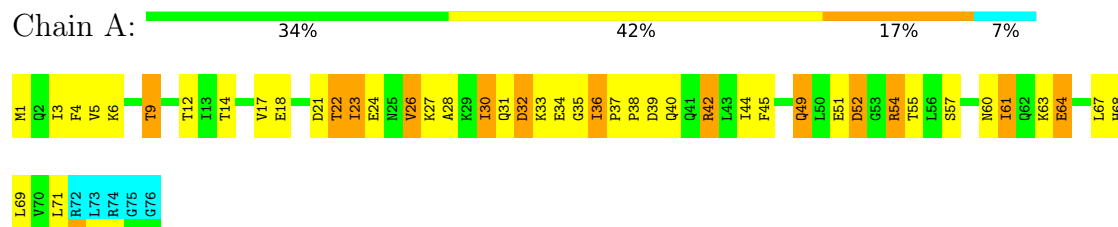
4.2.76 Score per residue for model 76

- Molecule 1: Ubiquitin



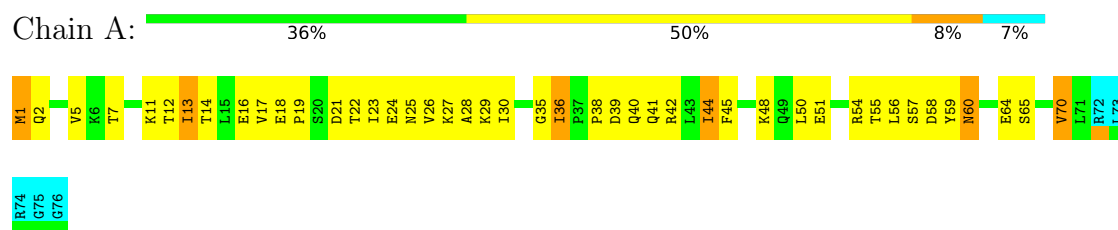
4.2.77 Score per residue for model 77

- Molecule 1: Ubiquitin



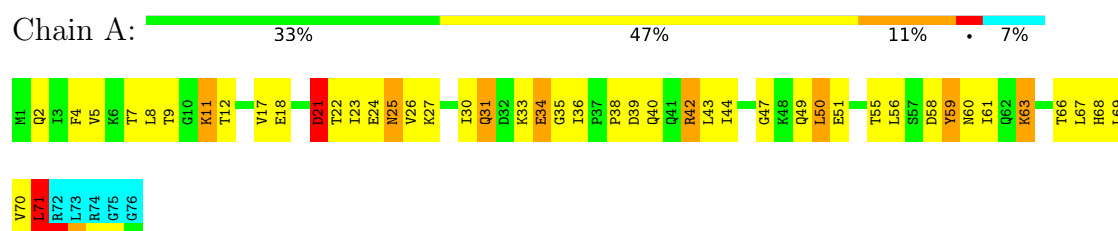
4.2.78 Score per residue for model 78

- Molecule 1: Ubiquitin



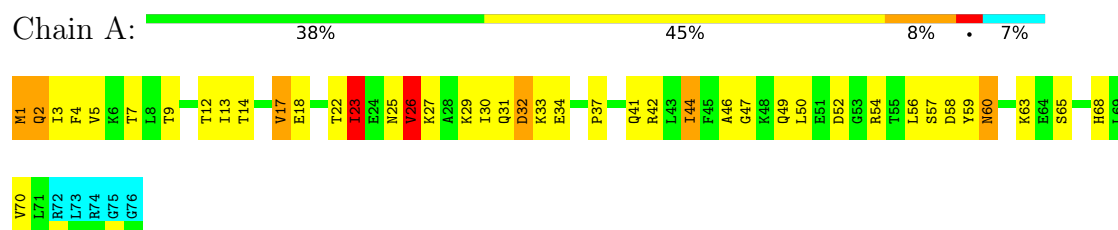
4.2.79 Score per residue for model 79

- Molecule 1: Ubiquitin



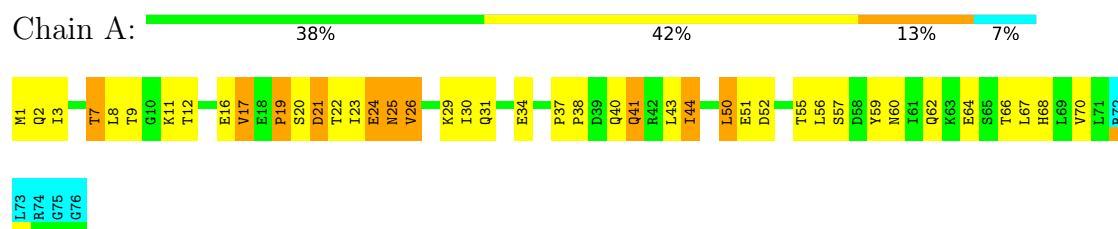
4.2.80 Score per residue for model 80

- Molecule 1: Ubiquitin



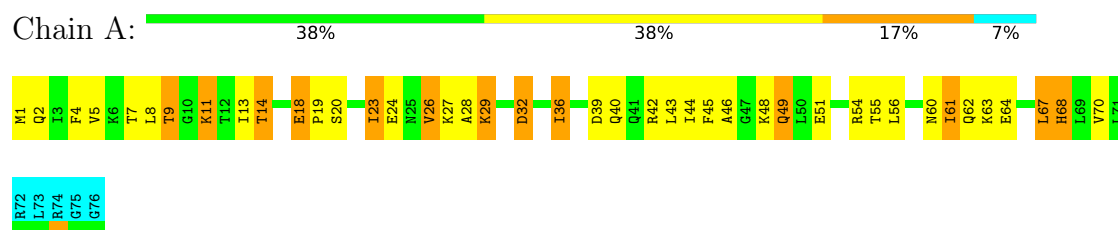
4.2.81 Score per residue for model 81

- Molecule 1: Ubiquitin



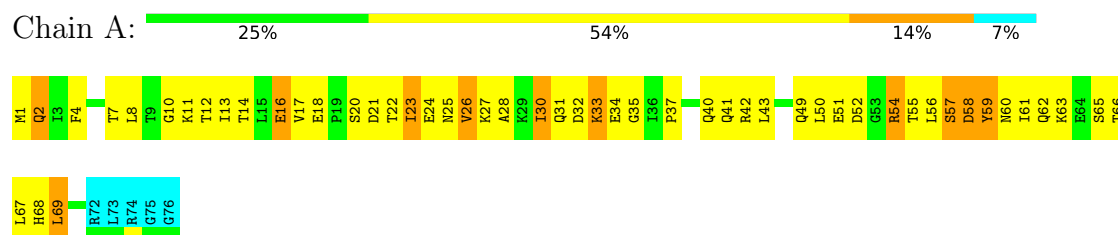
4.2.82 Score per residue for model 82

- Molecule 1: Ubiquitin



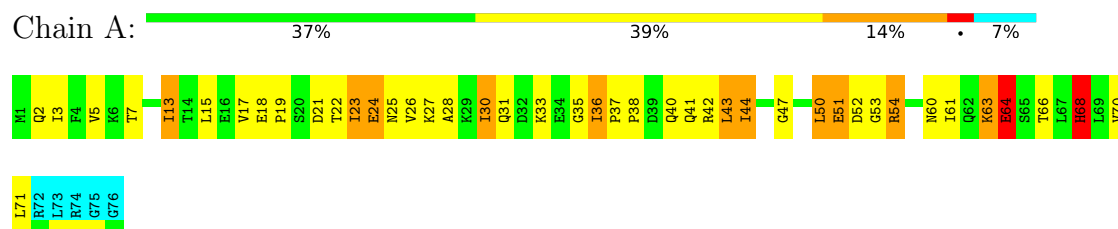
4.2.83 Score per residue for model 83

- Molecule 1: Ubiquitin



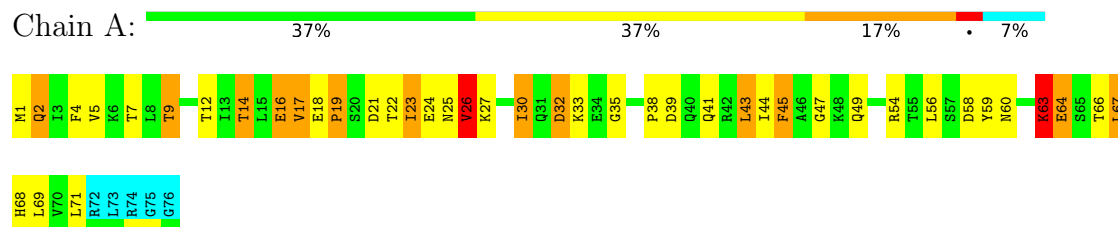
4.2.84 Score per residue for model 84

- Molecule 1: Ubiquitin



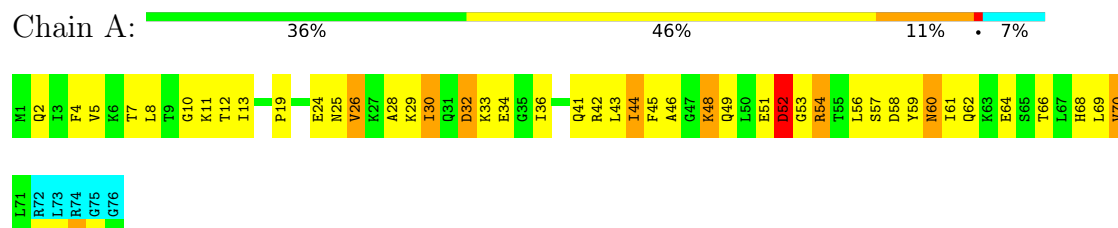
4.2.85 Score per residue for model 85

- Molecule 1: Ubiquitin



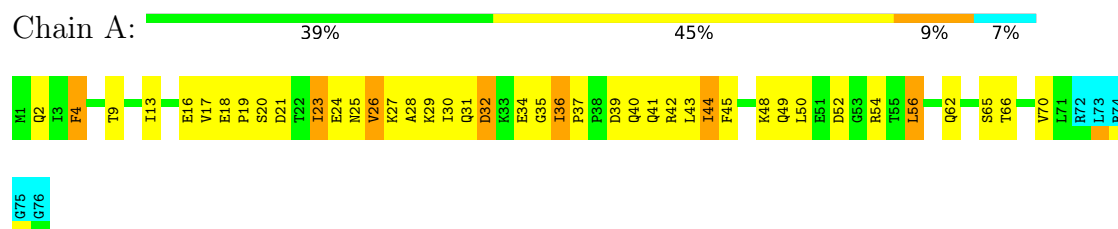
4.2.86 Score per residue for model 86

- Molecule 1: Ubiquitin



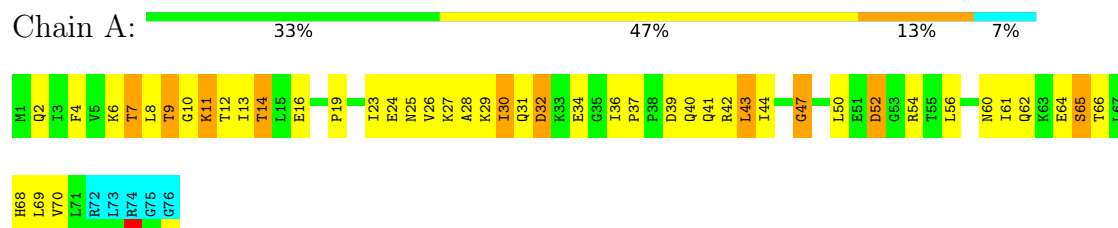
4.2.87 Score per residue for model 87

- Molecule 1: Ubiquitin



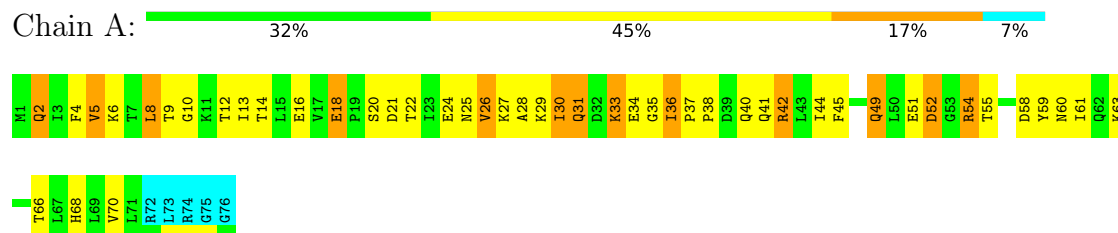
4.2.88 Score per residue for model 88

- Molecule 1: Ubiquitin



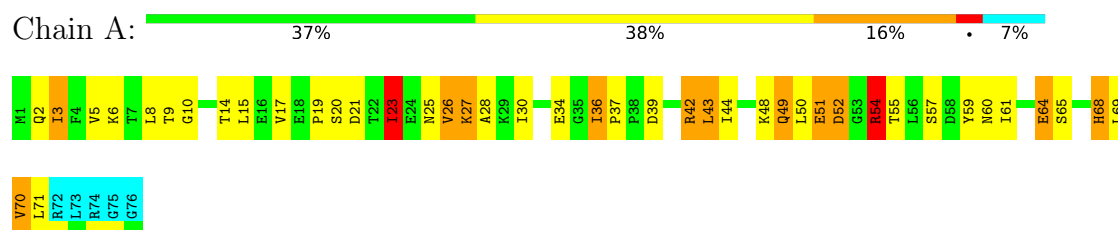
4.2.89 Score per residue for model 89

- Molecule 1: Ubiquitin



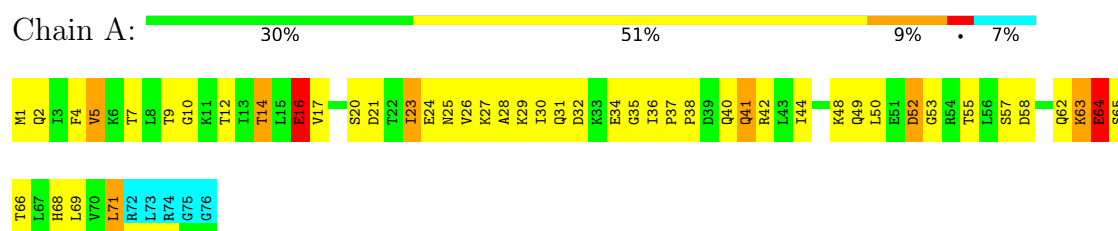
4.2.90 Score per residue for model 90

- Molecule 1: Ubiquitin



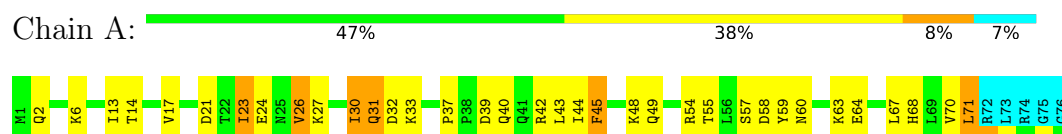
4.2.91 Score per residue for model 91

- Molecule 1: Ubiquitin



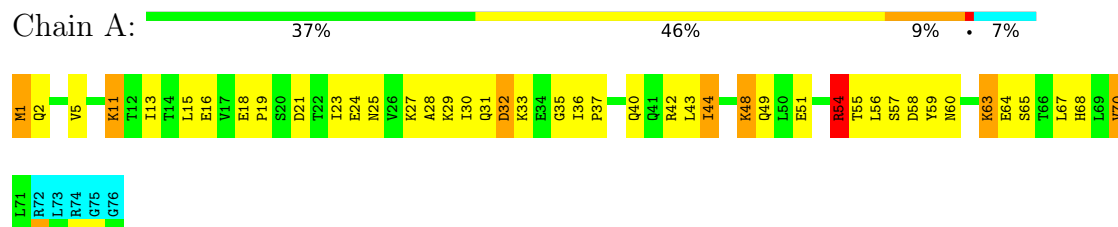
4.2.92 Score per residue for model 92

- Molecule 1: Ubiquitin



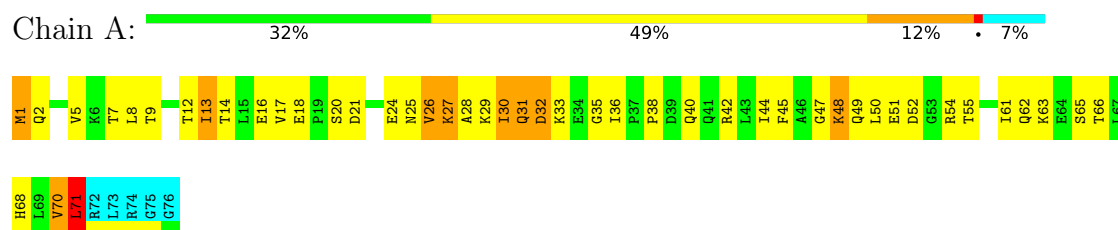
4.2.93 Score per residue for model 93

- Molecule 1: Ubiquitin



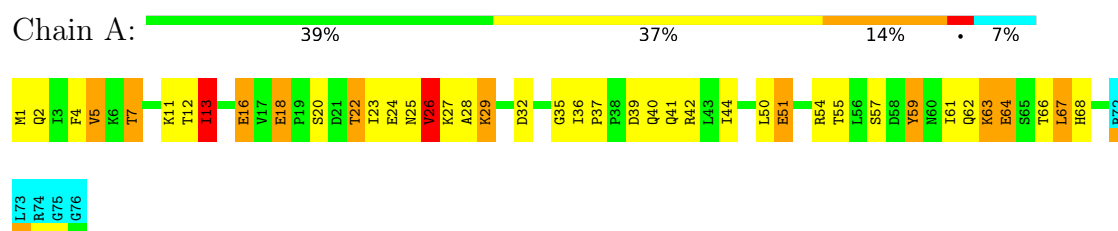
4.2.94 Score per residue for model 94

- Molecule 1: Ubiquitin



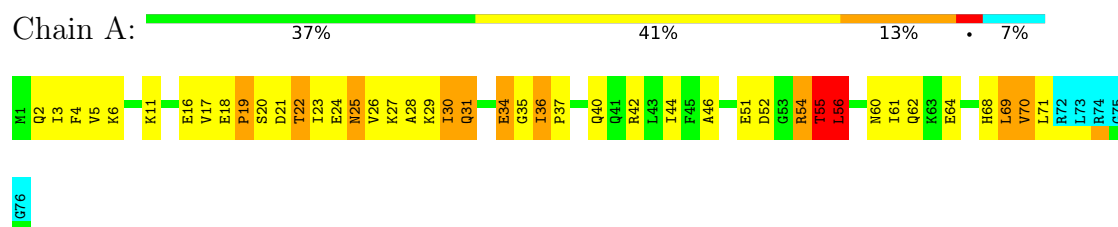
4.2.95 Score per residue for model 95

- Molecule 1: Ubiquitin



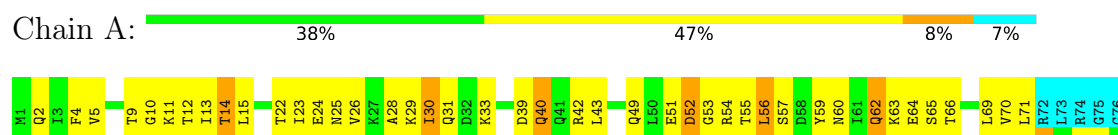
4.2.96 Score per residue for model 96

- Molecule 1: Ubiquitin



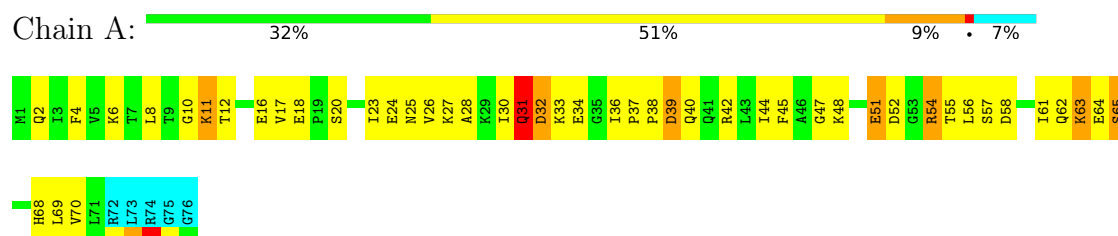
4.2.97 Score per residue for model 97

- Molecule 1: Ubiquitin



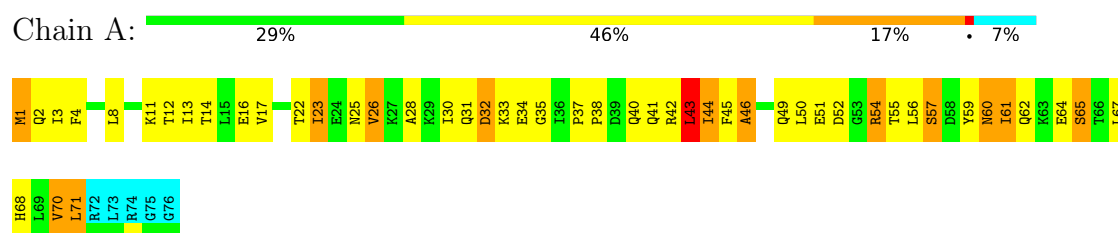
4.2.98 Score per residue for model 98

- Molecule 1: Ubiquitin



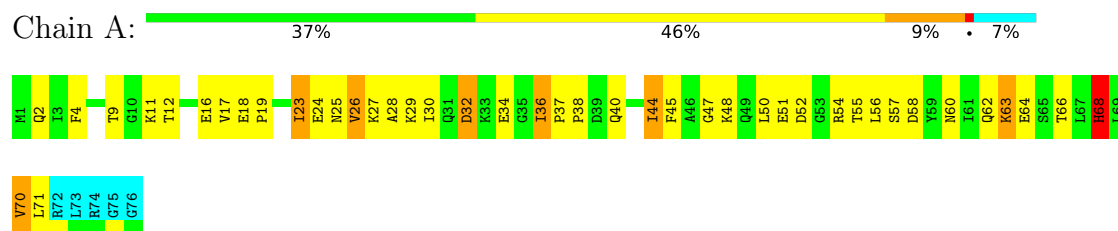
4.2.99 Score per residue for model 99

- Molecule 1: Ubiquitin



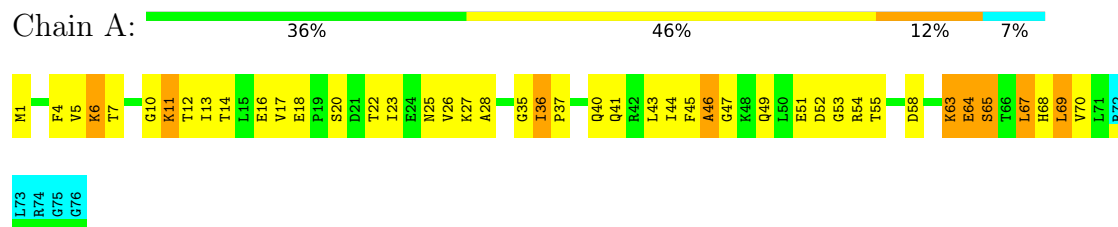
4.2.100 Score per residue for model 100

- Molecule 1: Ubiquitin



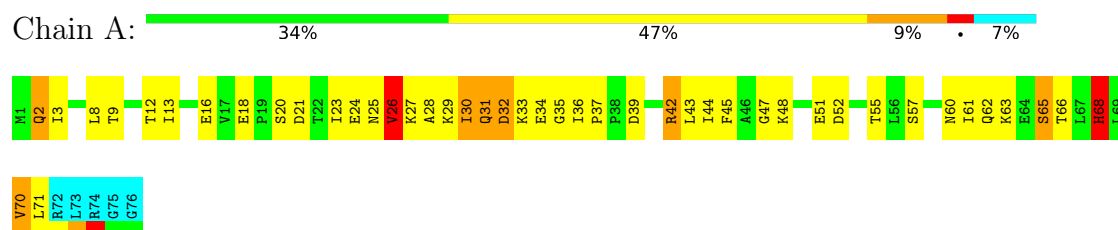
4.2.101 Score per residue for model 101

- Molecule 1: Ubiquitin



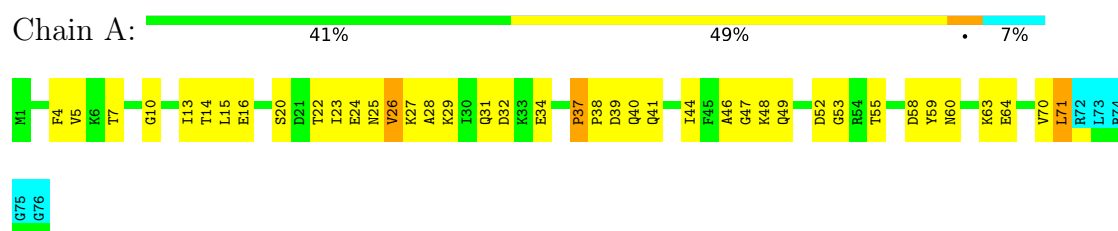
4.2.106 Score per residue for model 106

- Molecule 1: Ubiquitin



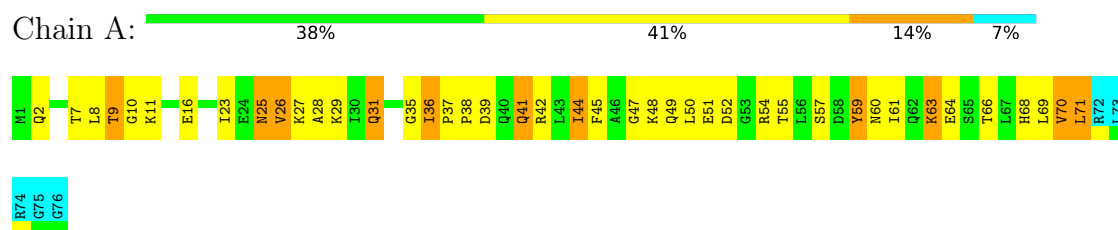
4.2.107 Score per residue for model 107

- Molecule 1: Ubiquitin



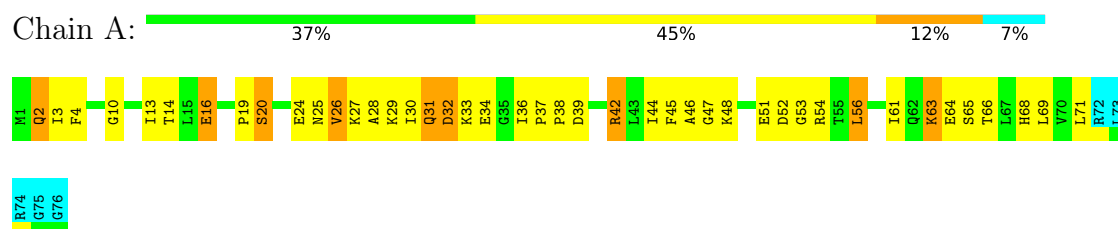
4.2.108 Score per residue for model 108

- Molecule 1: Ubiquitin



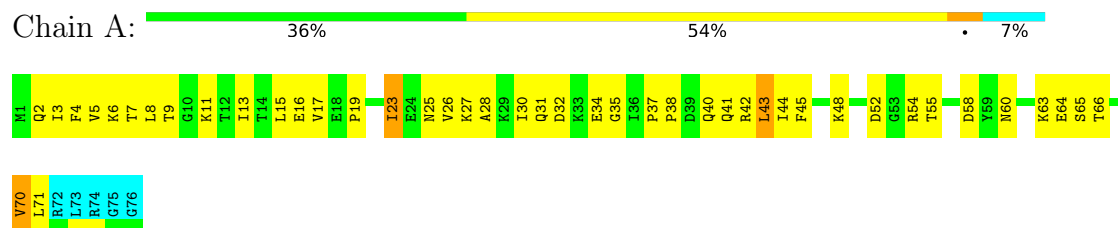
4.2.109 Score per residue for model 109

- Molecule 1: Ubiquitin



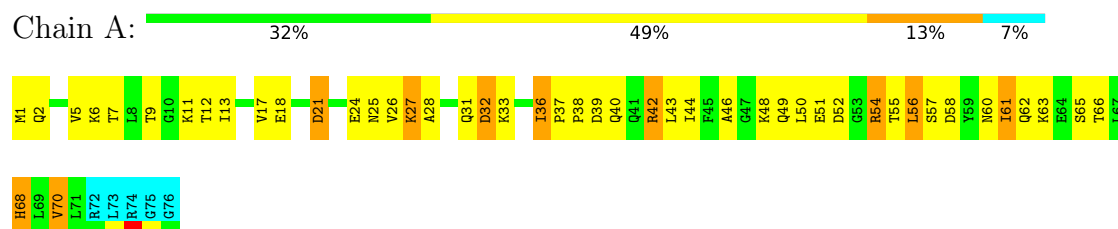
4.2.110 Score per residue for model 110

- Molecule 1: Ubiquitin



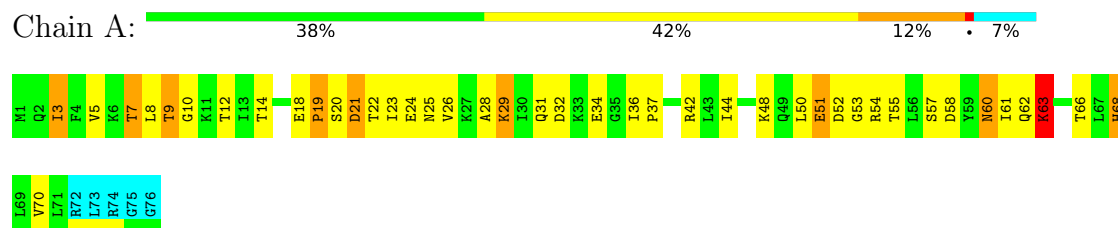
4.2.111 Score per residue for model 111

- Molecule 1: Ubiquitin



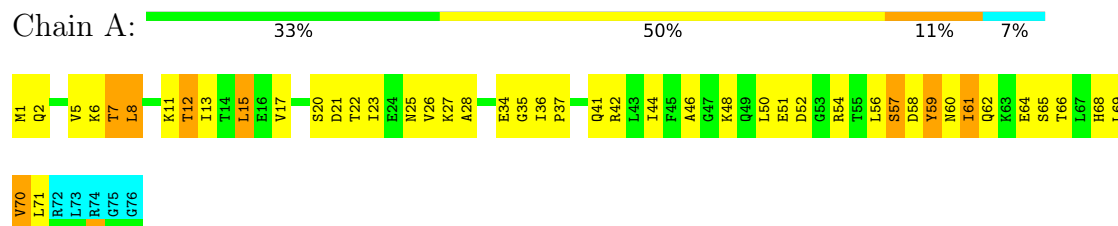
4.2.112 Score per residue for model 112

- Molecule 1: Ubiquitin



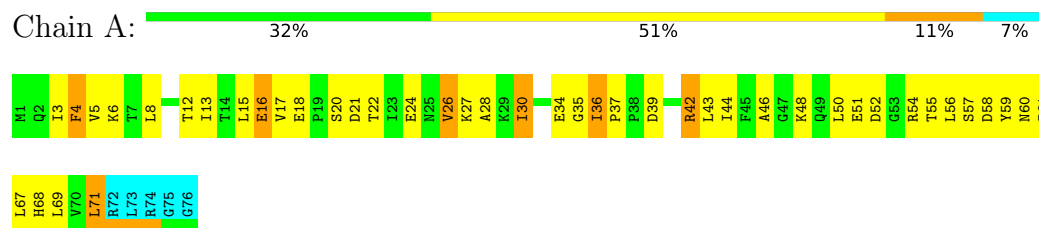
4.2.113 Score per residue for model 113

- Molecule 1: Ubiquitin



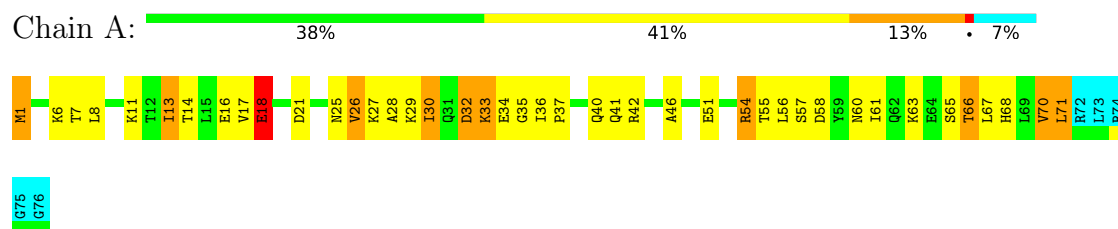
4.2.114 Score per residue for model 114

- Molecule 1: Ubiquitin



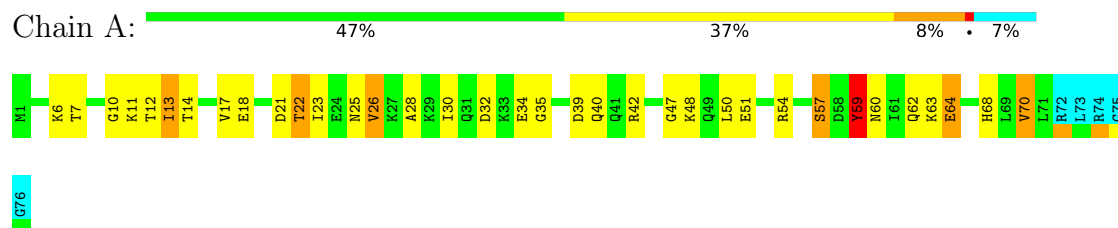
4.2.115 Score per residue for model 115

- Molecule 1: Ubiquitin



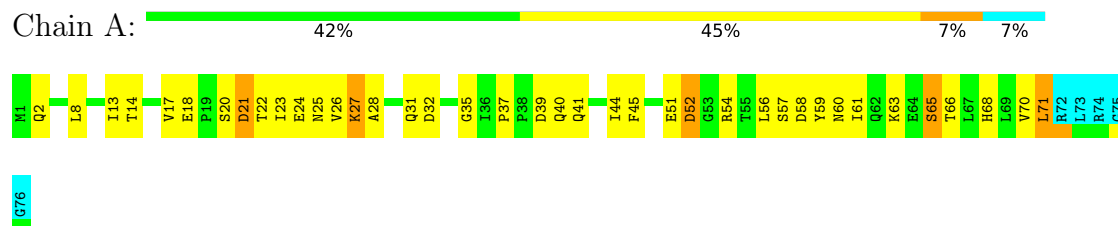
4.2.116 Score per residue for model 116

- Molecule 1: Ubiquitin



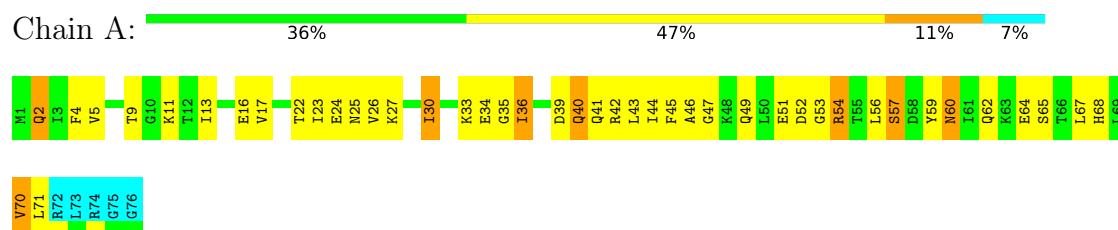
4.2.117 Score per residue for model 117

- Molecule 1: Ubiquitin



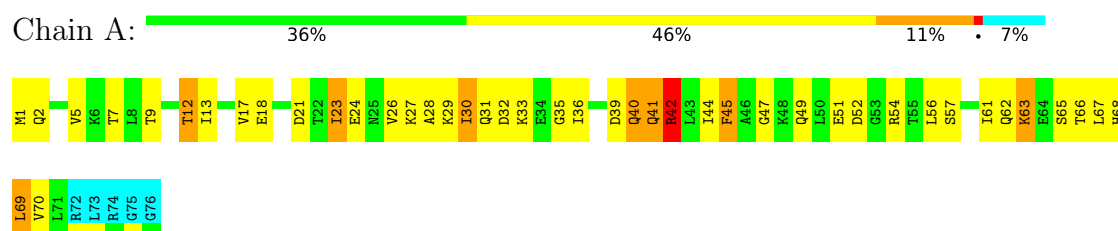
4.2.118 Score per residue for model 118

- Molecule 1: Ubiquitin



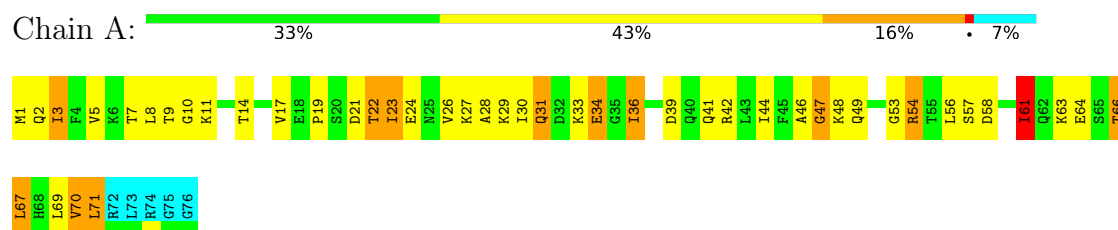
4.2.119 Score per residue for model 119

- Molecule 1: Ubiquitin



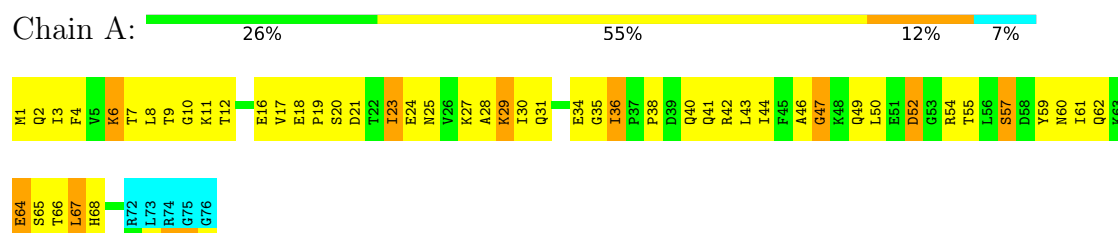
4.2.120 Score per residue for model 120

- Molecule 1: Ubiquitin



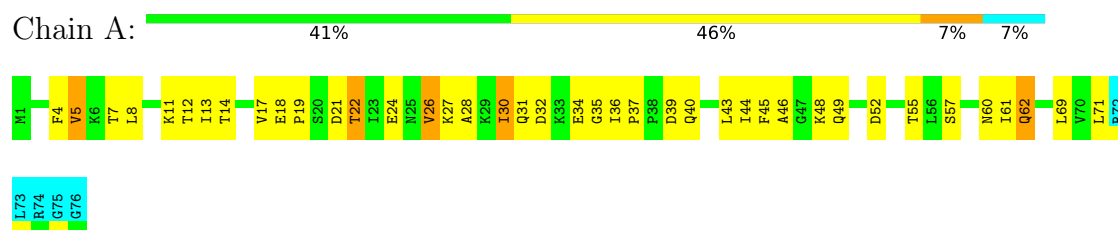
4.2.121 Score per residue for model 121

- Molecule 1: Ubiquitin



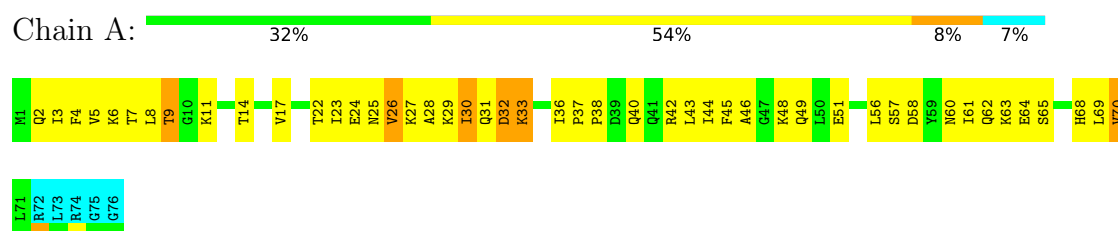
4.2.122 Score per residue for model 122

- Molecule 1: Ubiquitin



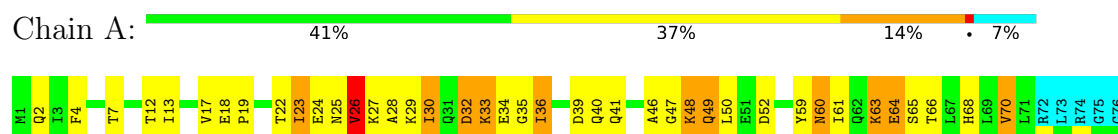
4.2.123 Score per residue for model 123

- Molecule 1: Ubiquitin



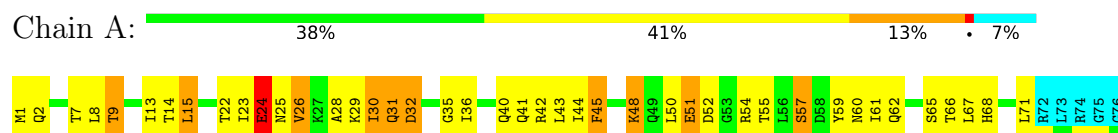
4.2.124 Score per residue for model 124

- Molecule 1: Ubiquitin



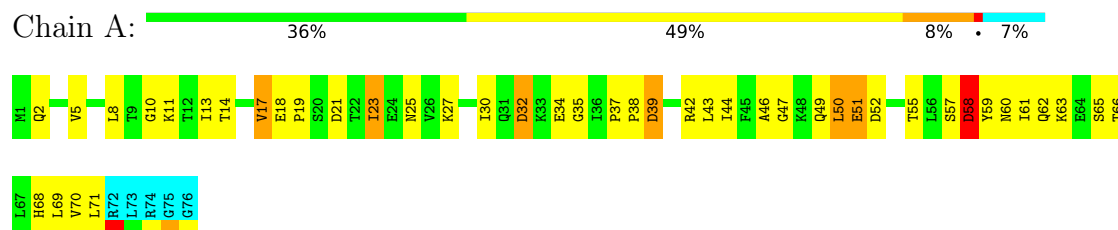
4.2.125 Score per residue for model 125

- Molecule 1: Ubiquitin



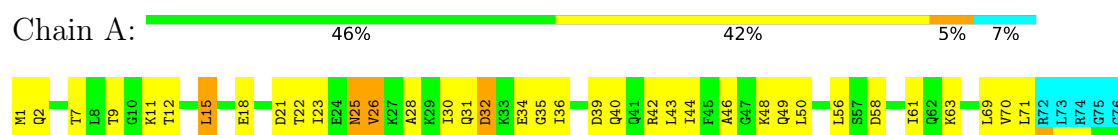
4.2.126 Score per residue for model 126

- Molecule 1: Ubiquitin



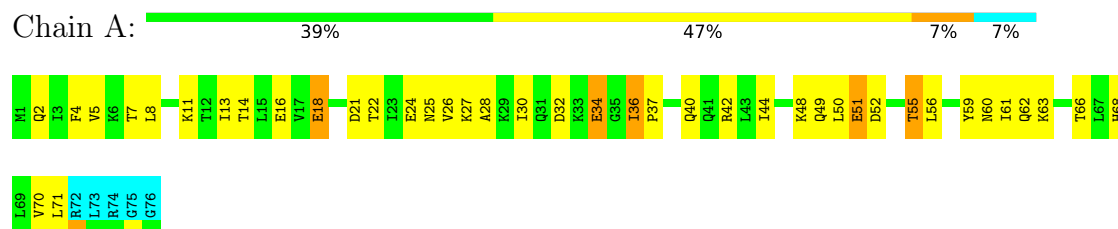
4.2.127 Score per residue for model 127

- Molecule 1: Ubiquitin



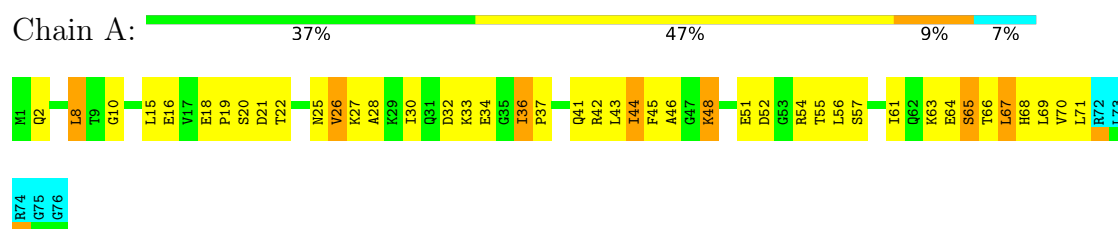
4.2.128 Score per residue for model 128

- Molecule 1: Ubiquitin



4.2.129 Score per residue for model 129

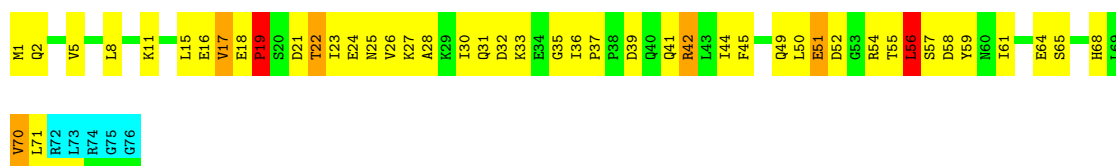
- Molecule 1: Ubiquitin



4.2.130 Score per residue for model 130

- Molecule 1: Ubiquitin

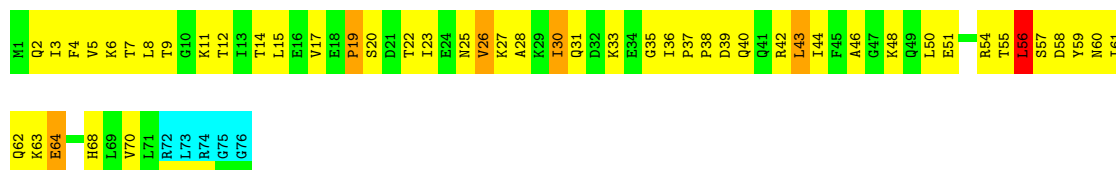




4.2.131 Score per residue for model 131

- Molecule 1: Ubiquitin

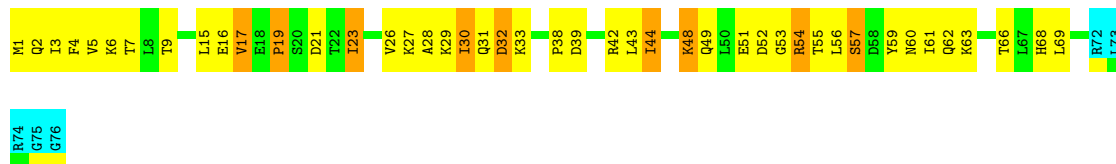
Chain A: 28% 58% 7% 7%



4.2.132 Score per residue for model 132

- Molecule 1: Ubiquitin

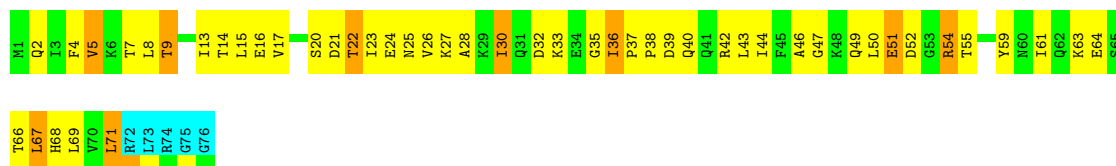
Chain A: 36% 46% 12% 7%



4.2.133 Score per residue for model 133

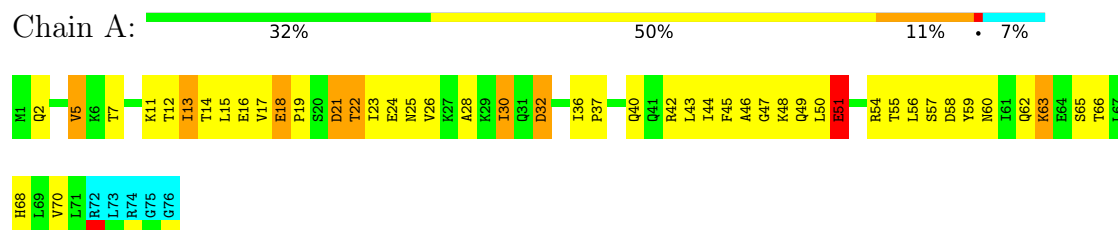
- Molecule 1: Ubiquitin

Chain A: 29% 53% 12% 7%



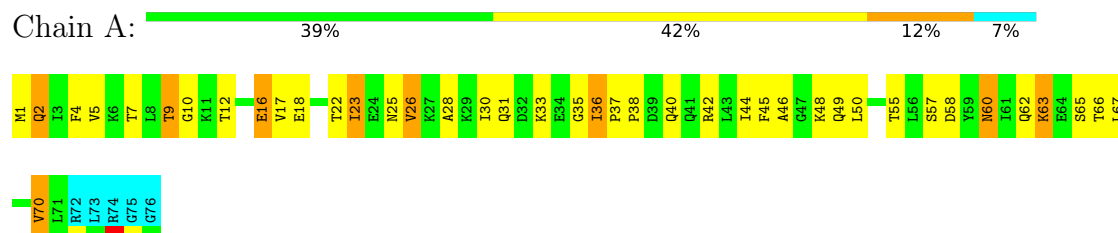
4.2.134 Score per residue for model 134

- Molecule 1: Ubiquitin



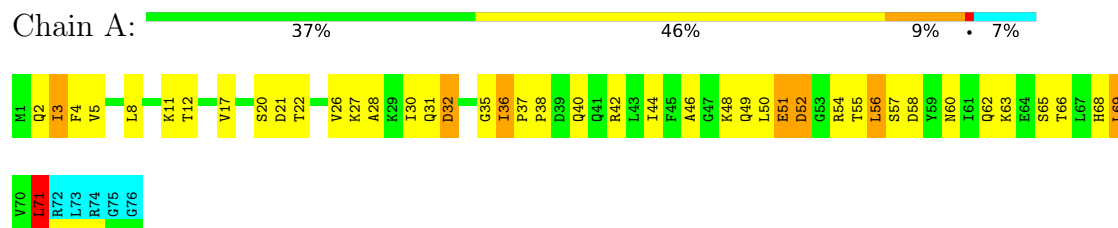
4.2.135 Score per residue for model 135

- Molecule 1: Ubiquitin



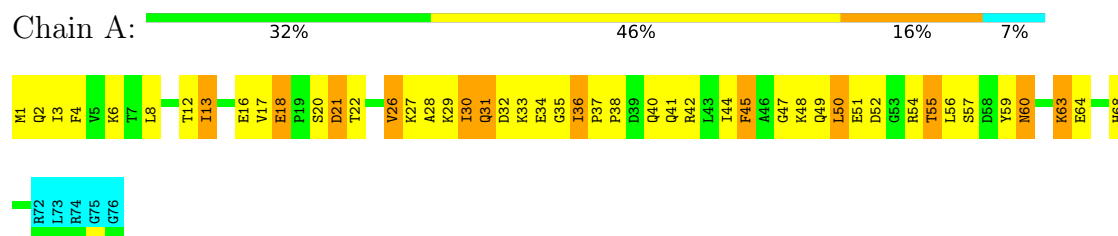
4.2.136 Score per residue for model 136

- Molecule 1: Ubiquitin



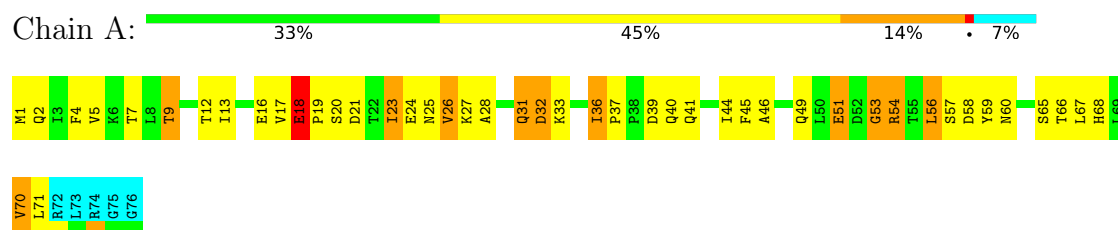
4.2.137 Score per residue for model 137

- Molecule 1: Ubiquitin



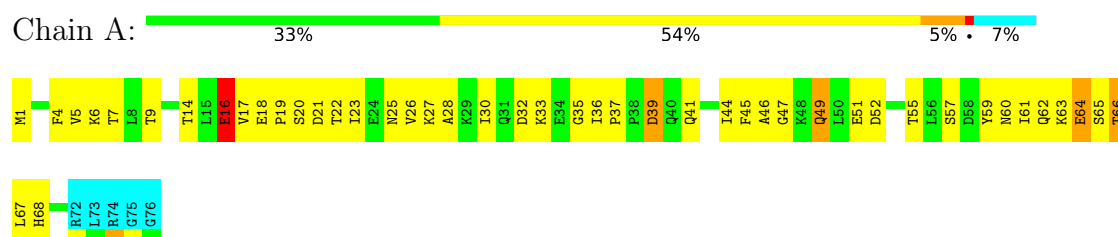
4.2.138 Score per residue for model 138

- Molecule 1: Ubiquitin



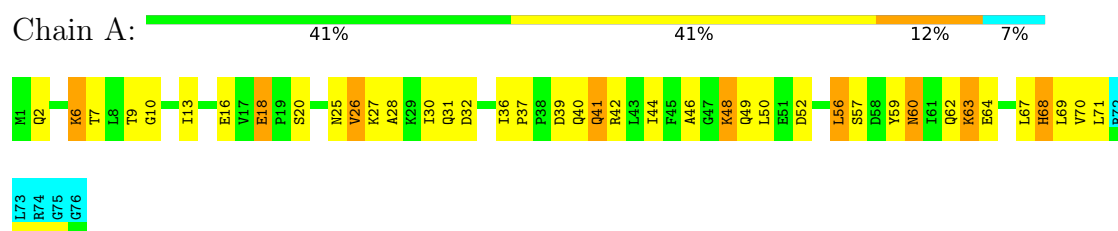
4.2.139 Score per residue for model 139

- Molecule 1: Ubiquitin



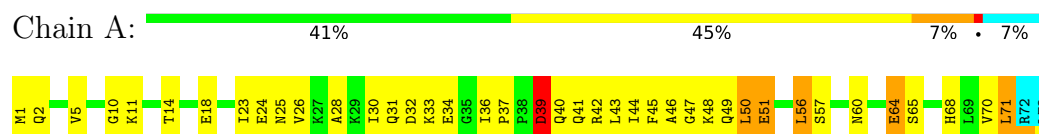
4.2.140 Score per residue for model 140

- Molecule 1: Ubiquitin



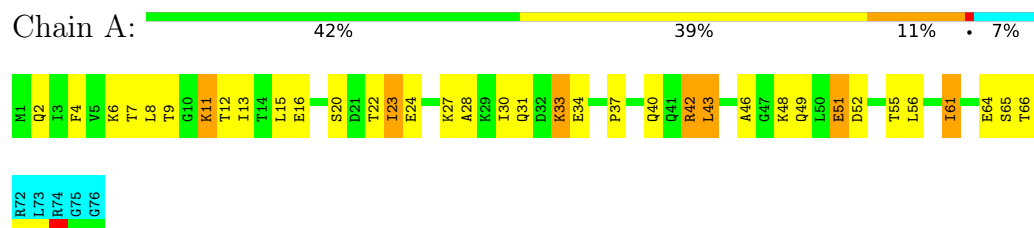
4.2.141 Score per residue for model 141

- Molecule 1: Ubiquitin



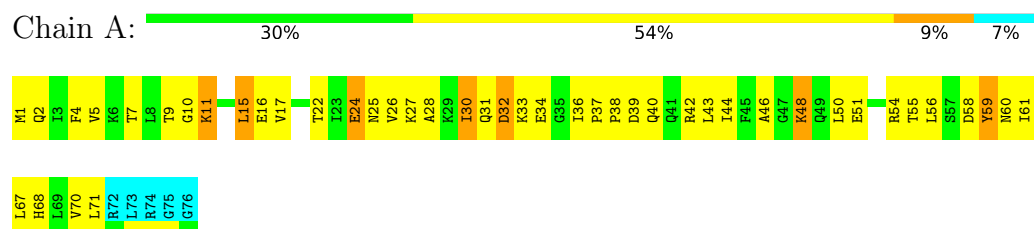
4.2.142 Score per residue for model 142

- Molecule 1: Ubiquitin



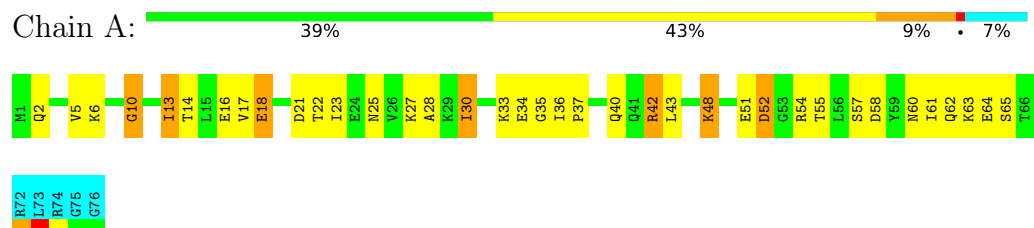
4.2.143 Score per residue for model 143

- Molecule 1: Ubiquitin



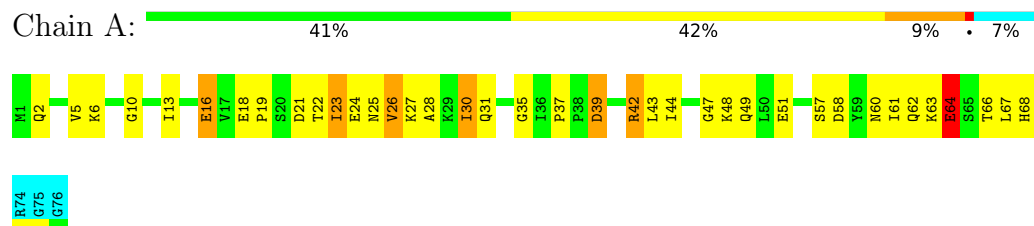
4.2.144 Score per residue for model 144

- Molecule 1: Ubiquitin



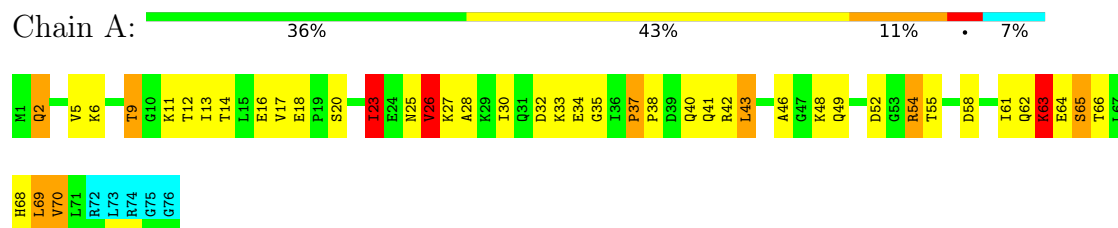
4.2.145 Score per residue for model 145

- Molecule 1: Ubiquitin



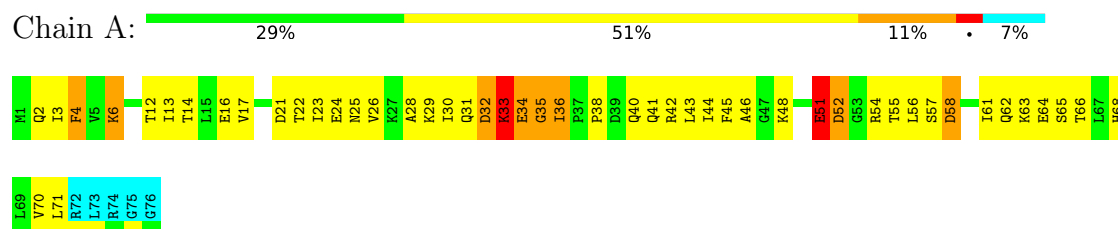
4.2.146 Score per residue for model 146

- Molecule 1: Ubiquitin



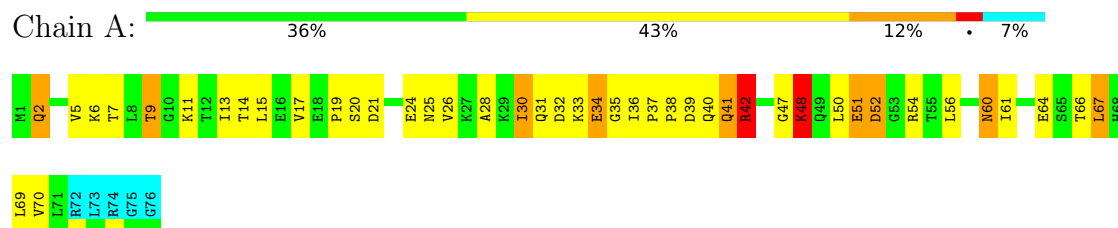
4.2.147 Score per residue for model 147

- Molecule 1: Ubiquitin



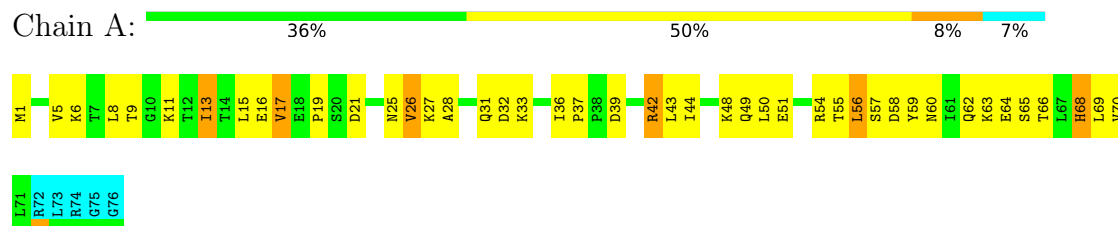
4.2.148 Score per residue for model 148

- Molecule 1: Ubiquitin



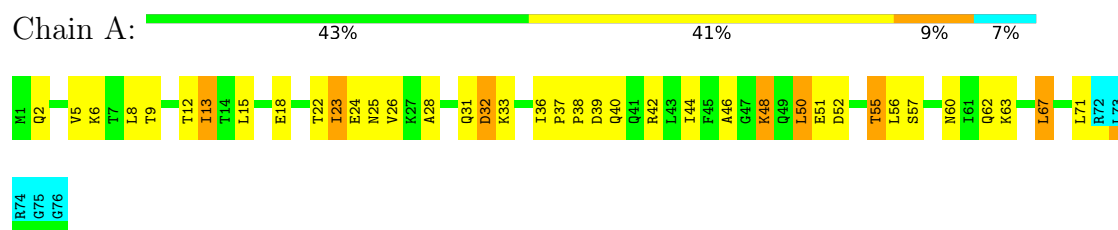
4.2.149 Score per residue for model 149

- Molecule 1: Ubiquitin



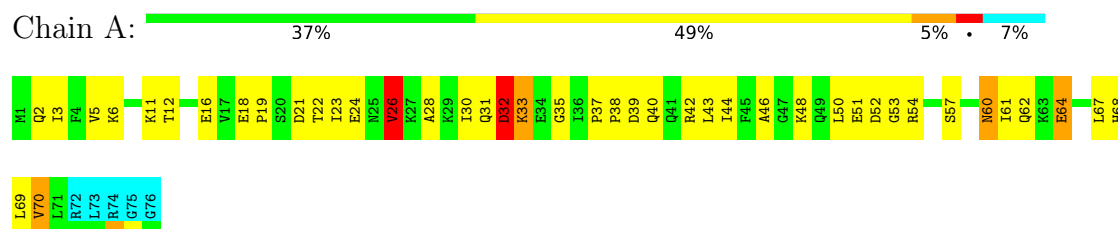
4.2.150 Score per residue for model 150

- Molecule 1: Ubiquitin



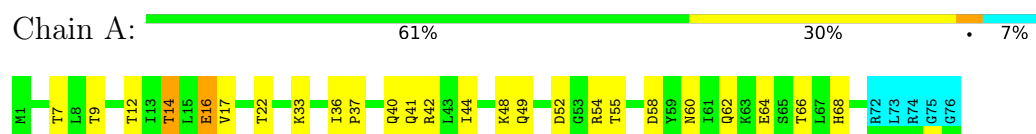
4.2.151 Score per residue for model 151

- Molecule 1: Ubiquitin



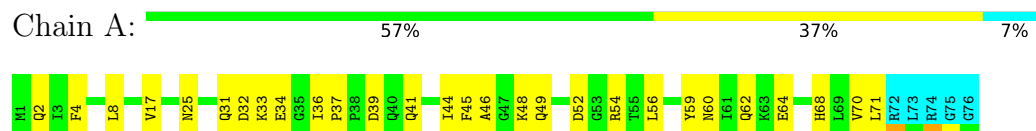
4.2.152 Score per residue for model 152

- Molecule 1: Ubiquitin



4.2.153 Score per residue for model 153

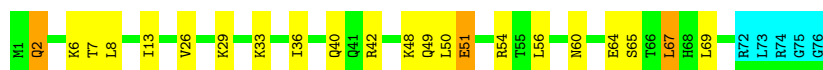
- Molecule 1: Ubiquitin



4.2.154 Score per residue for model 154

- Molecule 1: Ubiquitin

Chain A:  64% 25% 7%



4.2.155 Score per residue for model 155

- Molecule 1: Ubiquitin

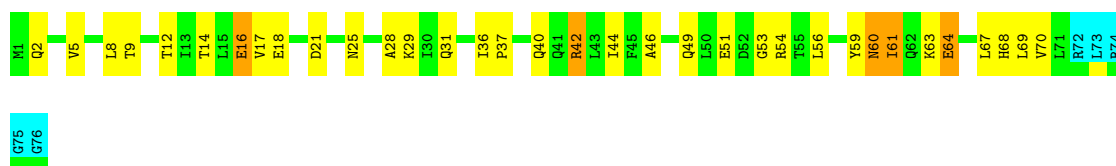
Chain A:  57% 36% 7%



4.2.156 Score per residue for model 156

- Molecule 1: Ubiquitin

Chain A:  49% 38% 7% 7%



4.2.157 Score per residue for model 157

- Molecule 1: Ubiquitin

Chain A:  58% 33% 7%



4.2.158 Score per residue for model 158

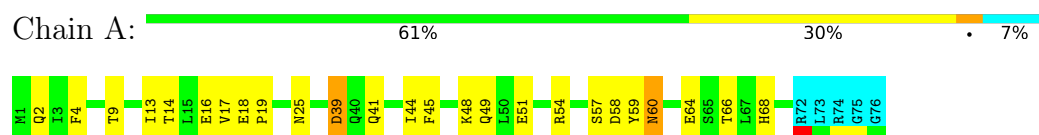
- Molecule 1: Ubiquitin

Chain A:  61% 33% 7%



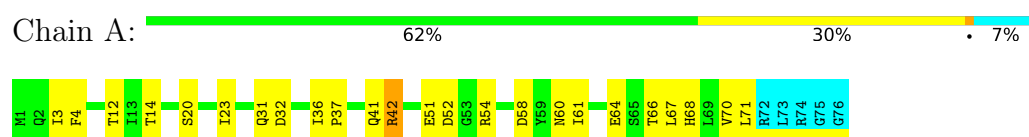
4.2.159 Score per residue for model 159

- Molecule 1: Ubiquitin



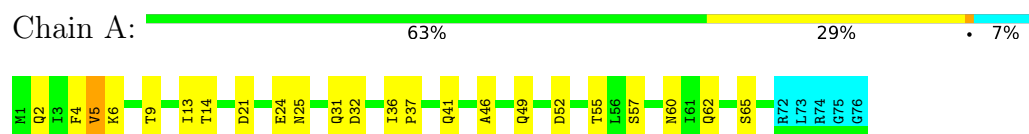
4.2.160 Score per residue for model 160

- Molecule 1: Ubiquitin



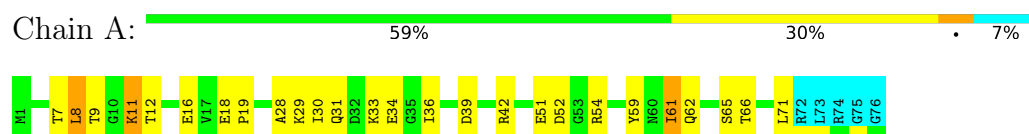
4.2.161 Score per residue for model 161

- Molecule 1: Ubiquitin



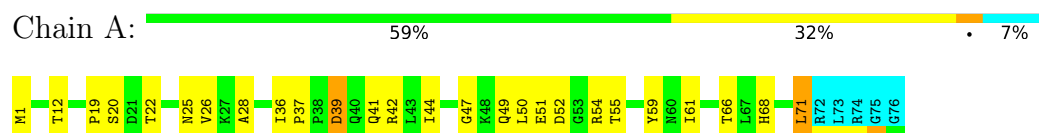
4.2.162 Score per residue for model 162

- Molecule 1: Ubiquitin



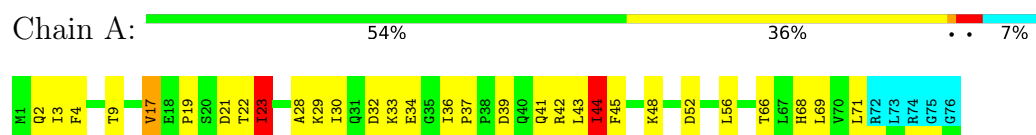
4.2.163 Score per residue for model 163

- Molecule 1: Ubiquitin



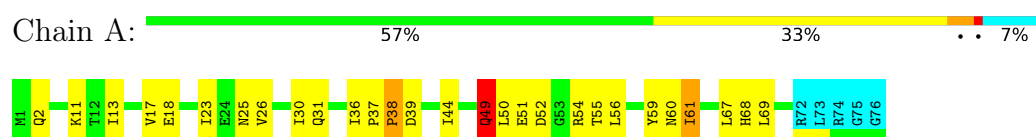
4.2.164 Score per residue for model 164

- Molecule 1: Ubiquitin



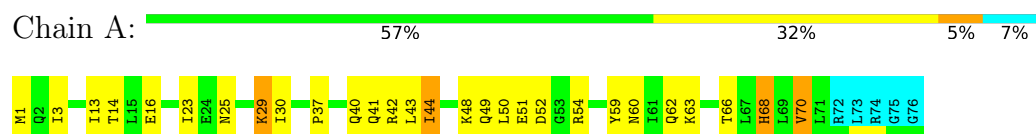
4.2.165 Score per residue for model 165

- Molecule 1: Ubiquitin



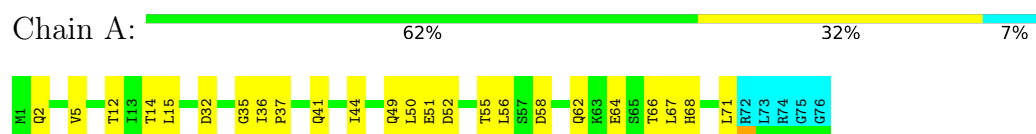
4.2.166 Score per residue for model 166

- Molecule 1: Ubiquitin



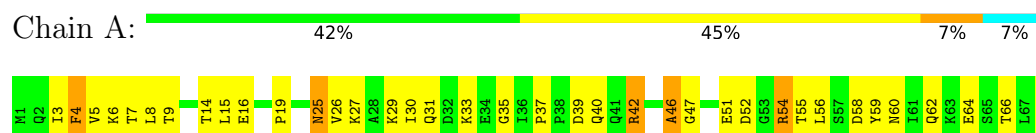
4.2.167 Score per residue for model 167

- Molecule 1: Ubiquitin



4.2.168 Score per residue for model 168

- Molecule 1: Ubiquitin





4.2.169 Score per residue for model 169

- Molecule 1: Ubiquitin

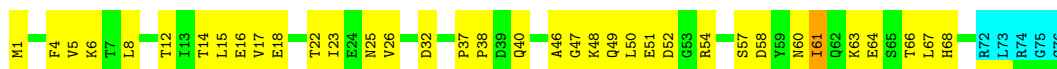
Chain A: 57% 32% 5% 7%



4.2.170 Score per residue for model 170

- Molecule 1: Ubiquitin

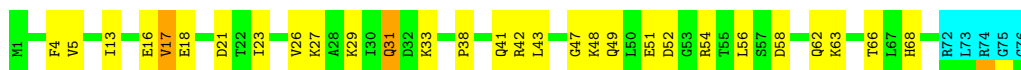
Chain A: 46% 46% 7%



4.2.171 Score per residue for model 171

- Molecule 1: Ubiquitin

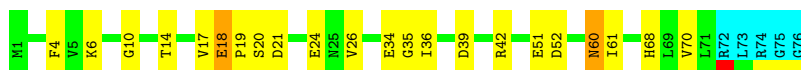
Chain A: 55% 36% 7%



4.2.172 Score per residue for model 172

- Molecule 1: Ubiquitin

Chain A: 64% 26% 7%



4.2.173 Score per residue for model 173

- Molecule 1: Ubiquitin

Chain A: 57% 33% 7%



4.2.174 Score per residue for model 174

- Molecule 1: Ubiquitin



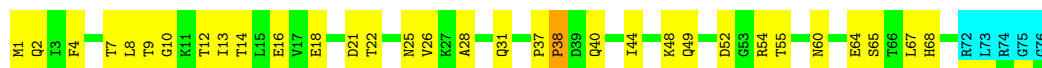
4.2.175 Score per residue for model 175

- Molecule 1: Ubiquitin



4.2.176 Score per residue for model 176

- Molecule 1: Ubiquitin



4.2.177 Score per residue for model 177

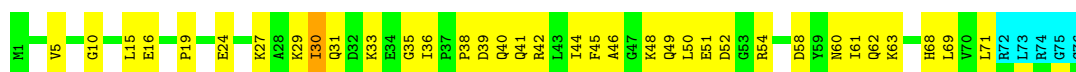
- Molecule 1: Ubiquitin



4.2.178 Score per residue for model 178

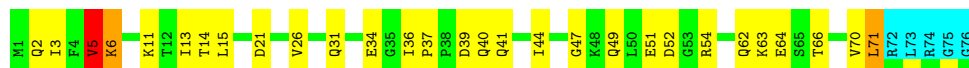
- Molecule 1: Ubiquitin





4.2.179 Score per residue for model 179

- Molecule 1: Ubiquitin



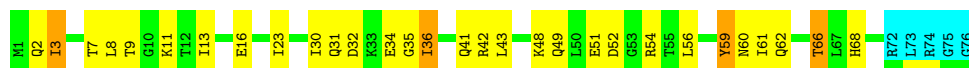
4.2.180 Score per residue for model 180

- Molecule 1: Ubiquitin



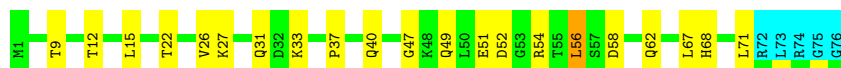
4.2.181 Score per residue for model 181

- Molecule 1: Ubiquitin



4.2.182 Score per residue for model 182

- Molecule 1: Ubiquitin



4.2.183 Score per residue for model 183

- Molecule 1: Ubiquitin





4.2.184 Score per residue for model 184

- Molecule 1: Ubiquitin

Chain A: 58% 28% 7% 7%



4.2.185 Score per residue for model 185

- Molecule 1: Ubiquitin

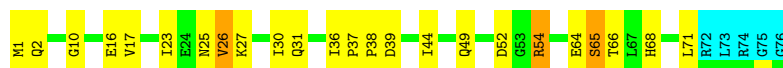
Chain A: 53% 36% 5% 7%



4.2.186 Score per residue for model 186

- Molecule 1: Ubiquitin

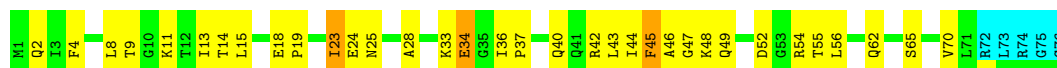
Chain A: 62% 28% 7%



4.2.187 Score per residue for model 187

- Molecule 1: Ubiquitin

Chain A: 49% 41% 7%



4.2.188 Score per residue for model 188

- Molecule 1: Ubiquitin

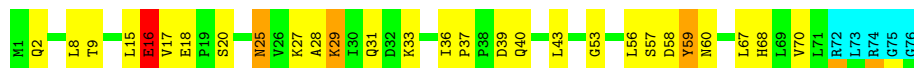
Chain A: 55% 34% 7%



4.2.189 Score per residue for model 189

- Molecule 1: Ubiquitin

Chain A: 57% 32% 7%



4.2.190 Score per residue for model 190

- Molecule 1: Ubiquitin

Chain A: 70% 18% 5% 7%



4.2.191 Score per residue for model 191

- Molecule 1: Ubiquitin

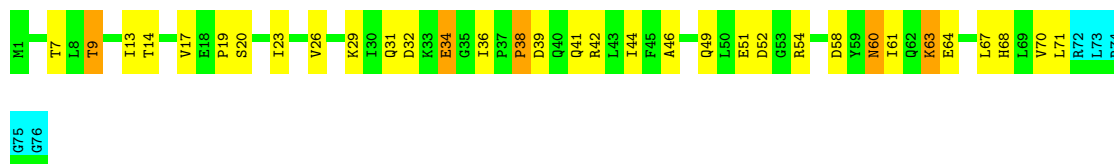
Chain A: 47% 42% 7%



4.2.192 Score per residue for model 192

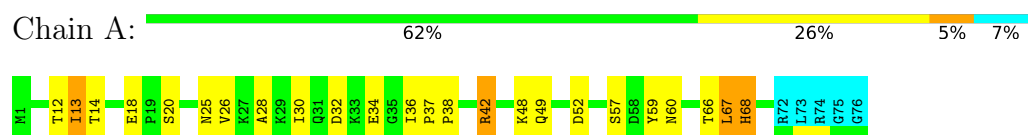
- Molecule 1: Ubiquitin

Chain A: 50% 37% 7% 7%



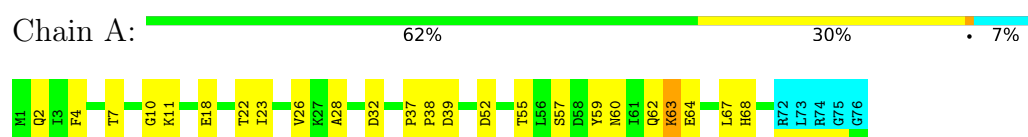
4.2.193 Score per residue for model 193

- Molecule 1: Ubiquitin



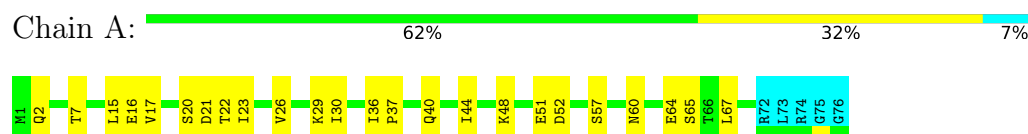
4.2.194 Score per residue for model 194

- Molecule 1: Ubiquitin



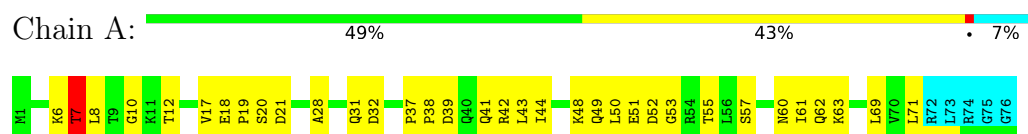
4.2.195 Score per residue for model 195

- Molecule 1: Ubiquitin



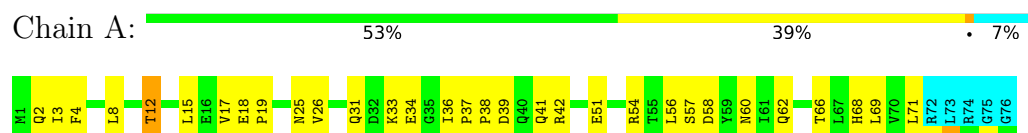
4.2.196 Score per residue for model 196

- Molecule 1: Ubiquitin



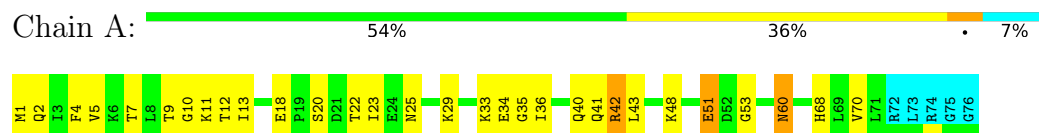
4.2.197 Score per residue for model 197

- Molecule 1: Ubiquitin



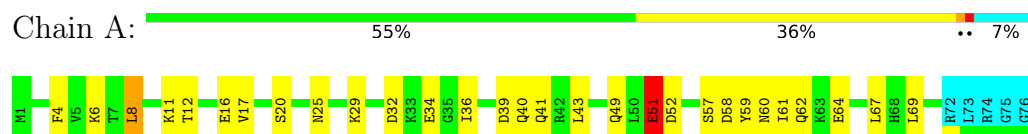
4.2.198 Score per residue for model 198

- Molecule 1: Ubiquitin



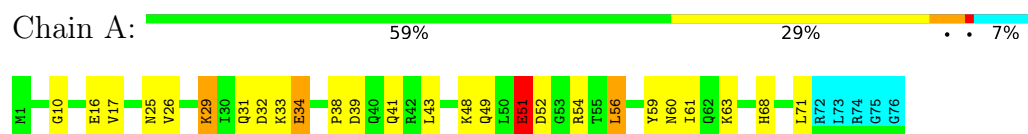
4.2.199 Score per residue for model 199

- Molecule 1: Ubiquitin



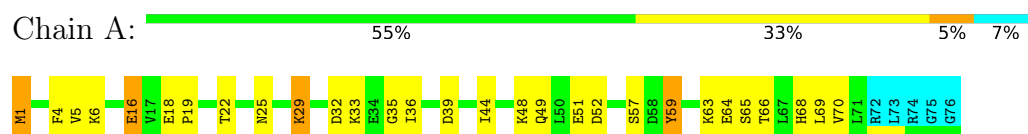
4.2.200 Score per residue for model 200

- Molecule 1: Ubiquitin



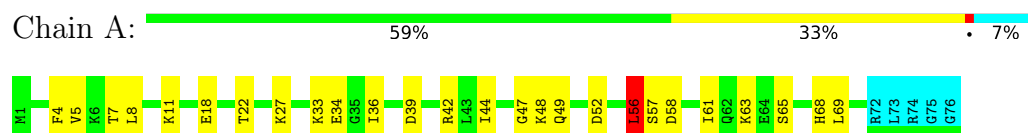
4.2.201 Score per residue for model 201

- Molecule 1: Ubiquitin



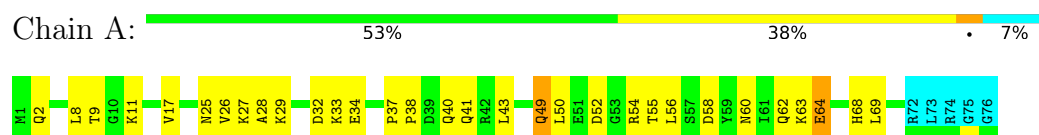
4.2.202 Score per residue for model 202

- Molecule 1: Ubiquitin



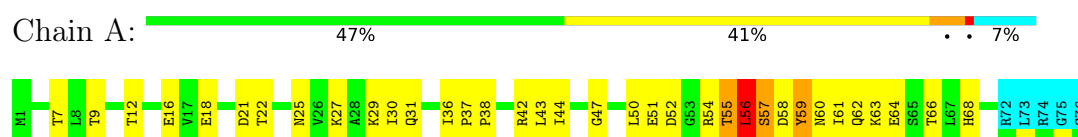
4.2.203 Score per residue for model 203

- Molecule 1: Ubiquitin



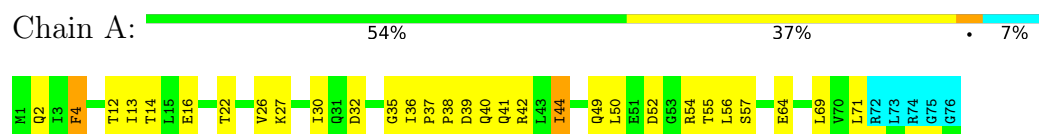
4.2.204 Score per residue for model 204

- Molecule 1: Ubiquitin



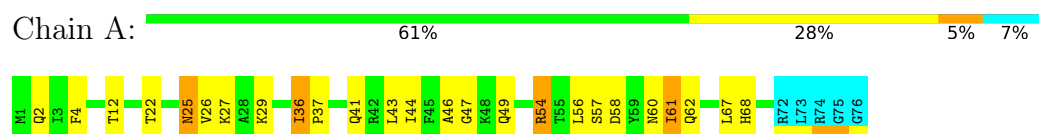
4.2.205 Score per residue for model 205

- Molecule 1: Ubiquitin



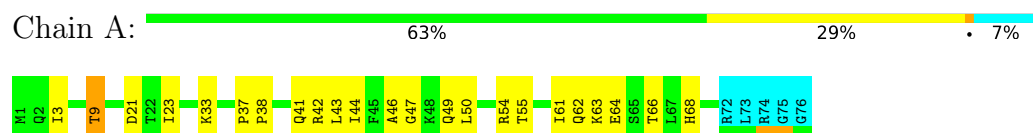
4.2.206 Score per residue for model 206

- Molecule 1: Ubiquitin



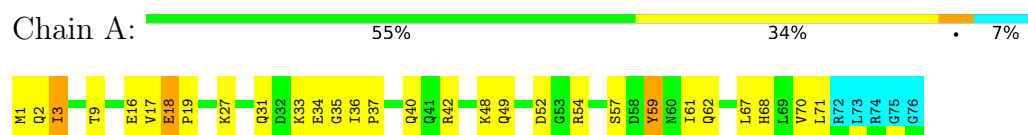
4.2.207 Score per residue for model 207

- Molecule 1: Ubiquitin



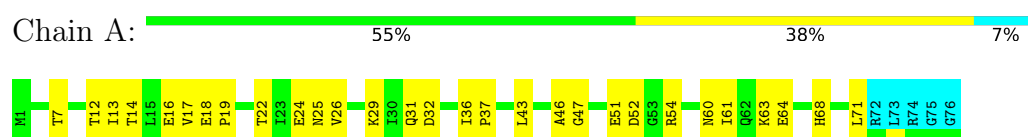
4.2.208 Score per residue for model 208

- Molecule 1: Ubiquitin



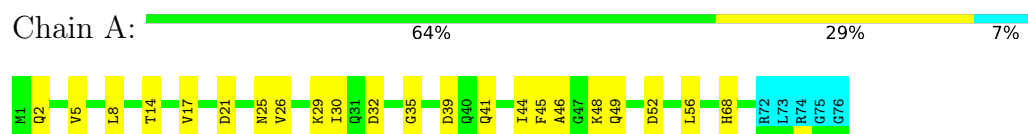
4.2.209 Score per residue for model 209

- Molecule 1: Ubiquitin



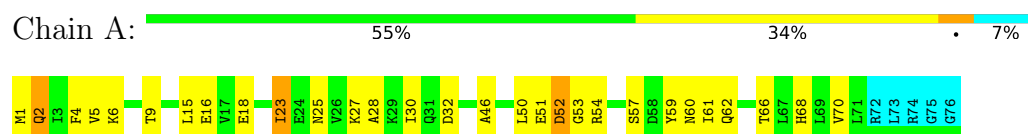
4.2.210 Score per residue for model 210 (medoid)

- Molecule 1: Ubiquitin



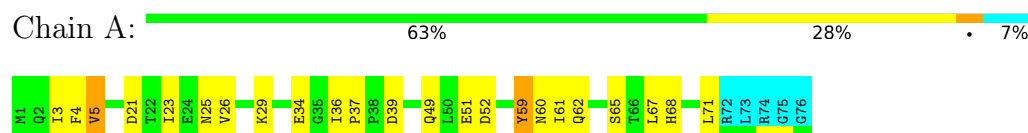
4.2.211 Score per residue for model 211

- Molecule 1: Ubiquitin



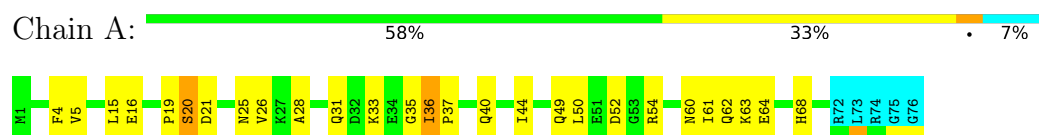
4.2.212 Score per residue for model 212

- Molecule 1: Ubiquitin



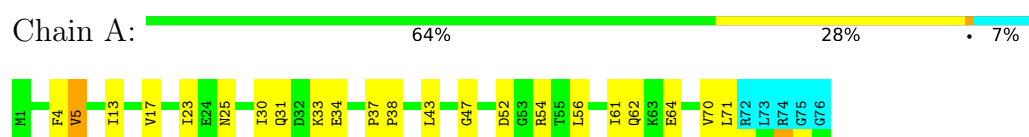
4.2.213 Score per residue for model 213

- Molecule 1: Ubiquitin



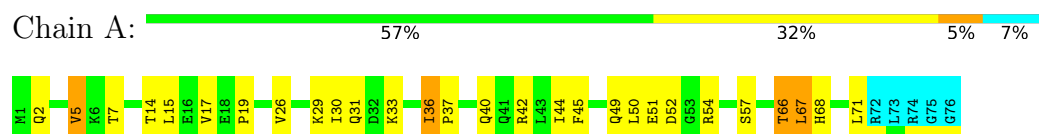
4.2.214 Score per residue for model 214

- Molecule 1: Ubiquitin



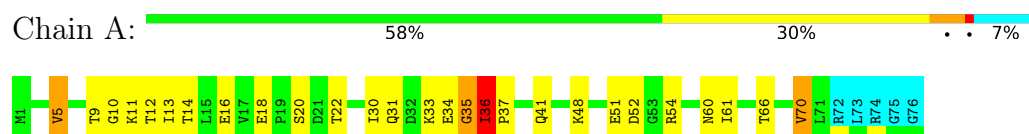
4.2.215 Score per residue for model 215

- Molecule 1: Ubiquitin



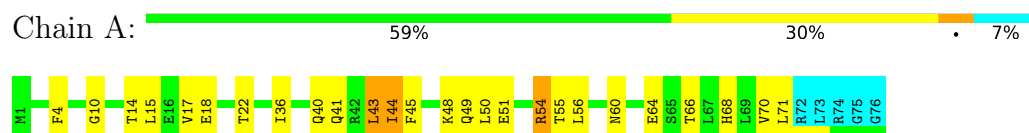
4.2.216 Score per residue for model 216

- Molecule 1: Ubiquitin



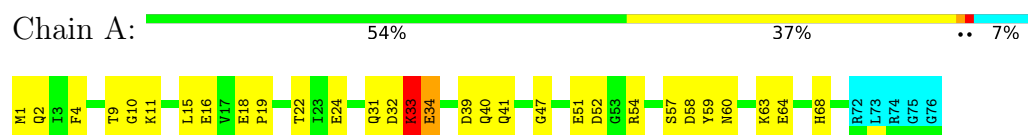
4.2.217 Score per residue for model 217

- Molecule 1: Ubiquitin



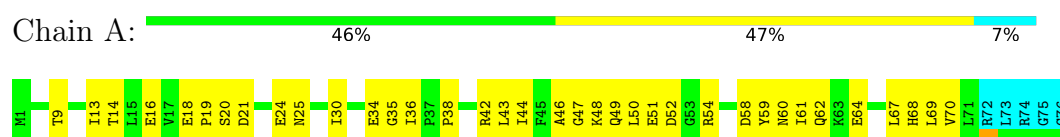
4.2.218 Score per residue for model 218

- Molecule 1: Ubiquitin



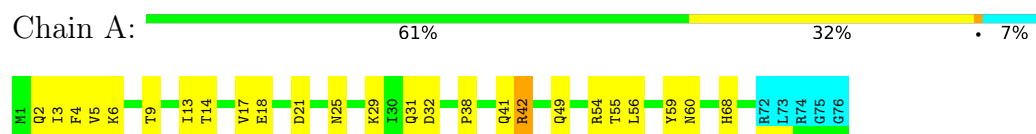
4.2.219 Score per residue for model 219

- Molecule 1: Ubiquitin



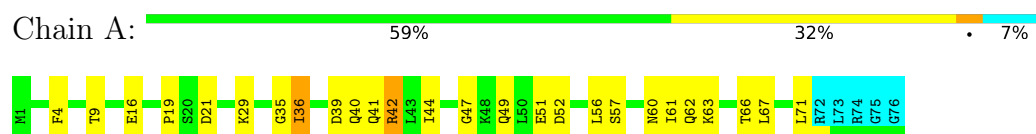
4.2.220 Score per residue for model 220

- Molecule 1: Ubiquitin



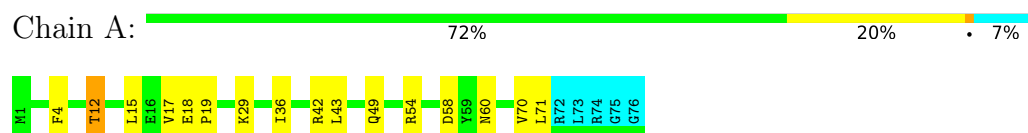
4.2.221 Score per residue for model 221

- Molecule 1: Ubiquitin



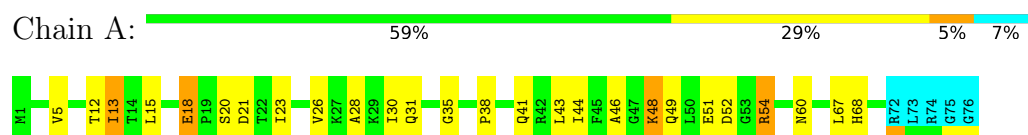
4.2.222 Score per residue for model 222

- Molecule 1: Ubiquitin



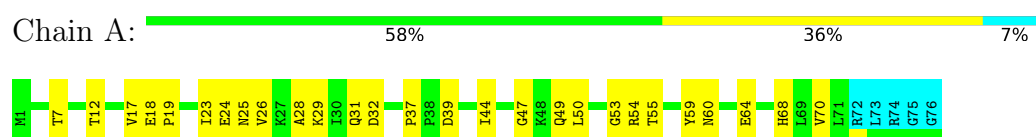
4.2.223 Score per residue for model 223

- Molecule 1: Ubiquitin



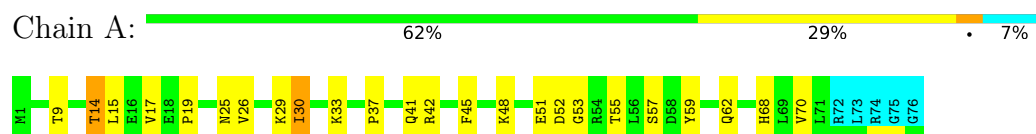
4.2.224 Score per residue for model 224

- Molecule 1: Ubiquitin



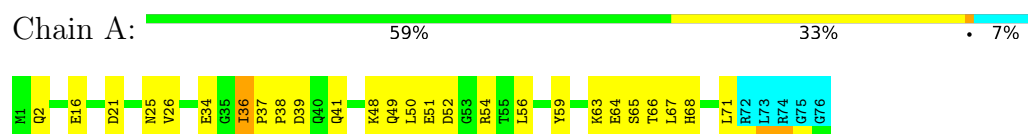
4.2.225 Score per residue for model 225

- Molecule 1: Ubiquitin



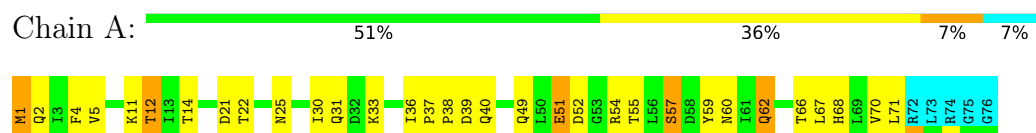
4.2.226 Score per residue for model 226

- Molecule 1: Ubiquitin



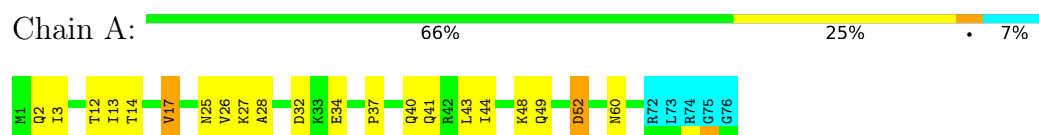
4.2.227 Score per residue for model 227

- Molecule 1: Ubiquitin



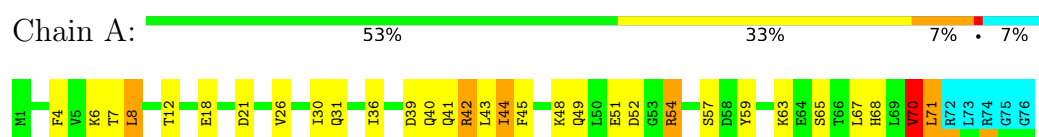
4.2.228 Score per residue for model 228

- Molecule 1: Ubiquitin



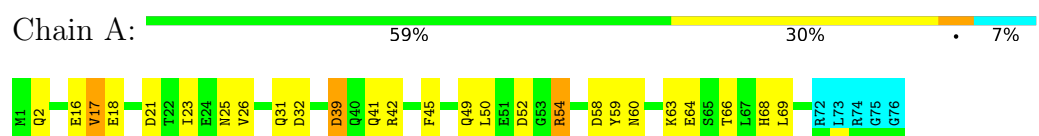
4.2.229 Score per residue for model 229

- Molecule 1: Ubiquitin



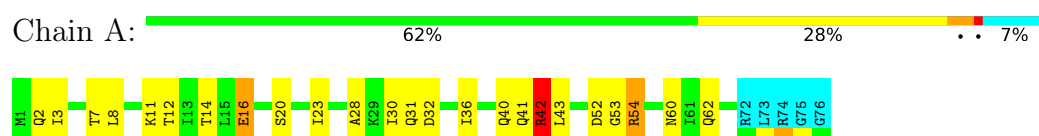
4.2.230 Score per residue for model 230

- Molecule 1: Ubiquitin



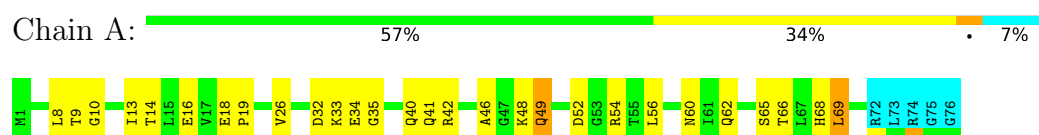
4.2.231 Score per residue for model 231

- Molecule 1: Ubiquitin



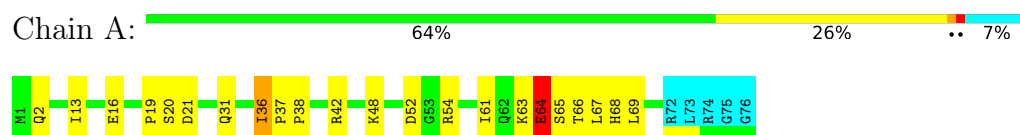
4.2.232 Score per residue for model 232

- Molecule 1: Ubiquitin



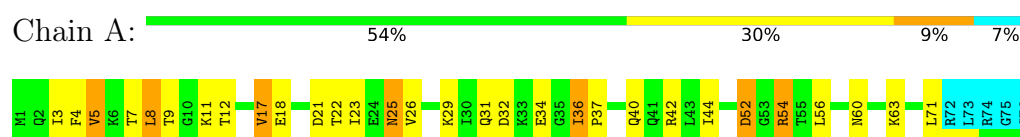
4.2.233 Score per residue for model 233

- Molecule 1: Ubiquitin



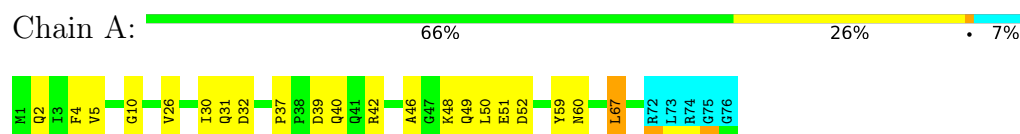
4.2.234 Score per residue for model 234

- Molecule 1: Ubiquitin



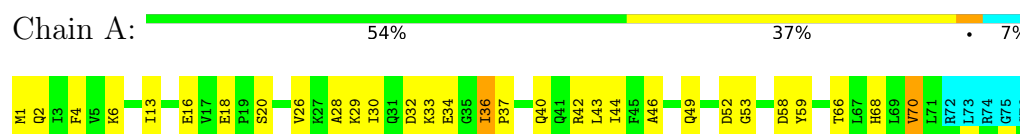
4.2.235 Score per residue for model 235

- Molecule 1: Ubiquitin



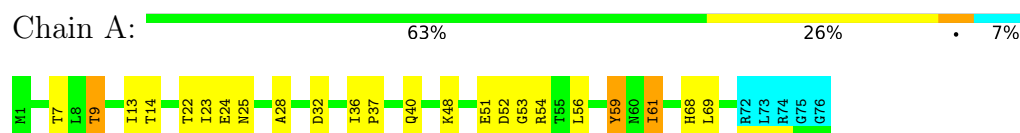
4.2.236 Score per residue for model 236

- Molecule 1: Ubiquitin



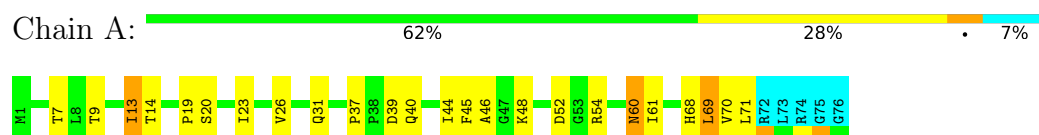
4.2.237 Score per residue for model 237

- Molecule 1: Ubiquitin



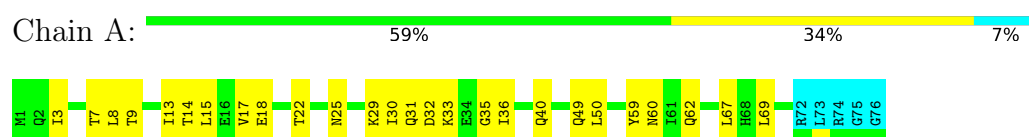
4.2.238 Score per residue for model 238

- Molecule 1: Ubiquitin



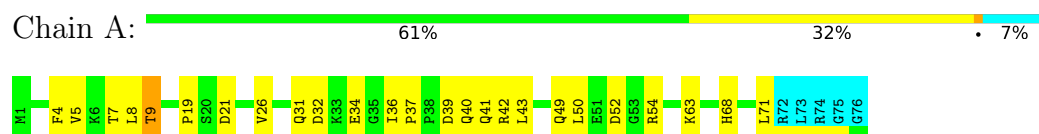
4.2.239 Score per residue for model 239

- Molecule 1: Ubiquitin



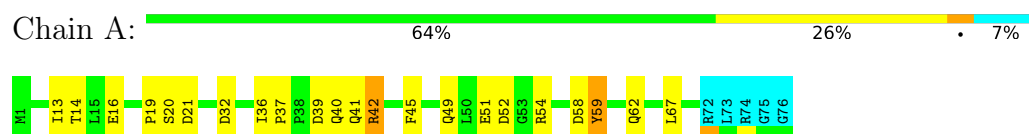
4.2.240 Score per residue for model 240

- Molecule 1: Ubiquitin



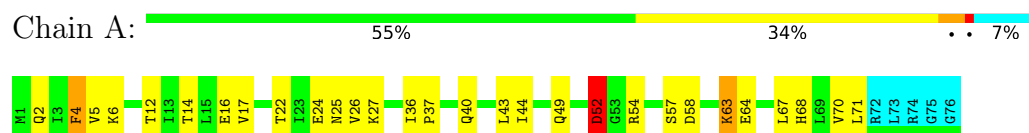
4.2.241 Score per residue for model 241

- Molecule 1: Ubiquitin



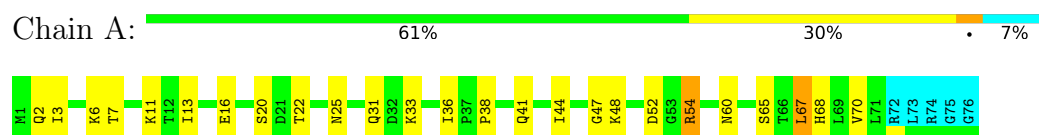
4.2.242 Score per residue for model 242

- Molecule 1: Ubiquitin



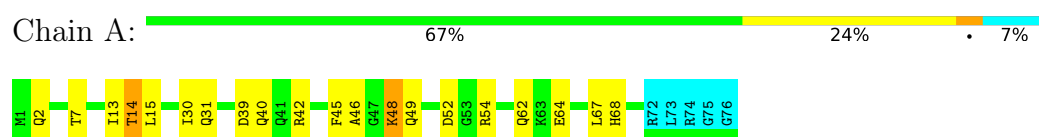
4.2.243 Score per residue for model 243

- Molecule 1: Ubiquitin



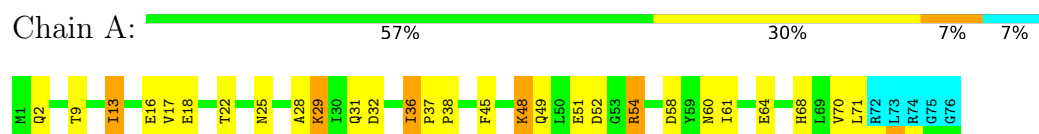
4.2.244 Score per residue for model 244

- Molecule 1: Ubiquitin



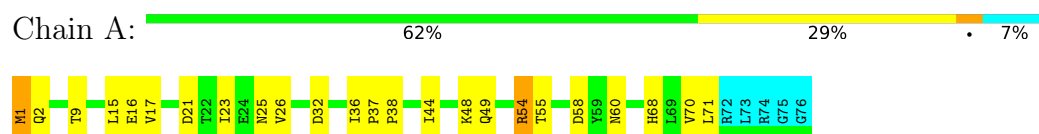
4.2.245 Score per residue for model 245

- Molecule 1: Ubiquitin



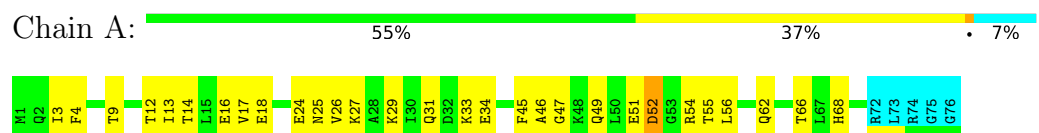
4.2.246 Score per residue for model 246

- Molecule 1: Ubiquitin



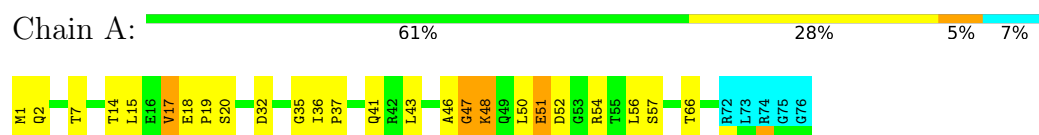
4.2.247 Score per residue for model 247

- Molecule 1: Ubiquitin



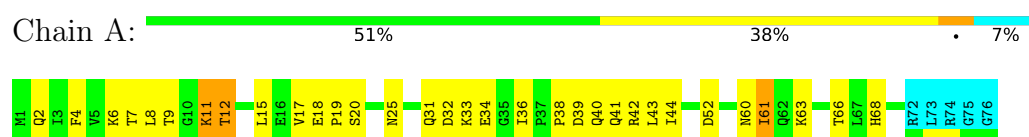
4.2.248 Score per residue for model 248

- Molecule 1: Ubiquitin



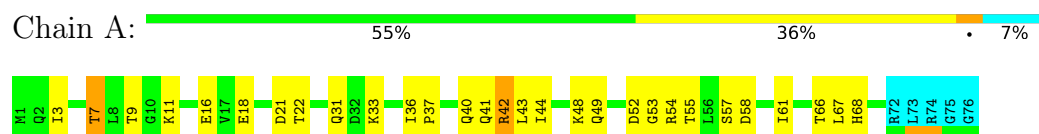
4.2.249 Score per residue for model 249

- Molecule 1: Ubiquitin



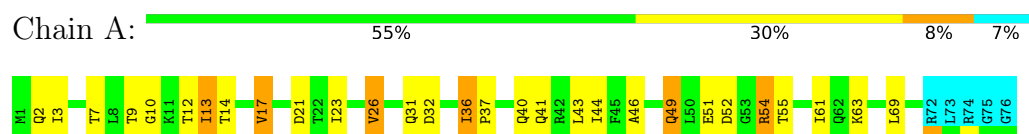
4.2.250 Score per residue for model 250

- Molecule 1: Ubiquitin



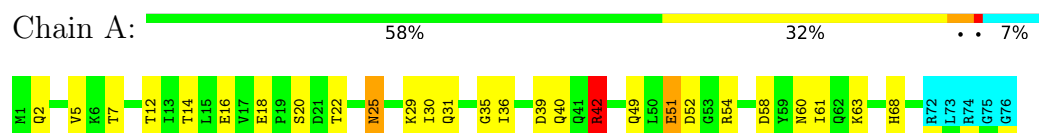
4.2.251 Score per residue for model 251

- Molecule 1: Ubiquitin



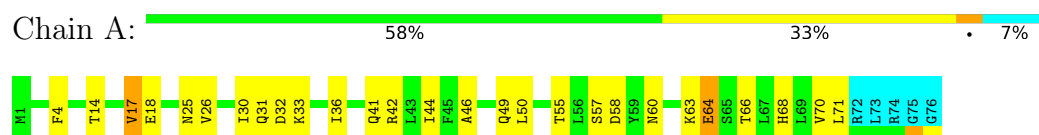
4.2.252 Score per residue for model 252

- Molecule 1: Ubiquitin



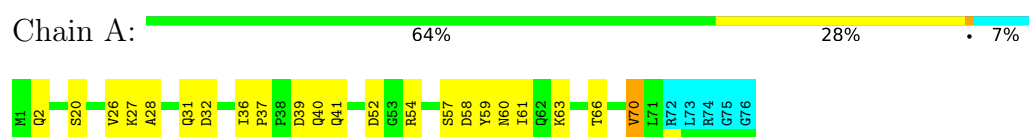
4.2.253 Score per residue for model 253

- Molecule 1: Ubiquitin



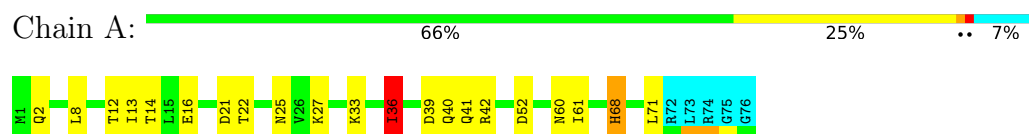
4.2.254 Score per residue for model 254

- Molecule 1: Ubiquitin



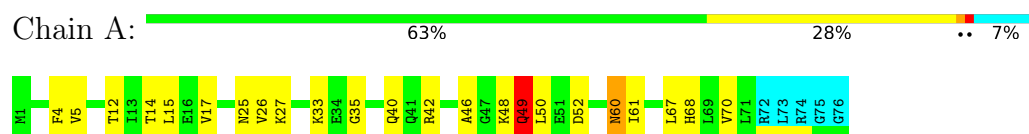
4.2.255 Score per residue for model 255

- Molecule 1: Ubiquitin



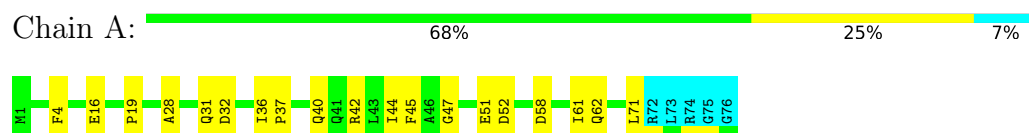
4.2.256 Score per residue for model 256

- Molecule 1: Ubiquitin



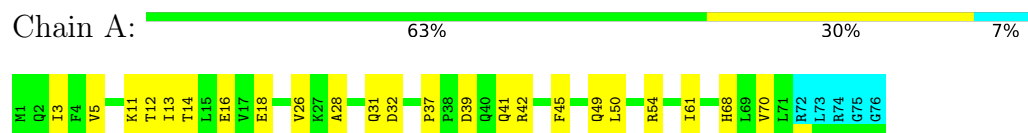
4.2.257 Score per residue for model 257

- Molecule 1: Ubiquitin



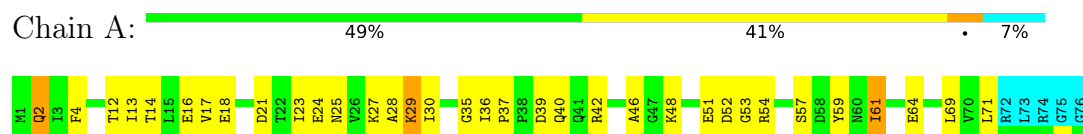
4.2.258 Score per residue for model 258

- Molecule 1: Ubiquitin



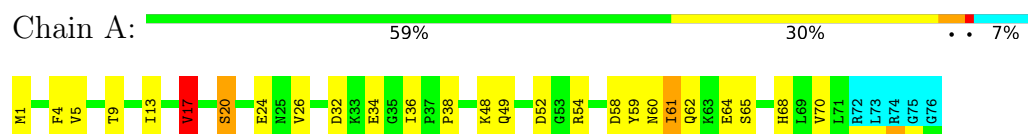
4.2.259 Score per residue for model 259

- Molecule 1: Ubiquitin



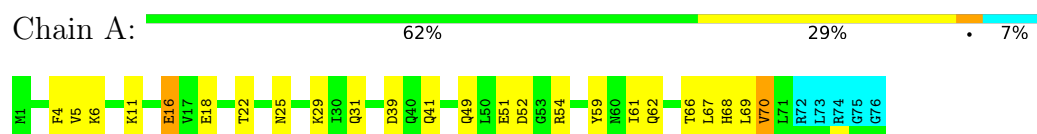
4.2.260 Score per residue for model 260

- Molecule 1: Ubiquitin



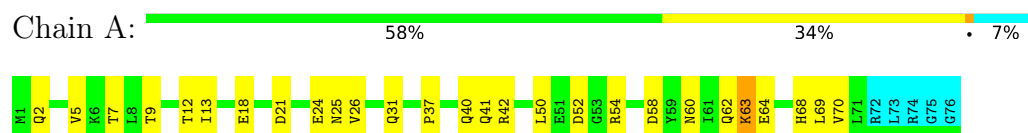
4.2.261 Score per residue for model 261

- Molecule 1: Ubiquitin



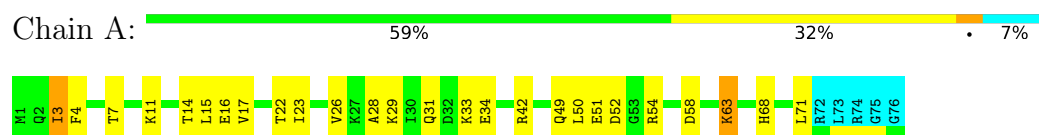
4.2.262 Score per residue for model 262

- Molecule 1: Ubiquitin



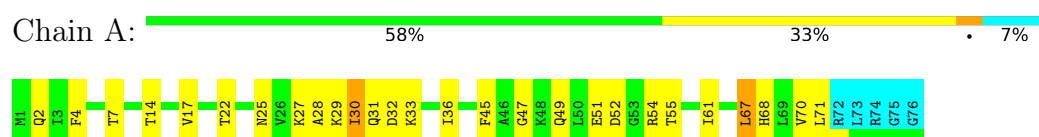
4.2.263 Score per residue for model 263

- Molecule 1: Ubiquitin



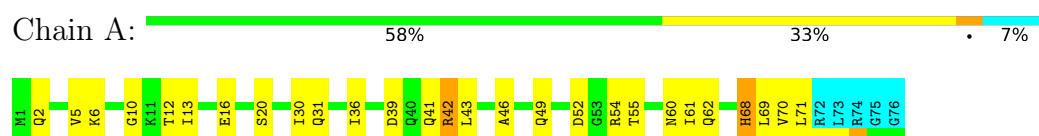
4.2.264 Score per residue for model 264

- Molecule 1: Ubiquitin



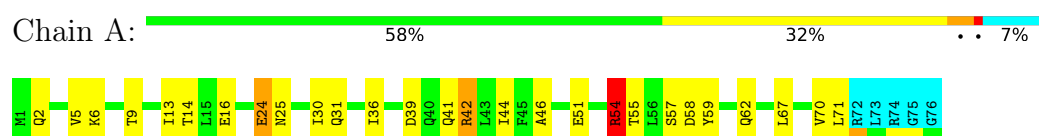
4.2.265 Score per residue for model 265

- Molecule 1: Ubiquitin



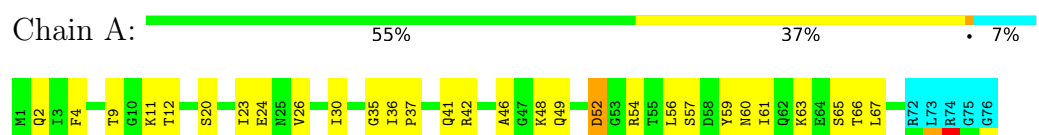
4.2.266 Score per residue for model 266

- Molecule 1: Ubiquitin



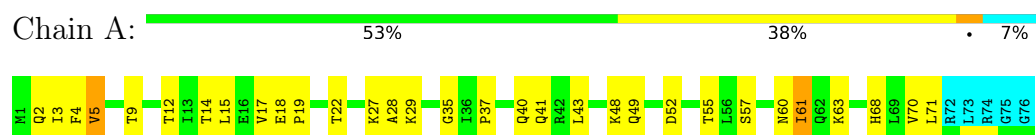
4.2.267 Score per residue for model 267

- Molecule 1: Ubiquitin



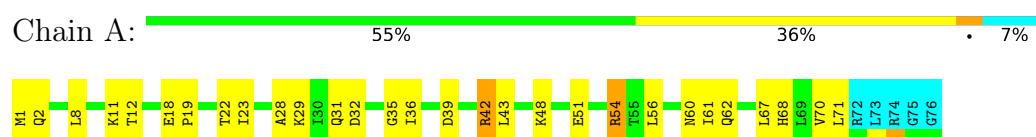
4.2.268 Score per residue for model 268

- Molecule 1: Ubiquitin



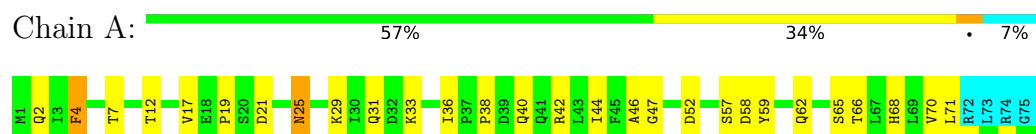
4.2.269 Score per residue for model 269

- Molecule 1: Ubiquitin



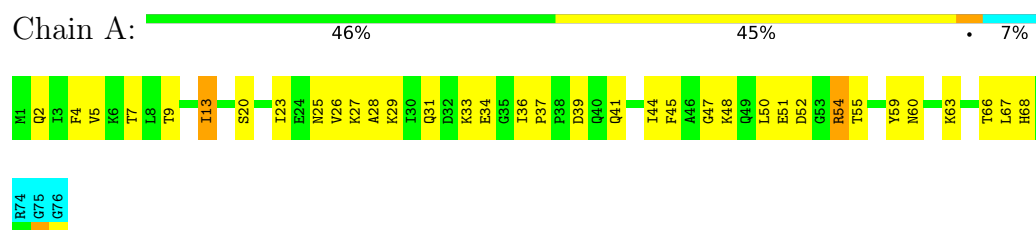
4.2.270 Score per residue for model 270

- Molecule 1: Ubiquitin



4.2.271 Score per residue for model 271

- Molecule 1: Ubiquitin



4.2.272 Score per residue for model 272

- Molecule 1: Ubiquitin





4.2.273 Score per residue for model 273

- Molecule 1: Ubiquitin



4.2.274 Score per residue for model 274

- Molecule 1: Ubiquitin



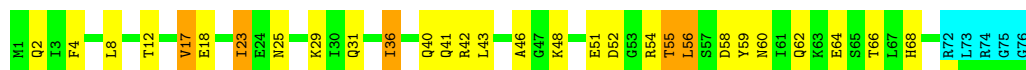
4.2.275 Score per residue for model 275

- Molecule 1: Ubiquitin



4.2.276 Score per residue for model 276

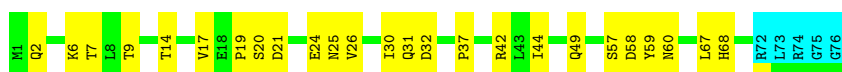
- Molecule 1: Ubiquitin



4.2.277 Score per residue for model 277

- Molecule 1: Ubiquitin





4.2.278 Score per residue for model 278

- Molecule 1: Ubiquitin



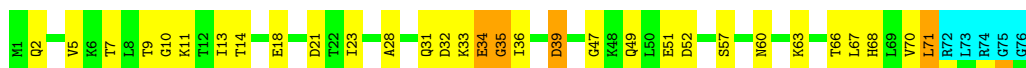
4.2.279 Score per residue for model 279

- Molecule 1: Ubiquitin



4.2.280 Score per residue for model 280

- Molecule 1: Ubiquitin



4.2.281 Score per residue for model 281

- Molecule 1: Ubiquitin



4.2.282 Score per residue for model 282

- Molecule 1: Ubiquitin





4.2.283 Score per residue for model 283

- Molecule 1: Ubiquitin

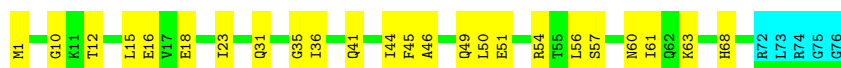
Chain A: 63% 28% 7%



4.2.284 Score per residue for model 284

- Molecule 1: Ubiquitin

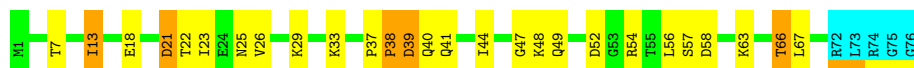
Chain A: 62% 32% 7%



4.2.285 Score per residue for model 285

- Molecule 1: Ubiquitin

Chain A: 58% 29% 7% 7%



4.2.286 Score per residue for model 286

- Molecule 1: Ubiquitin

Chain A: 64% 28% 7%



4.2.287 Score per residue for model 287

- Molecule 1: Ubiquitin

Chain A: 58% 33% 7%



4.2.288 Score per residue for model 288

- Molecule 1: Ubiquitin

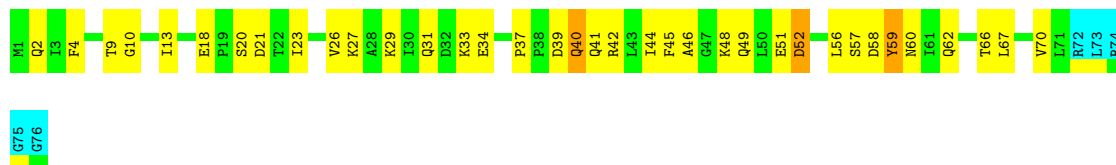
Chain A: 54% 37% 7%



4.2.289 Score per residue for model 289

- Molecule 1: Ubiquitin

Chain A: 46% 43% 7%



4.2.290 Score per residue for model 290

- Molecule 1: Ubiquitin

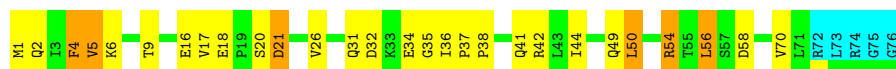
Chain A: 66% 26% 7%



4.2.291 Score per residue for model 291

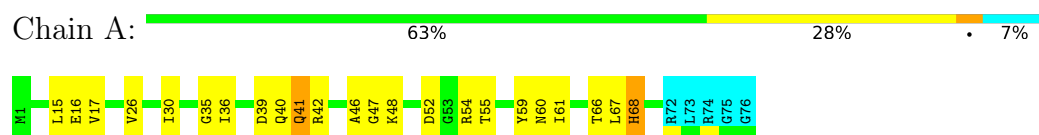
- Molecule 1: Ubiquitin

Chain A: 57% 29% 8% 7%



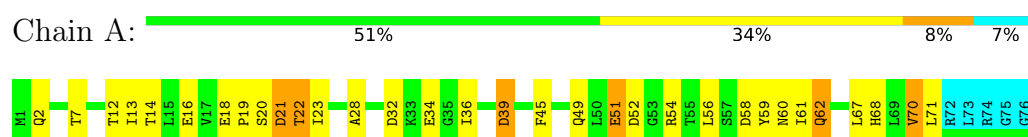
4.2.292 Score per residue for model 292

- Molecule 1: Ubiquitin



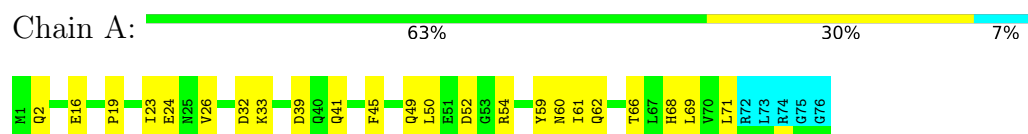
4.2.293 Score per residue for model 293

- Molecule 1: Ubiquitin



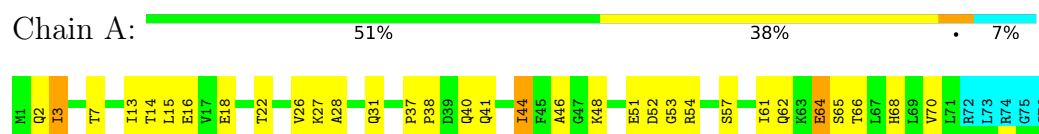
4.2.294 Score per residue for model 294

- Molecule 1: Ubiquitin



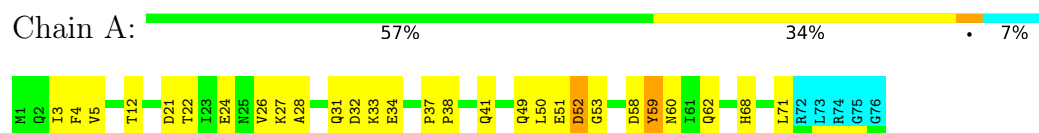
4.2.295 Score per residue for model 295

- Molecule 1: Ubiquitin



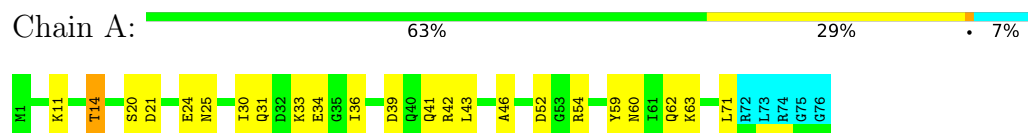
4.2.296 Score per residue for model 296

- Molecule 1: Ubiquitin



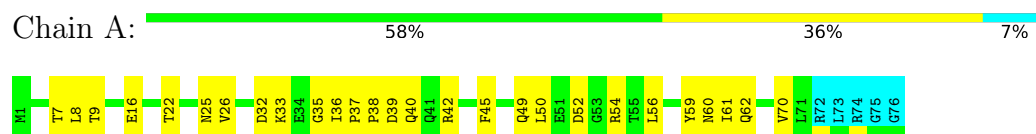
4.2.297 Score per residue for model 297

- Molecule 1: Ubiquitin



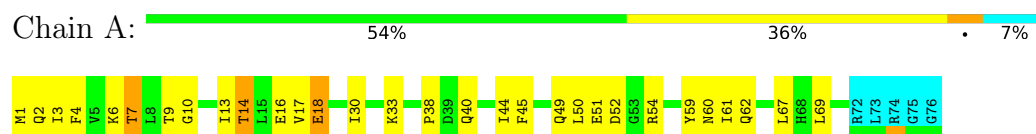
4.2.298 Score per residue for model 298

- Molecule 1: Ubiquitin



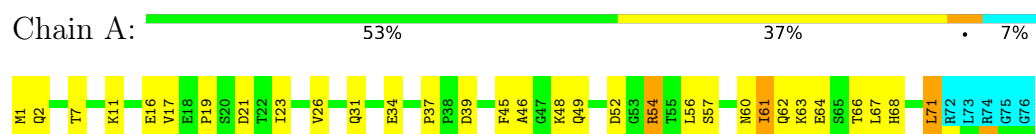
4.2.299 Score per residue for model 299

- Molecule 1: Ubiquitin



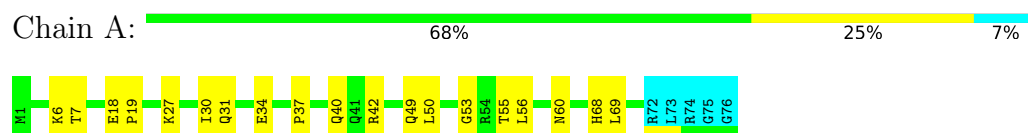
4.2.300 Score per residue for model 300

- Molecule 1: Ubiquitin



4.2.301 Score per residue for model 301

- Molecule 1: Ubiquitin



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 321 calculated structures, 301 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

Software name	Classification	Version
GROMOS	geometry optimization	
GROMOS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	426
Number of shifts mapped to atoms	426
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	42%

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.52±0.01	0±0/570 (0.0± 0.0%)	2.63±0.23	49±15/770 (6.3± 2.0%)
All	All	0.52	0/171570 (0.0%)	2.64	14628/231770 (6.3%)

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	2.9±2.1
All	All	0	877

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	35	GLY	CA-C-N	17.80	135.41	122.59	94	86
1	A	35	GLY	C-N-CA	17.80	135.41	122.59	94	86
1	A	32	ASP	CA-CB-CG	17.29	129.89	112.60	115	102
1	A	36	ILE	CA-C-O	-17.13	109.53	119.12	115	52
1	A	49	GLN	OE1-CD-NE2	-16.45	106.16	122.60	47	125
1	A	36	ILE	CA-C-N	15.83	131.06	119.66	42	90
1	A	36	ILE	C-N-CA	15.83	131.06	119.66	42	90
1	A	25	ASN	CA-CB-CG	15.80	128.40	112.60	65	104
1	A	26	VAL	CA-CB-CG1	14.82	135.60	110.40	55	32
1	A	25	ASN	OD1-CG-ND2	-14.42	108.18	122.60	83	57
1	A	57	SER	CA-C-O	-14.36	105.33	120.55	93	52
1	A	37	PRO	O-C-N	-14.28	114.44	121.15	130	44
1	A	61	ILE	CB-CA-C	14.22	126.59	111.23	46	69
1	A	52	ASP	CA-CB-CG	13.90	126.50	112.60	125	80
1	A	48	LYS	N-CA-C	13.75	131.31	108.90	256	76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	54	ARG	NE-CZ-NH2	13.72	131.55	119.20	11	66
1	A	14	THR	CA-C-N	13.71	142.25	123.05	99	46
1	A	14	THR	C-N-CA	13.71	142.25	123.05	99	46
1	A	2	GLN	OE1-CD-NE2	-13.54	109.06	122.60	76	111
1	A	52	ASP	N-CA-C	13.45	125.94	111.28	3	138
1	A	36	ILE	N-CA-C	13.43	120.18	108.63	10	46
1	A	42	ARG	CA-C-O	-13.12	105.72	120.81	146	43
1	A	62	GLN	OE1-CD-NE2	-13.04	109.56	122.60	270	115
1	A	37	PRO	N-CA-CB	13.01	109.98	103.22	46	88
1	A	55	THR	CA-C-N	12.98	137.31	120.44	103	47
1	A	55	THR	C-N-CA	12.98	137.31	120.44	103	47
1	A	61	ILE	N-CA-CB	12.97	124.86	110.72	95	21
1	A	58	ASP	CA-CB-CG	12.96	125.56	112.60	296	75
1	A	33	LYS	N-CA-C	12.84	124.97	110.97	111	44
1	A	28	ALA	N-CA-CB	12.84	129.16	110.16	22	131
1	A	21	ASP	CA-CB-CG	12.73	125.33	112.60	32	96
1	A	46	ALA	CB-CA-C	12.50	126.60	111.22	124	53
1	A	48	LYS	O-C-N	12.45	136.76	123.56	141	26
1	A	26	VAL	N-CA-CB	12.38	123.62	110.62	24	65
1	A	40	GLN	OE1-CD-NE2	-12.38	110.22	122.60	279	121
1	A	37	PRO	CA-C-N	12.37	132.10	119.24	109	102
1	A	37	PRO	C-N-CA	12.37	132.10	119.24	109	102
1	A	54	ARG	NH1-CZ-NH2	-12.33	103.27	119.30	279	42
1	A	67	LEU	O-C-N	-12.21	109.39	123.06	68	44
1	A	64	GLU	N-CA-CB	-11.89	100.61	114.17	81	24
1	A	60	ASN	CA-CB-CG	11.86	124.46	112.60	75	62
1	A	37	PRO	N-CA-C	11.85	121.84	110.47	137	46
1	A	12	THR	CA-C-O	-11.82	107.57	120.33	94	19
1	A	53	GLY	N-CA-C	11.79	127.49	114.40	112	21
1	A	2	GLN	CA-C-N	11.75	135.76	122.48	91	100
1	A	2	GLN	C-N-CA	11.75	135.76	122.48	91	100
1	A	65	SER	CA-C-N	11.74	138.30	121.50	110	40
1	A	65	SER	C-N-CA	11.74	138.30	121.50	110	40
1	A	60	ASN	OD1-CG-ND2	-11.67	110.93	122.60	284	101
1	A	19	PRO	N-CA-CB	11.63	114.57	103.52	27	58
1	A	45	PHE	CA-CB-CG	11.62	125.42	113.80	125	53
1	A	54	ARG	NE-CZ-NH1	11.60	133.10	121.50	45	43
1	A	51	GLU	CA-C-N	11.60	136.91	120.79	212	35
1	A	51	GLU	C-N-CA	11.60	136.91	120.79	212	35
1	A	51	GLU	CA-C-O	-11.54	108.00	120.80	10	18
1	A	55	THR	CA-C-O	-11.52	108.51	121.87	194	48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	50	LEU	N-CA-C	11.47	126.45	108.67	185	11
1	A	56	LEU	CA-C-O	-11.46	108.25	120.63	276	62
1	A	42	ARG	NE-CZ-NH2	11.41	129.47	119.20	106	52
1	A	68	HIS	CB-CA-C	11.33	128.77	110.19	115	22
1	A	70	VAL	CA-CB-CG2	11.33	129.66	110.40	118	30
1	A	34	GLU	CA-C-O	11.32	131.09	118.97	100	27
1	A	18	GLU	O-C-N	-11.31	113.39	121.65	44	32
1	A	17	VAL	CA-CB-CG1	11.25	129.53	110.40	51	46
1	A	26	VAL	CA-CB-CG2	11.18	129.40	110.40	151	97
1	A	29	LYS	CA-C-O	11.12	132.44	120.55	80	22
1	A	36	ILE	O-C-N	-11.10	113.67	121.55	148	30
1	A	27	LYS	CA-C-O	-11.09	108.79	120.55	87	108
1	A	13	ILE	CB-CA-C	11.00	126.39	110.33	78	35
1	A	31	GLN	OE1-CD-NE2	-10.97	111.63	122.60	213	91
1	A	37	PRO	CB-CA-C	10.96	121.47	111.17	1	23
1	A	38	PRO	CA-C-N	10.95	135.38	120.38	150	75
1	A	38	PRO	C-N-CA	10.95	135.38	120.38	150	75
1	A	22	THR	CA-CB-OG1	10.92	125.99	109.60	293	22
1	A	50	LEU	CA-C-O	-10.90	109.59	120.92	17	28
1	A	34	GLU	N-CA-C	10.88	126.73	113.23	11	33
1	A	61	ILE	N-CA-C	-10.87	94.54	108.89	12	31
1	A	58	ASP	CA-C-O	10.87	132.07	120.55	111	23
1	A	14	THR	CA-CB-CG2	10.84	128.93	110.50	192	24
1	A	12	THR	CA-CB-OG1	10.77	125.76	109.60	249	32
1	A	71	LEU	CB-CA-C	10.76	127.90	109.51	286	32
1	A	64	GLU	CA-C-O	10.73	129.73	119.00	27	25
1	A	44	ILE	N-CA-C	10.68	125.30	108.85	121	29
1	A	42	ARG	CD-NE-CZ	10.60	139.24	124.40	143	18
1	A	34	GLU	N-CA-CB	-10.53	96.99	111.00	121	14
1	A	8	LEU	N-CA-C	10.51	125.20	111.75	9	22
1	A	51	GLU	O-C-N	10.48	135.42	123.27	34	17
1	A	51	GLU	CB-CG-CD	-10.47	94.80	112.60	90	17
1	A	30	ILE	CA-C-N	10.45	134.70	120.38	58	64
1	A	30	ILE	C-N-CA	10.45	134.70	120.38	58	64
1	A	25	ASN	CA-C-N	10.42	133.90	120.56	145	9
1	A	25	ASN	C-N-CA	10.42	133.90	120.56	145	9
1	A	27	LYS	O-C-N	10.41	133.16	122.12	74	14
1	A	12	THR	CA-C-N	10.37	136.48	123.10	102	44
1	A	12	THR	C-N-CA	10.37	136.48	123.10	102	44
1	A	17	VAL	N-CA-C	10.34	121.14	108.53	147	56
1	A	24	GLU	N-CA-C	10.28	122.07	111.07	106	23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	41	GLN	OE1-CD-NE2	-10.19	112.41	122.60	181	76
1	A	70	VAL	O-C-N	-10.09	112.38	122.97	54	34
1	A	55	THR	CA-CB-OG1	10.09	124.73	109.60	132	16
1	A	64	GLU	N-CA-C	10.08	125.17	113.38	95	66
1	A	16	GLU	CB-CA-C	10.04	126.66	110.19	247	35
1	A	32	ASP	CA-C-N	9.97	133.81	120.65	260	12
1	A	32	ASP	C-N-CA	9.97	133.81	120.65	260	12
1	A	68	HIS	CA-C-N	9.96	135.79	122.84	171	43
1	A	68	HIS	C-N-CA	9.96	135.79	122.84	171	43
1	A	14	THR	N-CA-C	9.96	126.00	109.46	255	21
1	A	16	GLU	CA-C-N	9.96	135.56	122.51	219	68
1	A	16	GLU	C-N-CA	9.96	135.56	122.51	219	68
1	A	65	SER	CA-C-O	-9.95	110.92	121.87	65	28
1	A	25	ASN	N-CA-C	-9.95	100.44	111.28	91	32
1	A	5	VAL	CA-C-O	9.95	130.73	120.39	42	30
1	A	39	ASP	CA-CB-CG	-9.91	102.69	112.60	50	46
1	A	42	ARG	CA-C-N	9.89	136.89	123.05	207	40
1	A	42	ARG	C-N-CA	9.89	136.89	123.05	207	40
1	A	16	GLU	CA-C-O	9.87	130.81	120.54	107	36
1	A	28	ALA	N-CA-C	9.84	122.08	111.36	46	32
1	A	56	LEU	CA-C-N	9.82	133.80	120.54	276	57
1	A	56	LEU	C-N-CA	9.82	133.80	120.54	276	57
1	A	56	LEU	N-CA-CB	-9.82	95.31	109.94	59	3
1	A	24	GLU	CA-C-N	9.79	133.16	120.44	107	72
1	A	24	GLU	C-N-CA	9.79	133.16	120.44	107	72
1	A	13	ILE	CA-C-O	-9.79	113.95	121.68	117	31
1	A	25	ASN	CA-C-O	-9.78	110.18	120.55	71	33
1	A	63	LYS	CA-C-O	9.76	131.98	121.44	28	22
1	A	5	VAL	O-C-N	-9.76	113.57	123.03	131	56
1	A	4	PHE	CA-CB-CG	-9.76	104.04	113.80	40	43
1	A	20	SER	N-CA-C	9.75	125.00	113.20	129	31
1	A	29	LYS	N-CA-C	9.74	121.97	111.36	2	19
1	A	67	LEU	CA-C-N	9.73	136.45	122.24	95	25
1	A	67	LEU	C-N-CA	9.73	136.45	122.24	95	25
1	A	18	GLU	CA-C-N	9.71	130.38	119.32	145	51
1	A	18	GLU	C-N-CA	9.71	130.38	119.32	145	51
1	A	42	ARG	NH1-CZ-NH2	-9.70	106.69	119.30	215	22
1	A	40	GLN	CA-C-N	9.70	134.64	120.87	11	71
1	A	40	GLN	C-N-CA	9.70	134.64	120.87	11	71
1	A	54	ARG	CB-CA-C	9.69	125.91	109.53	46	29
1	A	57	SER	CA-C-N	9.63	133.19	120.28	54	58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	57	SER	C-N-CA	9.63	133.19	120.28	54	58
1	A	44	ILE	CA-CB-CG2	9.63	126.87	110.50	59	47
1	A	35	GLY	O-C-N	-9.63	110.38	122.41	60	34
1	A	55	THR	O-C-N	-9.61	111.89	122.85	147	28
1	A	2	GLN	N-CA-CB	9.60	125.83	110.46	211	5
1	A	17	VAL	CA-CB-CG2	9.59	126.70	110.40	130	26
1	A	30	ILE	O-C-N	-9.55	112.55	121.91	42	32
1	A	66	THR	N-CA-C	9.55	124.94	109.76	91	41
1	A	18	GLU	CB-CG-CD	9.54	128.82	112.60	137	14
1	A	65	SER	O-C-N	-9.54	111.78	122.84	4	28
1	A	42	ARG	N-CA-CB	9.54	124.61	110.49	90	7
1	A	23	ILE	N-CA-C	9.52	120.33	110.62	263	21
1	A	64	GLU	CA-C-N	9.51	135.10	121.02	130	7
1	A	64	GLU	C-N-CA	9.51	135.10	121.02	130	7
1	A	63	LYS	CA-C-N	9.50	136.04	122.08	6	42
1	A	63	LYS	C-N-CA	9.50	136.04	122.08	6	42
1	A	50	LEU	O-C-N	9.50	134.05	123.13	39	20
1	A	23	ILE	O-C-N	-9.49	112.29	121.87	70	4
1	A	9	THR	N-CA-C	9.48	124.67	113.20	34	38
1	A	59	TYR	CA-C-N	9.44	135.51	122.19	254	38
1	A	59	TYR	C-N-CA	9.44	135.51	122.19	254	38
1	A	68	HIS	CA-CB-CG	-9.40	104.40	113.80	207	54
1	A	48	LYS	CA-C-O	9.40	130.67	120.43	128	31
1	A	47	GLY	CA-C-N	9.39	136.22	122.99	163	27
1	A	47	GLY	C-N-CA	9.39	136.22	122.99	163	27
1	A	38	PRO	N-CA-CB	9.38	113.46	103.52	91	25
1	A	3	ILE	CA-C-O	9.36	130.90	121.63	183	19
1	A	17	VAL	CA-C-O	-9.35	111.37	121.28	10	39
1	A	39	ASP	CA-C-O	-9.34	109.54	120.10	25	21
1	A	60	ASN	CB-CA-C	9.32	125.41	111.80	39	61
1	A	33	LYS	CB-CG-CD	9.32	132.73	111.30	142	23
1	A	36	ILE	N-CA-CB	9.30	120.18	110.23	54	23
1	A	53	GLY	CA-C-N	9.24	135.22	122.19	30	13
1	A	53	GLY	C-N-CA	9.24	135.22	122.19	30	13
1	A	67	LEU	CB-CA-C	9.24	127.98	110.51	274	10
1	A	54	ARG	CD-NE-CZ	9.24	137.34	124.40	267	41
1	A	55	THR	N-CA-C	9.24	123.02	110.55	114	11
1	A	61	ILE	CB-CG1-CD1	9.23	133.18	113.80	143	29
1	A	52	ASP	N-CA-CB	-9.21	96.72	110.07	298	33
1	A	22	THR	N-CA-C	9.20	123.47	110.50	10	24
1	A	49	GLN	CB-CA-C	9.20	124.83	109.84	154	23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	48	LYS	CA-C-N	9.20	133.82	120.95	114	19
1	A	48	LYS	C-N-CA	9.20	133.82	120.95	114	19
1	A	17	VAL	O-C-N	-9.19	112.84	123.04	103	24
1	A	54	ARG	CA-C-O	9.17	132.65	121.56	133	17
1	A	19	PRO	CA-C-N	9.15	133.46	120.28	34	31
1	A	19	PRO	C-N-CA	9.15	133.46	120.28	34	31
1	A	9	THR	CA-CB-OG1	9.15	123.32	109.60	177	19
1	A	14	THR	CA-CB-OG1	9.14	123.31	109.60	242	18
1	A	68	HIS	CA-C-O	-9.13	110.91	121.68	124	27
1	A	28	ALA	CA-C-O	9.12	130.09	120.42	196	21
1	A	7	THR	CA-C-N	9.07	133.63	120.38	202	22
1	A	7	THR	C-N-CA	9.07	133.63	120.38	202	22
1	A	10	GLY	CA-C-O	-9.07	108.94	119.01	15	13
1	A	66	THR	CA-CB-CG2	9.05	125.88	110.50	232	44
1	A	60	ASN	CA-C-N	9.04	132.61	122.22	44	16
1	A	60	ASN	C-N-CA	9.04	132.61	122.22	44	16
1	A	68	HIS	CB-CG-CD2	-9.03	119.46	131.20	226	127
1	A	42	ARG	CB-CA-C	9.03	125.45	109.65	102	41
1	A	10	GLY	CA-C-N	9.02	133.68	120.87	90	36
1	A	10	GLY	C-N-CA	9.02	133.68	120.87	90	36
1	A	70	VAL	CA-C-N	9.02	135.44	123.00	89	21
1	A	70	VAL	C-N-CA	9.02	135.44	123.00	89	21
1	A	26	VAL	CA-C-N	9.00	132.34	120.28	29	43
1	A	26	VAL	C-N-CA	9.00	132.34	120.28	29	43
1	A	7	THR	CA-CB-CG2	8.98	125.77	110.50	51	29
1	A	68	HIS	CG-CD2-NE2	-8.98	98.22	107.20	301	4
1	A	54	ARG	O-C-N	-8.98	112.89	122.94	32	35
1	A	62	GLN	CA-C-O	8.97	133.28	121.89	35	10
1	A	26	VAL	CA-C-O	-8.96	110.51	120.46	106	20
1	A	36	ILE	CA-CB-CG1	8.96	125.63	110.40	174	38
1	A	50	LEU	CA-C-N	8.95	134.30	121.50	291	35
1	A	50	LEU	C-N-CA	8.95	134.30	121.50	291	35
1	A	5	VAL	N-CA-CB	8.94	121.67	111.21	50	23
1	A	49	GLN	CA-C-N	8.87	133.33	120.82	256	29
1	A	49	GLN	C-N-CA	8.87	133.33	120.82	256	29
1	A	70	VAL	CB-CA-C	8.84	124.43	110.82	216	23
1	A	54	ARG	N-CA-C	8.83	123.81	109.59	61	40
1	A	59	TYR	N-CA-C	8.83	124.11	113.16	259	23
1	A	66	THR	CA-C-O	8.82	129.59	120.24	11	15
1	A	31	GLN	CA-C-N	8.81	132.45	120.38	173	56
1	A	31	GLN	C-N-CA	8.81	132.45	120.38	173	56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	29	LYS	CB-CG-CD	8.80	131.53	111.30	33	1
1	A	23	ILE	CB-CA-C	8.79	123.56	112.04	84	14
1	A	1	MET	CA-C-N	8.79	133.35	120.87	121	14
1	A	1	MET	C-N-CA	8.79	133.35	120.87	121	14
1	A	69	LEU	CA-C-N	8.75	135.05	122.45	11	19
1	A	69	LEU	C-N-CA	8.75	135.05	122.45	11	19
1	A	11	LYS	CA-CB-CG	8.72	131.55	114.10	81	13
1	A	33	LYS	O-C-N	8.72	131.05	122.07	62	17
1	A	65	SER	N-CA-C	8.72	122.94	109.60	10	20
1	A	4	PHE	CA-C-N	8.71	134.68	123.10	274	15
1	A	4	PHE	C-N-CA	8.71	134.68	123.10	274	15
1	A	55	THR	N-CA-CB	8.70	124.81	110.63	130	14
1	A	61	ILE	CA-C-O	-8.68	111.81	121.36	288	12
1	A	55	THR	CA-CB-CG2	8.67	125.24	110.50	276	20
1	A	64	GLU	O-C-N	-8.66	113.33	121.56	27	10
1	A	42	ARG	NE-CZ-NH1	8.64	130.14	121.50	89	24
1	A	10	GLY	N-CA-C	8.63	126.14	114.92	46	10
1	A	2	GLN	CA-C-O	-8.63	110.48	120.49	2	20
1	A	29	LYS	O-C-N	-8.62	112.33	122.15	70	6
1	A	41	GLN	CB-CA-C	-8.62	95.83	110.22	291	9
1	A	60	ASN	N-CA-C	8.61	123.00	111.30	288	18
1	A	44	ILE	O-C-N	-8.60	113.91	123.20	152	29
1	A	18	GLU	CB-CA-C	8.59	121.86	108.63	299	39
1	A	66	THR	CB-CA-C	-8.59	96.91	110.14	125	28
1	A	11	LYS	CA-C-N	8.59	135.10	122.99	198	24
1	A	11	LYS	C-N-CA	8.59	135.10	122.99	198	24
1	A	71	LEU	CA-C-N	8.57	136.08	123.13	18	15
1	A	71	LEU	C-N-CA	8.57	136.08	123.13	18	15
1	A	7	THR	CA-C-O	-8.57	112.08	121.94	73	25
1	A	49	GLN	CG-CD-NE2	8.56	129.24	116.40	102	20
1	A	2	GLN	N-CA-C	8.56	123.80	109.76	66	29
1	A	30	ILE	CA-C-O	-8.54	112.07	120.95	21	28
1	A	25	ASN	O-C-N	-8.47	113.14	122.12	46	17
1	A	63	LYS	CG-CD-CE	8.47	130.78	111.30	60	7
1	A	45	PHE	CA-C-O	-8.46	110.13	120.54	87	17
1	A	30	ILE	CA-CB-CG1	8.46	124.79	110.40	84	9
1	A	31	GLN	N-CA-C	-8.42	102.04	111.14	181	18
1	A	57	SER	N-CA-C	8.42	120.46	111.28	204	46
1	A	6	LYS	CB-CA-C	8.42	123.62	109.48	66	24
1	A	39	ASP	N-CA-C	8.40	122.63	112.38	273	22
1	A	4	PHE	CA-C-O	-8.39	111.62	121.11	205	14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	34	GLU	O-C-N	-8.38	112.55	122.27	184	24
1	A	57	SER	N-CA-CB	8.38	122.57	110.16	115	9
1	A	34	GLU	CB-CG-CD	-8.37	98.37	112.60	109	17
1	A	7	THR	N-CA-C	8.37	121.40	110.43	152	29
1	A	57	SER	O-C-N	-8.37	110.91	122.46	122	23
1	A	48	LYS	CB-CG-CD	8.37	130.55	111.30	148	12
1	A	63	LYS	CB-CA-C	8.36	122.38	109.84	119	6
1	A	39	ASP	O-C-N	-8.34	111.26	122.43	280	28
1	A	58	ASP	CB-CA-C	8.34	124.63	110.79	204	12
1	A	4	PHE	O-C-N	-8.34	113.44	123.19	55	18
1	A	56	LEU	N-CA-C	8.33	121.41	111.33	234	20
1	A	18	GLU	CA-C-O	-8.30	111.06	120.03	140	26
1	A	68	HIS	N-CA-C	8.29	121.92	108.41	175	22
1	A	47	GLY	CA-C-O	-8.29	110.74	118.95	33	19
1	A	31	GLN	CA-C-O	-8.28	110.74	120.10	149	50
1	A	62	GLN	O-C-N	-8.27	113.68	123.03	122	4
1	A	26	VAL	CB-CA-C	-8.25	100.83	112.22	46	47
1	A	44	ILE	CB-CA-C	8.23	122.81	110.63	112	40
1	A	58	ASP	CA-C-N	8.23	137.26	121.54	59	19
1	A	58	ASP	C-N-CA	8.23	137.26	121.54	59	19
1	A	23	ILE	CA-C-O	-8.23	111.58	120.47	16	31
1	A	12	THR	CA-CB-CG2	8.22	124.48	110.50	79	27
1	A	70	VAL	N-CA-CB	-8.22	100.07	111.25	64	10
1	A	22	THR	O-C-N	-8.22	113.16	122.86	133	24
1	A	49	GLN	CA-C-O	-8.22	112.60	121.56	219	32
1	A	49	GLN	O-C-N	8.21	132.70	123.01	66	15
1	A	57	SER	CB-CA-C	-8.21	97.17	110.79	204	6
1	A	5	VAL	N-CA-C	8.20	119.65	108.17	58	22
1	A	48	LYS	N-CA-CB	8.19	123.41	110.55	238	20
1	A	62	GLN	N-CA-CB	-8.19	98.77	111.05	23	9
1	A	61	ILE	CA-C-N	8.18	138.47	122.03	59	9
1	A	61	ILE	C-N-CA	8.18	138.47	122.03	59	9
1	A	36	ILE	CB-CA-C	8.18	119.12	110.37	264	22
1	A	13	ILE	N-CA-CB	8.17	122.69	111.41	271	11
1	A	15	LEU	CB-CA-C	8.16	124.06	109.38	131	9
1	A	50	LEU	CB-CA-C	8.14	123.82	110.22	143	33
1	A	43	LEU	CD1-CG-CD2	-8.14	92.89	110.80	196	13
1	A	51	GLU	N-CA-C	8.13	122.66	109.40	188	31
1	A	1	MET	CA-CB-CG	8.12	130.34	114.10	103	16
1	A	15	LEU	CA-C-N	8.11	133.38	122.84	107	12
1	A	15	LEU	C-N-CA	8.11	133.38	122.84	107	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	13	ILE	CA-C-N	8.08	133.58	122.19	244	10
1	A	13	ILE	C-N-CA	8.08	133.58	122.19	244	10
1	A	41	GLN	N-CA-CB	-8.08	96.75	109.19	37	5
1	A	33	LYS	CA-C-N	8.07	135.88	121.92	7	30
1	A	33	LYS	C-N-CA	8.07	135.88	121.92	7	30
1	A	62	GLN	CG-CD-NE2	8.06	128.50	116.40	175	23
1	A	5	VAL	CB-CA-C	8.06	122.22	110.77	210	23
1	A	41	GLN	CA-C-N	8.06	134.13	122.77	125	11
1	A	41	GLN	C-N-CA	8.06	134.13	122.77	125	11
1	A	68	HIS	ND1-CG-CD2	8.06	114.16	106.10	301	20
1	A	44	ILE	CA-CB-CG1	8.05	124.08	110.40	205	46
1	A	49	GLN	N-CA-C	-8.03	97.92	109.96	83	17
1	A	46	ALA	CA-C-N	8.02	135.97	121.85	170	15
1	A	46	ALA	C-N-CA	8.02	135.97	121.85	170	15
1	A	26	VAL	N-CA-C	8.02	118.81	110.72	49	21
1	A	4	PHE	N-CA-C	-8.01	96.35	109.40	168	29
1	A	23	ILE	N-CA-CB	-8.01	100.46	110.47	102	5
1	A	41	GLN	N-CA-C	8.00	121.44	108.63	45	21
1	A	34	GLU	CA-C-N	7.98	133.64	121.51	141	14
1	A	34	GLU	C-N-CA	7.98	133.64	121.51	141	14
1	A	27	LYS	CA-C-N	-7.98	107.39	120.72	74	10
1	A	27	LYS	C-N-CA	-7.98	107.39	120.72	74	10
1	A	32	ASP	N-CA-C	7.96	119.95	111.28	23	24
1	A	27	LYS	CB-CA-C	-7.95	97.34	110.85	131	7
1	A	23	ILE	CB-CG1-CD1	7.93	130.46	113.80	64	12
1	A	1	MET	CB-CA-C	7.93	125.18	110.10	72	6
1	A	43	LEU	CB-CA-C	7.93	123.32	110.16	236	23
1	A	68	HIS	N-CA-CB	-7.91	97.39	110.68	243	19
1	A	61	ILE	O-C-N	-7.88	114.00	122.83	53	29
1	A	71	LEU	N-CA-C	7.88	122.08	109.24	122	16
1	A	32	ASP	CA-C-O	-7.88	112.12	120.63	119	17
1	A	16	GLU	O-C-N	-7.87	114.00	123.29	95	15
1	A	26	VAL	CG1-CB-CG2	-7.87	93.49	110.80	232	53
1	A	58	ASP	O-C-N	-7.86	113.78	122.12	145	15
1	A	12	THR	OG1-CB-CG2	-7.84	93.62	109.30	10	12
1	A	29	LYS	CA-C-N	7.84	131.55	120.42	198	23
1	A	29	LYS	C-N-CA	7.84	131.55	120.42	198	23
1	A	60	ASN	O-C-N	-7.84	112.78	122.57	281	10
1	A	11	LYS	N-CA-CB	-7.83	98.23	110.06	5	11
1	A	44	ILE	CA-C-N	7.83	135.42	122.73	139	18
1	A	44	ILE	C-N-CA	7.83	135.42	122.73	139	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	11	LYS	CA-C-O	7.83	130.48	121.47	59	13
1	A	59	TYR	CA-C-O	-7.83	110.35	119.59	36	14
1	A	11	LYS	CB-CG-CD	7.82	129.29	111.30	93	4
1	A	48	LYS	CA-CB-CG	7.82	129.73	114.10	137	10
1	A	41	GLN	O-C-N	-7.81	113.41	123.02	33	14
1	A	36	ILE	CB-CG1-CD1	7.81	130.20	113.80	63	5
1	A	13	ILE	CA-CB-CG1	7.80	123.67	110.40	34	27
1	A	67	LEU	N-CA-C	7.80	122.55	109.76	2	2
1	A	42	ARG	O-C-N	-7.80	113.76	123.27	20	8
1	A	40	GLN	O-C-N	-7.79	110.86	122.39	100	26
1	A	45	PHE	N-CA-CB	-7.79	97.73	110.81	174	7
1	A	66	THR	CA-CB-OG1	-7.79	97.92	109.60	270	16
1	A	15	LEU	N-CA-C	7.78	122.46	108.69	239	17
1	A	27	LYS	N-CA-C	-7.76	102.82	111.28	29	14
1	A	5	VAL	CA-C-N	7.76	133.13	122.19	91	26
1	A	5	VAL	C-N-CA	7.76	133.13	122.19	91	26
1	A	43	LEU	CA-C-N	7.75	133.10	123.10	145	18
1	A	43	LEU	C-N-CA	7.75	133.10	123.10	145	18
1	A	44	ILE	CA-C-O	7.75	128.69	120.48	150	10
1	A	14	THR	O-C-N	7.74	132.14	123.16	13	19
1	A	35	GLY	CA-C-O	7.73	128.56	119.13	60	20
1	A	18	GLU	N-CA-C	7.72	120.94	110.29	171	16
1	A	60	ASN	CA-C-O	7.72	130.73	121.08	64	13
1	A	39	ASP	N-CA-CB	-7.71	98.32	110.28	140	19
1	A	30	ILE	CB-CG1-CD1	7.71	129.98	113.80	45	47
1	A	13	ILE	O-C-N	7.71	131.00	123.14	118	16
1	A	32	ASP	CB-CA-C	7.69	123.93	110.85	57	7
1	A	60	ASN	N-CA-CB	-7.69	100.61	112.30	165	8
1	A	24	GLU	O-C-N	-7.67	113.41	122.15	40	30
1	A	12	THR	CB-CA-C	7.66	123.41	111.77	98	16
1	A	2	GLN	CB-CA-C	7.66	123.17	109.38	103	23
1	A	9	THR	CA-CB-CG2	7.64	123.50	110.50	260	11
1	A	6	LYS	N-CA-C	7.63	122.13	109.46	26	25
1	A	19	PRO	CA-C-O	7.63	129.00	118.86	209	4
1	A	59	TYR	N-CA-CB	-7.62	98.72	110.46	261	10
1	A	66	THR	O-C-N	-7.62	114.30	123.29	43	17
1	A	69	LEU	CD1-CG-CD2	-7.61	94.06	110.80	39	15
1	A	14	THR	CA-C-O	7.61	129.48	120.20	52	13
1	A	2	GLN	CB-CG-CD	7.61	125.53	112.60	10	13
1	A	52	ASP	O-C-N	-7.59	114.07	122.12	129	22
1	A	41	GLN	CA-CB-CG	7.59	129.29	114.10	29	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	46	ALA	N-CA-CB	-7.59	100.77	111.62	114	44
1	A	52	ASP	CA-C-O	-7.59	112.43	120.55	295	22
1	A	63	LYS	N-CA-C	7.59	120.94	110.24	97	13
1	A	41	GLN	CA-C-O	7.58	128.92	120.43	249	14
1	A	8	LEU	N-CA-CB	-7.58	97.67	110.49	90	11
1	A	47	GLY	N-CA-C	7.57	125.40	115.40	116	12
1	A	25	ASN	CB-CA-C	7.57	123.35	110.79	30	10
1	A	29	LYS	CB-CA-C	7.57	123.35	110.79	147	5
1	A	61	ILE	CA-CB-CG2	7.55	123.33	110.50	131	1
1	A	69	LEU	N-CA-CB	-7.54	98.02	110.68	301	11
1	A	20	SER	CA-C-O	-7.54	110.11	119.38	70	21
1	A	34	GLU	CA-CB-CG	7.54	129.17	114.10	113	16
1	A	52	ASP	CA-C-N	7.54	128.29	120.00	270	6
1	A	52	ASP	C-N-CA	7.54	128.29	120.00	270	6
1	A	16	GLU	N-CA-CB	7.53	122.40	110.57	140	15
1	A	14	THR	OG1-CB-CG2	-7.52	94.26	109.30	51	17
1	A	13	ILE	CA-CB-CG2	-7.51	97.74	110.50	133	11
1	A	51	GLU	CA-CB-CG	7.50	129.10	114.10	105	10
1	A	68	HIS	ND1-CE1-NE2	7.50	115.90	108.40	245	16
1	A	30	ILE	N-CA-C	7.50	119.17	110.62	166	40
1	A	43	LEU	N-CA-C	7.50	121.91	109.46	45	14
1	A	11	LYS	N-CA-C	7.49	120.61	108.32	121	21
1	A	64	GLU	CG-CD-OE2	-7.49	101.17	118.40	75	5
1	A	71	LEU	N-CA-CB	7.48	121.88	109.60	120	7
1	A	45	PHE	N-CA-C	7.48	121.73	109.24	86	13
1	A	28	ALA	CB-CA-C	7.47	123.39	110.68	73	17
1	A	6	LYS	CA-C-O	7.47	128.98	120.54	123	12
1	A	22	THR	OG1-CB-CG2	-7.46	94.38	109.30	206	8
1	A	6	LYS	CA-C-N	7.45	132.53	122.84	88	4
1	A	6	LYS	C-N-CA	7.45	132.53	122.84	88	4
1	A	38	PRO	O-C-N	7.44	130.22	122.18	62	6
1	A	2	GLN	O-C-N	7.44	131.27	122.94	211	18
1	A	64	GLU	CB-CA-C	7.44	123.68	111.26	109	15
1	A	16	GLU	N-CA-C	-7.42	96.42	108.52	247	5
1	A	11	LYS	CB-CA-C	7.42	121.77	109.53	179	16
1	A	24	GLU	CA-C-O	-7.42	112.69	120.55	219	11
1	A	30	ILE	N-CA-CB	-7.41	101.88	110.55	148	6
1	A	71	LEU	O-C-N	-7.41	114.58	123.10	7	24
1	A	33	LYS	N-CA-CB	-7.41	99.65	110.47	147	5
1	A	23	ILE	CA-CB-CG1	7.39	122.96	110.40	83	4
1	A	3	ILE	CA-CB-CG1	7.39	122.96	110.40	136	17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	20	SER	N-CA-CB	-7.38	98.93	110.44	96	7
1	A	8	LEU	CA-C-N	7.37	135.62	121.54	33	11
1	A	8	LEU	C-N-CA	7.37	135.62	121.54	33	11
1	A	58	ASP	N-CA-C	-7.37	103.33	111.36	123	14
1	A	19	PRO	N-CD-CG	7.36	114.24	103.20	172	3
1	A	1	MET	CB-CG-SD	7.34	134.72	112.70	103	1
1	A	64	GLU	CA-CB-CG	7.33	128.76	114.10	149	14
1	A	3	ILE	CB-CG1-CD1	7.32	129.16	113.80	50	6
1	A	1	MET	O-C-N	-7.31	111.31	123.00	1	3
1	A	4	PHE	N-CA-CB	-7.30	99.16	110.85	29	9
1	A	19	PRO	CA-N-CD	-7.30	101.78	112.00	248	7
1	A	28	ALA	O-C-N	-7.30	113.29	122.27	245	17
1	A	20	SER	CA-C-N	7.29	131.48	121.05	98	29
1	A	20	SER	C-N-CA	7.29	131.48	121.05	98	29
1	A	49	GLN	N-CA-CB	-7.29	99.05	110.06	201	9
1	A	10	GLY	O-C-N	7.29	130.85	122.33	14	5
1	A	68	HIS	O-C-N	-7.28	114.68	123.27	250	17
1	A	21	ASP	CA-C-N	7.27	133.46	121.39	38	6
1	A	21	ASP	C-N-CA	7.27	133.46	121.39	38	6
1	A	31	GLN	O-C-N	7.26	129.82	122.12	79	12
1	A	62	GLN	CA-C-N	7.26	131.14	120.90	275	14
1	A	62	GLN	C-N-CA	7.26	131.14	120.90	275	14
1	A	17	VAL	CB-CA-C	-7.25	101.84	111.70	39	17
1	A	22	THR	CA-C-O	-7.24	113.18	121.72	83	13
1	A	54	ARG	N-CA-CB	7.24	120.29	110.38	67	8
1	A	38	PRO	CB-CA-C	-7.23	101.59	111.85	196	4
1	A	27	LYS	CA-CB-CG	7.22	128.54	114.10	84	3
1	A	21	ASP	N-CA-C	7.22	120.42	110.24	128	8
1	A	65	SER	CA-CB-OG	-7.21	96.67	111.10	25	5
1	A	1	MET	CA-C-O	-7.21	108.54	120.80	113	3
1	A	15	LEU	O-C-N	-7.21	114.88	123.31	16	4
1	A	43	LEU	O-C-N	-7.20	114.77	123.27	268	5
1	A	27	LYS	N-CA-CB	-7.20	99.22	109.94	106	4
1	A	40	GLN	CA-C-O	-7.19	111.12	119.24	17	9
1	A	6	LYS	O-C-N	-7.19	114.08	123.21	45	11
1	A	26	VAL	O-C-N	-7.18	112.64	122.05	53	16
1	A	43	LEU	CA-C-O	7.18	128.26	120.43	51	16
1	A	3	ILE	N-CA-C	7.18	119.91	108.85	24	11
1	A	17	VAL	N-CA-CB	-7.17	104.42	112.45	4	13
1	A	21	ASP	O-C-N	-7.17	115.08	123.11	38	5
1	A	31	GLN	CB-CA-C	7.14	124.38	110.67	69	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	70	VAL	CA-C-O	7.13	128.94	121.67	130	10
1	A	65	SER	CB-CA-C	7.12	120.42	110.16	6	7
1	A	69	LEU	CA-C-O	-7.12	112.42	120.32	45	14
1	A	3	ILE	N-CA-CB	7.11	125.09	111.93	112	3
1	A	16	GLU	CA-CB-CG	7.11	128.32	114.10	25	13
1	A	13	ILE	N-CA-C	7.11	119.80	108.85	251	12
1	A	63	LYS	N-CA-CB	-7.10	98.49	110.49	137	13
1	A	51	GLU	CB-CA-C	7.09	120.96	109.90	90	17
1	A	17	VAL	CG1-CB-CG2	-7.09	95.20	110.80	209	4
1	A	55	THR	CB-CA-C	7.08	122.48	109.46	59	4
1	A	32	ASP	N-CA-CB	-7.08	98.64	110.39	164	16
1	A	8	LEU	CA-C-O	7.07	128.10	119.97	122	14
1	A	56	LEU	CB-CA-C	7.06	122.69	110.68	131	8
1	A	9	THR	CA-C-O	7.06	128.86	120.53	57	13
1	A	46	ALA	O-C-N	7.05	131.29	122.55	276	10
1	A	9	THR	OG1-CB-CG2	-7.04	95.23	109.30	60	8
1	A	54	ARG	CA-C-N	7.03	133.52	121.29	100	10
1	A	54	ARG	C-N-CA	7.03	133.52	121.29	100	10
1	A	32	ASP	OD1-CG-OD2	7.00	139.70	122.90	4	2
1	A	40	GLN	N-CA-CB	-7.00	100.10	110.53	92	5
1	A	28	ALA	CA-C-N	7.00	130.22	120.29	70	13
1	A	28	ALA	C-N-CA	7.00	130.22	120.29	70	13
1	A	62	GLN	CB-CA-C	6.99	124.13	110.30	2	7
1	A	40	GLN	CG-CD-NE2	6.99	126.88	116.40	127	11
1	A	31	GLN	CA-CB-CG	6.98	128.06	114.10	112	2
1	A	8	LEU	CB-CA-C	-6.97	99.00	110.85	4	9
1	A	30	ILE	CB-CA-C	-6.96	102.74	112.14	53	11
1	A	63	LYS	CA-CB-CG	6.95	127.99	114.10	101	12
1	A	62	GLN	N-CA-C	6.92	119.92	109.95	61	15
1	A	46	ALA	CA-C-O	-6.92	113.51	121.54	51	10
1	A	61	ILE	CA-CB-CG1	6.92	122.17	110.40	293	14
1	A	42	ARG	CB-CG-CD	6.91	127.19	111.30	46	6
1	A	15	LEU	CA-C-O	6.91	127.99	120.32	16	16
1	A	7	THR	CA-CB-OG1	6.90	119.96	109.60	148	19
1	A	14	THR	CB-CA-C	-6.90	98.49	109.80	210	13
1	A	56	LEU	O-C-N	6.89	129.42	122.12	52	12
1	A	14	THR	N-CA-CB	6.88	121.38	110.57	231	8
1	A	7	THR	O-C-N	6.88	130.80	122.68	76	17
1	A	33	LYS	CA-C-O	-6.88	112.60	120.24	99	16
1	A	48	LYS	CB-CA-C	6.87	122.50	109.37	144	8
1	A	70	VAL	CG1-CB-CG2	-6.87	95.68	110.80	72	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	30	ILE	CA-CB-CG2	6.87	122.18	110.50	180	15
1	A	45	PHE	CA-C-N	6.85	133.93	123.04	101	10
1	A	45	PHE	C-N-CA	6.85	133.93	123.04	101	10
1	A	12	THR	N-CA-C	6.84	120.14	110.23	258	9
1	A	44	ILE	N-CA-CB	-6.83	101.54	111.52	78	20
1	A	58	ASP	N-CA-CB	-6.83	100.09	110.26	59	7
1	A	64	GLU	CB-CG-CD	6.81	124.17	112.60	2	9
1	A	40	GLN	CB-CG-CD	6.80	124.15	112.60	270	4
1	A	5	VAL	CA-CB-CG1	6.79	121.94	110.40	58	2
1	A	71	LEU	CA-C-O	6.78	128.33	120.80	17	12
1	A	66	THR	OG1-CB-CG2	-6.78	95.73	109.30	215	7
1	A	6	LYS	N-CA-CB	-6.78	99.93	110.57	46	4
1	A	64	GLU	OE1-CD-OE2	-6.78	106.64	122.90	156	3
1	A	47	GLY	O-C-N	-6.77	114.17	122.23	204	14
1	A	59	TYR	CB-CA-C	6.77	121.39	110.09	51	8
1	A	38	PRO	CA-C-O	-6.76	109.32	119.86	98	10
1	A	67	LEU	N-CA-CB	-6.75	99.41	110.41	135	3
1	A	31	GLN	CB-CG-CD	-6.74	101.14	112.60	33	10
1	A	64	GLU	CG-CD-OE1	6.73	133.89	118.40	217	5
1	A	21	ASP	CB-CA-C	-6.70	100.75	110.06	151	12
1	A	66	THR	CA-C-N	6.68	131.94	122.72	105	4
1	A	66	THR	C-N-CA	6.68	131.94	122.72	105	4
1	A	59	TYR	O-C-N	-6.67	113.78	122.39	14	12
1	A	3	ILE	O-C-N	-6.67	115.48	123.02	183	13
1	A	54	ARG	CA-CB-CG	-6.67	100.77	114.10	39	4
1	A	34	GLU	CB-CA-C	-6.66	100.42	109.28	118	10
1	A	59	TYR	CB-CG-CD2	-6.66	110.81	120.80	143	1
1	A	23	ILE	CA-CB-CG2	6.64	121.79	110.50	133	22
1	A	40	GLN	N-CA-C	-6.63	104.21	112.90	14	10
1	A	44	ILE	CB-CG1-CD1	6.62	127.70	113.80	91	6
1	A	2	GLN	CG-CD-NE2	6.61	126.31	116.40	67	17
1	A	29	LYS	CG-CD-CE	6.61	126.50	111.30	100	5
1	A	52	ASP	CB-CA-C	6.61	121.38	110.81	240	12
1	A	24	GLU	CB-CG-CD	-6.60	101.38	112.60	185	10
1	A	57	SER	CA-CB-OG	6.60	124.30	111.10	284	7
1	A	45	PHE	CB-CG-CD1	-6.59	109.50	120.70	288	1
1	A	19	PRO	N-CA-C	6.59	126.04	112.47	130	8
1	A	60	ASN	CB-CG-ND2	6.58	126.27	116.40	152	11
1	A	67	LEU	CA-C-O	6.58	127.68	120.71	58	13
1	A	63	LYS	O-C-N	-6.57	114.95	122.97	25	8
1	A	11	LYS	O-C-N	-6.56	115.12	122.86	120	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	53	GLY	O-C-N	-6.55	113.29	122.27	288	8
1	A	40	GLN	CB-CA-C	6.53	123.71	110.38	229	8
1	A	18	GLU	N-CA-CB	6.51	117.29	109.74	158	11
1	A	16	GLU	CG-CD-OE1	-6.47	103.51	118.40	91	1
1	A	54	ARG	CB-CG-CD	6.47	126.18	111.30	18	7
1	A	29	LYS	CA-CB-CG	6.46	127.02	114.10	4	4
1	A	37	PRO	CA-C-O	-6.45	116.25	120.90	240	7
1	A	70	VAL	CA-CB-CG1	6.45	121.36	110.40	293	7
1	A	38	PRO	N-CD-CG	6.44	112.86	103.20	291	5
1	A	53	GLY	CA-C-O	-6.43	111.86	119.45	189	3
1	A	8	LEU	CD1-CG-CD2	-6.43	96.65	110.80	43	4
1	A	62	GLN	CA-CB-CG	6.43	126.97	114.10	296	2
1	A	41	GLN	CG-CD-NE2	6.43	126.04	116.40	120	16
1	A	69	LEU	N-CA-C	6.42	119.03	109.59	274	10
1	A	22	THR	CA-CB-CG2	6.40	121.39	110.50	37	8
1	A	63	LYS	CB-CG-CD	6.40	126.03	111.30	79	11
1	A	2	GLN	CA-CB-CG	6.40	126.90	114.10	121	12
1	A	33	LYS	CG-CD-CE	-6.38	96.61	111.30	50	12
1	A	19	PRO	CB-CA-C	6.38	121.00	111.68	4	4
1	A	45	PHE	O-C-N	6.36	131.42	123.28	247	5
1	A	31	GLN	N-CA-CB	-6.36	100.42	110.28	69	5
1	A	68	HIS	CB-CG-ND1	6.35	132.23	122.70	90	9
1	A	23	ILE	CA-C-N	6.34	128.78	120.28	238	11
1	A	23	ILE	C-N-CA	6.34	128.78	120.28	238	11
1	A	9	THR	O-C-N	-6.34	114.08	122.20	185	9
1	A	69	LEU	O-C-N	-6.34	114.98	122.96	85	10
1	A	51	GLU	N-CA-CB	-6.33	99.98	110.23	130	10
1	A	69	LEU	CB-CG-CD1	6.32	129.67	110.70	98	2
1	A	39	ASP	CA-C-N	6.32	129.26	120.29	51	4
1	A	39	ASP	C-N-CA	6.32	129.26	120.29	51	4
1	A	31	GLN	CG-CD-NE2	6.30	125.86	116.40	137	13
1	A	27	LYS	CG-CD-CE	6.29	125.77	111.30	43	4
1	A	43	LEU	N-CA-CB	-6.28	100.69	110.55	207	8
1	A	33	LYS	CB-CA-C	-6.27	100.25	110.79	15	9
1	A	27	LYS	CB-CG-CD	6.27	125.72	111.30	120	1
1	A	3	ILE	CB-CA-C	6.26	119.91	110.90	250	9
1	A	21	ASP	CB-CG-OD1	6.25	132.78	118.40	274	2
1	A	16	GLU	CB-CG-CD	6.25	123.22	112.60	114	7
1	A	62	GLN	CG-CD-OE1	6.22	133.25	120.80	81	2
1	A	33	LYS	CA-CB-CG	-6.21	101.69	114.10	168	7
1	A	5	VAL	CA-CB-CG2	6.19	120.92	110.40	91	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	1	MET	N-CA-CB	-6.18	99.99	110.50	76	5
1	A	22	THR	N-CA-CB	6.17	119.68	110.29	227	13
1	A	7	THR	OG1-CB-CG2	-6.17	96.95	109.30	196	11
1	A	50	LEU	N-CA-CB	-6.14	100.29	110.23	166	4
1	A	66	THR	N-CA-CB	-6.13	100.27	109.71	23	7
1	A	20	SER	O-C-N	-6.11	115.24	122.20	4	7
1	A	32	ASP	CB-CG-OD2	-6.09	104.39	118.40	28	2
1	A	8	LEU	O-C-N	-6.09	114.47	122.39	187	5
1	A	3	ILE	CA-CB-CG2	-6.08	100.16	110.50	23	2
1	A	22	THR	CA-C-N	6.08	130.08	120.47	218	5
1	A	22	THR	C-N-CA	6.08	130.08	120.47	218	5
1	A	45	PHE	CB-CA-C	6.06	122.48	110.42	298	1
1	A	19	PRO	O-C-N	-6.05	113.97	122.38	209	2
1	A	9	THR	CA-C-N	6.03	131.79	122.20	245	9
1	A	9	THR	C-N-CA	6.03	131.79	122.20	245	9
1	A	29	LYS	N-CA-CB	6.01	119.59	110.28	278	11
1	A	70	VAL	N-CA-C	-6.00	99.56	108.45	110	5
1	A	35	GLY	N-CA-C	6.00	123.94	115.30	85	15
1	A	32	ASP	O-C-N	-6.00	115.20	122.22	83	9
1	A	12	THR	O-C-N	-6.00	116.55	123.33	33	7
1	A	25	ASN	CB-CG-ND2	5.99	125.38	116.40	243	8
1	A	56	LEU	CA-CB-CG	5.97	137.21	116.30	204	1
1	A	21	ASP	N-CA-CB	-5.97	100.82	109.83	96	10
1	A	49	GLN	CA-CB-CG	5.97	126.04	114.10	124	9
1	A	56	LEU	CD1-CG-CD2	-5.96	97.68	110.80	55	8
1	A	65	SER	N-CA-CB	5.96	119.34	110.29	18	7
1	A	62	GLN	CB-CG-CD	5.95	122.71	112.60	59	4
1	A	40	GLN	CA-CB-CG	-5.92	102.26	114.10	21	2
1	A	9	THR	CB-CA-C	5.92	119.49	109.55	138	3
1	A	52	ASP	CB-CG-OD2	5.92	132.01	118.40	39	2
1	A	49	GLN	CB-CG-CD	5.91	122.66	112.60	42	9
1	A	59	TYR	CA-CB-CG	5.90	124.52	113.90	261	4
1	A	60	ASN	CB-CG-OD1	5.89	132.58	120.80	138	4
1	A	24	GLU	N-CA-CB	-5.89	101.17	109.94	147	7
1	A	68	HIS	CE1-NE2-CD2	5.86	114.86	109.00	301	3
1	A	17	VAL	CA-C-N	-5.86	112.99	122.48	111	3
1	A	17	VAL	C-N-CA	-5.86	112.99	122.48	111	3
1	A	34	GLU	CG-CD-OE2	5.85	131.86	118.40	35	1
1	A	39	ASP	CB-CG-OD2	-5.84	104.97	118.40	92	2
1	A	19	PRO	CA-CB-CG	-5.83	93.43	104.50	132	2
1	A	21	ASP	OD1-CG-OD2	-5.82	108.94	122.90	148	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	24	GLU	CB-CA-C	-5.81	101.76	110.88	87	6
1	A	37	PRO	N-CD-CG	5.81	111.91	103.20	288	9
1	A	20	SER	CB-CA-C	-5.76	98.43	110.17	185	1
1	A	1	MET	CG-SD-CE	5.75	113.56	100.90	65	4
1	A	69	LEU	CB-CA-C	5.75	119.30	110.62	72	1
1	A	42	ARG	N-CA-C	-5.75	97.79	108.02	25	2
1	A	67	LEU	CD1-CG-CD2	-5.74	98.17	110.80	274	6
1	A	32	ASP	CB-CG-OD1	-5.73	105.21	118.40	51	3
1	A	55	THR	OG1-CB-CG2	-5.73	97.83	109.30	102	2
1	A	6	LYS	CA-CB-CG	-5.70	102.70	114.10	42	2
1	A	50	LEU	CD1-CG-CD2	-5.68	98.30	110.80	284	5
1	A	25	ASN	N-CA-CB	5.68	119.09	110.28	54	6
1	A	15	LEU	CD1-CG-CD2	-5.68	98.30	110.80	11	5
1	A	6	LYS	CB-CG-CD	5.68	124.37	111.30	147	5
1	A	37	PRO	CA-N-CD	-5.68	104.05	112.00	267	1
1	A	59	TYR	CB-CG-CD1	-5.67	112.29	120.80	19	2
1	A	7	THR	CB-CA-C	-5.67	104.24	113.37	83	3
1	A	38	PRO	N-CA-C	5.66	122.02	113.81	84	4
1	A	15	LEU	CB-CG-CD2	5.66	127.67	110.70	142	1
1	A	46	ALA	N-CA-C	5.65	118.91	111.28	284	10
1	A	13	ILE	CG1-CB-CG2	5.64	127.61	110.70	279	2
1	A	21	ASP	CA-C-O	5.63	127.38	121.19	126	5
1	A	18	GLU	CA-CB-CG	-5.62	102.85	114.10	230	3
1	A	7	THR	N-CA-CB	5.61	119.57	110.43	101	3
1	A	12	THR	N-CA-CB	5.59	119.35	110.57	152	1
1	A	3	ILE	CA-C-N	-5.57	114.35	122.65	132	4
1	A	3	ILE	C-N-CA	-5.57	114.35	122.65	132	4
1	A	5	VAL	CG1-CB-CG2	5.57	123.04	110.80	144	4
1	A	13	ILE	CB-CG1-CD1	5.56	125.48	113.80	38	3
1	A	25	ASN	CB-CG-OD1	5.53	131.85	120.80	28	1
1	A	48	LYS	CG-CD-CE	-5.51	98.63	111.30	82	1
1	A	9	THR	N-CA-CB	5.45	118.77	110.44	225	2
1	A	1	MET	N-CA-C	-5.40	95.87	111.00	57	1
1	A	38	PRO	CA-N-CD	-5.39	104.46	112.00	63	6
1	A	40	GLN	CG-CD-OE1	5.38	131.57	120.80	6	1
1	A	22	THR	CB-CA-C	-5.38	99.05	109.76	116	3
1	A	18	GLU	CG-CD-OE1	-5.37	106.05	118.40	98	1
1	A	67	LEU	CB-CG-CD2	-5.36	94.63	110.70	176	1
1	A	15	LEU	CB-CG-CD1	5.35	126.74	110.70	50	1
1	A	54	ARG	CG-CD-NE	5.34	123.76	112.00	244	2
1	A	52	ASP	CB-CG-OD1	-5.31	106.19	118.40	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	69	LEU	CB-CG-CD2	5.29	126.58	110.70	205	1
1	A	24	GLU	CA-CB-CG	-5.29	103.52	114.10	14	2
1	A	71	LEU	CD1-CG-CD2	-5.29	99.16	110.80	57	1
1	A	36	ILE	CA-CB-CG2	5.26	119.44	110.50	28	3
1	A	16	GLU	OE1-CD-OE2	-5.25	110.30	122.90	51	2
1	A	20	SER	CA-CB-OG	5.17	121.44	111.10	213	3
1	A	6	LYS	CG-CD-CE	-5.17	99.42	111.30	201	1
1	A	11	LYS	CG-CD-CE	5.16	123.17	111.30	61	1
1	A	15	LEU	N-CA-CB	5.16	119.04	110.63	12	1
1	A	4	PHE	CB-CG-CD2	5.12	129.41	120.70	34	1
1	A	34	GLU	CG-CD-OE1	5.10	130.14	118.40	90	1
1	A	41	GLN	CB-CG-CD	5.09	121.25	112.60	29	1
1	A	67	LEU	CB-CG-CD1	5.04	125.82	110.70	176	1
1	A	33	LYS	CD-CE-NZ	5.03	128.00	111.90	2	1
1	A	4	PHE	CB-CA-C	-5.01	101.03	109.50	87	1
1	A	45	PHE	CD1-CG-CD2	5.01	126.12	118.60	229	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	51	GLU	Peptide,Sidechain,Mainchain	115
1	A	54	ARG	Mainchain,Sidechain	80
1	A	59	TYR	Sidechain,Mainchain	63
1	A	42	ARG	Sidechain,Mainchain	61
1	A	4	PHE	Peptide,Sidechain,Mainchain	47
1	A	45	PHE	Sidechain	28
1	A	65	SER	Mainchain,Peptide	26
1	A	41	GLN	Peptide,Mainchain	25
1	A	17	VAL	Mainchain,Peptide	23
1	A	68	HIS	Mainchain,Sidechain	22
1	A	71	LEU	Peptide,Mainchain	21
1	A	11	LYS	Mainchain,Peptide	13
1	A	64	GLU	Sidechain,Mainchain,Peptide	13
1	A	47	GLY	Mainchain,Peptide	12
1	A	7	THR	Mainchain,Peptide	12
1	A	21	ASP	Mainchain,Sidechain	11
1	A	13	ILE	Mainchain,Peptide	11
1	A	34	GLU	Sidechain,Mainchain,Peptide	11
1	A	57	SER	Mainchain,Peptide	10

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	23	ILE	Mainchain	10
1	A	33	LYS	Peptide,Mainchain	10
1	A	50	LEU	Peptide,Mainchain	10
1	A	48	LYS	Mainchain,Peptide	9
1	A	56	LEU	Mainchain,Peptide	9
1	A	29	LYS	Peptide,Mainchain	9
1	A	26	VAL	Peptide,Mainchain	8
1	A	6	LYS	Mainchain,Peptide	8
1	A	10	GLY	Peptide,Mainchain	8
1	A	55	THR	Mainchain,Peptide	7
1	A	58	ASP	Sidechain,Mainchain	7
1	A	52	ASP	Mainchain,Sidechain	7
1	A	20	SER	Peptide,Mainchain	7
1	A	53	GLY	Peptide,Mainchain	7
1	A	24	GLU	Mainchain,Peptide	7
1	A	35	GLY	Mainchain,Peptide	7
1	A	39	ASP	Mainchain	7
1	A	46	ALA	Mainchain,Peptide	7
1	A	1	MET	Peptide,Mainchain	6
1	A	62	GLN	Peptide,Mainchain	6
1	A	37	PRO	Peptide	6
1	A	15	LEU	Peptide,Mainchain	6
1	A	40	GLN	Peptide,Mainchain,Sidechain	6
1	A	5	VAL	Mainchain	5
1	A	18	GLU	Mainchain,Peptide	5
1	A	44	ILE	Mainchain	5
1	A	16	GLU	Mainchain	5
1	A	28	ALA	Mainchain	5
1	A	38	PRO	Mainchain	4
1	A	25	ASN	Peptide,Mainchain	4
1	A	70	VAL	Peptide	4
1	A	31	GLN	Mainchain	4
1	A	61	ILE	Mainchain	4
1	A	12	THR	Peptide,Mainchain	3
1	A	60	ASN	Mainchain	3
1	A	43	LEU	Mainchain	3
1	A	9	THR	Peptide,Mainchain	3
1	A	14	THR	Peptide,Mainchain	3
1	A	69	LEU	Mainchain	2
1	A	36	ILE	Mainchain	2
1	A	3	ILE	Mainchain	2
1	A	32	ASP	Sidechain,Mainchain	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	2	GLN	Peptide	2
1	A	27	LYS	Mainchain	2
1	A	8	LEU	Mainchain	2
1	A	30	ILE	Mainchain	2
1	A	63	LYS	Mainchain	1
1	A	67	LEU	Mainchain	1
1	A	49	GLN	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	563	586	586	1±1
All	All	169463	176386	176386	412

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ILE:HA	1:A:26:VAL:HG23	0.73	1.59	151	9
1:A:7:THR:HG22	1:A:69:LEU:HD23	0.71	1.61	154	3
1:A:68:HIS:CG	1:A:69:LEU:H	0.71	2.03	49	8
1:A:63:LYS:HE2	1:A:64:GLU:OE2	0.69	1.87	173	4
1:A:23:ILE:HG23	1:A:43:LEU:HD13	0.68	1.66	90	1
1:A:63:LYS:NZ	1:A:64:GLU:OE1	0.67	2.26	44	15
1:A:63:LYS:HE2	1:A:64:GLU:OE1	0.67	1.89	300	4
1:A:7:THR:HG21	1:A:34:GLU:CD	0.66	2.16	273	1
1:A:63:LYS:NZ	1:A:64:GLU:OE2	0.64	2.31	233	6
1:A:48:LYS:HE2	1:A:59:TYR:CE1	0.62	2.29	45	2
1:A:18:GLU:OE1	1:A:19:PRO:HD2	0.62	1.94	12	1
1:A:68:HIS:CG	1:A:69:LEU:N	0.62	2.68	105	7
1:A:15:LEU:HD11	1:A:29:LYS:CB	0.62	2.23	40	1
1:A:5:VAL:HG21	1:A:30:ILE:HD11	0.62	1.70	64	14
1:A:48:LYS:HE2	1:A:49:GLN:O	0.58	1.99	58	1
1:A:11:LYS:NZ	1:A:34:GLU:OE1	0.55	2.39	128	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:GLU:CD	1:A:27:LYS:HE3	0.55	2.26	117	1
1:A:49:GLN:HE21	1:A:51:GLU:CD	0.55	2.09	17	1
1:A:16:GLU:O	1:A:29:LYS:HE3	0.55	2.02	132	1
1:A:45:PHE:HB2	1:A:67:LEU:HD23	0.55	1.77	27	1
1:A:48:LYS:CE	1:A:59:TYR:CE1	0.55	2.89	143	1
1:A:48:LYS:NZ	1:A:51:GLU:OE2	0.55	2.40	134	2
1:A:27:LYS:HE3	1:A:52:ASP:OD1	0.54	2.02	65	1
1:A:16:GLU:OE1	1:A:16:GLU:HA	0.54	2.02	60	2
1:A:8:LEU:HD11	1:A:71:LEU:HD21	0.54	1.80	162	1
1:A:6:LYS:HE2	1:A:10:GLY:O	0.54	2.03	290	1
1:A:48:LYS:NZ	1:A:51:GLU:OE1	0.53	2.41	148	1
1:A:17:VAL:HG21	1:A:56:LEU:HD21	0.53	1.80	276	1
1:A:32:ASP:OD1	1:A:33:LYS:NZ	0.53	2.42	151	5
1:A:41:GLN:HA	1:A:69:LEU:HD11	0.53	1.78	37	1
1:A:1:MET:HG2	1:A:18:GLU:OE1	0.53	2.03	115	1
1:A:25:ASN:OD1	1:A:29:LYS:HE3	0.53	2.04	200	17
1:A:70:VAL:HG12	1:A:71:LEU:H	0.53	1.64	84	3
1:A:1:MET:N	1:A:18:GLU:OE2	0.53	2.41	57	13
1:A:16:GLU:N	1:A:16:GLU:CD	0.53	2.67	128	1
1:A:27:LYS:HZ2	1:A:52:ASP:CG	0.53	2.12	9	2
1:A:15:LEU:HD23	1:A:15:LEU:N	0.52	2.18	282	1
1:A:8:LEU:HD13	1:A:70:VAL:HG23	0.52	1.81	229	1
1:A:1:MET:N	1:A:16:GLU:OE2	0.52	2.42	5	2
1:A:69:LEU:O	1:A:69:LEU:HD23	0.52	2.05	146	1
1:A:18:GLU:OE1	1:A:18:GLU:HA	0.52	2.05	116	7
1:A:67:LEU:HD12	1:A:67:LEU:N	0.52	2.19	121	16
1:A:30:ILE:HB	1:A:41:GLN:HE22	0.52	1.64	3	1
1:A:43:LEU:HD12	1:A:43:LEU:N	0.51	2.19	188	3
1:A:8:LEU:HD13	1:A:70:VAL:HG13	0.51	1.82	29	1
1:A:71:LEU:CD1	1:A:71:LEU:N	0.51	2.74	50	1
1:A:36:ILE:N	1:A:36:ILE:HD13	0.51	2.21	236	5
1:A:63:LYS:NZ	1:A:64:GLU:CD	0.51	2.69	66	2
1:A:22:THR:O	1:A:26:VAL:HG23	0.50	2.05	195	2
1:A:15:LEU:HD22	1:A:15:LEU:N	0.50	2.21	61	1
1:A:16:GLU:H	1:A:16:GLU:CD	0.50	2.13	185	3
1:A:33:LYS:HA	1:A:33:LYS:HE3	0.50	1.81	1	1
1:A:11:LYS:NZ	1:A:34:GLU:OE2	0.50	2.39	79	6
1:A:24:GLU:OE1	1:A:27:LYS:CE	0.50	2.59	283	1
1:A:12:THR:C	1:A:13:ILE:CG2	0.50	2.85	78	1
1:A:63:LYS:HD2	1:A:63:LYS:C	0.49	2.32	45	2
1:A:1:MET:HG2	1:A:17:VAL:O	0.49	2.07	260	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:VAL:HG12	1:A:29:LYS:NZ	0.49	2.22	23	1
1:A:47:GLY:C	1:A:48:LYS:HG3	0.49	2.33	248	1
1:A:7:THR:HG21	1:A:34:GLU:OE1	0.49	2.08	273	1
1:A:59:TYR:O	1:A:60:ASN:C	0.49	2.54	157	1
1:A:17:VAL:HG21	1:A:56:LEU:CD1	0.49	2.37	169	2
1:A:70:VAL:C	1:A:71:LEU:HD12	0.49	2.32	208	1
1:A:17:VAL:HG12	1:A:29:LYS:HZ2	0.49	1.68	23	1
1:A:68:HIS:CD2	1:A:69:LEU:H	0.49	2.25	34	1
1:A:23:ILE:HA	1:A:26:VAL:HG12	0.49	1.85	21	1
1:A:50:LEU:HD22	1:A:59:TYR:CD1	0.49	2.43	22	1
1:A:63:LYS:HZ2	1:A:64:GLU:CD	0.49	2.16	66	1
1:A:23:ILE:N	1:A:23:ILE:HD13	0.48	2.23	135	3
1:A:43:LEU:HB3	1:A:50:LEU:HD12	0.48	1.86	40	1
1:A:50:LEU:HD22	1:A:59:TYR:CD2	0.48	2.43	61	5
1:A:25:ASN:OD1	1:A:29:LYS:CE	0.48	2.61	156	1
1:A:43:LEU:C	1:A:44:ILE:CG2	0.48	2.86	53	5
1:A:27:LYS:NZ	1:A:52:ASP:OD2	0.48	2.46	242	7
1:A:50:LEU:HD22	1:A:59:TYR:CG	0.48	2.44	19	3
1:A:15:LEU:HD11	1:A:29:LYS:HB3	0.48	1.84	40	1
1:A:15:LEU:HD11	1:A:29:LYS:HB2	0.48	1.85	40	1
1:A:3:ILE:HG12	1:A:17:VAL:HG21	0.48	1.85	19	2
1:A:25:ASN:OD1	1:A:29:LYS:HE2	0.48	2.08	206	4
1:A:45:PHE:CD2	1:A:61:ILE:HD11	0.47	2.43	99	1
1:A:36:ILE:HD11	1:A:69:LEU:HD21	0.47	1.86	190	1
1:A:44:ILE:N	1:A:44:ILE:HD13	0.47	2.25	6	2
1:A:61:ILE:HD13	1:A:67:LEU:HD21	0.47	1.87	77	1
1:A:44:ILE:HD13	1:A:44:ILE:H	0.47	1.69	6	1
1:A:48:LYS:HD3	1:A:48:LYS:C	0.47	2.34	93	1
1:A:15:LEU:HD11	1:A:30:ILE:HG12	0.47	1.86	125	1
1:A:51:GLU:CD	1:A:54:ARG:HE	0.47	2.18	299	1
1:A:5:VAL:HG22	1:A:67:LEU:HB2	0.47	1.85	235	3
1:A:1:MET:HE3	1:A:17:VAL:HG23	0.47	1.86	80	1
1:A:44:ILE:HA	1:A:48:LYS:O	0.47	2.09	123	2
1:A:8:LEU:HD22	1:A:71:LEU:H	0.47	1.69	184	1
1:A:27:LYS:HE3	1:A:41:GLN:HB2	0.47	1.86	57	1
1:A:8:LEU:HD23	1:A:8:LEU:H	0.47	1.70	203	1
1:A:17:VAL:HG12	1:A:21:ASP:OD2	0.46	2.10	6	1
1:A:63:LYS:CE	1:A:64:GLU:OE2	0.46	2.63	203	1
1:A:62:GLN:NE2	1:A:62:GLN:H	0.46	2.08	293	1
1:A:1:MET:N	1:A:16:GLU:OE1	0.46	2.46	132	3
1:A:39:ASP:OD2	1:A:40:GLN:NE2	0.46	2.49	289	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:LEU:HD22	1:A:61:ILE:HG21	0.46	1.86	3	1
1:A:12:THR:C	1:A:13:ILE:HG13	0.46	2.36	7	2
1:A:54:ARG:NH1	1:A:58:ASP:OD1	0.46	2.49	12	1
1:A:48:LYS:NZ	1:A:59:TYR:HA	0.46	2.26	22	1
1:A:45:PHE:CE2	1:A:61:ILE:HD13	0.46	2.45	147	1
1:A:8:LEU:O	1:A:8:LEU:HD23	0.46	2.10	234	1
1:A:67:LEU:CD1	1:A:67:LEU:N	0.46	2.79	144	1
1:A:13:ILE:HG22	1:A:14:THR:N	0.45	2.25	3	1
1:A:11:LYS:HZ3	1:A:34:GLU:CD	0.45	2.19	110	1
1:A:61:ILE:HD13	1:A:67:LEU:HD11	0.45	1.87	14	1
1:A:32:ASP:OD2	1:A:33:LYS:NZ	0.45	2.48	147	4
1:A:61:ILE:CD1	1:A:67:LEU:HD11	0.45	2.40	120	1
1:A:12:THR:C	1:A:13:ILE:HD12	0.45	2.36	150	1
1:A:1:MET:SD	1:A:1:MET:C	0.45	3.00	44	1
1:A:27:LYS:HE2	1:A:52:ASP:OD1	0.45	2.11	69	1
1:A:66:THR:C	1:A:67:LEU:HD22	0.45	2.37	76	1
1:A:43:LEU:HD23	1:A:68:HIS:O	0.45	2.12	84	1
1:A:23:ILE:HG21	1:A:50:LEU:HB3	0.45	1.87	100	1
1:A:71:LEU:HD12	1:A:71:LEU:N	0.45	2.26	229	2
1:A:62:GLN:O	1:A:63:LYS:C	0.45	2.60	16	2
1:A:1:MET:C	1:A:16:GLU:OE2	0.45	2.60	49	1
1:A:45:PHE:C	1:A:47:GLY:N	0.45	2.72	85	1
1:A:27:LYS:CE	1:A:38:PRO:O	0.45	2.64	111	1
1:A:31:GLN:HE21	1:A:32:ASP:N	0.45	2.10	98	1
1:A:63:LYS:HE3	1:A:64:GLU:OE2	0.45	2.12	242	1
1:A:51:GLU:CD	1:A:54:ARG:HH21	0.45	2.19	178	3
1:A:13:ILE:HG12	1:A:34:GLU:HG3	0.45	1.88	191	1
1:A:39:ASP:OD1	1:A:39:ASP:C	0.44	2.60	29	1
1:A:50:LEU:HD23	1:A:59:TYR:CD2	0.44	2.46	116	1
1:A:45:PHE:CD2	1:A:61:ILE:HD13	0.44	2.46	64	1
1:A:68:HIS:N	1:A:68:HIS:CD2	0.44	2.79	106	1
1:A:25:ASN:OD1	1:A:29:LYS:NZ	0.44	2.51	112	1
1:A:21:ASP:OD2	1:A:29:LYS:NZ	0.44	2.50	285	2
1:A:11:LYS:HE2	1:A:34:GLU:OE2	0.44	2.11	64	1
1:A:7:THR:HG23	1:A:69:LEU:HD23	0.44	1.90	196	1
1:A:46:ALA:O	1:A:48:LYS:HE2	0.44	2.12	51	1
1:A:54:ARG:HH11	1:A:54:ARG:HG3	0.44	1.72	90	1
1:A:54:ARG:HD2	1:A:59:TYR:CZ	0.44	2.47	104	1
1:A:23:ILE:O	1:A:26:VAL:HG23	0.44	2.12	146	1
1:A:5:VAL:HG21	1:A:30:ILE:CD1	0.44	2.42	77	1
1:A:67:LEU:N	1:A:67:LEU:CD1	0.44	2.80	283	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ILE:HB	1:A:52:ASP:HA	0.44	1.89	267	2
1:A:1:MET:N	1:A:18:GLU:OE1	0.44	2.51	58	2
1:A:71:LEU:N	1:A:71:LEU:HD12	0.44	2.28	50	1
1:A:32:ASP:OD1	1:A:33:LYS:HE2	0.44	2.13	123	1
1:A:63:LYS:HB2	1:A:64:GLU:OE2	0.44	2.13	9	1
1:A:54:ARG:HD3	1:A:58:ASP:CG	0.44	2.38	26	1
1:A:55:THR:O	1:A:56:LEU:C	0.44	2.60	96	1
1:A:66:THR:C	1:A:67:LEU:HD12	0.44	2.38	170	3
1:A:23:ILE:HG13	1:A:50:LEU:HD13	0.43	1.89	36	1
1:A:49:GLN:HE21	1:A:51:GLU:HG2	0.43	1.71	199	1
1:A:43:LEU:C	1:A:44:ILE:HG23	0.43	2.38	99	3
1:A:32:ASP:OD2	1:A:33:LYS:CE	0.43	2.67	50	1
1:A:43:LEU:C	1:A:44:ILE:HD12	0.43	2.39	129	1
1:A:19:PRO:HA	1:A:56:LEU:HD22	0.43	1.90	131	1
1:A:16:GLU:CD	1:A:16:GLU:N	0.43	2.76	185	1
1:A:32:ASP:C	1:A:33:LYS:HE2	0.43	2.37	218	1
1:A:45:PHE:O	1:A:46:ALA:C	0.43	2.62	122	3
1:A:63:LYS:O	1:A:63:LYS:HG3	0.43	2.14	234	1
1:A:16:GLU:OE1	1:A:33:LYS:NZ	0.43	2.52	3	1
1:A:1:MET:C	1:A:16:GLU:OE1	0.43	2.61	64	2
1:A:43:LEU:HD22	1:A:67:LEU:HD23	0.43	1.91	36	1
1:A:3:ILE:HG12	1:A:17:VAL:CG2	0.43	2.43	84	1
1:A:24:GLU:HA	1:A:27:LYS:HE2	0.43	1.89	3	1
1:A:68:HIS:CD2	1:A:68:HIS:N	0.43	2.87	255	3
1:A:68:HIS:CD2	1:A:69:LEU:N	0.43	2.87	71	2
1:A:67:LEU:N	1:A:67:LEU:CD2	0.42	2.81	76	1
1:A:23:ILE:HG21	1:A:50:LEU:HB2	0.42	1.90	124	1
1:A:44:ILE:HG22	1:A:68:HIS:ND1	0.42	2.30	11	1
1:A:5:VAL:HG21	1:A:43:LEU:HD21	0.42	1.91	31	1
1:A:63:LYS:CE	1:A:64:GLU:OE1	0.42	2.67	57	1
1:A:1:MET:CA	1:A:16:GLU:OE1	0.42	2.68	130	1
1:A:27:LYS:CE	1:A:52:ASP:OD1	0.42	2.67	10	1
1:A:63:LYS:HD2	1:A:63:LYS:O	0.42	2.14	67	1
1:A:67:LEU:HD22	1:A:67:LEU:N	0.42	2.29	76	1
1:A:23:ILE:CD1	1:A:56:LEU:HD12	0.42	2.44	29	1
1:A:23:ILE:HD12	1:A:54:ARG:O	0.42	2.14	56	1
1:A:57:SER:C	1:A:59:TYR:H	0.42	2.22	60	1
1:A:8:LEU:H	1:A:8:LEU:CD2	0.42	2.27	203	1
1:A:21:ASP:O	1:A:56:LEU:HD13	0.42	2.15	291	1
1:A:27:LYS:HE2	1:A:38:PRO:O	0.42	2.14	48	1
1:A:50:LEU:HD22	1:A:59:TYR:CE2	0.42	2.49	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:LYS:HE2	1:A:38:PRO:HB3	0.42	1.91	185	1
1:A:18:GLU:HB3	1:A:19:PRO:CD	0.41	2.44	39	1
1:A:27:LYS:HE3	1:A:41:GLN:CB	0.41	2.45	57	1
1:A:24:GLU:OE1	1:A:24:GLU:HA	0.41	2.15	125	1
1:A:23:ILE:HA	1:A:26:VAL:HG22	0.41	1.92	124	1
1:A:5:VAL:HB	1:A:13:ILE:HD12	0.41	1.91	223	1
1:A:6:LYS:CE	1:A:12:THR:OG1	0.41	2.68	18	1
1:A:12:THR:C	1:A:13:ILE:HG23	0.41	2.40	78	1
1:A:49:GLN:CD	1:A:49:GLN:H	0.41	2.23	165	1
1:A:51:GLU:OE1	1:A:54:ARG:NH2	0.41	2.52	200	2
1:A:18:GLU:O	1:A:21:ASP:HB2	0.41	2.16	293	1
1:A:50:LEU:CD2	1:A:59:TYR:CD1	0.41	3.04	95	1
1:A:11:LYS:HE3	1:A:34:GLU:OE2	0.41	2.14	142	1
1:A:44:ILE:HG22	1:A:49:GLN:HA	0.41	1.93	6	2
1:A:27:LYS:NZ	1:A:52:ASP:OD1	0.41	2.51	58	1
1:A:54:ARG:HD3	1:A:58:ASP:OD2	0.41	2.16	115	2
1:A:18:GLU:OE1	1:A:19:PRO:HD3	0.41	2.16	287	1
1:A:22:THR:HA	1:A:55:THR:HA	0.41	1.91	70	1
1:A:32:ASP:OD1	1:A:32:ASP:C	0.41	2.64	104	2
1:A:54:ARG:HE	1:A:58:ASP:CG	0.41	2.23	56	1
1:A:33:LYS:HA	1:A:33:LYS:NZ	0.41	2.31	67	1
1:A:54:ARG:N	1:A:54:ARG:HD3	0.41	2.30	98	1
1:A:71:LEU:HD22	1:A:71:LEU:N	0.41	2.31	136	1
1:A:44:ILE:HD13	1:A:49:GLN:HA	0.41	1.93	94	1
1:A:23:ILE:HG23	1:A:43:LEU:HD12	0.41	1.93	187	1
1:A:50:LEU:HD22	1:A:59:TYR:CE1	0.40	2.52	63	1
1:A:35:GLY:C	1:A:36:ILE:HD13	0.40	2.41	216	1
1:A:70:VAL:C	1:A:71:LEU:HD23	0.40	2.41	102	1
1:A:40:GLN:HA	1:A:40:GLN:NE2	0.40	2.31	123	1
1:A:18:GLU:HA	1:A:18:GLU:OE1	0.40	2.17	134	1
1:A:36:ILE:N	1:A:36:ILE:CD1	0.40	2.84	236	1
1:A:55:THR:O	1:A:58:ASP:HB2	0.40	2.17	253	1
1:A:7:THR:CG2	1:A:13:ILE:HD12	0.40	2.46	67	1
1:A:37:PRO:HB2	1:A:38:PRO:HD2	0.40	1.92	71	1
1:A:21:ASP:OD1	1:A:25:ASN:CG	0.40	2.64	79	1
1:A:27:LYS:HE2	1:A:41:GLN:HB2	0.40	1.93	206	1
1:A:49:GLN:O	1:A:49:GLN:HG2	0.40	2.16	256	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	70/76 (92%)	67±2 (96±3%)	3±2 (4±2%)	0±1 (0±1%)	31	76
All	All	21070/22876 (92%)	20213 (96%)	777 (4%)	80 (0%)	31	76

All 26 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	63	LYS	19
1	A	8	LEU	9
1	A	46	ALA	6
1	A	64	GLU	6
1	A	52	ASP	5
1	A	11	LYS	4
1	A	32	ASP	4
1	A	19	PRO	4
1	A	56	LEU	3
1	A	57	SER	2
1	A	47	GLY	2
1	A	60	ASN	2
1	A	29	LYS	1
1	A	37	PRO	1
1	A	17	VAL	1
1	A	38	PRO	1
1	A	9	THR	1
1	A	39	ASP	1
1	A	30	ILE	1
1	A	36	ILE	1
1	A	49	GLN	1
1	A	65	SER	1
1	A	35	GLY	1
1	A	10	GLY	1
1	A	45	PHE	1
1	A	51	GLU	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	65/68 (96%)	59±4 (91±6%)	6±4 (9±6%)	11	57
All	All	19565/20468 (96%)	17812 (91%)	1753 (9%)	11	57

All 64 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	70	VAL	96
1	A	23	ILE	91
1	A	26	VAL	78
1	A	36	ILE	75
1	A	9	THR	69
1	A	32	ASP	67
1	A	63	LYS	65
1	A	71	LEU	56
1	A	60	ASN	53
1	A	67	LEU	50
1	A	22	THR	49
1	A	13	ILE	47
1	A	31	GLN	43
1	A	30	ILE	43
1	A	1	MET	43
1	A	52	ASP	38
1	A	44	ILE	38
1	A	61	ILE	38
1	A	43	LEU	37
1	A	16	GLU	36
1	A	39	ASP	36
1	A	8	LEU	36
1	A	33	LYS	35
1	A	64	GLU	34
1	A	21	ASP	34
1	A	56	LEU	33
1	A	69	LEU	26
1	A	18	GLU	25
1	A	14	THR	25

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Mol	Chain	Res	Type	Models (Total)
1	A	2	GLN	25
1	A	66	THR	21
1	A	57	SER	19
1	A	38	PRO	19
1	A	20	SER	19
1	A	49	GLN	18
1	A	3	ILE	18
1	A	51	GLU	16
1	A	48	LYS	16
1	A	15	LEU	15
1	A	7	THR	13
1	A	54	ARG	13
1	A	5	VAL	13
1	A	12	THR	12
1	A	34	GLU	10
1	A	25	ASN	9
1	A	6	LYS	9
1	A	62	GLN	9
1	A	42	ARG	9
1	A	50	LEU	9
1	A	19	PRO	9
1	A	11	LYS	8
1	A	24	GLU	6
1	A	68	HIS	6
1	A	29	LYS	6
1	A	4	PHE	6
1	A	65	SER	4
1	A	58	ASP	4
1	A	41	GLN	3
1	A	55	THR	3
1	A	40	GLN	3
1	A	17	VAL	3
1	A	37	PRO	2
1	A	27	LYS	1
1	A	59	TYR	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 42% for the well-defined parts and 39% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	426
Number of shifts mapped to atoms	426
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	72	-0.23 ± 0.20	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	68	0.16 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	72	-0.30 ± 0.12	None needed (< 0.5 ppm)
^{15}N	71	1.31 ± 0.33	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 42%, i.e. 417 atoms were assigned a chemical shift out of a possible 995. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	350/353 (99%)	141/143 (99%)	142/142 (100%)	67/68 (99%)
Sidechain	67/606 (11%)	0/392 (0%)	67/193 (35%)	0/21 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/36 (0%)	0/18 (0%)	0/17 (0%)	0/1 (0%)
Overall	417/995 (42%)	141/553 (25%)	209/352 (59%)	67/90 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 39%, i.e. 423 atoms were assigned a chemical shift out of a possible 1071. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	355/380 (93%)	143/155 (92%)	144/152 (95%)	68/73 (93%)
Sidechain	68/655 (10%)	0/423 (0%)	68/205 (33%)	0/27 (0%)
Aromatic	0/36 (0%)	0/18 (0%)	0/17 (0%)	0/1 (0%)
Overall	423/1071 (39%)	143/596 (24%)	212/374 (57%)	68/101 (67%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

