



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 10:05 AM UTC

PDB ID : 2KOX / pdb_00002kox
Title : NMR residual dipolar couplings identify long range correlated motions in the backbone of the protein ubiquitin
Authors : Fenwick, R.B.; Richter, B.; Lee, D.; Walter, K.F.A.; Milovanovic, D.; Becker, S.; Lakomek, N.A.; Griesinger, C.; Salvatella, X.
Deposited on : 2009-10-02

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

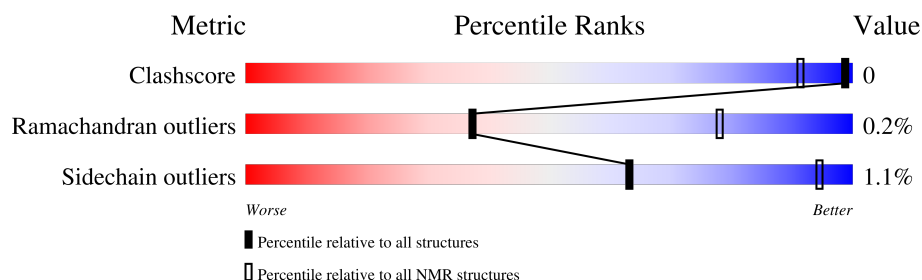
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	76	

2 Ensemble composition and analysis ⓘ

This entry contains 640 models. Model 76 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)	0.60	76

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 79 clusters and 27 single-model clusters were found.

Cluster number	Models
1	1, 39, 57, 61, 101, 103, 121, 144, 150, 151, 158, 163, 165, 167, 180, 184, 196, 213, 231, 233, 235, 238, 247, 251, 252, 253, 255, 262, 264, 268, 288, 293, 297, 315, 319, 330, 332, 333, 341, 366, 377, 379, 380, 405, 415, 423, 460, 469, 483, 507, 512, 547, 559, 564, 571, 572, 592, 603, 610
2	2, 24, 26, 33, 37, 47, 49, 62, 74, 81, 88, 111, 129, 154, 169, 175, 179, 204, 218, 256, 258, 276, 280, 282, 286, 303, 311, 320, 322, 335, 344, 350, 361, 363, 365, 367, 371, 384, 394, 404, 408, 427, 429, 435, 448, 452, 468, 470, 474, 529, 532, 534, 555, 567, 578, 596, 600, 602
3	8, 11, 21, 22, 31, 52, 54, 73, 106, 108, 116, 138, 149, 182, 189, 211, 214, 216, 246, 275, 342, 364, 417, 428, 440, 442, 445, 447, 472, 492, 504, 506, 509, 511, 519, 533, 566, 573, 583, 625, 631
4	12, 38, 40, 66, 69, 76, 78, 79, 86, 97, 102, 104, 142, 148, 161, 166, 200, 212, 230, 236, 245, 277, 300, 309, 339, 347, 358, 373, 374, 396, 426, 437, 449, 462, 481, 501, 524, 526, 554, 590, 626
5	27, 65, 159, 195, 234, 257, 287, 298, 325, 362, 383, 387, 389, 399, 424, 453, 461, 486, 488, 515, 517, 525, 550, 570, 579, 633
6	29, 48, 50, 60, 89, 91, 210, 217, 225, 227, 242, 281, 289, 321, 345, 355, 370, 432, 434, 496, 601
7	28, 117, 181, 220, 222, 278, 284, 292, 294, 348, 369, 410, 412, 458, 478, 538, 540, 588, 604, 613
8	16, 80, 92, 208, 274, 334, 398, 400, 457, 464, 466, 499, 530, 539, 560, 594, 623, 628
9	19, 23, 174, 190, 299, 316, 326, 329, 390, 403, 436, 454, 471, 518, 535, 561, 582

10	15, 99, 171, 215, 224, 237, 243, 279, 343, 407, 446, 476, 542, 574
11	30, 32, 94, 202, 266, 290, 418, 494, 522, 536, 544, 586, 609
12	93, 157, 176, 240, 285, 381, 402, 443, 562, 589, 605
13	9, 55, 59, 123, 125, 187, 191, 198, 441, 479, 599
14	14, 46, 115, 119, 183, 324, 414, 516, 597, 607, 632
15	13, 77, 114, 127, 141, 155, 178, 205, 306, 615, 634
16	44, 120, 130, 226, 267, 395, 521, 568, 581, 587
17	41, 64, 105, 192, 241, 254, 318, 508, 563, 618
18	25, 139, 239, 397, 455, 463, 503, 528, 617, 622
19	34, 98, 223, 351, 413, 477, 541, 619
20	5, 20, 43, 135, 168, 201, 259, 263
21	17, 96, 145, 209, 354, 386, 433, 465
22	56, 72, 110, 118, 248, 250, 378, 430
23	229, 357, 421, 489, 502, 553, 616
24	100, 134, 136, 170, 244, 495, 575
25	10, 513, 577, 595, 612, 640
26	90, 109, 301, 425, 491, 510
27	18, 71, 112, 199, 323, 451
28	85, 438, 556, 621, 624, 629
29	147, 328, 338, 392, 498, 580
30	295, 487, 551, 614, 638
31	68, 188, 375, 485, 549
32	107, 382, 450, 514, 639
33	143, 207, 271, 591
34	261, 393, 411, 475
35	3, 193, 490, 537
36	51, 132, 260, 576
37	133, 523, 565, 585
38	75, 439, 505, 636
39	356, 420, 484, 611
40	137, 269, 331, 598
41	83, 467, 531
42	6, 337, 401
43	352, 520, 584
44	177, 314, 497
45	58, 327, 391
46	221, 368, 543
47	340, 422, 569
48	95, 146, 630
49	265, 310, 593
50	87, 353, 409
51	70, 273
52	232, 552

53	482, 546
54	500, 627
55	128, 194
56	173, 493
57	186, 444
58	307, 637
59	473, 635
60	346, 388
61	122, 527
62	160, 406
63	164, 548
64	419, 606
65	67, 296
66	308, 372
67	203, 459
68	152, 317
69	249, 313
70	63, 219
71	124, 385
72	45, 126
73	270, 557
74	42, 185
75	172, 558
76	156, 431
77	140, 456
78	416, 480
79	283, 336
Single-model clusters	4; 7; 35; 36; 53; 82; 84; 113; 131; 153; 162; 197; 206; 228; 272; 291; 302; 304; 305; 31

3 Entry composition [i](#)

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

- Molecule 1 is a protein called Ubiquitin.

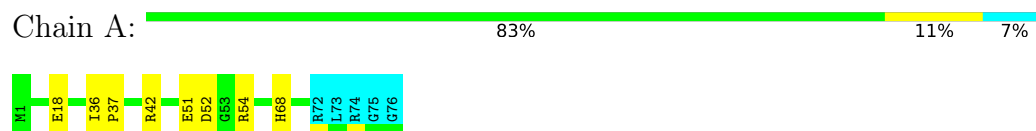
Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1231	378	629	105	118	1	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Ubiquitin

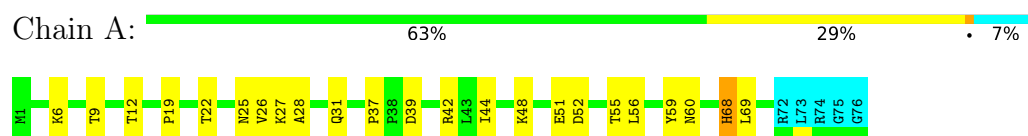


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

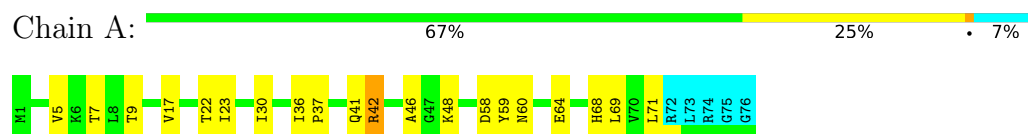
4.2.1 Score per residue for model 1

- Molecule 1: Ubiquitin



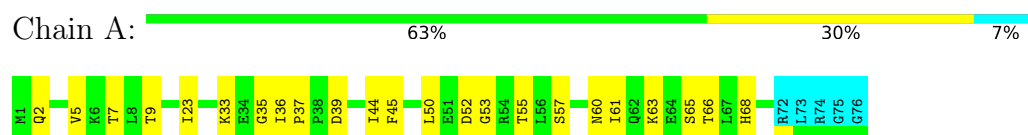
4.2.2 Score per residue for model 2

- Molecule 1: Ubiquitin



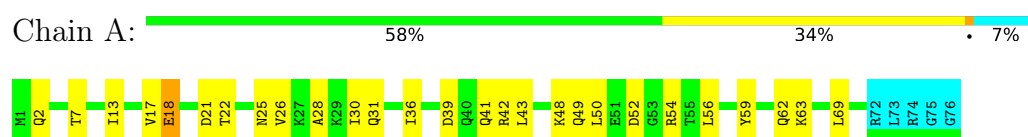
4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin



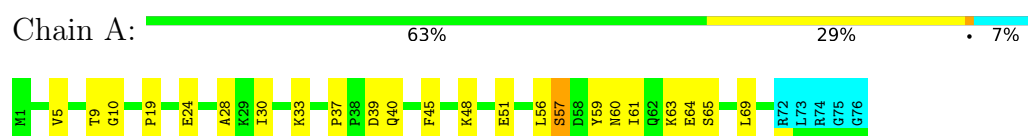
4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin



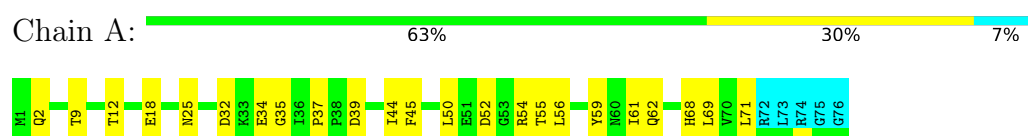
4.2.5 Score per residue for model 5

- Molecule 1: Ubiquitin



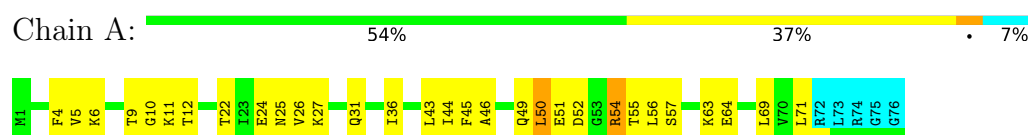
4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin



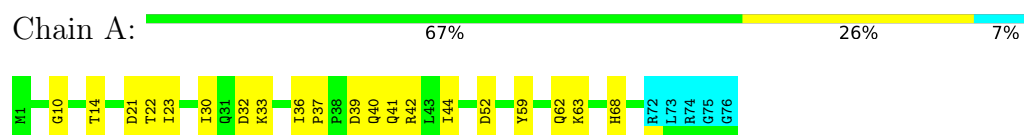
4.2.7 Score per residue for model 7

- Molecule 1: Ubiquitin



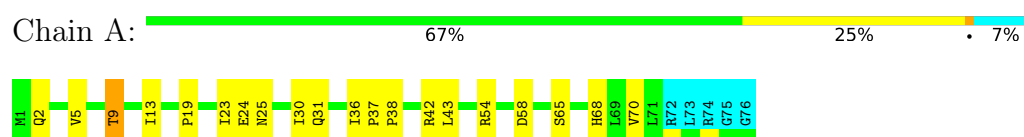
4.2.8 Score per residue for model 8

- Molecule 1: Ubiquitin



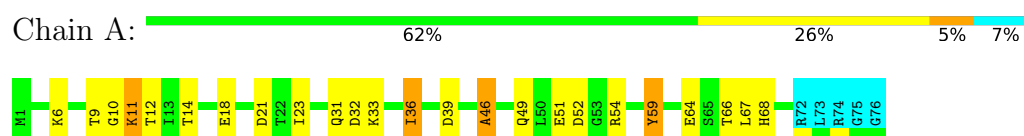
4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin



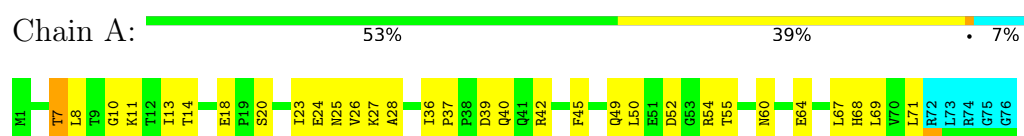
4.2.10 Score per residue for model 10

- Molecule 1: Ubiquitin



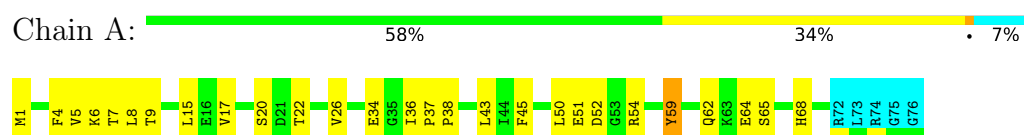
4.2.11 Score per residue for model 11

- Molecule 1: Ubiquitin



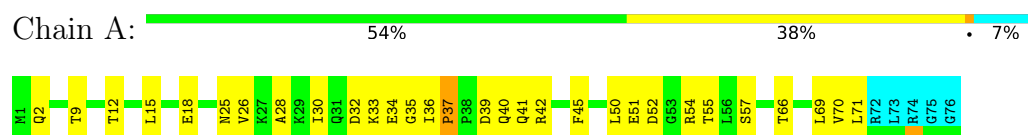
4.2.12 Score per residue for model 12

- Molecule 1: Ubiquitin



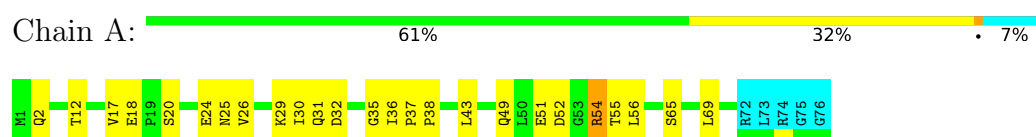
4.2.13 Score per residue for model 13

- Molecule 1: Ubiquitin



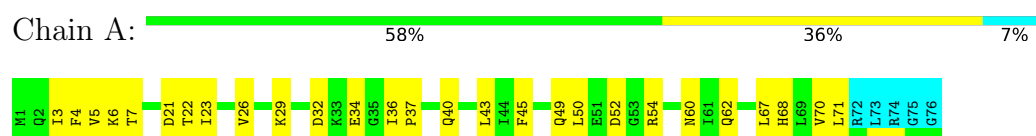
4.2.14 Score per residue for model 14

- Molecule 1: Ubiquitin



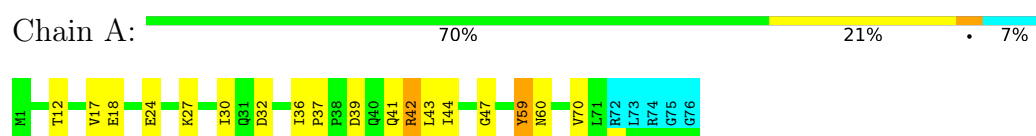
4.2.15 Score per residue for model 15

- Molecule 1: Ubiquitin



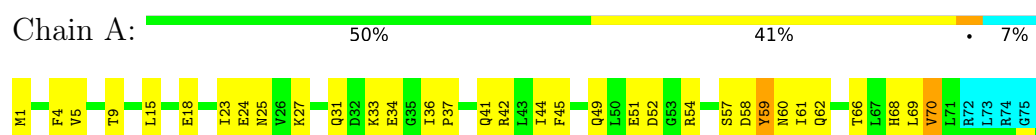
4.2.16 Score per residue for model 16

- Molecule 1: Ubiquitin



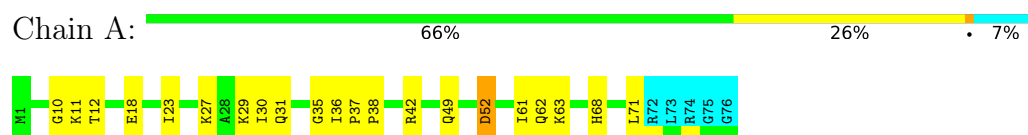
4.2.17 Score per residue for model 17

- Molecule 1: Ubiquitin



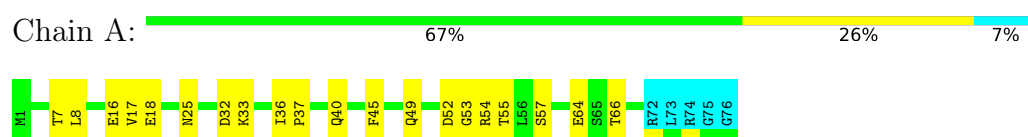
4.2.18 Score per residue for model 18

- Molecule 1: Ubiquitin



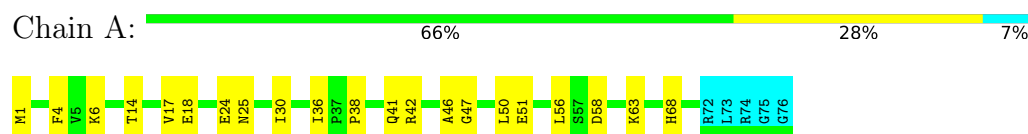
4.2.19 Score per residue for model 19

- Molecule 1: Ubiquitin



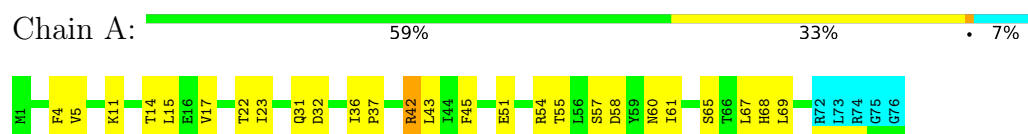
4.2.20 Score per residue for model 20

- Molecule 1: Ubiquitin



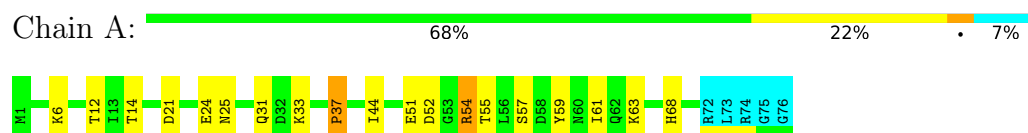
4.2.21 Score per residue for model 21

- Molecule 1: Ubiquitin



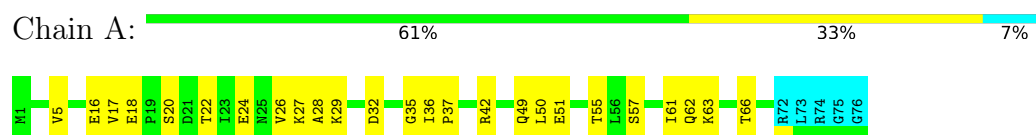
4.2.22 Score per residue for model 22

- Molecule 1: Ubiquitin



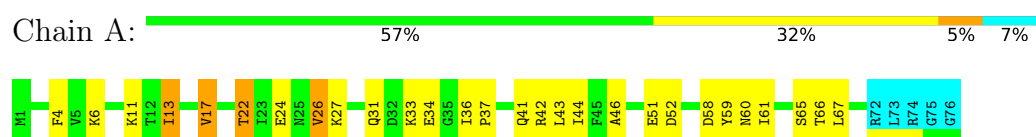
4.2.23 Score per residue for model 23

- Molecule 1: Ubiquitin



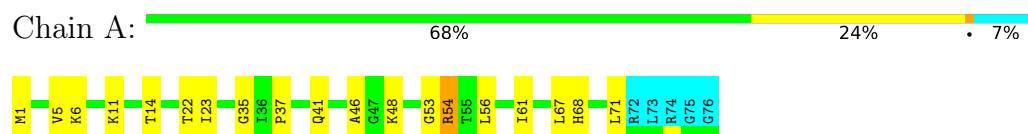
4.2.24 Score per residue for model 24

- Molecule 1: Ubiquitin



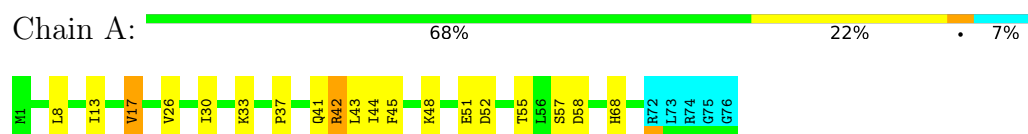
4.2.25 Score per residue for model 25

- Molecule 1: Ubiquitin



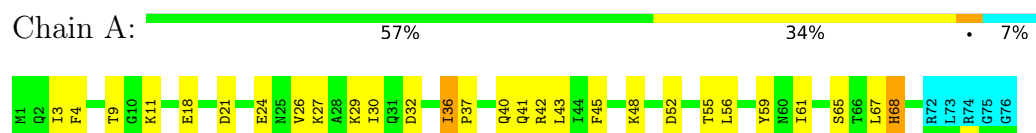
4.2.26 Score per residue for model 26

- Molecule 1: Ubiquitin



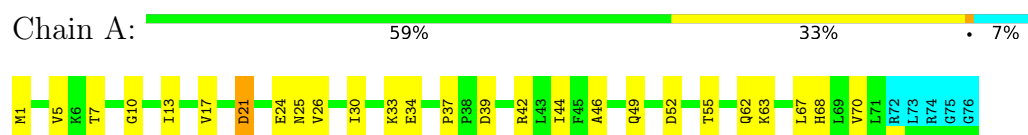
4.2.27 Score per residue for model 27

- Molecule 1: Ubiquitin



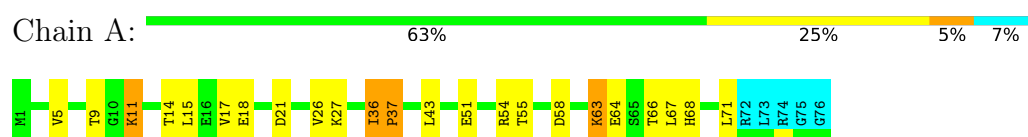
4.2.28 Score per residue for model 28

- Molecule 1: Ubiquitin



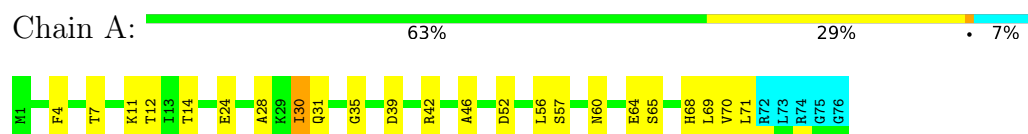
4.2.29 Score per residue for model 29

- Molecule 1: Ubiquitin



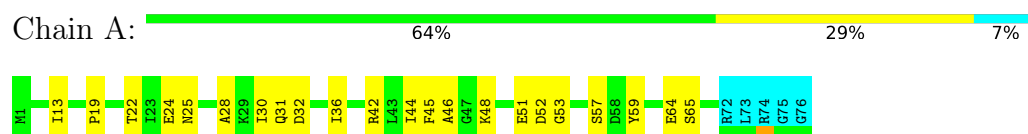
4.2.30 Score per residue for model 30

- Molecule 1: Ubiquitin



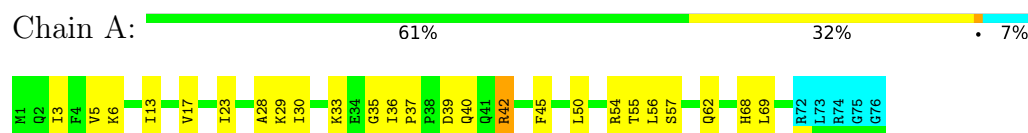
4.2.31 Score per residue for model 31

- Molecule 1: Ubiquitin



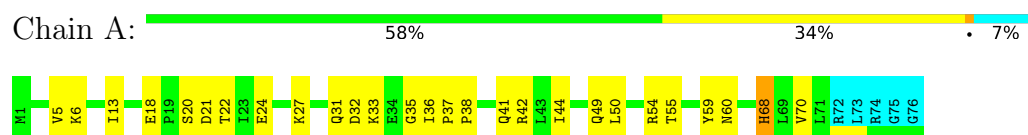
4.2.32 Score per residue for model 32

- Molecule 1: Ubiquitin



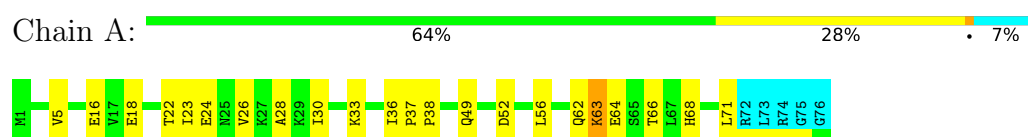
4.2.33 Score per residue for model 33

- Molecule 1: Ubiquitin



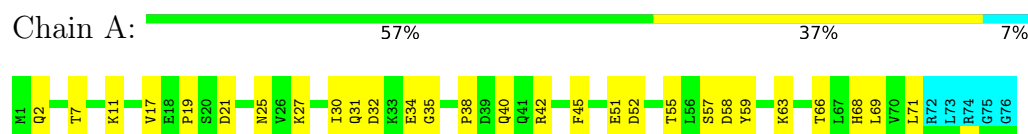
4.2.34 Score per residue for model 34

- Molecule 1: Ubiquitin



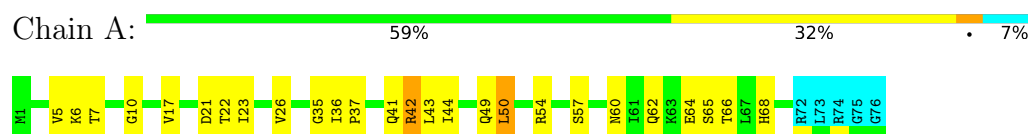
4.2.35 Score per residue for model 35

- Molecule 1: Ubiquitin



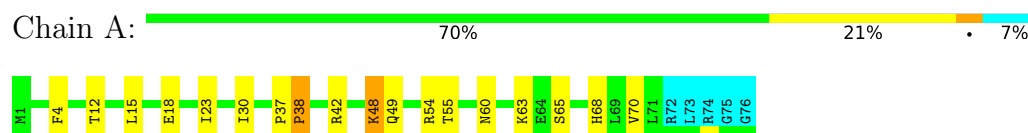
4.2.36 Score per residue for model 36

- Molecule 1: Ubiquitin



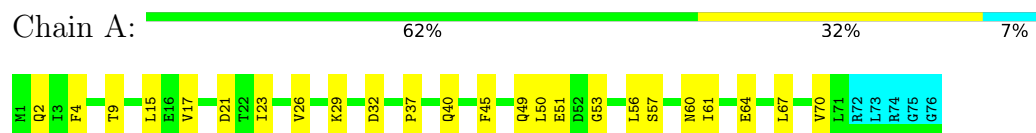
4.2.37 Score per residue for model 37

- Molecule 1: Ubiquitin



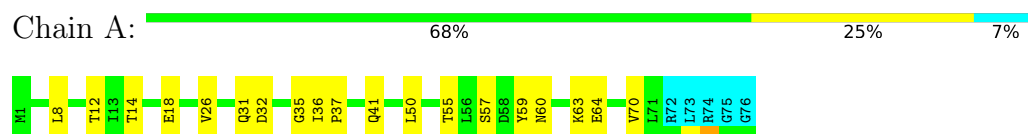
4.2.38 Score per residue for model 38

- Molecule 1: Ubiquitin



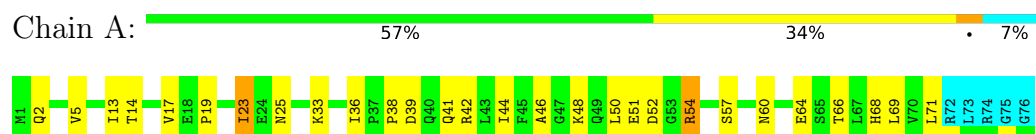
4.2.39 Score per residue for model 39

- Molecule 1: Ubiquitin



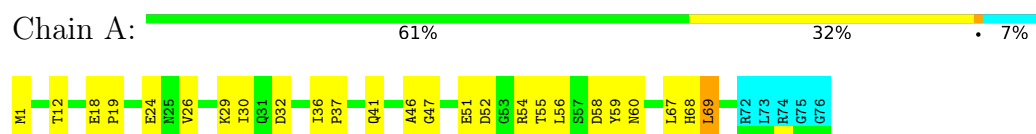
4.2.40 Score per residue for model 40

- Molecule 1: Ubiquitin



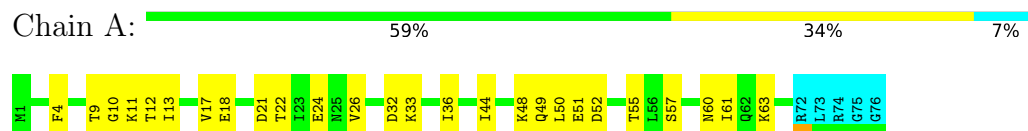
4.2.41 Score per residue for model 41

- Molecule 1: Ubiquitin



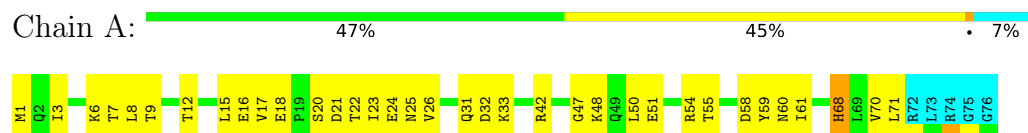
4.2.42 Score per residue for model 42

- Molecule 1: Ubiquitin



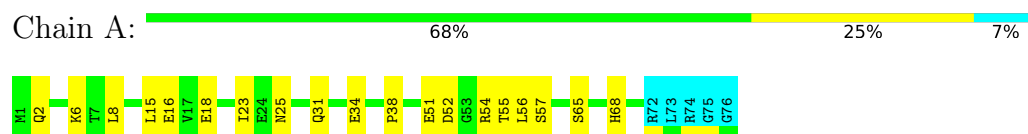
4.2.43 Score per residue for model 43

- Molecule 1: Ubiquitin



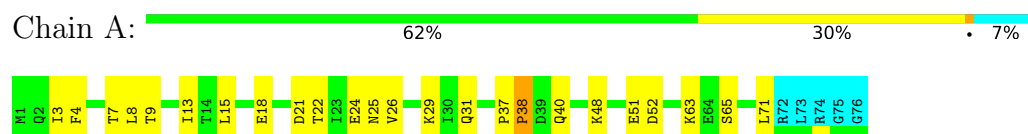
4.2.44 Score per residue for model 44

- Molecule 1: Ubiquitin



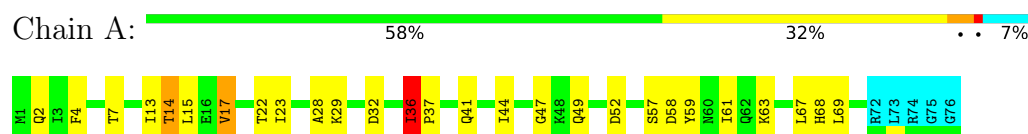
4.2.45 Score per residue for model 45

- Molecule 1: Ubiquitin



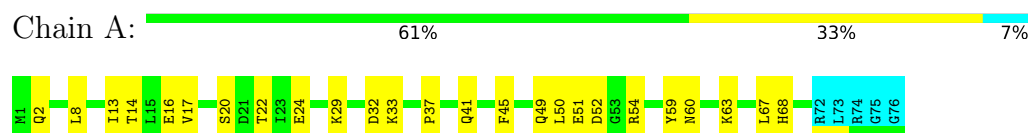
4.2.46 Score per residue for model 46

- Molecule 1: Ubiquitin



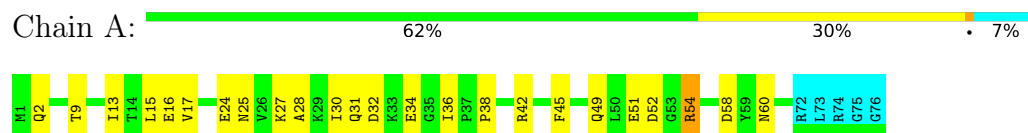
4.2.47 Score per residue for model 47

- Molecule 1: Ubiquitin



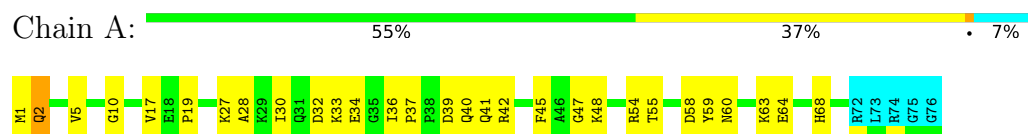
4.2.48 Score per residue for model 48

- Molecule 1: Ubiquitin



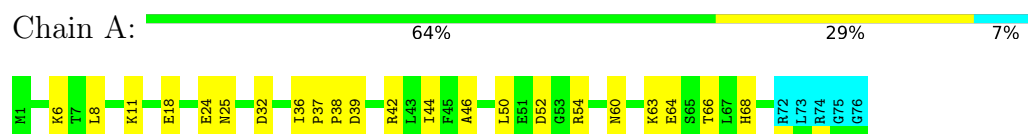
4.2.49 Score per residue for model 49

- Molecule 1: Ubiquitin



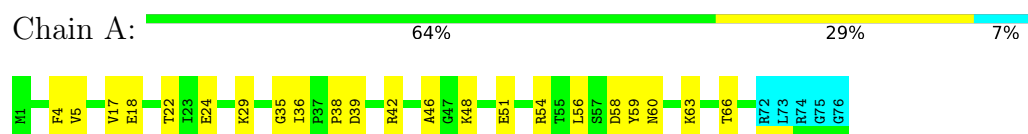
4.2.50 Score per residue for model 50

- Molecule 1: Ubiquitin



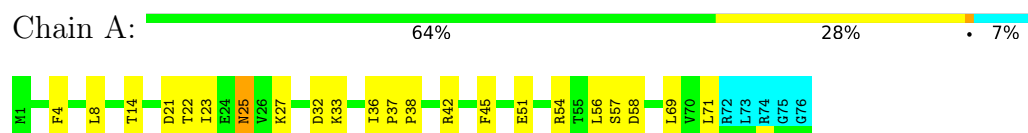
4.2.51 Score per residue for model 51

- Molecule 1: Ubiquitin



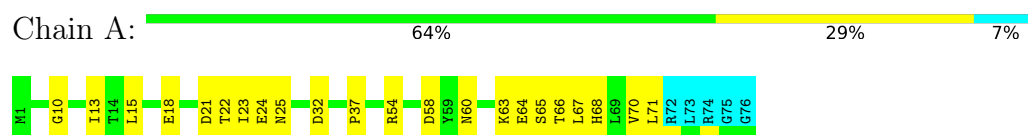
4.2.52 Score per residue for model 52

- Molecule 1: Ubiquitin



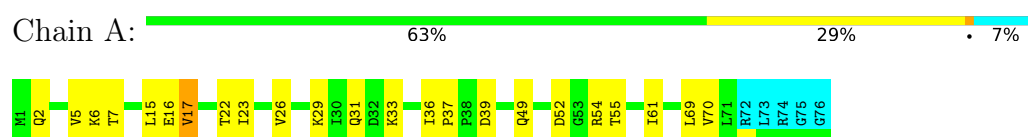
4.2.53 Score per residue for model 53

- Molecule 1: Ubiquitin



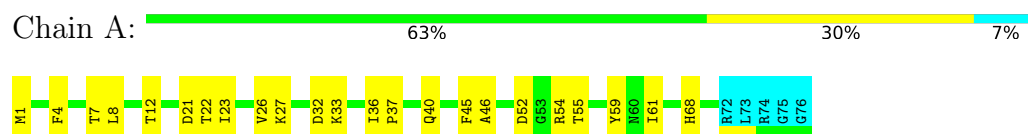
4.2.54 Score per residue for model 54

- Molecule 1: Ubiquitin



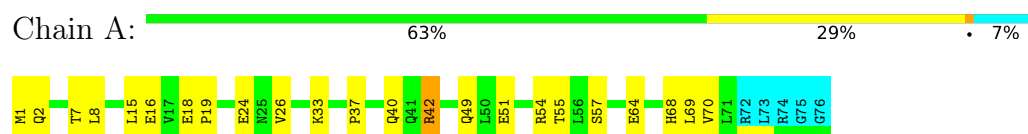
4.2.55 Score per residue for model 55

- Molecule 1: Ubiquitin



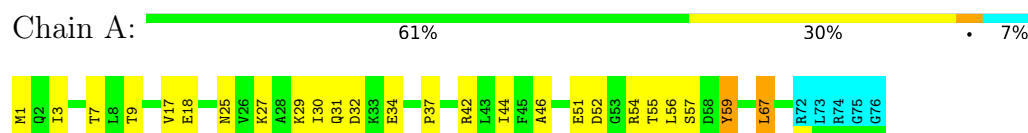
4.2.56 Score per residue for model 56

- Molecule 1: Ubiquitin



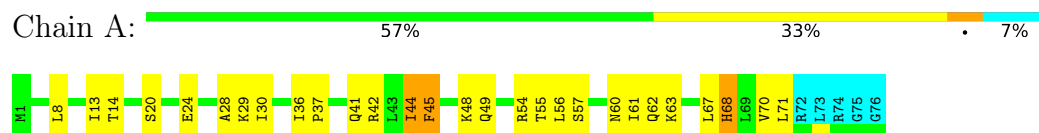
4.2.57 Score per residue for model 57

- Molecule 1: Ubiquitin



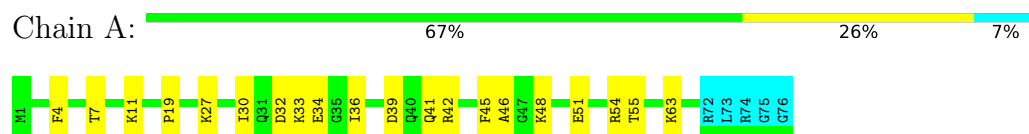
4.2.58 Score per residue for model 58

- Molecule 1: Ubiquitin



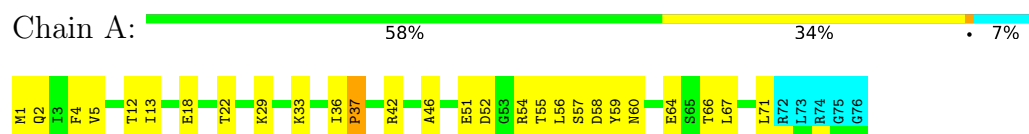
4.2.59 Score per residue for model 59

- Molecule 1: Ubiquitin



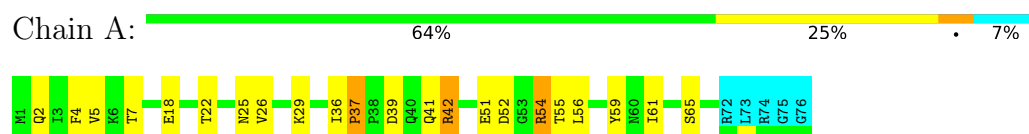
4.2.60 Score per residue for model 60

- Molecule 1: Ubiquitin



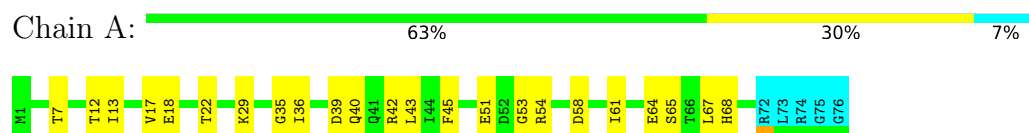
4.2.61 Score per residue for model 61

- Molecule 1: Ubiquitin



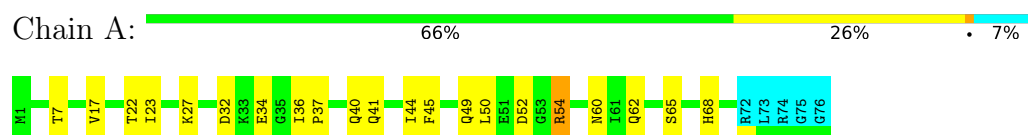
4.2.62 Score per residue for model 62

- Molecule 1: Ubiquitin



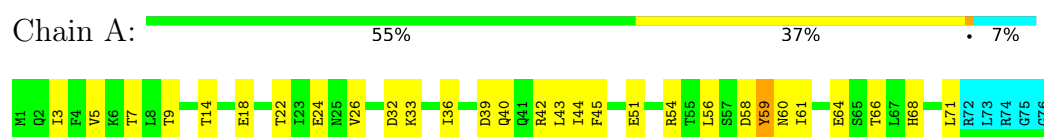
4.2.63 Score per residue for model 63

- Molecule 1: Ubiquitin



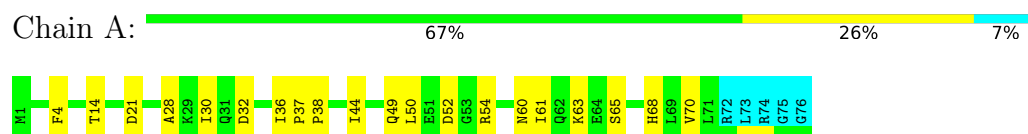
4.2.64 Score per residue for model 64

- Molecule 1: Ubiquitin



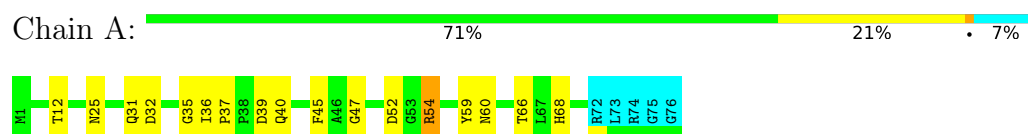
4.2.65 Score per residue for model 65

- Molecule 1: Ubiquitin



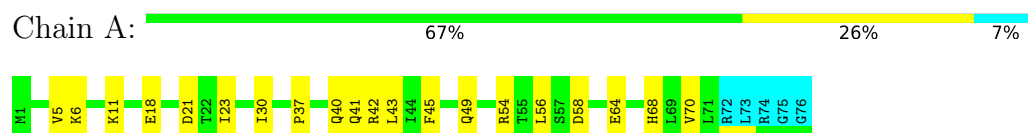
4.2.66 Score per residue for model 66

- Molecule 1: Ubiquitin



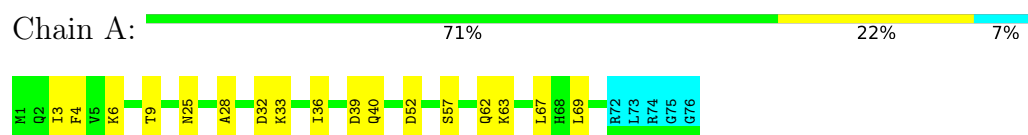
4.2.67 Score per residue for model 67

- Molecule 1: Ubiquitin



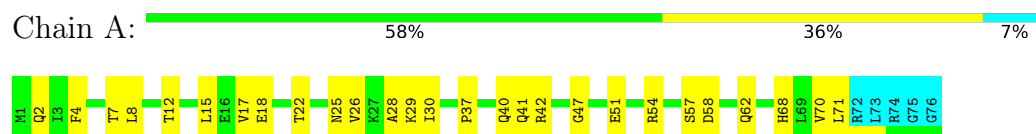
4.2.68 Score per residue for model 68

- Molecule 1: Ubiquitin



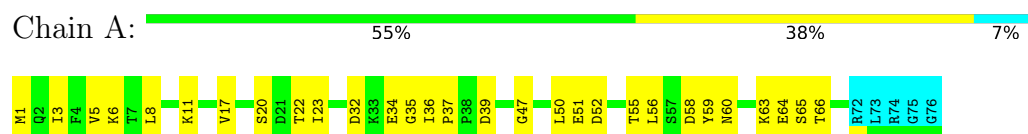
4.2.69 Score per residue for model 69

- Molecule 1: Ubiquitin



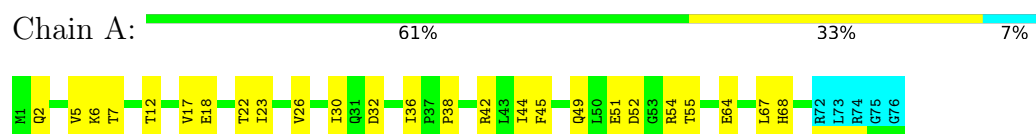
4.2.70 Score per residue for model 70

- Molecule 1: Ubiquitin



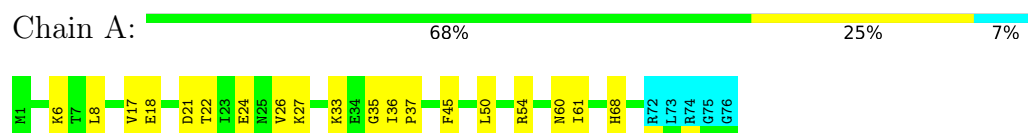
4.2.71 Score per residue for model 71

- Molecule 1: Ubiquitin



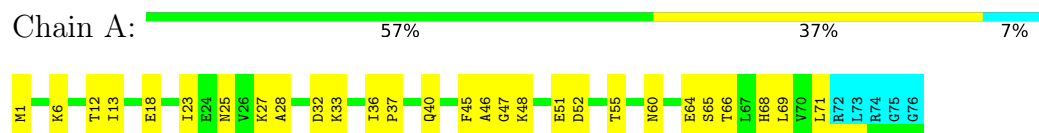
4.2.72 Score per residue for model 72

- Molecule 1: Ubiquitin



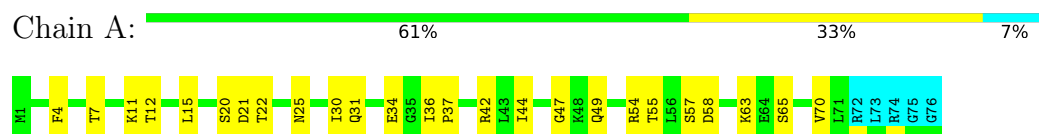
4.2.73 Score per residue for model 73

- Molecule 1: Ubiquitin



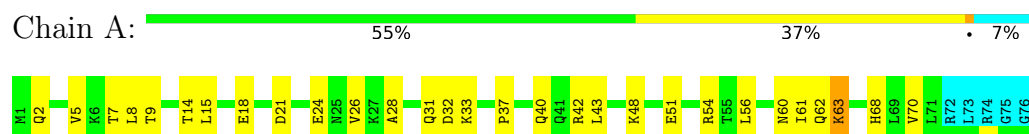
4.2.74 Score per residue for model 74

- Molecule 1: Ubiquitin



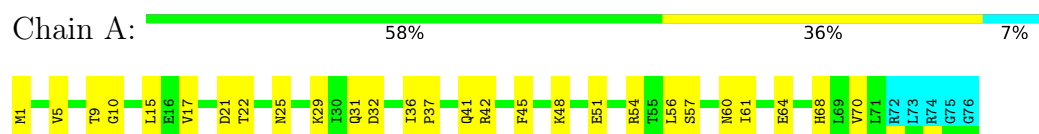
4.2.75 Score per residue for model 75

- Molecule 1: Ubiquitin



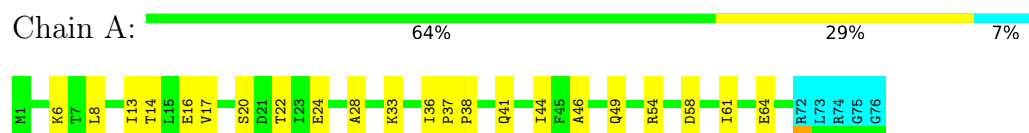
4.2.76 Score per residue for model 76 (medoid)

- Molecule 1: Ubiquitin



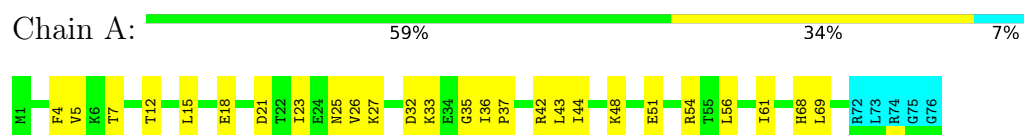
4.2.77 Score per residue for model 77

- Molecule 1: Ubiquitin



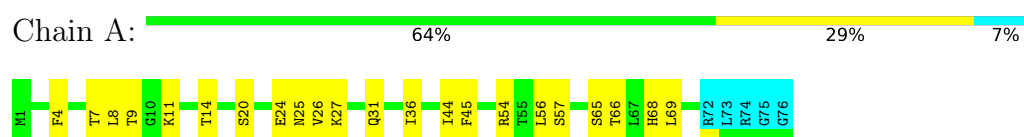
4.2.78 Score per residue for model 78

- Molecule 1: Ubiquitin



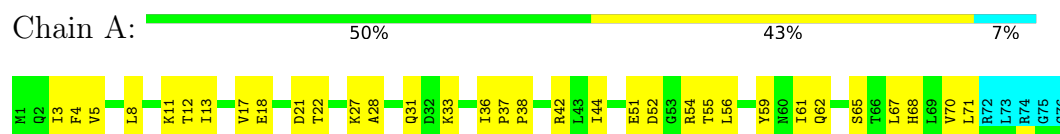
4.2.79 Score per residue for model 79

- Molecule 1: Ubiquitin



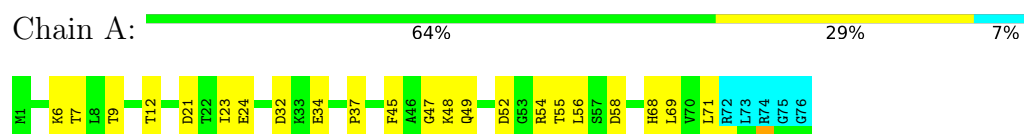
4.2.80 Score per residue for model 80

- Molecule 1: Ubiquitin



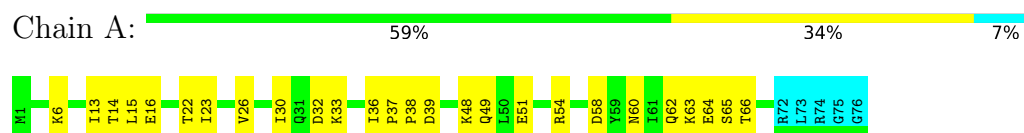
4.2.81 Score per residue for model 81

- Molecule 1: Ubiquitin



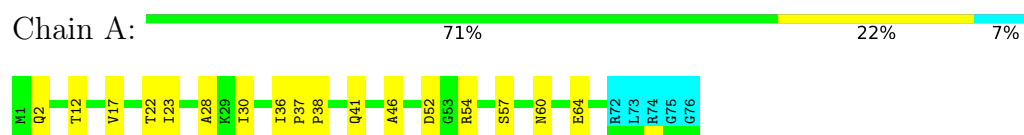
4.2.82 Score per residue for model 82

- Molecule 1: Ubiquitin



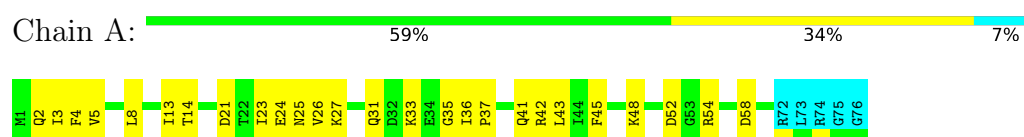
4.2.83 Score per residue for model 83

- Molecule 1: Ubiquitin



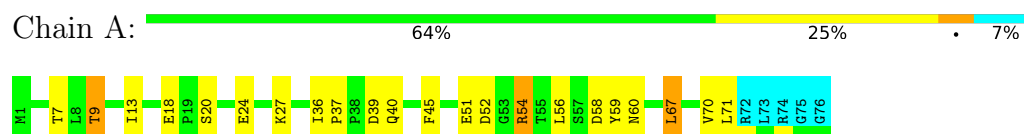
4.2.84 Score per residue for model 84

- Molecule 1: Ubiquitin



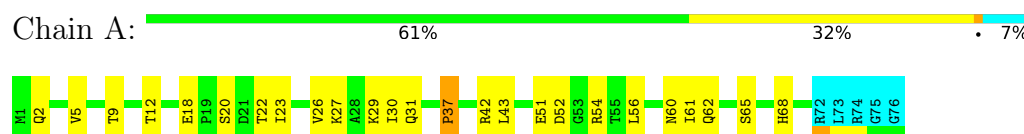
4.2.85 Score per residue for model 85

- Molecule 1: Ubiquitin



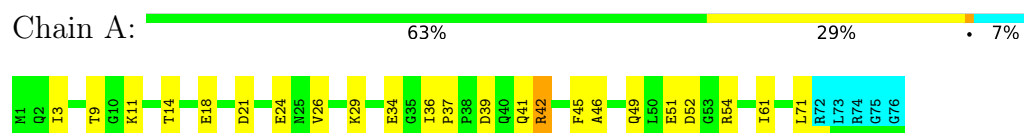
4.2.86 Score per residue for model 86

- Molecule 1: Ubiquitin



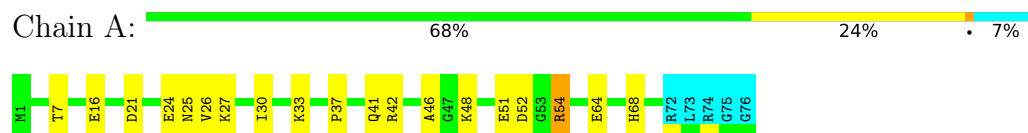
4.2.87 Score per residue for model 87

- Molecule 1: Ubiquitin



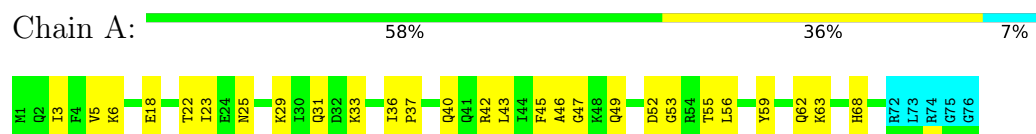
4.2.88 Score per residue for model 88

- Molecule 1: Ubiquitin



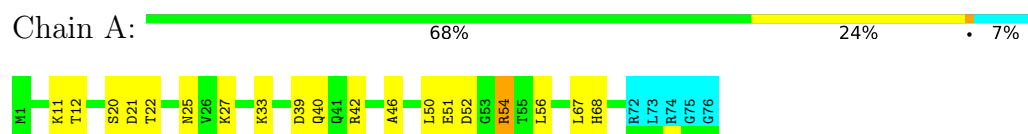
4.2.89 Score per residue for model 89

- Molecule 1: Ubiquitin



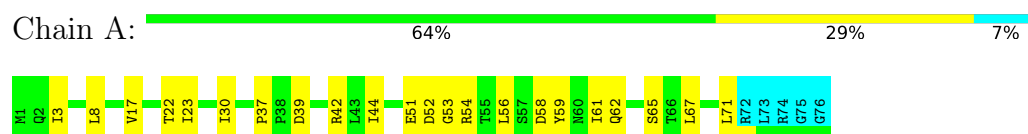
4.2.90 Score per residue for model 90

- Molecule 1: Ubiquitin



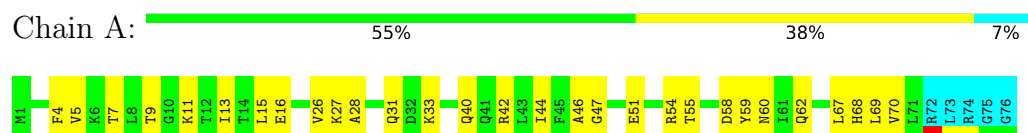
4.2.91 Score per residue for model 91

- Molecule 1: Ubiquitin



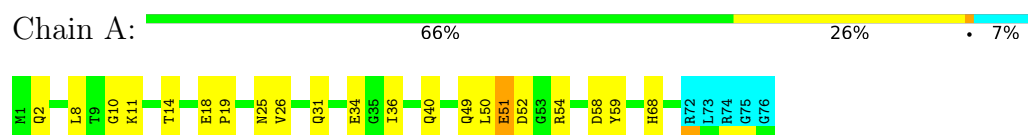
4.2.92 Score per residue for model 92

- Molecule 1: Ubiquitin



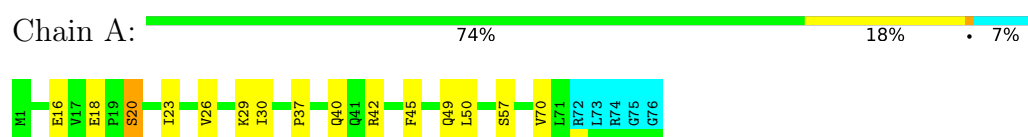
4.2.93 Score per residue for model 93

- Molecule 1: Ubiquitin



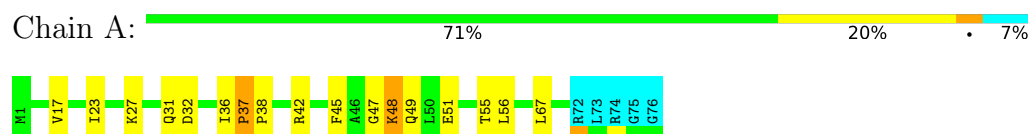
4.2.94 Score per residue for model 94

- Molecule 1: Ubiquitin



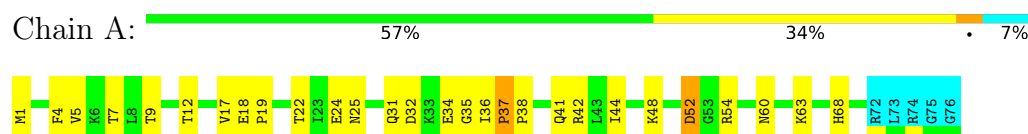
4.2.95 Score per residue for model 95

- Molecule 1: Ubiquitin



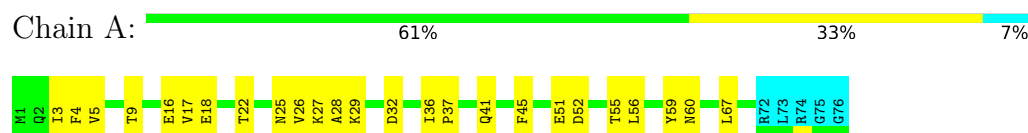
4.2.96 Score per residue for model 96

- Molecule 1: Ubiquitin



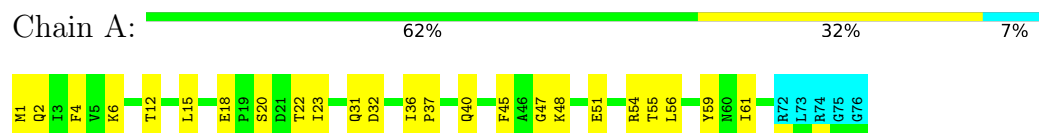
4.2.97 Score per residue for model 97

- Molecule 1: Ubiquitin



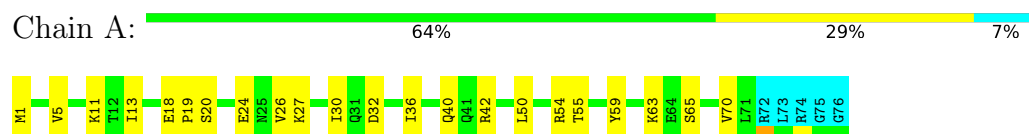
4.2.98 Score per residue for model 98

- Molecule 1: Ubiquitin



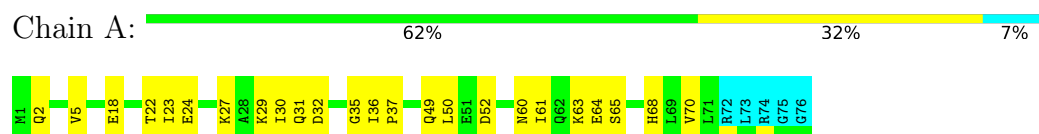
4.2.99 Score per residue for model 99

- Molecule 1: Ubiquitin



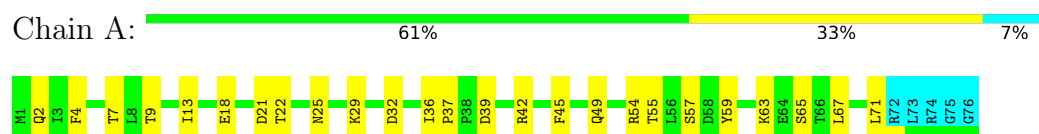
4.2.100 Score per residue for model 100

- Molecule 1: Ubiquitin



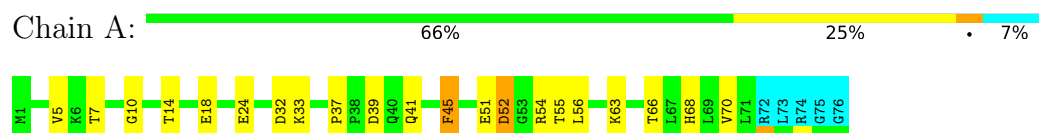
4.2.101 Score per residue for model 101

- Molecule 1: Ubiquitin



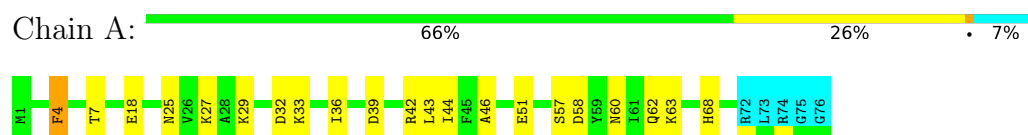
4.2.102 Score per residue for model 102

- Molecule 1: Ubiquitin



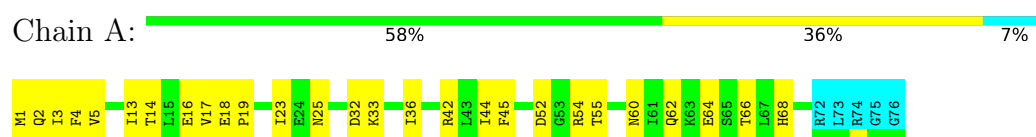
4.2.103 Score per residue for model 103

- Molecule 1: Ubiquitin



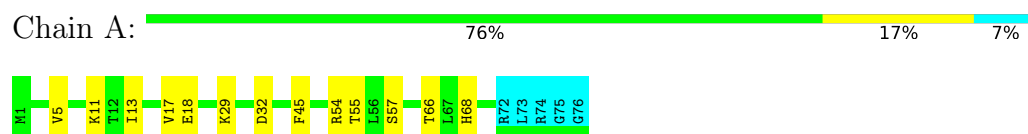
4.2.104 Score per residue for model 104

- Molecule 1: Ubiquitin



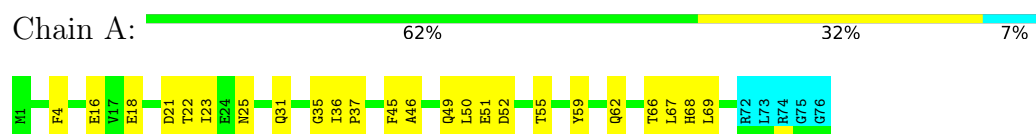
4.2.105 Score per residue for model 105

- Molecule 1: Ubiquitin



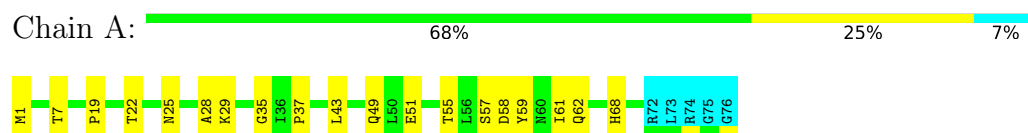
4.2.106 Score per residue for model 106

- Molecule 1: Ubiquitin



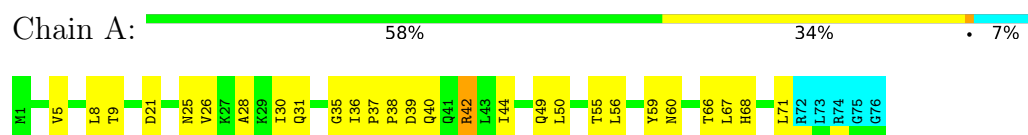
4.2.107 Score per residue for model 107

- Molecule 1: Ubiquitin



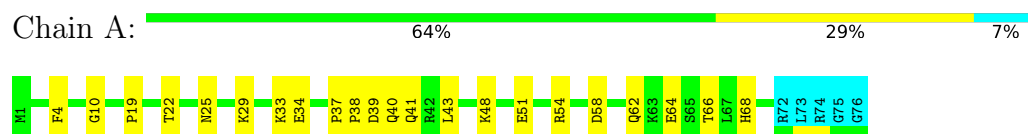
4.2.108 Score per residue for model 108

- Molecule 1: Ubiquitin



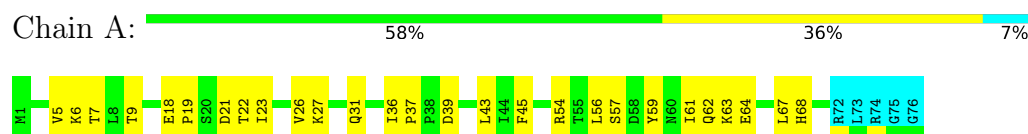
4.2.109 Score per residue for model 109

- Molecule 1: Ubiquitin



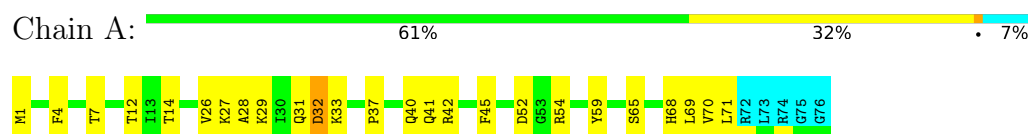
4.2.110 Score per residue for model 110

- Molecule 1: Ubiquitin



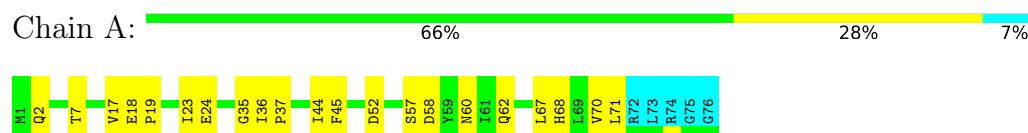
4.2.111 Score per residue for model 111

- Molecule 1: Ubiquitin



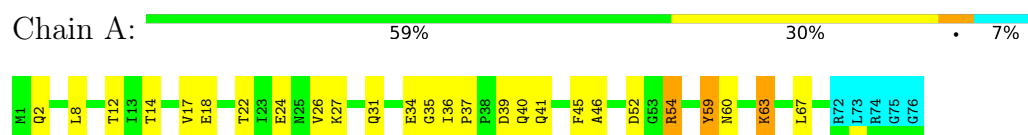
4.2.112 Score per residue for model 112

- Molecule 1: Ubiquitin



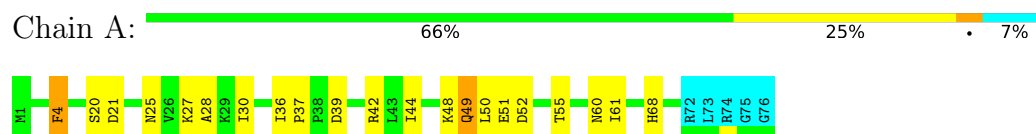
4.2.113 Score per residue for model 113

- Molecule 1: Ubiquitin



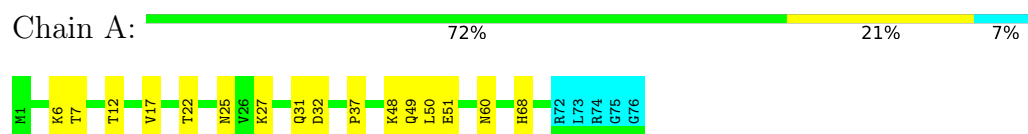
4.2.114 Score per residue for model 114

- Molecule 1: Ubiquitin



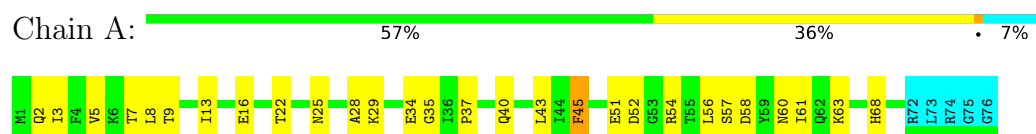
4.2.115 Score per residue for model 115

- Molecule 1: Ubiquitin



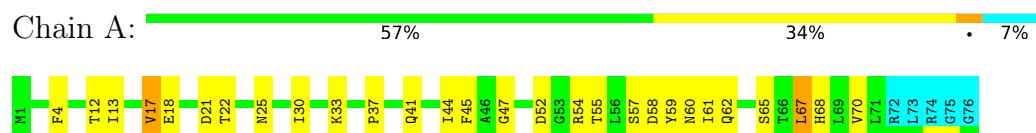
4.2.116 Score per residue for model 116

- Molecule 1: Ubiquitin



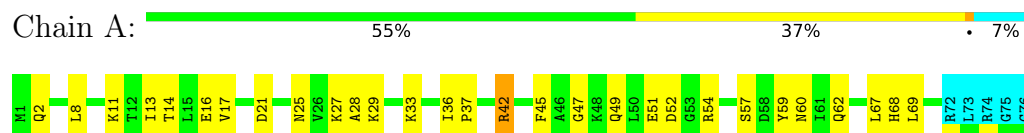
4.2.117 Score per residue for model 117

- Molecule 1: Ubiquitin



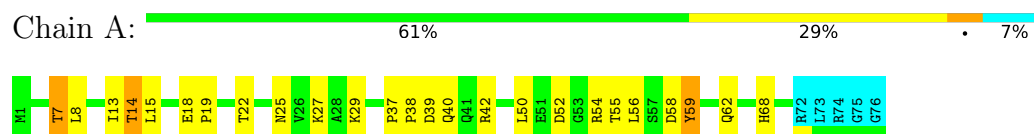
4.2.118 Score per residue for model 118

- Molecule 1: Ubiquitin



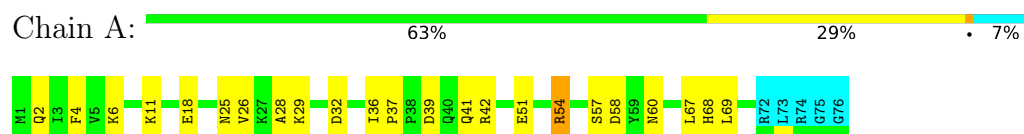
4.2.119 Score per residue for model 119

- Molecule 1: Ubiquitin



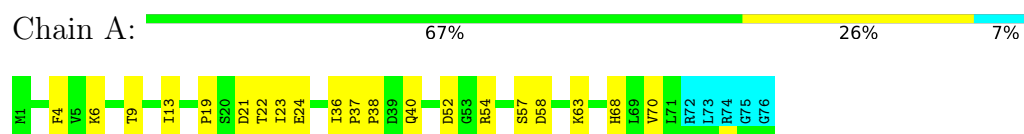
4.2.120 Score per residue for model 120

- Molecule 1: Ubiquitin



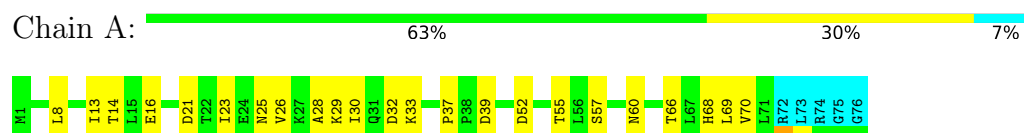
4.2.121 Score per residue for model 121

- Molecule 1: Ubiquitin



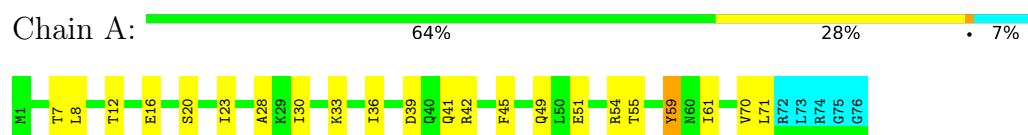
4.2.122 Score per residue for model 122

- Molecule 1: Ubiquitin



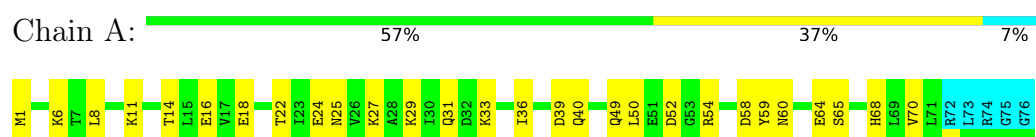
4.2.123 Score per residue for model 123

- Molecule 1: Ubiquitin



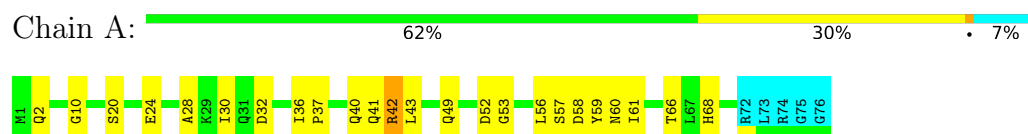
4.2.124 Score per residue for model 124

- Molecule 1: Ubiquitin



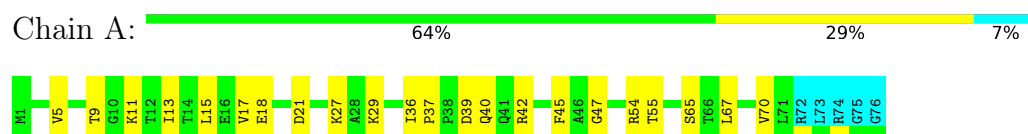
4.2.125 Score per residue for model 125

- Molecule 1: Ubiquitin



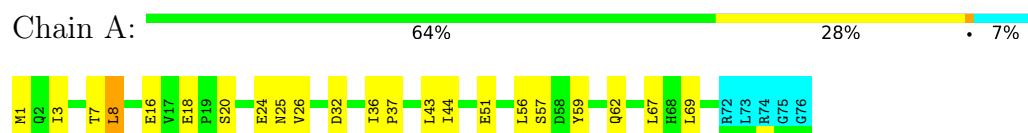
4.2.126 Score per residue for model 126

- Molecule 1: Ubiquitin



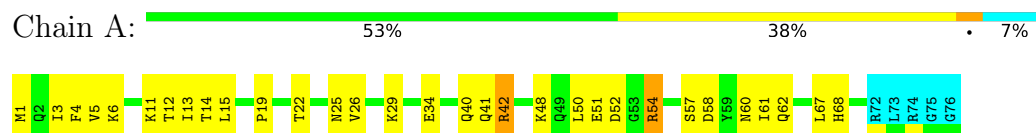
4.2.127 Score per residue for model 127

- Molecule 1: Ubiquitin



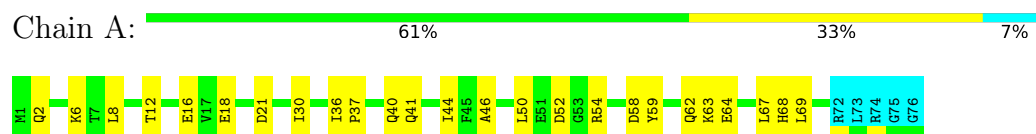
4.2.128 Score per residue for model 128

- Molecule 1: Ubiquitin



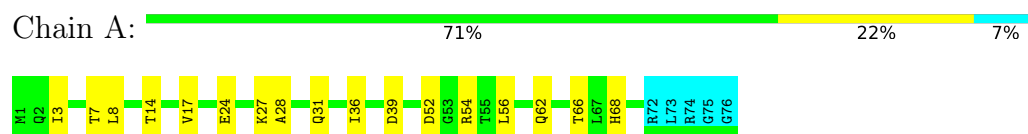
4.2.129 Score per residue for model 129

- Molecule 1: Ubiquitin



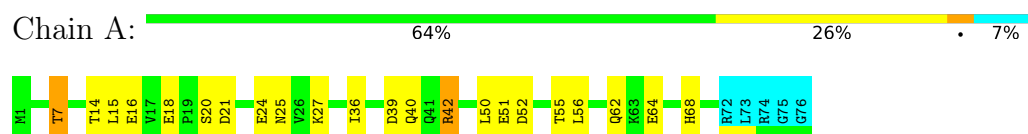
4.2.130 Score per residue for model 130

- Molecule 1: Ubiquitin



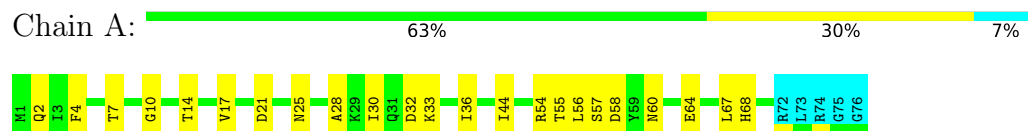
4.2.131 Score per residue for model 131

- Molecule 1: Ubiquitin



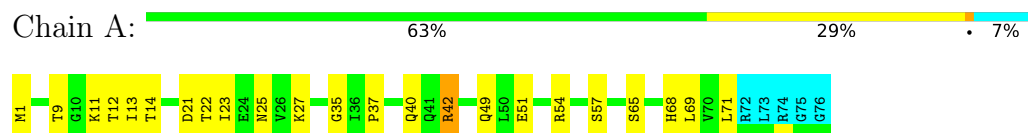
4.2.132 Score per residue for model 132

- Molecule 1: Ubiquitin



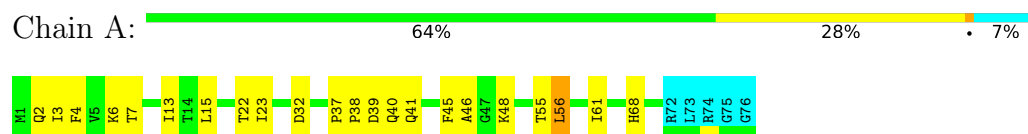
4.2.133 Score per residue for model 133

- Molecule 1: Ubiquitin



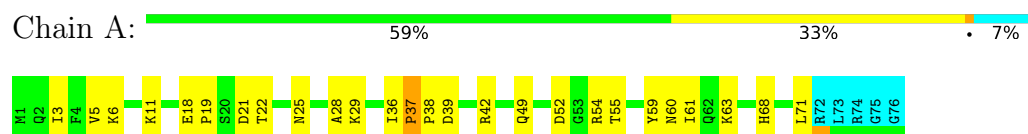
4.2.134 Score per residue for model 134

- Molecule 1: Ubiquitin



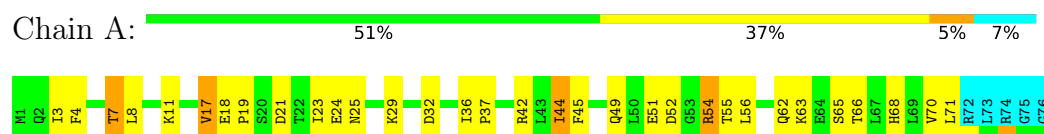
4.2.135 Score per residue for model 135

- Molecule 1: Ubiquitin



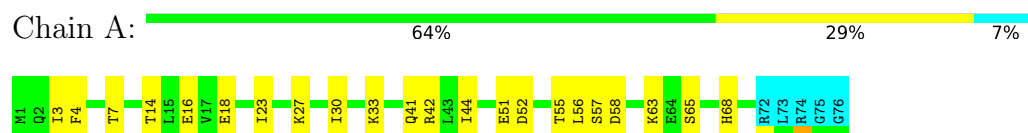
4.2.136 Score per residue for model 136

- Molecule 1: Ubiquitin



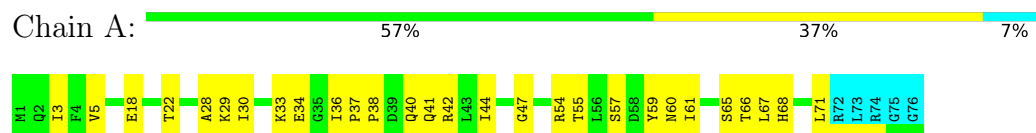
4.2.137 Score per residue for model 137

- Molecule 1: Ubiquitin



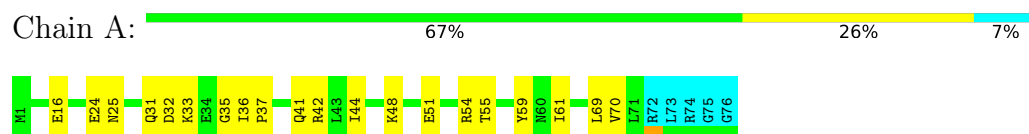
4.2.138 Score per residue for model 138

- Molecule 1: Ubiquitin



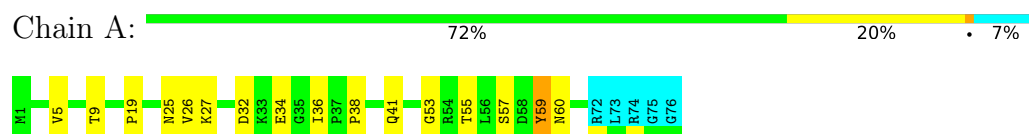
4.2.139 Score per residue for model 139

- Molecule 1: Ubiquitin



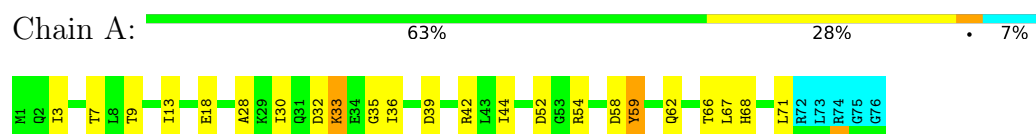
4.2.140 Score per residue for model 140

- Molecule 1: Ubiquitin



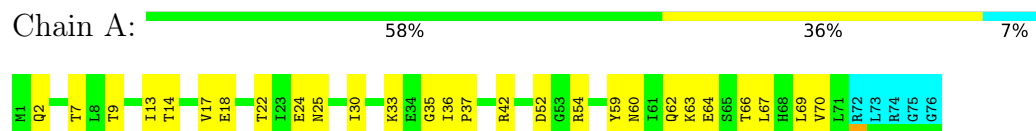
4.2.141 Score per residue for model 141

- Molecule 1: Ubiquitin



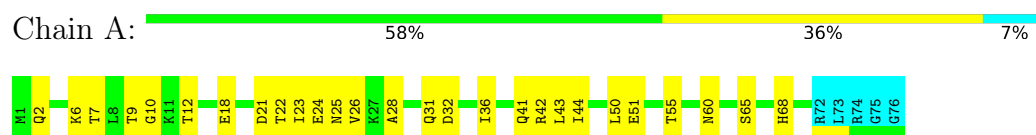
4.2.142 Score per residue for model 142

- Molecule 1: Ubiquitin



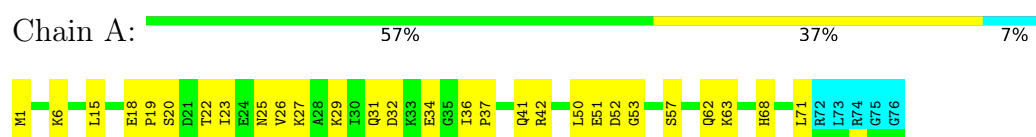
4.2.143 Score per residue for model 143

- Molecule 1: Ubiquitin



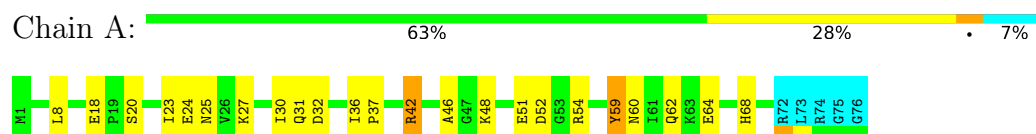
4.2.144 Score per residue for model 144

- Molecule 1: Ubiquitin



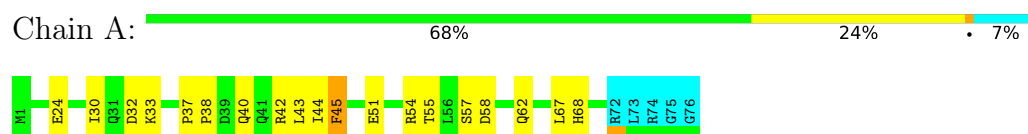
4.2.145 Score per residue for model 145

- Molecule 1: Ubiquitin



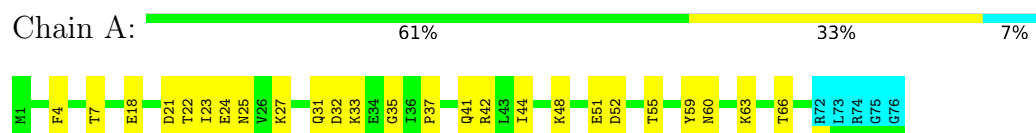
4.2.146 Score per residue for model 146

- Molecule 1: Ubiquitin



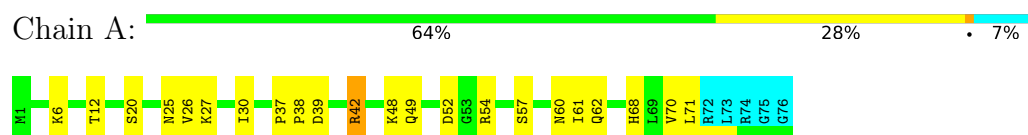
4.2.147 Score per residue for model 147

- Molecule 1: Ubiquitin



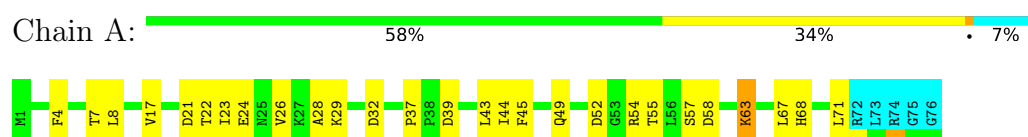
4.2.148 Score per residue for model 148

- Molecule 1: Ubiquitin



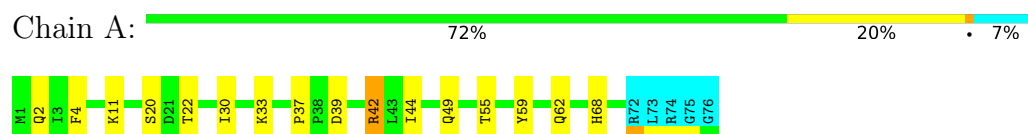
4.2.149 Score per residue for model 149

- Molecule 1: Ubiquitin



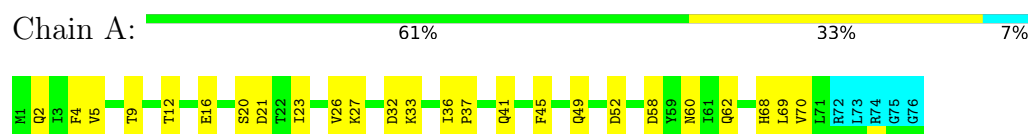
4.2.150 Score per residue for model 150

- Molecule 1: Ubiquitin



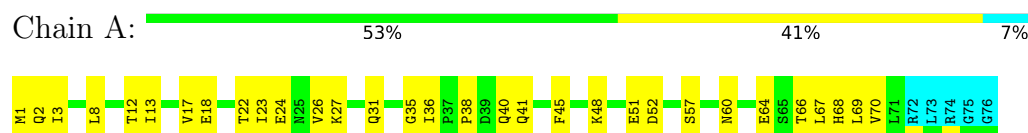
4.2.151 Score per residue for model 151

- Molecule 1: Ubiquitin



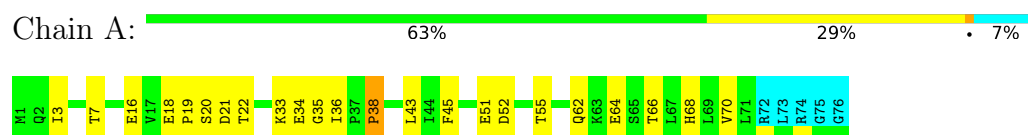
4.2.152 Score per residue for model 152

- Molecule 1: Ubiquitin



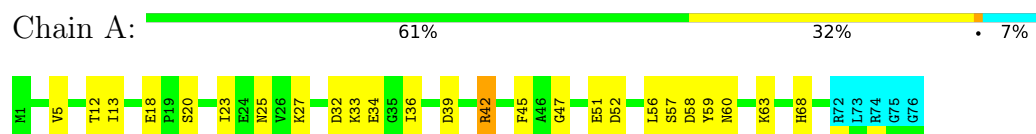
4.2.153 Score per residue for model 153

- Molecule 1: Ubiquitin



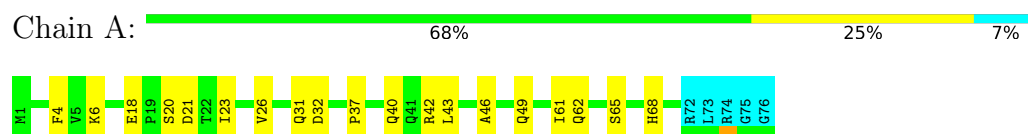
4.2.154 Score per residue for model 154

- Molecule 1: Ubiquitin



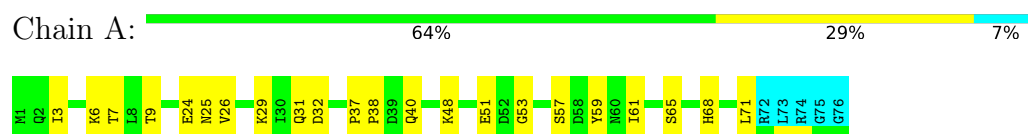
4.2.155 Score per residue for model 155

- Molecule 1: Ubiquitin



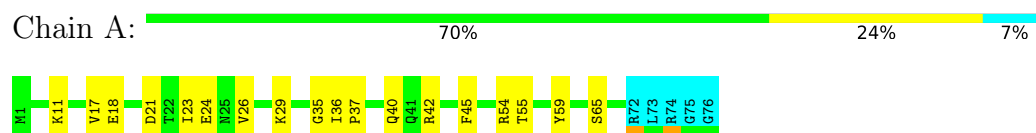
4.2.156 Score per residue for model 156

- Molecule 1: Ubiquitin



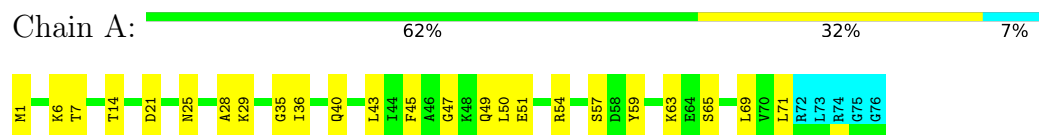
4.2.157 Score per residue for model 157

- Molecule 1: Ubiquitin



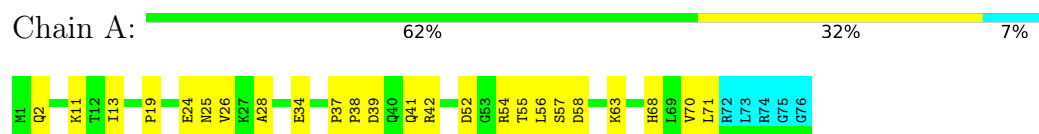
4.2.158 Score per residue for model 158

- Molecule 1: Ubiquitin



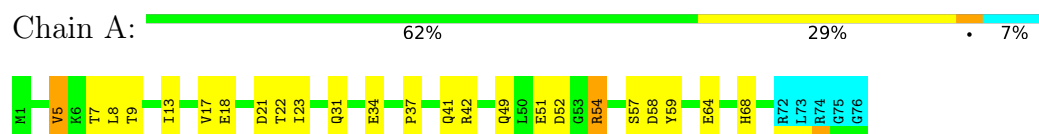
4.2.159 Score per residue for model 159

- Molecule 1: Ubiquitin



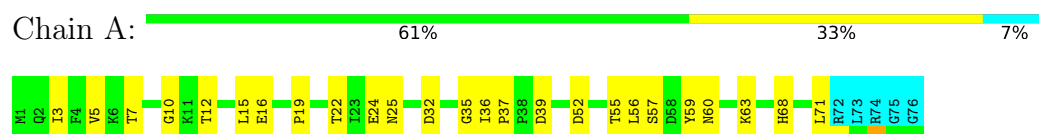
4.2.160 Score per residue for model 160

- Molecule 1: Ubiquitin



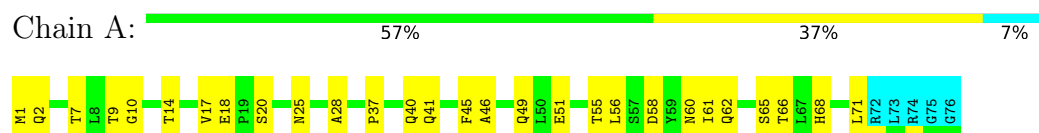
4.2.161 Score per residue for model 161

- Molecule 1: Ubiquitin



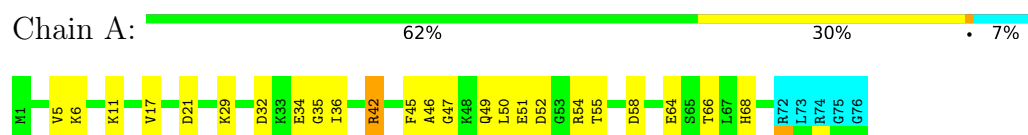
4.2.162 Score per residue for model 162

- Molecule 1: Ubiquitin



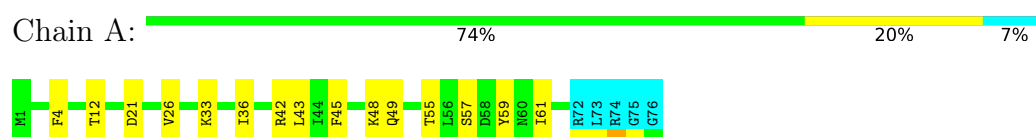
4.2.163 Score per residue for model 163

- Molecule 1: Ubiquitin



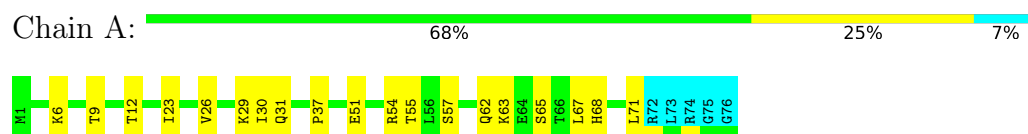
4.2.164 Score per residue for model 164

- Molecule 1: Ubiquitin



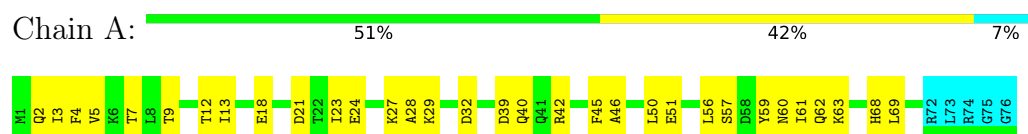
4.2.165 Score per residue for model 165

- Molecule 1: Ubiquitin



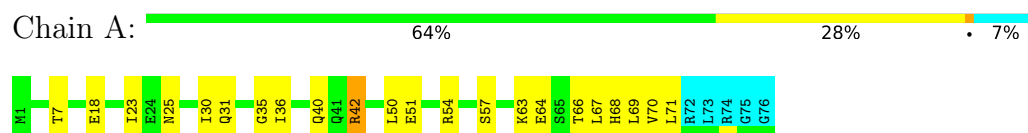
4.2.166 Score per residue for model 166

- Molecule 1: Ubiquitin



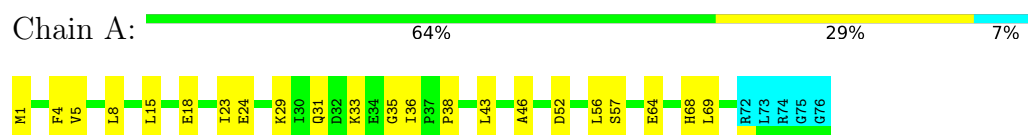
4.2.167 Score per residue for model 167

- Molecule 1: Ubiquitin



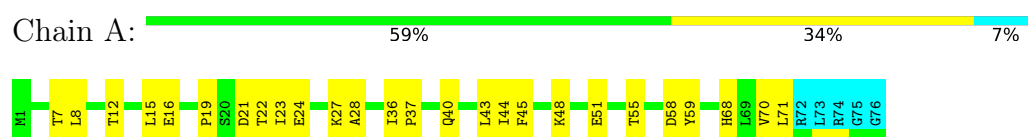
4.2.168 Score per residue for model 168

- Molecule 1: Ubiquitin



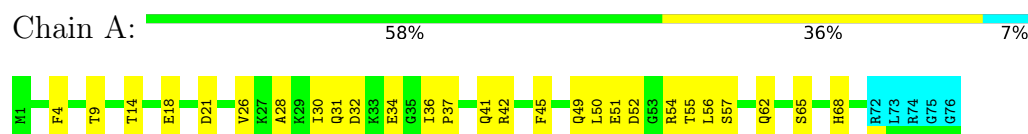
4.2.169 Score per residue for model 169

- Molecule 1: Ubiquitin



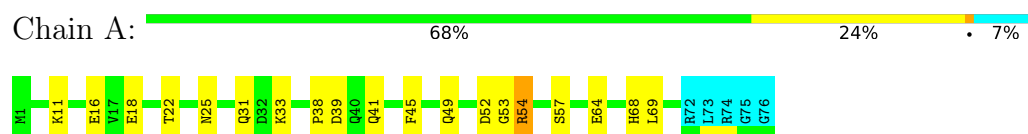
4.2.170 Score per residue for model 170

- Molecule 1: Ubiquitin



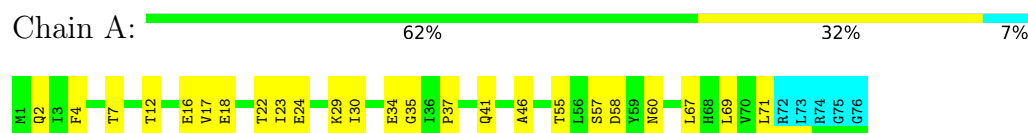
4.2.171 Score per residue for model 171

- Molecule 1: Ubiquitin



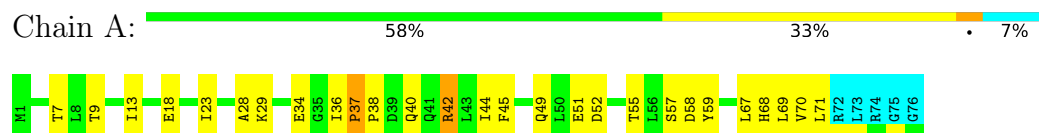
4.2.172 Score per residue for model 172

- Molecule 1: Ubiquitin



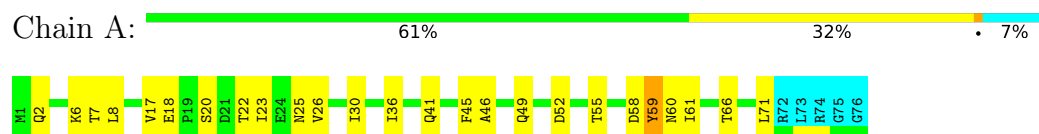
4.2.173 Score per residue for model 173

- Molecule 1: Ubiquitin



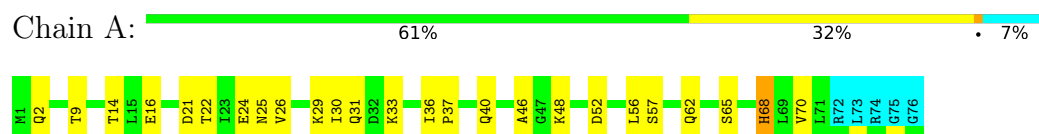
4.2.174 Score per residue for model 174

- Molecule 1: Ubiquitin



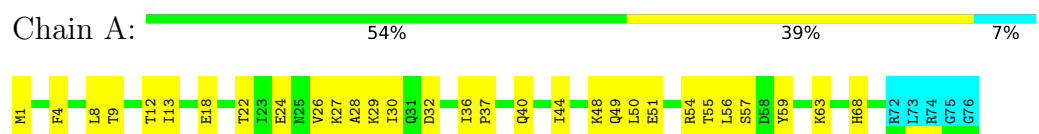
4.2.175 Score per residue for model 175

- Molecule 1: Ubiquitin



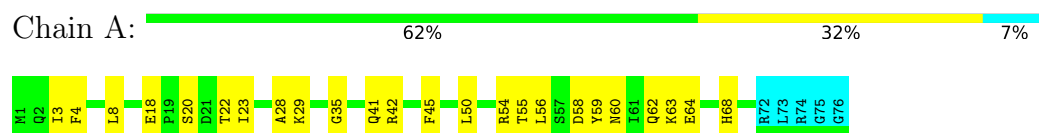
4.2.176 Score per residue for model 176

- Molecule 1: Ubiquitin



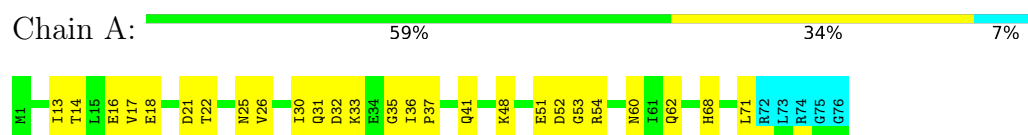
4.2.177 Score per residue for model 177

- Molecule 1: Ubiquitin



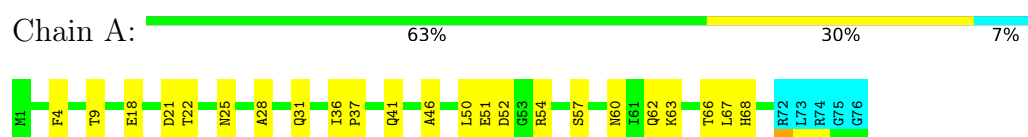
4.2.178 Score per residue for model 178

- Molecule 1: Ubiquitin



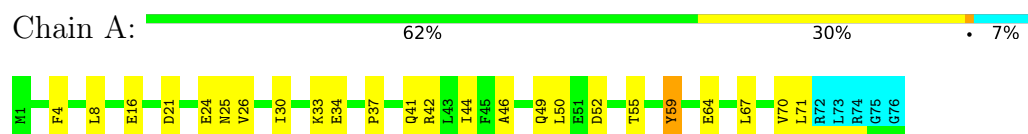
4.2.179 Score per residue for model 179

- Molecule 1: Ubiquitin



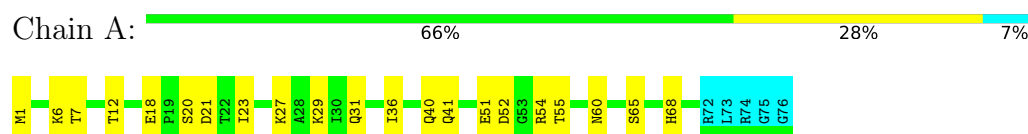
4.2.180 Score per residue for model 180

- Molecule 1: Ubiquitin



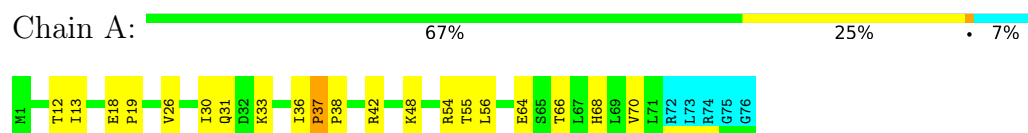
4.2.181 Score per residue for model 181

- Molecule 1: Ubiquitin



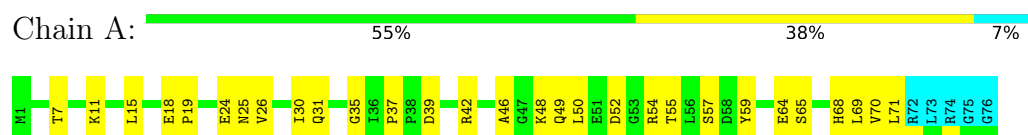
4.2.182 Score per residue for model 182

- Molecule 1: Ubiquitin



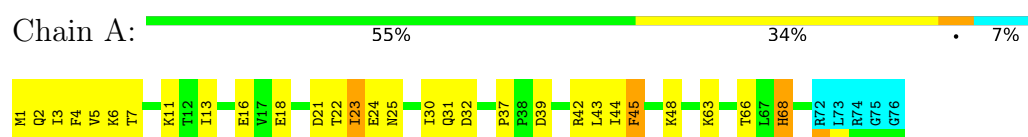
4.2.183 Score per residue for model 183

- Molecule 1: Ubiquitin



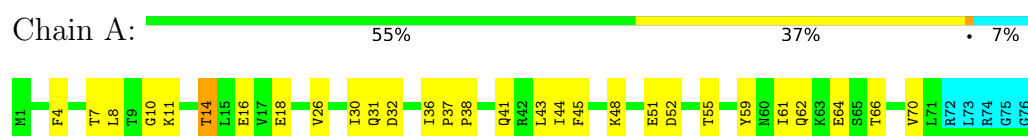
4.2.184 Score per residue for model 184

- Molecule 1: Ubiquitin



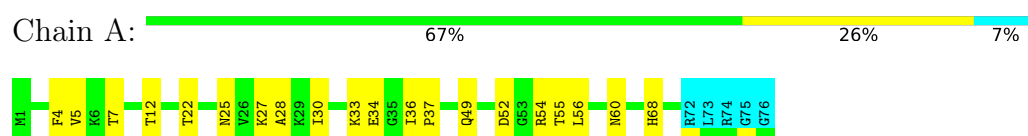
4.2.185 Score per residue for model 185

- Molecule 1: Ubiquitin



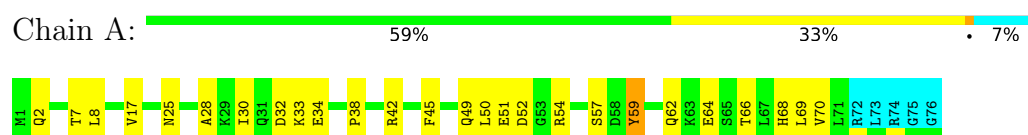
4.2.186 Score per residue for model 186

- Molecule 1: Ubiquitin



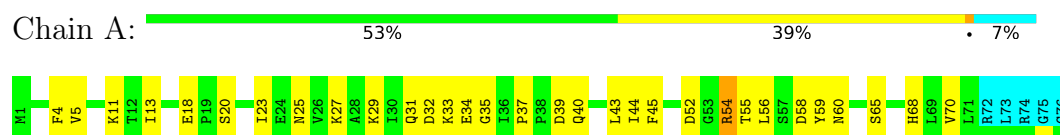
4.2.187 Score per residue for model 187

- Molecule 1: Ubiquitin



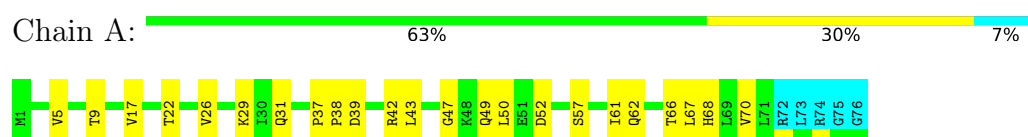
4.2.188 Score per residue for model 188

- Molecule 1: Ubiquitin



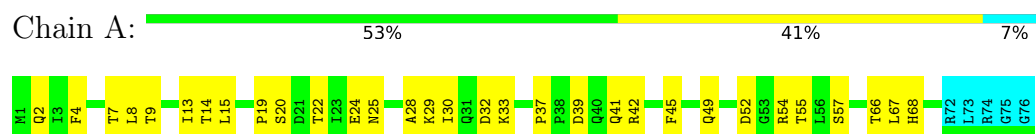
4.2.189 Score per residue for model 189

- Molecule 1: Ubiquitin



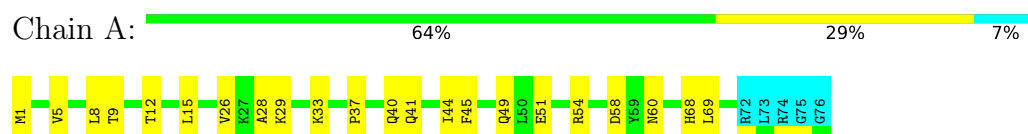
4.2.190 Score per residue for model 190

- Molecule 1: Ubiquitin



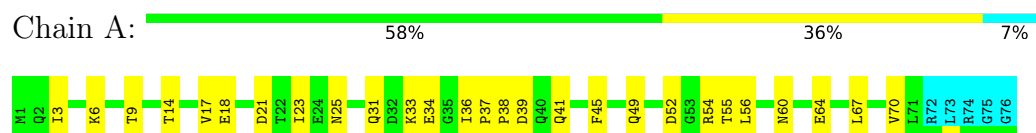
4.2.191 Score per residue for model 191

- Molecule 1: Ubiquitin



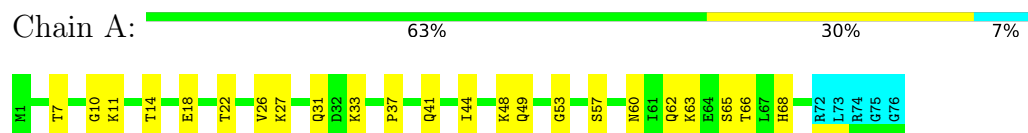
4.2.192 Score per residue for model 192

- Molecule 1: Ubiquitin



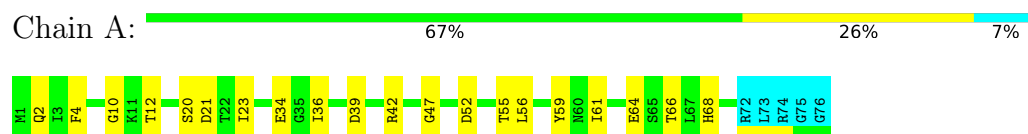
4.2.193 Score per residue for model 193

- Molecule 1: Ubiquitin



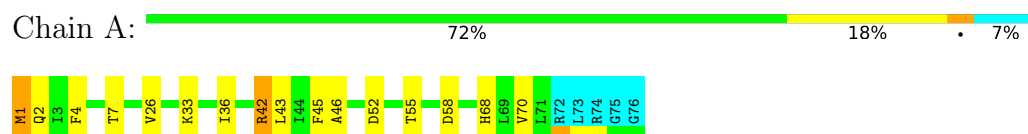
4.2.194 Score per residue for model 194

- Molecule 1: Ubiquitin



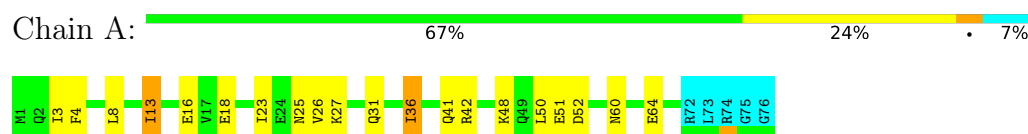
4.2.195 Score per residue for model 195

- Molecule 1: Ubiquitin



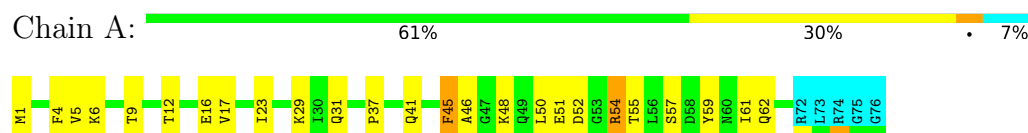
4.2.196 Score per residue for model 196

- Molecule 1: Ubiquitin



4.2.197 Score per residue for model 197

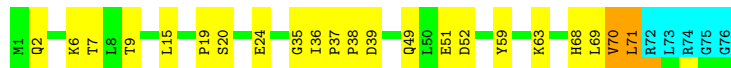
- Molecule 1: Ubiquitin



4.2.198 Score per residue for model 198

- Molecule 1: Ubiquitin

Chain A:  64% 26% 7%



4.2.199 Score per residue for model 199

- Molecule 1: Ubiquitin

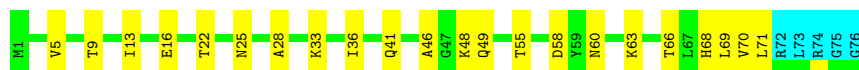
Chain A:  67% 24% 7%



4.2.200 Score per residue for model 200

- Molecule 1: Ubiquitin

Chain A:  64% 29% 7%



4.2.201 Score per residue for model 201

- Molecule 1: Ubiquitin

Chain A:  63% 30% 7%



4.2.202 Score per residue for model 202

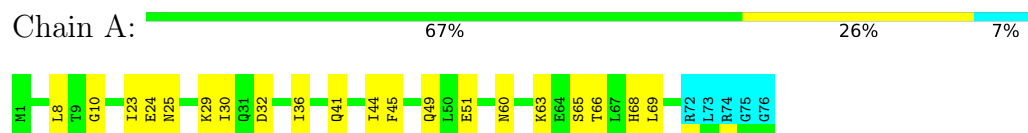
- Molecule 1: Ubiquitin

Chain A:  66% 26% 7%



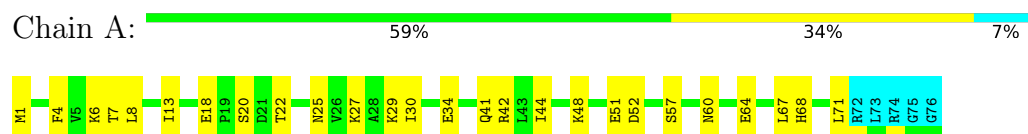
4.2.203 Score per residue for model 203

- Molecule 1: Ubiquitin



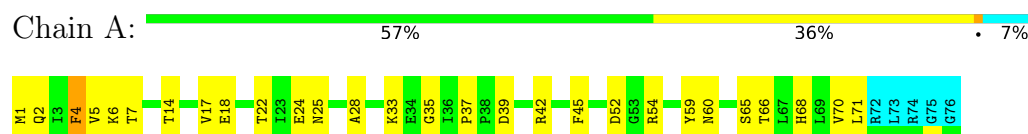
4.2.204 Score per residue for model 204

- Molecule 1: Ubiquitin



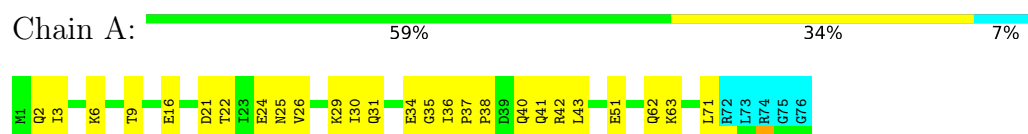
4.2.205 Score per residue for model 205

- Molecule 1: Ubiquitin



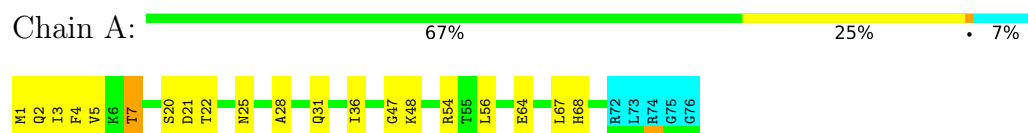
4.2.206 Score per residue for model 206

- Molecule 1: Ubiquitin



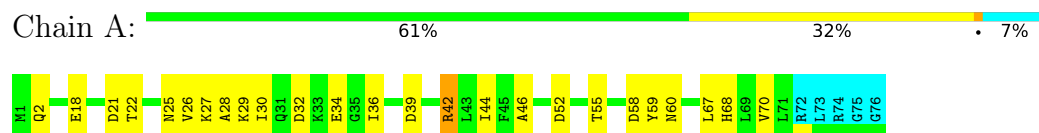
4.2.207 Score per residue for model 207

- Molecule 1: Ubiquitin



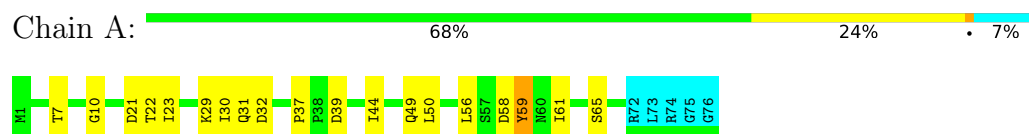
4.2.208 Score per residue for model 208

- Molecule 1: Ubiquitin



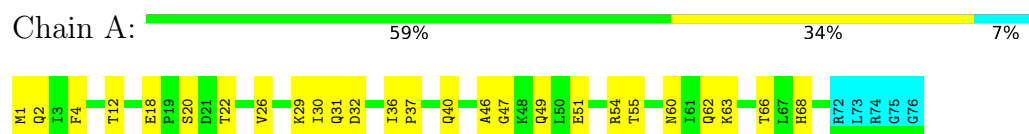
4.2.209 Score per residue for model 209

- Molecule 1: Ubiquitin



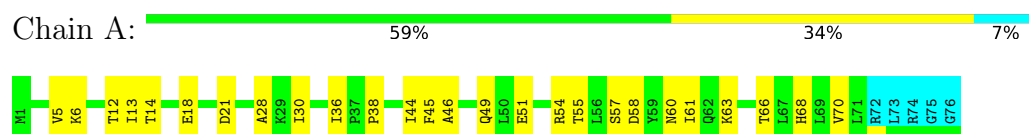
4.2.210 Score per residue for model 210

- Molecule 1: Ubiquitin



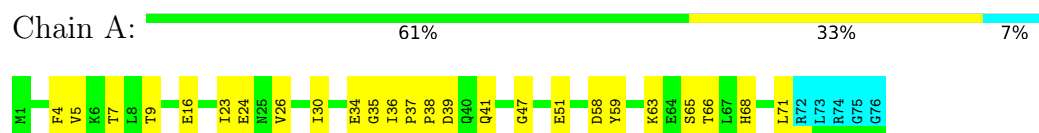
4.2.211 Score per residue for model 211

- Molecule 1: Ubiquitin



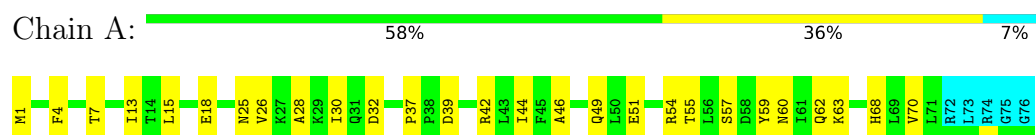
4.2.212 Score per residue for model 212

- Molecule 1: Ubiquitin



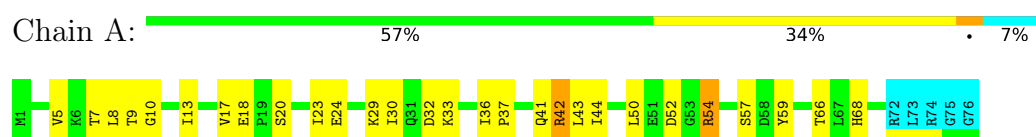
4.2.213 Score per residue for model 213

- Molecule 1: Ubiquitin



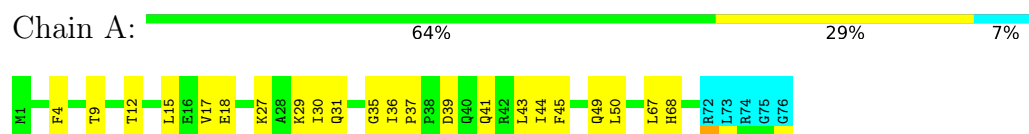
4.2.214 Score per residue for model 214

- Molecule 1: Ubiquitin



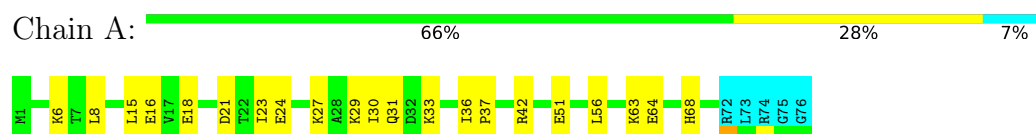
4.2.215 Score per residue for model 215

- Molecule 1: Ubiquitin



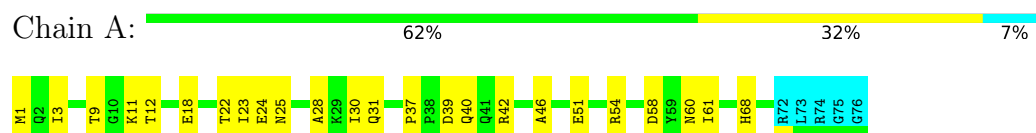
4.2.216 Score per residue for model 216

- Molecule 1: Ubiquitin



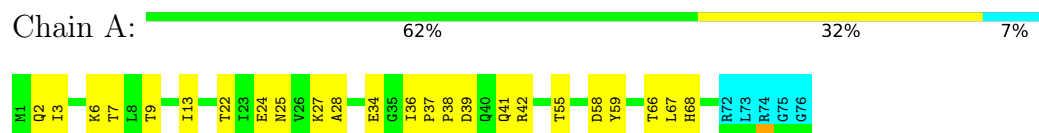
4.2.217 Score per residue for model 217

- Molecule 1: Ubiquitin



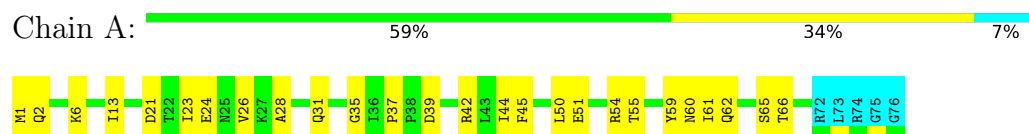
4.2.218 Score per residue for model 218

- Molecule 1: Ubiquitin



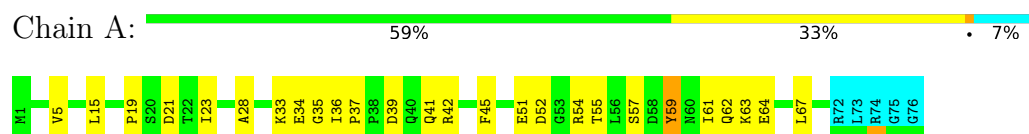
4.2.219 Score per residue for model 219

- Molecule 1: Ubiquitin



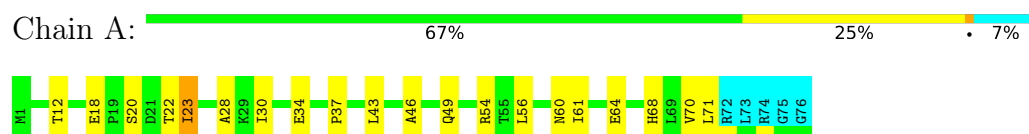
4.2.220 Score per residue for model 220

- Molecule 1: Ubiquitin



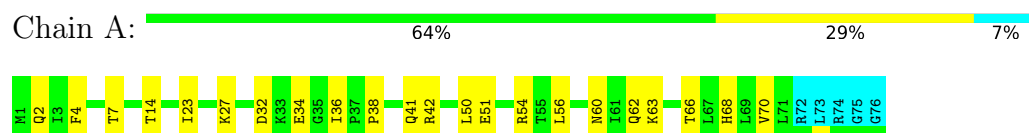
4.2.221 Score per residue for model 221

- Molecule 1: Ubiquitin



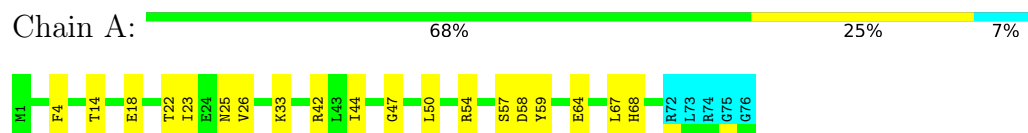
4.2.222 Score per residue for model 222

- Molecule 1: Ubiquitin



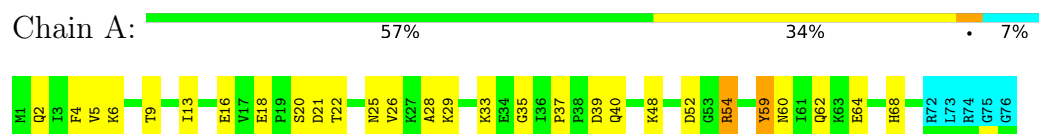
4.2.223 Score per residue for model 223

- Molecule 1: Ubiquitin



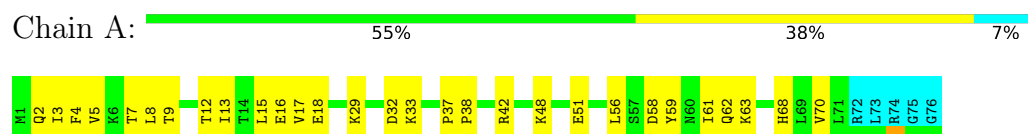
4.2.224 Score per residue for model 224

- Molecule 1: Ubiquitin



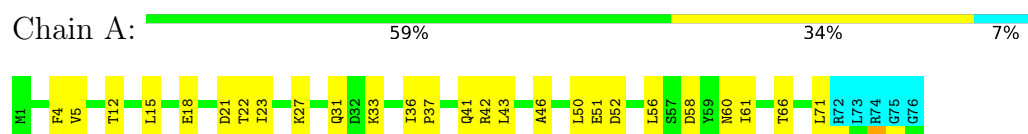
4.2.225 Score per residue for model 225

- Molecule 1: Ubiquitin



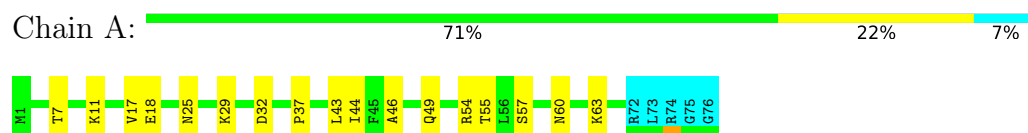
4.2.226 Score per residue for model 226

- Molecule 1: Ubiquitin



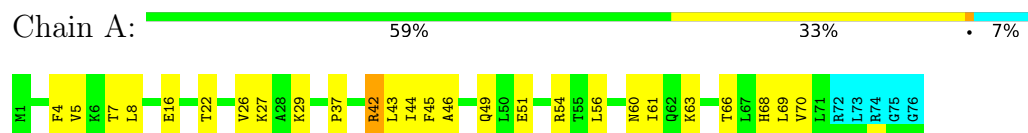
4.2.227 Score per residue for model 227

- Molecule 1: Ubiquitin



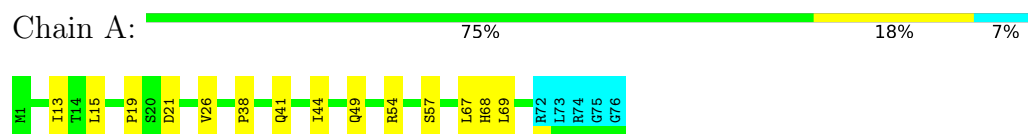
4.2.228 Score per residue for model 228

- Molecule 1: Ubiquitin



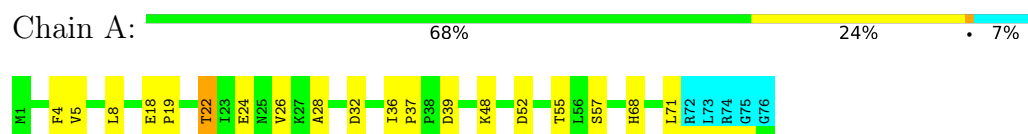
4.2.229 Score per residue for model 229

- Molecule 1: Ubiquitin



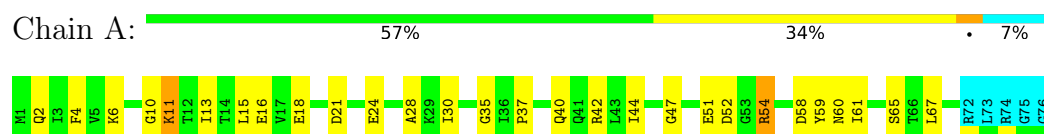
4.2.230 Score per residue for model 230

- Molecule 1: Ubiquitin



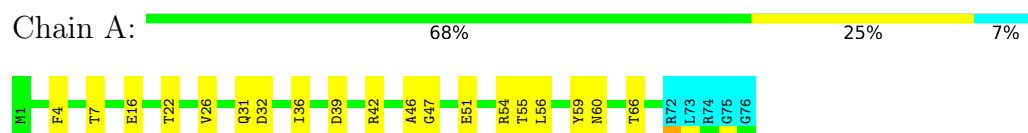
4.2.231 Score per residue for model 231

- Molecule 1: Ubiquitin



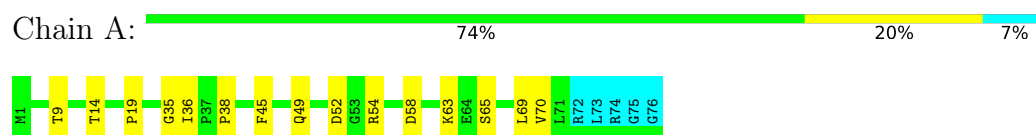
4.2.232 Score per residue for model 232

- Molecule 1: Ubiquitin



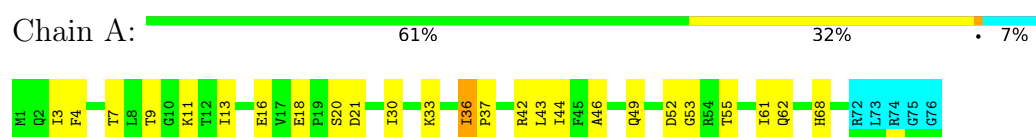
4.2.233 Score per residue for model 233

- Molecule 1: Ubiquitin



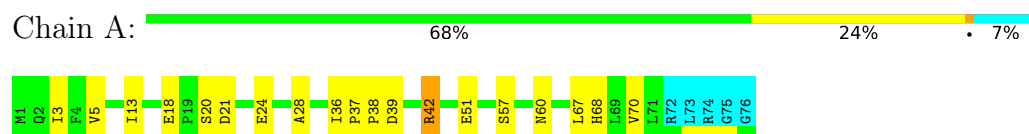
4.2.234 Score per residue for model 234

- Molecule 1: Ubiquitin



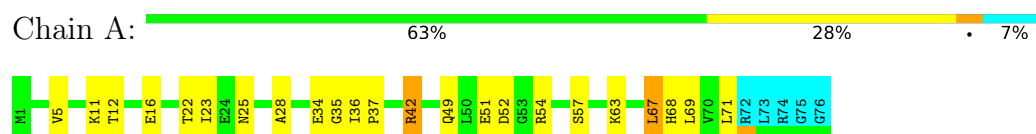
4.2.235 Score per residue for model 235

- Molecule 1: Ubiquitin



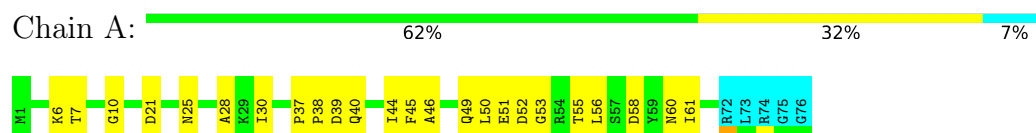
4.2.236 Score per residue for model 236

- Molecule 1: Ubiquitin



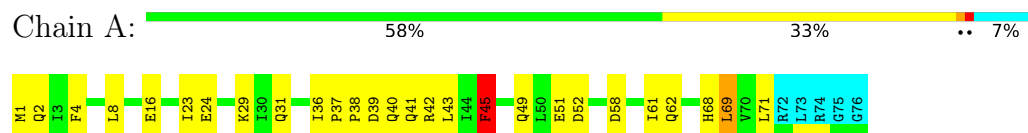
4.2.237 Score per residue for model 237

- Molecule 1: Ubiquitin



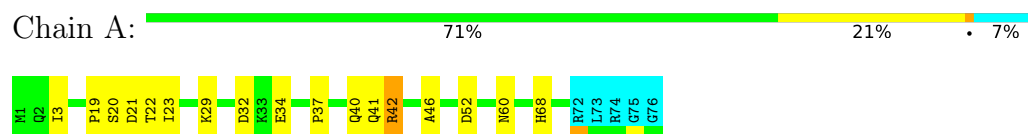
4.2.238 Score per residue for model 238

- Molecule 1: Ubiquitin



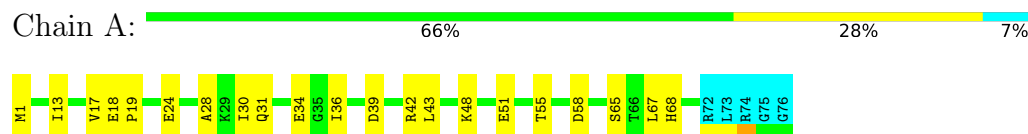
4.2.239 Score per residue for model 239

- Molecule 1: Ubiquitin



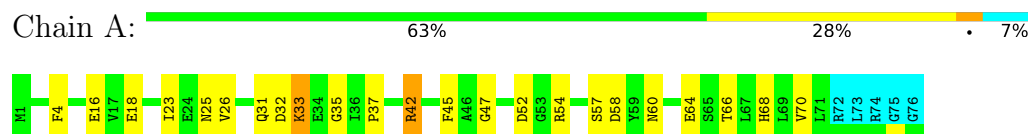
4.2.240 Score per residue for model 240

- Molecule 1: Ubiquitin



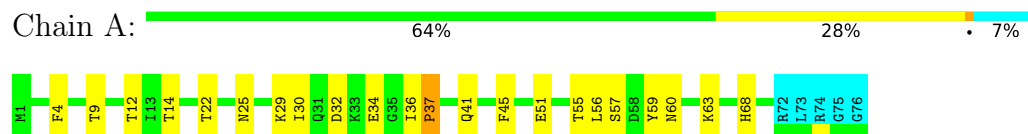
4.2.241 Score per residue for model 241

- Molecule 1: Ubiquitin



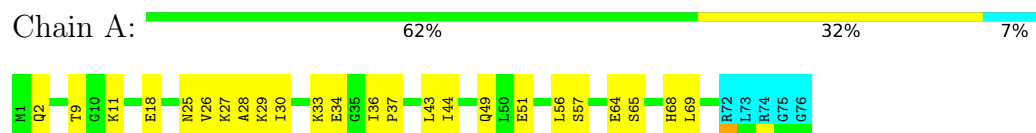
4.2.242 Score per residue for model 242

- Molecule 1: Ubiquitin



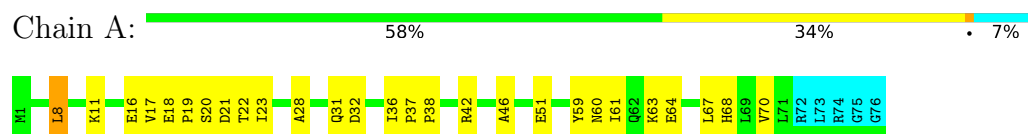
4.2.243 Score per residue for model 243

- Molecule 1: Ubiquitin



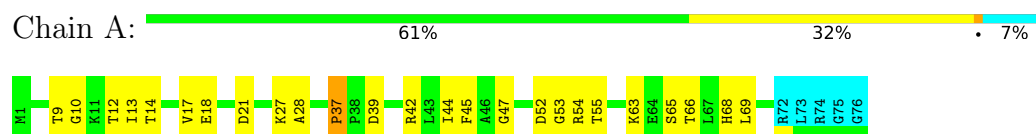
4.2.244 Score per residue for model 244

- Molecule 1: Ubiquitin



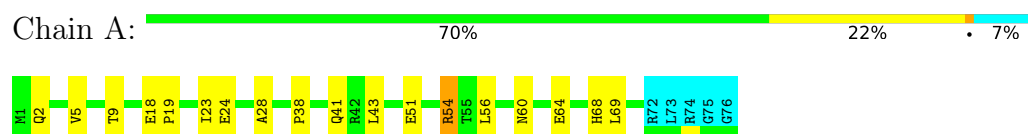
4.2.245 Score per residue for model 245

- Molecule 1: Ubiquitin



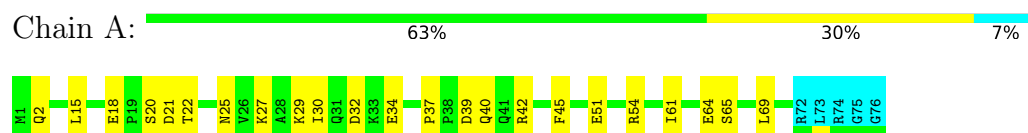
4.2.246 Score per residue for model 246

- Molecule 1: Ubiquitin



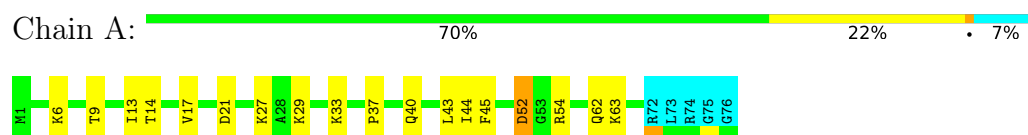
4.2.247 Score per residue for model 247

- Molecule 1: Ubiquitin



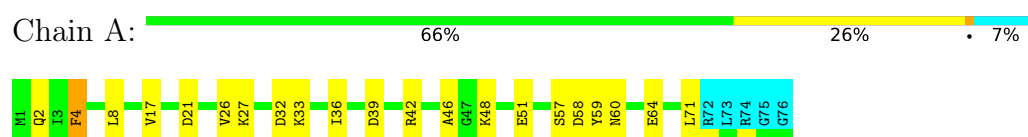
4.2.248 Score per residue for model 248

- Molecule 1: Ubiquitin



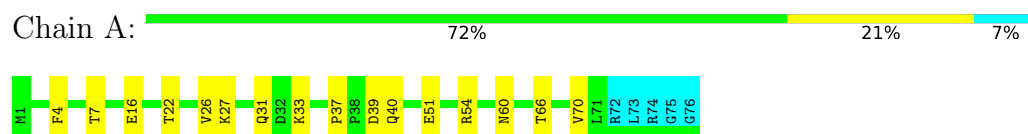
4.2.249 Score per residue for model 249

- Molecule 1: Ubiquitin



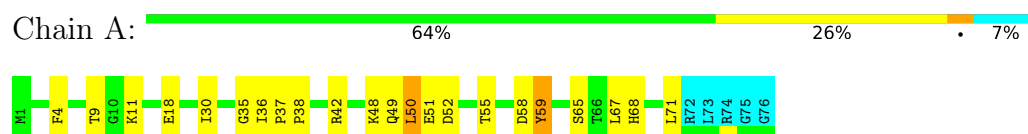
4.2.250 Score per residue for model 250

- Molecule 1: Ubiquitin



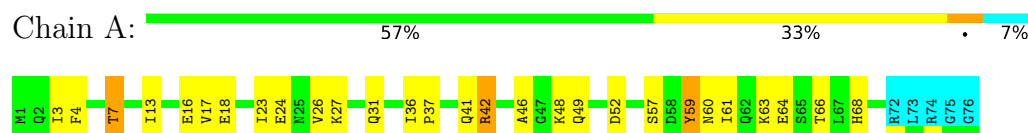
4.2.251 Score per residue for model 251

- Molecule 1: Ubiquitin



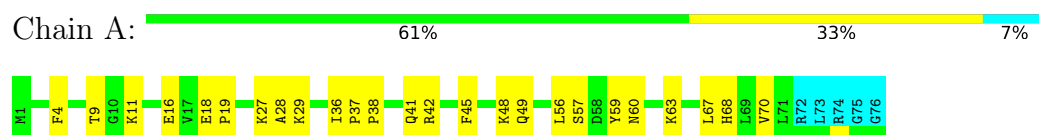
4.2.252 Score per residue for model 252

- Molecule 1: Ubiquitin



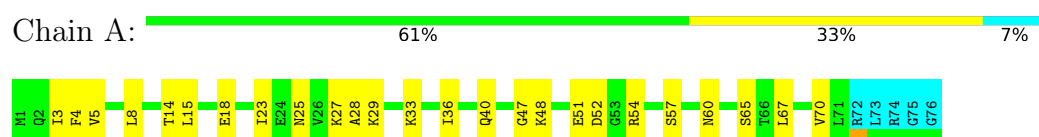
4.2.253 Score per residue for model 253

- Molecule 1: Ubiquitin



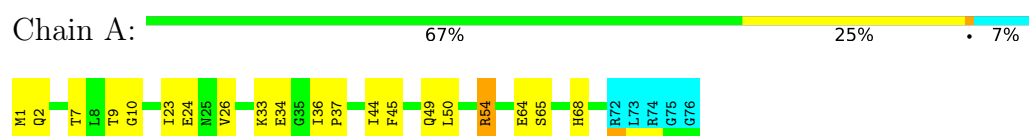
4.2.254 Score per residue for model 254

- Molecule 1: Ubiquitin



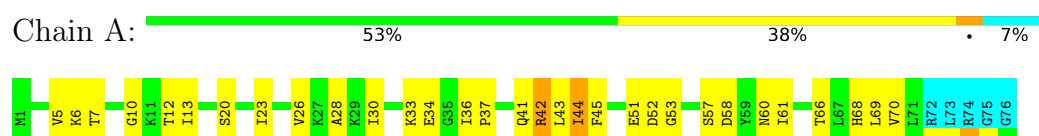
4.2.255 Score per residue for model 255

- Molecule 1: Ubiquitin



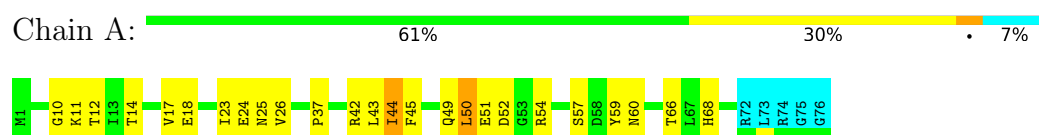
4.2.256 Score per residue for model 256

- Molecule 1: Ubiquitin



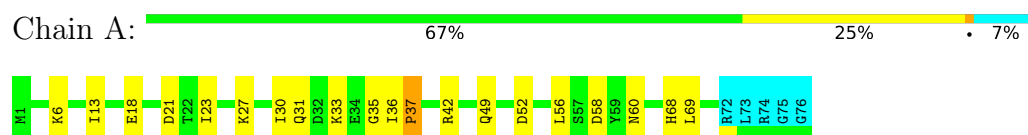
4.2.257 Score per residue for model 257

- Molecule 1: Ubiquitin



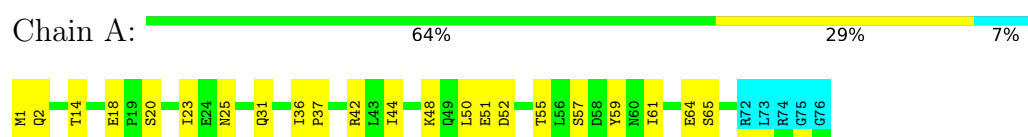
4.2.258 Score per residue for model 258

- Molecule 1: Ubiquitin



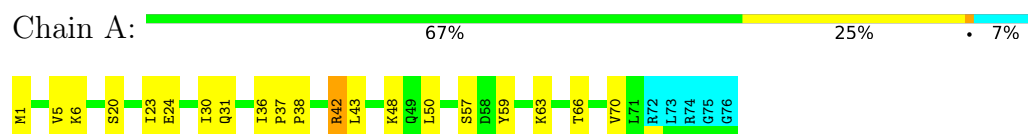
4.2.259 Score per residue for model 259

- Molecule 1: Ubiquitin



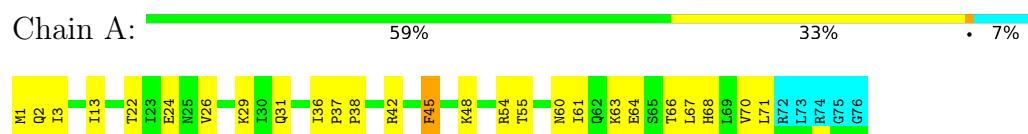
4.2.260 Score per residue for model 260

- Molecule 1: Ubiquitin



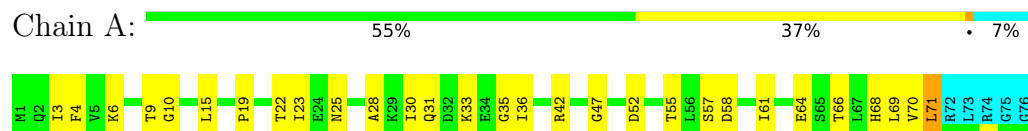
4.2.261 Score per residue for model 261

- Molecule 1: Ubiquitin



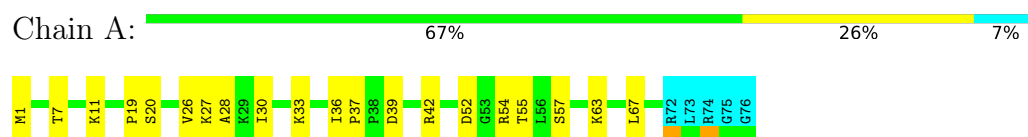
4.2.262 Score per residue for model 262

- Molecule 1: Ubiquitin



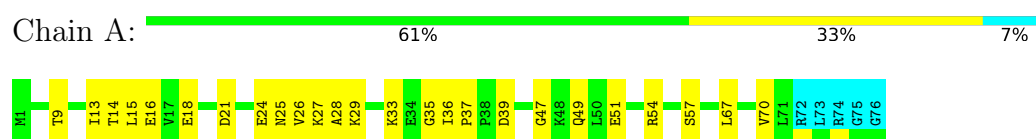
4.2.263 Score per residue for model 263

- Molecule 1: Ubiquitin



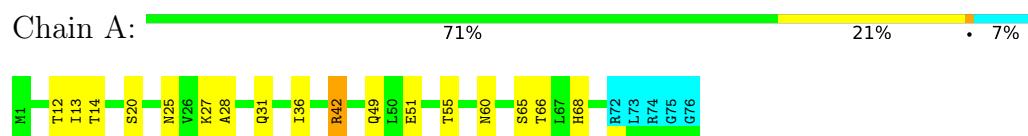
4.2.264 Score per residue for model 264

- Molecule 1: Ubiquitin



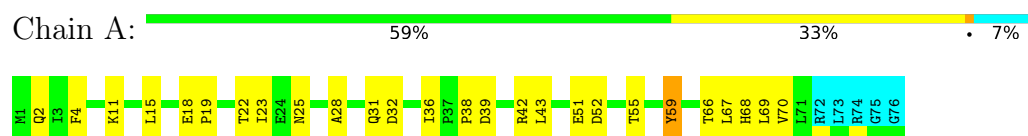
4.2.265 Score per residue for model 265

- Molecule 1: Ubiquitin



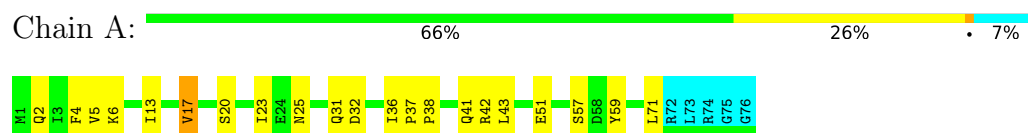
4.2.266 Score per residue for model 266

- Molecule 1: Ubiquitin



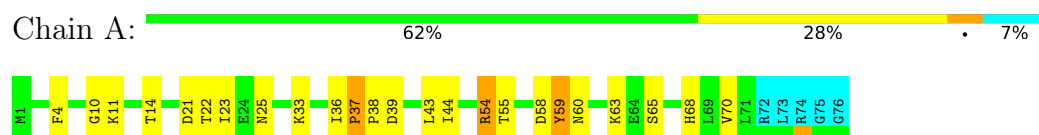
4.2.267 Score per residue for model 267

- Molecule 1: Ubiquitin



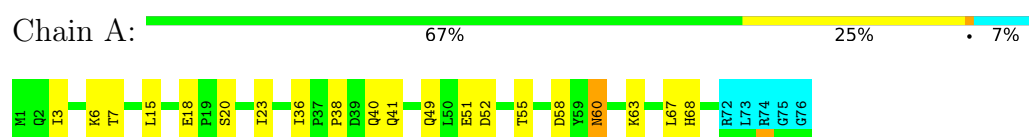
4.2.268 Score per residue for model 268

- Molecule 1: Ubiquitin



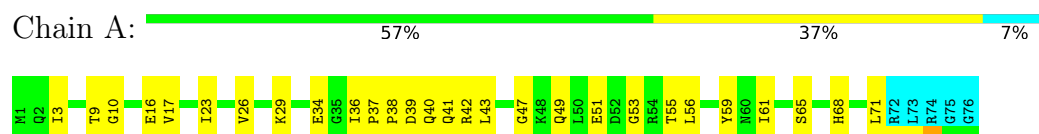
4.2.269 Score per residue for model 269

- Molecule 1: Ubiquitin



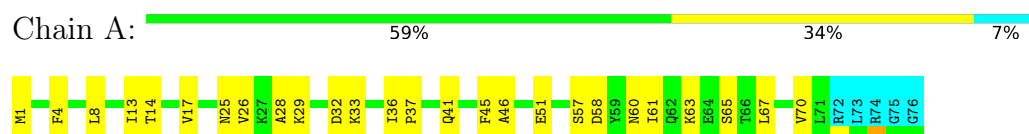
4.2.270 Score per residue for model 270

- Molecule 1: Ubiquitin



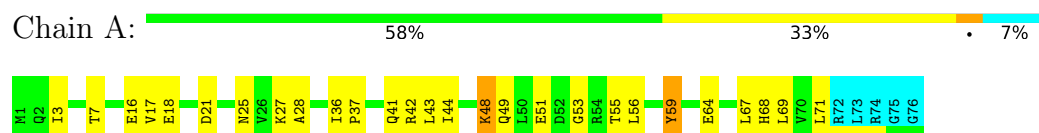
4.2.271 Score per residue for model 271

- Molecule 1: Ubiquitin



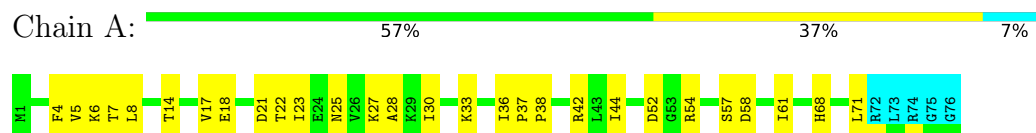
4.2.272 Score per residue for model 272

- Molecule 1: Ubiquitin



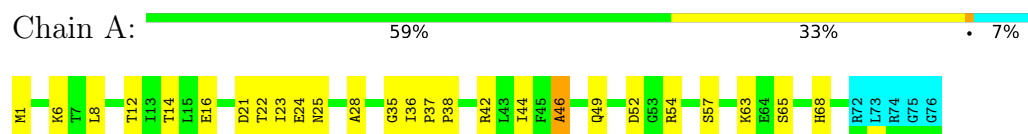
4.2.273 Score per residue for model 273

- Molecule 1: Ubiquitin



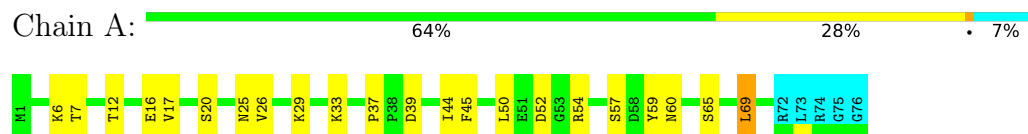
4.2.274 Score per residue for model 274

- Molecule 1: Ubiquitin



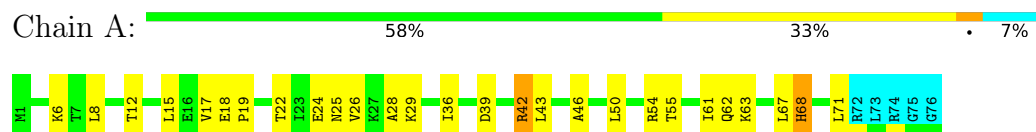
4.2.275 Score per residue for model 275

- Molecule 1: Ubiquitin



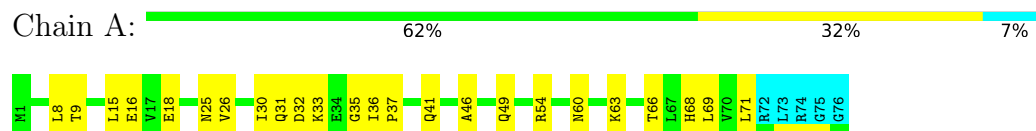
4.2.276 Score per residue for model 276

- Molecule 1: Ubiquitin



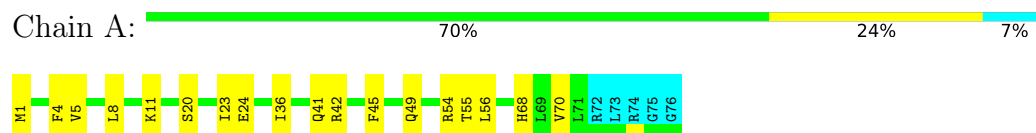
4.2.277 Score per residue for model 277

- Molecule 1: Ubiquitin



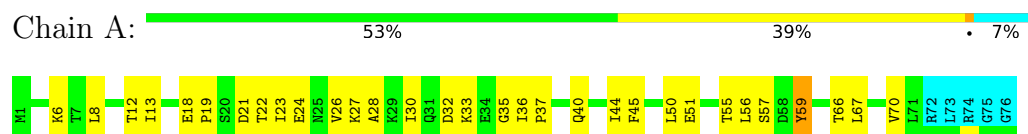
4.2.278 Score per residue for model 278

- Molecule 1: Ubiquitin



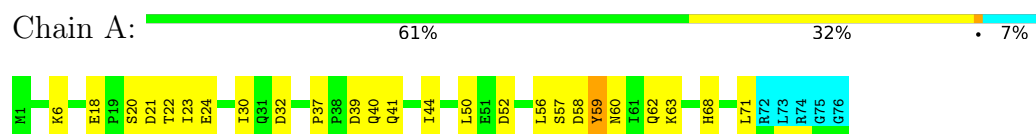
4.2.279 Score per residue for model 279

- Molecule 1: Ubiquitin



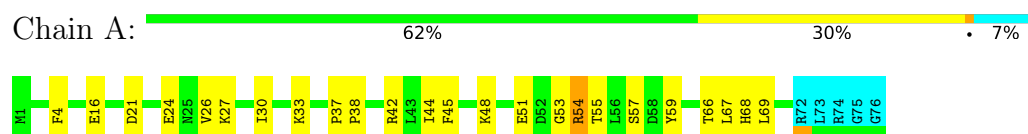
4.2.280 Score per residue for model 280

- Molecule 1: Ubiquitin



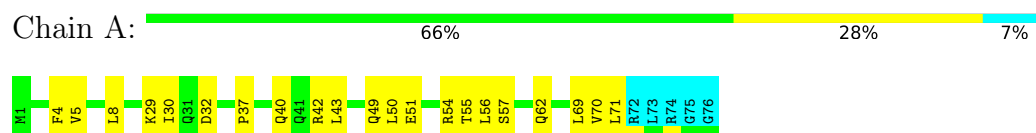
4.2.281 Score per residue for model 281

- Molecule 1: Ubiquitin



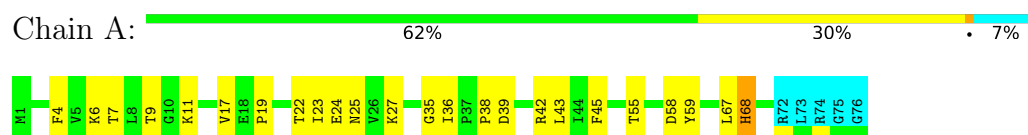
4.2.282 Score per residue for model 282

- Molecule 1: Ubiquitin



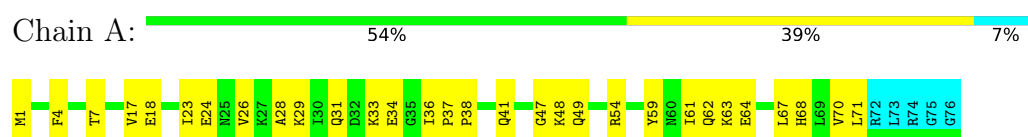
4.2.283 Score per residue for model 283

- Molecule 1: Ubiquitin



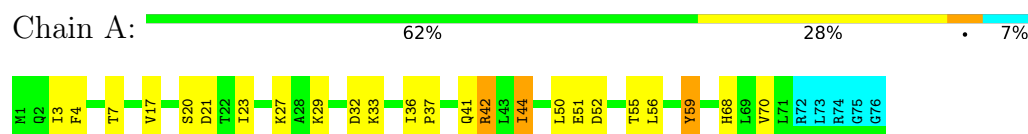
4.2.284 Score per residue for model 284

- Molecule 1: Ubiquitin



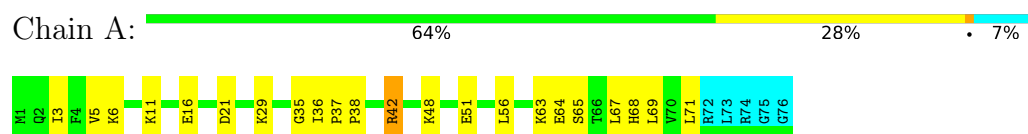
4.2.285 Score per residue for model 285

- Molecule 1: Ubiquitin



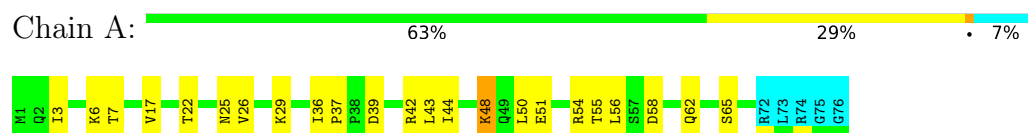
4.2.286 Score per residue for model 286

- Molecule 1: Ubiquitin



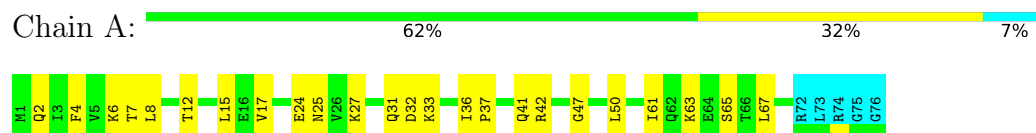
4.2.287 Score per residue for model 287

- Molecule 1: Ubiquitin



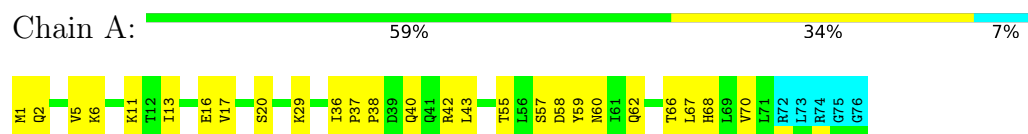
4.2.288 Score per residue for model 288

- Molecule 1: Ubiquitin



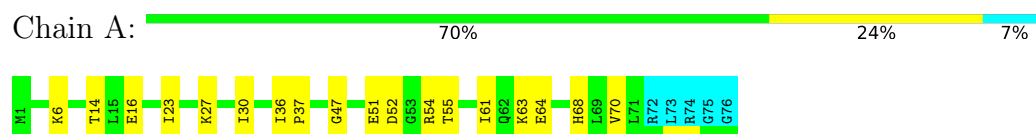
4.2.289 Score per residue for model 289

- Molecule 1: Ubiquitin



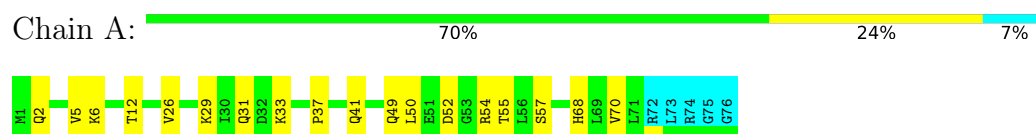
4.2.290 Score per residue for model 290

- Molecule 1: Ubiquitin



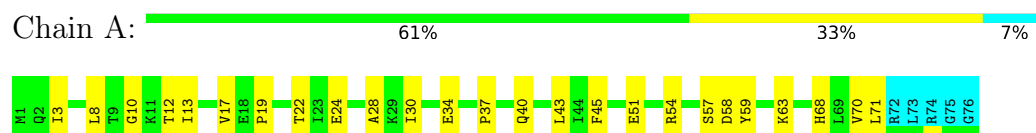
4.2.291 Score per residue for model 291

- Molecule 1: Ubiquitin



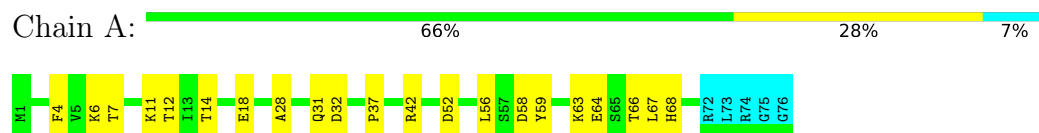
4.2.292 Score per residue for model 292

- Molecule 1: Ubiquitin



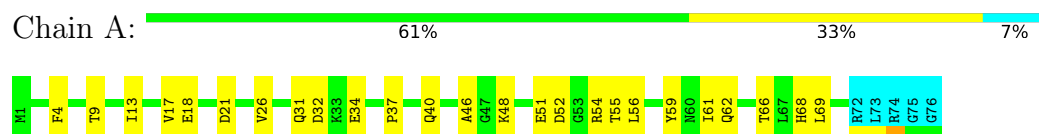
4.2.293 Score per residue for model 293

- Molecule 1: Ubiquitin



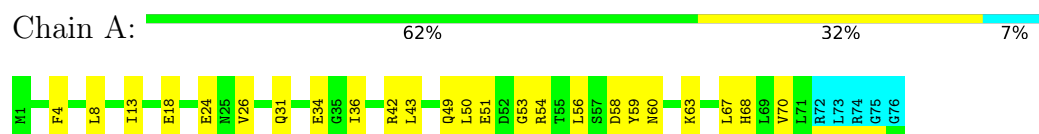
4.2.294 Score per residue for model 294

- Molecule 1: Ubiquitin



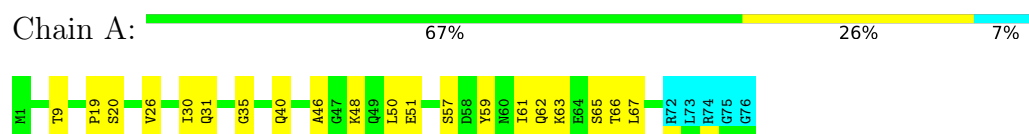
4.2.295 Score per residue for model 295

- Molecule 1: Ubiquitin



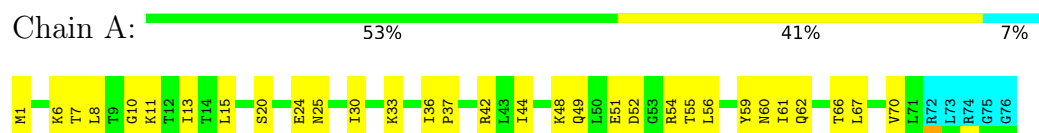
4.2.296 Score per residue for model 296

- Molecule 1: Ubiquitin



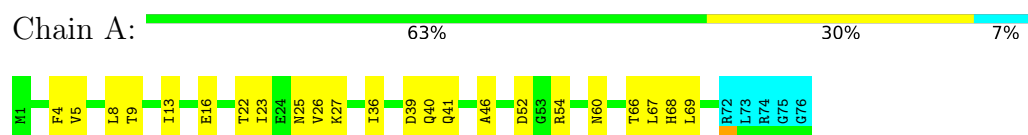
4.2.297 Score per residue for model 297

- Molecule 1: Ubiquitin



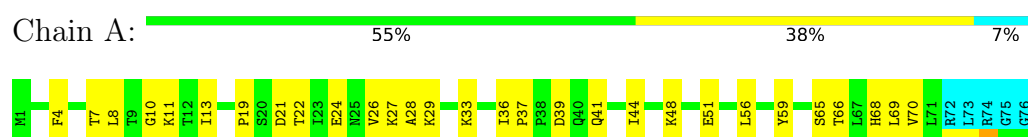
4.2.298 Score per residue for model 298

- Molecule 1: Ubiquitin



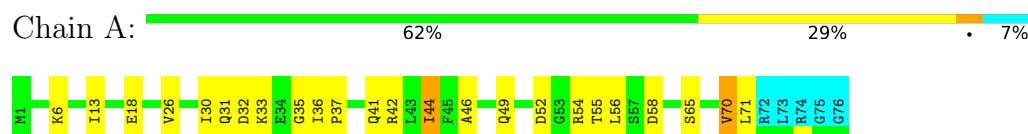
4.2.299 Score per residue for model 299

- Molecule 1: Ubiquitin



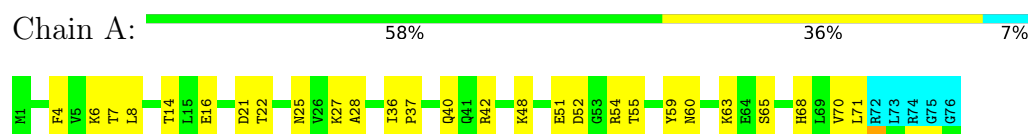
4.2.300 Score per residue for model 300

- Molecule 1: Ubiquitin



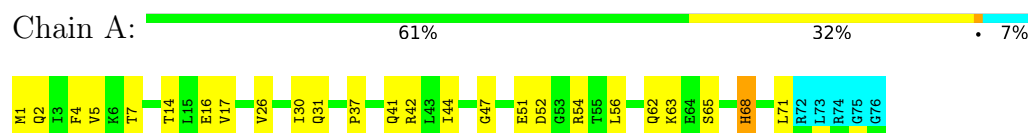
4.2.301 Score per residue for model 301

- Molecule 1: Ubiquitin



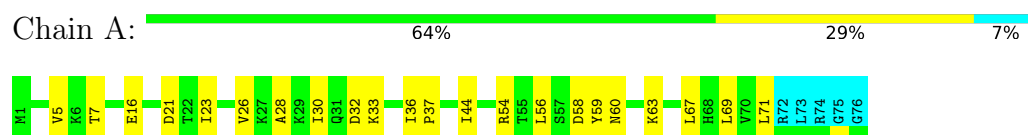
4.2.302 Score per residue for model 302

- Molecule 1: Ubiquitin



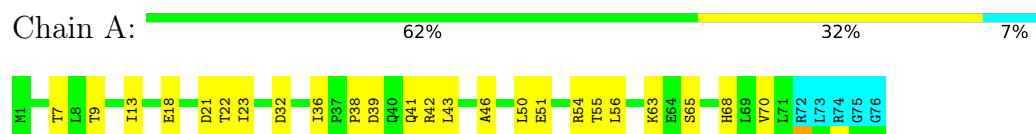
4.2.303 Score per residue for model 303

- Molecule 1: Ubiquitin



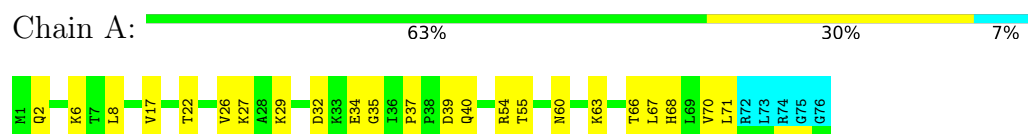
4.2.304 Score per residue for model 304

- Molecule 1: Ubiquitin



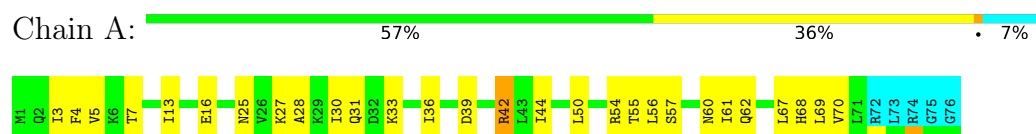
4.2.305 Score per residue for model 305

- Molecule 1: Ubiquitin



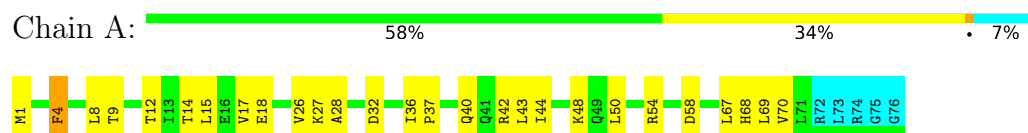
4.2.306 Score per residue for model 306

- Molecule 1: Ubiquitin



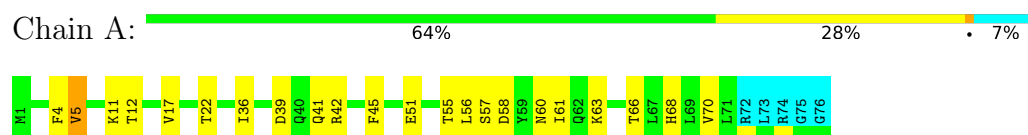
4.2.307 Score per residue for model 307

- Molecule 1: Ubiquitin



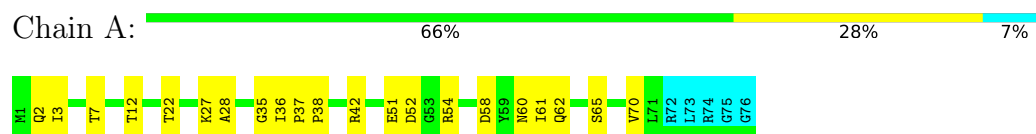
4.2.308 Score per residue for model 308

- Molecule 1: Ubiquitin



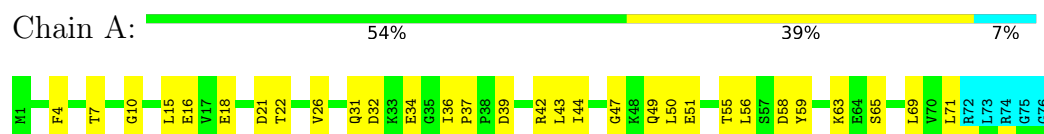
4.2.309 Score per residue for model 309

- Molecule 1: Ubiquitin



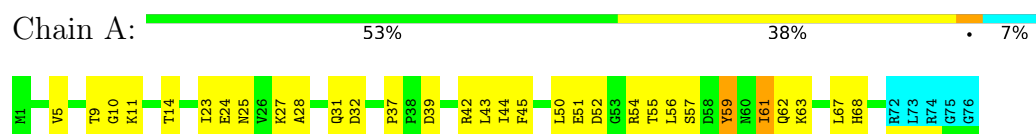
4.2.310 Score per residue for model 310

- Molecule 1: Ubiquitin



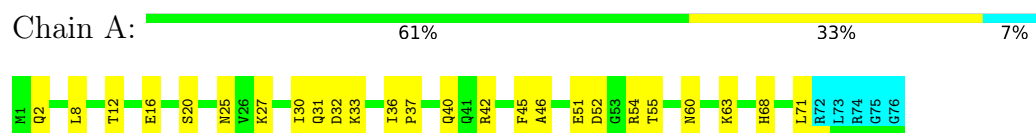
4.2.311 Score per residue for model 311

- Molecule 1: Ubiquitin



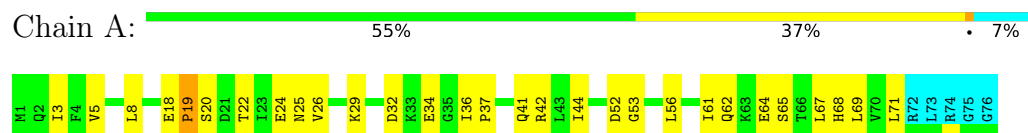
4.2.312 Score per residue for model 312

- Molecule 1: Ubiquitin



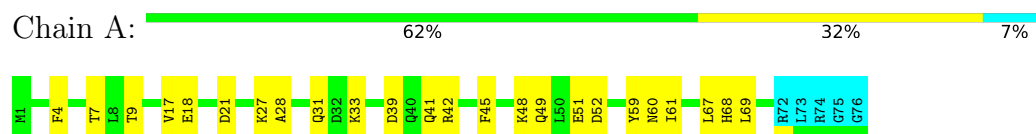
4.2.313 Score per residue for model 313

- Molecule 1: Ubiquitin



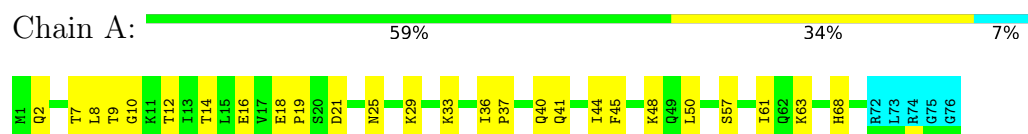
4.2.314 Score per residue for model 314

- Molecule 1: Ubiquitin



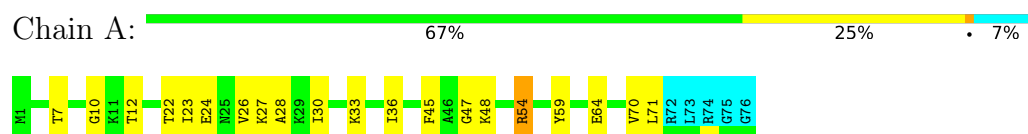
4.2.315 Score per residue for model 315

- Molecule 1: Ubiquitin



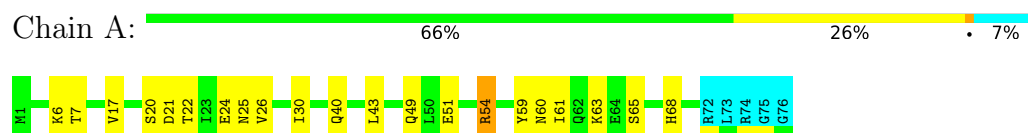
4.2.316 Score per residue for model 316

- Molecule 1: Ubiquitin



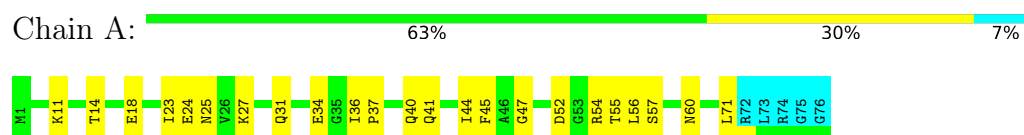
4.2.317 Score per residue for model 317

- Molecule 1: Ubiquitin



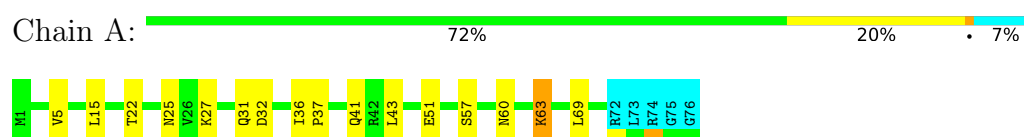
4.2.318 Score per residue for model 318

- Molecule 1: Ubiquitin



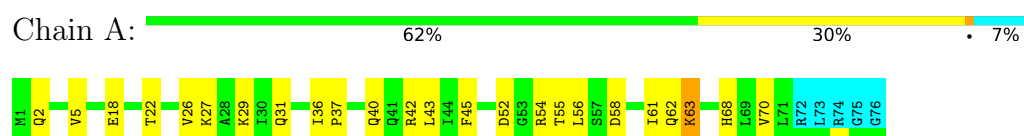
4.2.319 Score per residue for model 319

- Molecule 1: Ubiquitin



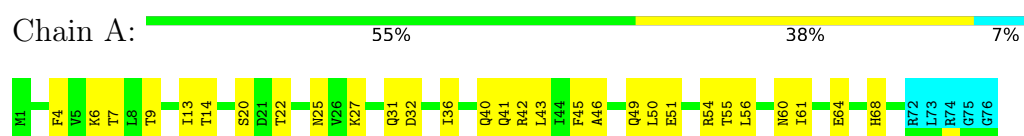
4.2.320 Score per residue for model 320

- Molecule 1: Ubiquitin



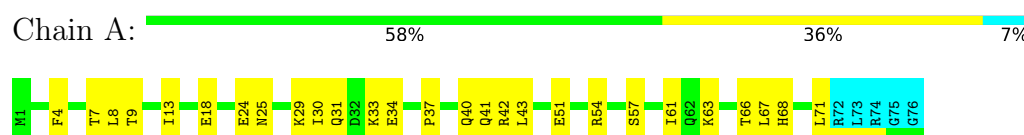
4.2.321 Score per residue for model 321

- Molecule 1: Ubiquitin



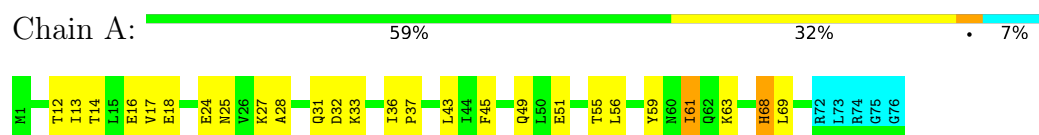
4.2.322 Score per residue for model 322

- Molecule 1: Ubiquitin



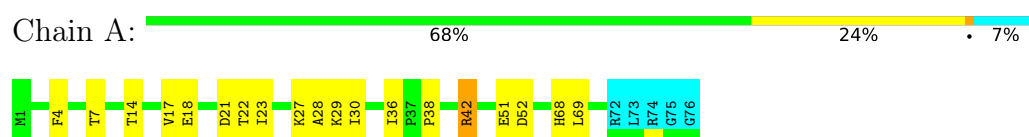
4.2.323 Score per residue for model 323

- Molecule 1: Ubiquitin



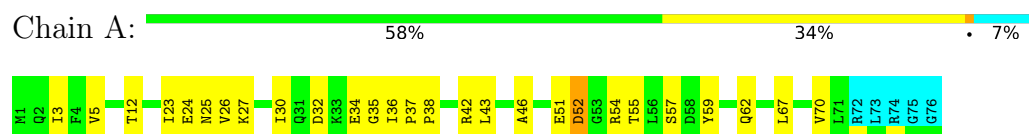
4.2.324 Score per residue for model 324

- Molecule 1: Ubiquitin



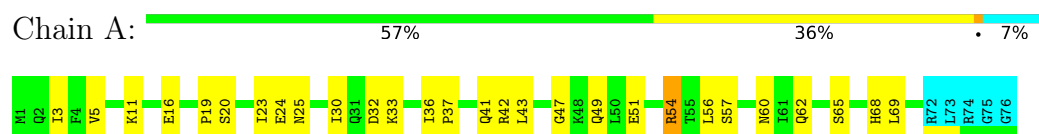
4.2.325 Score per residue for model 325

- Molecule 1: Ubiquitin



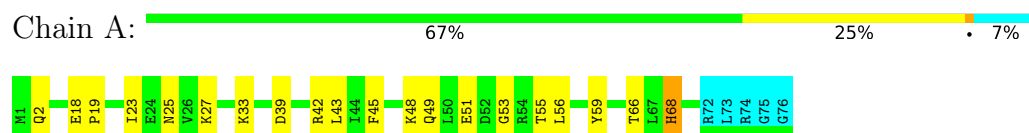
4.2.326 Score per residue for model 326

- Molecule 1: Ubiquitin



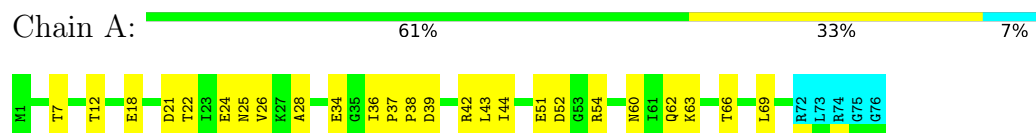
4.2.327 Score per residue for model 327

- Molecule 1: Ubiquitin



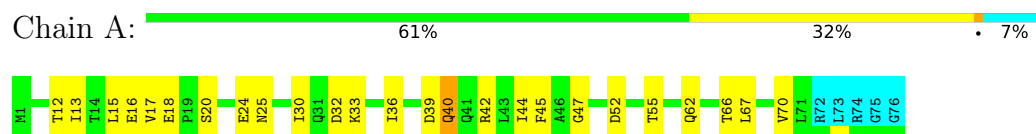
4.2.328 Score per residue for model 328

- Molecule 1: Ubiquitin



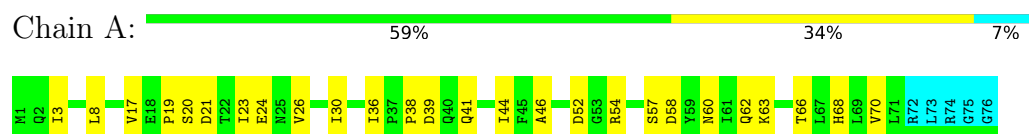
4.2.329 Score per residue for model 329

- Molecule 1: Ubiquitin



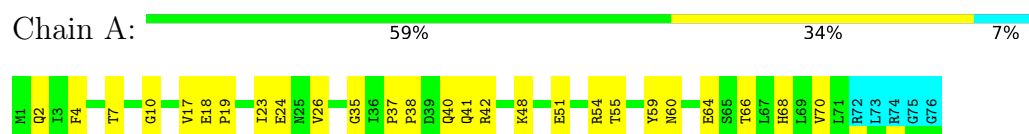
4.2.330 Score per residue for model 330

- Molecule 1: Ubiquitin



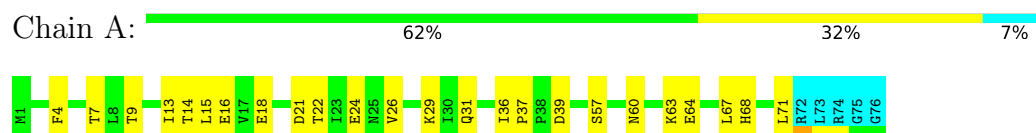
4.2.331 Score per residue for model 331

- Molecule 1: Ubiquitin



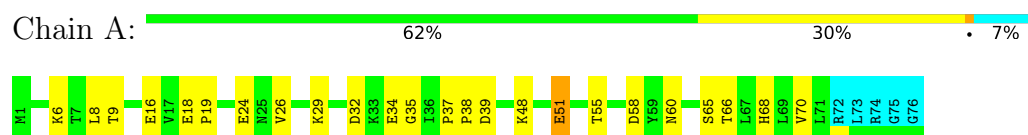
4.2.332 Score per residue for model 332

- Molecule 1: Ubiquitin



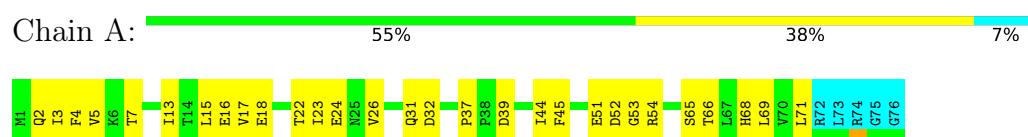
4.2.333 Score per residue for model 333

- Molecule 1: Ubiquitin



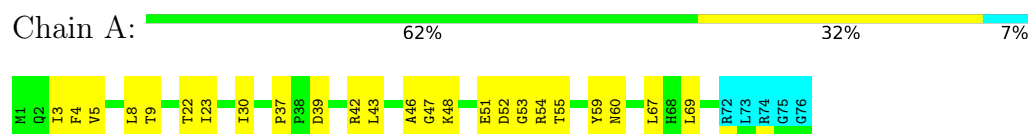
4.2.334 Score per residue for model 334

- Molecule 1: Ubiquitin



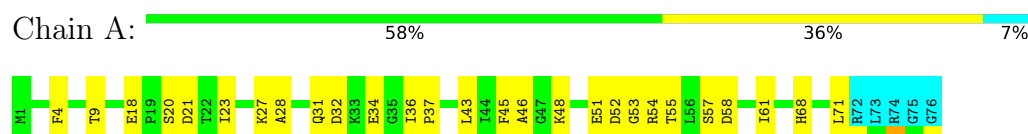
4.2.335 Score per residue for model 335

- Molecule 1: Ubiquitin



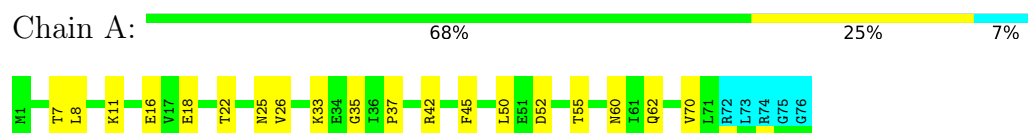
4.2.336 Score per residue for model 336

- Molecule 1: Ubiquitin



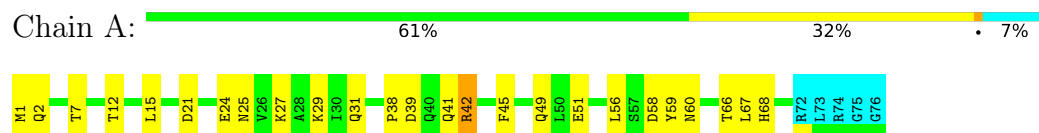
4.2.337 Score per residue for model 337

- Molecule 1: Ubiquitin



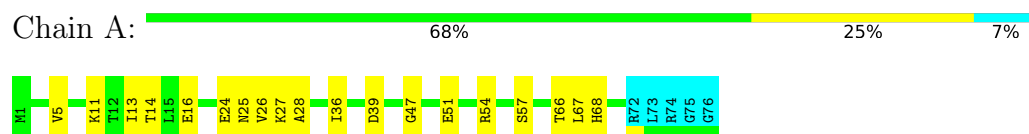
4.2.338 Score per residue for model 338

- Molecule 1: Ubiquitin



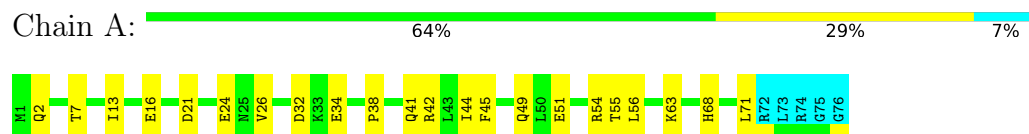
4.2.339 Score per residue for model 339

- Molecule 1: Ubiquitin



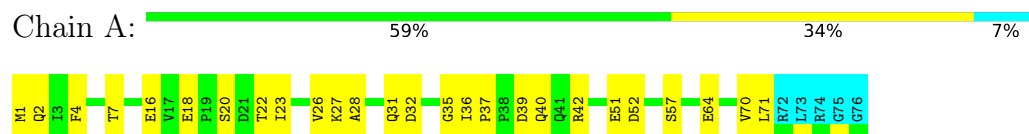
4.2.340 Score per residue for model 340

- Molecule 1: Ubiquitin



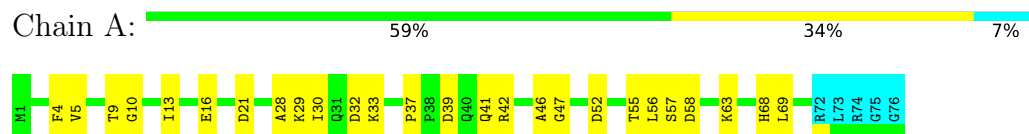
4.2.341 Score per residue for model 341

- Molecule 1: Ubiquitin



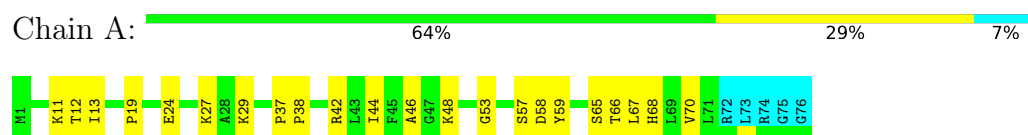
4.2.342 Score per residue for model 342

- Molecule 1: Ubiquitin



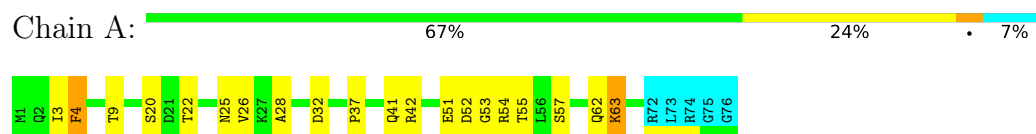
4.2.343 Score per residue for model 343

- Molecule 1: Ubiquitin



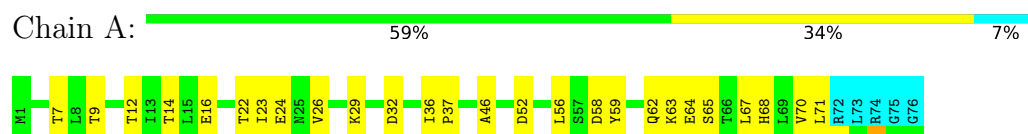
4.2.344 Score per residue for model 344

- Molecule 1: Ubiquitin



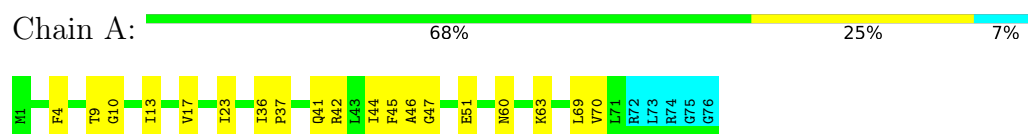
4.2.345 Score per residue for model 345

- Molecule 1: Ubiquitin



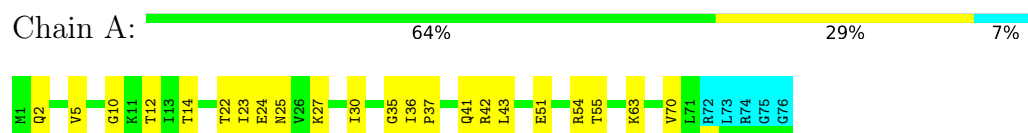
4.2.346 Score per residue for model 346

- Molecule 1: Ubiquitin



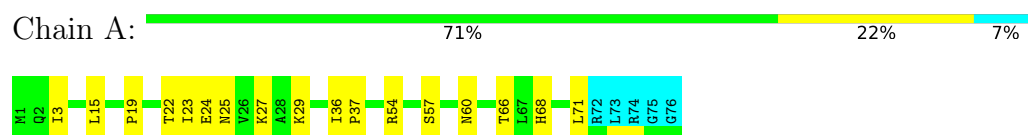
4.2.347 Score per residue for model 347

- Molecule 1: Ubiquitin



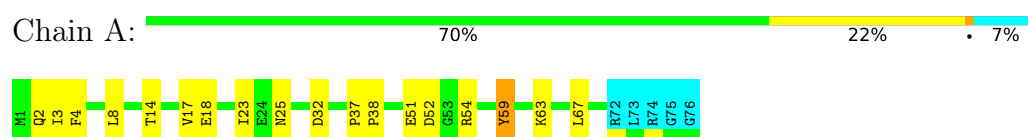
4.2.348 Score per residue for model 348

- Molecule 1: Ubiquitin



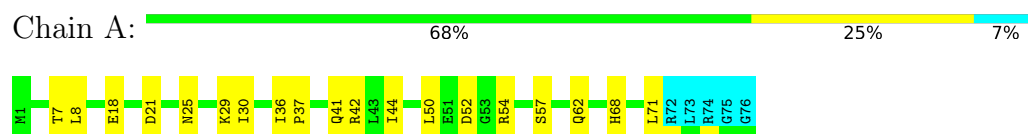
4.2.349 Score per residue for model 349

- Molecule 1: Ubiquitin



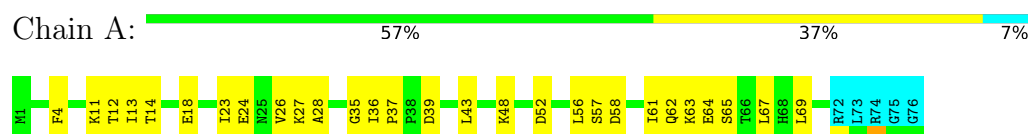
4.2.350 Score per residue for model 350

- Molecule 1: Ubiquitin



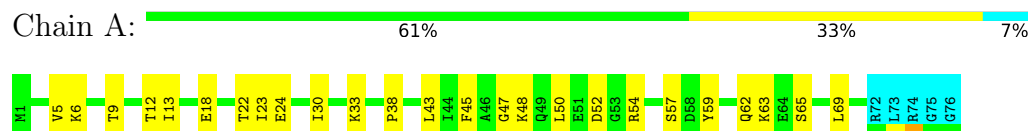
4.2.351 Score per residue for model 351

- Molecule 1: Ubiquitin



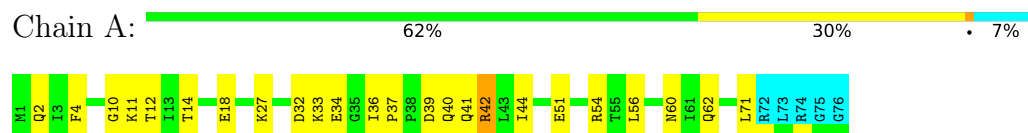
4.2.352 Score per residue for model 352

- Molecule 1: Ubiquitin



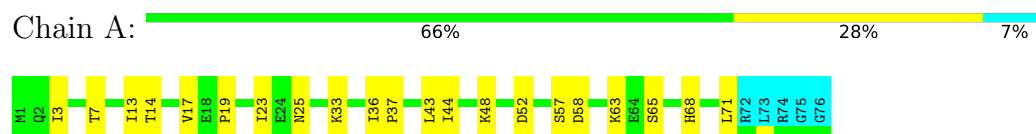
4.2.353 Score per residue for model 353

- Molecule 1: Ubiquitin



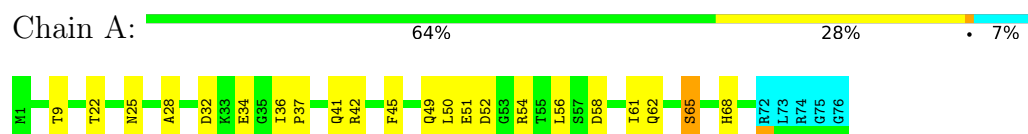
4.2.354 Score per residue for model 354

- Molecule 1: Ubiquitin



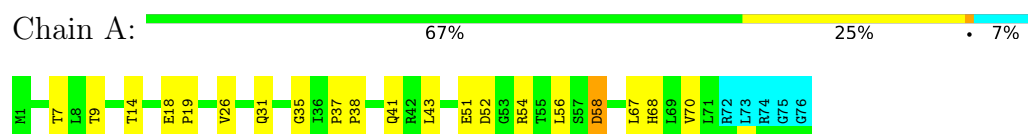
4.2.355 Score per residue for model 355

- Molecule 1: Ubiquitin



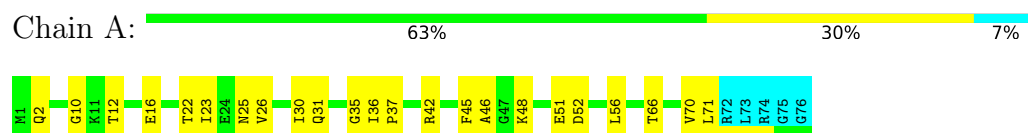
4.2.356 Score per residue for model 356

- Molecule 1: Ubiquitin



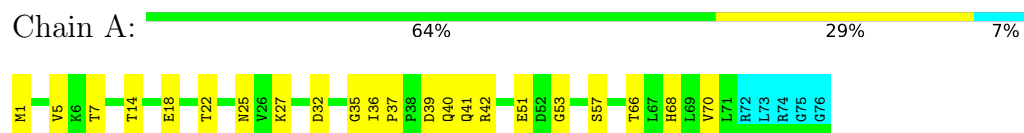
4.2.357 Score per residue for model 357

- Molecule 1: Ubiquitin



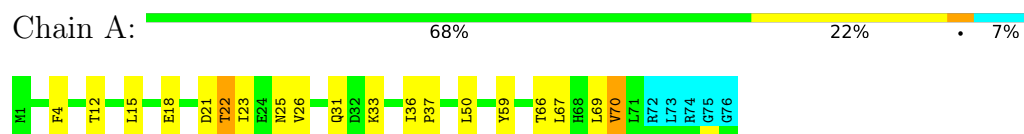
4.2.358 Score per residue for model 358

- Molecule 1: Ubiquitin



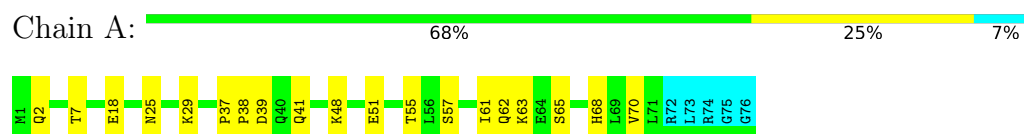
4.2.359 Score per residue for model 359

- Molecule 1: Ubiquitin



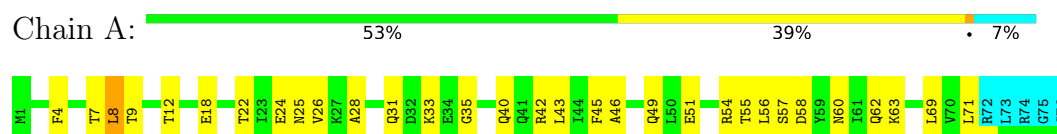
4.2.360 Score per residue for model 360

- Molecule 1: Ubiquitin



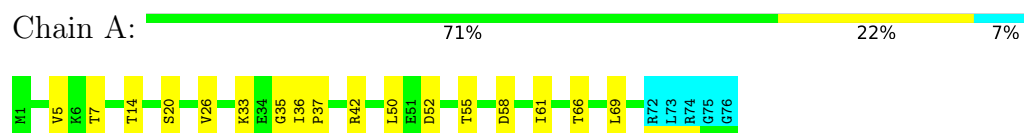
4.2.361 Score per residue for model 361

- Molecule 1: Ubiquitin



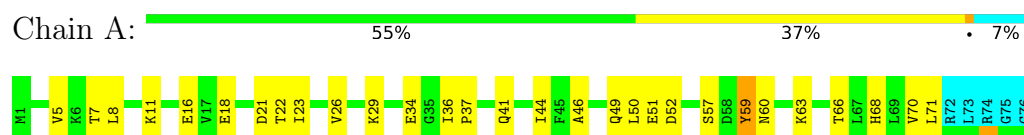
4.2.362 Score per residue for model 362

- Molecule 1: Ubiquitin



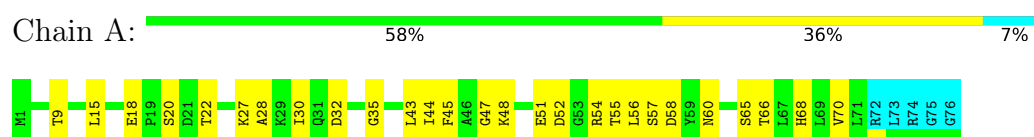
4.2.363 Score per residue for model 363

- Molecule 1: Ubiquitin



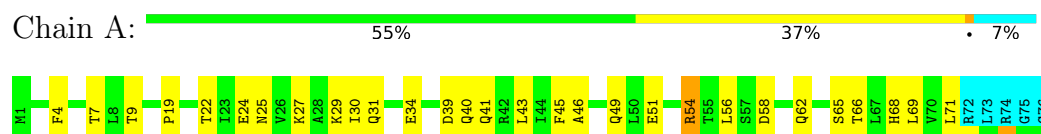
4.2.364 Score per residue for model 364

- Molecule 1: Ubiquitin



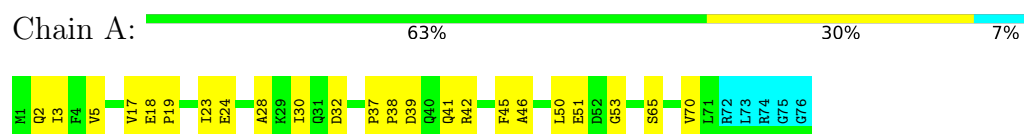
4.2.365 Score per residue for model 365

- Molecule 1: Ubiquitin



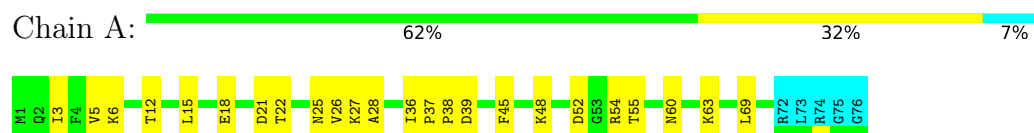
4.2.366 Score per residue for model 366

- Molecule 1: Ubiquitin



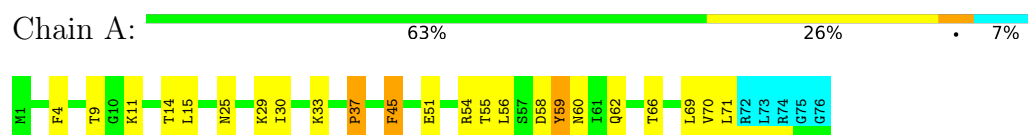
4.2.367 Score per residue for model 367

- Molecule 1: Ubiquitin



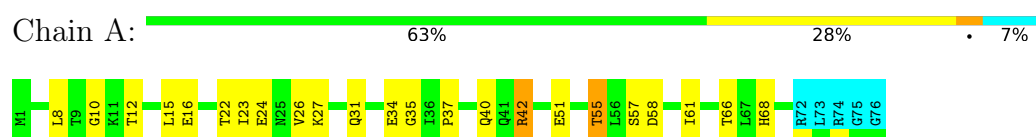
4.2.368 Score per residue for model 368

- Molecule 1: Ubiquitin



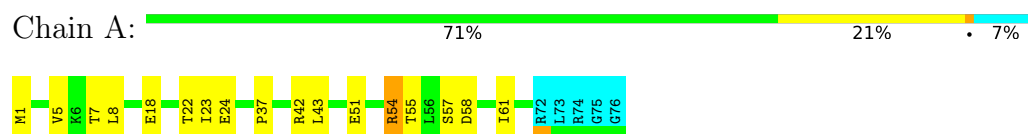
4.2.369 Score per residue for model 369

- Molecule 1: Ubiquitin



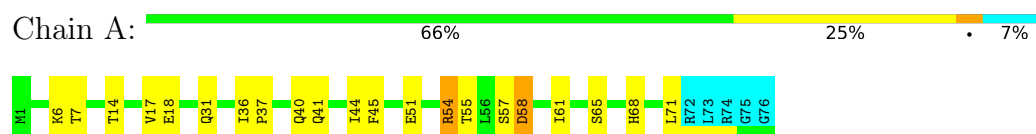
4.2.370 Score per residue for model 370

- Molecule 1: Ubiquitin



4.2.371 Score per residue for model 371

- Molecule 1: Ubiquitin



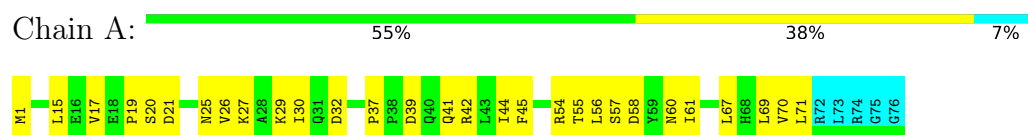
4.2.372 Score per residue for model 372

- Molecule 1: Ubiquitin



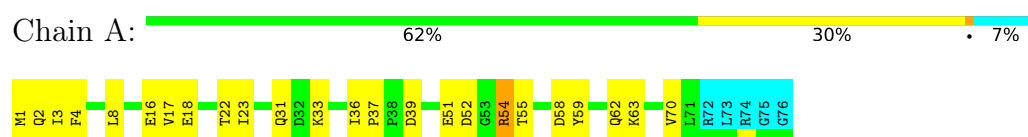
4.2.373 Score per residue for model 373

- Molecule 1: Ubiquitin



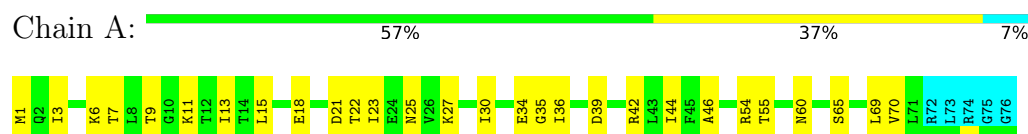
4.2.374 Score per residue for model 374

- Molecule 1: Ubiquitin



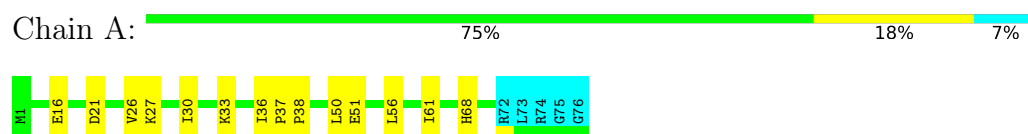
4.2.375 Score per residue for model 375

- Molecule 1: Ubiquitin



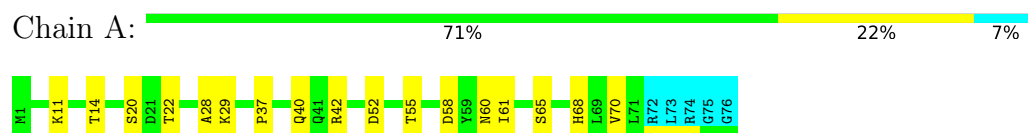
4.2.376 Score per residue for model 376

- Molecule 1: Ubiquitin



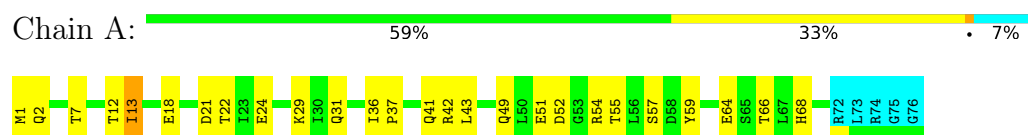
4.2.377 Score per residue for model 377

- Molecule 1: Ubiquitin



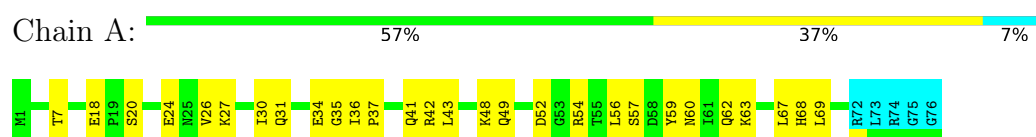
4.2.378 Score per residue for model 378

- Molecule 1: Ubiquitin



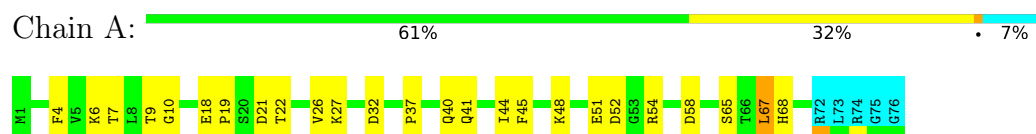
4.2.379 Score per residue for model 379

- Molecule 1: Ubiquitin



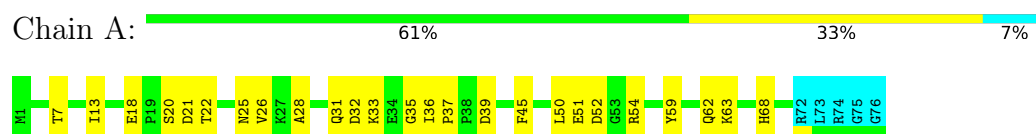
4.2.380 Score per residue for model 380

- Molecule 1: Ubiquitin



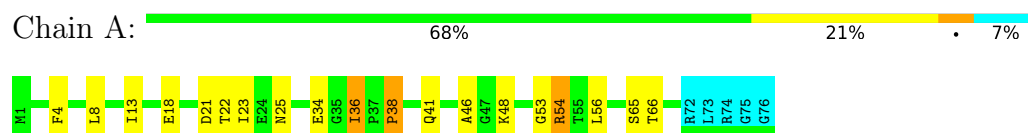
4.2.381 Score per residue for model 381

- Molecule 1: Ubiquitin



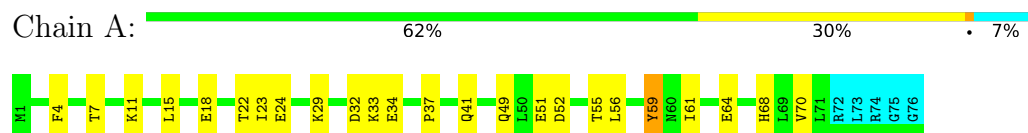
4.2.382 Score per residue for model 382

- Molecule 1: Ubiquitin



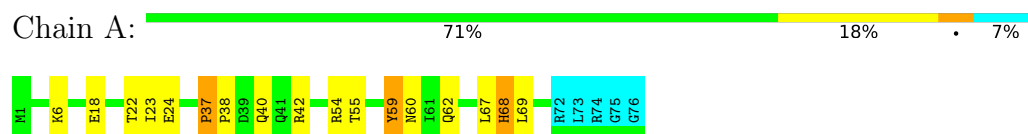
4.2.383 Score per residue for model 383

- Molecule 1: Ubiquitin



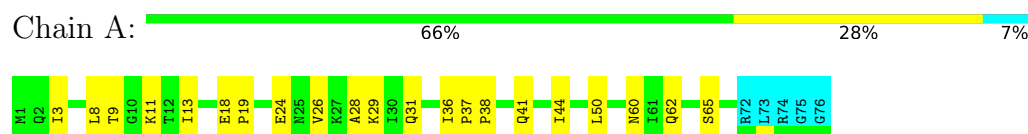
4.2.384 Score per residue for model 384

- Molecule 1: Ubiquitin



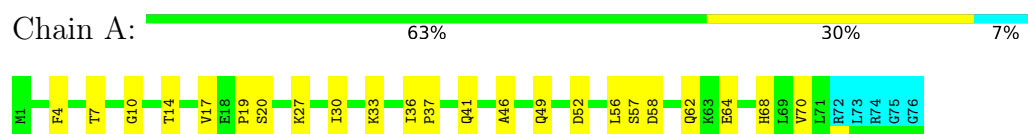
4.2.385 Score per residue for model 385

- Molecule 1: Ubiquitin



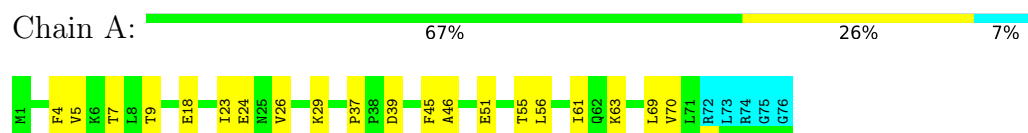
4.2.386 Score per residue for model 386

- Molecule 1: Ubiquitin



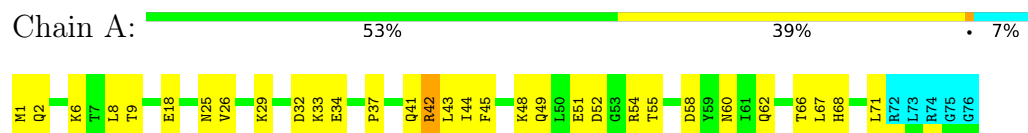
4.2.387 Score per residue for model 387

- Molecule 1: Ubiquitin



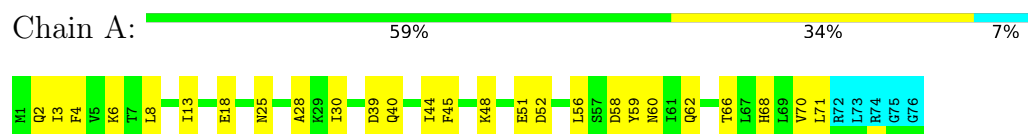
4.2.388 Score per residue for model 388

- Molecule 1: Ubiquitin



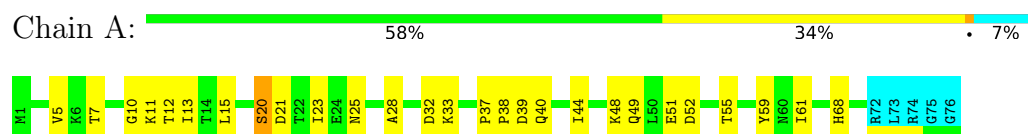
4.2.389 Score per residue for model 389

- Molecule 1: Ubiquitin



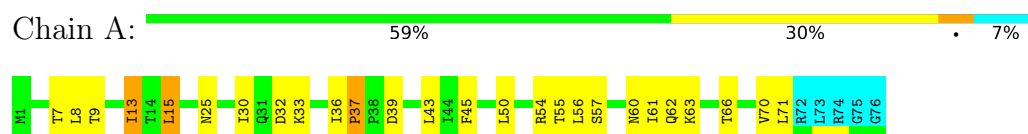
4.2.390 Score per residue for model 390

- Molecule 1: Ubiquitin



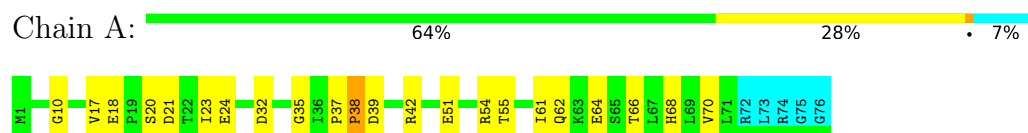
4.2.391 Score per residue for model 391

- Molecule 1: Ubiquitin



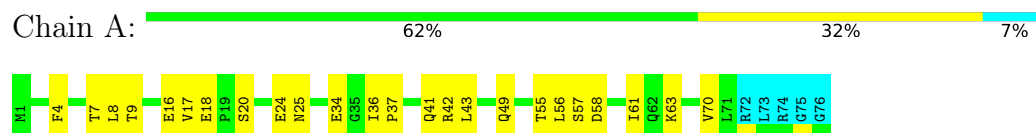
4.2.392 Score per residue for model 392

- Molecule 1: Ubiquitin



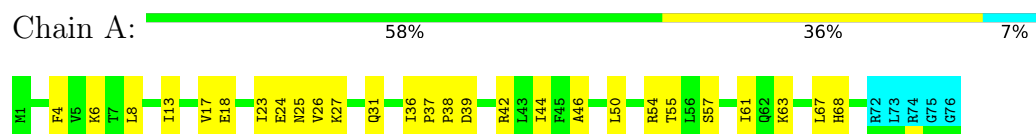
4.2.393 Score per residue for model 393

- Molecule 1: Ubiquitin



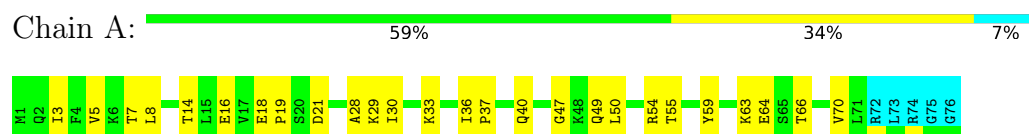
4.2.394 Score per residue for model 394

- Molecule 1: Ubiquitin



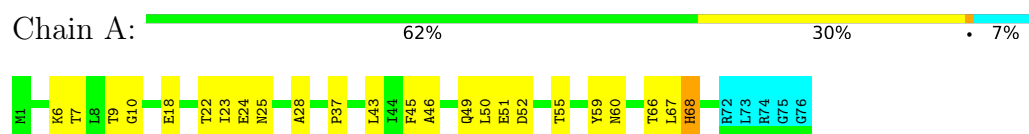
4.2.395 Score per residue for model 395

- Molecule 1: Ubiquitin



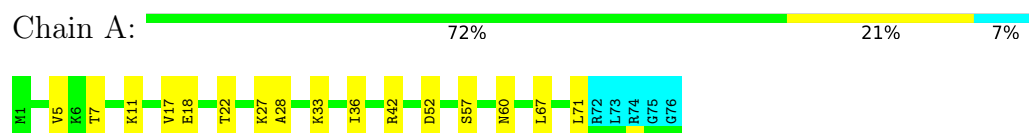
4.2.396 Score per residue for model 396

- Molecule 1: Ubiquitin



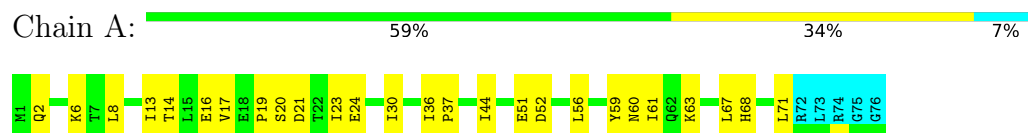
4.2.397 Score per residue for model 397

- Molecule 1: Ubiquitin



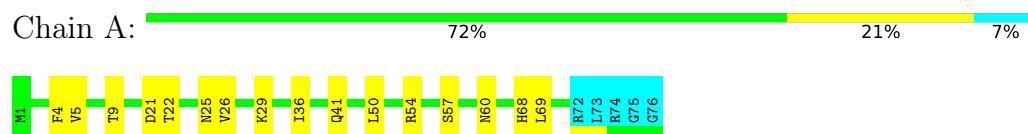
4.2.398 Score per residue for model 398

- Molecule 1: Ubiquitin



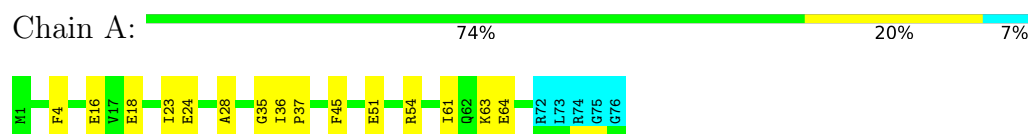
4.2.399 Score per residue for model 399

- Molecule 1: Ubiquitin



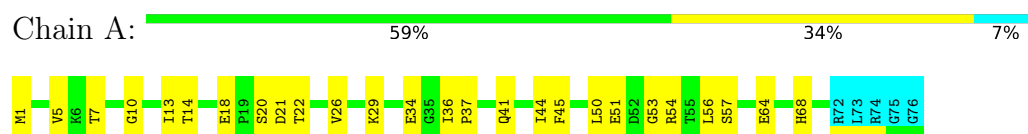
4.2.400 Score per residue for model 400

- Molecule 1: Ubiquitin



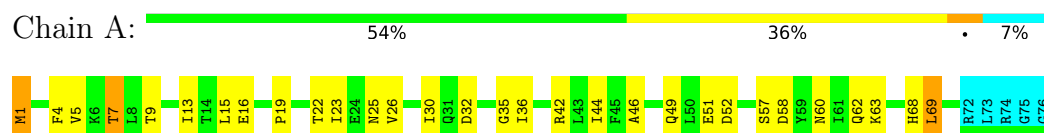
4.2.401 Score per residue for model 401

- Molecule 1: Ubiquitin



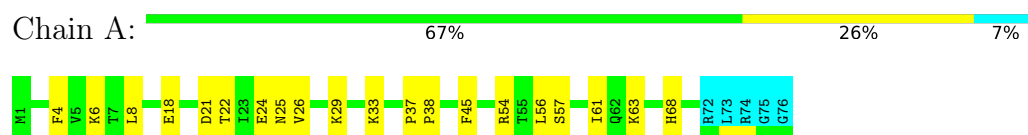
4.2.402 Score per residue for model 402

- Molecule 1: Ubiquitin



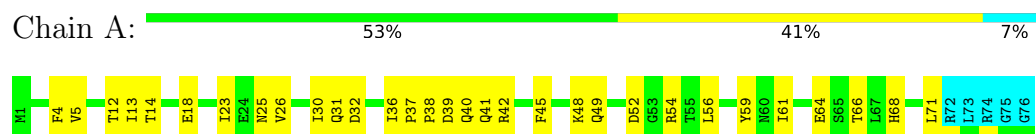
4.2.403 Score per residue for model 403

- Molecule 1: Ubiquitin



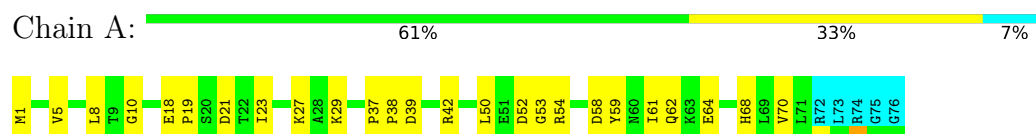
4.2.404 Score per residue for model 404

- Molecule 1: Ubiquitin



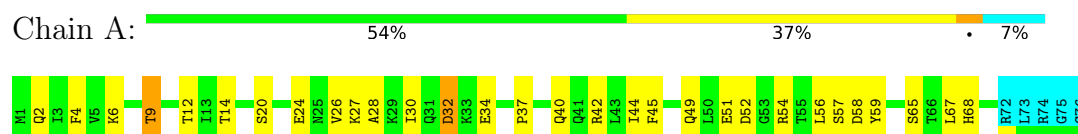
4.2.405 Score per residue for model 405

- Molecule 1: Ubiquitin



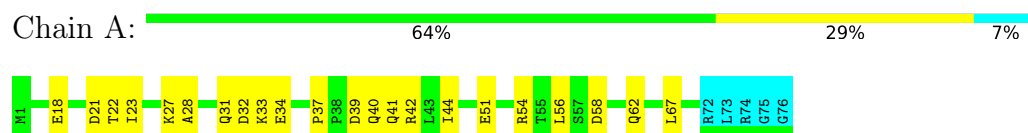
4.2.406 Score per residue for model 406

- Molecule 1: Ubiquitin



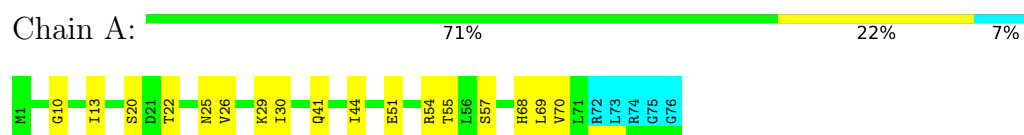
4.2.407 Score per residue for model 407

- Molecule 1: Ubiquitin



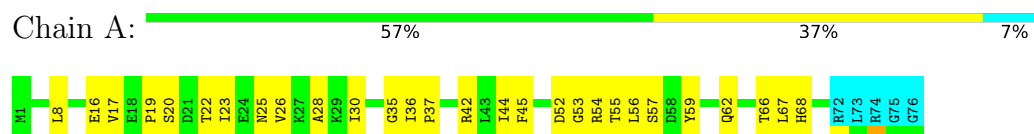
4.2.408 Score per residue for model 408

- Molecule 1: Ubiquitin



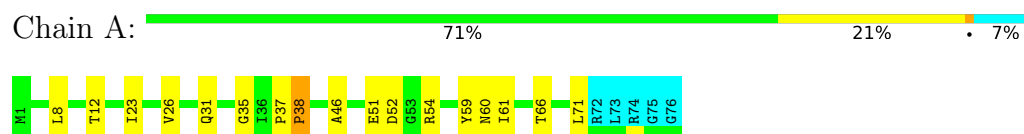
4.2.409 Score per residue for model 409

- Molecule 1: Ubiquitin



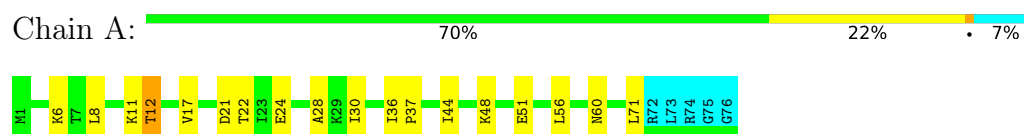
4.2.410 Score per residue for model 410

- Molecule 1: Ubiquitin



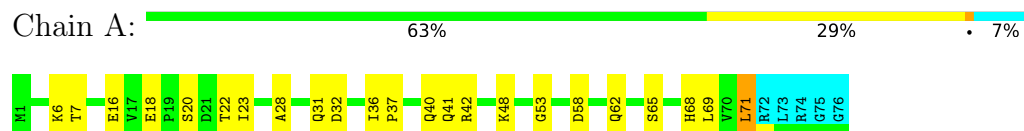
4.2.411 Score per residue for model 411

- Molecule 1: Ubiquitin



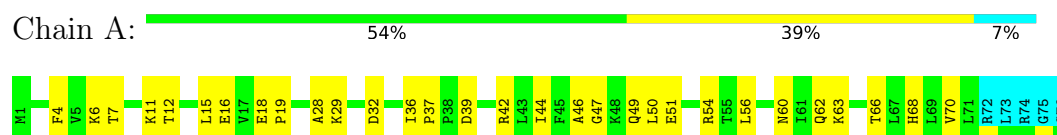
4.2.412 Score per residue for model 412

- Molecule 1: Ubiquitin



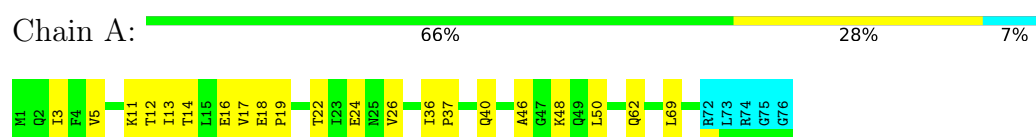
4.2.413 Score per residue for model 413

- Molecule 1: Ubiquitin



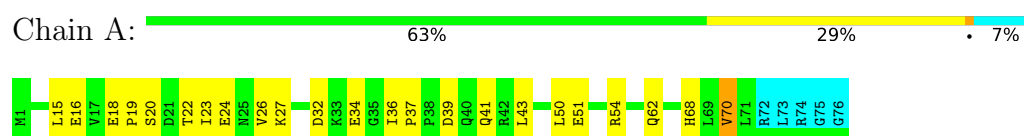
4.2.414 Score per residue for model 414

- Molecule 1: Ubiquitin



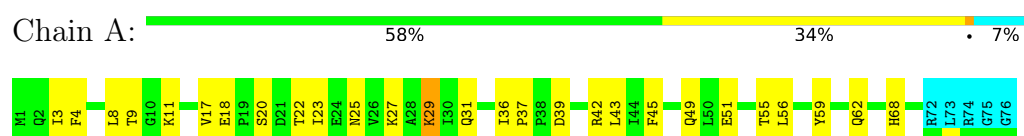
4.2.415 Score per residue for model 415

- Molecule 1: Ubiquitin



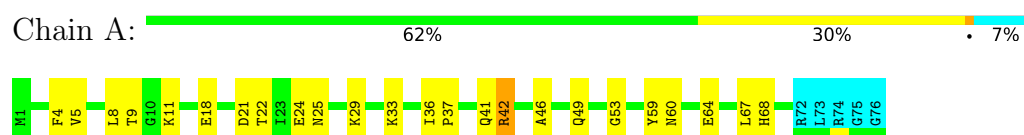
4.2.416 Score per residue for model 416

- Molecule 1: Ubiquitin



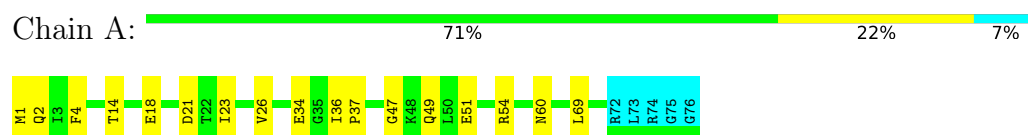
4.2.417 Score per residue for model 417

- Molecule 1: Ubiquitin



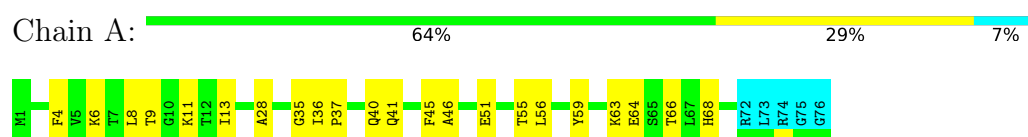
4.2.418 Score per residue for model 418

- Molecule 1: Ubiquitin



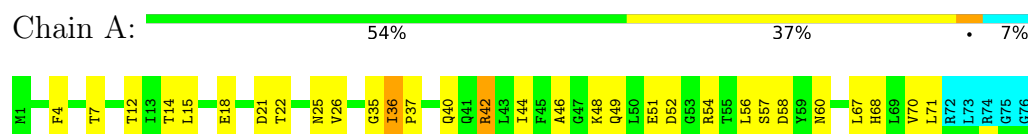
4.2.419 Score per residue for model 419

- Molecule 1: Ubiquitin



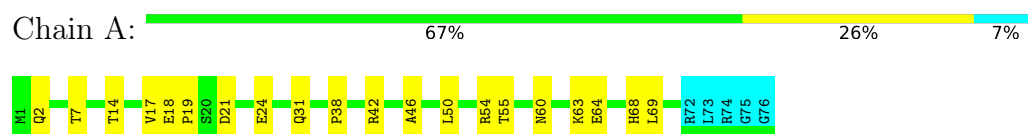
4.2.420 Score per residue for model 420

- Molecule 1: Ubiquitin



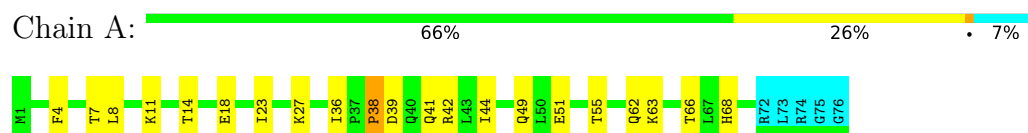
4.2.421 Score per residue for model 421

- Molecule 1: Ubiquitin



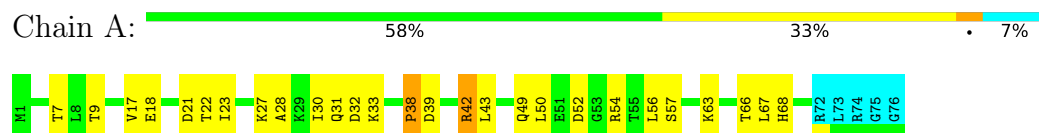
4.2.422 Score per residue for model 422

- Molecule 1: Ubiquitin



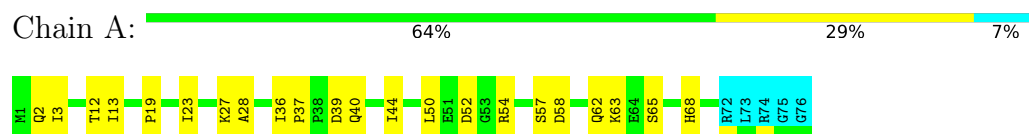
4.2.423 Score per residue for model 423

- Molecule 1: Ubiquitin



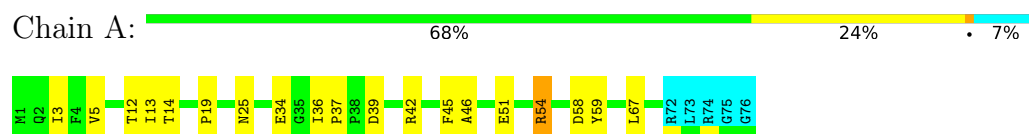
4.2.424 Score per residue for model 424

- Molecule 1: Ubiquitin



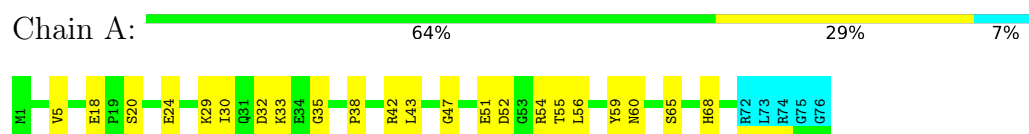
4.2.425 Score per residue for model 425

- Molecule 1: Ubiquitin



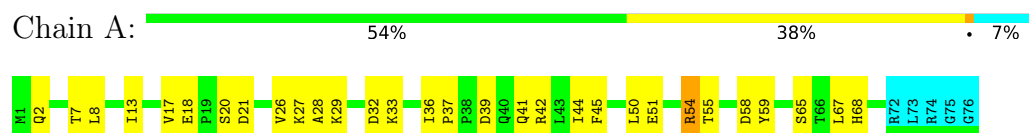
4.2.426 Score per residue for model 426

- Molecule 1: Ubiquitin



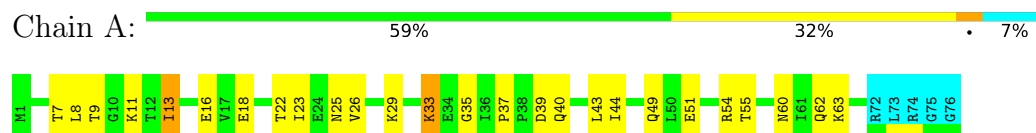
4.2.427 Score per residue for model 427

- Molecule 1: Ubiquitin



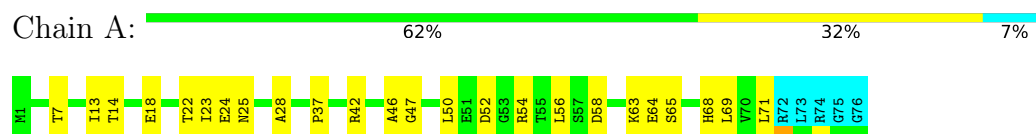
4.2.428 Score per residue for model 428

- Molecule 1: Ubiquitin



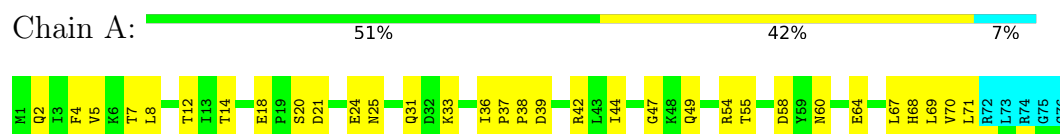
4.2.429 Score per residue for model 429

- Molecule 1: Ubiquitin



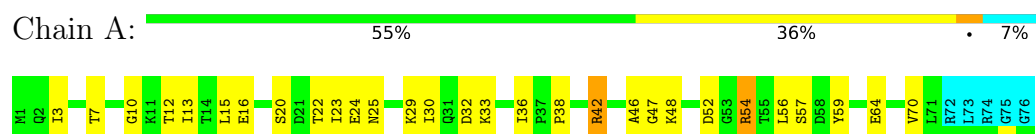
4.2.430 Score per residue for model 430

- Molecule 1: Ubiquitin



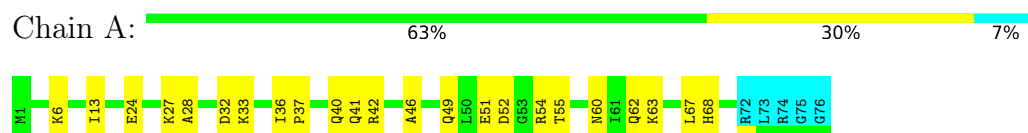
4.2.431 Score per residue for model 431

- Molecule 1: Ubiquitin



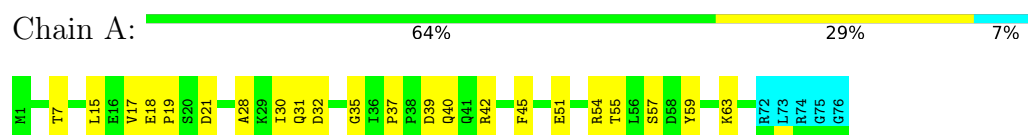
4.2.432 Score per residue for model 432

- Molecule 1: Ubiquitin



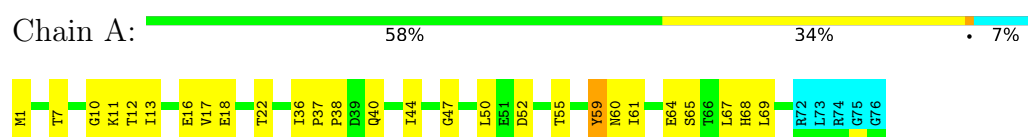
4.2.433 Score per residue for model 433

- Molecule 1: Ubiquitin



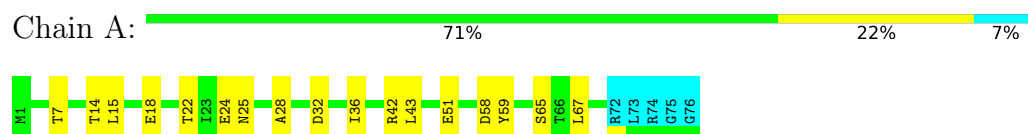
4.2.434 Score per residue for model 434

- Molecule 1: Ubiquitin



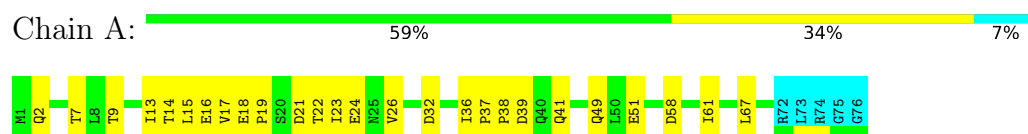
4.2.435 Score per residue for model 435

- Molecule 1: Ubiquitin



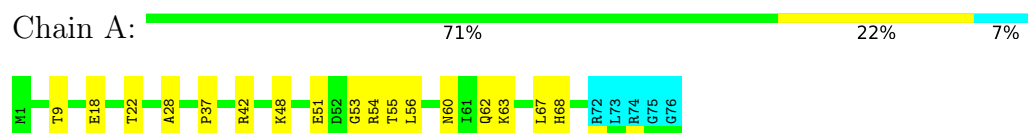
4.2.436 Score per residue for model 436

- Molecule 1: Ubiquitin



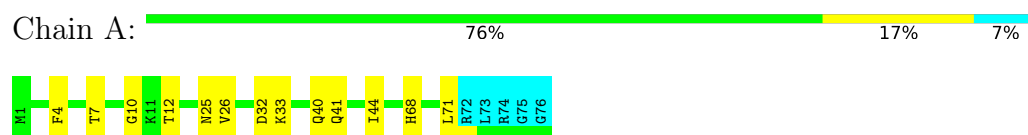
4.2.437 Score per residue for model 437

- Molecule 1: Ubiquitin



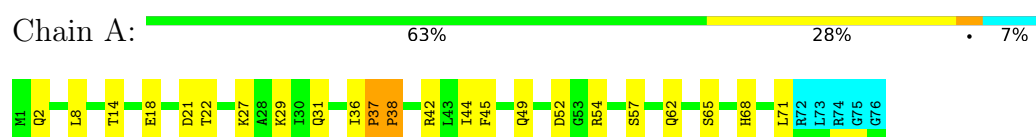
4.2.438 Score per residue for model 438

- Molecule 1: Ubiquitin



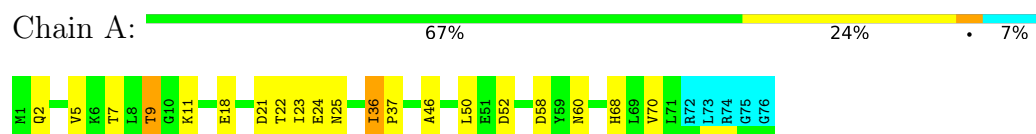
4.2.439 Score per residue for model 439

- Molecule 1: Ubiquitin



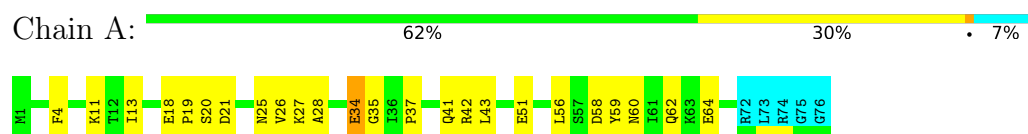
4.2.440 Score per residue for model 440

- Molecule 1: Ubiquitin



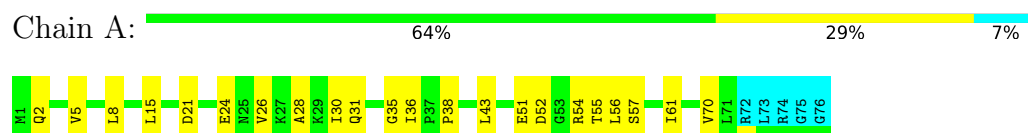
4.2.441 Score per residue for model 441

- Molecule 1: Ubiquitin



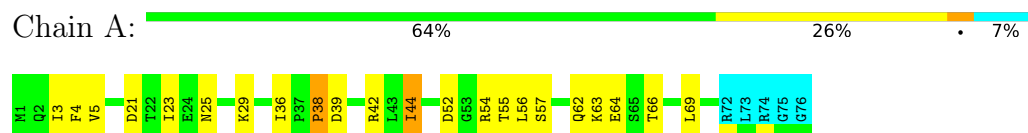
4.2.442 Score per residue for model 442

- Molecule 1: Ubiquitin



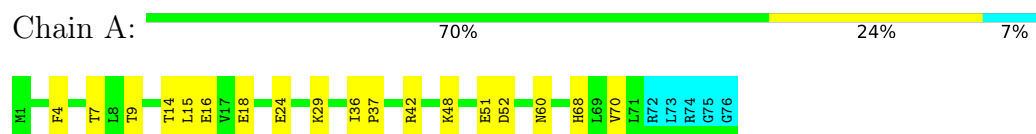
4.2.443 Score per residue for model 443

- Molecule 1: Ubiquitin



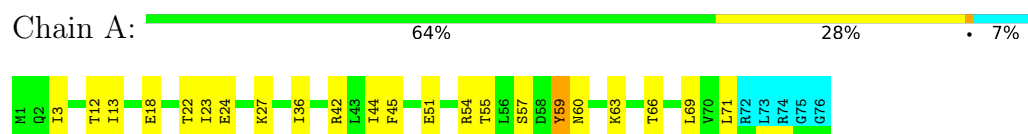
4.2.444 Score per residue for model 444

- Molecule 1: Ubiquitin



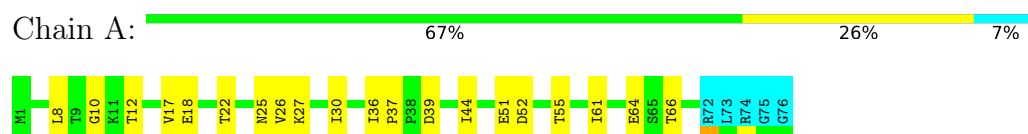
4.2.445 Score per residue for model 445

- Molecule 1: Ubiquitin



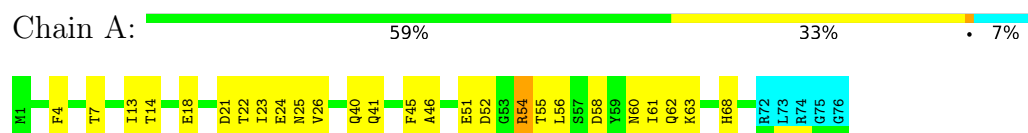
4.2.446 Score per residue for model 446

- Molecule 1: Ubiquitin



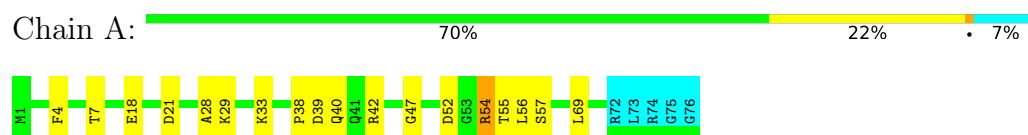
4.2.447 Score per residue for model 447

- Molecule 1: Ubiquitin



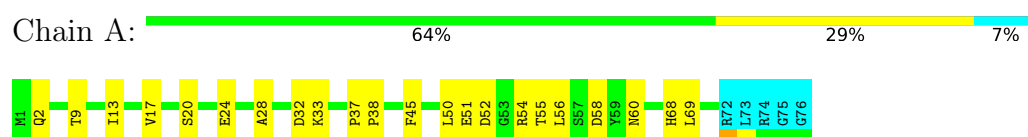
4.2.448 Score per residue for model 448

- Molecule 1: Ubiquitin



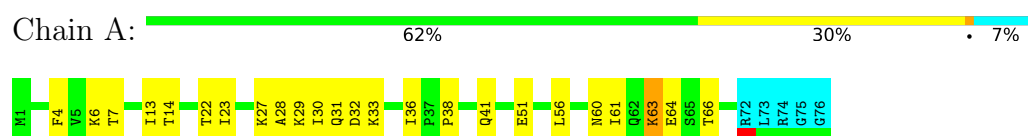
4.2.449 Score per residue for model 449

- Molecule 1: Ubiquitin



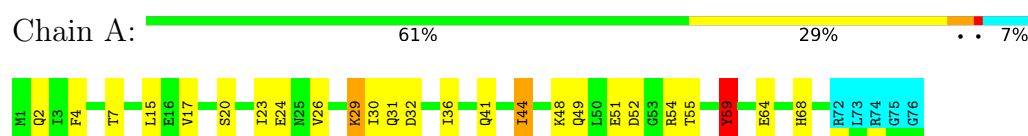
4.2.450 Score per residue for model 450

- Molecule 1: Ubiquitin



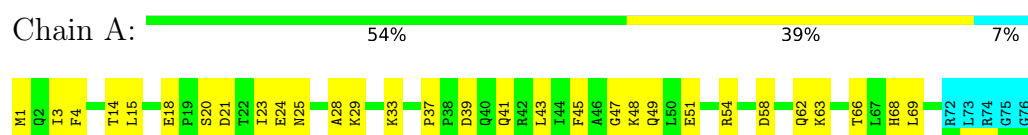
4.2.451 Score per residue for model 451

- Molecule 1: Ubiquitin



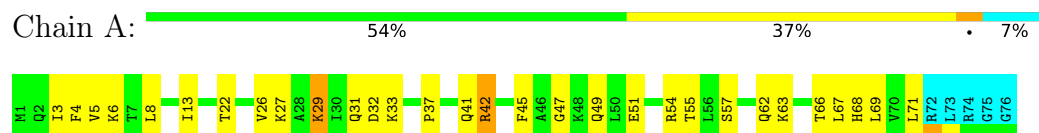
4.2.452 Score per residue for model 452

- Molecule 1: Ubiquitin



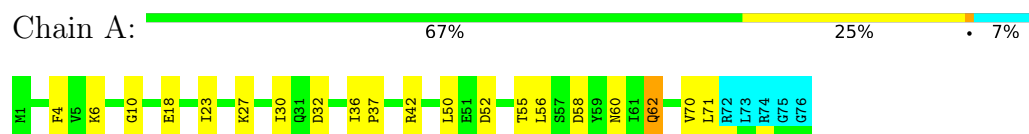
4.2.453 Score per residue for model 453

- Molecule 1: Ubiquitin



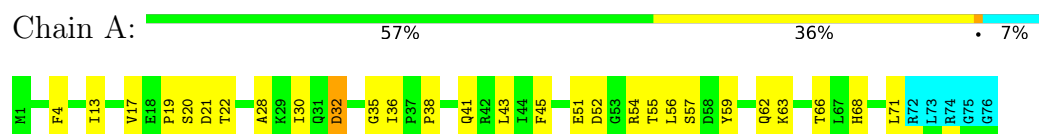
4.2.454 Score per residue for model 454

- Molecule 1: Ubiquitin



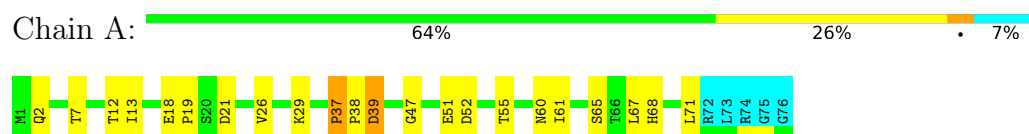
4.2.455 Score per residue for model 455

- Molecule 1: Ubiquitin



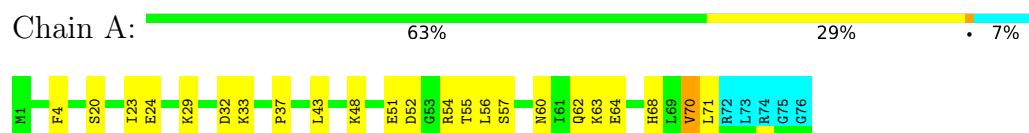
4.2.456 Score per residue for model 456

- Molecule 1: Ubiquitin



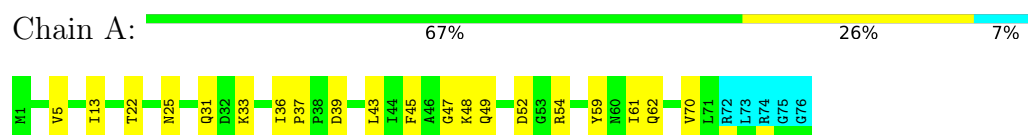
4.2.457 Score per residue for model 457

- Molecule 1: Ubiquitin



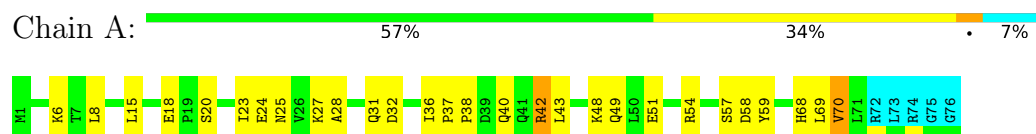
4.2.458 Score per residue for model 458

- Molecule 1: Ubiquitin



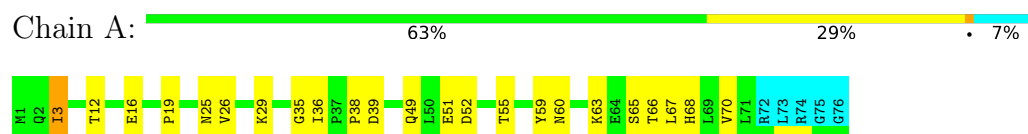
4.2.459 Score per residue for model 459

- Molecule 1: Ubiquitin



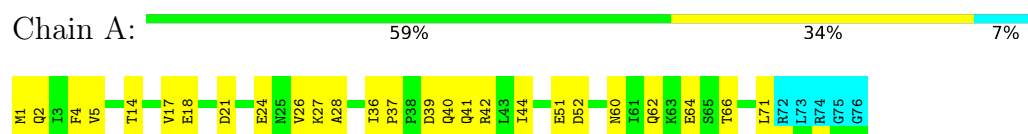
4.2.460 Score per residue for model 460

- Molecule 1: Ubiquitin



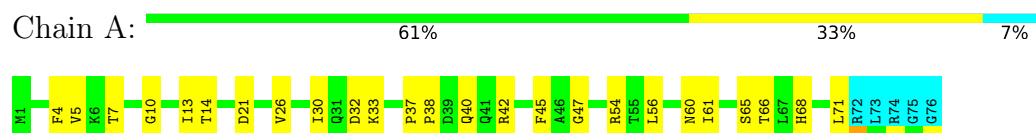
4.2.461 Score per residue for model 461

- Molecule 1: Ubiquitin



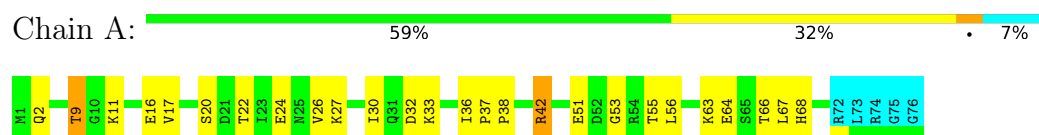
4.2.462 Score per residue for model 462

- Molecule 1: Ubiquitin



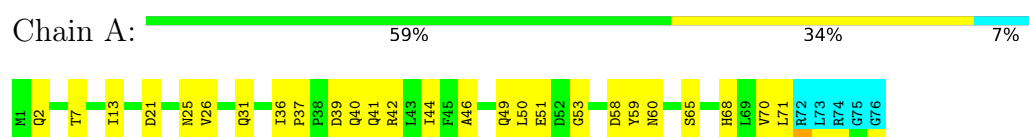
4.2.463 Score per residue for model 463

- Molecule 1: Ubiquitin



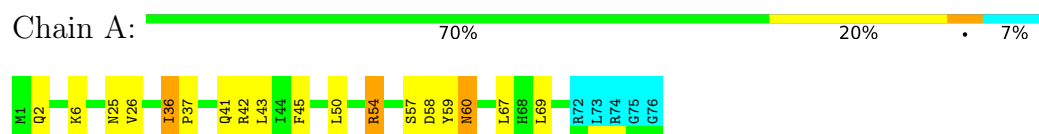
4.2.464 Score per residue for model 464

- Molecule 1: Ubiquitin



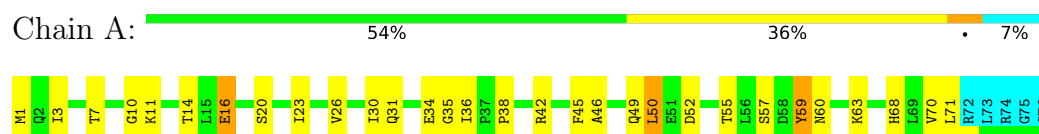
4.2.465 Score per residue for model 465

- Molecule 1: Ubiquitin



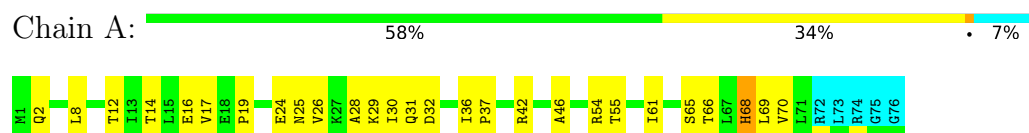
4.2.466 Score per residue for model 466

- Molecule 1: Ubiquitin



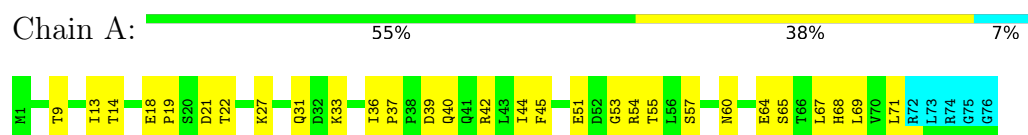
4.2.467 Score per residue for model 467

- Molecule 1: Ubiquitin



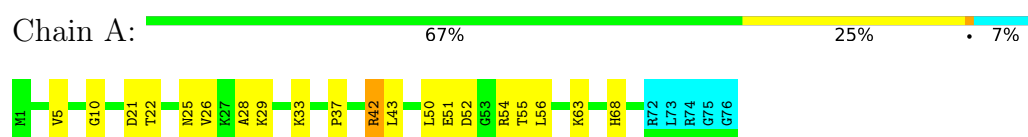
4.2.468 Score per residue for model 468

- Molecule 1: Ubiquitin



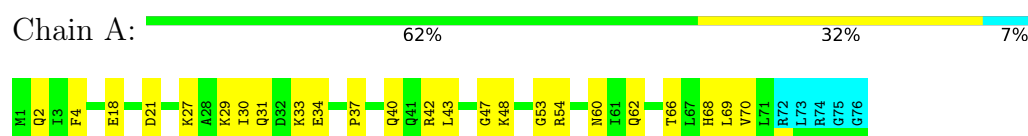
4.2.469 Score per residue for model 469

- Molecule 1: Ubiquitin



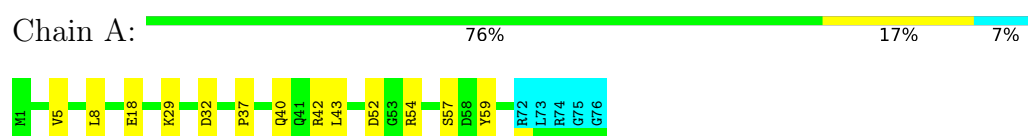
4.2.470 Score per residue for model 470

- Molecule 1: Ubiquitin



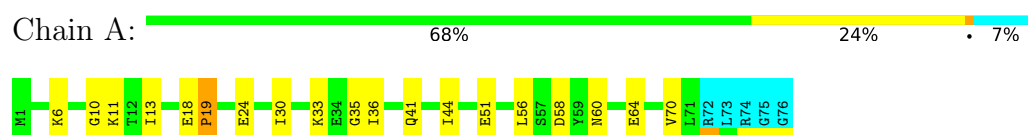
4.2.471 Score per residue for model 471

- Molecule 1: Ubiquitin



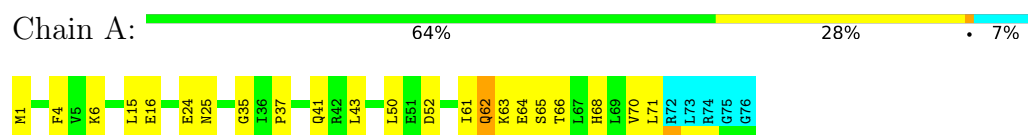
4.2.472 Score per residue for model 472

- Molecule 1: Ubiquitin



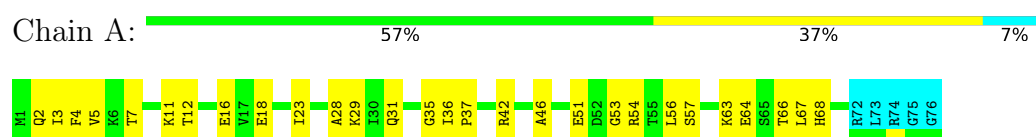
4.2.473 Score per residue for model 473

- Molecule 1: Ubiquitin



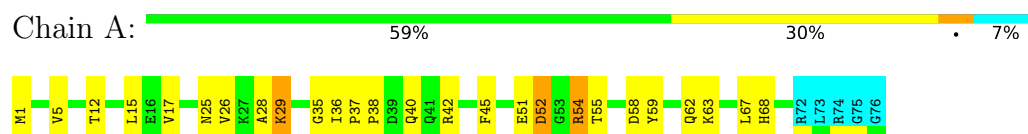
4.2.474 Score per residue for model 474

- Molecule 1: Ubiquitin



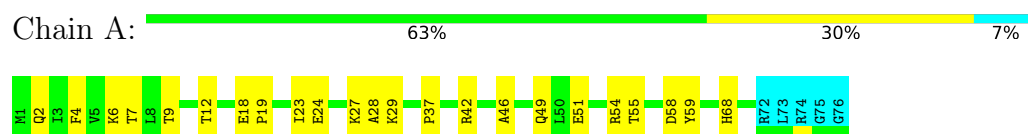
4.2.475 Score per residue for model 475

- Molecule 1: Ubiquitin



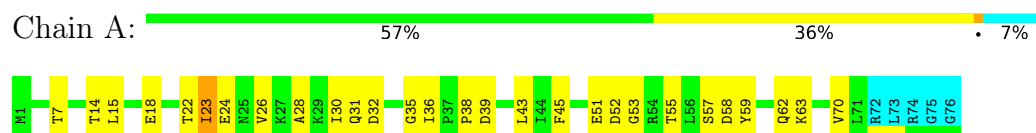
4.2.476 Score per residue for model 476

- Molecule 1: Ubiquitin



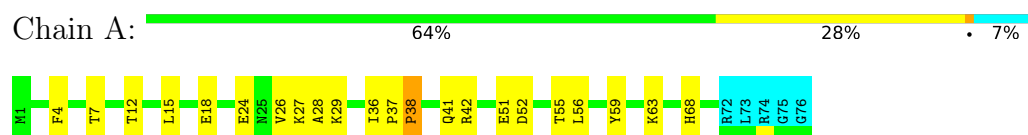
4.2.477 Score per residue for model 477

- Molecule 1: Ubiquitin



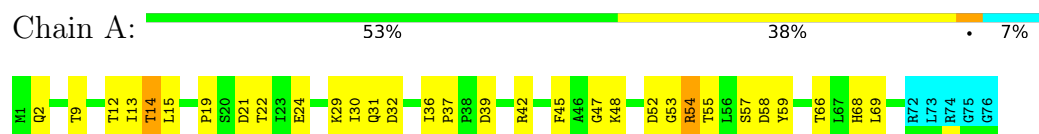
4.2.478 Score per residue for model 478

- Molecule 1: Ubiquitin



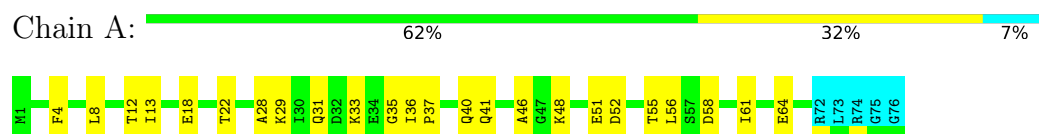
4.2.479 Score per residue for model 479

- Molecule 1: Ubiquitin



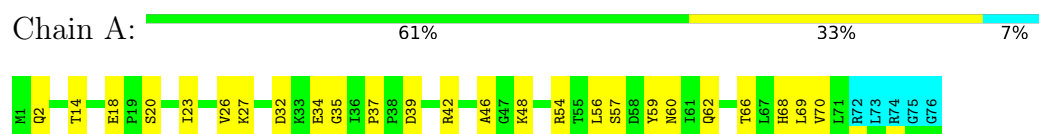
4.2.480 Score per residue for model 480

- Molecule 1: Ubiquitin



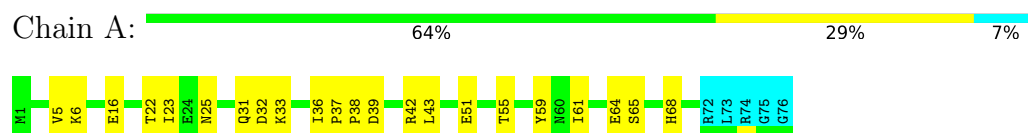
4.2.481 Score per residue for model 481

- Molecule 1: Ubiquitin



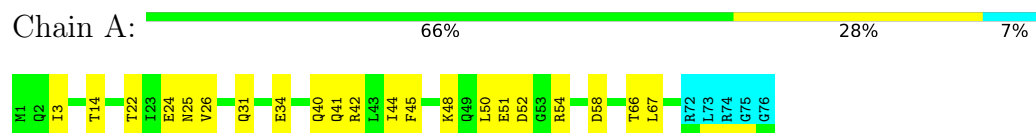
4.2.482 Score per residue for model 482

- Molecule 1: Ubiquitin



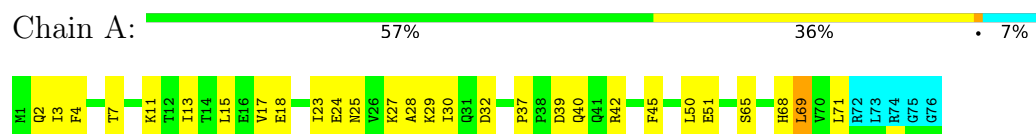
4.2.483 Score per residue for model 483

- Molecule 1: Ubiquitin



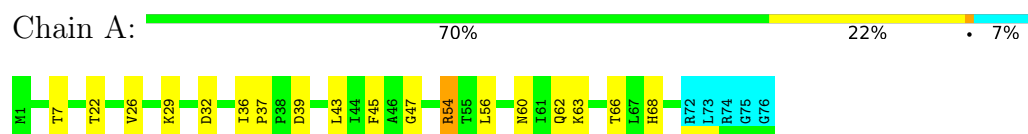
4.2.484 Score per residue for model 484

- Molecule 1: Ubiquitin



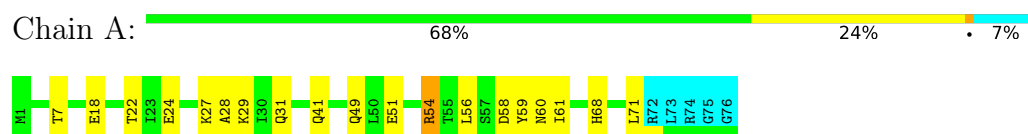
4.2.485 Score per residue for model 485

- Molecule 1: Ubiquitin



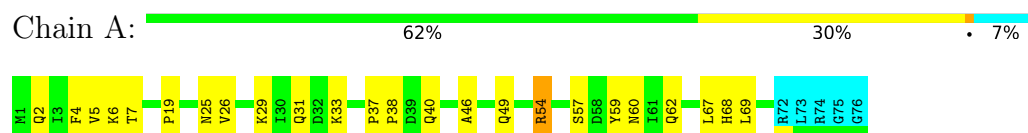
4.2.486 Score per residue for model 486

- Molecule 1: Ubiquitin



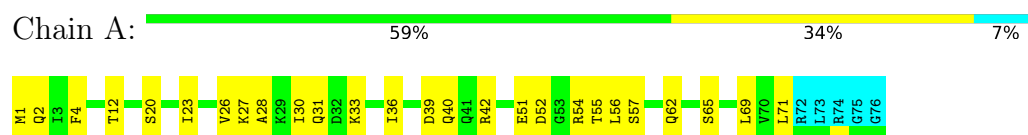
4.2.487 Score per residue for model 487

- Molecule 1: Ubiquitin



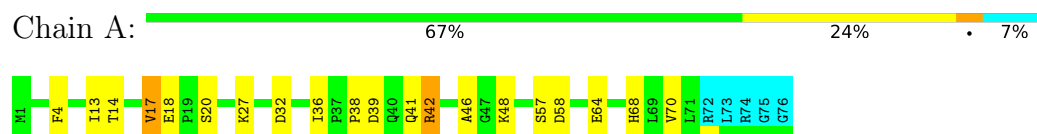
4.2.488 Score per residue for model 488

- Molecule 1: Ubiquitin



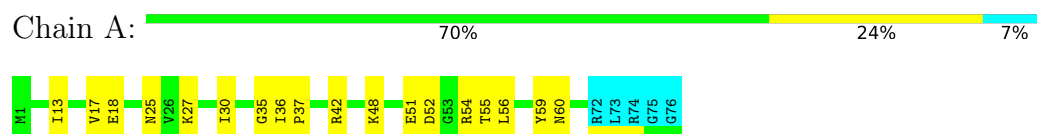
4.2.489 Score per residue for model 489

- Molecule 1: Ubiquitin



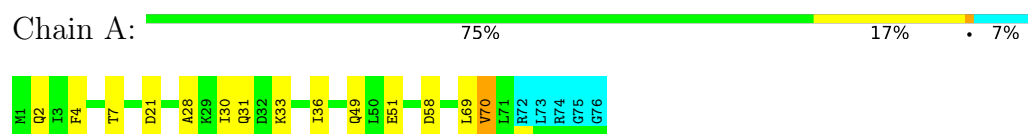
4.2.490 Score per residue for model 490

- Molecule 1: Ubiquitin



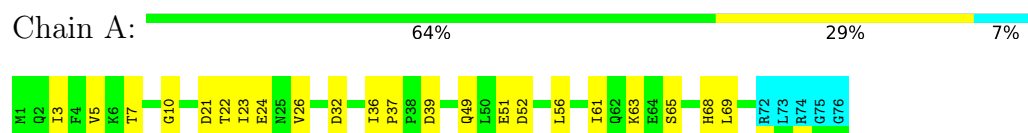
4.2.491 Score per residue for model 491

- Molecule 1: Ubiquitin



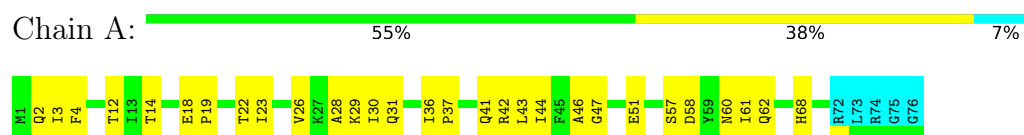
4.2.492 Score per residue for model 492

- Molecule 1: Ubiquitin



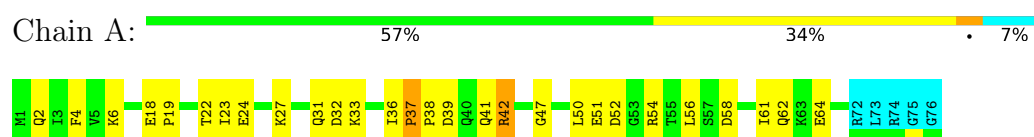
4.2.493 Score per residue for model 493

- Molecule 1: Ubiquitin



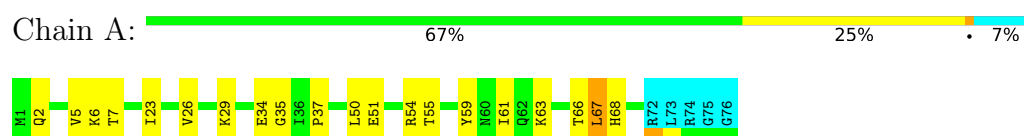
4.2.494 Score per residue for model 494

- Molecule 1: Ubiquitin



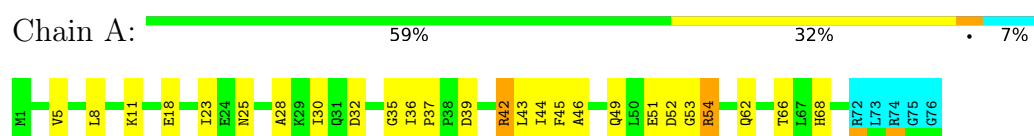
4.2.495 Score per residue for model 495

- Molecule 1: Ubiquitin



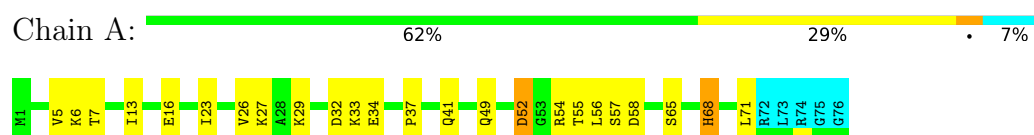
4.2.496 Score per residue for model 496

- Molecule 1: Ubiquitin



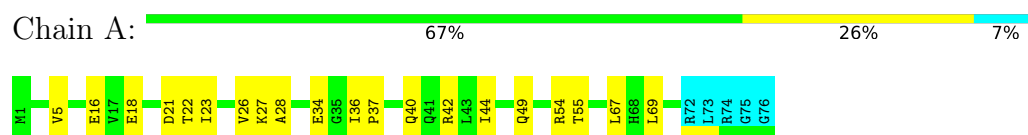
4.2.497 Score per residue for model 497

- Molecule 1: Ubiquitin



4.2.498 Score per residue for model 498

- Molecule 1: Ubiquitin



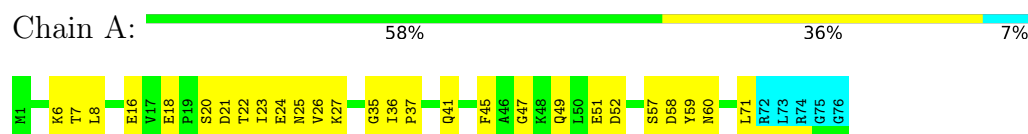
4.2.499 Score per residue for model 499

- Molecule 1: Ubiquitin



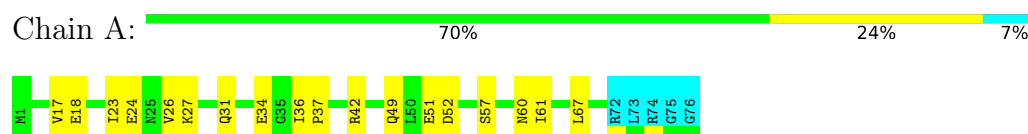
4.2.500 Score per residue for model 500

- Molecule 1: Ubiquitin



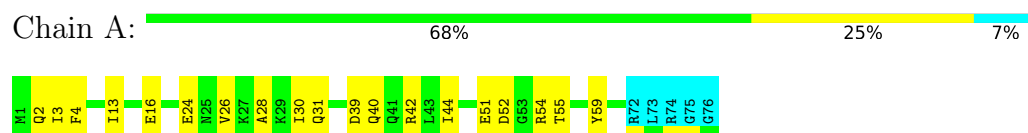
4.2.501 Score per residue for model 501

- Molecule 1: Ubiquitin



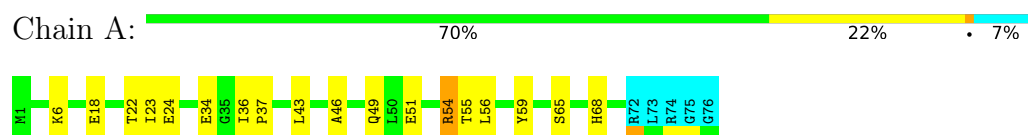
4.2.502 Score per residue for model 502

- Molecule 1: Ubiquitin



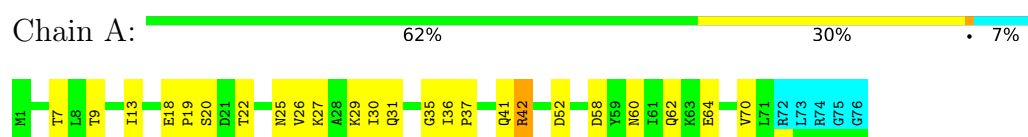
4.2.503 Score per residue for model 503

- Molecule 1: Ubiquitin



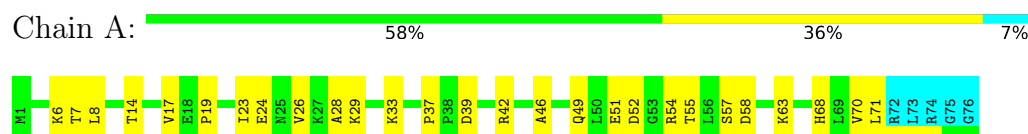
4.2.504 Score per residue for model 504

- Molecule 1: Ubiquitin



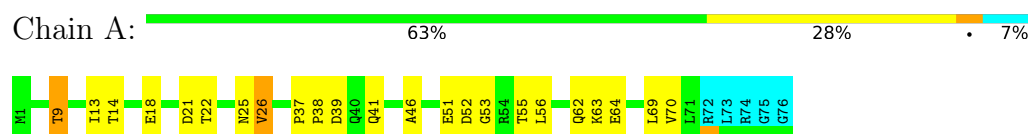
4.2.505 Score per residue for model 505

- Molecule 1: Ubiquitin



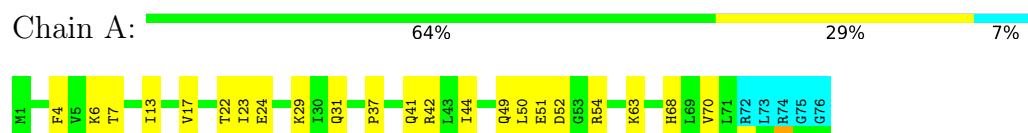
4.2.506 Score per residue for model 506

- Molecule 1: Ubiquitin



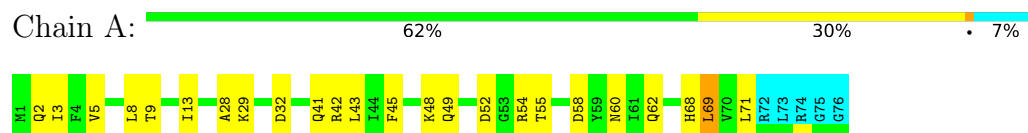
4.2.507 Score per residue for model 507

- Molecule 1: Ubiquitin



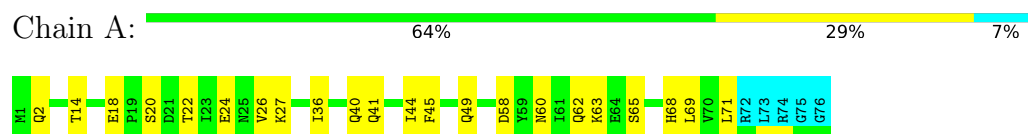
4.2.508 Score per residue for model 508

- Molecule 1: Ubiquitin



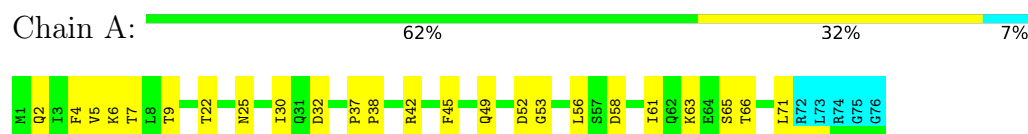
4.2.509 Score per residue for model 509

- Molecule 1: Ubiquitin



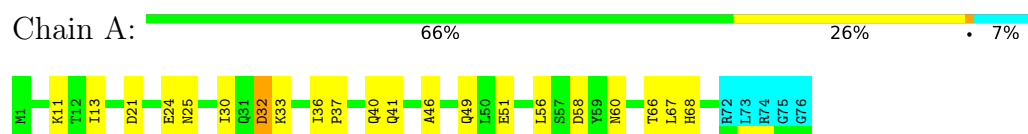
4.2.510 Score per residue for model 510

- Molecule 1: Ubiquitin



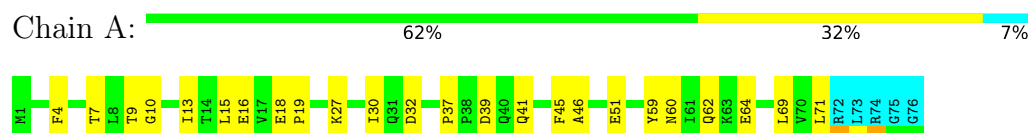
4.2.511 Score per residue for model 511

- Molecule 1: Ubiquitin



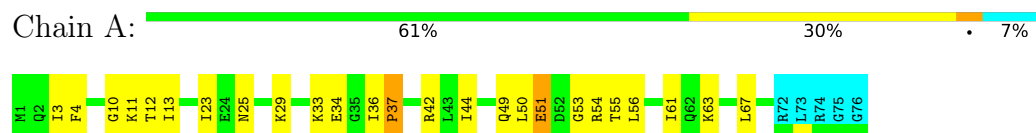
4.2.512 Score per residue for model 512

- Molecule 1: Ubiquitin



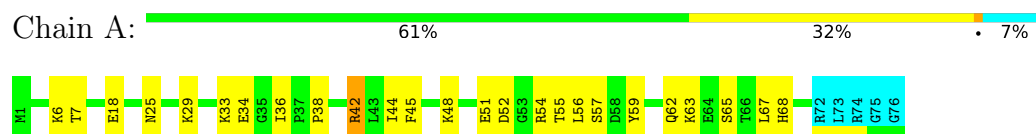
4.2.513 Score per residue for model 513

- Molecule 1: Ubiquitin



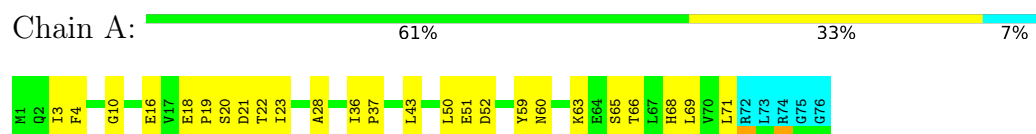
4.2.514 Score per residue for model 514

- Molecule 1: Ubiquitin



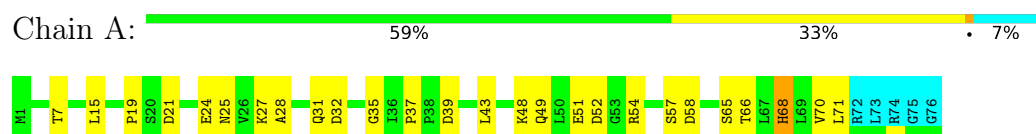
4.2.515 Score per residue for model 515

- Molecule 1: Ubiquitin



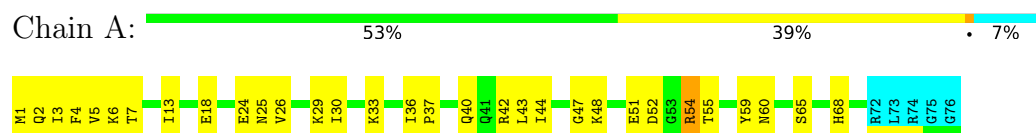
4.2.516 Score per residue for model 516

- Molecule 1: Ubiquitin



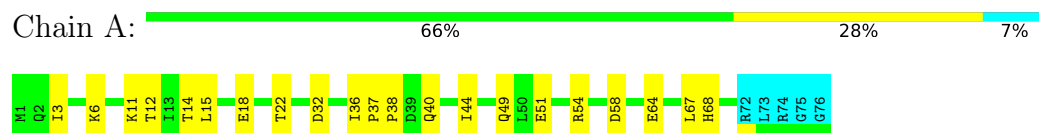
4.2.517 Score per residue for model 517

- Molecule 1: Ubiquitin



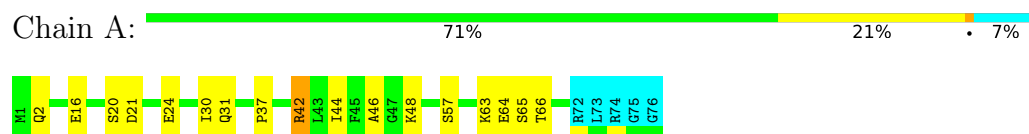
4.2.518 Score per residue for model 518

- Molecule 1: Ubiquitin



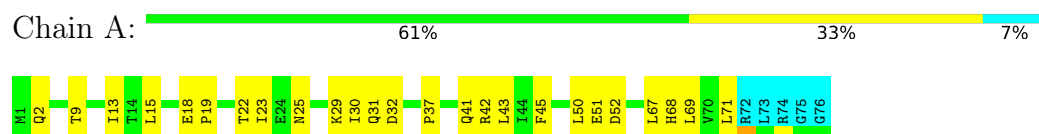
4.2.519 Score per residue for model 519

- Molecule 1: Ubiquitin



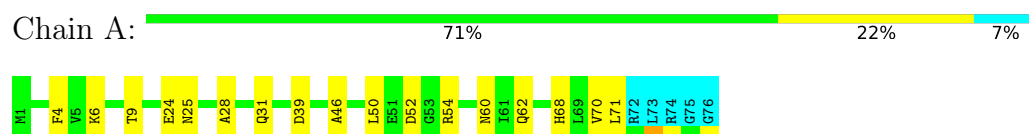
4.2.520 Score per residue for model 520

- Molecule 1: Ubiquitin



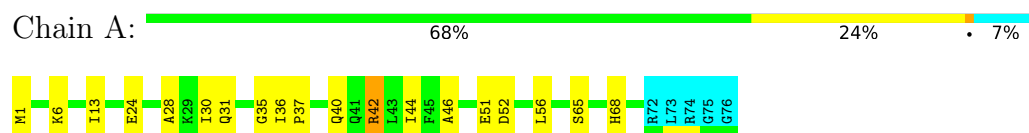
4.2.521 Score per residue for model 521

- Molecule 1: Ubiquitin



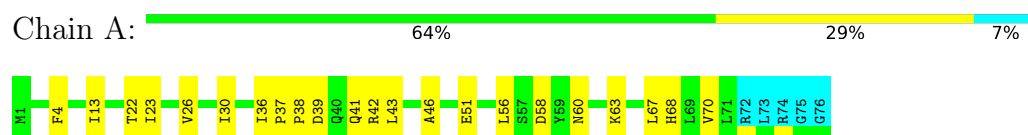
4.2.522 Score per residue for model 522

- Molecule 1: Ubiquitin



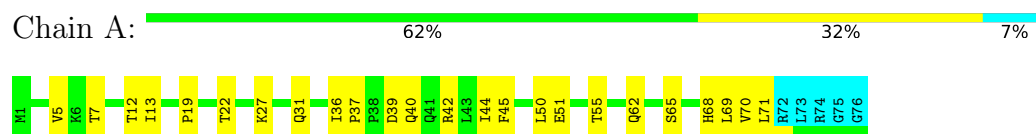
4.2.523 Score per residue for model 523

- Molecule 1: Ubiquitin



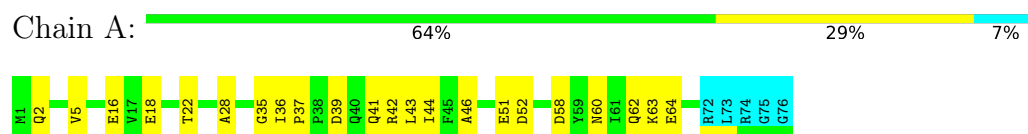
4.2.524 Score per residue for model 524

- Molecule 1: Ubiquitin



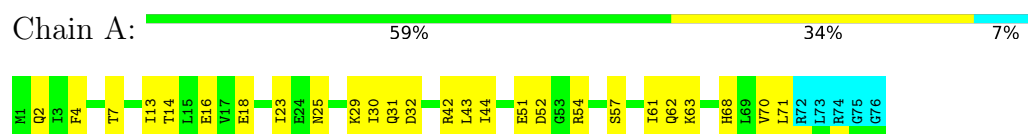
4.2.525 Score per residue for model 525

- Molecule 1: Ubiquitin



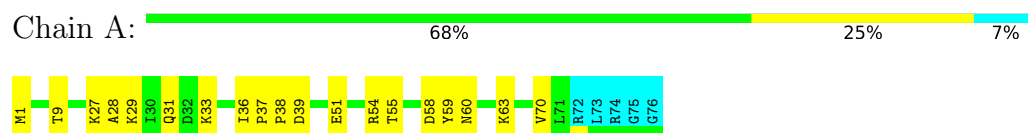
4.2.526 Score per residue for model 526

- Molecule 1: Ubiquitin



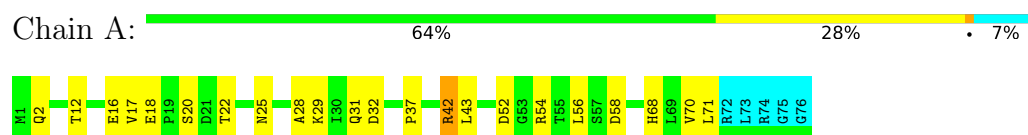
4.2.527 Score per residue for model 527

- Molecule 1: Ubiquitin



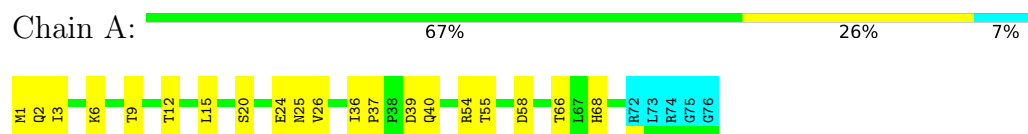
4.2.528 Score per residue for model 528

- Molecule 1: Ubiquitin



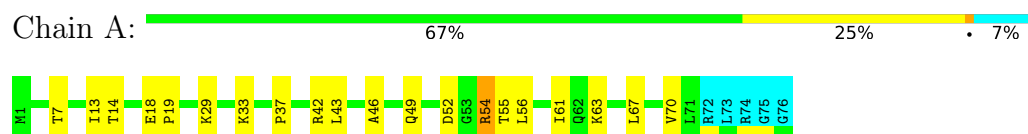
4.2.529 Score per residue for model 529

- Molecule 1: Ubiquitin



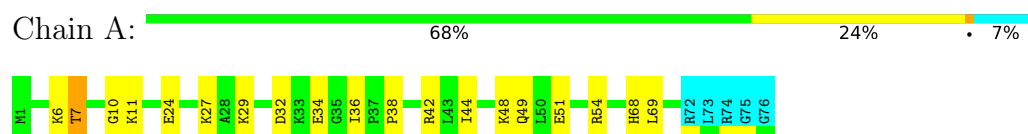
4.2.530 Score per residue for model 530

- Molecule 1: Ubiquitin



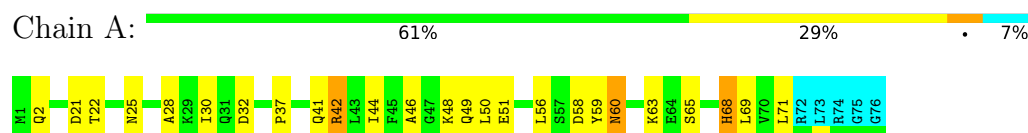
4.2.531 Score per residue for model 531

- Molecule 1: Ubiquitin



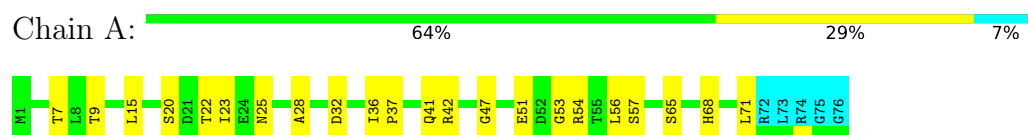
4.2.532 Score per residue for model 532

- Molecule 1: Ubiquitin



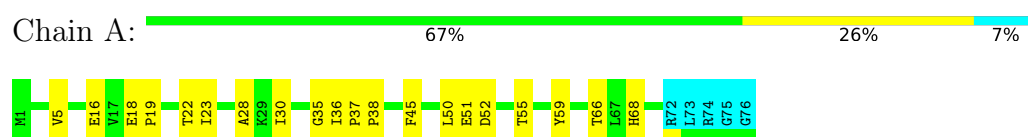
4.2.533 Score per residue for model 533

- Molecule 1: Ubiquitin



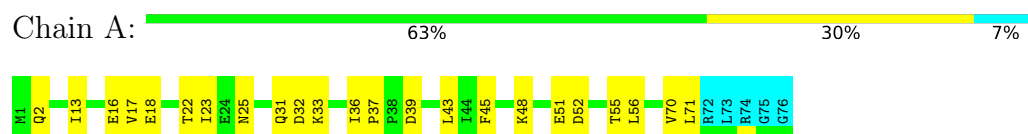
4.2.534 Score per residue for model 534

- Molecule 1: Ubiquitin



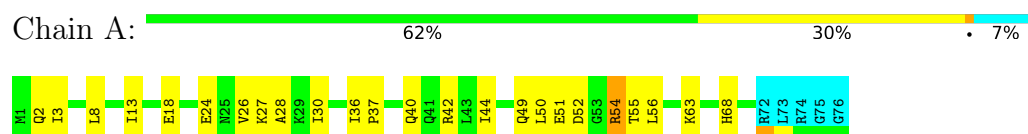
4.2.535 Score per residue for model 535

- Molecule 1: Ubiquitin



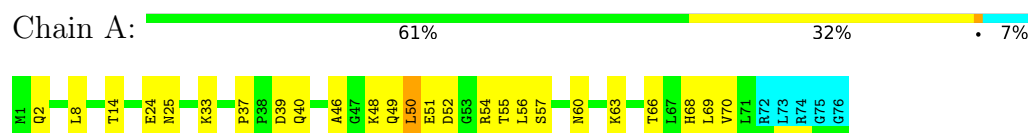
4.2.536 Score per residue for model 536

- Molecule 1: Ubiquitin



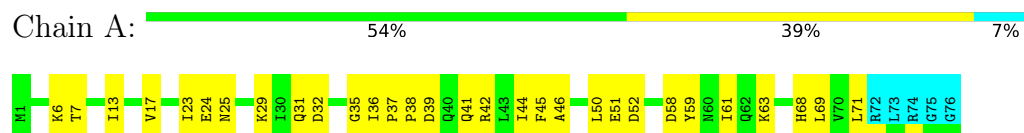
4.2.537 Score per residue for model 537

- Molecule 1: Ubiquitin



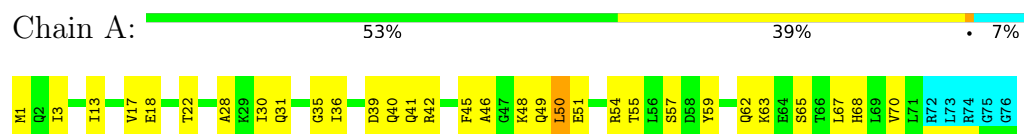
4.2.538 Score per residue for model 538

- Molecule 1: Ubiquitin



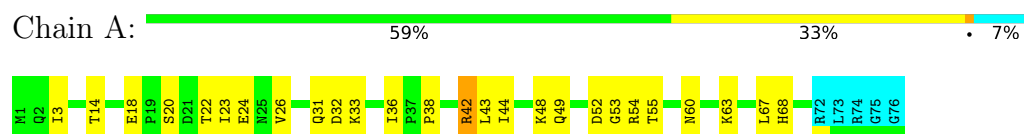
4.2.539 Score per residue for model 539

- Molecule 1: Ubiquitin



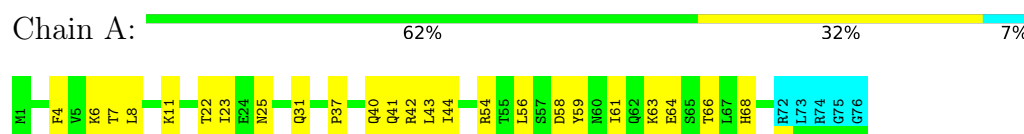
4.2.540 Score per residue for model 540

- Molecule 1: Ubiquitin



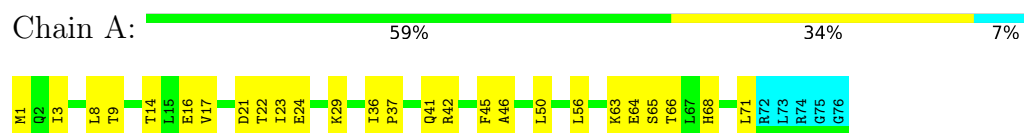
4.2.541 Score per residue for model 541

- Molecule 1: Ubiquitin



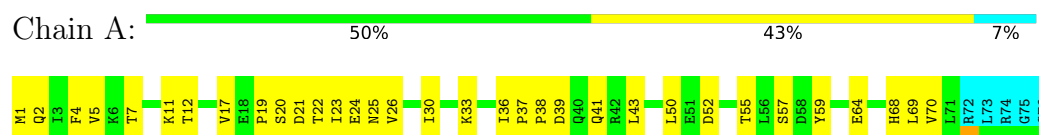
4.2.542 Score per residue for model 542

- Molecule 1: Ubiquitin



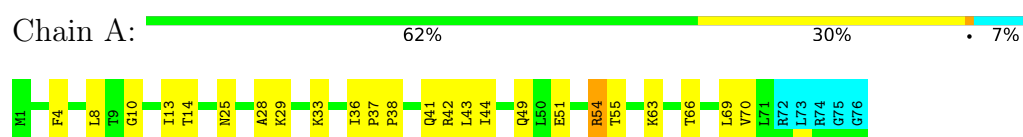
4.2.543 Score per residue for model 543

- Molecule 1: Ubiquitin



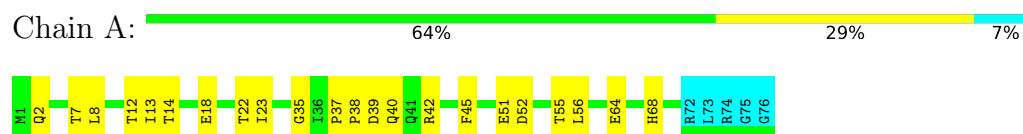
4.2.544 Score per residue for model 544

- Molecule 1: Ubiquitin



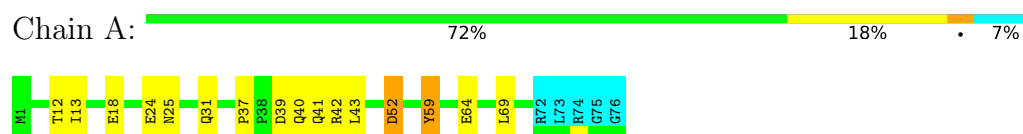
4.2.545 Score per residue for model 545

- Molecule 1: Ubiquitin



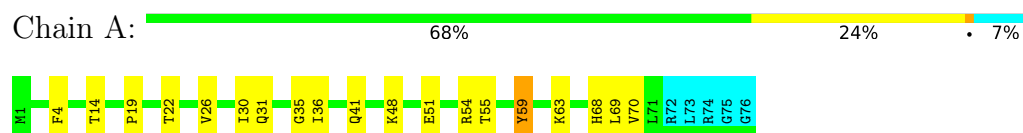
4.2.546 Score per residue for model 546

- Molecule 1: Ubiquitin



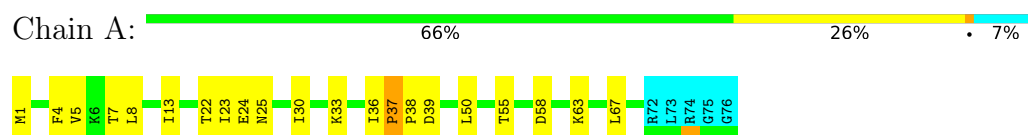
4.2.547 Score per residue for model 547

- Molecule 1: Ubiquitin



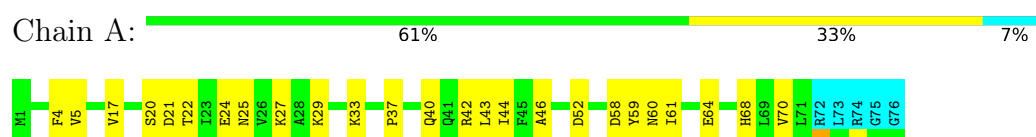
4.2.548 Score per residue for model 548

- Molecule 1: Ubiquitin



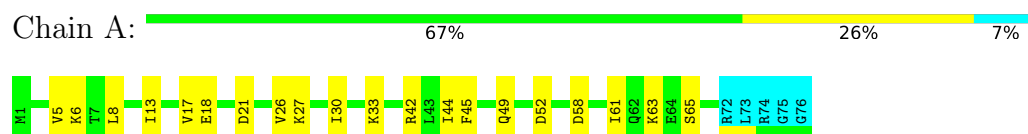
4.2.549 Score per residue for model 549

- Molecule 1: Ubiquitin



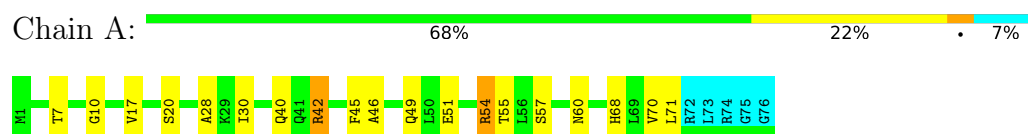
4.2.550 Score per residue for model 550

- Molecule 1: Ubiquitin



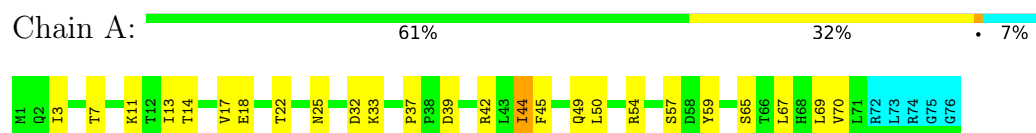
4.2.551 Score per residue for model 551

- Molecule 1: Ubiquitin



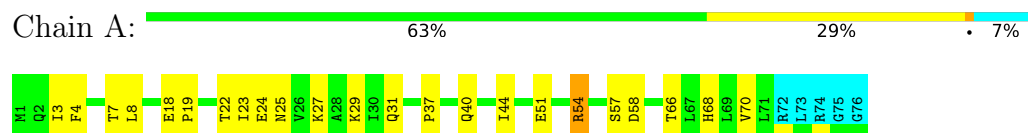
4.2.552 Score per residue for model 552

- Molecule 1: Ubiquitin



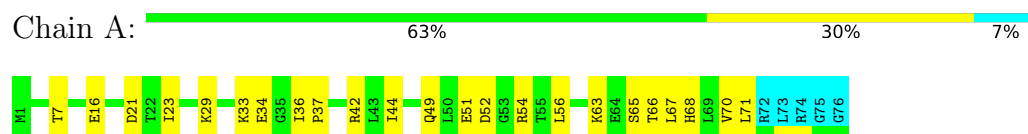
4.2.553 Score per residue for model 553

- Molecule 1: Ubiquitin



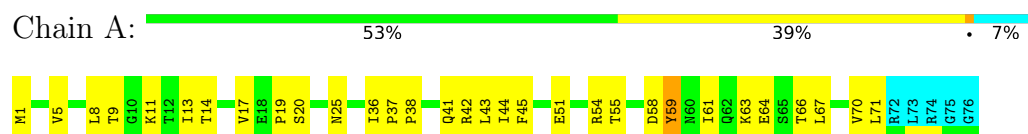
4.2.554 Score per residue for model 554

- Molecule 1: Ubiquitin



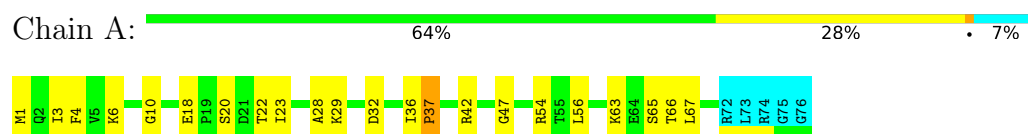
4.2.555 Score per residue for model 555

- Molecule 1: Ubiquitin



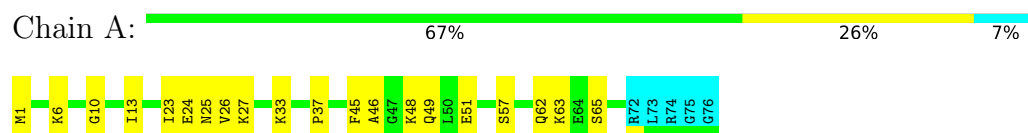
4.2.556 Score per residue for model 556

- Molecule 1: Ubiquitin



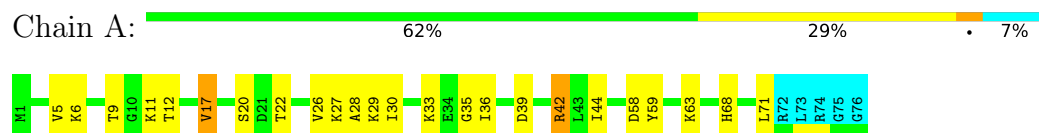
4.2.557 Score per residue for model 557

- Molecule 1: Ubiquitin



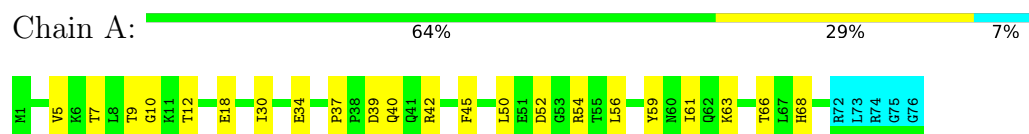
4.2.558 Score per residue for model 558

- Molecule 1: Ubiquitin



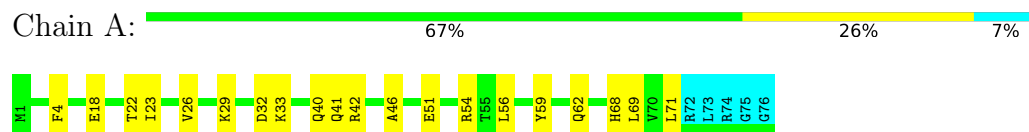
4.2.559 Score per residue for model 559

- Molecule 1: Ubiquitin



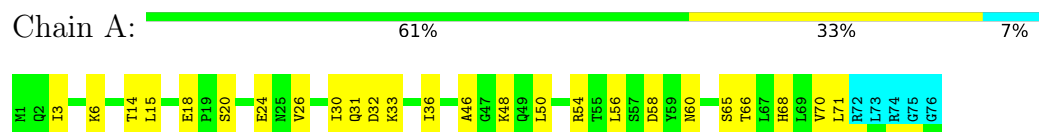
4.2.560 Score per residue for model 560

- Molecule 1: Ubiquitin



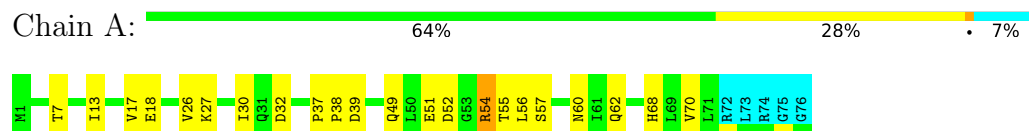
4.2.561 Score per residue for model 561

- Molecule 1: Ubiquitin



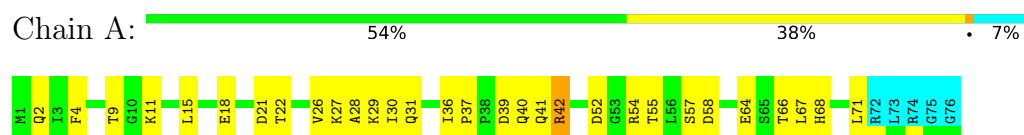
4.2.562 Score per residue for model 562

- Molecule 1: Ubiquitin



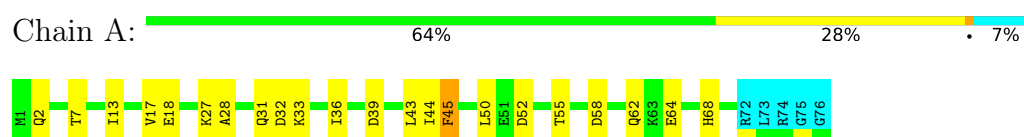
4.2.563 Score per residue for model 563

- Molecule 1: Ubiquitin



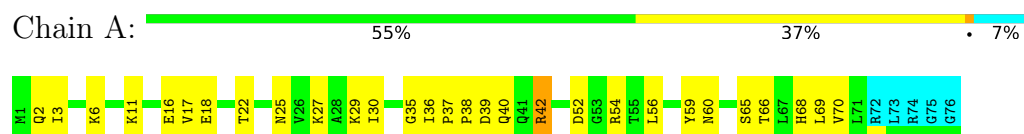
4.2.564 Score per residue for model 564

- Molecule 1: Ubiquitin



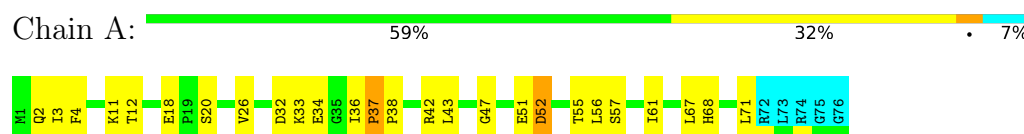
4.2.565 Score per residue for model 565

- Molecule 1: Ubiquitin



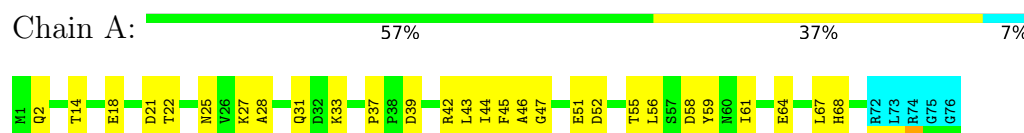
4.2.566 Score per residue for model 566

- Molecule 1: Ubiquitin



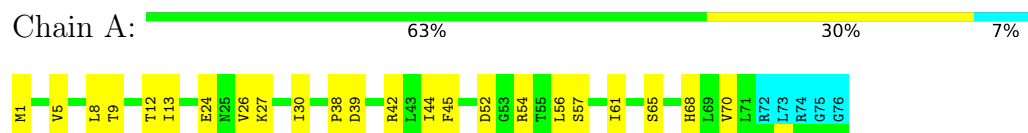
4.2.567 Score per residue for model 567

- Molecule 1: Ubiquitin



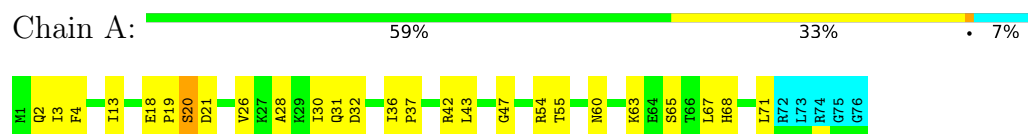
4.2.568 Score per residue for model 568

- Molecule 1: Ubiquitin



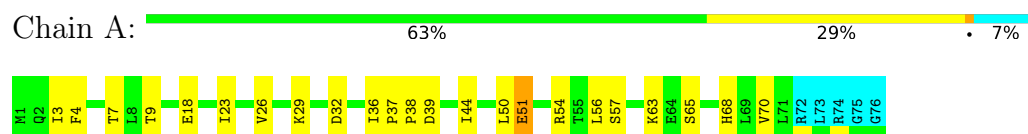
4.2.569 Score per residue for model 569

- Molecule 1: Ubiquitin



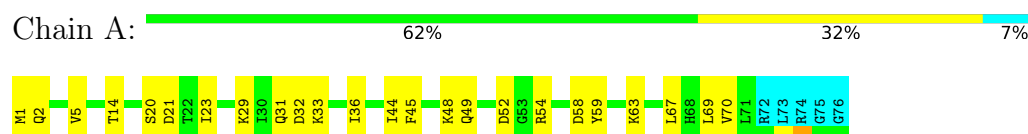
4.2.570 Score per residue for model 570

- Molecule 1: Ubiquitin



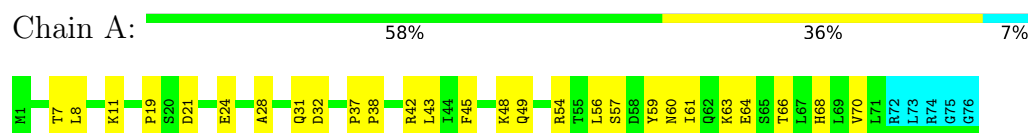
4.2.571 Score per residue for model 571

- Molecule 1: Ubiquitin



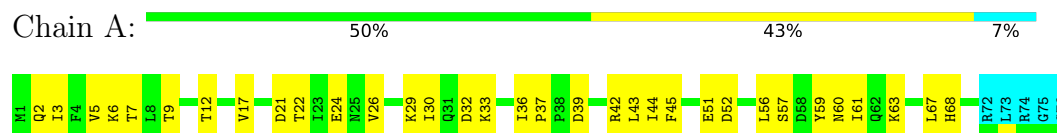
4.2.572 Score per residue for model 572

- Molecule 1: Ubiquitin



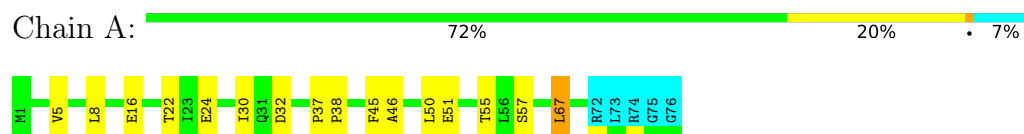
4.2.573 Score per residue for model 573

- Molecule 1: Ubiquitin



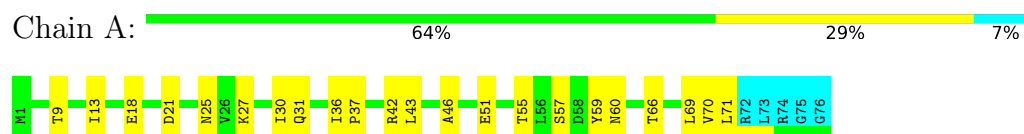
4.2.574 Score per residue for model 574

- Molecule 1: Ubiquitin



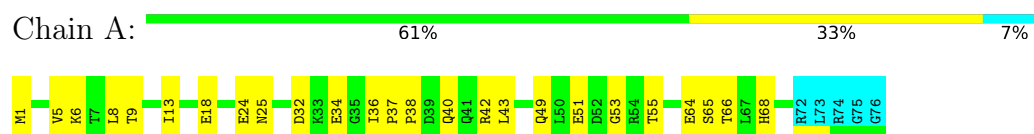
4.2.575 Score per residue for model 575

- Molecule 1: Ubiquitin



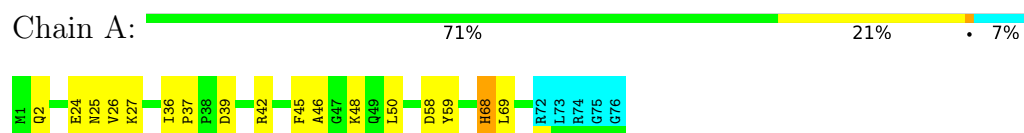
4.2.576 Score per residue for model 576

- Molecule 1: Ubiquitin



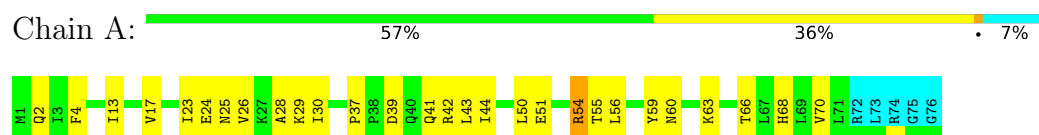
4.2.577 Score per residue for model 577

- Molecule 1: Ubiquitin



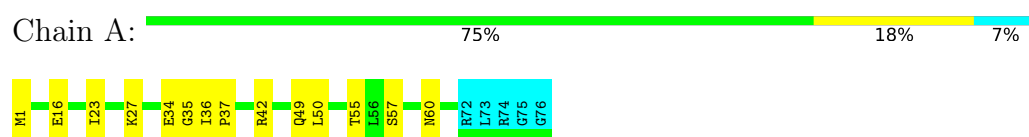
4.2.578 Score per residue for model 578

- Molecule 1: Ubiquitin



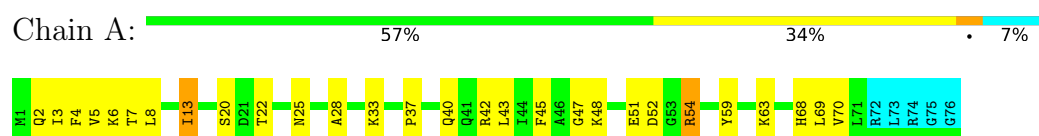
4.2.579 Score per residue for model 579

- Molecule 1: Ubiquitin



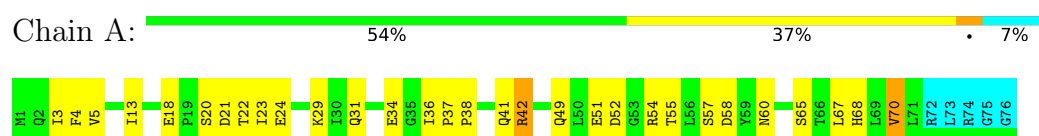
4.2.580 Score per residue for model 580

- Molecule 1: Ubiquitin



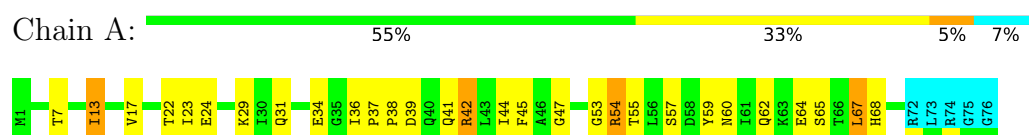
4.2.581 Score per residue for model 581

- Molecule 1: Ubiquitin



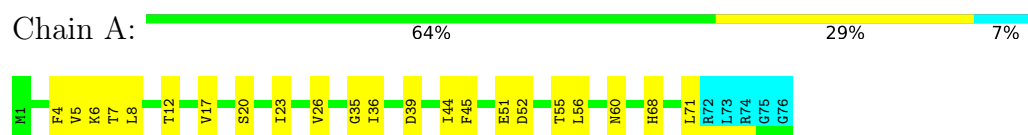
4.2.582 Score per residue for model 582

- Molecule 1: Ubiquitin



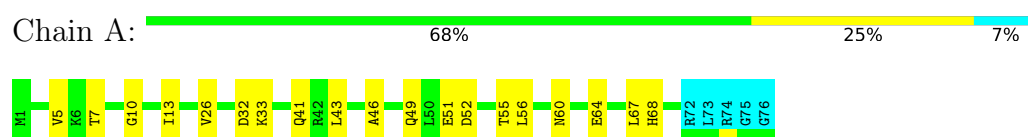
4.2.583 Score per residue for model 583

- Molecule 1: Ubiquitin



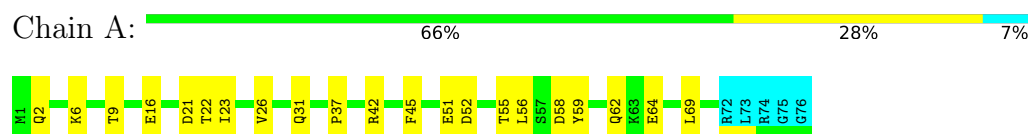
4.2.584 Score per residue for model 584

- Molecule 1: Ubiquitin



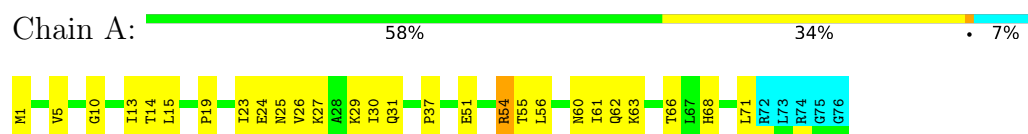
4.2.585 Score per residue for model 585

- Molecule 1: Ubiquitin



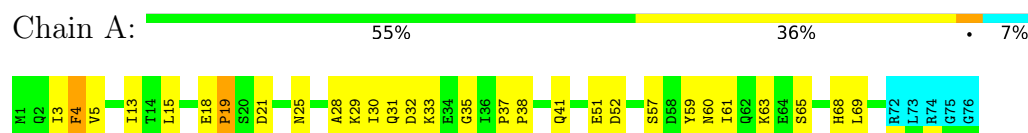
4.2.586 Score per residue for model 586

- Molecule 1: Ubiquitin



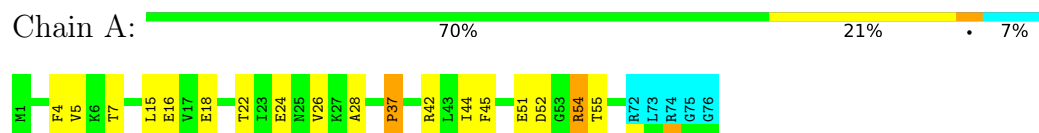
4.2.587 Score per residue for model 587

- Molecule 1: Ubiquitin



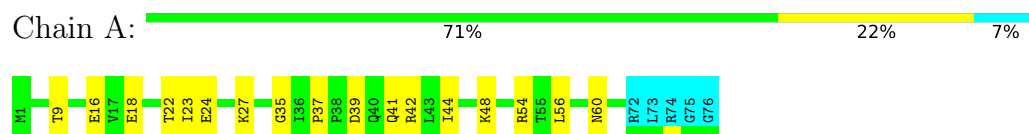
4.2.588 Score per residue for model 588

- Molecule 1: Ubiquitin



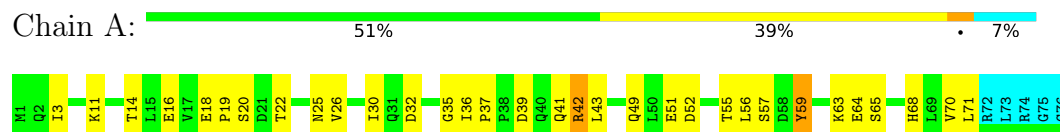
4.2.589 Score per residue for model 589

- Molecule 1: Ubiquitin



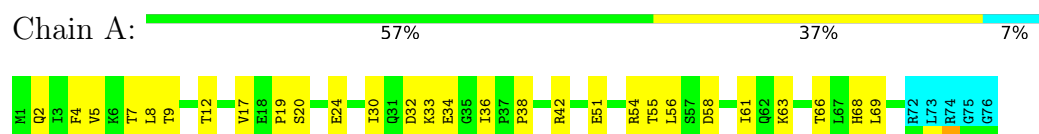
4.2.590 Score per residue for model 590

- Molecule 1: Ubiquitin



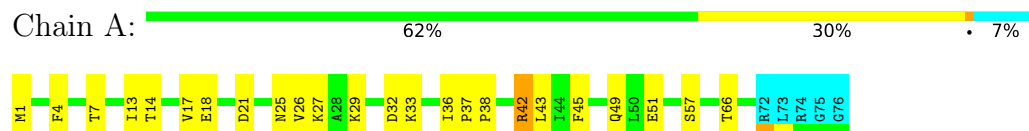
4.2.591 Score per residue for model 591

- Molecule 1: Ubiquitin



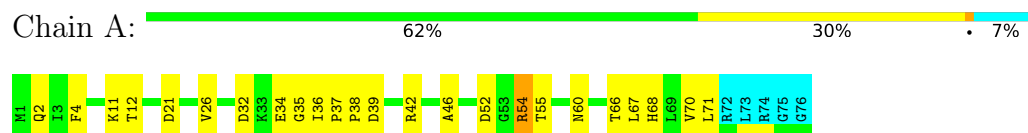
4.2.592 Score per residue for model 592

- Molecule 1: Ubiquitin



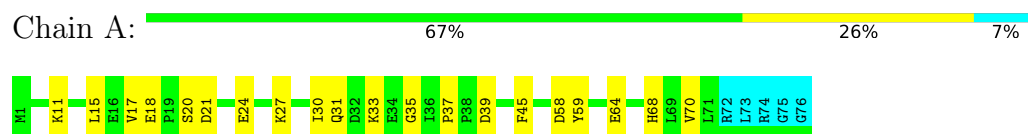
4.2.593 Score per residue for model 593

- Molecule 1: Ubiquitin



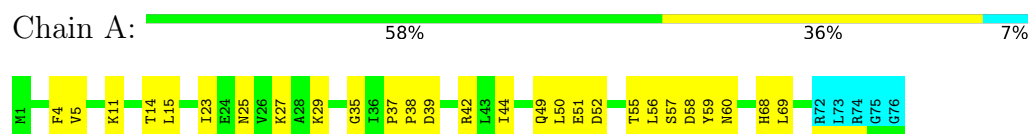
4.2.594 Score per residue for model 594

- Molecule 1: Ubiquitin



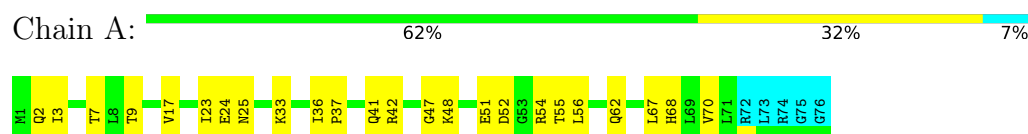
4.2.595 Score per residue for model 595

- Molecule 1: Ubiquitin



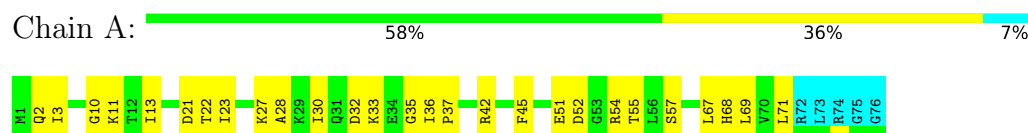
4.2.596 Score per residue for model 596

- Molecule 1: Ubiquitin



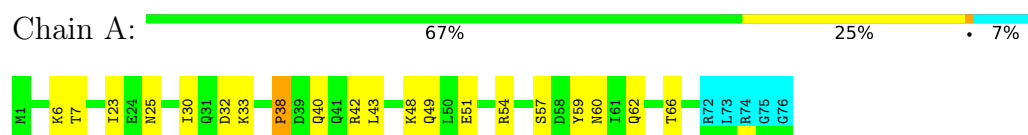
4.2.597 Score per residue for model 597

- Molecule 1: Ubiquitin



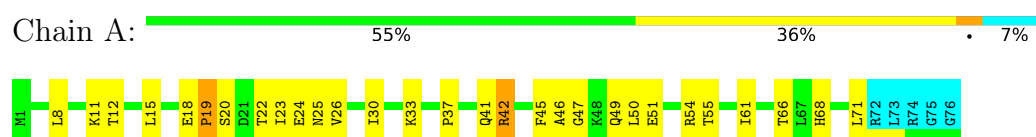
4.2.598 Score per residue for model 598

- Molecule 1: Ubiquitin



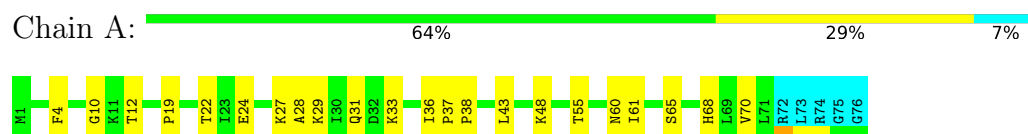
4.2.599 Score per residue for model 599

- Molecule 1: Ubiquitin



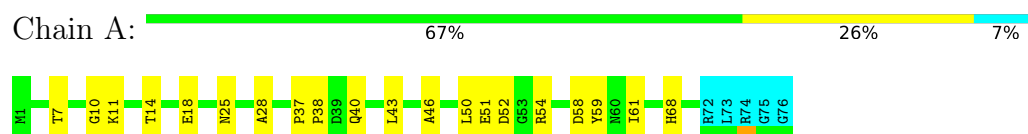
4.2.600 Score per residue for model 600

- Molecule 1: Ubiquitin



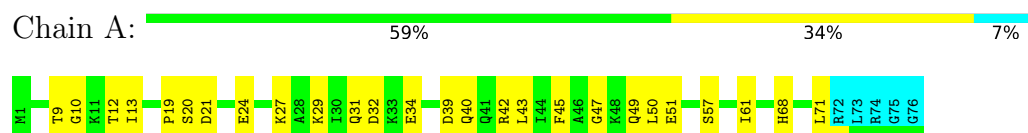
4.2.601 Score per residue for model 601

- Molecule 1: Ubiquitin



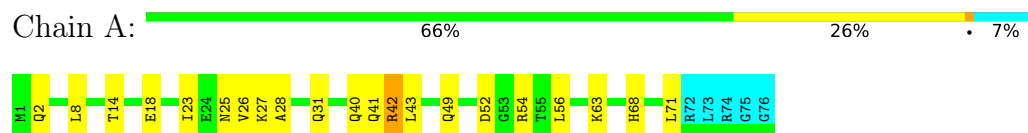
4.2.602 Score per residue for model 602

- Molecule 1: Ubiquitin



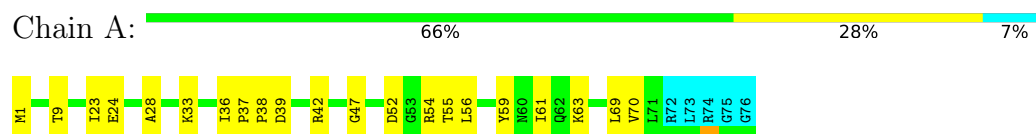
4.2.603 Score per residue for model 603

- Molecule 1: Ubiquitin



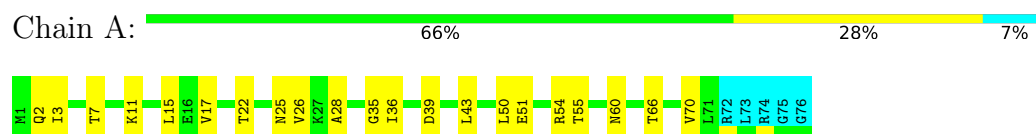
4.2.604 Score per residue for model 604

- Molecule 1: Ubiquitin



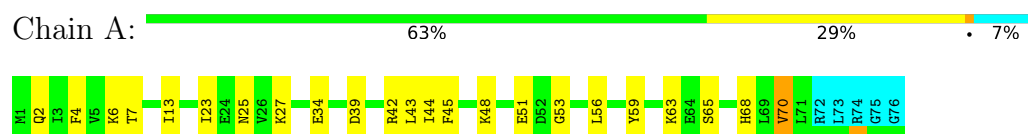
4.2.605 Score per residue for model 605

- Molecule 1: Ubiquitin



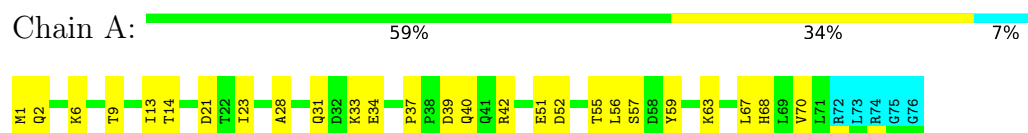
4.2.606 Score per residue for model 606

- Molecule 1: Ubiquitin



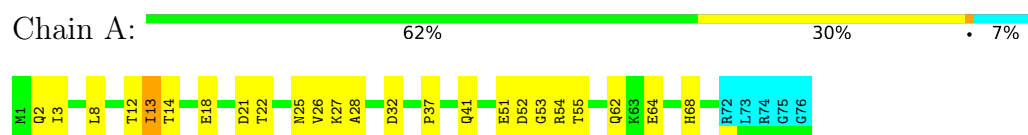
4.2.607 Score per residue for model 607

- Molecule 1: Ubiquitin



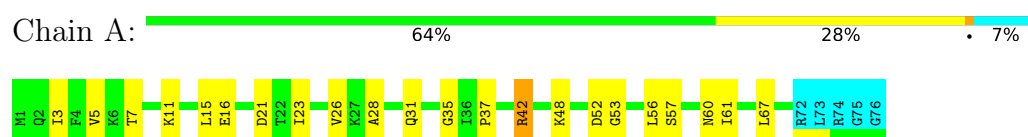
4.2.608 Score per residue for model 608

- Molecule 1: Ubiquitin



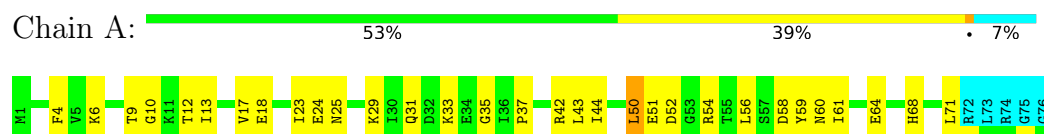
4.2.609 Score per residue for model 609

- Molecule 1: Ubiquitin



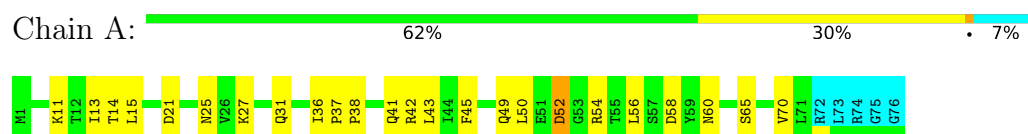
4.2.610 Score per residue for model 610

- Molecule 1: Ubiquitin



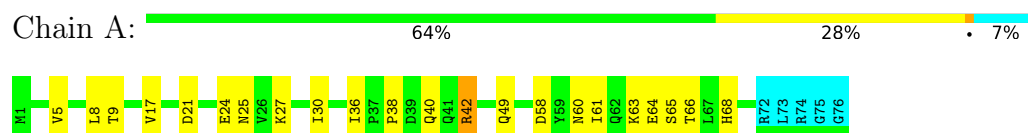
4.2.611 Score per residue for model 611

- Molecule 1: Ubiquitin



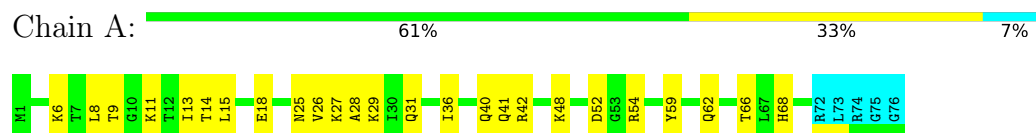
4.2.612 Score per residue for model 612

- Molecule 1: Ubiquitin



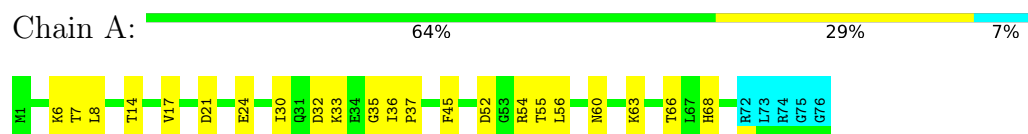
4.2.613 Score per residue for model 613

- Molecule 1: Ubiquitin



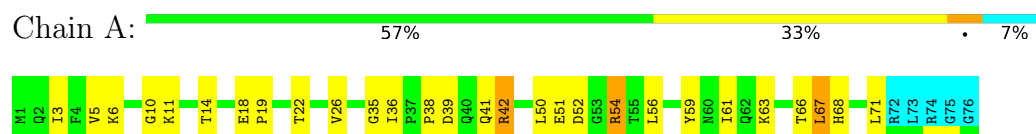
4.2.614 Score per residue for model 614

- Molecule 1: Ubiquitin



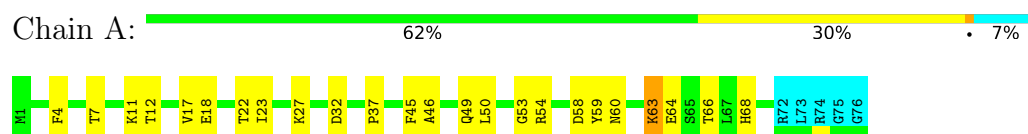
4.2.615 Score per residue for model 615

- Molecule 1: Ubiquitin



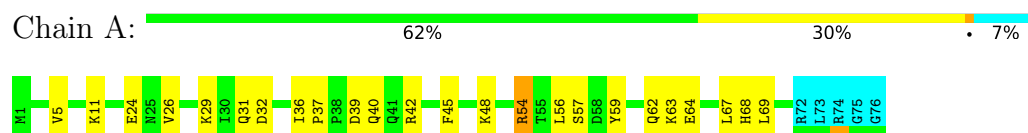
4.2.616 Score per residue for model 616

- Molecule 1: Ubiquitin



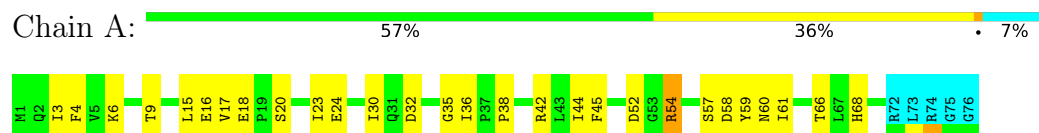
4.2.617 Score per residue for model 617

- Molecule 1: Ubiquitin



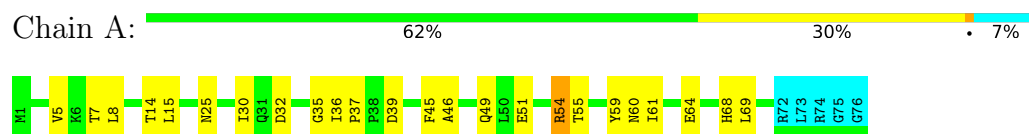
4.2.618 Score per residue for model 618

- Molecule 1: Ubiquitin



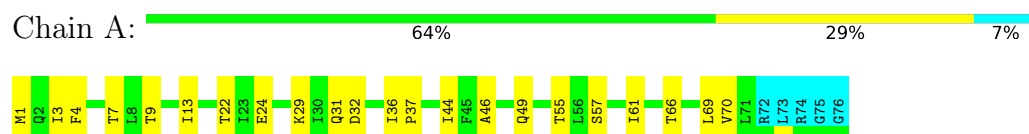
4.2.619 Score per residue for model 619

- Molecule 1: Ubiquitin



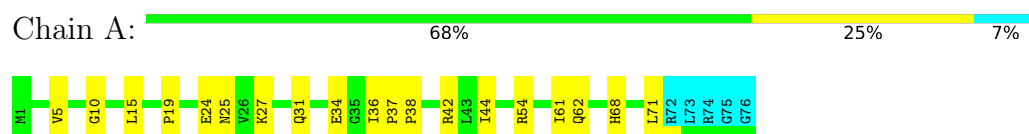
4.2.620 Score per residue for model 620

- Molecule 1: Ubiquitin



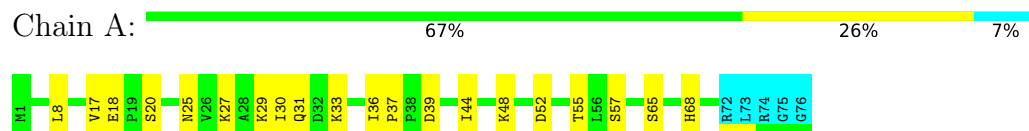
4.2.621 Score per residue for model 621

- Molecule 1: Ubiquitin



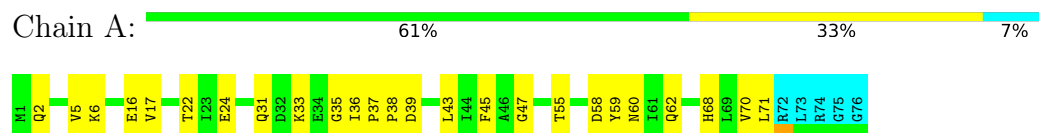
4.2.622 Score per residue for model 622

- Molecule 1: Ubiquitin



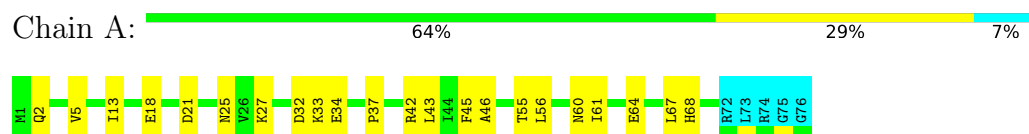
4.2.623 Score per residue for model 623

- Molecule 1: Ubiquitin



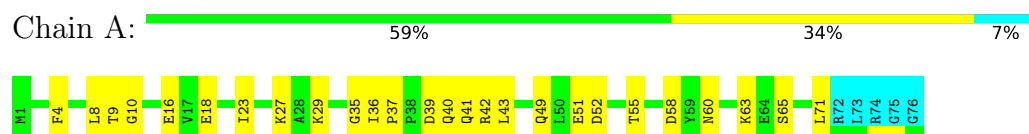
4.2.624 Score per residue for model 624

- Molecule 1: Ubiquitin



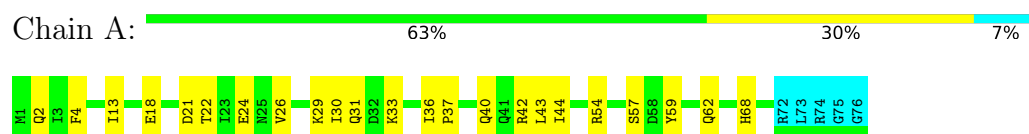
4.2.625 Score per residue for model 625

- Molecule 1: Ubiquitin



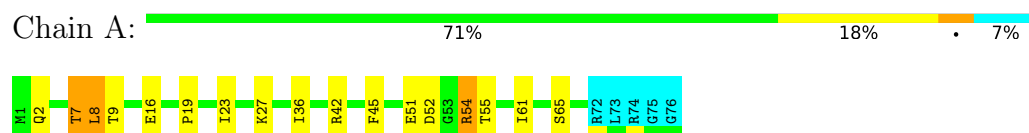
4.2.626 Score per residue for model 626

- Molecule 1: Ubiquitin



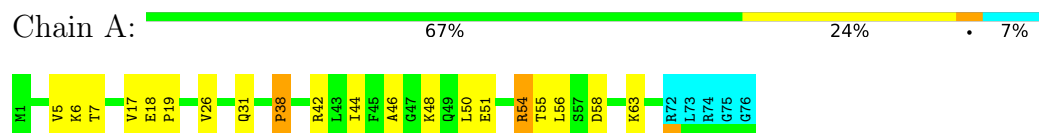
4.2.627 Score per residue for model 627

- Molecule 1: Ubiquitin



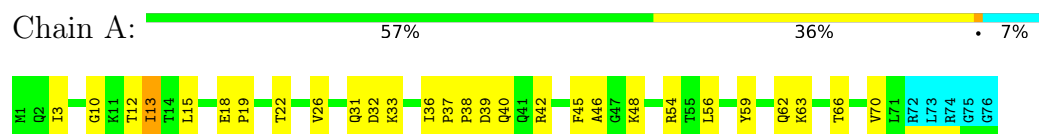
4.2.628 Score per residue for model 628

- Molecule 1: Ubiquitin



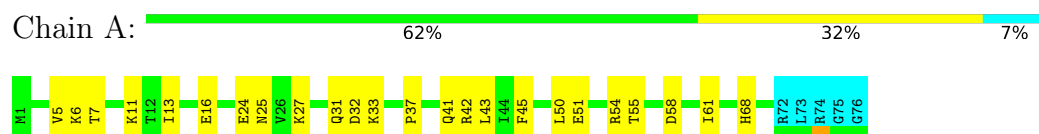
4.2.629 Score per residue for model 629

- Molecule 1: Ubiquitin



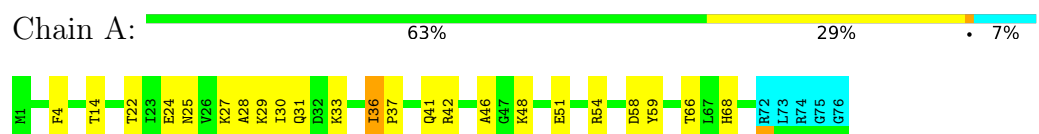
4.2.630 Score per residue for model 630

- Molecule 1: Ubiquitin



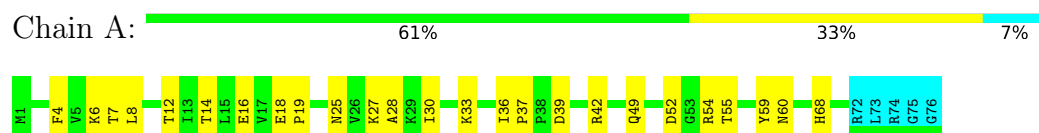
4.2.631 Score per residue for model 631

- Molecule 1: Ubiquitin



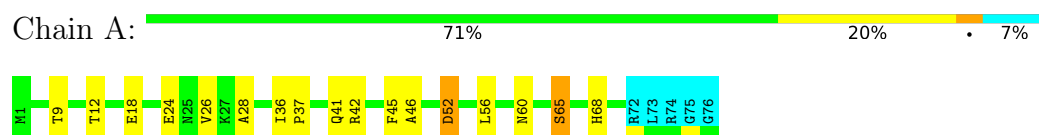
4.2.632 Score per residue for model 632

- Molecule 1: Ubiquitin



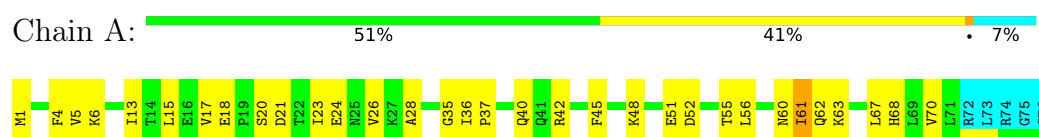
4.2.633 Score per residue for model 633

- Molecule 1: Ubiquitin



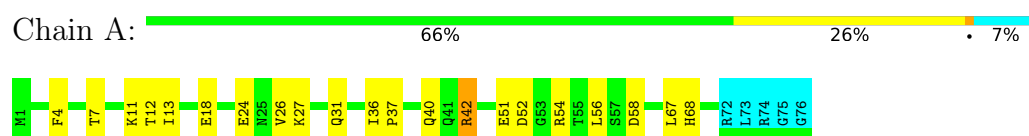
4.2.634 Score per residue for model 634

- Molecule 1: Ubiquitin



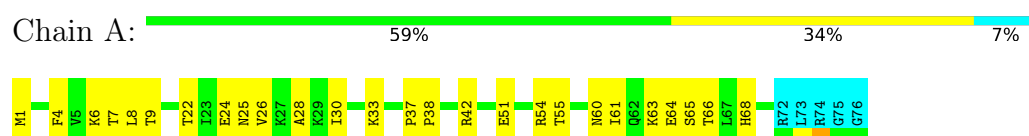
4.2.635 Score per residue for model 635

- Molecule 1: Ubiquitin



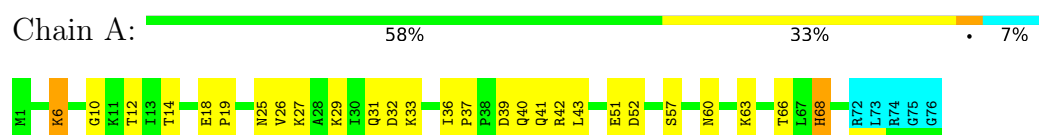
4.2.636 Score per residue for model 636

- Molecule 1: Ubiquitin



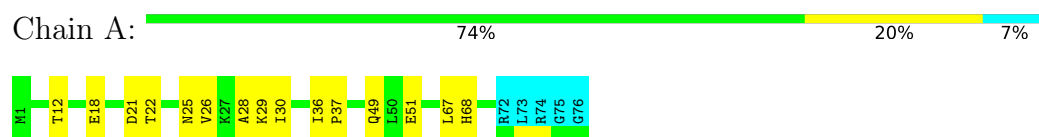
4.2.637 Score per residue for model 637

- Molecule 1: Ubiquitin



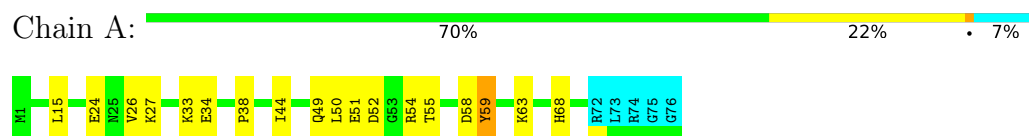
4.2.638 Score per residue for model 638

- Molecule 1: Ubiquitin



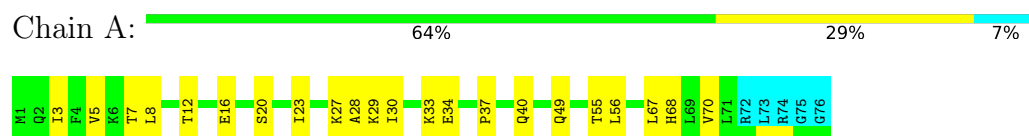
4.2.639 Score per residue for model 639

- Molecule 1: Ubiquitin



4.2.640 Score per residue for model 640

- Molecule 1: Ubiquitin



5 Refinement protocol and experimental data overview

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

Of the 640 calculated structures, 640 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CHARMM	structure solution	c34b1
CHARMM	refinement	c34b1

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.87±0.06	8±3/570 (1.5± 0.5%)	2.19±0.07	24±6/770 (3.1± 0.7%)
All	All	1.87	5390/364800 (1.5%)	2.19	15147/492800 (3.1%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.8±0.8
All	All	0	538

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	37	PRO	CA-C	15.44	1.60	1.51	275	141
1	A	17	VAL	N-CA	12.92	1.60	1.46	414	17
1	A	41	GLN	CA-CB	12.66	1.71	1.53	584	16
1	A	18	GLU	N-CA	-11.21	1.38	1.46	213	10
1	A	17	VAL	CA-C	-11.05	1.43	1.52	174	46
1	A	36	ILE	CA-C	-10.37	1.44	1.53	621	84
1	A	42	ARG	CD-NE	9.87	1.60	1.46	551	102
1	A	41	GLN	N-CA	-9.84	1.33	1.46	613	14
1	A	3	ILE	CA-C	-9.83	1.41	1.52	87	27
1	A	61	ILE	CA-C	9.74	1.64	1.52	42	37
1	A	60	ASN	C-N	9.71	1.44	1.33	261	22
1	A	36	ILE	N-CA	9.63	1.53	1.46	600	47
1	A	16	GLU	CA-C	-9.61	1.40	1.52	414	38
1	A	68	HIS	ND1-CE1	9.38	1.42	1.32	245	136
1	A	44	ILE	CA-C	9.38	1.64	1.52	281	30
1	A	20	SER	C-N	9.35	1.46	1.33	297	31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	35	GLY	C-N	9.26	1.42	1.33	455	56
1	A	12	THR	CA-C	-9.12	1.41	1.52	608	33
1	A	59	TYR	CA-C	-9.11	1.41	1.52	283	8
1	A	20	SER	N-CA	-9.01	1.34	1.46	204	14
1	A	15	LEU	CA-C	-8.98	1.41	1.52	75	32
1	A	50	LEU	N-CA	-8.95	1.34	1.46	520	10
1	A	54	ARG	CD-NE	8.85	1.58	1.46	130	91
1	A	23	ILE	C-N	8.85	1.45	1.33	383	14
1	A	31	GLN	CA-C	8.76	1.64	1.52	296	20
1	A	67	LEU	N-CA	-8.76	1.35	1.45	62	17
1	A	57	SER	CA-C	-8.75	1.41	1.52	466	15
1	A	36	ILE	CA-CB	-8.75	1.44	1.53	269	30
1	A	63	LYS	CA-C	-8.73	1.40	1.52	245	24
1	A	50	LEU	C-N	8.72	1.45	1.33	362	10
1	A	18	GLU	C-N	-8.67	1.23	1.34	418	18
1	A	16	GLU	CA-CB	8.66	1.65	1.53	197	29
1	A	15	LEU	N-CA	-8.63	1.35	1.46	262	13
1	A	49	GLN	CA-C	-8.61	1.42	1.52	498	23
1	A	56	LEU	CA-CB	8.58	1.67	1.53	186	12
1	A	71	LEU	CA-CB	8.55	1.65	1.53	404	15
1	A	26	VAL	CA-CB	-8.50	1.43	1.54	165	38
1	A	71	LEU	CA-C	-8.50	1.42	1.52	64	23
1	A	50	LEU	CA-CB	8.48	1.65	1.53	15	23
1	A	18	GLU	CA-CB	8.47	1.64	1.54	332	34
1	A	23	ILE	CA-CB	-8.44	1.44	1.54	316	42
1	A	68	HIS	CE1-NE2	8.43	1.41	1.32	559	20
1	A	4	PHE	CA-C	8.42	1.62	1.52	556	27
1	A	7	THR	CA-C	-8.39	1.42	1.52	107	18
1	A	59	TYR	CA-CB	8.35	1.67	1.53	27	13
1	A	66	THR	CA-C	-8.28	1.42	1.52	365	36
1	A	70	VAL	CA-C	-8.27	1.42	1.52	266	26
1	A	22	THR	N-CA	8.26	1.56	1.45	223	13
1	A	43	LEU	N-CA	-8.26	1.36	1.46	158	25
1	A	26	VAL	C-N	8.24	1.44	1.33	122	13
1	A	43	LEU	CA-C	-8.22	1.42	1.52	503	30
1	A	32	ASP	CA-C	8.21	1.63	1.52	95	30
1	A	42	ARG	CA-C	-8.20	1.42	1.52	335	31
1	A	25	ASN	N-CA	-8.17	1.36	1.46	344	15
1	A	58	ASP	CA-CB	8.17	1.66	1.53	300	16
1	A	58	ASP	CA-C	8.16	1.64	1.52	561	18
1	A	26	VAL	CA-C	8.14	1.63	1.52	560	24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	23	ILE	CA-C	8.13	1.63	1.52	203	30
1	A	6	LYS	CA-CB	8.09	1.63	1.52	305	13
1	A	5	VAL	N-CA	-8.09	1.36	1.46	510	13
1	A	5	VAL	CA-CB	-8.07	1.43	1.54	311	27
1	A	57	SER	CA-CB	8.04	1.65	1.53	590	18
1	A	4	PHE	N-CA	-8.03	1.36	1.46	308	25
1	A	6	LYS	CA-C	-8.02	1.43	1.52	388	28
1	A	49	GLN	N-CA	-8.01	1.35	1.46	432	16
1	A	48	LYS	CA-C	-8.01	1.43	1.52	622	27
1	A	7	THR	N-CA	-7.99	1.36	1.45	635	12
1	A	59	TYR	C-N	7.97	1.45	1.33	5	11
1	A	51	GLU	CA-C	7.93	1.62	1.52	61	22
1	A	13	ILE	CA-CB	7.93	1.62	1.53	586	23
1	A	45	PHE	N-CA	7.92	1.56	1.46	327	22
1	A	69	LEU	CA-CB	7.90	1.66	1.53	73	33
1	A	70	VAL	C-N	7.90	1.44	1.33	123	7
1	A	14	THR	CA-C	-7.87	1.42	1.52	526	36
1	A	4	PHE	C-N	7.84	1.43	1.33	382	7
1	A	60	ASN	CA-C	-7.84	1.43	1.53	128	17
1	A	34	GLU	N-CA	7.84	1.54	1.46	483	3
1	A	11	LYS	CA-CB	7.83	1.62	1.52	543	15
1	A	16	GLU	N-CA	-7.82	1.37	1.46	376	13
1	A	14	THR	C-N	7.81	1.44	1.33	462	13
1	A	53	GLY	CA-C	-7.81	1.41	1.51	616	12
1	A	37	PRO	C-N	7.80	1.40	1.33	258	15
1	A	13	ILE	N-CA	7.80	1.54	1.46	381	12
1	A	49	GLN	CA-CB	7.77	1.63	1.53	10	26
1	A	19	PRO	C-N	7.77	1.44	1.33	386	9
1	A	62	GLN	CA-CB	7.76	1.65	1.53	416	15
1	A	68	HIS	CD2-NE2	7.75	1.46	1.37	188	23
1	A	56	LEU	CA-C	7.74	1.62	1.52	85	23
1	A	2	GLN	CA-C	-7.74	1.43	1.52	202	23
1	A	28	ALA	C-N	7.74	1.44	1.33	429	15
1	A	44	ILE	CA-CB	7.72	1.63	1.54	502	24
1	A	35	GLY	CA-C	-7.71	1.41	1.51	496	18
1	A	54	ARG	N-CA	-7.71	1.35	1.45	470	13
1	A	67	LEU	CA-C	-7.71	1.43	1.52	435	21
1	A	44	ILE	C-O	-7.68	1.16	1.24	17	15
1	A	62	GLN	CA-C	-7.65	1.43	1.52	477	25
1	A	54	ARG	CA-C	7.65	1.63	1.52	10	27
1	A	45	PHE	CA-C	-7.63	1.43	1.52	151	29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	68	HIS	N-CA	-7.62	1.36	1.46	487	15
1	A	41	GLN	CA-C	-7.62	1.43	1.52	441	21
1	A	23	ILE	N-CA	-7.61	1.37	1.46	37	13
1	A	50	LEU	CA-C	7.60	1.62	1.52	366	18
1	A	69	LEU	CA-C	-7.60	1.43	1.52	246	34
1	A	55	THR	C-N	7.60	1.43	1.33	605	17
1	A	9	THR	C-N	7.59	1.43	1.33	355	18
1	A	3	ILE	CA-CB	7.59	1.66	1.54	414	6
1	A	27	LYS	C-N	7.57	1.43	1.33	55	17
1	A	13	ILE	CA-C	-7.57	1.43	1.52	352	24
1	A	20	SER	CA-C	-7.55	1.42	1.52	481	16
1	A	34	GLU	CA-CB	7.55	1.64	1.54	186	16
1	A	52	ASP	N-CA	-7.54	1.37	1.46	241	15
1	A	12	THR	N-CA	-7.54	1.37	1.46	488	10
1	A	25	ASN	CA-C	-7.53	1.43	1.52	266	18
1	A	71	LEU	N-CA	-7.53	1.36	1.46	488	10
1	A	42	ARG	NE-CZ	7.52	1.41	1.33	470	23
1	A	18	GLU	C-O	-7.50	1.17	1.24	33	5
1	A	64	GLU	N-CA	-7.50	1.35	1.46	504	8
1	A	17	VAL	C-O	-7.49	1.16	1.24	83	4
1	A	34	GLU	CA-C	-7.49	1.42	1.52	514	14
1	A	56	LEU	C-N	7.48	1.44	1.34	134	17
1	A	28	ALA	N-CA	-7.47	1.37	1.46	264	20
1	A	60	ASN	CA-CB	7.46	1.65	1.53	396	26
1	A	65	SER	CA-C	-7.46	1.43	1.52	79	27
1	A	68	HIS	CA-C	-7.45	1.44	1.52	514	22
1	A	66	THR	CA-CB	-7.45	1.43	1.53	138	6
1	A	53	GLY	N-CA	7.45	1.55	1.45	237	9
1	A	29	LYS	C-N	-7.42	1.24	1.33	23	31
1	A	21	ASP	N-CA	-7.42	1.36	1.46	258	10
1	A	32	ASP	N-CA	-7.41	1.37	1.46	48	20
1	A	56	LEU	N-CA	-7.40	1.37	1.46	280	11
1	A	30	ILE	CA-C	7.39	1.62	1.52	146	19
1	A	28	ALA	CA-C	7.36	1.62	1.52	597	17
1	A	30	ILE	CA-CB	-7.35	1.45	1.54	262	26
1	A	33	LYS	N-CA	-7.34	1.37	1.46	448	17
1	A	63	LYS	C-N	7.34	1.43	1.33	301	7
1	A	36	ILE	C-N	7.34	1.42	1.33	138	25
1	A	52	ASP	CA-C	7.34	1.62	1.52	54	23
1	A	18	GLU	CA-C	-7.33	1.43	1.52	545	26
1	A	21	ASP	C-N	7.32	1.43	1.33	587	22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	66	THR	C-N	7.31	1.43	1.33	125	8
1	A	5	VAL	CA-C	-7.30	1.43	1.52	60	24
1	A	11	LYS	CA-C	-7.30	1.43	1.52	118	18
1	A	66	THR	N-CA	-7.29	1.37	1.46	419	19
1	A	64	GLU	CA-C	-7.28	1.42	1.53	518	15
1	A	30	ILE	N-CA	-7.28	1.37	1.46	16	14
1	A	43	LEU	CA-CB	7.28	1.64	1.53	14	18
1	A	40	GLN	N-CA	7.27	1.55	1.46	89	8
1	A	29	LYS	CA-CB	7.27	1.64	1.53	103	9
1	A	25	ASN	CA-CB	7.26	1.65	1.53	382	20
1	A	45	PHE	CA-CB	7.25	1.66	1.53	187	11
1	A	40	GLN	CA-C	-7.23	1.43	1.52	560	17
1	A	16	GLU	C-N	7.22	1.43	1.33	137	13
1	A	21	ASP	CA-C	7.22	1.62	1.52	492	28
1	A	37	PRO	CA-CB	7.22	1.60	1.53	433	15
1	A	69	LEU	N-CA	-7.22	1.37	1.46	488	26
1	A	10	GLY	C-N	7.21	1.43	1.33	621	16
1	A	27	LYS	CA-C	7.21	1.62	1.52	612	21
1	A	68	HIS	CG-CD2	7.21	1.43	1.35	251	9
1	A	30	ILE	C-N	7.21	1.43	1.33	206	19
1	A	64	GLU	CA-CB	7.20	1.65	1.53	70	20
1	A	55	THR	N-CA	7.20	1.54	1.45	390	20
1	A	17	VAL	CA-CB	-7.20	1.44	1.54	583	9
1	A	59	TYR	N-CA	-7.19	1.36	1.46	327	9
1	A	3	ILE	N-CA	7.19	1.54	1.46	587	18
1	A	25	ASN	C-N	7.18	1.43	1.33	200	11
1	A	33	LYS	CA-C	7.18	1.62	1.52	34	24
1	A	44	ILE	N-CA	7.17	1.54	1.46	532	15
1	A	8	LEU	CA-C	7.17	1.62	1.52	505	13
1	A	22	THR	CA-C	-7.16	1.43	1.52	174	21
1	A	24	GLU	CA-CB	7.15	1.64	1.53	348	10
1	A	17	VAL	C-N	7.14	1.42	1.33	539	6
1	A	45	PHE	C-N	7.13	1.42	1.33	616	11
1	A	24	GLU	CA-C	7.13	1.61	1.52	58	33
1	A	43	LEU	C-N	7.13	1.43	1.33	238	13
1	A	47	GLY	CA-C	-7.12	1.41	1.51	207	16
1	A	39	ASP	N-CA	-7.11	1.37	1.46	637	10
1	A	33	LYS	CA-CB	7.11	1.64	1.53	573	14
1	A	39	ASP	CA-C	7.11	1.61	1.52	339	12
1	A	51	GLU	CA-CB	7.10	1.62	1.53	42	22
1	A	27	LYS	CA-CB	7.09	1.65	1.53	18	14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	68	HIS	CA-CB	7.09	1.62	1.53	638	12
1	A	19	PRO	C-O	-7.08	1.16	1.24	356	3
1	A	65	SER	N-CA	7.08	1.54	1.45	467	11
1	A	55	THR	CA-C	-7.07	1.44	1.52	131	23
1	A	8	LEU	N-CA	7.07	1.55	1.46	471	9
1	A	68	HIS	CB-CG	-7.06	1.40	1.50	234	16
1	A	40	GLN	C-N	7.05	1.43	1.33	210	15
1	A	53	GLY	C-N	7.04	1.43	1.33	336	13
1	A	48	LYS	C-N	7.03	1.42	1.33	281	15
1	A	67	LEU	C-N	7.03	1.43	1.33	244	9
1	A	11	LYS	C-N	7.02	1.42	1.33	29	9
1	A	52	ASP	CA-CB	7.02	1.64	1.53	61	12
1	A	46	ALA	CA-C	7.02	1.62	1.53	221	13
1	A	31	GLN	CA-CB	7.00	1.64	1.53	302	23
1	A	9	THR	CA-C	-6.99	1.43	1.52	385	13
1	A	53	GLY	C-O	6.99	1.30	1.24	576	4
1	A	19	PRO	N-CA	-6.95	1.38	1.47	380	6
1	A	8	LEU	CA-CB	6.94	1.65	1.53	118	18
1	A	64	GLU	C-N	6.93	1.43	1.33	5	17
1	A	1	MET	N-CA	6.93	1.59	1.46	307	9
1	A	61	ILE	N-CA	-6.93	1.38	1.46	61	14
1	A	38	PRO	CA-CB	6.91	1.63	1.53	356	8
1	A	13	ILE	C-N	6.91	1.42	1.33	121	8
1	A	3	ILE	C-N	6.90	1.42	1.33	80	8
1	A	2	GLN	N-CA	-6.89	1.37	1.45	535	17
1	A	62	GLN	C-N	6.89	1.42	1.33	155	14
1	A	42	ARG	N-CA	-6.88	1.38	1.46	114	26
1	A	44	ILE	C-N	6.87	1.42	1.33	389	14
1	A	48	LYS	N-CA	6.86	1.54	1.45	261	11
1	A	47	GLY	C-N	6.86	1.42	1.33	49	12
1	A	55	THR	CA-CB	6.85	1.64	1.53	21	3
1	A	21	ASP	CA-CB	6.84	1.64	1.53	220	12
1	A	61	ILE	CA-CB	-6.83	1.45	1.54	355	21
1	A	34	GLU	C-N	6.83	1.42	1.33	57	10
1	A	51	GLU	N-CA	6.79	1.54	1.46	625	14
1	A	24	GLU	C-N	6.78	1.42	1.33	503	16
1	A	2	GLN	C-N	6.75	1.42	1.33	565	12
1	A	26	VAL	N-CA	6.73	1.54	1.46	317	12
1	A	7	THR	CA-CB	6.73	1.63	1.53	156	10
1	A	70	VAL	N-CA	-6.71	1.38	1.46	58	22
1	A	12	THR	C-O	6.71	1.32	1.24	559	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	46	ALA	CA-CB	6.71	1.63	1.53	523	10
1	A	42	ARG	C-N	6.70	1.42	1.33	379	11
1	A	46	ALA	C-N	6.69	1.42	1.33	521	12
1	A	70	VAL	CA-CB	-6.67	1.45	1.53	152	26
1	A	65	SER	CA-CB	6.66	1.64	1.53	581	14
1	A	68	HIS	CG-ND1	-6.63	1.30	1.38	115	14
1	A	54	ARG	C-N	6.63	1.42	1.33	565	11
1	A	48	LYS	CA-CB	6.63	1.61	1.53	431	9
1	A	27	LYS	N-CA	6.62	1.54	1.46	432	12
1	A	14	THR	CA-CB	6.62	1.63	1.53	254	9
1	A	20	SER	CA-CB	6.62	1.64	1.53	90	10
1	A	32	ASP	CA-CB	6.61	1.63	1.53	449	19
1	A	61	ILE	C-N	6.61	1.42	1.33	309	14
1	A	31	GLN	N-CA	6.58	1.54	1.46	252	13
1	A	31	GLN	C-N	6.56	1.42	1.34	267	10
1	A	14	THR	N-CA	-6.55	1.38	1.46	619	12
1	A	25	ASN	C-O	-6.55	1.16	1.24	435	4
1	A	54	ARG	CA-CB	6.54	1.64	1.53	85	14
1	A	35	GLY	N-CA	6.54	1.55	1.45	428	11
1	A	68	HIS	C-N	6.54	1.42	1.33	457	15
1	A	69	LEU	C-N	-6.53	1.25	1.33	346	7
1	A	54	ARG	NE-CZ	6.51	1.40	1.33	316	11
1	A	29	LYS	CA-C	6.51	1.61	1.52	271	32
1	A	40	GLN	CA-CB	6.48	1.63	1.53	45	12
1	A	22	THR	C-N	6.47	1.42	1.33	507	15
1	A	23	ILE	C-O	-6.47	1.16	1.24	556	5
1	A	39	ASP	CA-CB	6.47	1.64	1.53	194	9
1	A	8	LEU	C-N	6.46	1.42	1.33	446	9
1	A	57	SER	N-CA	6.46	1.54	1.46	455	14
1	A	16	GLU	CG-CD	6.46	1.68	1.52	414	2
1	A	2	GLN	CA-CB	6.45	1.61	1.53	218	10
1	A	70	VAL	C-O	-6.44	1.17	1.24	304	6
1	A	5	VAL	C-N	6.42	1.42	1.33	508	12
1	A	15	LEU	C-N	6.41	1.42	1.33	229	12
1	A	63	LYS	CA-CB	6.41	1.64	1.53	625	9
1	A	42	ARG	C-O	-6.41	1.16	1.23	145	1
1	A	67	LEU	CA-CB	6.39	1.63	1.53	638	19
1	A	47	GLY	N-CA	6.39	1.54	1.45	46	3
1	A	63	LYS	N-CA	6.38	1.54	1.46	301	15
1	A	45	PHE	C-O	-6.38	1.16	1.24	538	3
1	A	71	LEU	C-N	6.37	1.42	1.33	133	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	32	ASP	C-O	-6.35	1.16	1.24	31	6
1	A	32	ASP	C-N	6.35	1.41	1.33	584	14
1	A	61	ILE	C-O	-6.33	1.17	1.24	458	3
1	A	24	GLU	N-CA	-6.32	1.38	1.46	152	18
1	A	9	THR	N-CA	6.31	1.53	1.46	162	9
1	A	68	HIS	C-O	-6.31	1.17	1.24	622	5
1	A	1	MET	C-N	6.28	1.42	1.33	375	9
1	A	39	ASP	C-N	6.28	1.42	1.33	423	8
1	A	49	GLN	C-N	6.28	1.41	1.33	77	9
1	A	65	SER	C-N	6.28	1.41	1.33	539	7
1	A	4	PHE	CA-CB	6.27	1.63	1.53	335	5
1	A	4	PHE	C-O	-6.25	1.16	1.23	383	3
1	A	37	PRO	N-CD	-6.25	1.39	1.47	418	4
1	A	10	GLY	CA-C	6.23	1.60	1.51	299	12
1	A	29	LYS	N-CA	6.21	1.54	1.46	15	14
1	A	58	ASP	N-CA	6.20	1.54	1.46	82	11
1	A	7	THR	C-N	6.20	1.42	1.34	184	14
1	A	15	LEU	CB-CG	6.18	1.65	1.53	69	2
1	A	52	ASP	C-N	6.17	1.42	1.33	231	6
1	A	58	ASP	C-N	6.14	1.42	1.33	369	6
1	A	19	PRO	CA-CB	6.13	1.62	1.53	543	10
1	A	19	PRO	N-CD	-6.12	1.39	1.47	555	8
1	A	6	LYS	N-CA	-6.12	1.38	1.46	155	16
1	A	15	LEU	CA-CB	6.12	1.63	1.53	144	7
1	A	27	LYS	C-O	-6.11	1.16	1.24	348	2
1	A	29	LYS	C-O	-6.10	1.17	1.24	565	3
1	A	5	VAL	C-O	-6.10	1.17	1.24	586	7
1	A	6	LYS	C-N	6.09	1.41	1.33	181	9
1	A	38	PRO	N-CA	-6.09	1.39	1.47	148	9
1	A	9	THR	CA-CB	6.09	1.61	1.53	234	9
1	A	69	LEU	C-O	-6.08	1.16	1.23	468	4
1	A	12	THR	CA-CB	6.07	1.61	1.53	211	7
1	A	22	THR	CA-CB	6.07	1.63	1.53	415	3
1	A	51	GLU	C-N	6.06	1.41	1.33	418	16
1	A	56	LEU	C-O	-6.03	1.17	1.24	365	5
1	A	12	THR	C-N	6.03	1.41	1.33	559	11
1	A	11	LYS	N-CA	-6.02	1.38	1.45	531	3
1	A	66	THR	CB-OG1	-6.01	1.34	1.43	561	3
1	A	13	ILE	CB-CG1	5.99	1.65	1.53	85	1
1	A	50	LEU	CB-CG	5.99	1.65	1.53	279	5
1	A	15	LEU	C-O	-5.98	1.16	1.24	533	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	38	PRO	C-N	5.98	1.42	1.33	51	9
1	A	1	MET	CA-CB	5.98	1.65	1.53	548	3
1	A	33	LYS	C-N	5.96	1.41	1.33	381	3
1	A	20	SER	C-O	-5.93	1.16	1.24	207	1
1	A	19	PRO	CA-C	5.93	1.61	1.52	356	3
1	A	16	GLU	C-O	-5.92	1.17	1.24	436	8
1	A	36	ILE	C-O	-5.88	1.17	1.24	556	2
1	A	14	THR	C-O	5.87	1.30	1.23	87	2
1	A	48	LYS	C-O	-5.85	1.17	1.24	547	5
1	A	62	GLN	N-CA	-5.82	1.38	1.45	345	10
1	A	57	SER	C-N	5.80	1.41	1.33	493	10
1	A	24	GLU	C-O	-5.79	1.17	1.24	442	5
1	A	55	THR	C-O	-5.78	1.16	1.23	368	2
1	A	65	SER	C-O	5.76	1.30	1.23	9	2
1	A	28	ALA	CA-CB	5.75	1.62	1.53	240	5
1	A	10	GLY	N-CA	5.75	1.53	1.45	346	3
1	A	58	ASP	C-O	-5.75	1.17	1.24	425	2
1	A	3	ILE	CB-CG1	5.75	1.65	1.53	166	1
1	A	30	ILE	CB-CG1	5.69	1.64	1.53	217	2
1	A	41	GLN	C-N	5.69	1.41	1.33	436	7
1	A	40	GLN	C-O	-5.67	1.16	1.24	468	1
1	A	12	THR	CB-OG1	-5.66	1.34	1.43	292	1
1	A	61	ILE	CB-CG1	5.66	1.64	1.53	559	1
1	A	51	GLU	C-O	-5.64	1.17	1.23	91	2
1	A	42	ARG	CA-CB	5.62	1.63	1.53	344	5
1	A	31	GLN	C-O	-5.61	1.17	1.24	113	3
1	A	69	LEU	CB-CG	5.59	1.64	1.53	492	1
1	A	67	LEU	C-O	-5.58	1.17	1.24	58	1
1	A	33	LYS	C-O	-5.58	1.17	1.24	59	2
1	A	46	ALA	N-CA	-5.56	1.38	1.46	304	2
1	A	38	PRO	N-CD	5.56	1.55	1.47	45	7
1	A	21	ASP	C-O	5.55	1.30	1.23	247	2
1	A	42	ARG	CZ-NH2	-5.53	1.26	1.33	4	2
1	A	4	PHE	CG-CD1	5.52	1.50	1.38	389	1
1	A	13	ILE	C-O	-5.52	1.18	1.24	279	2
1	A	30	ILE	C-O	-5.49	1.17	1.24	526	1
1	A	43	LEU	C-O	5.46	1.30	1.24	226	4
1	A	26	VAL	C-O	-5.46	1.17	1.24	415	6
1	A	52	ASP	C-O	-5.44	1.17	1.24	11	1
1	A	44	ILE	CB-CG1	5.43	1.64	1.53	127	1
1	A	56	LEU	CB-CG	5.42	1.64	1.53	573	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	59	TYR	CZ-OH	5.41	1.49	1.38	213	2
1	A	22	THR	C-O	-5.40	1.16	1.23	615	1
1	A	45	PHE	CB-CG	5.38	1.63	1.50	371	1
1	A	60	ASN	C-O	5.37	1.30	1.23	244	2
1	A	63	LYS	C-O	5.35	1.30	1.23	580	2
1	A	38	PRO	C-O	5.35	1.30	1.24	119	3
1	A	49	GLN	C-O	-5.32	1.17	1.23	125	1
1	A	65	SER	CB-OG	5.32	1.52	1.42	439	1
1	A	60	ASN	N-CA	-5.30	1.38	1.46	226	2
1	A	14	THR	CB-OG1	-5.29	1.35	1.43	22	1
1	A	6	LYS	C-O	-5.29	1.17	1.24	22	3
1	A	41	GLN	C-O	5.28	1.30	1.23	497	1
1	A	57	SER	C-O	-5.28	1.17	1.24	254	1
1	A	23	ILE	CB-CG1	5.28	1.64	1.53	256	1
1	A	38	PRO	CA-C	5.27	1.59	1.52	475	4
1	A	43	LEU	CB-CG	5.25	1.64	1.53	64	1
1	A	37	PRO	C-O	-5.25	1.18	1.24	395	2
1	A	62	GLN	C-O	-5.25	1.17	1.23	453	1
1	A	71	LEU	C-O	-5.23	1.17	1.24	162	1
1	A	42	ARG	CZ-NH1	5.21	1.40	1.32	234	1
1	A	66	THR	C-O	-5.17	1.17	1.24	328	5
1	A	54	ARG	CZ-NH1	-5.16	1.25	1.32	278	1
1	A	36	ILE	CB-CG1	5.15	1.63	1.53	591	1
1	A	22	THR	CB-OG1	-5.14	1.35	1.43	4	2
1	A	3	ILE	C-O	5.13	1.29	1.24	508	1
1	A	28	ALA	C-O	5.09	1.30	1.24	390	1
1	A	46	ALA	C-O	-5.08	1.17	1.23	420	1
1	A	2	GLN	C-O	-5.05	1.17	1.23	142	1
1	A	67	LEU	CB-CG	5.05	1.63	1.53	495	1
1	A	8	LEU	CB-CG	-5.04	1.43	1.53	26	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	37	PRO	O-C-N	-17.58	113.22	121.31	288	39
1	A	18	GLU	O-C-N	-15.17	112.00	121.71	474	119
1	A	37	PRO	CA-C-O	-13.02	111.53	120.90	89	103
1	A	39	ASP	CA-CB-CG	12.76	125.36	112.60	335	113
1	A	36	ILE	CA-C-O	-12.16	111.97	119.15	251	112
1	A	52	ASP	N-CA-C	11.96	125.46	111.11	160	190

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	41	GLN	OE1-CD-NE2	-11.54	111.06	122.60	174	54
1	A	7	THR	CA-C-N	11.49	135.67	120.28	127	82
1	A	7	THR	C-N-CA	11.49	135.67	120.28	127	82
1	A	68	HIS	CA-CB-CG	-11.41	102.39	113.80	534	96
1	A	36	ILE	CA-C-N	11.34	132.06	120.38	185	132
1	A	36	ILE	C-N-CA	11.34	132.06	120.38	185	132
1	A	18	GLU	CA-C-N	11.20	130.98	119.56	484	140
1	A	18	GLU	C-N-CA	11.20	130.98	119.56	484	140
1	A	60	ASN	CA-CB-CG	-11.19	101.41	112.60	623	102
1	A	33	LYS	N-CA-C	11.16	123.01	111.07	383	137
1	A	52	ASP	CA-CB-CG	-11.15	101.45	112.60	61	82
1	A	37	PRO	N-CA-C	11.07	121.10	110.47	41	205
1	A	36	ILE	O-C-N	-11.05	113.70	121.55	570	84
1	A	51	GLU	CA-C-N	11.05	134.81	120.44	185	285
1	A	51	GLU	C-N-CA	11.05	134.81	120.44	185	285
1	A	37	PRO	CA-C-N	11.01	133.60	119.84	15	214
1	A	37	PRO	C-N-CA	11.01	133.60	119.84	15	214
1	A	36	ILE	N-CA-C	11.00	119.73	108.95	46	44
1	A	58	ASP	CA-CB-CG	-10.98	101.62	112.60	429	98
1	A	25	ASN	CA-CB-CG	-10.55	102.05	112.60	565	90
1	A	35	GLY	CA-C-N	10.55	130.18	122.59	347	34
1	A	35	GLY	C-N-CA	10.55	130.18	122.59	347	34
1	A	40	GLN	OE1-CD-NE2	-10.53	112.07	122.60	247	29
1	A	30	ILE	O-C-N	-10.37	111.81	121.87	317	55
1	A	32	ASP	CA-CB-CG	10.27	122.87	112.60	496	65
1	A	36	ILE	CB-CA-C	-10.22	99.77	110.71	200	54
1	A	4	PHE	CA-CB-CG	-10.10	103.70	113.80	359	120
1	A	61	ILE	N-CA-CB	10.09	121.85	112.06	5	26
1	A	30	ILE	N-CA-C	10.06	120.08	110.42	240	45
1	A	37	PRO	N-CA-CB	9.96	108.77	103.19	367	27
1	A	38	PRO	CA-C-N	9.96	133.62	120.28	592	49
1	A	38	PRO	C-N-CA	9.96	133.62	120.28	592	49
1	A	31	GLN	CA-C-N	9.94	133.59	120.28	252	64
1	A	31	GLN	C-N-CA	9.94	133.59	120.28	252	64
1	A	22	THR	N-CA-CB	9.93	124.47	110.17	352	121
1	A	14	THR	O-C-N	-9.93	111.56	123.27	248	40
1	A	23	ILE	O-C-N	-9.89	111.89	121.87	177	46
1	A	70	VAL	O-C-N	-9.79	112.80	122.98	9	63
1	A	39	ASP	N-CA-C	9.77	124.74	113.01	308	42
1	A	21	ASP	CA-CB-CG	-9.77	102.83	112.60	80	55
1	A	54	ARG	NE-CZ-NH2	-9.77	110.41	119.20	32	57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	26	VAL	N-CA-C	9.76	119.79	110.42	281	55
1	A	57	SER	N-CA-C	9.72	123.09	111.33	159	105
1	A	30	ILE	N-CA-CB	9.68	121.87	110.55	479	15
1	A	18	GLU	CA-C-O	-9.66	112.30	120.71	241	60
1	A	25	ASN	N-CA-C	9.59	121.73	111.28	52	34
1	A	2	GLN	OE1-CD-NE2	-9.54	113.06	122.60	259	42
1	A	42	ARG	NE-CZ-NH2	9.49	127.74	119.20	125	40
1	A	27	LYS	O-C-N	-9.49	112.06	122.12	222	33
1	A	8	LEU	N-CA-C	9.49	121.62	111.28	374	48
1	A	27	LYS	N-CA-C	9.48	121.62	111.28	454	70
1	A	13	ILE	O-C-N	-9.46	112.97	123.18	517	35
1	A	5	VAL	O-C-N	-9.46	113.05	123.26	442	50
1	A	7	THR	N-CA-C	9.35	122.59	110.53	464	27
1	A	29	LYS	N-CA-C	9.32	121.04	111.07	345	40
1	A	21	ASP	N-CA-C	9.32	123.93	110.24	294	17
1	A	34	GLU	O-C-N	-9.31	111.47	122.27	503	38
1	A	40	GLN	N-CA-C	-9.22	101.34	112.59	131	35
1	A	26	VAL	O-C-N	-9.21	112.94	121.87	442	52
1	A	56	LEU	CA-C-N	9.16	132.93	120.38	401	118
1	A	56	LEU	C-N-CA	9.16	132.93	120.38	401	118
1	A	32	ASP	CA-C-N	9.14	132.87	120.44	561	30
1	A	32	ASP	C-N-CA	9.14	132.87	120.44	561	30
1	A	39	ASP	CA-C-O	9.14	130.04	119.35	351	25
1	A	24	GLU	N-CA-C	9.14	120.85	111.07	492	61
1	A	32	ASP	CA-C-O	9.12	130.22	120.55	485	25
1	A	49	GLN	OE1-CD-NE2	-9.12	113.48	122.60	251	41
1	A	63	LYS	CA-C-O	9.03	129.98	120.95	402	20
1	A	50	LEU	O-C-N	-8.97	112.89	123.03	255	31
1	A	52	ASP	O-C-N	-8.96	112.62	122.12	35	30
1	A	44	ILE	O-C-N	-8.95	113.71	123.20	536	52
1	A	49	GLN	O-C-N	-8.94	112.31	122.86	135	32
1	A	36	ILE	N-CA-CB	8.94	118.39	110.08	49	20
1	A	71	LEU	CA-C-N	8.92	133.80	121.05	508	46
1	A	71	LEU	C-N-CA	8.92	133.80	121.05	508	46
1	A	45	PHE	O-C-N	-8.91	112.99	123.41	205	20
1	A	13	ILE	N-CA-CB	8.90	120.42	110.72	160	32
1	A	40	GLN	CA-C-N	-8.88	110.05	122.93	129	21
1	A	40	GLN	C-N-CA	-8.88	110.05	122.93	129	21
1	A	55	THR	CA-C-N	8.87	132.52	120.54	102	98
1	A	55	THR	C-N-CA	8.87	132.52	120.54	102	98
1	A	61	ILE	O-C-N	-8.87	113.01	122.68	62	22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	42	ARG	NE-CZ-NH1	8.85	130.34	121.50	239	39
1	A	65	SER	N-CA-C	8.84	122.38	110.35	30	38
1	A	52	ASP	CA-C-O	-8.81	111.08	120.42	614	19
1	A	6	LYS	O-C-N	-8.79	112.98	123.10	165	43
1	A	28	ALA	CA-C-N	8.79	131.87	120.44	118	81
1	A	28	ALA	C-N-CA	8.79	131.87	120.44	118	81
1	A	68	HIS	CE1-NE2-CD2	-8.77	100.23	109.00	515	189
1	A	24	GLU	CA-C-O	8.70	129.77	120.55	317	29
1	A	7	THR	O-C-N	-8.70	112.75	122.84	440	38
1	A	29	LYS	CA-C-O	8.65	129.91	119.97	554	28
1	A	71	LEU	CA-C-O	8.64	129.53	120.54	551	12
1	A	9	THR	N-CA-C	-8.62	101.75	112.88	12	30
1	A	33	LYS	O-C-N	-8.62	112.78	122.09	480	24
1	A	63	LYS	N-CA-C	8.61	122.99	110.42	542	85
1	A	7	THR	CA-C-O	-8.61	112.97	122.01	436	7
1	A	15	LEU	O-C-N	-8.60	113.25	123.31	169	16
1	A	17	VAL	O-C-N	-8.57	113.67	122.75	163	52
1	A	27	LYS	CA-C-N	8.56	132.44	120.29	375	64
1	A	27	LYS	C-N-CA	8.56	132.44	120.29	375	64
1	A	8	LEU	CA-C-N	8.55	131.74	120.28	411	10
1	A	8	LEU	C-N-CA	8.55	131.74	120.28	411	10
1	A	19	PRO	O-C-N	-8.54	112.95	122.18	296	6
1	A	46	ALA	N-CA-C	8.54	123.17	112.24	208	71
1	A	10	GLY	O-C-N	-8.53	112.44	122.50	401	21
1	A	60	ASN	CA-C-N	8.52	132.01	122.22	5	28
1	A	60	ASN	C-N-CA	8.52	132.01	122.22	5	28
1	A	39	ASP	O-C-N	-8.50	112.46	122.15	299	18
1	A	71	LEU	N-CA-C	8.49	122.76	110.10	183	27
1	A	67	LEU	O-C-N	-8.49	113.68	123.27	297	60
1	A	23	ILE	CA-C-N	8.47	131.63	120.28	415	98
1	A	23	ILE	C-N-CA	8.47	131.63	120.28	415	98
1	A	25	ASN	OD1-CG-ND2	-8.47	114.13	122.60	107	39
1	A	66	THR	O-C-N	-8.47	113.70	123.27	190	33
1	A	70	VAL	CA-C-O	8.45	128.59	120.31	54	19
1	A	55	THR	O-C-N	-8.43	113.51	123.03	569	48
1	A	56	LEU	CA-C-O	8.39	129.45	120.55	386	15
1	A	57	SER	O-C-N	-8.39	113.23	122.12	279	24
1	A	45	PHE	CA-CB-CG	8.37	122.17	113.80	509	63
1	A	48	LYS	CA-C-N	8.37	133.38	120.75	388	30
1	A	48	LYS	C-N-CA	8.37	133.38	120.75	388	30
1	A	45	PHE	CA-C-N	8.37	134.53	122.40	63	56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	45	PHE	C-N-CA	8.37	134.53	122.40	63	56
1	A	31	GLN	N-CA-C	8.36	120.47	111.36	124	35
1	A	47	GLY	CA-C-O	8.32	128.26	119.02	16	26
1	A	25	ASN	CA-C-N	8.31	131.19	120.56	404	43
1	A	25	ASN	C-N-CA	8.31	131.19	120.56	404	43
1	A	28	ALA	N-CA-C	8.31	120.33	111.28	179	62
1	A	24	GLU	CA-C-N	8.30	131.23	120.44	393	78
1	A	24	GLU	C-N-CA	8.30	131.23	120.44	393	78
1	A	22	THR	N-CA-C	8.29	121.48	110.53	54	21
1	A	12	THR	CB-CA-C	-8.29	98.11	110.62	242	7
1	A	14	THR	N-CA-CB	8.28	123.55	110.55	190	20
1	A	15	LEU	CA-C-O	8.26	129.28	120.36	168	10
1	A	6	LYS	N-CA-C	8.23	122.55	107.99	81	20
1	A	59	TYR	CA-C-N	8.21	134.75	122.68	176	66
1	A	59	TYR	C-N-CA	8.21	134.75	122.68	176	66
1	A	37	PRO	CB-CA-C	-8.20	103.68	111.39	273	16
1	A	4	PHE	O-C-N	-8.21	113.61	123.29	444	37
1	A	57	SER	CA-C-N	8.20	131.26	120.28	252	59
1	A	57	SER	C-N-CA	8.20	131.26	120.28	252	59
1	A	56	LEU	N-CA-C	8.20	120.21	111.28	356	31
1	A	61	ILE	CB-CA-C	8.19	123.71	111.26	221	24
1	A	23	ILE	N-CA-C	-8.19	102.27	110.62	303	30
1	A	69	LEU	O-C-N	-8.18	114.03	123.27	158	14
1	A	44	ILE	N-CA-CB	8.16	122.67	111.41	461	16
1	A	34	GLU	CA-C-O	8.15	128.24	119.03	270	20
1	A	50	LEU	N-CA-C	8.13	121.54	109.59	449	18
1	A	21	ASP	CA-C-O	8.12	130.16	121.55	519	26
1	A	26	VAL	CA-C-O	8.11	129.45	120.85	174	31
1	A	35	GLY	O-C-N	-8.10	114.47	122.41	341	16
1	A	35	GLY	CA-C-O	8.09	127.62	119.04	587	22
1	A	66	THR	CA-C-O	8.09	128.81	120.24	327	35
1	A	13	ILE	CA-C-O	8.09	129.18	120.53	256	20
1	A	15	LEU	CA-C-N	8.08	133.52	122.77	415	13
1	A	15	LEU	C-N-CA	8.08	133.52	122.77	415	13
1	A	10	GLY	CA-C-O	8.07	128.06	118.86	316	14
1	A	54	ARG	NE-CZ-NH1	8.07	129.57	121.50	428	43
1	A	44	ILE	CB-CA-C	8.05	122.55	110.63	445	8
1	A	55	THR	N-CA-C	8.04	122.42	110.52	137	30
1	A	59	TYR	N-CA-C	-8.04	103.49	113.38	549	25
1	A	51	GLU	O-C-N	-8.04	113.51	122.84	551	14
1	A	41	GLN	O-C-N	-8.04	113.88	122.96	314	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	32	ASP	N-CA-C	8.02	120.94	111.71	510	40
1	A	68	HIS	ND1-CE1-NE2	8.02	116.42	108.40	415	103
1	A	30	ILE	CA-C-O	-8.00	111.83	120.47	562	19
1	A	26	VAL	CA-C-N	8.00	131.00	120.28	588	43
1	A	26	VAL	C-N-CA	8.00	131.00	120.28	588	43
1	A	8	LEU	O-C-N	-8.00	113.65	122.12	508	21
1	A	50	LEU	CA-C-O	7.99	128.91	120.36	595	23
1	A	51	GLU	CA-C-O	7.96	129.64	120.80	630	27
1	A	71	LEU	CB-CA-C	7.96	122.63	109.89	473	13
1	A	63	LYS	CA-C-N	7.96	133.66	122.36	590	43
1	A	63	LYS	C-N-CA	7.96	133.66	122.36	590	43
1	A	17	VAL	CB-CA-C	-7.95	100.75	111.80	434	14
1	A	54	ARG	O-C-N	-7.94	114.06	123.27	380	33
1	A	48	LYS	N-CA-C	7.94	122.03	110.28	343	14
1	A	21	ASP	O-C-N	-7.94	113.64	123.01	378	33
1	A	24	GLU	O-C-N	-7.92	113.72	122.12	509	38
1	A	55	THR	N-CA-CB	7.92	123.14	110.46	139	81
1	A	66	THR	CA-C-N	7.91	133.30	122.77	73	22
1	A	66	THR	C-N-CA	7.91	133.30	122.77	73	22
1	A	42	ARG	CB-CA-C	7.91	122.80	110.14	128	3
1	A	62	GLN	OE1-CD-NE2	-7.91	114.69	122.60	23	40
1	A	7	THR	CA-CB-OG1	7.90	121.46	109.60	609	32
1	A	16	GLU	O-C-N	-7.88	114.07	123.13	502	21
1	A	53	GLY	CA-C-N	7.87	134.95	122.59	412	6
1	A	53	GLY	C-N-CA	7.87	134.95	122.59	412	6
1	A	26	VAL	N-CA-CB	7.87	119.76	110.55	78	30
1	A	35	GLY	N-CA-C	7.86	125.81	115.36	593	9
1	A	49	GLN	CB-CA-C	7.85	121.47	110.16	82	9
1	A	14	THR	CA-C-O	7.85	128.84	120.36	439	15
1	A	22	THR	CA-C-N	7.85	131.21	120.46	62	51
1	A	22	THR	C-N-CA	7.85	131.21	120.46	62	51
1	A	69	LEU	CA-C-O	7.83	128.68	120.30	41	29
1	A	64	GLU	O-C-N	-7.83	113.18	122.58	450	9
1	A	65	SER	CA-C-N	7.83	132.87	122.30	117	14
1	A	65	SER	C-N-CA	7.83	132.87	122.30	117	14
1	A	57	SER	N-CA-CB	7.83	122.28	110.22	227	17
1	A	13	ILE	N-CA-C	7.82	120.35	108.71	292	14
1	A	4	PHE	CA-C-O	7.81	128.90	120.38	583	21
1	A	41	GLN	CB-CA-C	-7.80	96.32	109.65	631	20
1	A	29	LYS	CA-C-N	7.80	130.54	120.56	560	53
1	A	29	LYS	C-N-CA	7.80	130.54	120.56	560	53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	70	VAL	CA-C-N	7.79	131.78	120.71	121	8
1	A	70	VAL	C-N-CA	7.79	131.78	120.71	121	8
1	A	49	GLN	CA-C-O	-7.75	112.56	121.47	94	23
1	A	68	HIS	CA-C-N	7.75	133.07	122.77	148	16
1	A	68	HIS	C-N-CA	7.75	133.07	122.77	148	16
1	A	64	GLU	N-CA-C	7.74	122.19	111.74	567	22
1	A	68	HIS	CG-CD2-NE2	7.73	114.93	107.20	475	83
1	A	68	HIS	O-C-N	-7.72	113.75	122.86	125	23
1	A	3	ILE	N-CA-C	-7.72	97.45	108.65	287	5
1	A	31	GLN	N-CA-CB	7.72	121.47	110.12	631	10
1	A	42	ARG	O-C-N	-7.71	114.02	123.04	560	37
1	A	50	LEU	CA-C-N	7.69	132.87	121.72	42	22
1	A	50	LEU	C-N-CA	7.69	132.87	121.72	42	22
1	A	60	ASN	O-C-N	-7.68	113.37	122.58	353	10
1	A	55	THR	CA-C-O	7.68	131.03	121.66	162	11
1	A	25	ASN	O-C-N	-7.67	112.06	122.33	20	23
1	A	69	LEU	CA-C-N	7.64	132.56	122.93	509	20
1	A	69	LEU	C-N-CA	7.64	132.56	122.93	509	20
1	A	68	HIS	CB-CG-CD2	-7.64	121.26	131.20	28	18
1	A	31	GLN	OE1-CD-NE2	-7.63	114.97	122.60	521	47
1	A	63	LYS	O-C-N	-7.61	113.68	122.97	555	13
1	A	19	PRO	N-CA-C	-7.61	104.68	114.03	524	16
1	A	58	ASP	CA-C-O	7.61	128.72	119.97	527	24
1	A	22	THR	O-C-N	-7.59	114.19	122.85	53	45
1	A	40	GLN	N-CA-CB	-7.59	99.48	110.65	296	13
1	A	54	ARG	NH1-CZ-NH2	-7.59	109.43	119.30	424	9
1	A	57	SER	CA-C-O	7.59	128.59	120.55	110	20
1	A	28	ALA	CA-C-O	7.58	128.59	120.55	525	19
1	A	38	PRO	N-CA-C	7.58	124.80	113.81	555	32
1	A	25	ASN	CA-C-O	7.56	128.44	120.42	266	21
1	A	43	LEU	CA-C-O	7.56	129.08	120.54	378	28
1	A	26	VAL	CB-CA-C	-7.55	101.95	112.14	170	20
1	A	41	GLN	N-CA-C	7.55	121.44	110.42	278	40
1	A	55	THR	CA-CB-OG1	7.55	120.92	109.60	163	37
1	A	2	GLN	CA-C-O	-7.54	113.34	121.56	259	16
1	A	13	ILE	CB-CA-C	-7.53	102.73	111.09	526	22
1	A	5	VAL	N-CA-C	7.53	118.74	107.75	102	13
1	A	18	GLU	N-CA-CB	7.53	119.14	110.03	420	10
1	A	5	VAL	CA-C-O	7.51	127.86	120.27	168	26
1	A	3	ILE	O-C-N	-7.51	114.61	122.95	620	19
1	A	60	ASN	OD1-CG-ND2	-7.50	115.10	122.60	332	54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	40	GLN	CG-CD-OE1	7.50	135.80	120.80	369	2
1	A	11	LYS	O-C-N	-7.48	114.03	122.86	236	33
1	A	58	ASP	CA-C-N	7.47	134.14	122.26	581	4
1	A	58	ASP	C-N-CA	7.47	134.14	122.26	581	4
1	A	43	LEU	CA-C-N	7.47	133.32	122.94	549	20
1	A	43	LEU	C-N-CA	7.47	133.32	122.94	549	20
1	A	54	ARG	CD-NE-CZ	7.47	134.85	124.40	321	4
1	A	59	TYR	CB-CA-C	-7.46	97.96	110.56	626	9
1	A	9	THR	CA-C-N	7.44	131.83	121.26	192	15
1	A	9	THR	C-N-CA	7.44	131.83	121.26	192	15
1	A	66	THR	CA-CB-OG1	7.44	120.76	109.60	481	6
1	A	41	GLN	CA-C-O	7.43	128.39	120.36	326	17
1	A	20	SER	CB-CA-C	-7.42	101.93	111.50	590	11
1	A	49	GLN	N-CA-CB	7.42	120.88	109.97	243	14
1	A	44	ILE	CA-C-O	7.41	128.17	120.39	300	28
1	A	30	ILE	CA-C-N	7.41	130.07	120.44	243	52
1	A	30	ILE	C-N-CA	7.41	130.07	120.44	243	52
1	A	59	TYR	O-C-N	-7.40	113.09	122.34	5	14
1	A	12	THR	CA-C-N	7.40	132.25	122.93	186	16
1	A	12	THR	C-N-CA	7.40	132.25	122.93	186	16
1	A	52	ASP	N-CA-CB	-7.39	98.93	109.94	226	6
1	A	45	PHE	CB-CA-C	7.39	122.36	109.80	219	9
1	A	58	ASP	O-C-N	-7.38	114.30	122.12	21	20
1	A	18	GLU	CB-CA-C	7.37	120.06	109.08	61	12
1	A	50	LEU	N-CA-CB	7.37	122.12	110.55	350	8
1	A	39	ASP	CA-C-N	7.36	130.01	120.44	479	15
1	A	39	ASP	C-N-CA	7.36	130.01	120.44	479	15
1	A	20	SER	N-CA-C	-7.36	105.17	112.97	551	20
1	A	51	GLU	N-CA-C	7.35	121.67	109.46	501	26
1	A	65	SER	CB-CA-C	-7.35	98.43	109.90	300	19
1	A	15	LEU	N-CA-CB	7.33	121.62	110.70	520	4
1	A	60	ASN	N-CA-CB	7.33	122.88	110.49	384	12
1	A	46	ALA	CB-CA-C	-7.33	101.49	111.89	249	6
1	A	43	LEU	O-C-N	-7.32	114.87	123.22	378	20
1	A	10	GLY	N-CA-C	-7.32	105.22	115.32	209	13
1	A	1	MET	CG-SD-CE	-7.32	84.80	100.90	28	56
1	A	32	ASP	O-C-N	-7.32	114.36	122.12	392	35
1	A	6	LYS	CA-C-O	7.30	128.59	120.70	98	26
1	A	11	LYS	N-CA-C	7.30	121.61	108.69	552	17
1	A	70	VAL	N-CA-CB	7.29	121.47	111.41	124	21
1	A	5	VAL	CB-CA-C	7.29	120.14	111.32	583	12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	10	GLY	CA-C-N	7.28	131.21	120.87	396	15
1	A	10	GLY	C-N-CA	7.28	131.21	120.87	396	15
1	A	61	ILE	N-CA-C	7.28	118.35	107.51	290	17
1	A	67	LEU	N-CA-C	-7.27	98.39	109.95	289	32
1	A	7	THR	N-CA-CB	7.27	120.75	110.36	81	51
1	A	29	LYS	O-C-N	-7.27	113.33	122.27	554	33
1	A	2	GLN	O-C-N	-7.26	114.69	123.19	596	25
1	A	42	ARG	CA-C-O	7.25	127.93	120.24	126	12
1	A	42	ARG	CD-NE-CZ	-7.25	114.25	124.40	236	10
1	A	65	SER	N-CA-CB	7.25	120.63	109.97	80	24
1	A	71	LEU	O-C-N	-7.24	113.84	122.96	357	20
1	A	56	LEU	O-C-N	-7.21	114.47	122.12	603	22
1	A	20	SER	N-CA-CB	7.21	121.78	110.46	379	8
1	A	40	GLN	O-C-N	-7.19	113.69	122.25	358	19
1	A	49	GLN	CA-C-N	7.18	132.22	120.94	423	22
1	A	49	GLN	C-N-CA	7.18	132.22	120.94	423	22
1	A	45	PHE	CA-C-O	7.18	127.85	120.24	574	16
1	A	3	ILE	CA-C-O	-7.18	113.52	121.92	116	16
1	A	20	SER	CA-C-O	7.17	127.72	119.18	47	13
1	A	64	GLU	N-CA-CB	-7.17	101.31	112.41	461	4
1	A	58	ASP	N-CA-C	7.15	119.98	111.33	320	33
1	A	41	GLN	N-CA-CB	-7.15	98.65	110.23	356	7
1	A	66	THR	N-CA-CB	7.14	122.33	110.47	260	23
1	A	48	LYS	O-C-N	-7.13	114.84	123.19	114	25
1	A	59	TYR	CA-C-O	7.13	127.70	119.35	559	15
1	A	51	GLU	CB-CG-CD	7.13	124.73	112.60	294	7
1	A	48	LYS	CA-C-O	7.13	128.42	120.43	470	16
1	A	3	ILE	N-CA-CB	7.13	124.42	112.44	334	28
1	A	65	SER	O-C-N	-7.13	114.89	123.16	633	16
1	A	9	THR	CA-C-O	7.12	128.23	119.11	6	29
1	A	18	GLU	N-CA-C	-7.12	100.21	110.40	407	32
1	A	31	GLN	O-C-N	-7.12	114.57	122.12	486	20
1	A	25	ASN	CB-CG-ND2	7.12	127.07	116.40	271	8
1	A	25	ASN	N-CA-CB	7.11	120.68	110.16	624	19
1	A	60	ASN	N-CA-C	7.10	121.28	111.90	447	25
1	A	34	GLU	N-CA-C	7.10	122.81	113.30	406	11
1	A	43	LEU	N-CA-CB	7.10	121.69	110.55	541	10
1	A	41	GLN	CB-CG-CD	-7.09	100.55	112.60	318	27
1	A	46	ALA	O-C-N	-7.08	114.08	122.58	628	14
1	A	27	LYS	CA-C-O	7.08	128.09	119.31	446	19
1	A	8	LEU	CA-C-O	7.08	128.11	119.97	295	26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	23	ILE	CA-C-O	7.07	128.30	120.95	298	16
1	A	1	MET	O-C-N	-7.06	111.70	123.00	378	7
1	A	11	LYS	N-CA-CB	7.06	120.34	109.97	185	7
1	A	38	PRO	N-CA-CB	7.05	110.53	103.48	506	9
1	A	46	ALA	CA-C-O	7.05	129.90	121.65	343	17
1	A	21	ASP	CA-C-N	7.05	130.88	120.87	592	8
1	A	21	ASP	C-N-CA	7.05	130.88	120.87	592	8
1	A	9	THR	CA-CB-OG1	7.02	120.13	109.60	126	17
1	A	8	LEU	CB-CA-C	-7.02	97.64	110.63	632	7
1	A	64	GLU	CB-CG-CD	-7.02	100.67	112.60	316	4
1	A	61	ILE	CA-C-O	7.00	129.38	120.76	24	14
1	A	17	VAL	CA-C-O	-7.00	114.32	121.67	130	22
1	A	53	GLY	N-CA-C	7.00	122.38	114.67	499	11
1	A	67	LEU	N-CA-CB	7.00	121.48	110.56	434	10
1	A	32	ASP	CB-CA-C	6.99	121.85	110.88	76	6
1	A	9	THR	N-CA-CB	6.99	120.76	110.56	85	22
1	A	64	GLU	CA-C-N	6.98	130.63	120.71	321	33
1	A	64	GLU	C-N-CA	6.98	130.63	120.71	321	33
1	A	12	THR	N-CA-CB	6.98	121.51	110.55	225	31
1	A	28	ALA	O-C-N	-6.97	114.73	122.12	605	22
1	A	40	GLN	CA-C-O	6.97	127.47	119.18	15	26
1	A	47	GLY	O-C-N	-6.96	113.55	122.39	318	17
1	A	5	VAL	N-CA-CB	6.95	121.00	111.41	401	15
1	A	61	ILE	CA-C-N	6.95	135.46	123.03	494	6
1	A	61	ILE	C-N-CA	6.95	135.46	123.03	494	6
1	A	70	VAL	N-CA-C	-6.94	98.12	108.46	325	18
1	A	69	LEU	N-CA-C	6.94	120.55	109.24	595	7
1	A	4	PHE	N-CA-C	-6.93	97.05	108.76	61	4
1	A	65	SER	CA-C-O	-6.92	114.21	121.55	100	14
1	A	19	PRO	CB-CA-C	-6.90	102.05	111.85	313	5
1	A	64	GLU	CB-CA-C	6.88	122.75	111.26	104	13
1	A	58	ASP	N-CA-CB	6.88	120.23	110.12	427	9
1	A	11	LYS	CA-C-O	6.88	127.94	120.58	511	13
1	A	22	THR	CA-CB-OG1	6.87	119.91	109.60	91	27
1	A	62	GLN	CA-C-O	6.87	129.93	121.89	234	6
1	A	31	GLN	CA-C-O	6.87	127.83	120.55	258	16
1	A	25	ASN	CB-CA-C	-6.87	99.39	110.79	236	10
1	A	64	GLU	CA-C-O	6.85	128.56	119.59	12	17
1	A	2	GLN	CA-C-N	6.84	132.33	123.03	261	13
1	A	2	GLN	C-N-CA	6.84	132.33	123.03	261	13
1	A	68	HIS	N-CA-CB	6.84	121.80	110.52	639	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	59	TYR	CB-CG-CD2	6.81	131.01	120.80	595	2
1	A	34	GLU	N-CA-CB	-6.81	100.66	110.80	576	9
1	A	28	ALA	N-CA-CB	6.81	119.88	110.01	240	7
1	A	46	ALA	N-CA-CB	-6.81	101.36	111.71	493	5
1	A	12	THR	CA-C-O	6.81	128.05	120.43	69	18
1	A	54	ARG	N-CA-CB	6.80	121.17	110.56	615	6
1	A	33	LYS	CA-C-O	-6.79	113.29	120.55	271	18
1	A	70	VAL	CB-CA-C	6.79	118.81	110.73	54	8
1	A	67	LEU	CA-C-N	-6.79	113.64	123.00	345	2
1	A	67	LEU	C-N-CA	-6.79	113.64	123.00	345	2
1	A	34	GLU	CB-CA-C	-6.78	98.16	109.55	255	8
1	A	41	GLN	CG-CD-NE2	6.78	126.57	116.40	455	9
1	A	46	ALA	CA-C-N	6.78	135.08	121.93	577	15
1	A	46	ALA	C-N-CA	6.78	135.08	121.93	577	15
1	A	44	ILE	N-CA-C	6.78	117.66	108.17	502	15
1	A	62	GLN	O-C-N	-6.77	115.35	122.94	189	17
1	A	15	LEU	N-CA-C	6.76	120.90	110.42	332	10
1	A	2	GLN	N-CA-CB	-6.76	99.85	110.06	327	10
1	A	49	GLN	N-CA-C	6.76	120.10	109.96	18	21
1	A	1	MET	CB-CA-C	6.75	122.92	110.10	217	3
1	A	23	ILE	CB-CA-C	-6.74	102.92	112.22	8	10
1	A	16	GLU	CA-C-N	-6.74	113.86	123.03	632	9
1	A	16	GLU	C-N-CA	-6.74	113.86	123.03	632	9
1	A	4	PHE	CB-CA-C	-6.73	98.99	110.16	190	2
1	A	36	ILE	CA-CB-CG1	6.73	121.84	110.40	346	3
1	A	33	LYS	CB-CA-C	-6.71	100.31	110.90	68	10
1	A	66	THR	N-CA-C	6.70	119.20	108.41	19	12
1	A	11	LYS	CG-CD-CE	6.69	126.69	111.30	297	1
1	A	62	GLN	N-CA-CB	-6.68	100.11	110.46	617	4
1	A	2	GLN	CB-CG-CD	-6.68	101.25	112.60	532	11
1	A	60	ASN	CB-CA-C	6.67	120.69	111.63	17	11
1	A	19	PRO	CA-C-N	6.66	132.79	121.14	263	23
1	A	19	PRO	C-N-CA	6.66	132.79	121.14	263	23
1	A	9	THR	O-C-N	-6.66	112.71	122.43	217	10
1	A	48	LYS	N-CA-CB	6.66	121.28	110.43	207	1
1	A	60	ASN	CA-C-O	6.65	129.40	121.08	103	7
1	A	2	GLN	N-CA-C	6.65	119.57	108.73	218	15
1	A	2	GLN	CB-CA-C	-6.64	98.29	109.65	360	6
1	A	27	LYS	N-CA-CB	6.64	119.88	110.12	369	14
1	A	29	LYS	CB-CA-C	-6.63	99.58	110.85	285	4
1	A	16	GLU	CA-C-O	6.60	127.58	120.32	238	15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	54	ARG	N-CA-C	-6.60	100.19	110.42	615	24
1	A	7	THR	CA-CB-CG2	-6.60	99.28	110.50	250	2
1	A	68	HIS	CA-C-O	6.58	127.63	120.32	201	14
1	A	14	THR	CB-CA-C	-6.55	98.38	109.72	52	8
1	A	59	TYR	CB-CG-CD1	-6.54	110.98	120.80	595	4
1	A	47	GLY	CA-C-N	6.53	132.02	123.00	434	8
1	A	47	GLY	C-N-CA	6.53	132.02	123.00	434	8
1	A	3	ILE	CA-CB-CG2	-6.53	99.40	110.50	156	5
1	A	32	ASP	N-CA-CB	-6.52	100.53	110.12	140	13
1	A	41	GLN	CA-CB-CG	-6.50	101.09	114.10	271	4
1	A	39	ASP	CB-CA-C	-6.50	98.33	110.36	448	6
1	A	3	ILE	CA-C-N	6.48	132.14	123.00	513	5
1	A	3	ILE	C-N-CA	6.48	132.14	123.00	513	5
1	A	14	THR	CA-CB-OG1	6.47	119.31	109.60	132	4
1	A	6	LYS	CA-C-N	6.44	132.69	120.97	411	7
1	A	6	LYS	C-N-CA	6.44	132.69	120.97	411	7
1	A	29	LYS	CG-CD-CE	6.44	126.11	111.30	388	2
1	A	20	SER	O-C-N	-6.44	114.69	122.22	90	9
1	A	61	ILE	CA-CB-CG2	6.43	121.43	110.50	320	2
1	A	9	THR	CB-CA-C	-6.42	96.96	110.45	294	6
1	A	5	VAL	CA-C-N	6.42	129.98	120.87	49	13
1	A	5	VAL	C-N-CA	6.42	129.98	120.87	49	13
1	A	19	PRO	CA-C-O	6.41	126.98	118.90	436	3
1	A	14	THR	CA-C-N	6.41	132.61	122.62	467	3
1	A	14	THR	C-N-CA	6.41	132.61	122.62	467	3
1	A	22	THR	CA-C-O	6.40	128.53	121.56	500	14
1	A	9	THR	CA-CB-CG2	-6.39	99.63	110.50	101	8
1	A	63	LYS	CG-CD-CE	6.39	126.00	111.30	452	3
1	A	19	PRO	N-CD-CG	6.39	112.78	103.20	1	3
1	A	39	ASP	N-CA-CB	-6.39	100.42	109.94	298	5
1	A	53	GLY	O-C-N	-6.38	113.94	122.48	343	6
1	A	1	MET	N-CA-CB	-6.37	99.67	110.50	586	5
1	A	20	SER	CA-C-N	6.36	130.36	120.75	488	20
1	A	20	SER	C-N-CA	6.36	130.36	120.75	488	20
1	A	68	HIS	CB-CG-ND1	6.36	132.24	122.70	315	6
1	A	62	GLN	CA-C-N	6.35	129.86	120.90	128	45
1	A	62	GLN	C-N-CA	6.35	129.86	120.90	128	45
1	A	42	ARG	N-CA-CB	6.35	120.56	110.65	479	5
1	A	24	GLU	CB-CA-C	-6.33	100.90	110.90	406	5
1	A	19	PRO	N-CA-CB	-6.33	97.46	103.41	244	7
1	A	59	TYR	CA-CB-CG	-6.33	102.51	113.90	10	22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	13	ILE	CA-C-N	6.32	129.84	120.87	456	14
1	A	13	ILE	C-N-CA	6.32	129.84	120.87	456	14
1	A	47	GLY	N-CA-C	6.29	123.70	115.40	493	10
1	A	20	SER	CA-CB-OG	6.28	123.66	111.10	265	1
1	A	22	THR	OG1-CB-CG2	-6.27	96.76	109.30	301	1
1	A	12	THR	O-C-N	-6.26	115.90	123.29	325	26
1	A	68	HIS	ND1-CG-CD2	-6.26	99.84	106.10	576	3
1	A	42	ARG	NH1-CZ-NH2	-6.25	111.18	119.30	468	13
1	A	33	LYS	N-CA-CB	-6.24	100.93	109.98	256	8
1	A	45	PHE	N-CA-CB	-6.24	100.33	110.81	104	4
1	A	67	LEU	CA-C-O	6.23	128.15	121.11	152	12
1	A	31	GLN	CB-CA-C	-6.21	100.48	110.79	311	5
1	A	4	PHE	N-CA-CB	6.21	120.32	110.57	117	7
1	A	66	THR	CB-CA-C	-6.20	100.03	110.19	592	7
1	A	6	LYS	CA-CB-CG	-6.19	101.71	114.10	518	3
1	A	40	GLN	CG-CD-NE2	6.19	125.69	116.40	438	2
1	A	62	GLN	CG-CD-NE2	-6.19	107.11	116.40	146	5
1	A	65	SER	CA-CB-OG	6.19	123.47	111.10	587	1
1	A	15	LEU	CD1-CG-CD2	6.18	124.41	110.80	220	1
1	A	48	LYS	CB-CA-C	6.17	120.39	110.16	379	5
1	A	63	LYS	CB-CA-C	-6.16	99.49	109.72	413	3
1	A	3	ILE	CB-CA-C	-6.12	102.08	111.31	518	3
1	A	54	ARG	CA-CB-CG	6.10	126.31	114.10	61	1
1	A	24	GLU	CB-CG-CD	-6.10	102.23	112.60	461	5
1	A	49	GLN	CB-CG-CD	-6.10	102.23	112.60	297	16
1	A	6	LYS	N-CA-CB	6.09	120.13	110.57	300	8
1	A	45	PHE	N-CA-C	-6.09	99.43	108.99	203	8
1	A	21	ASP	N-CA-CB	6.08	119.01	109.83	609	13
1	A	54	ARG	CA-C-N	6.08	133.61	122.92	287	4
1	A	54	ARG	C-N-CA	6.08	133.61	122.92	287	4
1	A	63	LYS	N-CA-CB	6.07	118.63	109.34	129	13
1	A	2	GLN	CG-CD-NE2	6.07	125.50	116.40	315	7
1	A	68	HIS	CB-CA-C	-6.06	100.09	110.22	302	5
1	A	42	ARG	CG-CD-NE	-6.06	98.67	112.00	579	15
1	A	51	GLU	CB-CA-C	6.05	120.27	109.38	247	5
1	A	13	ILE	CA-CB-CG2	-6.04	100.23	110.50	304	6
1	A	62	GLN	CB-CG-CD	6.04	122.86	112.60	201	9
1	A	58	ASP	CB-CA-C	-6.04	97.59	110.32	623	13
1	A	38	PRO	O-C-N	6.03	130.00	122.22	574	6
1	A	31	GLN	CG-CD-NE2	-6.03	107.36	116.40	48	2
1	A	28	ALA	CB-CA-C	-6.03	100.78	110.79	449	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	24	GLU	N-CA-CB	-6.01	101.29	110.12	33	10
1	A	3	ILE	CA-CB-CG1	6.00	120.60	110.40	615	5
1	A	60	ASN	CB-CG-OD1	5.99	132.77	120.80	437	1
1	A	43	LEU	N-CA-C	5.98	118.70	109.07	435	5
1	A	40	GLN	CB-CG-CD	5.97	122.75	112.60	305	4
1	A	62	GLN	N-CA-C	5.97	118.29	109.69	355	10
1	A	71	LEU	N-CA-CB	5.96	120.14	110.43	165	6
1	A	66	THR	CA-CB-CG2	5.93	120.58	110.50	106	3
1	A	13	ILE	CA-CB-CG1	5.93	120.48	110.40	46	7
1	A	70	VAL	CA-CB-CG2	5.92	120.46	110.40	299	4
1	A	62	GLN	CG-CD-OE1	5.92	132.63	120.80	118	1
1	A	27	LYS	CB-CA-C	-5.91	100.98	110.79	454	2
1	A	4	PHE	CB-CG-CD1	-5.90	110.67	120.70	549	3
1	A	43	LEU	CB-CA-C	5.90	119.51	109.53	598	8
1	A	34	GLU	CB-CG-CD	5.90	122.63	112.60	153	4
1	A	36	ILE	CA-CB-CG2	-5.90	100.47	110.50	253	3
1	A	44	ILE	CA-CB-CG1	5.89	120.42	110.40	211	8
1	A	16	GLU	CB-CA-C	-5.89	100.65	110.19	196	6
1	A	23	ILE	CA-CB-CG2	5.89	120.51	110.50	585	3
1	A	14	THR	OG1-CB-CG2	-5.89	97.52	109.30	223	4
1	A	67	LEU	CB-CA-C	-5.89	99.11	109.71	523	5
1	A	31	GLN	CB-CG-CD	-5.89	102.59	112.60	108	7
1	A	69	LEU	N-CA-CB	5.89	120.01	110.77	515	2
1	A	54	ARG	CG-CD-NE	-5.89	99.05	112.00	186	14
1	A	1	MET	CA-C-N	5.89	131.42	122.65	529	10
1	A	1	MET	C-N-CA	5.89	131.42	122.65	529	10
1	A	33	LYS	CB-CG-CD	5.88	124.82	111.30	600	1
1	A	23	ILE	N-CA-CB	5.87	117.81	110.47	523	6
1	A	9	THR	OG1-CB-CG2	-5.87	97.56	109.30	57	2
1	A	30	ILE	CB-CA-C	5.87	120.06	112.14	165	6
1	A	29	LYS	N-CA-CB	5.86	118.93	110.20	313	6
1	A	55	THR	CA-CB-CG2	-5.83	100.58	110.50	220	1
1	A	38	PRO	N-CD-CG	5.83	111.95	103.20	376	5
1	A	38	PRO	CB-CA-C	5.82	121.17	111.56	14	6
1	A	8	LEU	N-CA-CB	5.81	118.66	110.12	337	8
1	A	68	HIS	N-CA-C	5.81	118.13	109.59	21	2
1	A	14	THR	N-CA-C	-5.81	100.43	109.72	79	3
1	A	63	LYS	CB-CG-CD	5.80	124.65	111.30	342	2
1	A	70	VAL	CA-CB-CG1	5.79	120.25	110.40	562	4
1	A	16	GLU	N-CA-C	-5.79	99.47	108.90	589	3
1	A	69	LEU	CB-CA-C	5.77	120.01	110.78	313	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	44	ILE	CA-CB-CG2	5.76	120.28	110.50	532	4
1	A	57	SER	CB-CA-C	-5.74	101.86	110.88	179	3
1	A	41	GLN	CA-C-N	5.74	131.09	123.00	61	7
1	A	41	GLN	C-N-CA	5.74	131.09	123.00	61	7
1	A	59	TYR	N-CA-CB	5.74	118.98	110.49	607	3
1	A	17	VAL	N-CA-C	-5.72	100.35	108.65	373	10
1	A	12	THR	N-CA-C	-5.72	99.33	109.06	434	7
1	A	17	VAL	N-CA-CB	5.71	121.20	112.06	314	3
1	A	6	LYS	CB-CA-C	-5.71	100.83	110.19	288	8
1	A	42	ARG	N-CA-C	-5.71	100.88	109.95	576	8
1	A	12	THR	CA-CB-OG1	5.69	118.13	109.60	513	4
1	A	48	LYS	CA-CB-CG	5.69	125.47	114.10	457	2
1	A	42	ARG	CA-C-N	5.69	130.33	122.77	187	3
1	A	42	ARG	C-N-CA	5.69	130.33	122.77	187	3
1	A	52	ASP	CA-C-N	5.68	132.55	121.41	26	2
1	A	52	ASP	C-N-CA	5.68	132.55	121.41	26	2
1	A	16	GLU	CB-CG-CD	5.67	122.24	112.60	244	8
1	A	27	LYS	CB-CG-CD	5.67	124.34	111.30	249	1
1	A	22	THR	CA-CB-CG2	-5.66	100.87	110.50	334	3
1	A	56	LEU	N-CA-CB	-5.65	101.52	110.22	154	1
1	A	33	LYS	CA-C-N	5.65	131.38	122.11	453	3
1	A	33	LYS	C-N-CA	5.65	131.38	122.11	453	3
1	A	26	VAL	CA-CB-CG1	5.65	120.00	110.40	467	2
1	A	56	LEU	CB-CA-C	-5.61	101.48	110.79	222	2
1	A	11	LYS	CB-CA-C	5.61	119.00	109.53	417	3
1	A	11	LYS	CA-C-N	5.60	129.87	122.42	363	5
1	A	11	LYS	C-N-CA	5.60	129.87	122.42	363	5
1	A	54	ARG	CA-C-O	-5.56	114.83	121.89	80	6
1	A	4	PHE	CA-C-N	-5.56	115.78	122.90	80	5
1	A	4	PHE	C-N-CA	-5.56	115.78	122.90	80	5
1	A	50	LEU	CB-CA-C	-5.56	101.92	110.26	449	2
1	A	54	ARG	CB-CA-C	5.54	118.94	109.80	273	3
1	A	5	VAL	CA-CB-CG2	-5.53	101.00	110.40	634	2
1	A	23	ILE	CA-CB-CG1	5.53	119.80	110.40	151	2
1	A	21	ASP	CB-CA-C	-5.52	100.21	109.65	301	5
1	A	52	ASP	CB-CA-C	-5.52	102.22	110.88	142	6
1	A	69	LEU	CD1-CG-CD2	-5.52	98.66	110.80	277	2
1	A	45	PHE	CB-CG-CD2	-5.50	111.35	120.70	257	2
1	A	6	LYS	CB-CG-CD	5.50	123.94	111.30	500	1
1	A	31	GLN	CA-CB-CG	-5.49	103.13	114.10	453	1
1	A	27	LYS	CG-CD-CE	5.48	123.91	111.30	298	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	40	GLN	CA-CB-CG	-5.45	103.20	114.10	546	1
1	A	55	THR	CB-CA-C	-5.45	100.67	110.36	576	5
1	A	16	GLU	N-CA-CB	5.45	119.36	110.37	345	3
1	A	7	THR	CB-CA-C	-5.44	101.09	111.48	477	1
1	A	14	THR	CA-CB-CG2	5.44	119.74	110.50	552	2
1	A	51	GLU	N-CA-CB	5.43	120.73	111.66	295	2
1	A	49	GLN	CG-CD-OE1	-5.40	110.00	120.80	93	1
1	A	15	LEU	CB-CA-C	-5.38	99.22	109.66	338	1
1	A	26	VAL	CA-CB-CG2	-5.38	101.26	110.40	270	4
1	A	4	PHE	CB-CG-CD2	5.37	129.83	120.70	79	2
1	A	12	THR	CA-CB-CG2	5.37	119.62	110.50	22	2
1	A	60	ASN	CB-CG-ND2	5.34	124.41	116.40	573	1
1	A	42	ARG	CA-CB-CG	5.33	124.76	114.10	217	1
1	A	17	VAL	CA-C-N	5.33	128.05	120.49	36	2
1	A	17	VAL	C-N-CA	5.33	128.05	120.49	36	2
1	A	18	GLU	CB-CG-CD	-5.32	103.55	112.60	489	3
1	A	30	ILE	CA-CB-CG2	5.30	119.50	110.50	511	3
1	A	67	LEU	CD1-CG-CD2	-5.30	99.15	110.80	540	1
1	A	16	GLU	CA-CB-CG	5.28	124.66	114.10	54	1
1	A	48	LYS	CG-CD-CE	5.26	123.40	111.30	27	1
1	A	22	THR	CB-CA-C	-5.25	99.30	109.76	380	1
1	A	12	THR	OG1-CB-CG2	-5.24	98.81	109.30	413	1
1	A	2	GLN	CG-CD-OE1	5.23	131.26	120.80	461	1
1	A	45	PHE	CD1-CG-CD2	5.22	126.43	118.60	406	2
1	A	66	THR	OG1-CB-CG2	-5.22	98.86	109.30	586	1
1	A	55	THR	OG1-CB-CG2	-5.18	98.93	109.30	165	2
1	A	17	VAL	CA-CB-CG2	5.17	119.19	110.40	302	1
1	A	5	VAL	CA-CB-CG1	5.16	119.18	110.40	226	2
1	A	23	ILE	CB-CG1-CD1	5.16	124.63	113.80	221	1
1	A	30	ILE	CA-CB-CG1	-5.15	101.64	110.40	547	1
1	A	49	GLN	CG-CD-NE2	5.14	124.11	116.40	93	1
1	A	2	GLN	CA-CB-CG	5.13	124.36	114.10	494	2
1	A	34	GLU	CA-C-N	5.11	129.19	120.91	28	2
1	A	34	GLU	C-N-CA	5.11	129.19	120.91	28	2
1	A	38	PRO	CA-CB-CG	-5.10	94.80	104.50	153	1
1	A	24	GLU	CA-CB-CG	5.10	124.31	114.10	600	1
1	A	53	GLY	CA-C-O	5.07	125.49	119.10	533	1
1	A	57	SER	CA-CB-OG	5.06	121.22	111.10	121	1
1	A	17	VAL	CA-CB-CG1	-5.04	101.83	110.40	591	1
1	A	54	ARG	CB-CG-CD	5.04	122.89	111.30	254	1
1	A	29	LYS	CB-CG-CD	5.04	122.89	111.30	253	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	40	GLN	CB-CA-C	-5.01	102.95	111.02	390	1
1	A	37	PRO	N-CD-CG	5.01	110.72	103.20	527	1
1	A	44	ILE	CA-C-N	-5.00	114.98	122.39	610	1
1	A	44	ILE	C-N-CA	-5.00	114.98	122.39	610	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	42	ARG	Sidechain	171
1	A	54	ARG	Sidechain	157
1	A	59	TYR	Sidechain	121
1	A	45	PHE	Sidechain	25
1	A	4	PHE	Sidechain	18
1	A	68	HIS	Sidechain	17
1	A	9	THR	Peptide	6
1	A	51	GLU	Peptide	6
1	A	17	VAL	Peptide	3
1	A	41	GLN	Peptide	3
1	A	20	SER	Mainchain,Peptide	2
1	A	49	GLN	Peptide	1
1	A	8	LEU	Peptide	1
1	A	33	LYS	Peptide	1
1	A	61	ILE	Peptide	1
1	A	37	PRO	Peptide	1
1	A	34	GLU	Peptide	1
1	A	16	GLU	Peptide	1
1	A	32	ASP	Mainchain	1
1	A	71	LEU	Peptide	1

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	563	586	586	0±0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	360320	375040	375040	65

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

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:ILE:HD12	1:A:67:LEU:HD22	0.59	1.74	483	1
1:A:23:ILE:HG23	1:A:43:LEU:HD12	0.54	1.77	267	2
1:A:22:THR:O	1:A:26:VAL:HG23	0.53	2.04	359	3
1:A:51:GLU:CD	1:A:54:ARG:HE	0.52	2.12	544	2
1:A:30:ILE:HG21	1:A:69:LEU:HD22	0.51	1.83	30	1
1:A:23:ILE:HD13	1:A:56:LEU:HD12	0.50	1.82	533	1
1:A:18:GLU:O	1:A:56:LEU:HD12	0.49	2.08	4	1
1:A:36:ILE:HD13	1:A:71:LEU:HD11	0.49	1.84	226	2
1:A:15:LEU:HD22	1:A:29:LYS:HG2	0.49	1.85	451	1
1:A:54:ARG:HH11	1:A:58:ASP:CG	0.48	2.16	371	1
1:A:50:LEU:HD22	1:A:59:TYR:CG	0.48	2.44	70	2
1:A:22:THR:HA	1:A:55:THR:HA	0.47	1.86	369	3
1:A:23:ILE:HB	1:A:52:ASP:HA	0.47	1.87	497	1
1:A:15:LEU:HD21	1:A:30:ILE:HG13	0.47	1.86	13	1
1:A:50:LEU:HD22	1:A:59:TYR:CD2	0.47	2.45	251	3
1:A:69:LEU:HD23	1:A:69:LEU:C	0.46	2.35	238	1
1:A:44:ILE:HD12	1:A:70:VAL:HG21	0.46	1.86	300	6
1:A:56:LEU:HD23	1:A:61:ILE:HD12	0.46	1.88	311	1
1:A:26:VAL:HG21	1:A:56:LEU:HD11	0.46	1.88	387	1
1:A:61:ILE:HG21	1:A:67:LEU:HD21	0.45	1.88	436	1
1:A:45:PHE:CE2	1:A:61:ILE:HG12	0.45	2.47	238	1
1:A:45:PHE:HB3	1:A:50:LEU:HD21	0.45	1.89	524	1
1:A:43:LEU:HD21	1:A:67:LEU:HD23	0.45	1.88	567	1
1:A:43:LEU:C	1:A:44:ILE:HD12	0.45	2.37	188	1
1:A:8:LEU:HD11	1:A:71:LEU:H	0.44	1.73	174	1
1:A:61:ILE:HG21	1:A:67:LEU:HD11	0.44	1.90	311	1
1:A:6:LYS:HB2	1:A:68:HIS:CD2	0.43	2.48	384	2
1:A:3:ILE:HD12	1:A:67:LEU:HD13	0.43	1.90	460	1
1:A:17:VAL:HG21	1:A:56:LEU:CD2	0.43	2.44	449	1
1:A:5:VAL:CG1	1:A:69:LEU:HB2	0.43	2.43	191	1
1:A:42:ARG:HB2	1:A:70:VAL:HG23	0.42	1.90	241	3
1:A:43:LEU:CD2	1:A:69:LEU:HD13	0.42	2.44	319	1
1:A:7:THR:HG22	1:A:69:LEU:HD23	0.42	1.91	402	3
1:A:11:LYS:HZ3	1:A:34:GLU:CD	0.42	2.23	441	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:LEU:HD11	1:A:67:LEU:HD22	0.42	1.91	539	1
1:A:54:ARG:HH21	1:A:58:ASP:CG	0.41	2.22	356	1
1:A:13:ILE:HD12	1:A:33:LYS:HG2	0.41	1.92	428	1
1:A:61:ILE:HD13	1:A:67:LEU:HD21	0.41	1.93	634	1
1:A:50:LEU:HD22	1:A:59:TYR:CD1	0.41	2.50	639	2
1:A:51:GLU:CD	1:A:54:ARG:HH21	0.41	2.24	93	1
1:A:36:ILE:HD12	1:A:36:ILE:H	0.41	1.76	46	1
1:A:56:LEU:HG	1:A:61:ILE:HD12	0.41	1.93	226	1
1:A:15:LEU:HD22	1:A:29:LYS:HB3	0.41	1.91	475	1
1:A:45:PHE:HB2	1:A:67:LEU:HD22	0.40	1.92	261	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	70/76 (92%)	68±1 (98±2%)	2±1 (2±2%)	0±0 (0±1%)	37	78
All	All	44800/48640 (92%)	43711 (98%)	977 (2%)	112 (0%)	37	78

All 17 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	29
1	A	52	ASP	16
1	A	11	LYS	12
1	A	37	PRO	11
1	A	50	LEU	10
1	A	7	THR	10
1	A	46	ALA	6
1	A	60	ASN	4
1	A	19	PRO	3
1	A	64	GLU	2
1	A	12	THR	2
1	A	38	PRO	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	8	LEU	1
1	A	45	PHE	1
1	A	65	SER	1
1	A	70	VAL	1
1	A	10	GLY	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	65/68 (96%)	64±1 (99±1%)	1±1 (1±1%)	63 94
All	All	41600/43520 (96%)	41126 (99%)	474 (1%)	63 94

All 51 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	38	PRO	63
1	A	70	VAL	28
1	A	13	ILE	28
1	A	19	PRO	26
1	A	37	PRO	25
1	A	67	LEU	22
1	A	17	VAL	21
1	A	71	LEU	17
1	A	44	ILE	17
1	A	36	ILE	15
1	A	7	THR	13
1	A	8	LEU	13
1	A	48	LYS	12
1	A	52	ASP	12
1	A	14	THR	12
1	A	20	SER	12
1	A	69	LEU	10
1	A	2	GLN	10
1	A	1	MET	7
1	A	63	LYS	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	11	LYS	7
1	A	65	SER	7
1	A	23	ILE	6
1	A	62	GLN	6
1	A	57	SER	5
1	A	21	ASP	5
1	A	12	THR	5
1	A	29	LYS	5
1	A	56	LEU	5
1	A	9	THR	5
1	A	32	ASP	5
1	A	68	HIS	4
1	A	59	TYR	4
1	A	50	LEU	4
1	A	33	LYS	3
1	A	5	VAL	3
1	A	49	GLN	3
1	A	39	ASP	3
1	A	15	LEU	3
1	A	66	THR	2
1	A	25	ASN	2
1	A	3	ILE	2
1	A	60	ASN	2
1	A	41	GLN	1
1	A	43	LEU	1
1	A	40	GLN	1
1	A	58	ASP	1
1	A	6	LYS	1
1	A	24	GLU	1
1	A	45	PHE	1
1	A	42	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided