



# Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 12:42 am BST

PDB ID : 2LJ5  
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](mailto: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.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

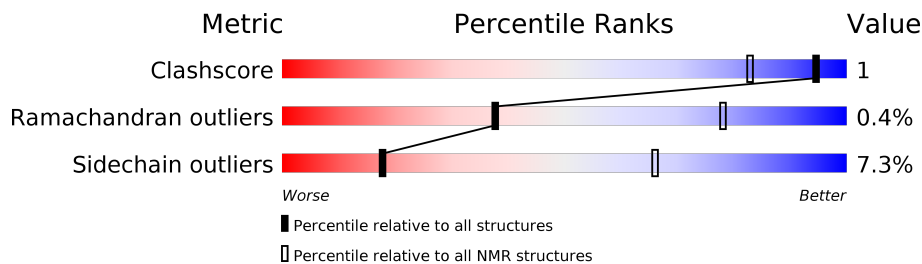
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 46%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	

## 2 Ensemble composition and analysis i

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)	0.35	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

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.

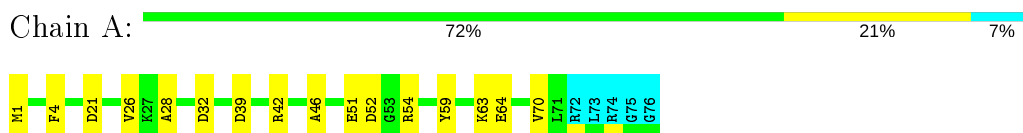
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	76	1231	378	629	105	118	1	0

## 4 Residue-property plots i

### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Ubiquitin

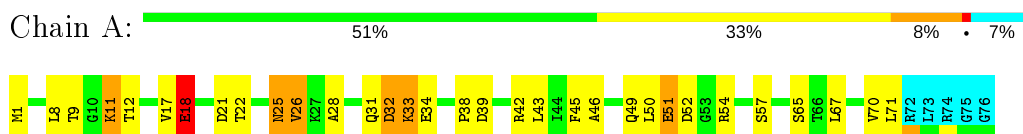


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

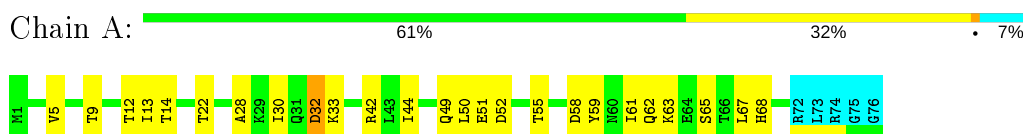
#### 4.2.1 Score per residue for model 1

- Molecule 1: Ubiquitin



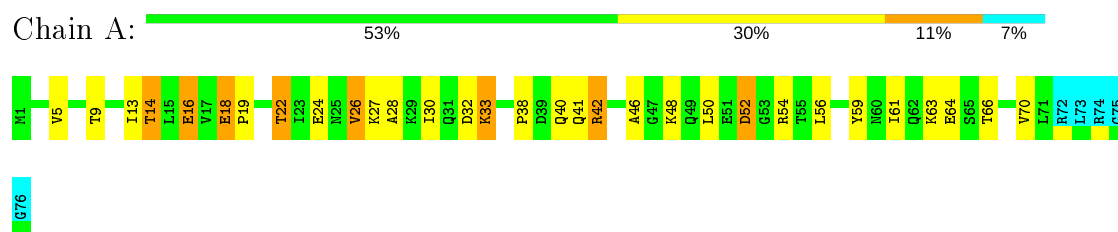
#### 4.2.2 Score per residue for model 2

- Molecule 1: Ubiquitin



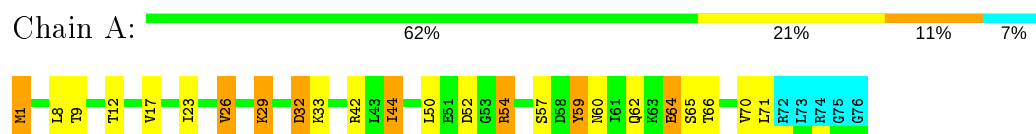
### 4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin



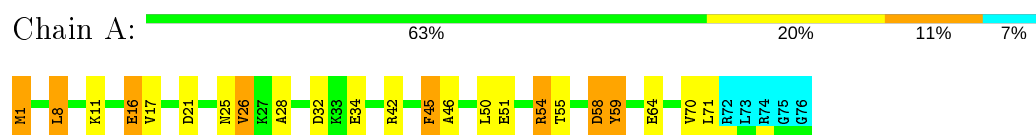
### 4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin



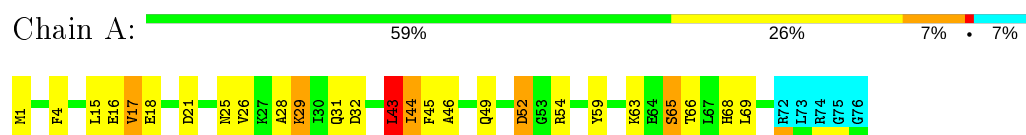
### 4.2.5 Score per residue for model 5

- Molecule 1: Ubiquitin



### 4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin



### 4.2.7 Score per residue for model 7

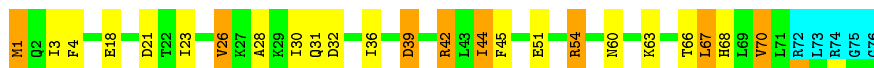
- Molecule 1: Ubiquitin





#### 4.2.8 Score per residue for model 8

- Molecule 1: Ubiquitin



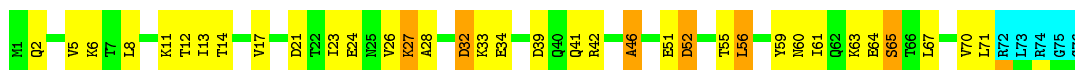
#### 4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin



#### 4.2.10 Score per residue for model 10

- Molecule 1: Ubiquitin



#### 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



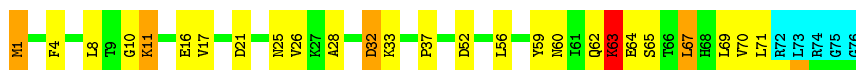
#### 4.2.14 Score per residue for model 14

- Molecule 1: Ubiquitin



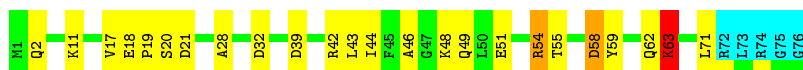
#### 4.2.15 Score per residue for model 15

- Molecule 1: Ubiquitin



#### 4.2.16 Score per residue for model 16

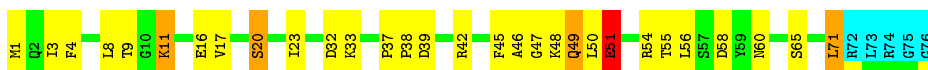
- Molecule 1: Ubiquitin



#### 4.2.17 Score per residue for model 17

- Molecule 1: Ubiquitin





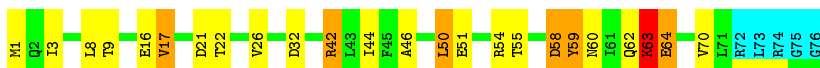
#### 4.2.18 Score per residue for model 18

- Molecule 1: Ubiquitin



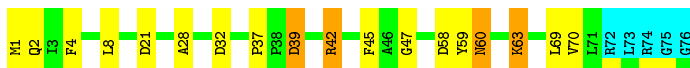
#### 4.2.19 Score per residue for model 19

- Molecule 1: Ubiquitin



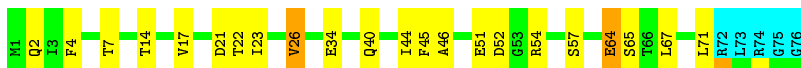
#### 4.2.20 Score per residue for model 20

- 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



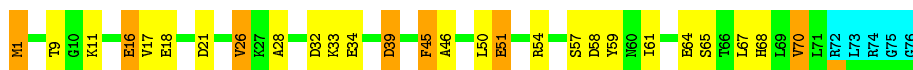
#### 4.2.24 Score per residue for model 24

- Molecule 1: Ubiquitin



#### 4.2.25 Score per residue for model 25

- Molecule 1: Ubiquitin



#### 4.2.26 Score per residue for model 26

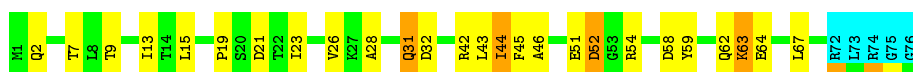
- Molecule 1: Ubiquitin



#### 4.2.27 Score per residue for model 27

- Molecule 1: Ubiquitin





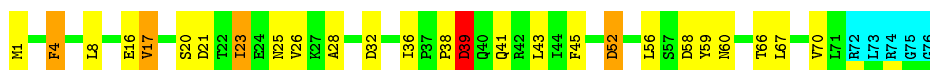
#### 4.2.28 Score per residue for model 28

- Molecule 1: Ubiquitin



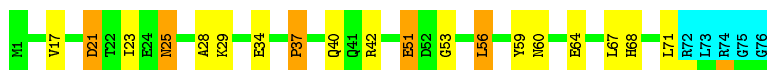
#### 4.2.29 Score per residue for model 29

- Molecule 1: Ubiquitin



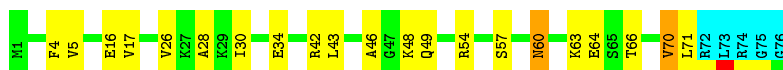
#### 4.2.30 Score per residue for model 30

- 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





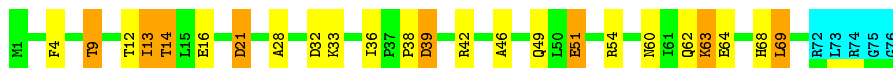
#### 4.2.33 Score per residue for model 33

- Molecule 1: Ubiquitin



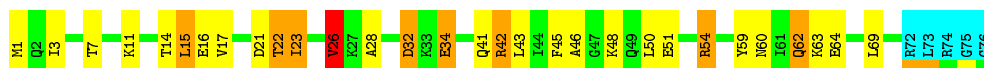
#### 4.2.34 Score per residue for model 34

- 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

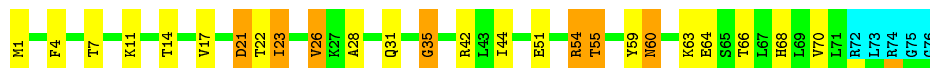
- Molecule 1: Ubiquitin





#### 4.2.38 Score per residue for model 38

- Molecule 1: Ubiquitin



#### 4.2.39 Score per residue for model 39

- Molecule 1: Ubiquitin



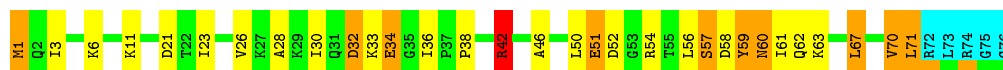
#### 4.2.40 Score per residue for model 40

- Molecule 1: Ubiquitin



#### 4.2.41 Score per residue for model 41

- Molecule 1: Ubiquitin



#### 4.2.42 Score per residue for model 42

- Molecule 1: Ubiquitin





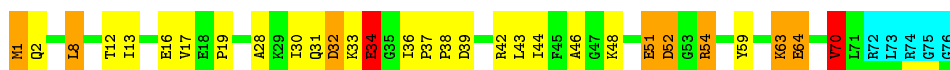
#### 4.2.43 Score per residue for model 43

- Molecule 1: Ubiquitin



#### 4.2.44 Score per residue for model 44

- Molecule 1: Ubiquitin



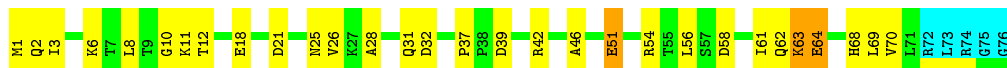
#### 4.2.45 Score per residue for model 45

- Molecule 1: Ubiquitin



#### 4.2.46 Score per residue for model 46

- Molecule 1: Ubiquitin



#### 4.2.47 Score per residue for model 47

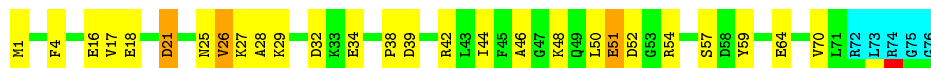
- Molecule 1: Ubiquitin





#### 4.2.48 Score per residue for model 48

- Molecule 1: Ubiquitin



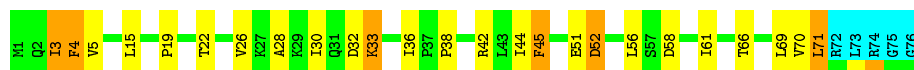
#### 4.2.49 Score per residue for model 49

- Molecule 1: Ubiquitin



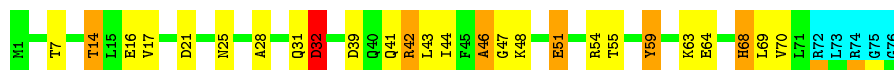
#### 4.2.50 Score per residue for model 50

- Molecule 1: Ubiquitin



#### 4.2.51 Score per residue for model 51

- Molecule 1: Ubiquitin

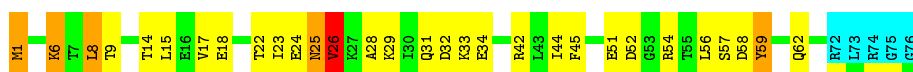


#### 4.2.52 Score per residue for model 52

- 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



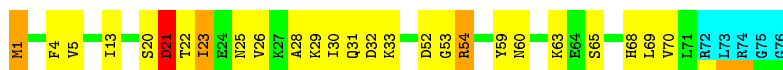
#### 4.2.55 Score per residue for model 55

- Molecule 1: Ubiquitin



#### 4.2.56 Score per residue for model 56

- Molecule 1: Ubiquitin



#### 4.2.57 Score per residue for model 57

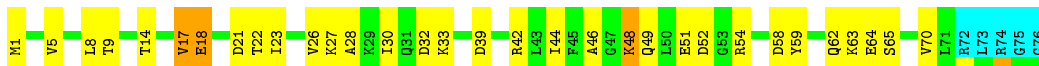
- Molecule 1: Ubiquitin





#### 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

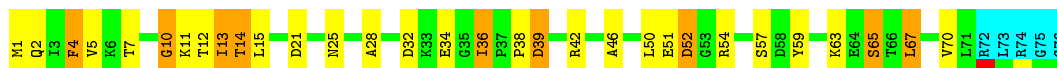
- Molecule 1: Ubiquitin





#### 4.2.63 Score per residue for model 63

- Molecule 1: Ubiquitin



#### 4.2.64 Score per residue for model 64

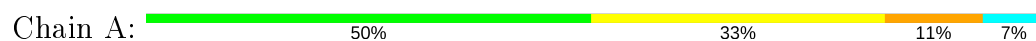
- Molecule 1: Ubiquitin



G76

#### 4.2.65 Score per residue for model 65

- Molecule 1: Ubiquitin



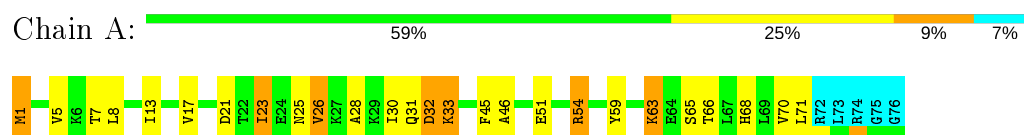
#### 4.2.66 Score per residue for model 66

- Molecule 1: Ubiquitin



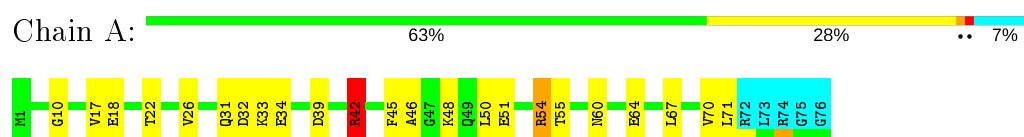
## 4.2.67 Score per residue for model 67

- Molecule 1: Ubiquitin



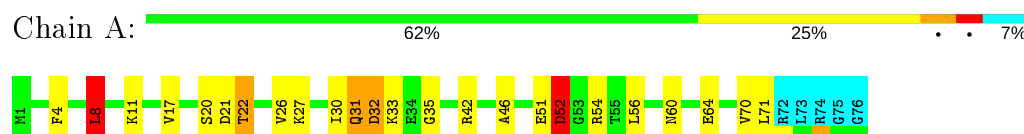
## 4.2.68 Score per residue for model 68

- Molecule 1: Ubiquitin



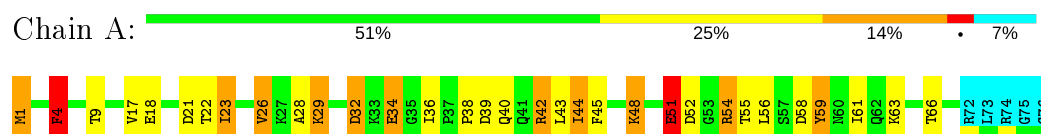
## 4.2.69 Score per residue for model 69

- Molecule 1: Ubiquitin



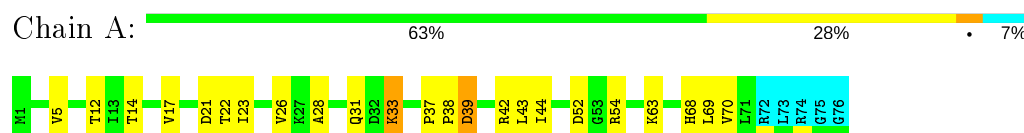
## 4.2.70 Score per residue for model 70

- Molecule 1: Ubiquitin



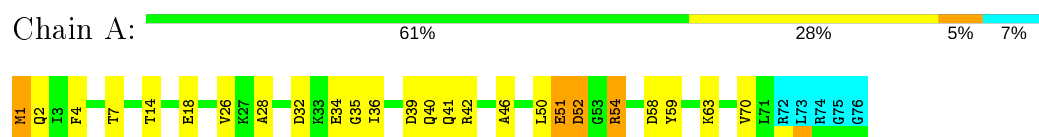
## 4.2.71 Score per residue for model 71

- Molecule 1: Ubiquitin



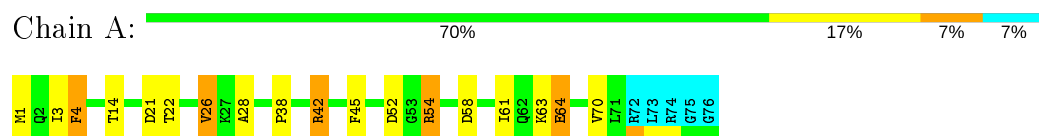
#### 4.2.72 Score per residue for model 72

- Molecule 1: Ubiquitin



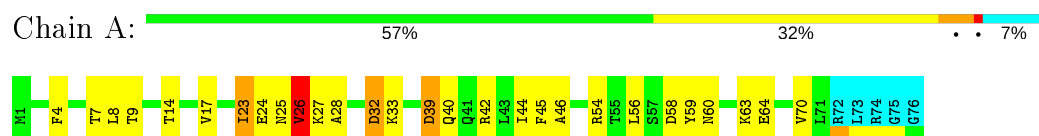
#### 4.2.73 Score per residue for model 73

- Molecule 1: Ubiquitin



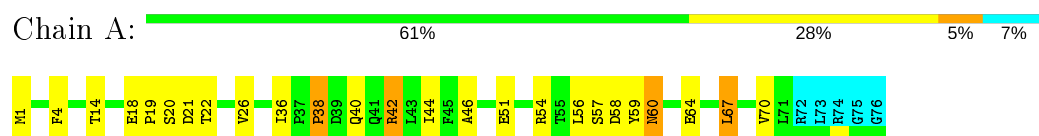
#### 4.2.74 Score per residue for model 74

- Molecule 1: Ubiquitin



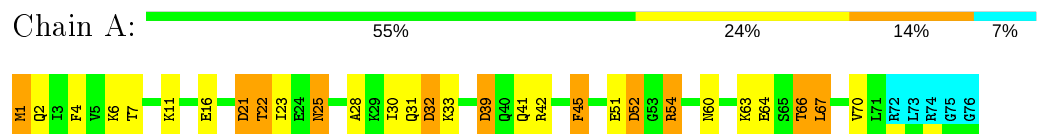
#### 4.2.75 Score per residue for model 75

- Molecule 1: Ubiquitin



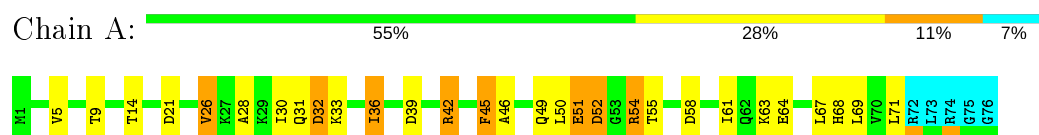
#### 4.2.76 Score per residue for model 76

- Molecule 1: Ubiquitin



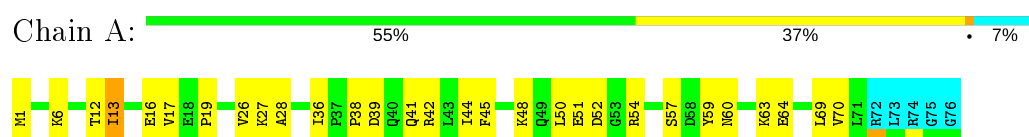
## 4.2.77 Score per residue for model 77

- Molecule 1: Ubiquitin



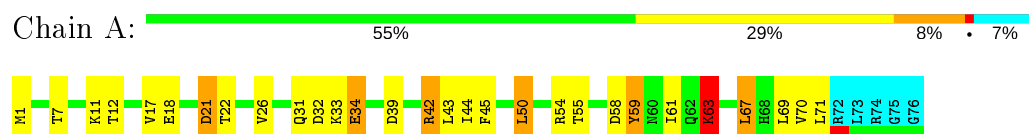
## 4.2.78 Score per residue for model 78

- Molecule 1: Ubiquitin



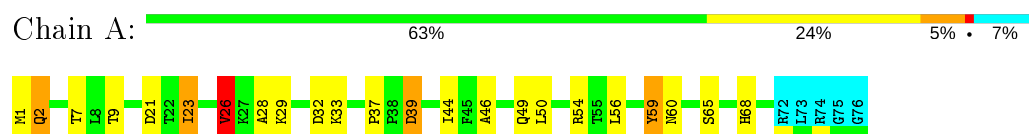
## 4.2.79 Score per residue for model 79

- Molecule 1: Ubiquitin



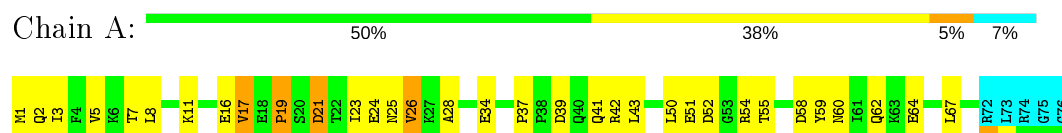
## 4.2.80 Score per residue for model 80

- Molecule 1: Ubiquitin



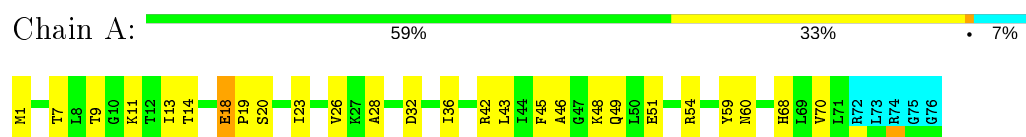
## 4.2.81 Score per residue for model 81

- Molecule 1: Ubiquitin



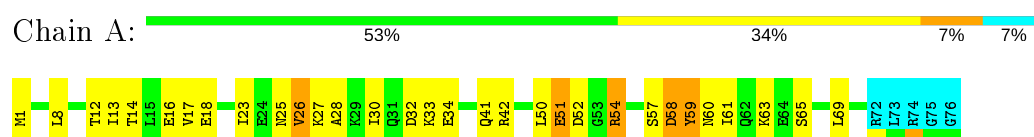
## 4.2.82 Score per residue for model 82

- Molecule 1: Ubiquitin



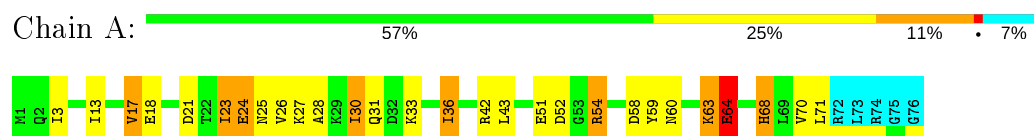
## 4.2.83 Score per residue for model 83

- Molecule 1: Ubiquitin



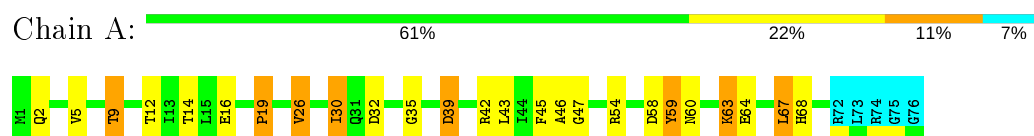
## 4.2.84 Score per residue for model 84

- Molecule 1: Ubiquitin



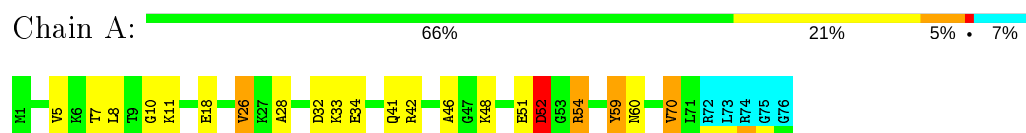
## 4.2.85 Score per residue for model 85

- Molecule 1: Ubiquitin



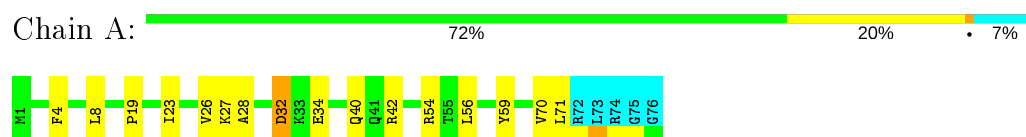
## 4.2.86 Score per residue for model 86

- Molecule 1: Ubiquitin



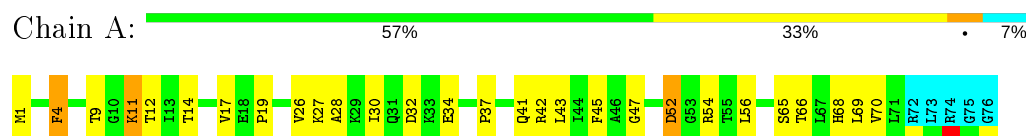
## 4.2.87 Score per residue for model 87

- Molecule 1: Ubiquitin



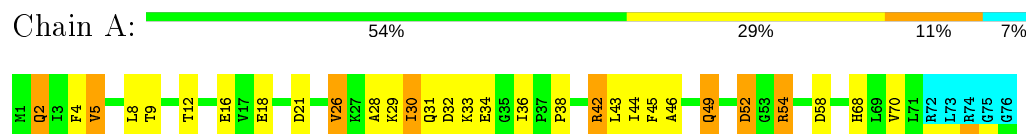
## 4.2.88 Score per residue for model 88

- Molecule 1: Ubiquitin



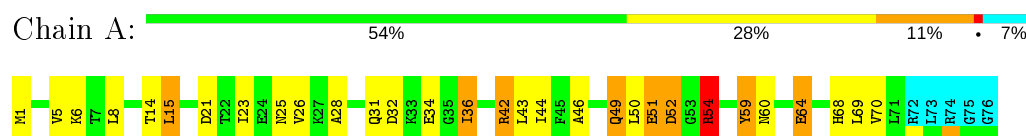
## 4.2.89 Score per residue for model 89

- Molecule 1: Ubiquitin



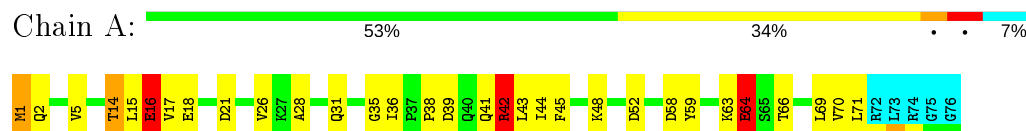
## 4.2.90 Score per residue for model 90

- Molecule 1: Ubiquitin



## 4.2.91 Score per residue for model 91

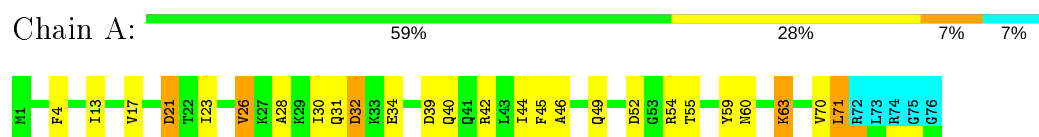
- Molecule 1: Ubiquitin





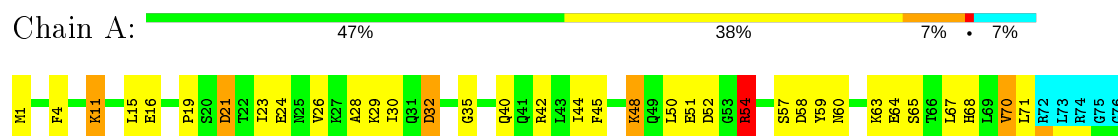
### 4.2.92 Score per residue for model 92

- Molecule 1: Ubiquitin



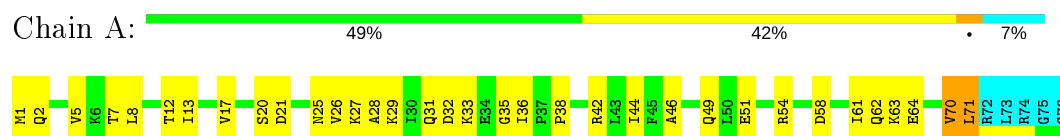
### 4.2.93 Score per residue for model 93

- Molecule 1: Ubiquitin



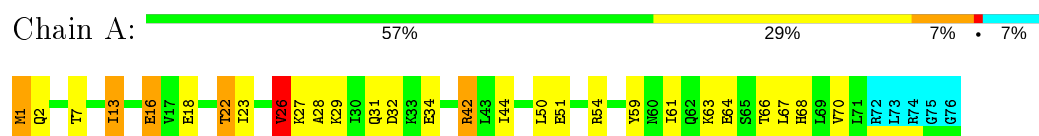
### 4.2.94 Score per residue for model 94

- Molecule 1: Ubiquitin



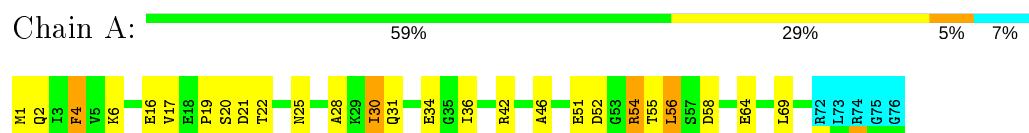
### 4.2.95 Score per residue for model 95

- Molecule 1: Ubiquitin



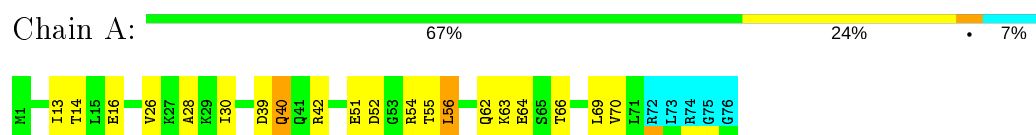
### 4.2.96 Score per residue for model 96

- Molecule 1: Ubiquitin



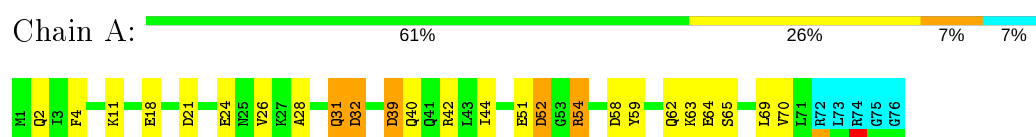
## 4.2.97 Score per residue for model 97

- Molecule 1: Ubiquitin



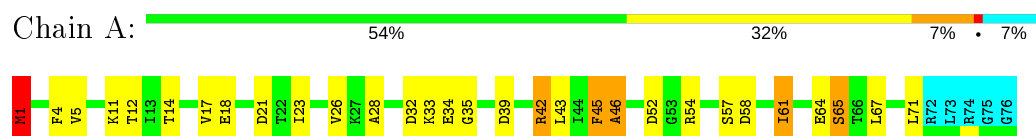
## 4.2.98 Score per residue for model 98

- Molecule 1: Ubiquitin



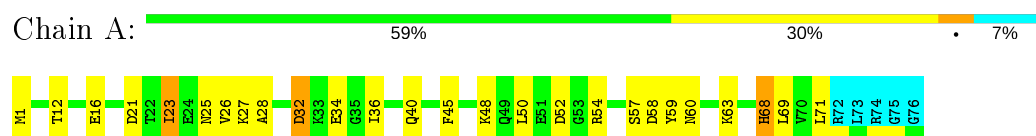
## 4.2.99 Score per residue for model 99

- Molecule 1: Ubiquitin



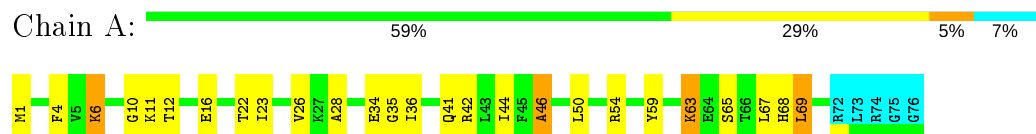
## 4.2.100 Score per residue for model 100

- Molecule 1: Ubiquitin



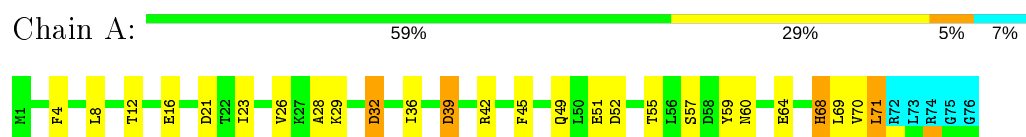
## 4.2.101 Score per residue for model 101

- Molecule 1: Ubiquitin



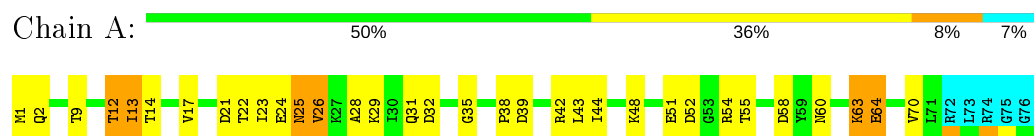
### 4.2.102 Score per residue for model 102

- Molecule 1: Ubiquitin



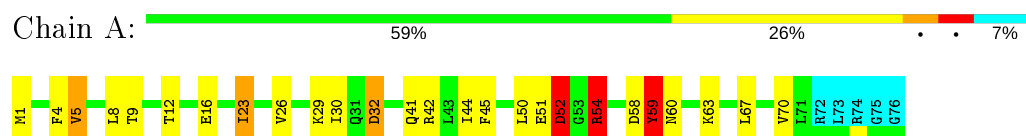
### 4.2.103 Score per residue for model 103

- Molecule 1: Ubiquitin



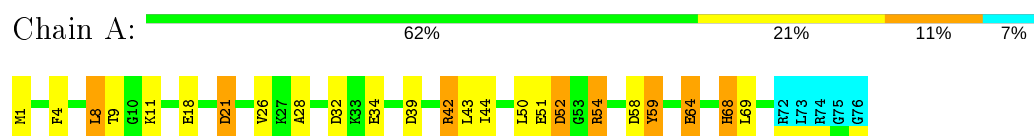
### 4.2.104 Score per residue for model 104

- Molecule 1: Ubiquitin



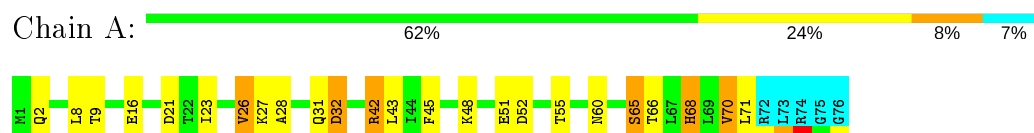
### 4.2.105 Score per residue for model 105

- Molecule 1: Ubiquitin



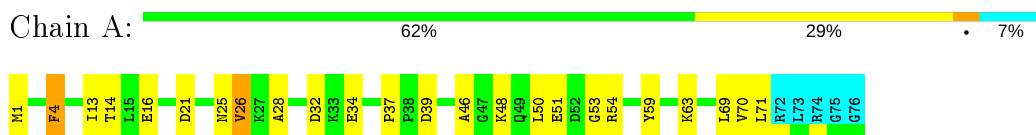
### 4.2.106 Score per residue for model 106

- Molecule 1: Ubiquitin



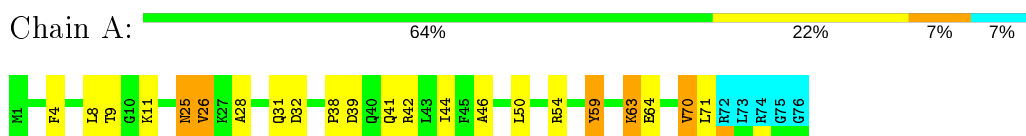
## 4.2.107 Score per residue for model 107

- Molecule 1: Ubiquitin



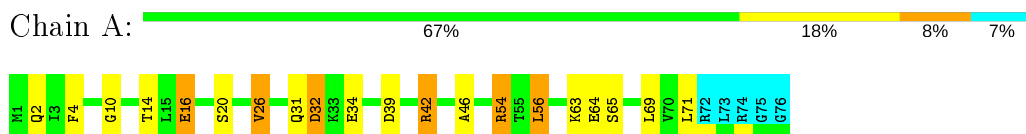
## 4.2.108 Score per residue for model 108

- Molecule 1: Ubiquitin



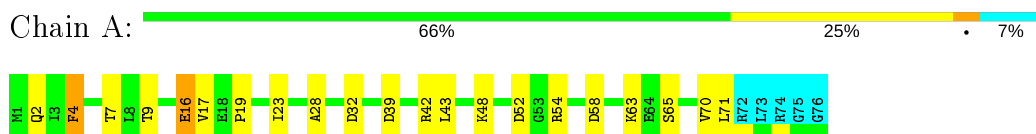
## 4.2.109 Score per residue for model 109

- Molecule 1: Ubiquitin



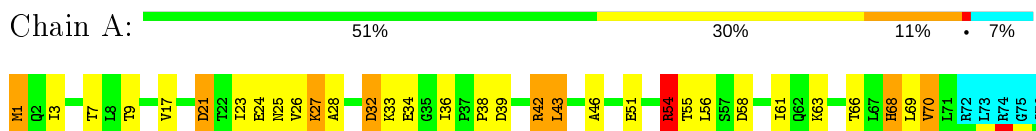
## 4.2.110 Score per residue for model 110

- Molecule 1: Ubiquitin



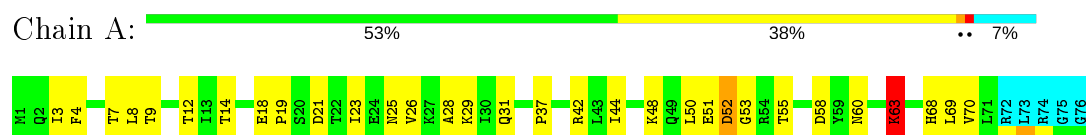
## 4.2.111 Score per residue for model 111

- Molecule 1: Ubiquitin



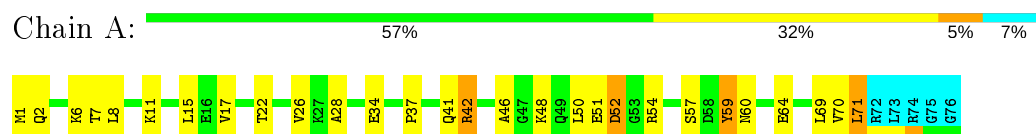
#### 4.2.112 Score per residue for model 112

- Molecule 1: Ubiquitin



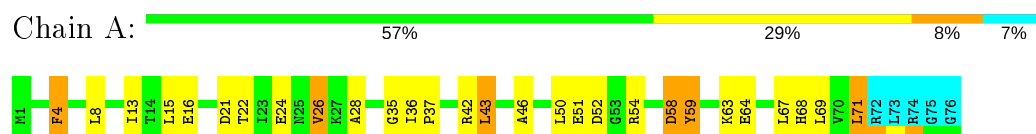
#### 4.2.113 Score per residue for model 113

- Molecule 1: Ubiquitin



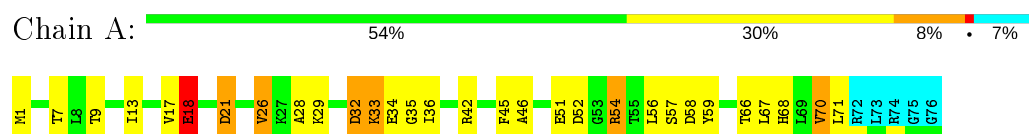
#### 4.2.114 Score per residue for model 114

- Molecule 1: Ubiquitin



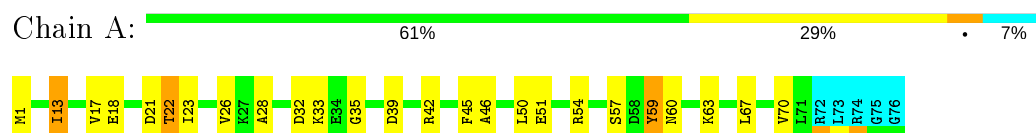
#### 4.2.115 Score per residue for model 115

- Molecule 1: Ubiquitin



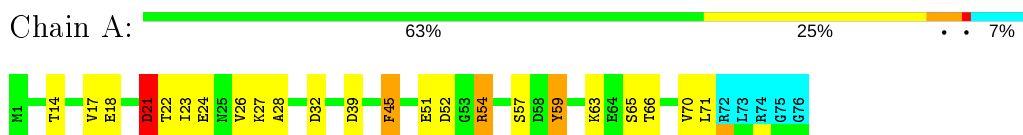
#### 4.2.116 Score per residue for model 116

- Molecule 1: Ubiquitin



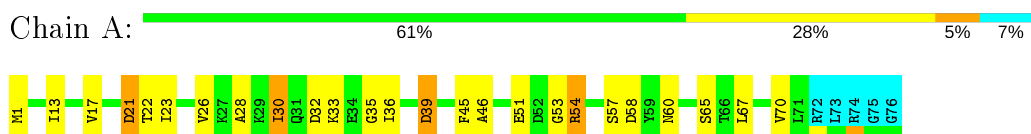
## 4.2.117 Score per residue for model 117

- Molecule 1: Ubiquitin



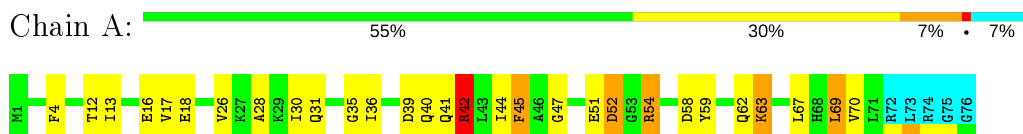
## 4.2.118 Score per residue for model 118

- Molecule 1: Ubiquitin



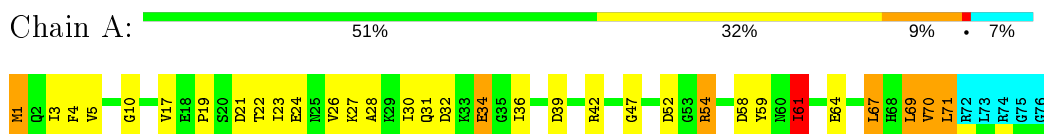
## 4.2.119 Score per residue for model 119

- Molecule 1: Ubiquitin



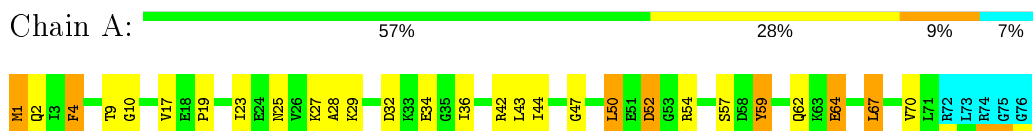
## 4.2.120 Score per residue for model 120

- Molecule 1: Ubiquitin



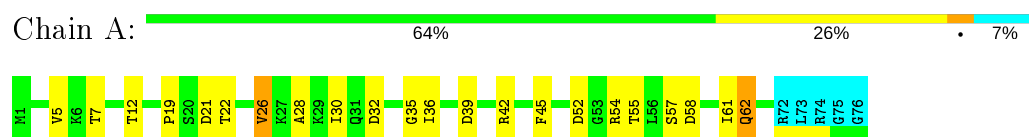
## 4.2.121 Score per residue for model 121

- Molecule 1: Ubiquitin



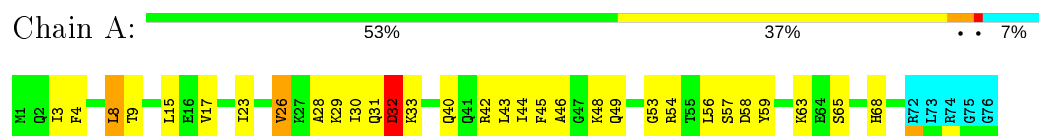
## 4.2.122 Score per residue for model 122

- Molecule 1: Ubiquitin



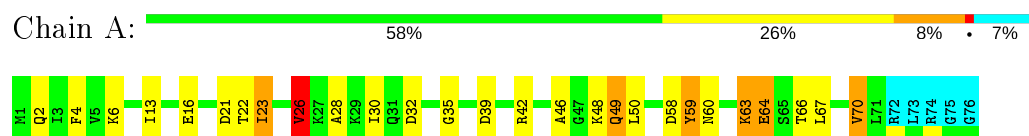
## 4.2.123 Score per residue for model 123

- Molecule 1: Ubiquitin



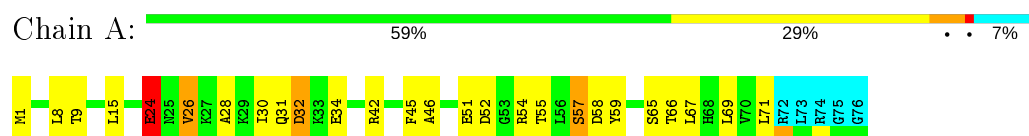
## 4.2.124 Score per residue for model 124

- Molecule 1: Ubiquitin



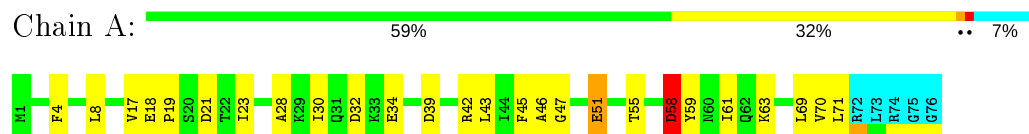
## 4.2.125 Score per residue for model 125

- Molecule 1: Ubiquitin



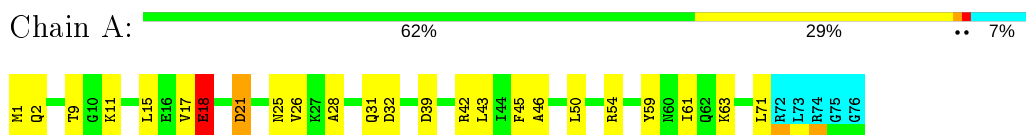
## 4.2.126 Score per residue for model 126

- Molecule 1: Ubiquitin



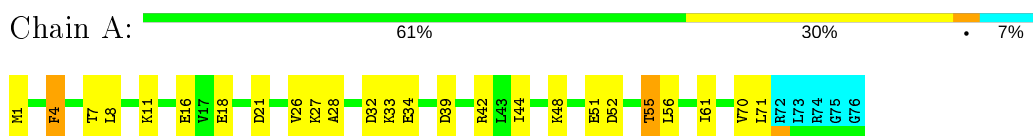
## 4.2.127 Score per residue for model 127

- Molecule 1: Ubiquitin



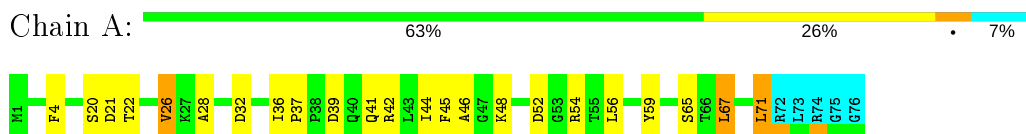
## 4.2.128 Score per residue for model 128

- Molecule 1: Ubiquitin



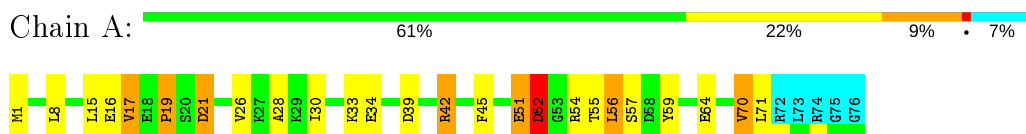
## 4.2.129 Score per residue for model 129

- Molecule 1: Ubiquitin



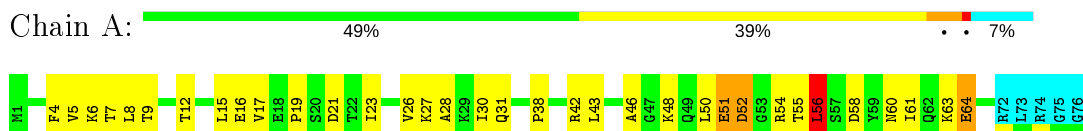
## 4.2.130 Score per residue for model 130

- Molecule 1: Ubiquitin



## 4.2.131 Score per residue for model 131

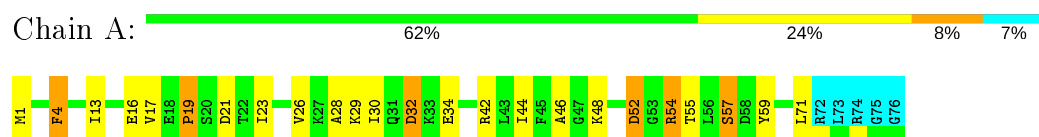
- Molecule 1: Ubiquitin





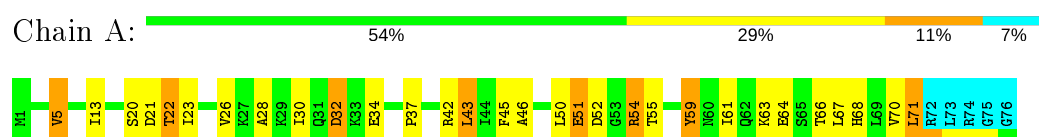
#### 4.2.132 Score per residue for model 132

- Molecule 1: Ubiquitin



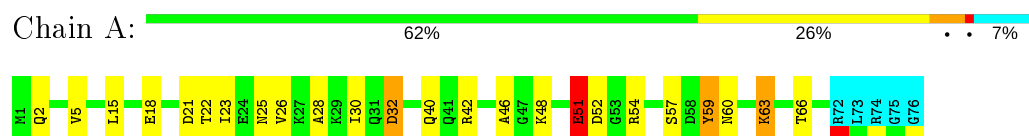
#### 4.2.133 Score per residue for model 133

- Molecule 1: Ubiquitin



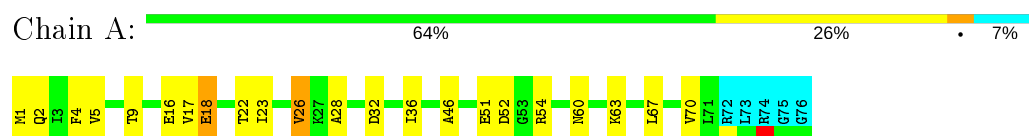
#### 4.2.134 Score per residue for model 134

- Molecule 1: Ubiquitin



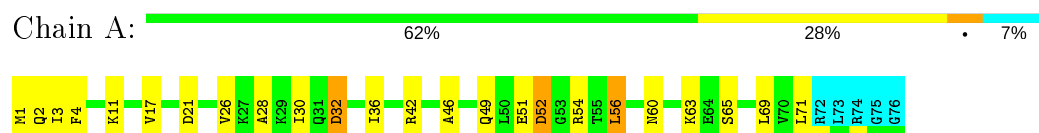
#### 4.2.135 Score per residue for model 135

- Molecule 1: Ubiquitin



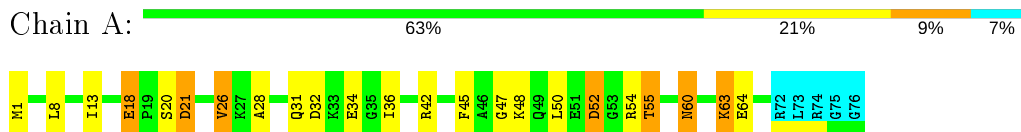
#### 4.2.136 Score per residue for model 136

- Molecule 1: Ubiquitin



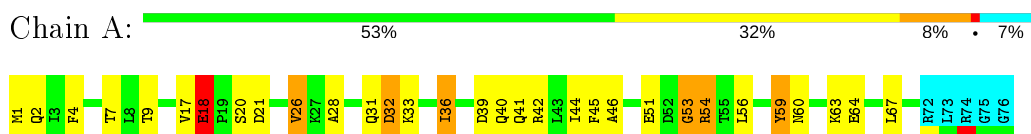
## 4.2.137 Score per residue for model 137

- Molecule 1: Ubiquitin



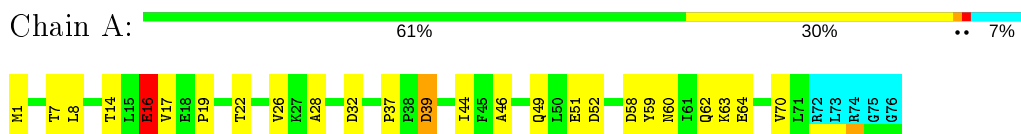
## 4.2.138 Score per residue for model 138

- Molecule 1: Ubiquitin



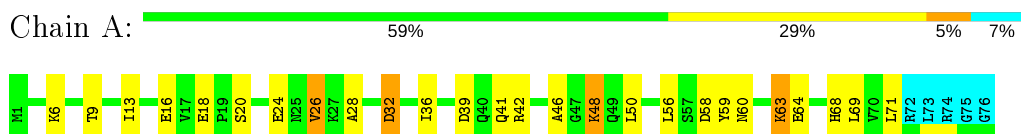
## 4.2.139 Score per residue for model 139

- Molecule 1: Ubiquitin



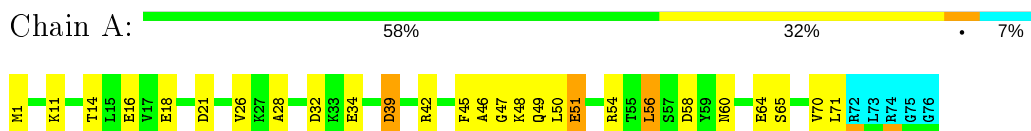
## 4.2.140 Score per residue for model 140

- Molecule 1: Ubiquitin



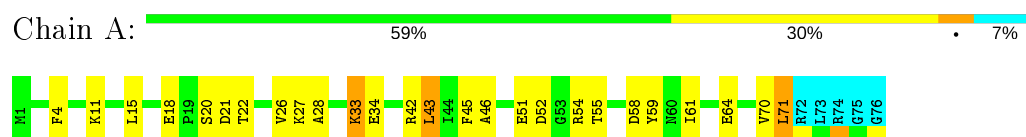
## 4.2.141 Score per residue for model 141

- Molecule 1: Ubiquitin



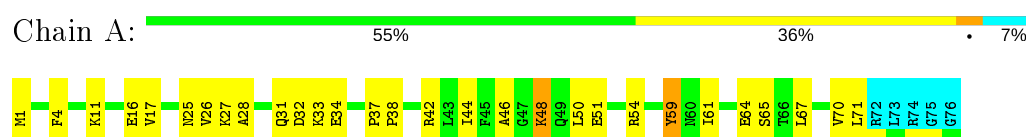
## 4.2.142 Score per residue for model 142

- Molecule 1: Ubiquitin



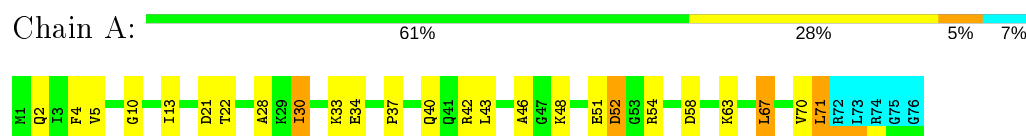
## 4.2.143 Score per residue for model 143

- Molecule 1: Ubiquitin



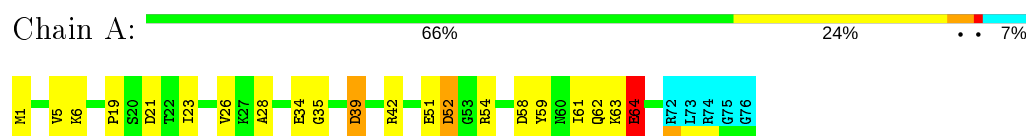
## 4.2.144 Score per residue for model 144

- Molecule 1: Ubiquitin



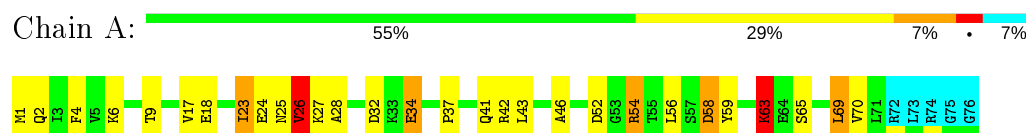
## 4.2.145 Score per residue for model 145

- Molecule 1: Ubiquitin



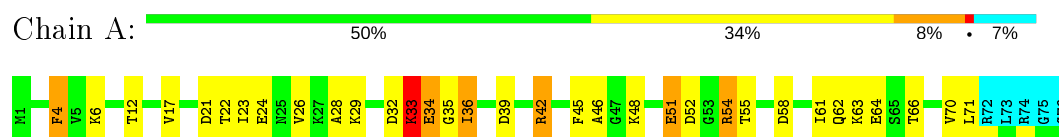
## 4.2.146 Score per residue for model 146

- Molecule 1: Ubiquitin



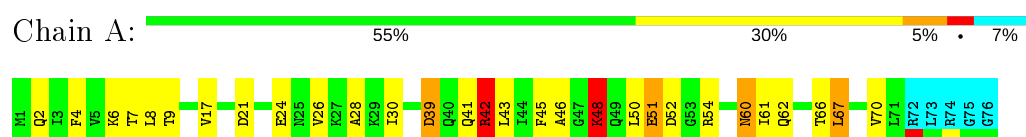
## 4.2.147 Score per residue for model 147

- Molecule 1: Ubiquitin



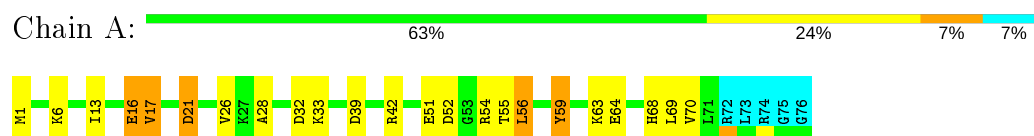
## 4.2.148 Score per residue for model 148

- Molecule 1: Ubiquitin



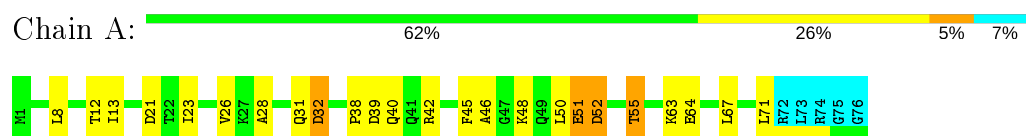
## 4.2.149 Score per residue for model 149

- Molecule 1: Ubiquitin



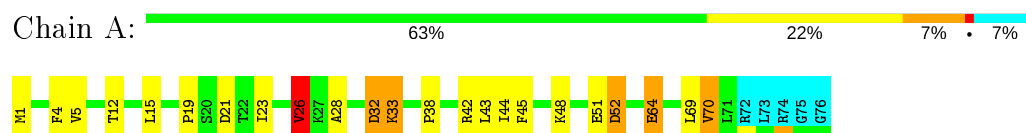
## 4.2.150 Score per residue for model 150

- Molecule 1: Ubiquitin



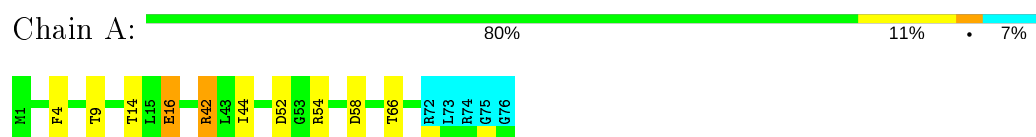
## 4.2.151 Score per residue for model 151

- Molecule 1: Ubiquitin



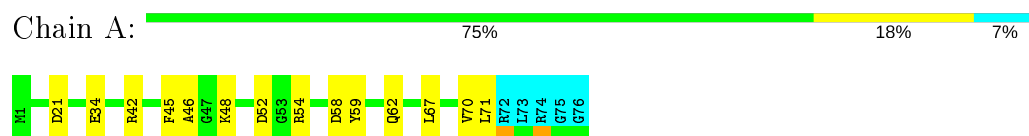
## 4.2.152 Score per residue for model 152

- Molecule 1: Ubiquitin



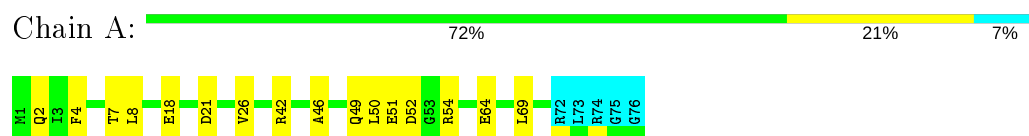
## 4.2.153 Score per residue for model 153

- Molecule 1: Ubiquitin



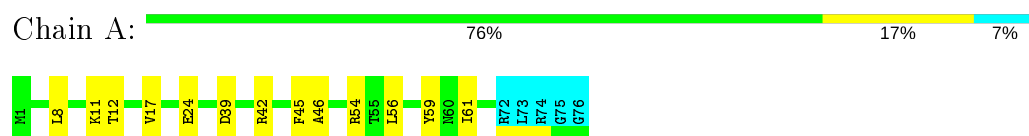
## 4.2.154 Score per residue for model 154

- Molecule 1: Ubiquitin



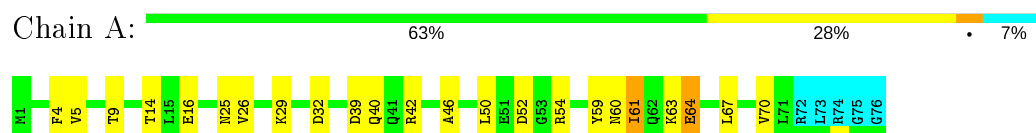
## 4.2.155 Score per residue for model 155

- Molecule 1: Ubiquitin



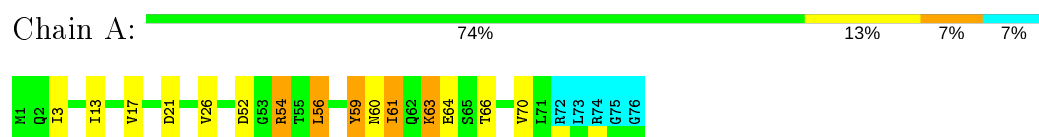
## 4.2.156 Score per residue for model 156

- Molecule 1: Ubiquitin



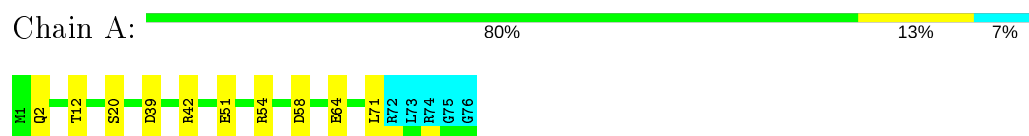
## 4.2.157 Score per residue for model 157

- Molecule 1: Ubiquitin



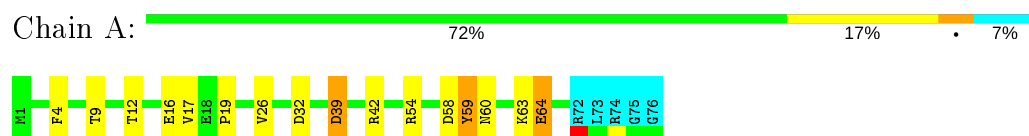
## 4.2.158 Score per residue for model 158

- Molecule 1: Ubiquitin



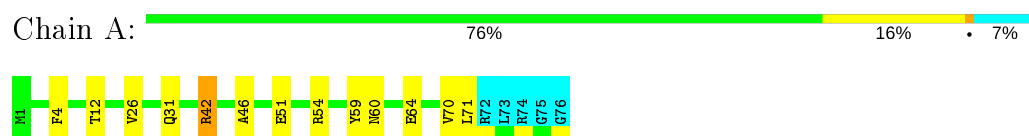
## 4.2.159 Score per residue for model 159

- Molecule 1: Ubiquitin



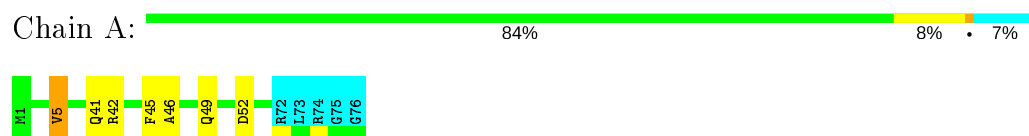
## 4.2.160 Score per residue for model 160

- Molecule 1: Ubiquitin



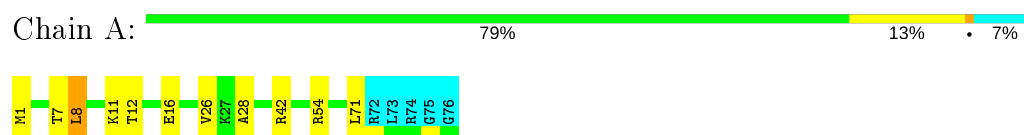
## 4.2.161 Score per residue for model 161

- Molecule 1: Ubiquitin



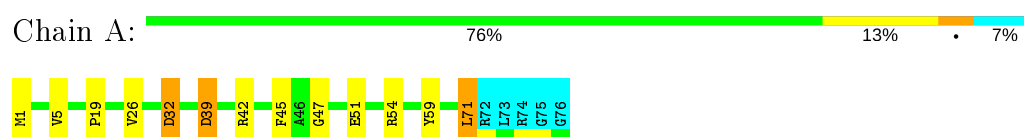
#### 4.2.162 Score per residue for model 162

- Molecule 1: Ubiquitin



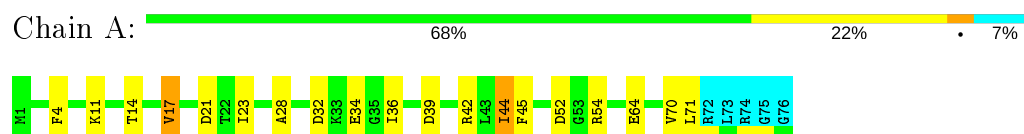
#### 4.2.163 Score per residue for model 163

- Molecule 1: Ubiquitin



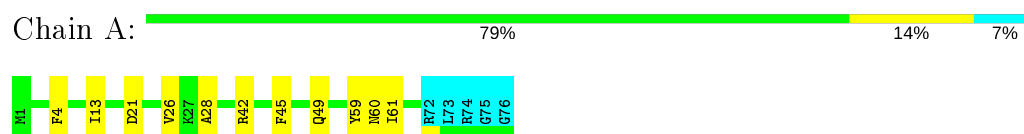
#### 4.2.164 Score per residue for model 164

- Molecule 1: Ubiquitin



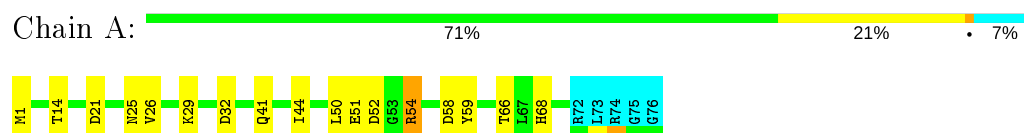
#### 4.2.165 Score per residue for model 165

- Molecule 1: Ubiquitin



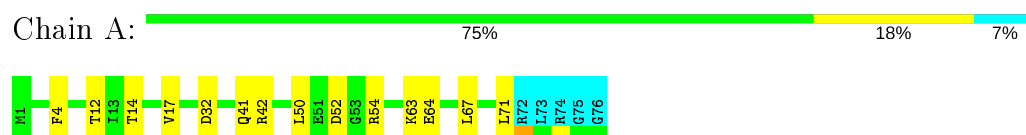
#### 4.2.166 Score per residue for model 166

- Molecule 1: Ubiquitin



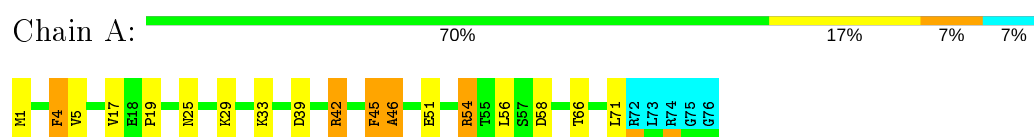
#### 4.2.167 Score per residue for model 167

- Molecule 1: Ubiquitin



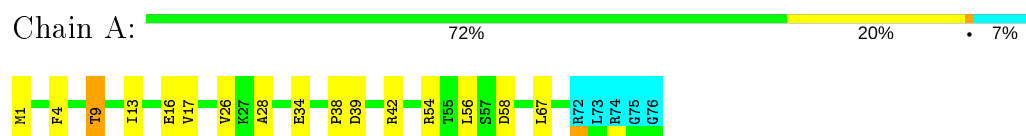
#### 4.2.168 Score per residue for model 168

- Molecule 1: Ubiquitin



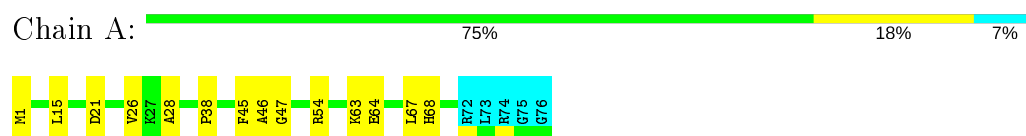
#### 4.2.169 Score per residue for model 169

- Molecule 1: Ubiquitin



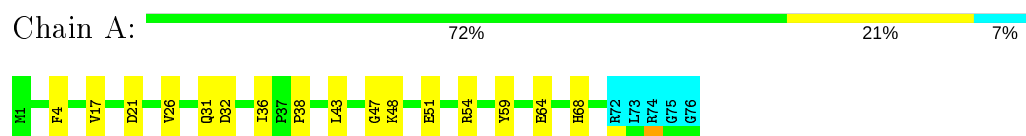
#### 4.2.170 Score per residue for model 170

- Molecule 1: Ubiquitin



#### 4.2.171 Score per residue for model 171

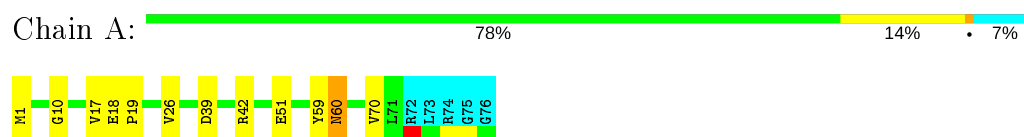
- Molecule 1: Ubiquitin





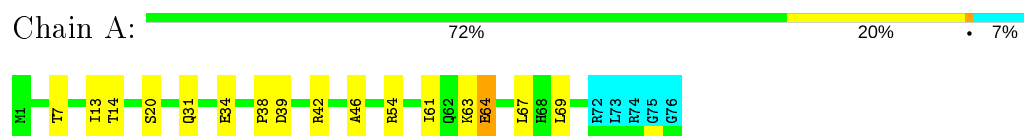
## 4.2.172 Score per residue for model 172

- Molecule 1: Ubiquitin



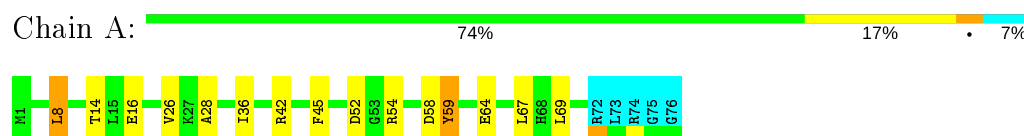
## 4.2.173 Score per residue for model 173

- Molecule 1: Ubiquitin



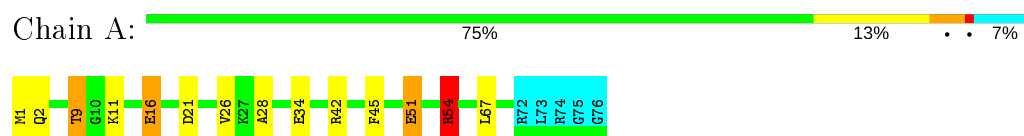
## 4.2.174 Score per residue for model 174

- Molecule 1: Ubiquitin



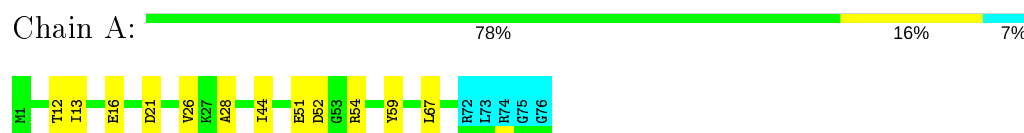
## 4.2.175 Score per residue for model 175

- Molecule 1: Ubiquitin



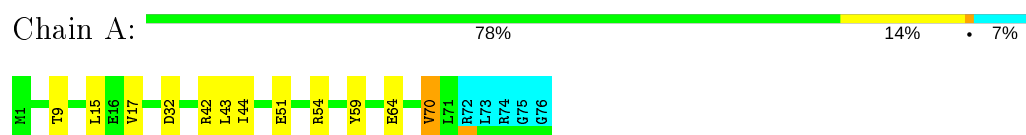
## 4.2.176 Score per residue for model 176

- Molecule 1: Ubiquitin



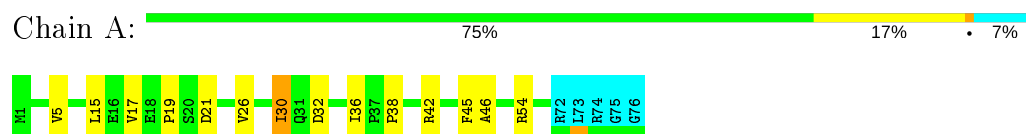
## 4.2.177 Score per residue for model 177

- Molecule 1: Ubiquitin



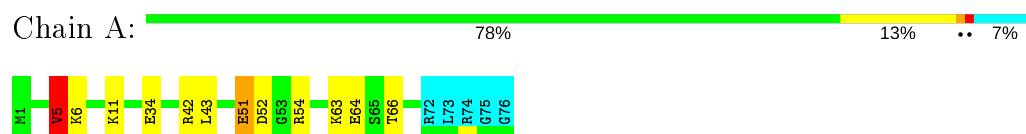
## 4.2.178 Score per residue for model 178

- Molecule 1: Ubiquitin



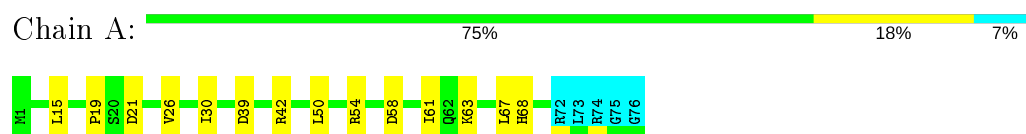
## 4.2.179 Score per residue for model 179

- Molecule 1: Ubiquitin



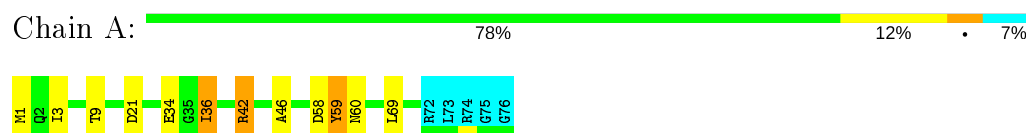
## 4.2.180 Score per residue for model 180

- Molecule 1: Ubiquitin



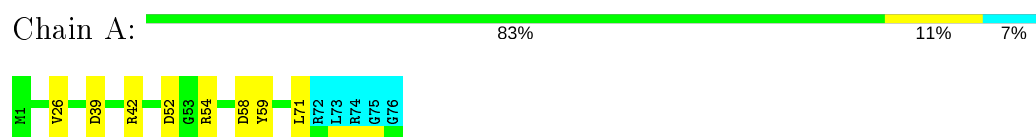
## 4.2.181 Score per residue for model 181

- Molecule 1: Ubiquitin



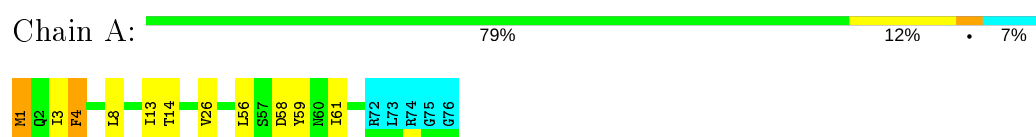
## 4.2.182 Score per residue for model 182

- Molecule 1: Ubiquitin



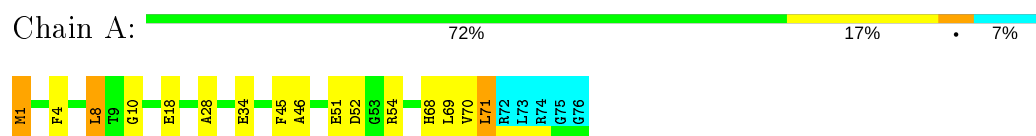
## 4.2.183 Score per residue for model 183

- Molecule 1: Ubiquitin



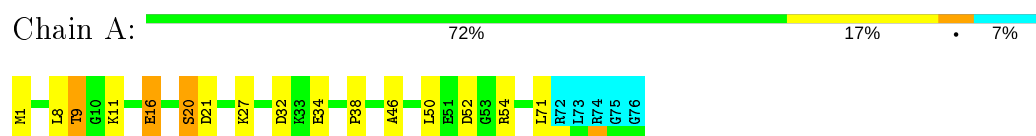
## 4.2.184 Score per residue for model 184

- Molecule 1: Ubiquitin



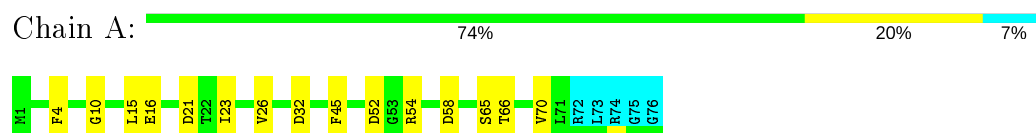
## 4.2.185 Score per residue for model 185

- Molecule 1: Ubiquitin



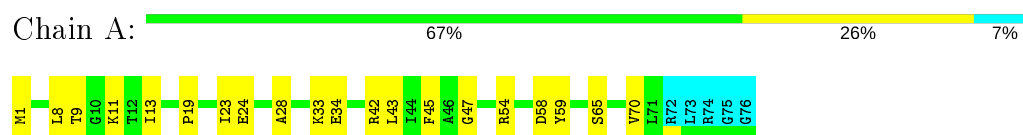
## 4.2.186 Score per residue for model 186

- Molecule 1: Ubiquitin



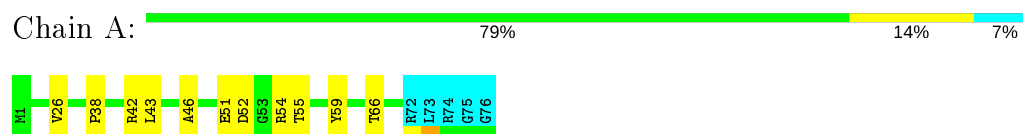
## 4.2.187 Score per residue for model 187

- Molecule 1: Ubiquitin



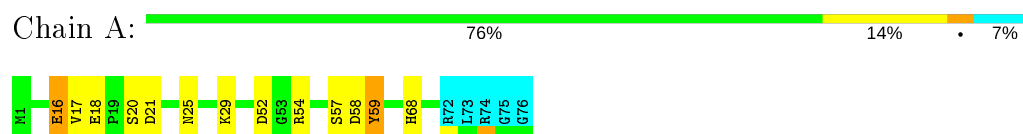
## 4.2.188 Score per residue for model 188

- Molecule 1: Ubiquitin



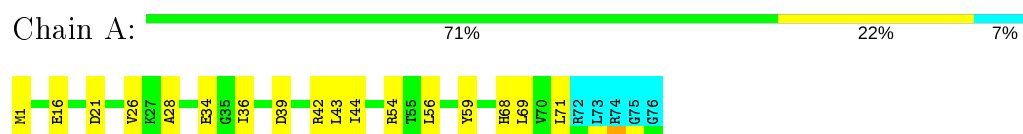
## 4.2.189 Score per residue for model 189

- Molecule 1: Ubiquitin



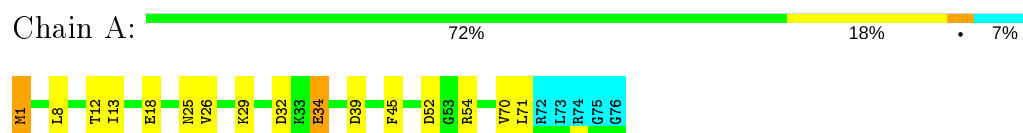
## 4.2.190 Score per residue for model 190

- Molecule 1: Ubiquitin



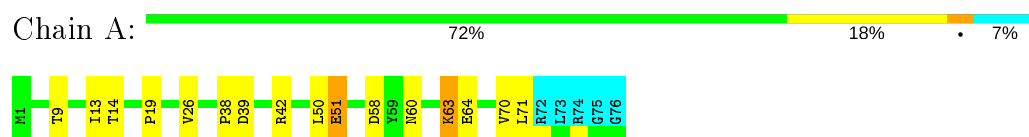
## 4.2.191 Score per residue for model 191

- Molecule 1: Ubiquitin



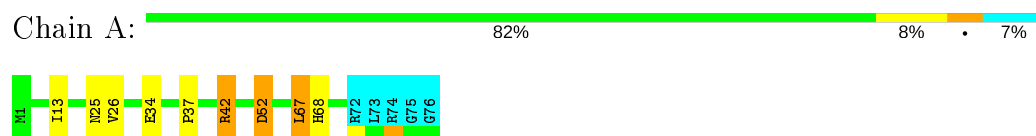
## 4.2.192 Score per residue for model 192

- Molecule 1: Ubiquitin



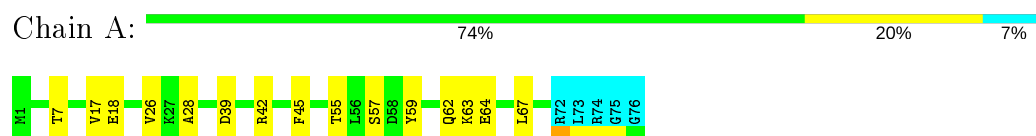
## 4.2.193 Score per residue for model 193

- Molecule 1: Ubiquitin



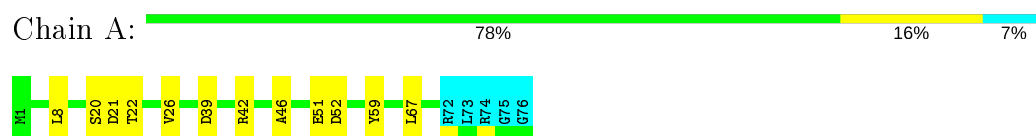
## 4.2.194 Score per residue for model 194

- Molecule 1: Ubiquitin



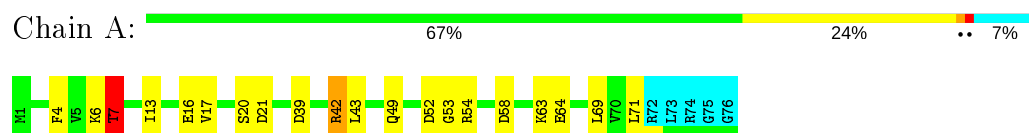
## 4.2.195 Score per residue for model 195

- Molecule 1: Ubiquitin



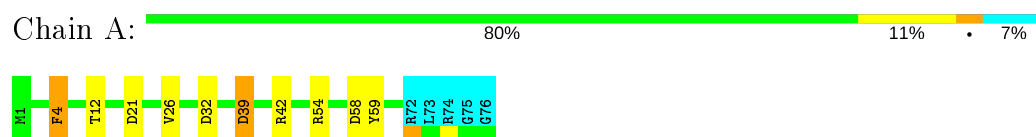
## 4.2.196 Score per residue for model 196

- Molecule 1: Ubiquitin



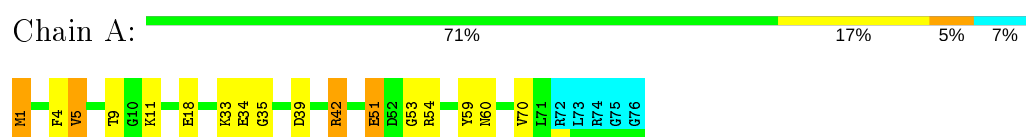
## 4.2.197 Score per residue for model 197

- Molecule 1: Ubiquitin



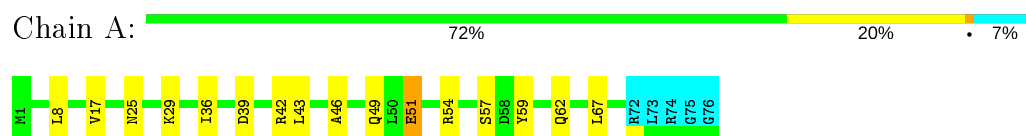
## 4.2.198 Score per residue for model 198

- Molecule 1: Ubiquitin



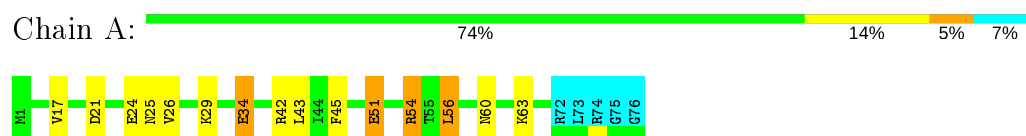
## 4.2.199 Score per residue for model 199

- Molecule 1: Ubiquitin



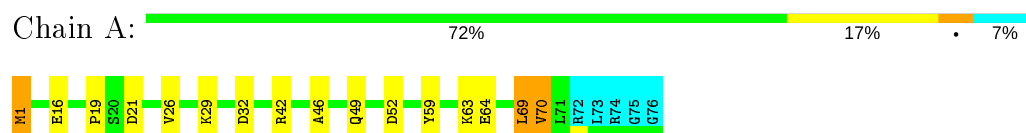
## 4.2.200 Score per residue for model 200

- Molecule 1: Ubiquitin



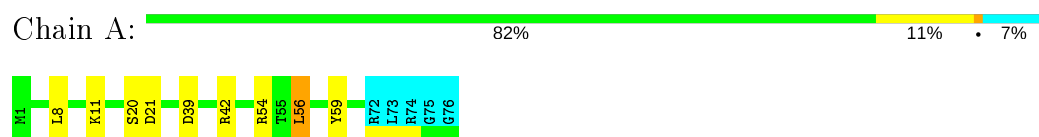
## 4.2.201 Score per residue for model 201

- Molecule 1: Ubiquitin



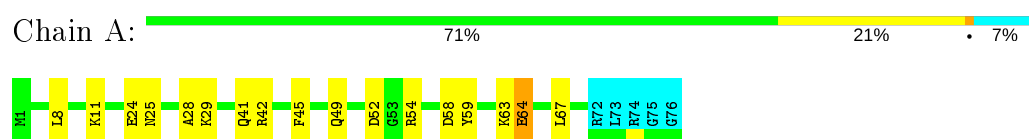
#### 4.2.202 Score per residue for model 202

- Molecule 1: Ubiquitin



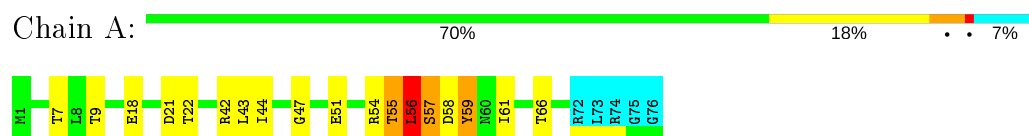
#### 4.2.203 Score per residue for model 203

- Molecule 1: Ubiquitin



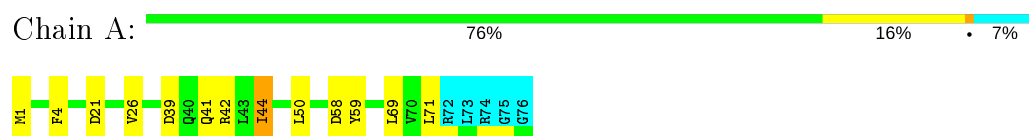
#### 4.2.204 Score per residue for model 204

- Molecule 1: Ubiquitin



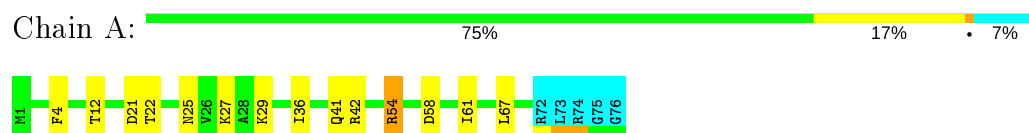
#### 4.2.205 Score per residue for model 205

- Molecule 1: Ubiquitin



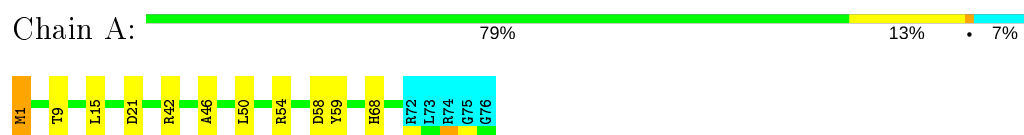
#### 4.2.206 Score per residue for model 206

- Molecule 1: Ubiquitin



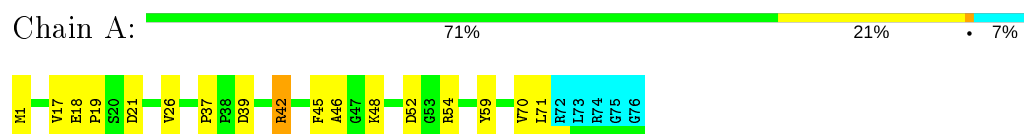
## 4.2.207 Score per residue for model 207

- Molecule 1: Ubiquitin



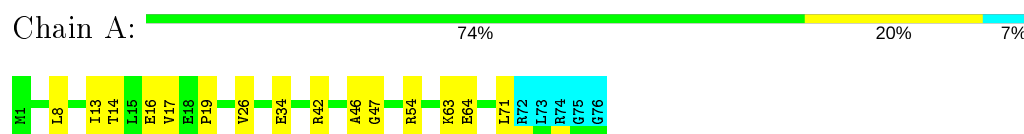
## 4.2.208 Score per residue for model 208

- Molecule 1: Ubiquitin



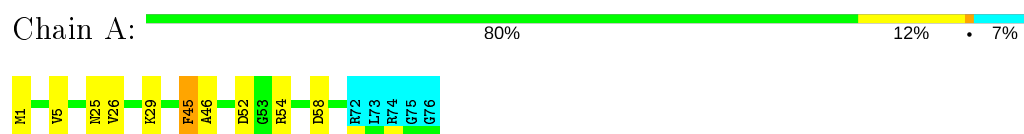
## 4.2.209 Score per residue for model 209

- Molecule 1: Ubiquitin



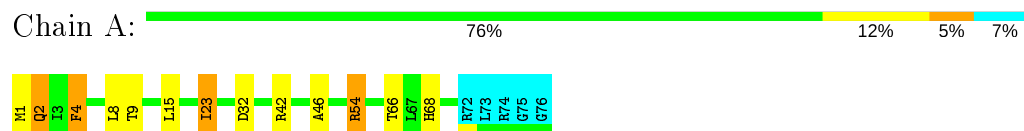
## 4.2.210 Score per residue for model 210 (medoid)

- Molecule 1: Ubiquitin



## 4.2.211 Score per residue for model 211

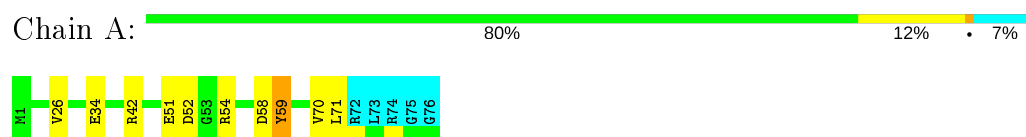
- Molecule 1: Ubiquitin





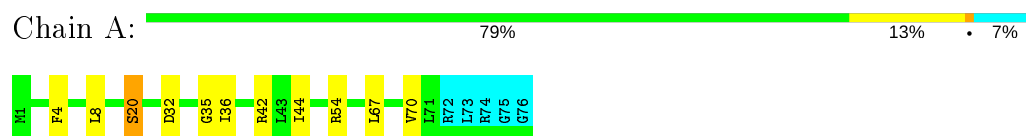
#### 4.2.212 Score per residue for model 212

- Molecule 1: Ubiquitin



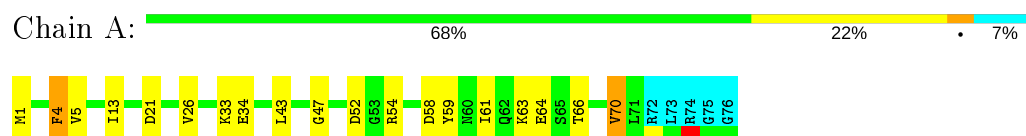
#### 4.2.213 Score per residue for model 213

- Molecule 1: Ubiquitin



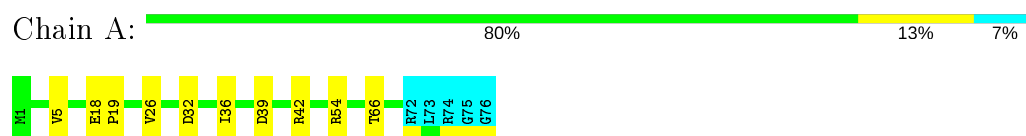
#### 4.2.214 Score per residue for model 214

- Molecule 1: Ubiquitin



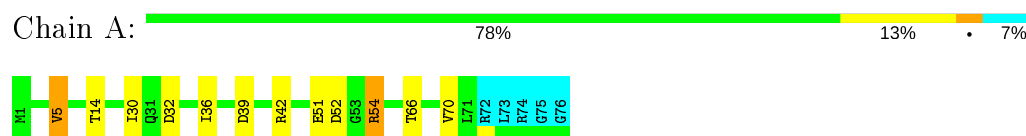
#### 4.2.215 Score per residue for model 215

- Molecule 1: Ubiquitin



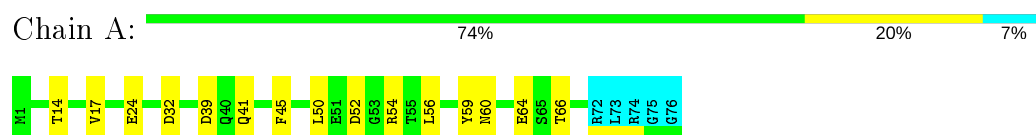
#### 4.2.216 Score per residue for model 216

- Molecule 1: Ubiquitin



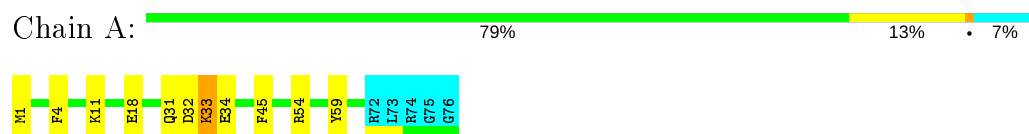
## 4.2.217 Score per residue for model 217

- Molecule 1: Ubiquitin



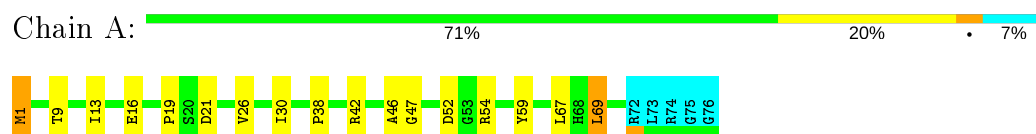
## 4.2.218 Score per residue for model 218

- Molecule 1: Ubiquitin



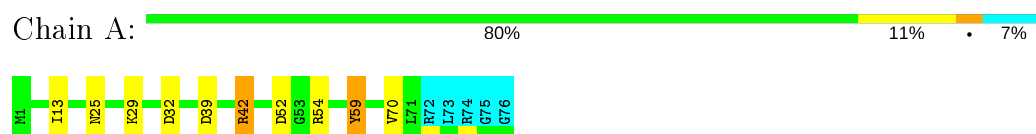
## 4.2.219 Score per residue for model 219

- Molecule 1: Ubiquitin



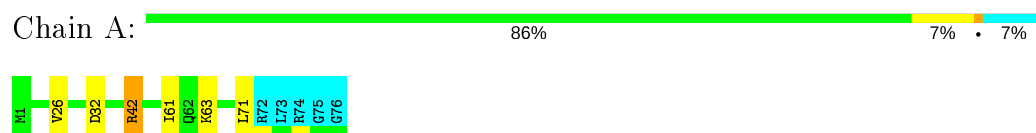
## 4.2.220 Score per residue for model 220

- Molecule 1: Ubiquitin



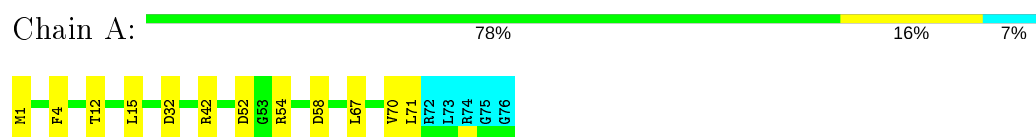
## 4.2.221 Score per residue for model 221

- Molecule 1: Ubiquitin



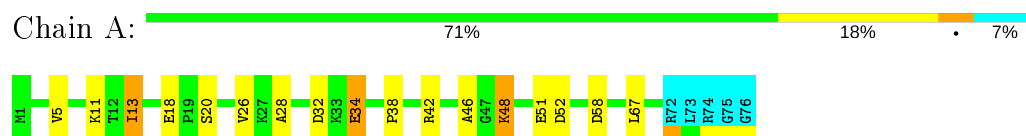
#### 4.2.222 Score per residue for model 222

- Molecule 1: Ubiquitin



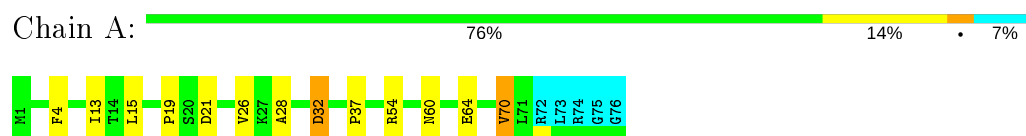
#### 4.2.223 Score per residue for model 223

- Molecule 1: Ubiquitin



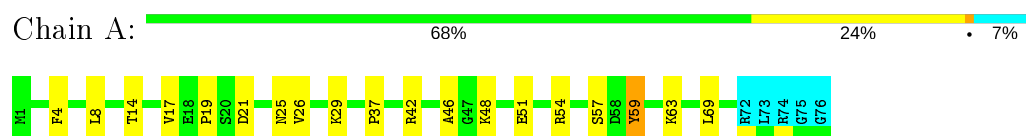
#### 4.2.224 Score per residue for model 224

- Molecule 1: Ubiquitin



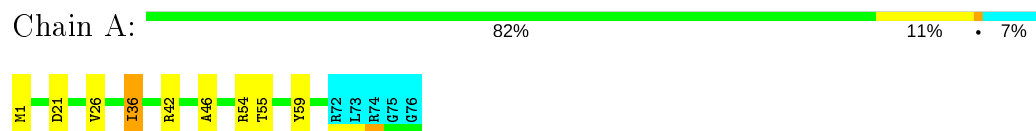
#### 4.2.225 Score per residue for model 225

- Molecule 1: Ubiquitin



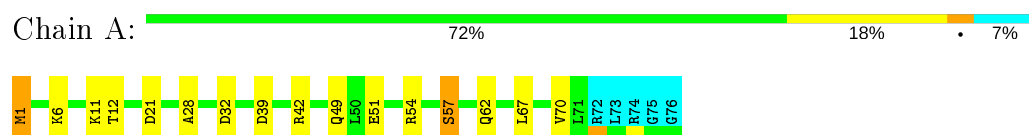
#### 4.2.226 Score per residue for model 226

- Molecule 1: Ubiquitin



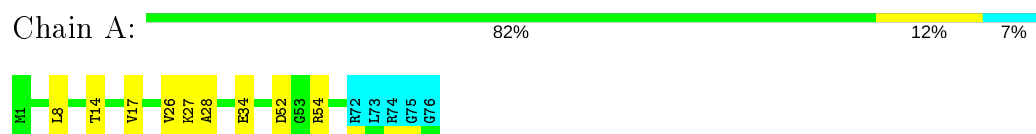
## 4.2.227 Score per residue for model 227

- Molecule 1: Ubiquitin



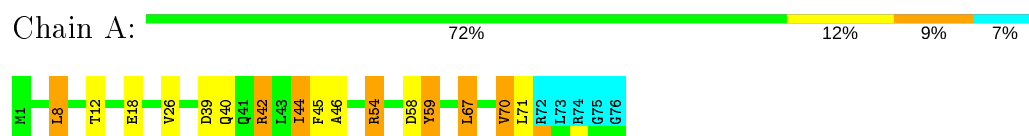
## 4.2.228 Score per residue for model 228

- Molecule 1: Ubiquitin



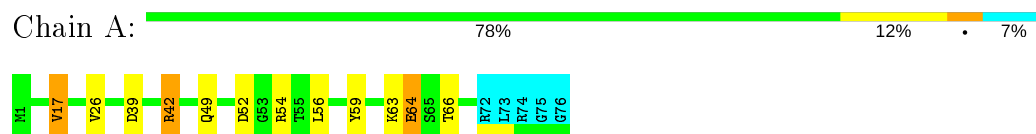
## 4.2.229 Score per residue for model 229

- Molecule 1: Ubiquitin



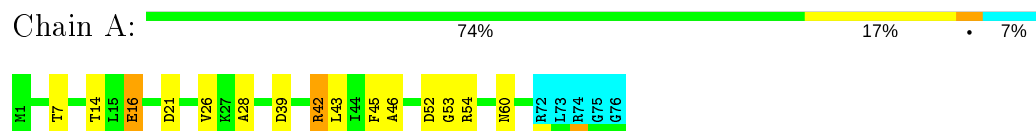
## 4.2.230 Score per residue for model 230

- Molecule 1: Ubiquitin



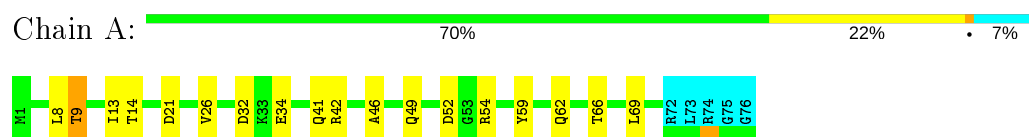
## 4.2.231 Score per residue for model 231

- Molecule 1: Ubiquitin



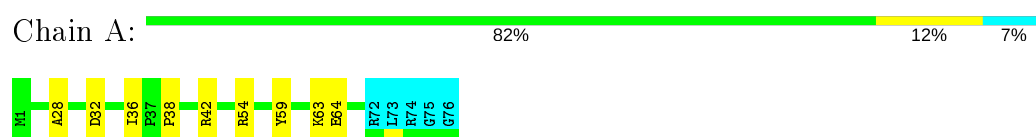
## 4.2.232 Score per residue for model 232

- Molecule 1: Ubiquitin



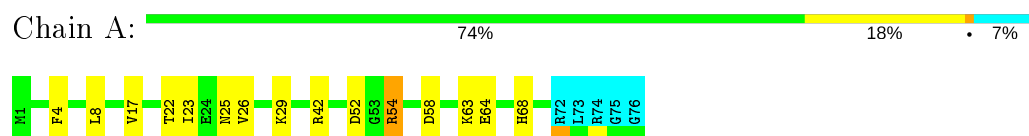
## 4.2.233 Score per residue for model 233

- Molecule 1: Ubiquitin



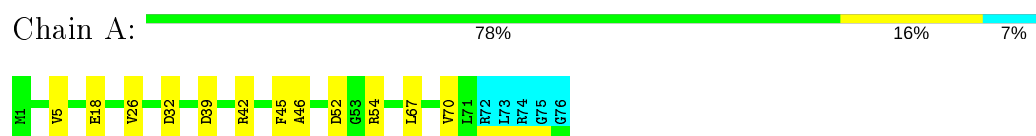
## 4.2.234 Score per residue for model 234

- Molecule 1: Ubiquitin



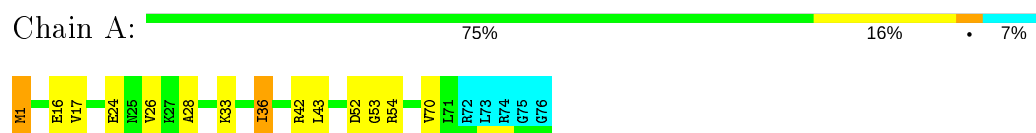
## 4.2.235 Score per residue for model 235

- Molecule 1: Ubiquitin



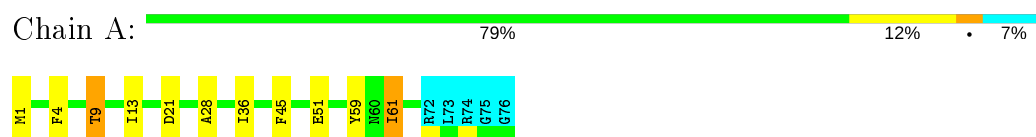
## 4.2.236 Score per residue for model 236

- Molecule 1: Ubiquitin



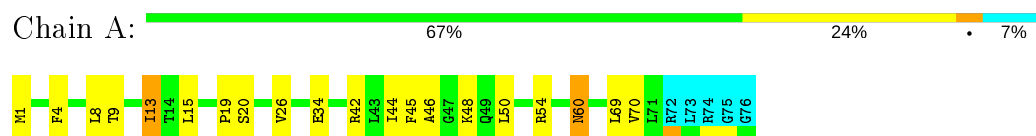
## 4.2.237 Score per residue for model 237

- Molecule 1: Ubiquitin



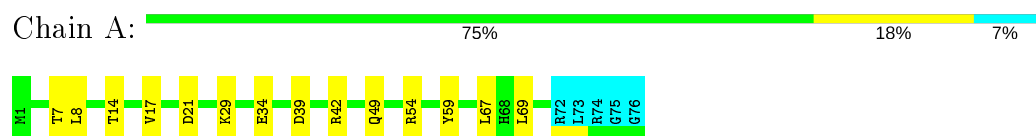
## 4.2.238 Score per residue for model 238

- Molecule 1: Ubiquitin



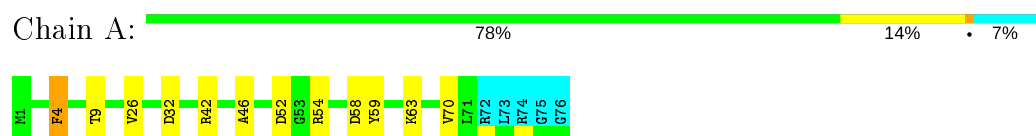
## 4.2.239 Score per residue for model 239

- Molecule 1: Ubiquitin



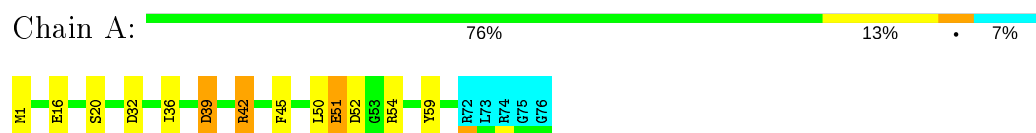
## 4.2.240 Score per residue for model 240

- Molecule 1: Ubiquitin



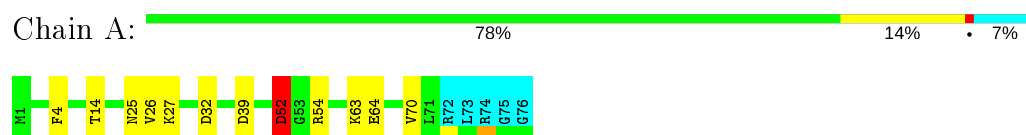
## 4.2.241 Score per residue for model 241

- Molecule 1: Ubiquitin



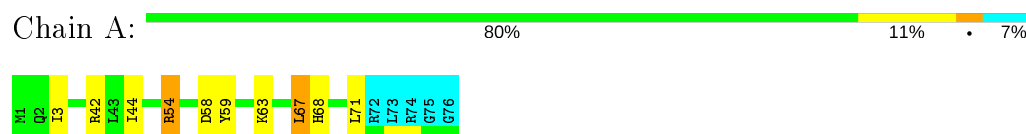
## 4.2.242 Score per residue for model 242

- Molecule 1: Ubiquitin



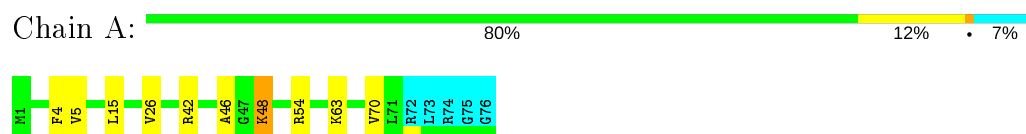
## 4.2.243 Score per residue for model 243

- Molecule 1: Ubiquitin



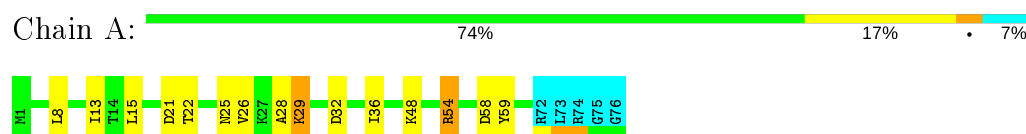
## 4.2.244 Score per residue for model 244

- Molecule 1: Ubiquitin



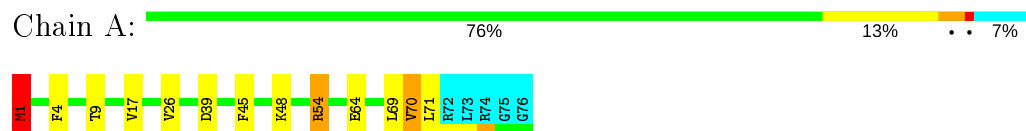
## 4.2.245 Score per residue for model 245

- Molecule 1: Ubiquitin



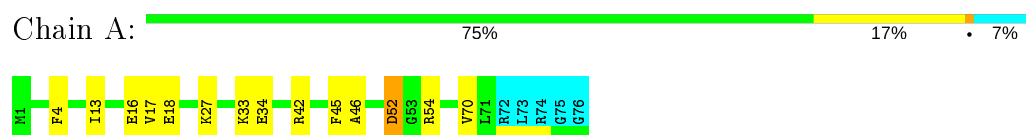
## 4.2.246 Score per residue for model 246

- Molecule 1: Ubiquitin



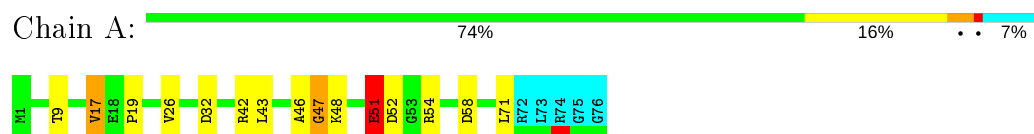
## 4.2.247 Score per residue for model 247

- Molecule 1: Ubiquitin



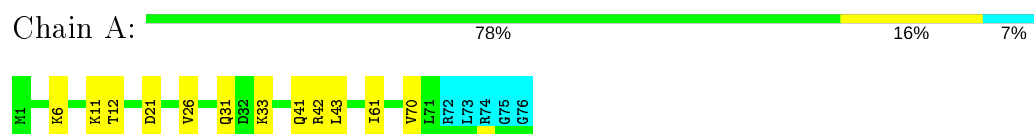
## 4.2.248 Score per residue for model 248

- Molecule 1: Ubiquitin



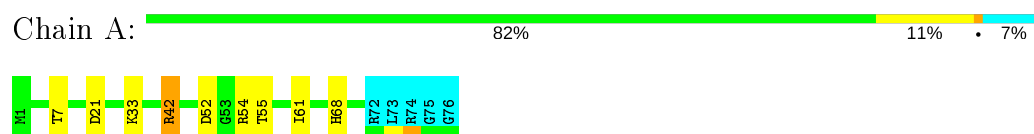
## 4.2.249 Score per residue for model 249

- Molecule 1: Ubiquitin



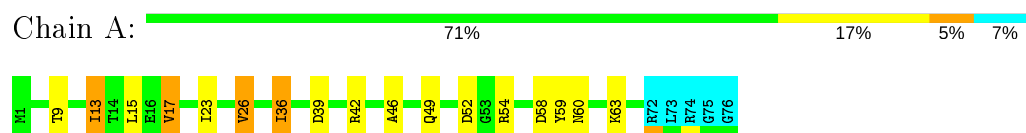
## 4.2.250 Score per residue for model 250

- Molecule 1: Ubiquitin



## 4.2.251 Score per residue for model 251

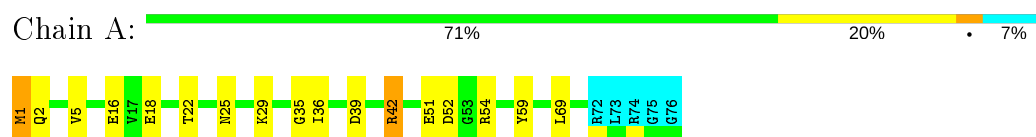
- Molecule 1: Ubiquitin





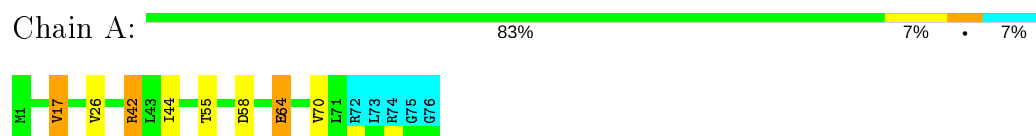
## 4.2.252 Score per residue for model 252

- Molecule 1: Ubiquitin



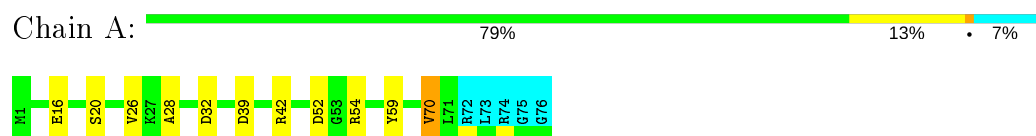
## 4.2.253 Score per residue for model 253

- Molecule 1: Ubiquitin



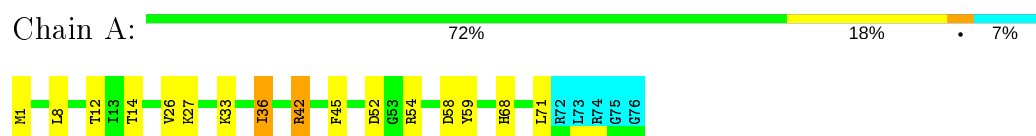
## 4.2.254 Score per residue for model 254

- Molecule 1: Ubiquitin



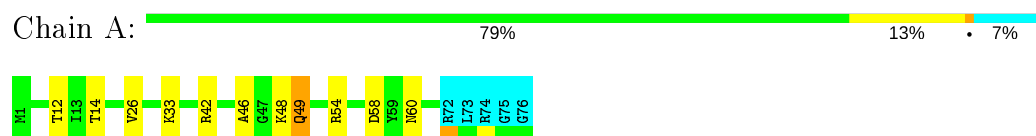
## 4.2.255 Score per residue for model 255

- Molecule 1: Ubiquitin



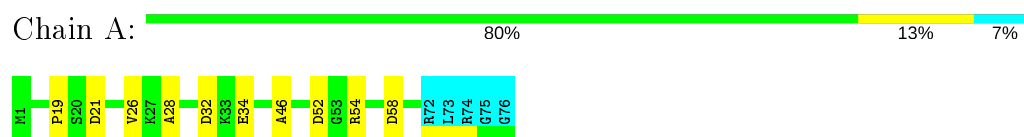
## 4.2.256 Score per residue for model 256

- Molecule 1: Ubiquitin



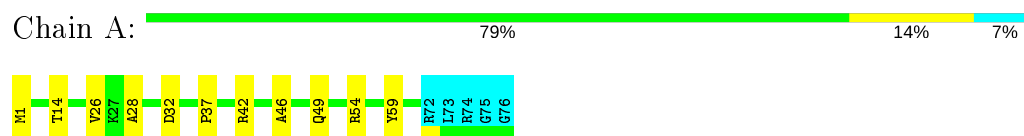
## 4.2.257 Score per residue for model 257

- Molecule 1: Ubiquitin



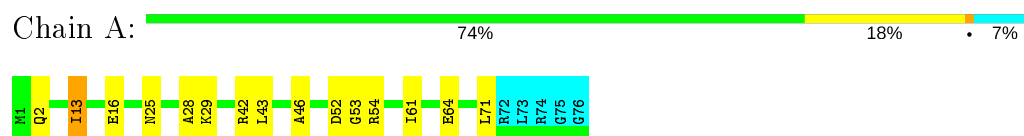
## 4.2.258 Score per residue for model 258

- Molecule 1: Ubiquitin



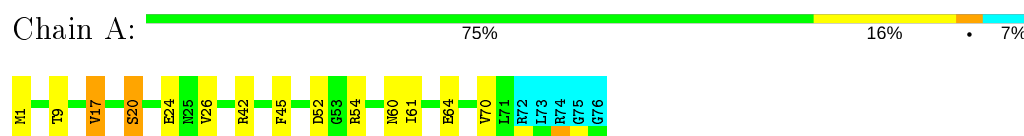
## 4.2.259 Score per residue for model 259

- Molecule 1: Ubiquitin



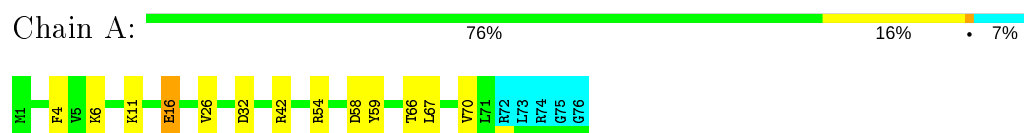
## 4.2.260 Score per residue for model 260

- Molecule 1: Ubiquitin



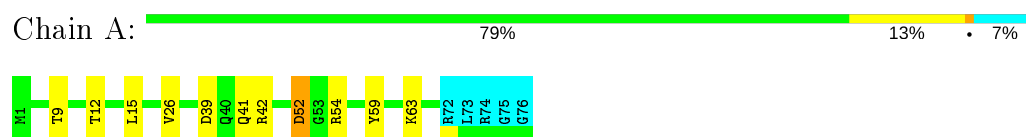
## 4.2.261 Score per residue for model 261

- Molecule 1: Ubiquitin



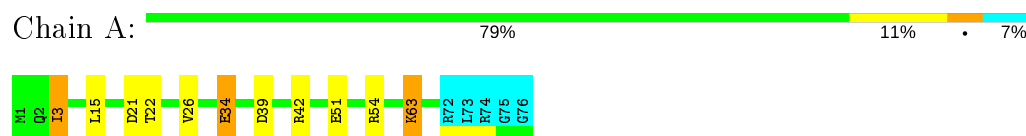
## 4.2.262 Score per residue for model 262

- Molecule 1: Ubiquitin



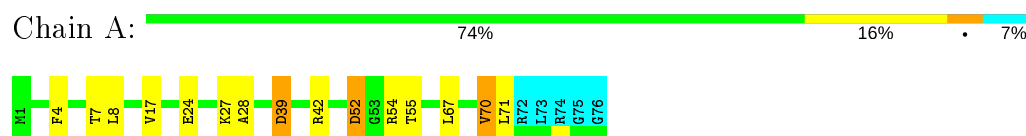
## 4.2.263 Score per residue for model 263

- Molecule 1: Ubiquitin



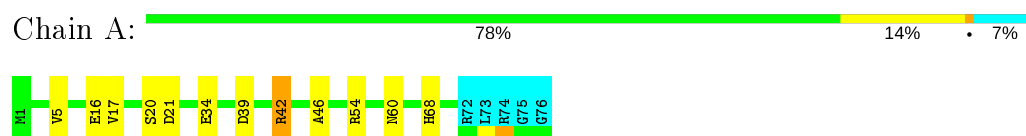
## 4.2.264 Score per residue for model 264

- Molecule 1: Ubiquitin



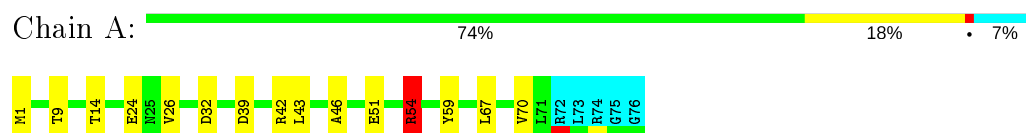
## 4.2.265 Score per residue for model 265

- Molecule 1: Ubiquitin



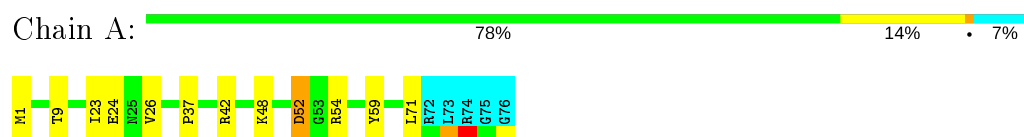
## 4.2.266 Score per residue for model 266

- Molecule 1: Ubiquitin



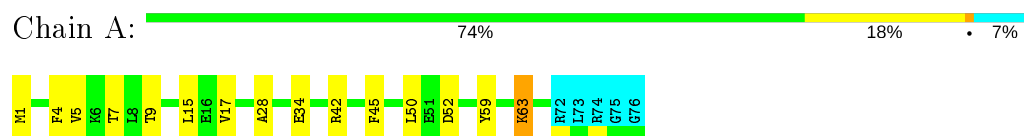
## 4.2.267 Score per residue for model 267

- Molecule 1: Ubiquitin



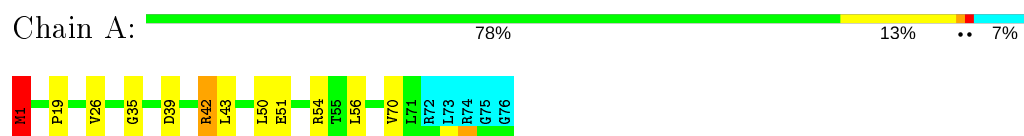
## 4.2.268 Score per residue for model 268

- Molecule 1: Ubiquitin



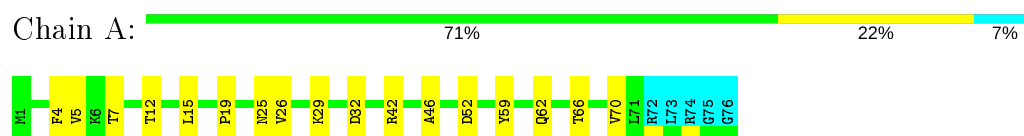
## 4.2.269 Score per residue for model 269

- Molecule 1: Ubiquitin



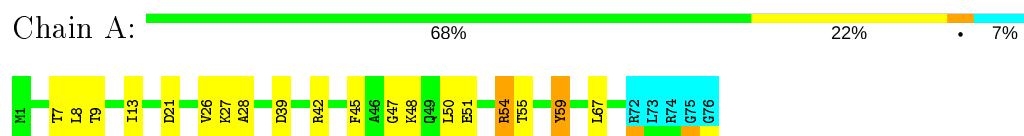
## 4.2.270 Score per residue for model 270

- Molecule 1: Ubiquitin



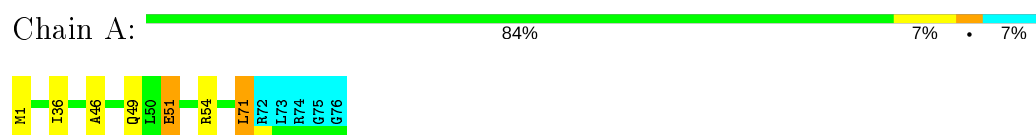
## 4.2.271 Score per residue for model 271

- Molecule 1: Ubiquitin



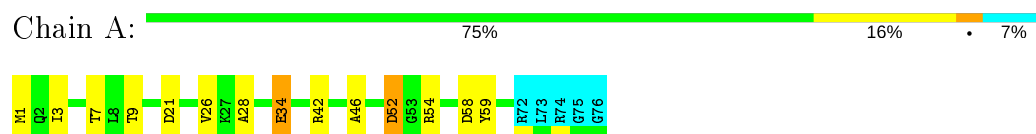
## 4.2.272 Score per residue for model 272

- Molecule 1: Ubiquitin



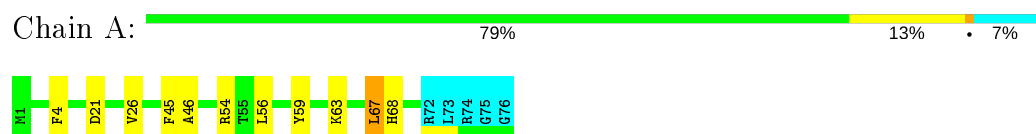
## 4.2.273 Score per residue for model 273

- Molecule 1: Ubiquitin



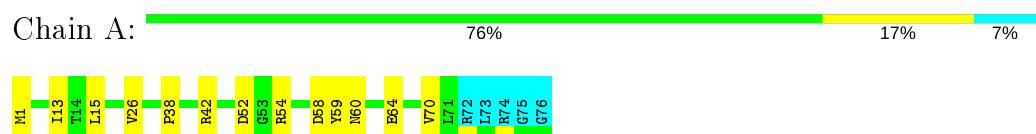
## 4.2.274 Score per residue for model 274

- Molecule 1: Ubiquitin



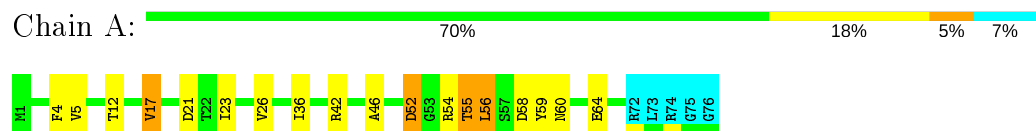
## 4.2.275 Score per residue for model 275

- Molecule 1: Ubiquitin



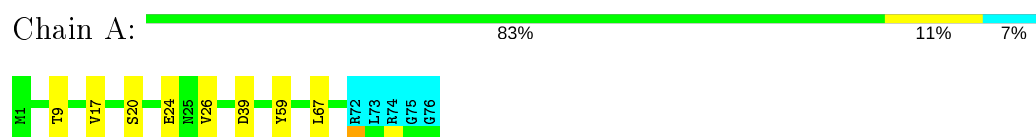
## 4.2.276 Score per residue for model 276

- Molecule 1: Ubiquitin



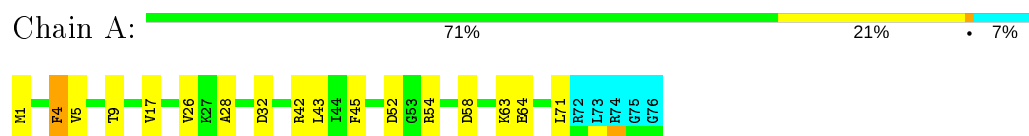
## 4.2.277 Score per residue for model 277

- Molecule 1: Ubiquitin



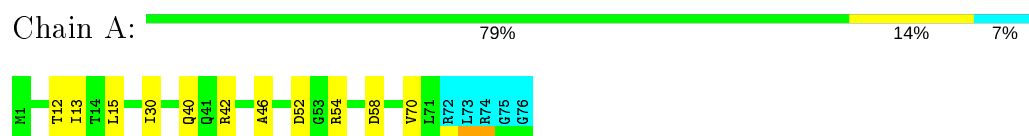
## 4.2.278 Score per residue for model 278

- Molecule 1: Ubiquitin



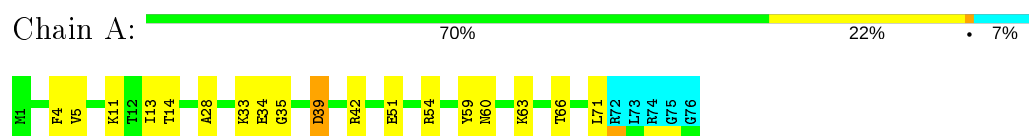
## 4.2.279 Score per residue for model 279

- Molecule 1: Ubiquitin



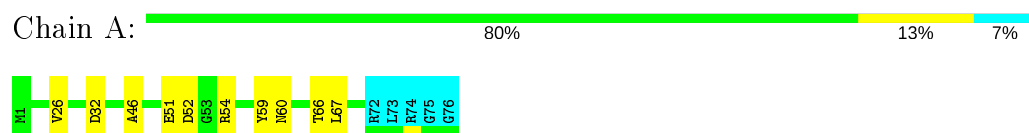
## 4.2.280 Score per residue for model 280

- Molecule 1: Ubiquitin



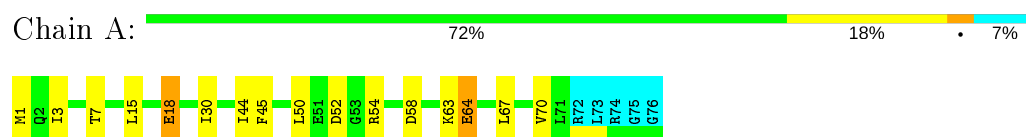
## 4.2.281 Score per residue for model 281

- Molecule 1: Ubiquitin



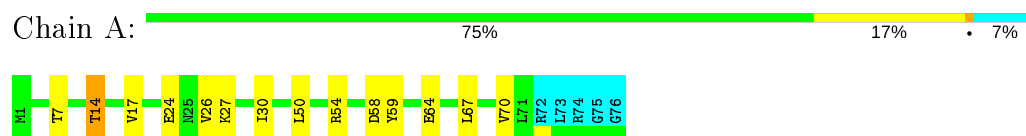
## 4.2.282 Score per residue for model 282

- Molecule 1: Ubiquitin



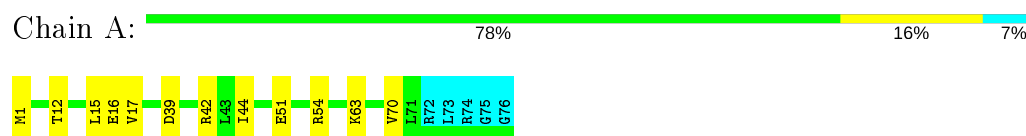
## 4.2.283 Score per residue for model 283

- Molecule 1: Ubiquitin



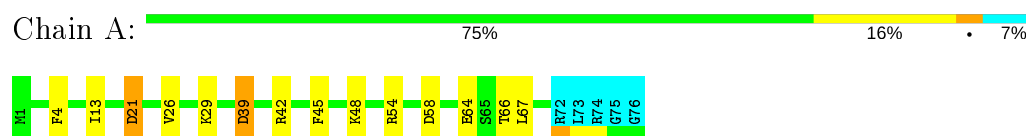
## 4.2.284 Score per residue for model 284

- Molecule 1: Ubiquitin



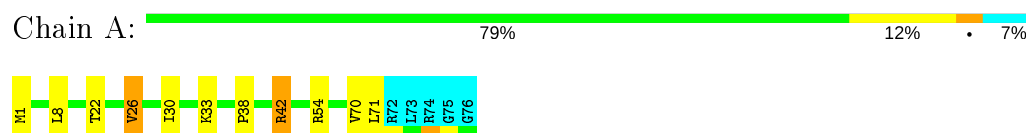
## 4.2.285 Score per residue for model 285

- Molecule 1: Ubiquitin



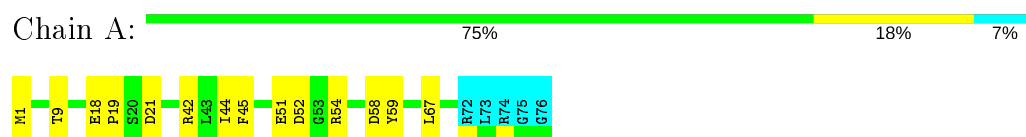
## 4.2.286 Score per residue for model 286

- Molecule 1: Ubiquitin



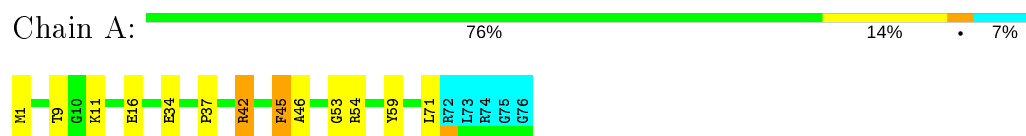
## 4.2.287 Score per residue for model 287

- Molecule 1: Ubiquitin



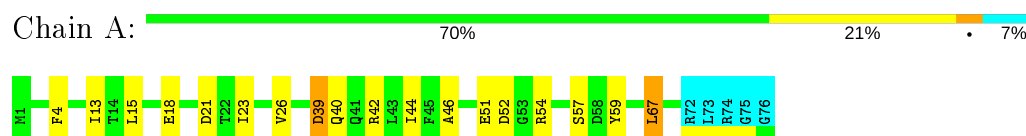
## 4.2.288 Score per residue for model 288

- Molecule 1: Ubiquitin



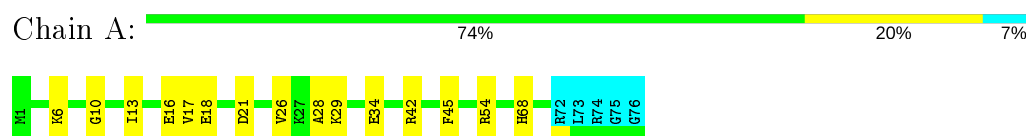
## 4.2.289 Score per residue for model 289

- Molecule 1: Ubiquitin



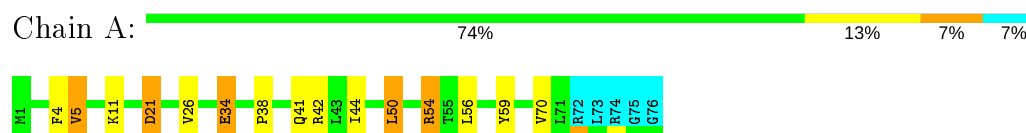
## 4.2.290 Score per residue for model 290

- Molecule 1: Ubiquitin



## 4.2.291 Score per residue for model 291

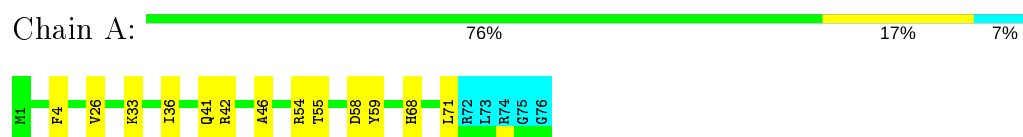
- Molecule 1: Ubiquitin





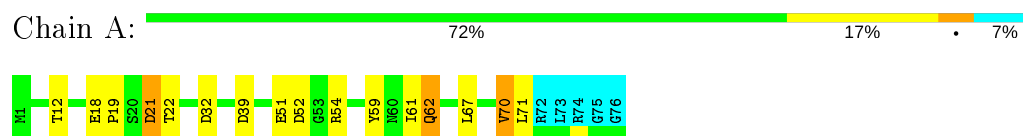
#### 4.2.292 Score per residue for model 292

- Molecule 1: Ubiquitin



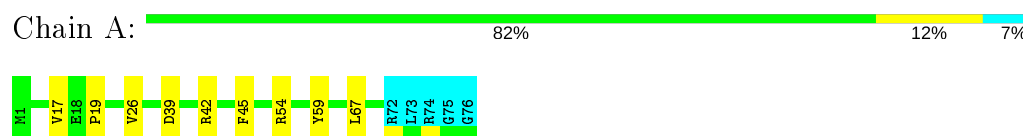
#### 4.2.293 Score per residue for model 293

- Molecule 1: Ubiquitin



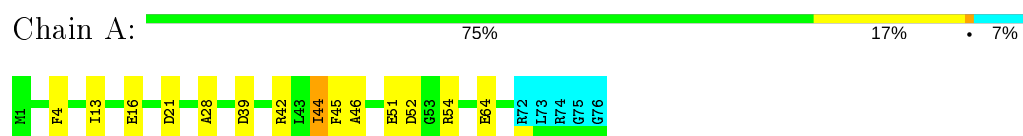
#### 4.2.294 Score per residue for model 294

- Molecule 1: Ubiquitin



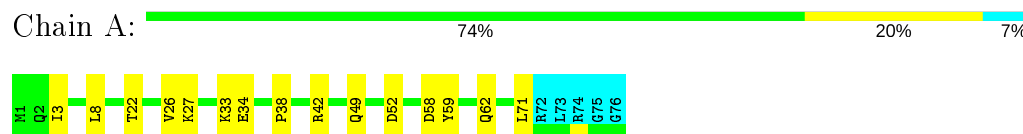
#### 4.2.295 Score per residue for model 295

- Molecule 1: Ubiquitin



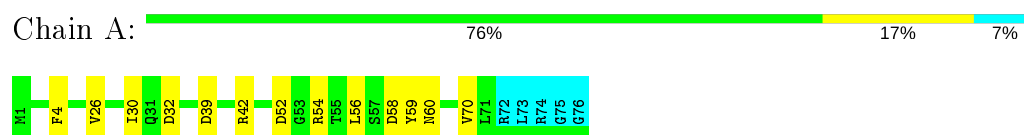
#### 4.2.296 Score per residue for model 296

- Molecule 1: Ubiquitin



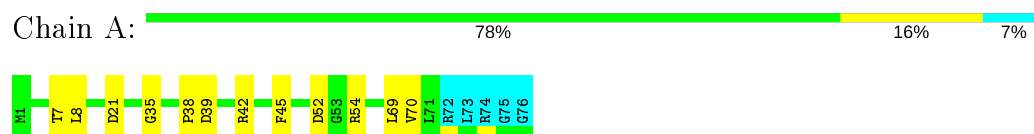
#### 4.2.297 Score per residue for model 297

- Molecule 1: Ubiquitin



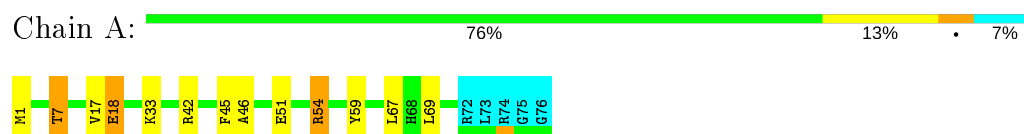
#### 4.2.298 Score per residue for model 298

- Molecule 1: Ubiquitin



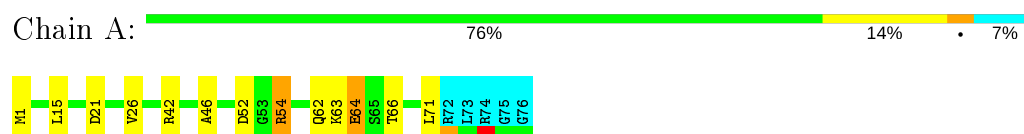
#### 4.2.299 Score per residue for model 299

- Molecule 1: Ubiquitin



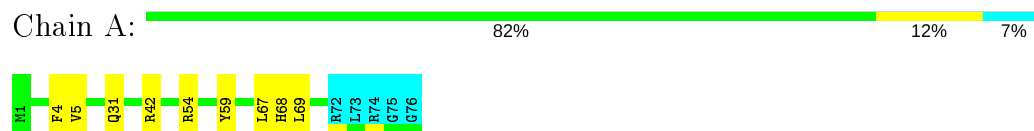
#### 4.2.300 Score per residue for model 300

- Molecule 1: Ubiquitin



#### 4.2.301 Score per residue for model 301

- Molecule 1: Ubiquitin



## 5 Refinement protocol and experimental data overview (i)

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 6 of this report.

Chemical shift file(s)	input_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)	46%

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

COVALENT-GEOMETRY INFOmissingINFO

### 5.1 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	378

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:63:LYS:NZ	1:A:64:GLU:OE2	0.63	2.31	233	7
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:7:THR:HG21	1:A:34:GLU:CD	0.60	2.16	273	1
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	5
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:HA	1:A:16:GLU:OE1	0.54	2.02	60	1
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	2
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	3
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	14
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:HD23	1:A:69:LEU:O	0.52	2.05	146	1
1:A:18:GLU:HA	1:A:18:GLU:OE1	0.52	2.05	116	3
1:A:67:LEU:HD12	1:A:67:LEU:N	0.52	2.19	121	7
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	2
1:A:8:LEU:HD13	1:A:70:VAL:HG13	0.51	1.82	29	1
1:A:71:LEU:N	1:A:71:LEU:CD1	0.51	2.74	50	1

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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	0.51	2.26	117	1
1:A:36:ILE:N	1:A:36:ILE:HD13	0.51	2.21	236	4
1:A:49:GLN:HE21	1:A:51:GLU:CD	0.50	2.09	17	1
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:43:LEU:N	1:A:43:LEU:HD12	0.50	2.21	106	1
1:A:11:LYS:NZ	1:A:34:GLU:OE2	0.50	2.39	79	8
1:A:33:LYS:HE3	1:A:33:LYS:HA	0.50	1.81	1	1
1:A:24:GLU:OE1	1:A:27:LYS:CE	0.50	2.59	283	1
1:A:1:MET:HG2	1:A:17:VAL:O	0.49	2.07	260	1
1:A:17:VAL:HG12	1:A:29:LYS:NZ	0.49	2.22	23	1
1:A:63:LYS:HZ3	1:A:64:GLU:CD	0.49	2.10	66	1
1:A:7:THR:HG21	1:A:34:GLU:OE1	0.49	2.08	273	1
1:A:17:VAL:HG21	1:A:56:LEU:CD1	0.49	2.37	169	2
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:23:ILE:HD13	1:A:23:ILE:N	0.48	2.23	135	2
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:27:LYS:NZ	1:A:52:ASP:OD2	0.48	2.46	242	6
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:16:GLU:CD	1:A:16:GLU:N	0.48	2.67	128	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:27:LYS:HZ2	1:A:52:ASP:CG	0.48	2.12	9	1
1:A:18:GLU:OE1	1:A:18:GLU:HA	0.48	2.09	3	5
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:HD13	1:A:44:ILE:N	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:H	1:A:44:ILE:HD13	0.47	1.69	6	1
1:A:15:LEU:HD11	1:A:30:ILE:HG12	0.47	1.86	125	1
1:A:5:VAL:HG22	1:A:67:LEU:HB2	0.47	1.85	235	3
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:H	1:A:8:LEU:HD23	0.47	1.70	203	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:H	1:A:62:GLN:NE2	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
1:A:56:LEU:HD22	1:A:61:ILE:HG21	0.46	1.86	3	1
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:63:LYS:NZ	1:A:64:GLU:CD	0.46	2.69	66	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	2
1:A:67:LEU:N	1:A:67:LEU:HD12	0.46	2.26	299	9
1:A:16:GLU:H	1:A:16:GLU:CD	0.46	2.13	185	1
1:A:13:ILE:HG22	1:A:14:THR:N	0.45	2.25	3	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:12:THR:C	1:A:13:ILE:CG2	0.45	2.85	78	1
1:A:61:ILE:CD1	1:A:67:LEU:HD11	0.45	2.40	120	1
1:A:27:LYS:HE2	1:A:52:ASP:OD1	0.45	2.11	69	1
1:A:17:VAL:HG12	1:A:29:LYS:HZ2	0.45	1.72	23	1
1:A:43:LEU:HD23	1:A:68:HIS:O	0.45	2.12	84	1
1:A:1:MET:N	1:A:17:VAL:O	0.45	2.47	236	1
1:A:63:LYS:C	1:A:63:LYS:HD2	0.45	2.32	45	1
1:A:71:LEU:N	1:A:71:LEU:HD12	0.45	2.26	229	2
1:A:23:ILE:HG21	1:A:50:LEU:HB3	0.45	1.87	100	1
1:A:70:VAL:C	1:A:71:LEU:HD12	0.45	2.32	208	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:13:ILE:HG12	1:A:34:GLU:HG3	0.45	1.88	191	1
1:A:50:LEU:HD23	1:A:59:TYR:CD2	0.44	2.46	116	1
1:A:59:TYR:O	1:A:60:ASN:C	0.44	2.54	157	1
1:A:47:GLY:C	1:A:48:LYS:HG3	0.44	2.33	248	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	3
1:A:25:ASN:OD1	1:A:29:LYS:NZ	0.44	2.51	112	1
1:A:71:LEU:HD12	1:A:71:LEU:N	0.44	2.27	192	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ALA:O	1:A:48:LYS:HE2	0.44	2.12	51	1
1:A:1:MET:N	1:A:18:GLU:OE1	0.44	2.51	58	1
1:A:27:LYS:NZ	1:A:52:ASP:OD1	0.44	2.50	78	2
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:23:ILE:HB	1:A:52:ASP:HA	0.44	1.89	267	2
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: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:32:ASP:OD2	1:A:33:LYS:CE	0.43	2.67	50	1
1:A:19:PRO:HA	1:A:56:LEU:HD22	0.43	1.90	131	1
1:A:27:LYS:HZ3	1:A:52:ASP:CG	0.43	2.17	264	1
1:A:63:LYS:HG3	1:A:63:LYS:O	0.43	2.14	234	1
1:A:16:GLU:OE1	1:A:33:LYS:NZ	0.43	2.52	3	1
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	1
1:A:68:HIS:CD2	1:A:69:LEU:N	0.43	2.87	71	2
1:A:43:LEU:C	1:A:44:ILE:CG2	0.42	2.86	53	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:36:ILE:HD13	1:A:36:ILE:N	0.42	2.30	181	1
1:A:23:ILE:N	1:A:23:ILE:HD13	0.42	2.28	164	1
1:A:1:MET:CA	1:A:16:GLU:OE1	0.42	2.68	130	1
1:A:48:LYS:C	1:A:48:LYS:HD3	0.42	2.34	93	1
1:A:67:LEU:N	1:A:67:LEU:CD1	0.42	2.83	170	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:N	1:A:67:LEU:HD22	0.42	2.29	76	1
1:A:51:GLU:CD	1:A:54:ARG:HE	0.42	2.18	299	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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:45:PHE:C	1:A:47:GLY:N	0.41	2.72	85	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: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:12:THR:C	1:A:13:ILE:HG13	0.41	2.36	7	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:12:THR:C	1:A:13:ILE:HD12	0.41	2.36	150	1
1:A:22:THR:HA	1:A:55:THR:HA	0.41	1.91	70	1
1:A:33:LYS:NZ	1:A:33:LYS:HA	0.41	2.31	67	1
1:A:54:ARG:HD3	1:A:54:ARG:N	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:39:ASP:OD1	1:A:39:ASP:C	0.40	2.60	29	1
1:A:50:LEU:HD22	1:A:59:TYR:CE1	0.40	2.52	63	1
1:A:66:THR:C	1:A:67:LEU:HD22	0.40	2.37	76	1
1:A:1:MET:SD	1:A:1:MET:C	0.40	3.00	44	1
1:A:40:GLN:NE2	1:A:40:GLN:HA	0.40	2.31	123	1
1:A:11:LYS:HZ1	1:A:34:GLU:CD	0.40	2.19	25	1
1:A:49:GLN:HG2	1:A:49:GLN:O	0.40	2.16	256	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:62:GLN:O	1:A:63:LYS:C	0.40	2.60	16	1
1:A:1:MET:C	1:A:16:GLU:OE2	0.40	2.60	49	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:16:GLU:OE1	1:A:16:GLU:HA	0.40	2.16	89	1
1:A:27:LYS:HE2	1:A:41:GLN:HB2	0.40	1.93	206	1



## 5.2 Torsion angles [i](#)

### 5.2.1 Protein backbone [i](#)

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%)	38	78
All	All	21070/22876 (92%)	20213 (96%)	777 (4%)	80 (0%)	38	78

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

### 5.2.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	65/68 (96%)	60±3 (93±5%)	5±3 (7±5%)	18 66
All	All	19565/20468 (96%)	18129 (93%)	1436 (7%)	18 66

All 65 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	63	LYS	82
1	A	32	ASP	70
1	A	1	MET	67
1	A	52	ASP	64
1	A	9	THR	55
1	A	60	ASN	54
1	A	70	VAL	52
1	A	31	GLN	51
1	A	26	VAL	51
1	A	36	ILE	51
1	A	23	ILE	49
1	A	39	ASP	43
1	A	71	LEU	40
1	A	22	THR	39
1	A	67	LEU	39
1	A	21	ASP	39
1	A	13	ILE	37
1	A	16	GLU	31
1	A	43	LEU	29
1	A	33	LYS	28
1	A	8	LEU	27
1	A	56	LEU	25
1	A	64	GLU	23
1	A	69	LEU	23
1	A	18	GLU	22
1	A	44	ILE	21
1	A	57	SER	21
1	A	30	ILE	19
1	A	14	THR	18

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Mol	Chain	Res	Type	Models (Total)
1	A	49	GLN	17
1	A	54	ARG	17
1	A	20	SER	16
1	A	38	PRO	14
1	A	2	GLN	13
1	A	48	LYS	13
1	A	61	ILE	12
1	A	6	LYS	12
1	A	42	ARG	12
1	A	25	ASN	11
1	A	62	GLN	11
1	A	51	GLU	10
1	A	11	LYS	9
1	A	4	PHE	9
1	A	7	THR	9
1	A	12	THR	9
1	A	58	ASP	8
1	A	19	PRO	8
1	A	15	LEU	8
1	A	3	ILE	6
1	A	68	HIS	5
1	A	5	VAL	5
1	A	66	THR	4
1	A	24	GLU	4
1	A	65	SER	4
1	A	34	GLU	3
1	A	40	GLN	3
1	A	41	GLN	2
1	A	50	LEU	2
1	A	17	VAL	2
1	A	55	THR	2
1	A	29	LYS	2
1	A	59	TYR	1
1	A	27	LYS	1
1	A	45	PHE	1
1	A	37	PRO	1

### 5.2.3 RNA

There are no RNA molecules in this entry.

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

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

### 5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.5 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.6 Other polymers [i](#)

There are no such molecules in this entry.

### 5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 46% for the well-defined parts and 44% for the entire structure.

### 6.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 6.1.1 Bookkeeping [i](#)

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

#### 6.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
<sup>13</sup> C <sub>α</sub>	72	-0.22 $\pm$ 0.12	None needed (< 0.5 ppm)
<sup>13</sup> C <sub>β</sub>	68	0.16 $\pm$ 0.17	None needed (< 0.5 ppm)
<sup>13</sup> C'	72	-0.30 $\pm$ 0.14	None needed (< 0.5 ppm)
<sup>15</sup> N	71	1.31 $\pm$ 0.54	Should be applied

#### 6.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 46%, i.e. 413 atoms were assigned a chemical shift out of a possible 892. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	346/349 (99%)	137/139 (99%)	142/142 (100%)	67/68 (99%)
Sidechain	67/510 (13%)	0/296 (0%)	67/193 (35%)	0/21 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/33 (0%)	0/18 (0%)	0/14 (0%)	0/1 (0%)
Overall	413/892 (46%)	137/453 (30%)	209/349 (60%)	67/90 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 44%, i.e. 419 atoms were assigned a chemical shift out of a possible 962. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	351/374 (94%)	139/149 (93%)	144/152 (95%)	68/73 (93%)
Sidechain	68/555 (12%)	0/323 (0%)	68/205 (33%)	0/27 (0%)
Aromatic	0/33 (0%)	0/18 (0%)	0/14 (0%)	0/1 (0%)
Overall	419/962 (44%)	139/490 (28%)	212/371 (57%)	68/101 (67%)

#### 6.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 6.1.5 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.

Random coil index (RCI) for chain A:

