



Full wwPDB NMR Structure Validation Report ⓘ

Apr 28, 2016 – 12:53 AM BST

PDB ID : 2KOX
Title : NMR residual dipolar couplings identify long range correlated motions in the backbone of the protein ubiquitin
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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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

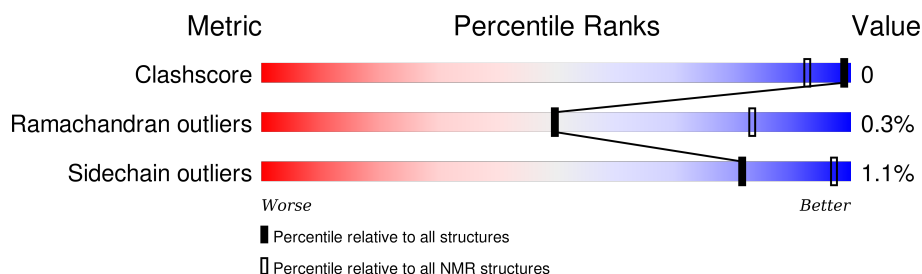
1 Overall quality at a glance

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 | 114402 | 11133 |
| Ramachandran outliers | 111179 | 9975 |
| Sidechain outliers | 111093 | 9958 |

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 | 89% • 7% |

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) | 0.35 | 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.

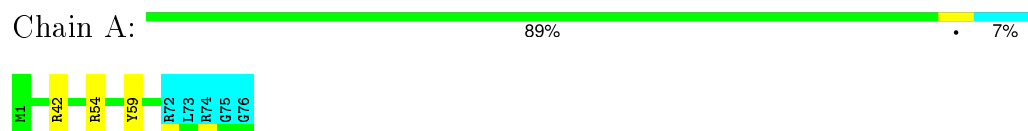
| Mol | Chain | Residues | Atoms | | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|--|-------|
| 1 | A | 76 | Total | C | H | N | O | S | | 0 |
| | | | 1231 | 378 | 629 | 105 | 118 | 1 | | |

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Ubiquitin

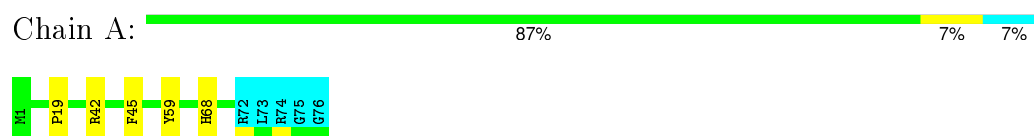


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

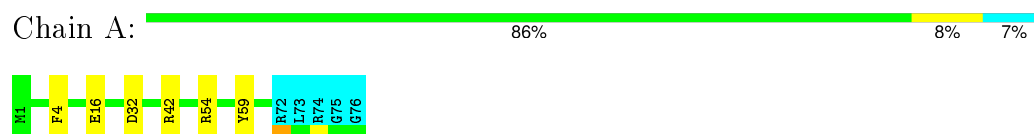
4.2.1 Score per residue for model 1

- Molecule 1: Ubiquitin




4.2.2 Score per residue for model 2

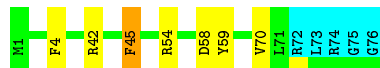
- Molecule 1: Ubiquitin



4.2.3 Score per residue for model 3


- Molecule 1: Ubiquitin

Chain A:  84% 8% 7%



4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin

Chain A:  87% 7% 7%



4.2.5 Score per residue for model 5


- Molecule 1: Ubiquitin

Chain A:  76% 17% 7%



4.2.6 Score per residue for model 6


- Molecule 1: Ubiquitin

Chain A:  88% 7% 7%



4.2.7 Score per residue for model 7


- Molecule 1: Ubiquitin

Chain A:  86% 7% 7%



4.2.8 Score per residue for model 8


- Molecule 1: Ubiquitin

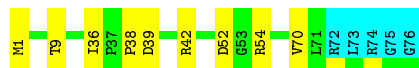
Chain A:  88% 5% 7%



4.2.9 Score per residue for model 9


- Molecule 1: Ubiquitin

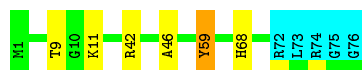
Chain A:  82% 12% 7%



4.2.10 Score per residue for model 10


- Molecule 1: Ubiquitin

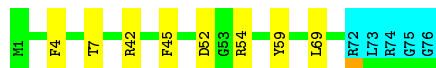
Chain A:  86% 7% 7%



4.2.11 Score per residue for model 11


- Molecule 1: Ubiquitin

Chain A:  83% 11% 7%



4.2.12 Score per residue for model 12

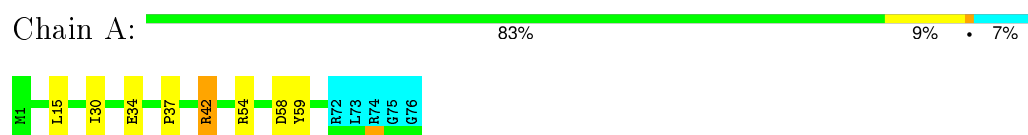
- Molecule 1: Ubiquitin

Chain A:  83% 8% 7%



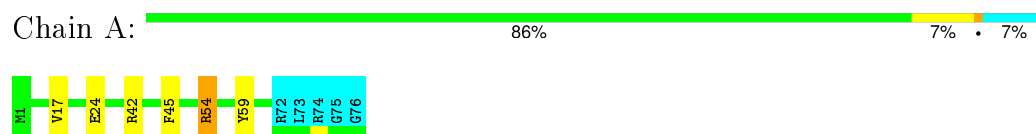
4.2.13 Score per residue for model 13

- Molecule 1: Ubiquitin



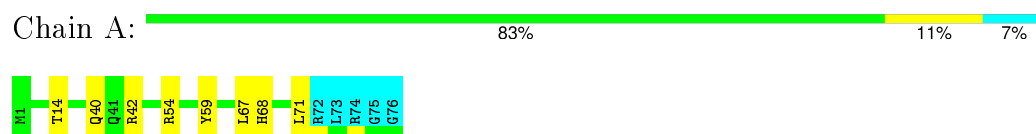
4.2.14 Score per residue for model 14

- Molecule 1: Ubiquitin



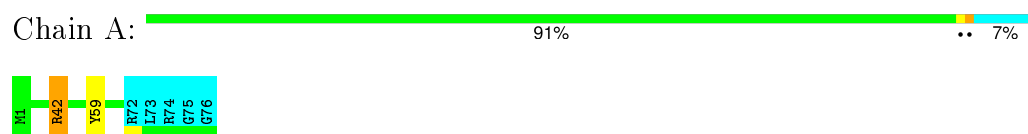
4.2.15 Score per residue for model 15

- Molecule 1: Ubiquitin



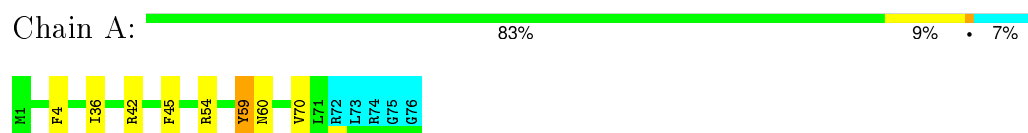
4.2.16 Score per residue for model 16

- Molecule 1: Ubiquitin



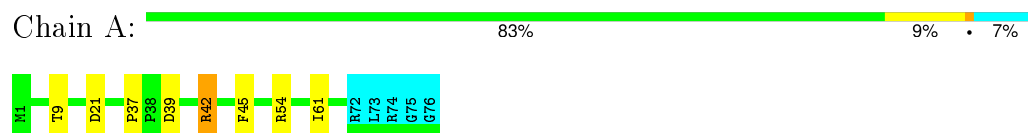
4.2.17 Score per residue for model 17

- Molecule 1: Ubiquitin



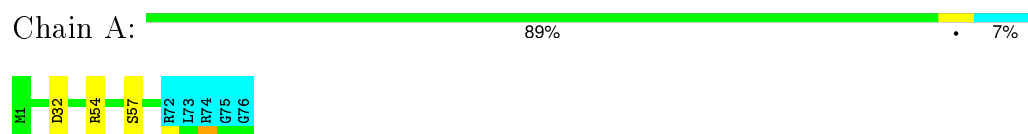
4.2.18 Score per residue for model 18

- Molecule 1: Ubiquitin



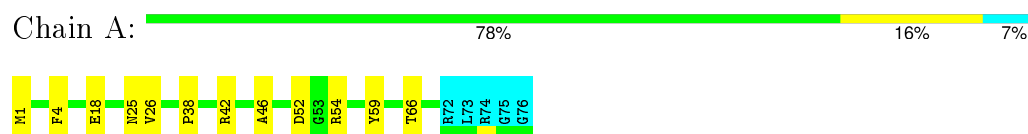
4.2.19 Score per residue for model 19

- Molecule 1: Ubiquitin



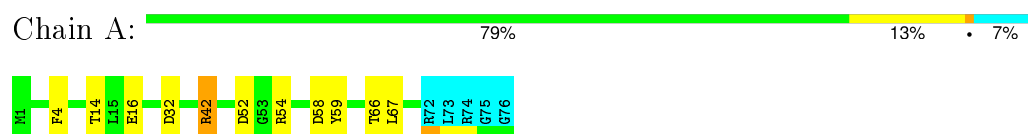
4.2.20 Score per residue for model 20

- Molecule 1: Ubiquitin



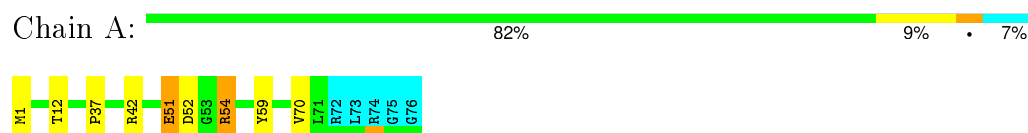
4.2.21 Score per residue for model 21

- Molecule 1: Ubiquitin



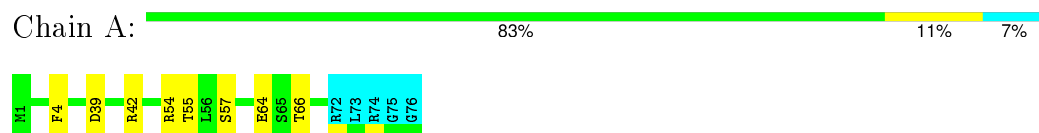
4.2.22 Score per residue for model 22

- Molecule 1: Ubiquitin



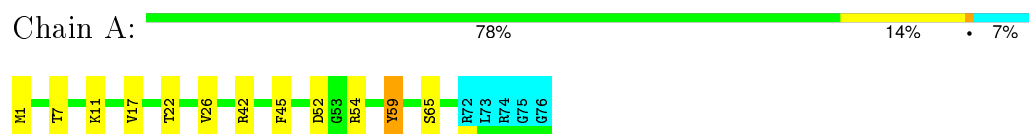
4.2.23 Score per residue for model 23

- Molecule 1: Ubiquitin



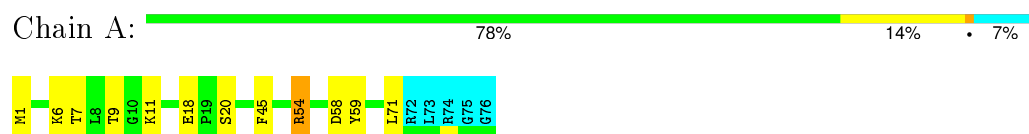
4.2.24 Score per residue for model 24

- Molecule 1: Ubiquitin



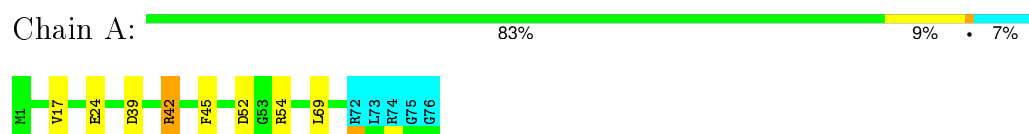
4.2.25 Score per residue for model 25

- Molecule 1: Ubiquitin



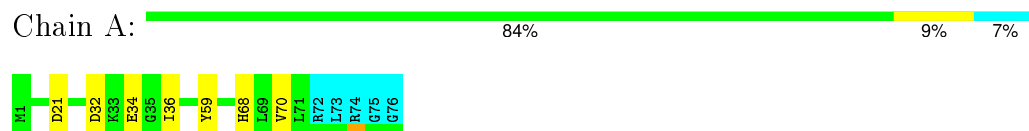
4.2.26 Score per residue for model 26

- Molecule 1: Ubiquitin



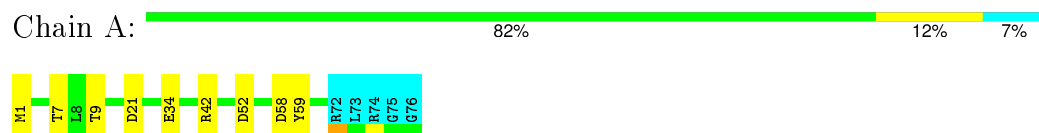
4.2.27 Score per residue for model 27

- Molecule 1: Ubiquitin



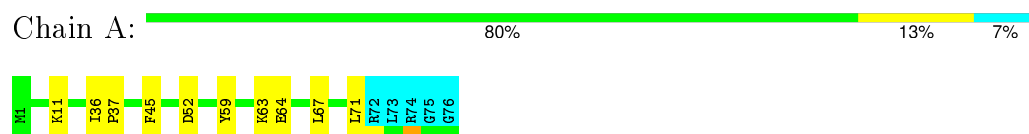
4.2.28 Score per residue for model 28

- Molecule 1: Ubiquitin



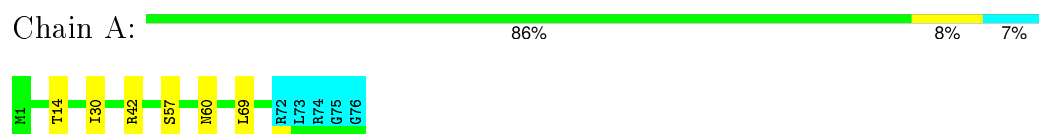
4.2.29 Score per residue for model 29

- Molecule 1: Ubiquitin



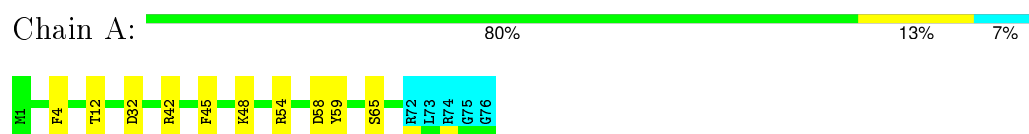
4.2.30 Score per residue for model 30

- Molecule 1: Ubiquitin



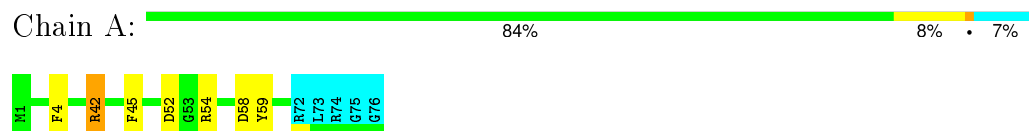
4.2.31 Score per residue for model 31

- Molecule 1: Ubiquitin



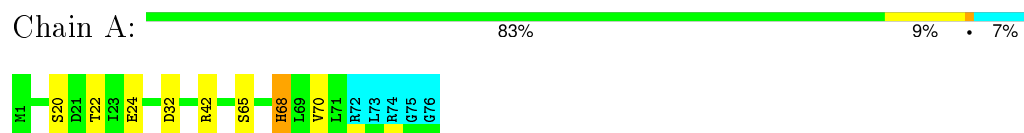
4.2.32 Score per residue for model 32

- Molecule 1: Ubiquitin



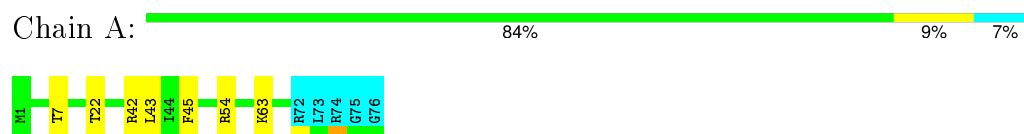
4.2.33 Score per residue for model 33

- Molecule 1: Ubiquitin



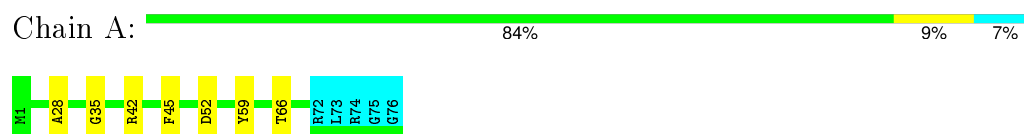
4.2.34 Score per residue for model 34

- Molecule 1: Ubiquitin



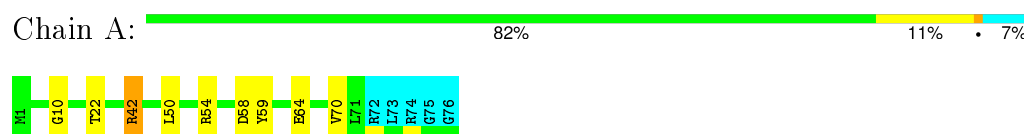
4.2.35 Score per residue for model 35

- Molecule 1: Ubiquitin



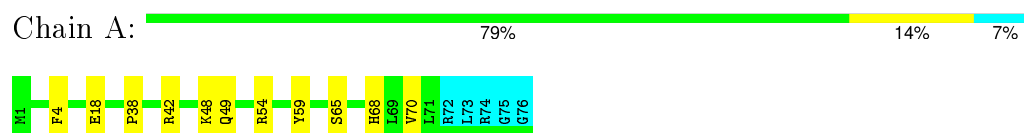
4.2.36 Score per residue for model 36

- Molecule 1: Ubiquitin



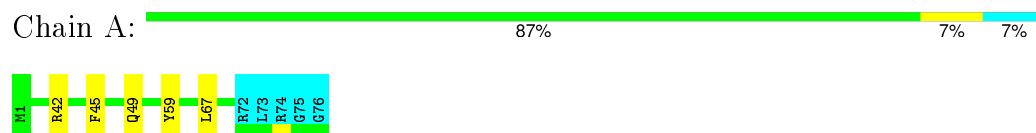
4.2.37 Score per residue for model 37

- Molecule 1: Ubiquitin



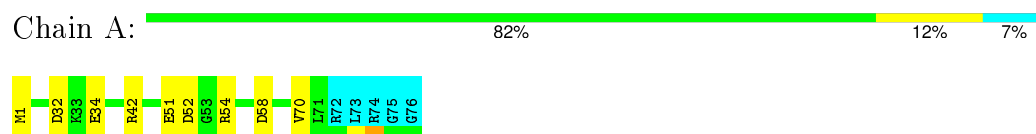
4.2.38 Score per residue for model 38

- Molecule 1: Ubiquitin



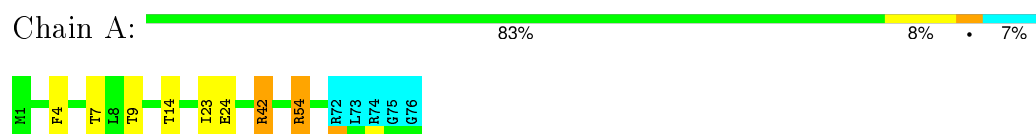
4.2.39 Score per residue for model 39

- Molecule 1: Ubiquitin



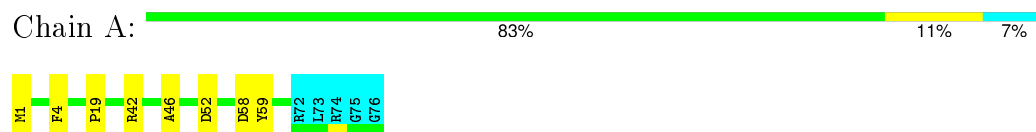
4.2.40 Score per residue for model 40

- Molecule 1: Ubiquitin



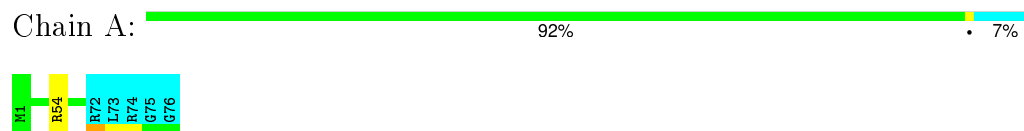
4.2.41 Score per residue for model 41

- Molecule 1: Ubiquitin



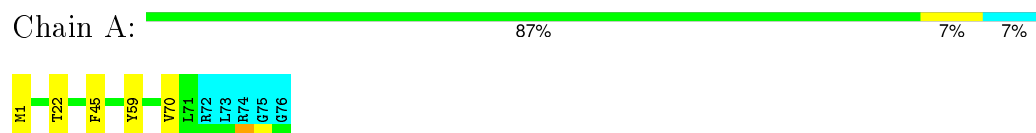
4.2.42 Score per residue for model 42

- Molecule 1: Ubiquitin



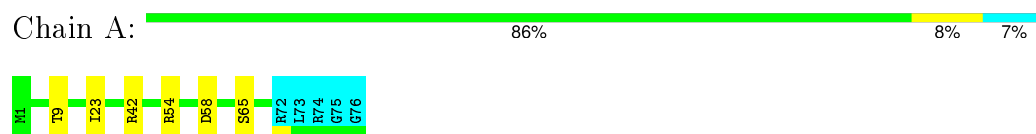
4.2.43 Score per residue for model 43

- Molecule 1: Ubiquitin



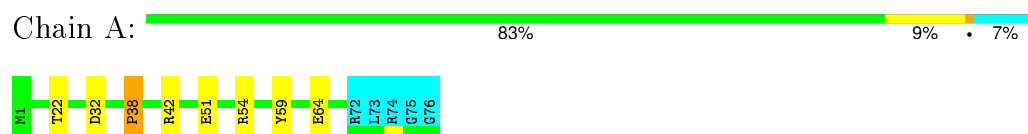
4.2.44 Score per residue for model 44

- Molecule 1: Ubiquitin



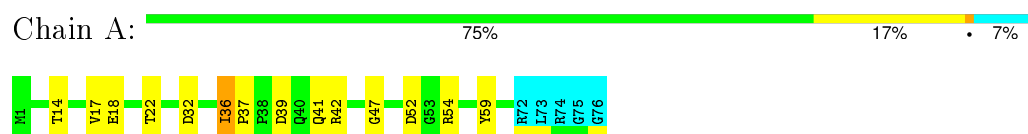
4.2.45 Score per residue for model 45

- Molecule 1: Ubiquitin



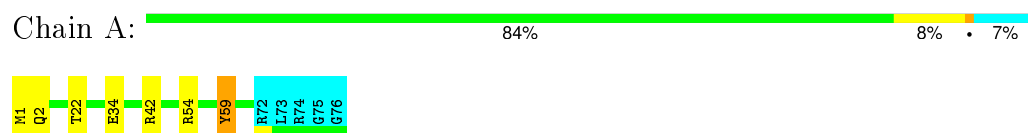
4.2.46 Score per residue for model 46

- Molecule 1: Ubiquitin



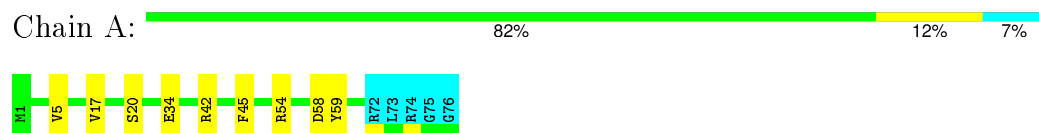
4.2.47 Score per residue for model 47

- Molecule 1: Ubiquitin



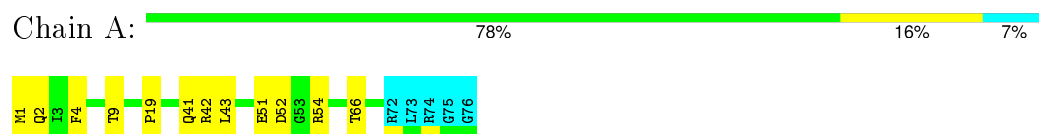
4.2.48 Score per residue for model 48

- Molecule 1: Ubiquitin



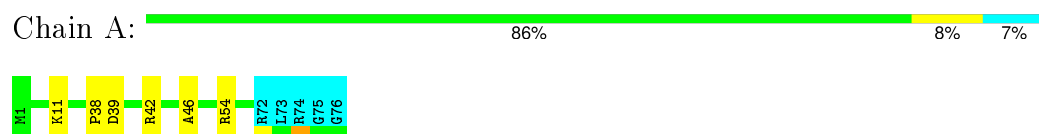
4.2.49 Score per residue for model 49

- Molecule 1: Ubiquitin



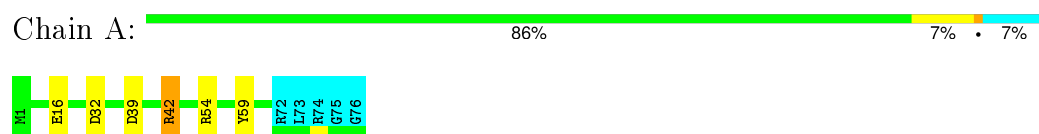
4.2.50 Score per residue for model 50

- Molecule 1: Ubiquitin



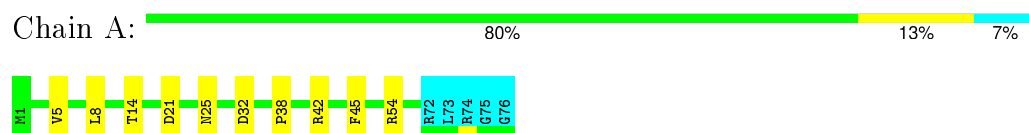
4.2.51 Score per residue for model 51

- Molecule 1: Ubiquitin



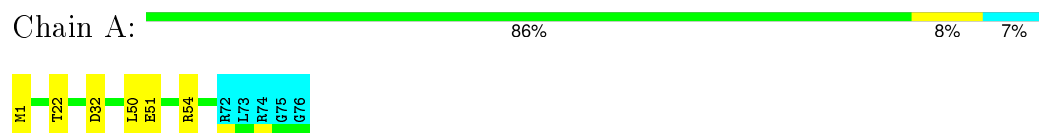
4.2.52 Score per residue for model 52

- Molecule 1: Ubiquitin



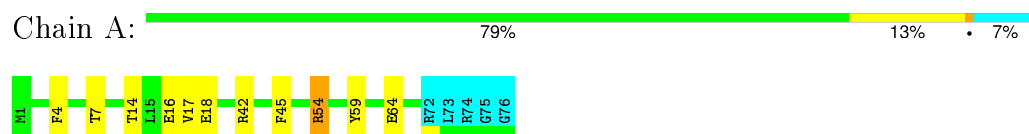
4.2.53 Score per residue for model 53

- Molecule 1: Ubiquitin



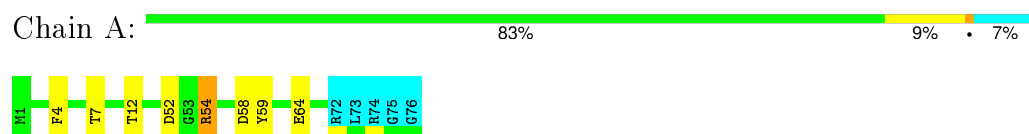
4.2.54 Score per residue for model 54

- Molecule 1: Ubiquitin



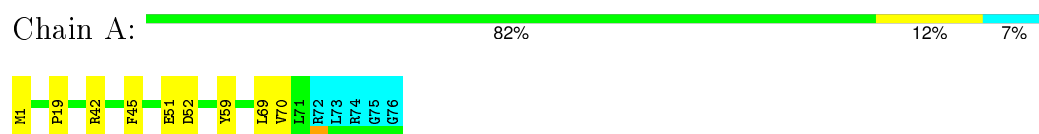
4.2.55 Score per residue for model 55

- Molecule 1: Ubiquitin



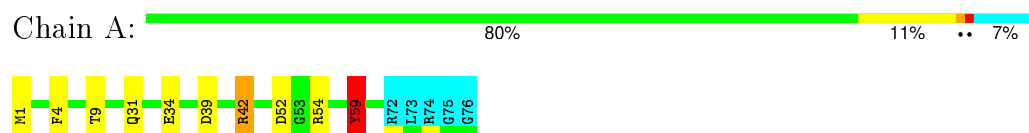
4.2.56 Score per residue for model 56

- Molecule 1: Ubiquitin



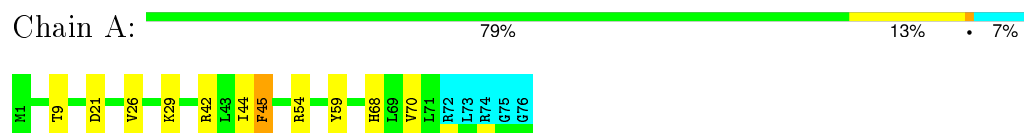
4.2.57 Score per residue for model 57

- Molecule 1: Ubiquitin



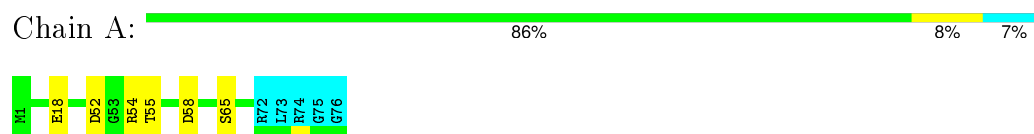
4.2.58 Score per residue for model 58

- Molecule 1: Ubiquitin



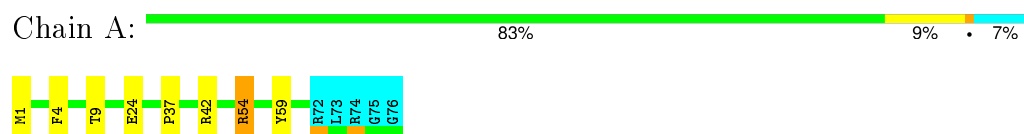
4.2.59 Score per residue for model 59

- Molecule 1: Ubiquitin



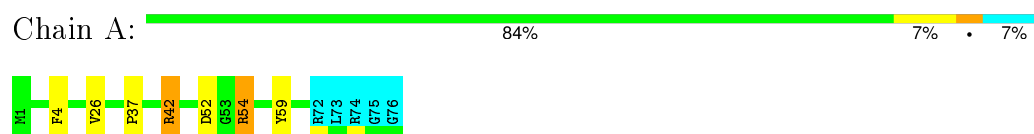
4.2.60 Score per residue for model 60

- Molecule 1: Ubiquitin



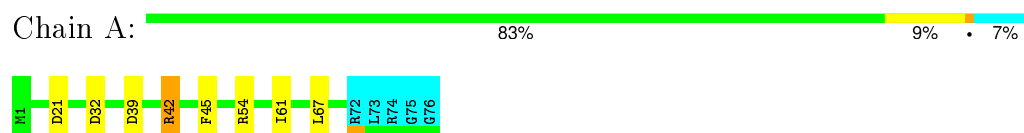
4.2.61 Score per residue for model 61

- Molecule 1: Ubiquitin



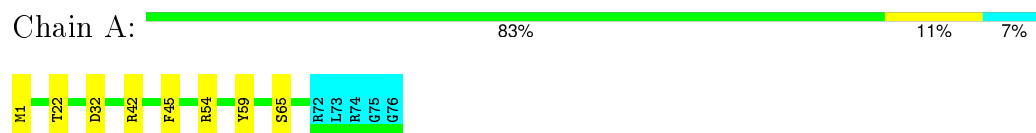
4.2.62 Score per residue for model 62

- Molecule 1: Ubiquitin



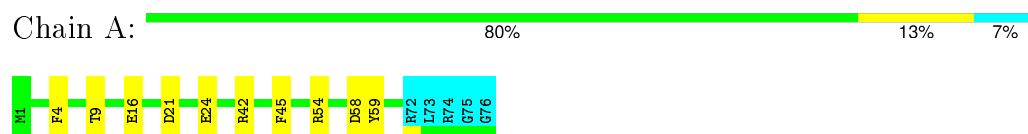
4.2.63 Score per residue for model 63

- Molecule 1: Ubiquitin



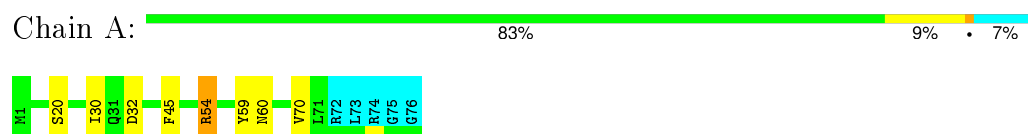
4.2.64 Score per residue for model 64

- Molecule 1: Ubiquitin



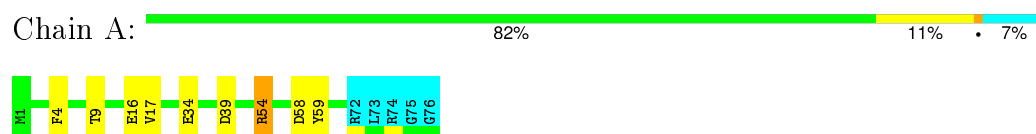
4.2.65 Score per residue for model 65

- Molecule 1: Ubiquitin



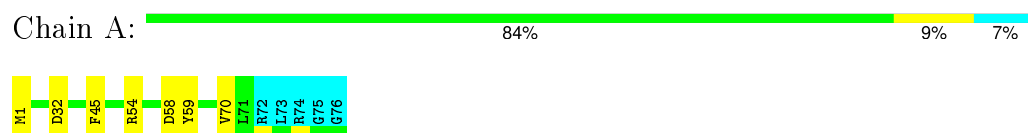
4.2.66 Score per residue for model 66

- Molecule 1: Ubiquitin



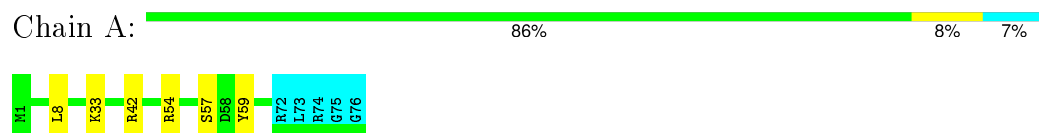
4.2.67 Score per residue for model 67

- Molecule 1: Ubiquitin



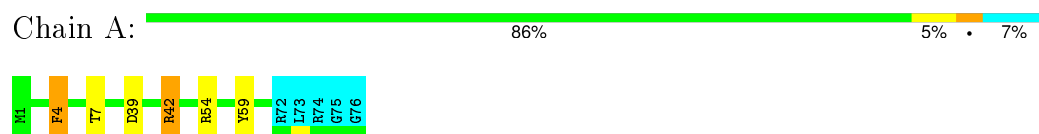
4.2.68 Score per residue for model 68

- Molecule 1: Ubiquitin



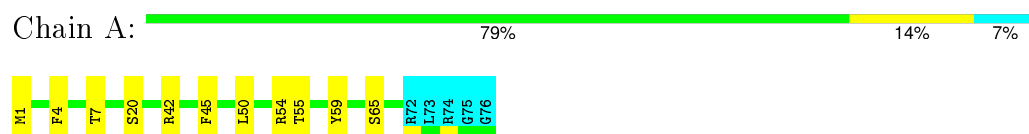
4.2.69 Score per residue for model 69

- Molecule 1: Ubiquitin



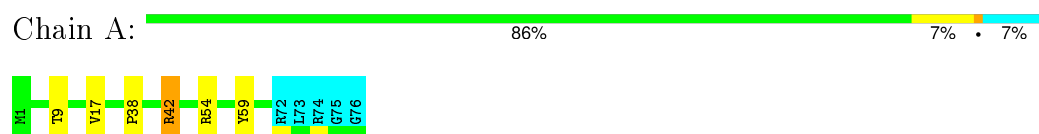
4.2.70 Score per residue for model 70

- Molecule 1: Ubiquitin



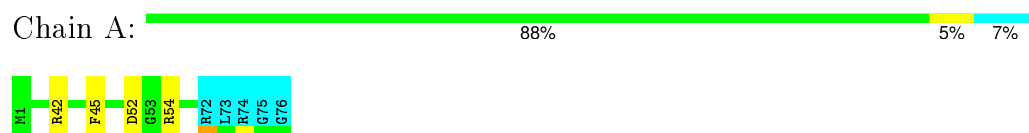
4.2.71 Score per residue for model 71

- 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

Chain A:  84% 9% 7%



4.2.74 Score per residue for model 74


- Molecule 1: Ubiquitin

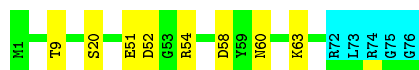
Chain A:  80% 11% 7%



4.2.75 Score per residue for model 75

- Molecule 1: Ubiquitin

Chain A:  83% 11% 7%



4.2.76 Score per residue for model 76 (medoid)


- Molecule 1: Ubiquitin

Chain A:  80% 13% 7%



4.2.77 Score per residue for model 77


- Molecule 1: Ubiquitin

Chain A:  82% 12% 7%



4.2.78 Score per residue for model 78


- Molecule 1: Ubiquitin

Chain A:  83% 9% 7%



4.2.79 Score per residue for model 79


- Molecule 1: Ubiquitin

Chain A:  83% 11% 7%



4.2.80 Score per residue for model 80


- Molecule 1: Ubiquitin

Chain A:  83% 11% 7%



4.2.81 Score per residue for model 81


- Molecule 1: Ubiquitin

Chain A:  88% 5% 7%



4.2.82 Score per residue for model 82

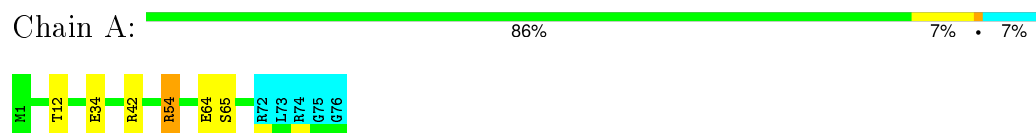
- Molecule 1: Ubiquitin

Chain A:  87% 7% 7%



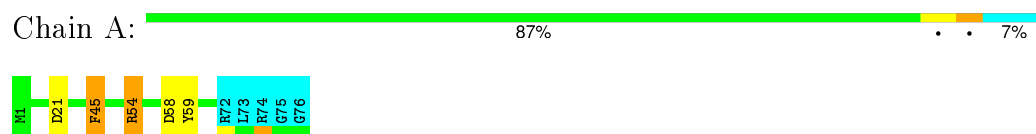
4.2.83 Score per residue for model 83

- Molecule 1: Ubiquitin



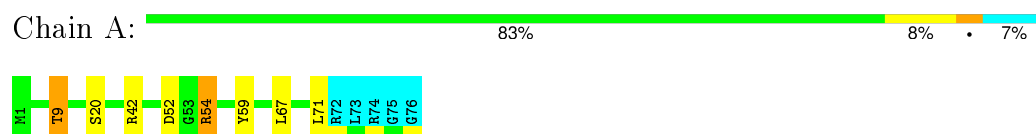
4.2.84 Score per residue for model 84

- Molecule 1: Ubiquitin



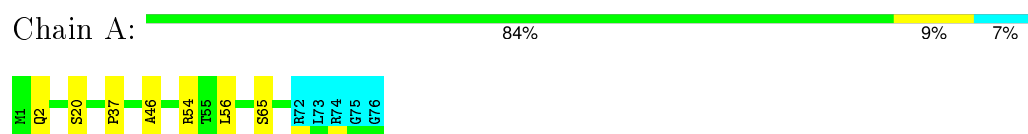
4.2.85 Score per residue for model 85

- Molecule 1: Ubiquitin



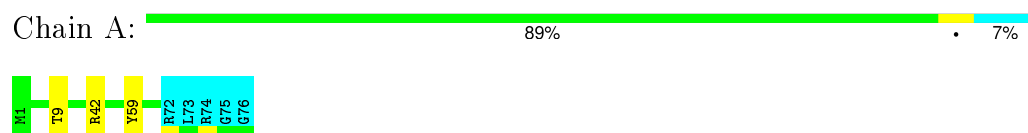
4.2.86 Score per residue for model 86

- Molecule 1: Ubiquitin



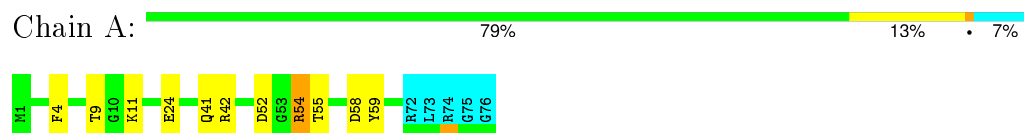
4.2.87 Score per residue for model 87

- Molecule 1: Ubiquitin



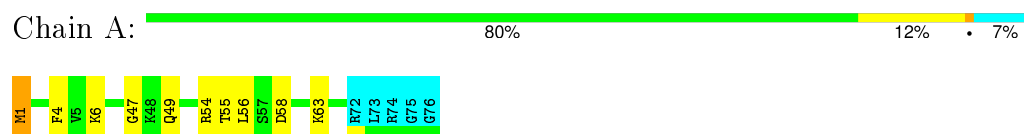
4.2.88 Score per residue for model 88

- Molecule 1: Ubiquitin



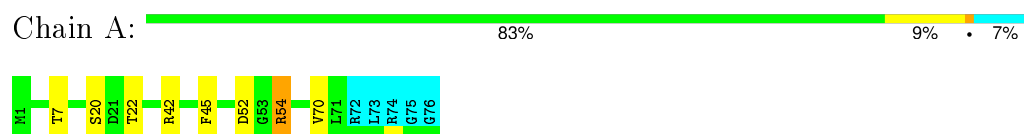
4.2.89 Score per residue for model 89

- Molecule 1: Ubiquitin



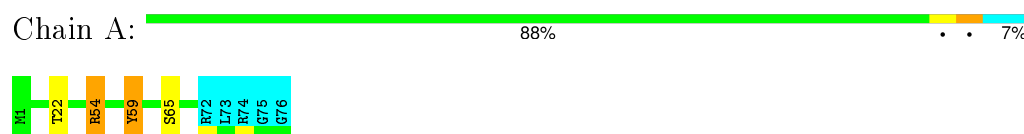
4.2.90 Score per residue for model 90

- Molecule 1: Ubiquitin



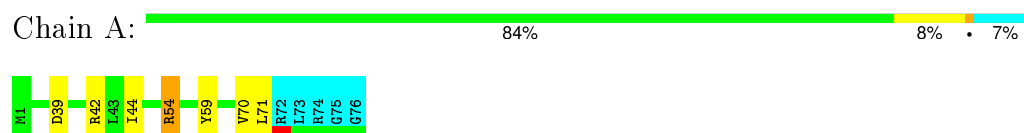
4.2.91 Score per residue for model 91

- Molecule 1: Ubiquitin



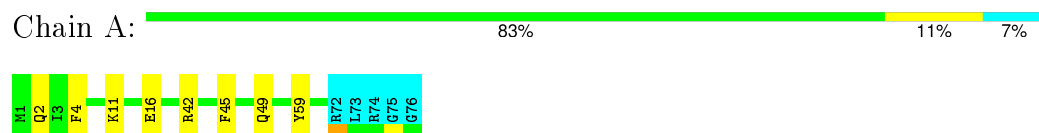
4.2.92 Score per residue for model 92

- Molecule 1: Ubiquitin



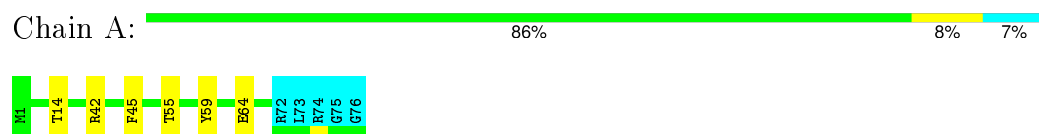
4.2.93 Score per residue for model 93

- Molecule 1: Ubiquitin



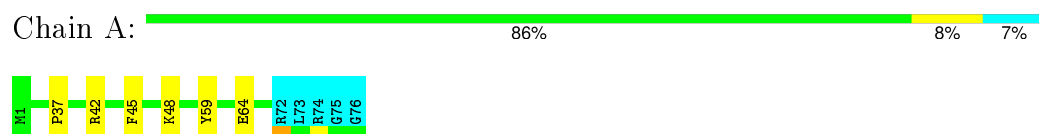
4.2.94 Score per residue for model 94

- Molecule 1: Ubiquitin



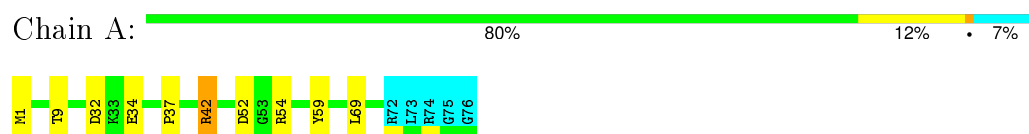
4.2.95 Score per residue for model 95

- Molecule 1: Ubiquitin



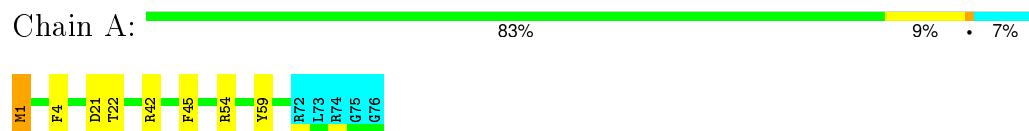
4.2.96 Score per residue for model 96

- 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

Chain A:  88% . . 7%



4.2.99 Score per residue for model 99


- Molecule 1: Ubiquitin

Chain A:  88% . . 7%



4.2.100 Score per residue for model 100


- Molecule 1: Ubiquitin

Chain A:  78% 16% 7%



4.2.101 Score per residue for model 101

- Molecule 1: Ubiquitin

Chain A:  86% 8% 7%



4.2.102 Score per residue for model 102

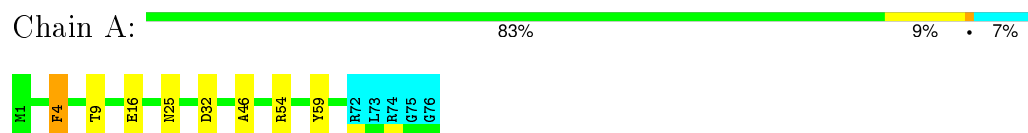
- Molecule 1: Ubiquitin

Chain A:  86% 8% 7%



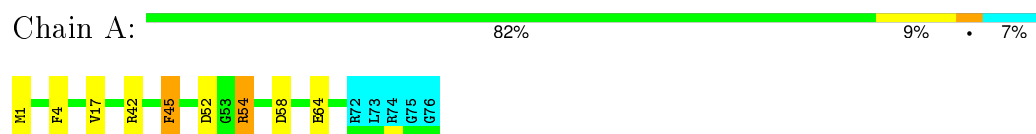
4.2.103 Score per residue for model 103

- Molecule 1: Ubiquitin



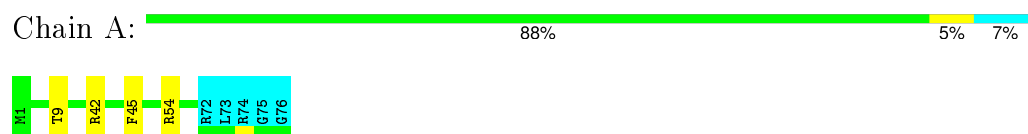
4.2.104 Score per residue for model 104

- Molecule 1: Ubiquitin



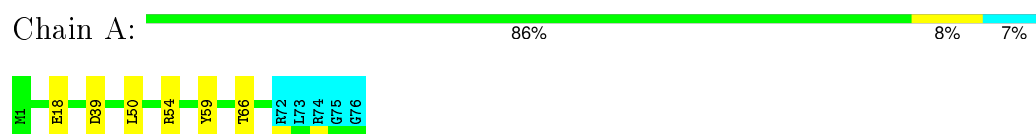
4.2.105 Score per residue for model 105

- Molecule 1: Ubiquitin



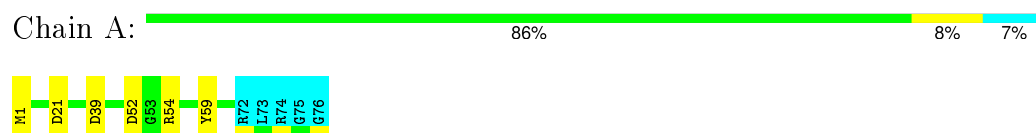
4.2.106 Score per residue for model 106

- Molecule 1: Ubiquitin




4.2.107 Score per residue for model 107

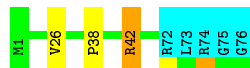
- Molecule 1: Ubiquitin



4.2.108 Score per residue for model 108


- Molecule 1: Ubiquitin

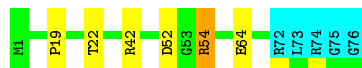
Chain A:  89% 7%



4.2.109 Score per residue for model 109


- Molecule 1: Ubiquitin

Chain A:  86% 7% 7%



4.2.110 Score per residue for model 110


- Molecule 1: Ubiquitin

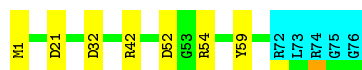
Chain A:  86% 8% 7%



4.2.111 Score per residue for model 111


- Molecule 1: Ubiquitin

Chain A:  84% 9% 7%



4.2.112 Score per residue for model 112

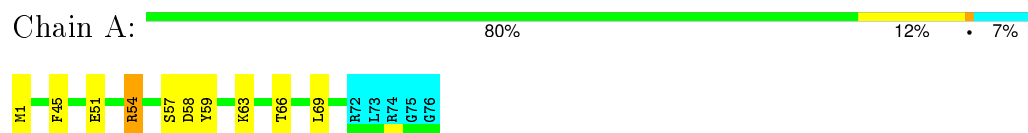
- Molecule 1: Ubiquitin

Chain A:  84% 9% 7%



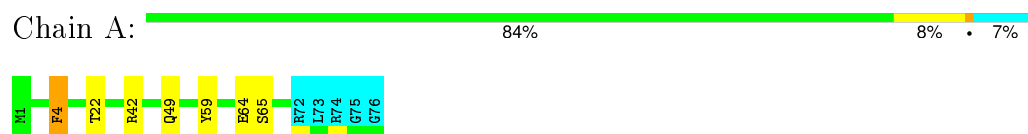
4.2.113 Score per residue for model 113

- Molecule 1: Ubiquitin



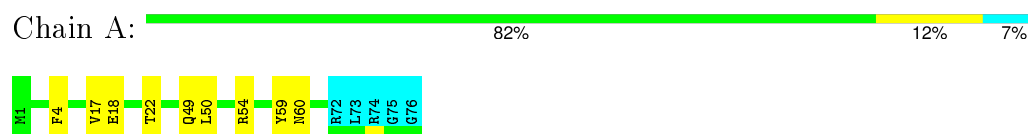
4.2.114 Score per residue for model 114

- Molecule 1: Ubiquitin



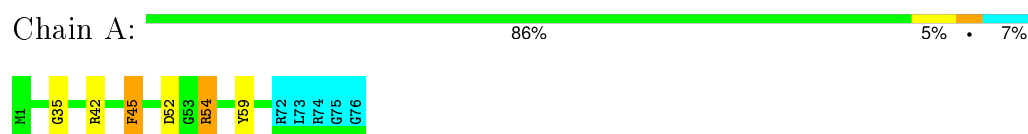
4.2.115 Score per residue for model 115

- Molecule 1: Ubiquitin



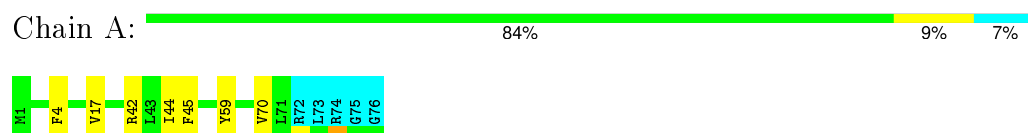
4.2.116 Score per residue for model 116

- Molecule 1: Ubiquitin



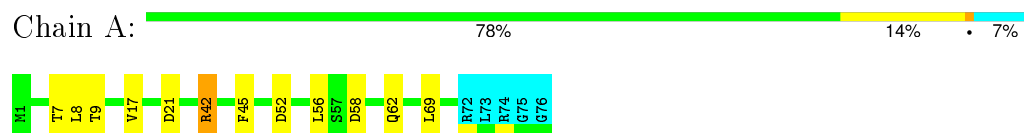
4.2.117 Score per residue for model 117

- Molecule 1: Ubiquitin



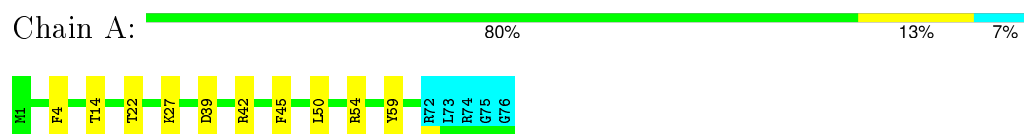
4.2.118 Score per residue for model 118

- Molecule 1: Ubiquitin



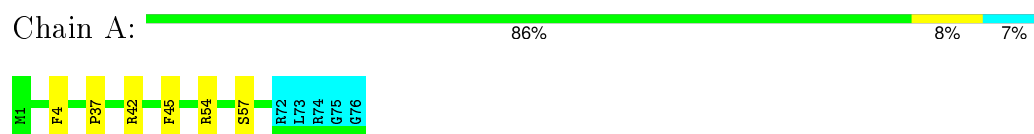
4.2.119 Score per residue for model 119

- Molecule 1: Ubiquitin



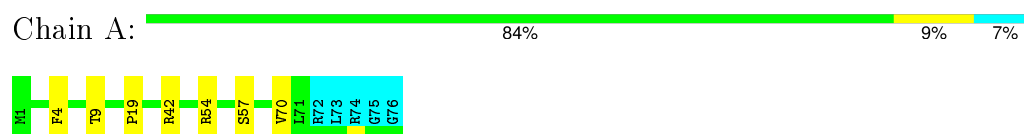
4.2.120 Score per residue for model 120

- Molecule 1: Ubiquitin



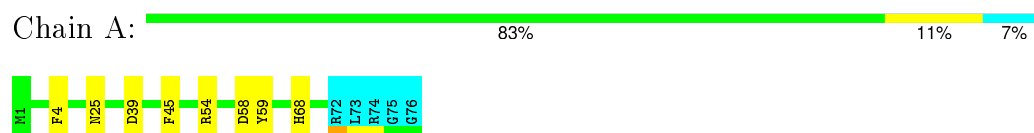
4.2.121 Score per residue for model 121

- Molecule 1: Ubiquitin



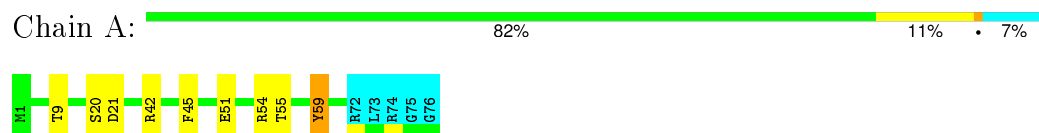
4.2.122 Score per residue for model 122

- Molecule 1: Ubiquitin



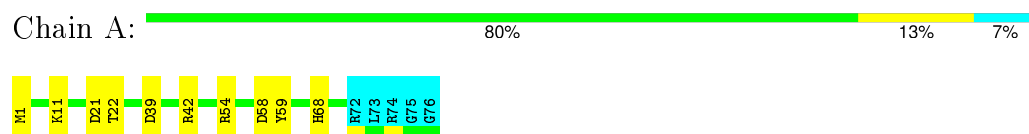
4.2.123 Score per residue for model 123

- Molecule 1: Ubiquitin



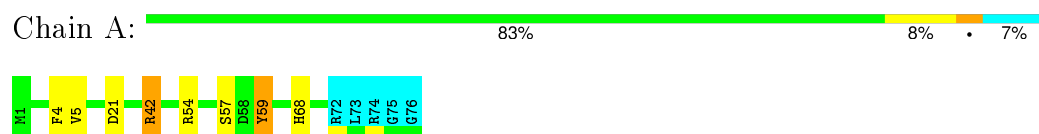
4.2.124 Score per residue for model 124

- Molecule 1: Ubiquitin



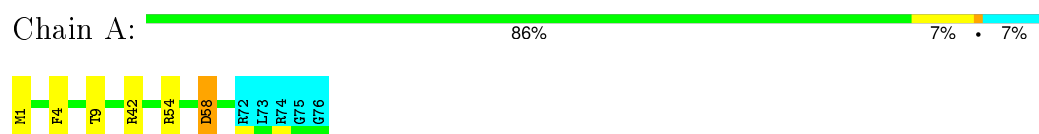
4.2.125 Score per residue for model 125

- Molecule 1: Ubiquitin



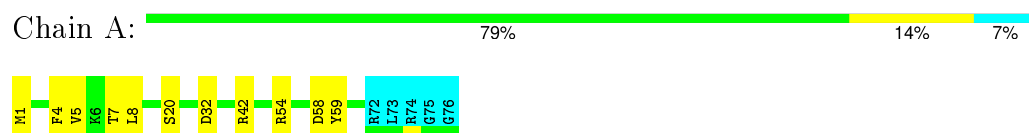
4.2.126 Score per residue for model 126

- 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

Chain A:  89% • • 7%



4.2.129 Score per residue for model 129


- Molecule 1: Ubiquitin

Chain A:  86% 7% • 7%



4.2.130 Score per residue for model 130


- Molecule 1: Ubiquitin

Chain A:  83% 11% 7%



4.2.131 Score per residue for model 131


- Molecule 1: Ubiquitin

Chain A:  82% 11% • 7%



4.2.132 Score per residue for model 132

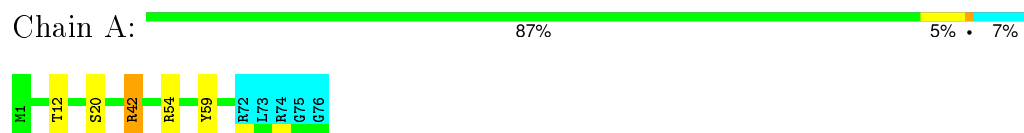
- Molecule 1: Ubiquitin

Chain A:  82% 12% 7%



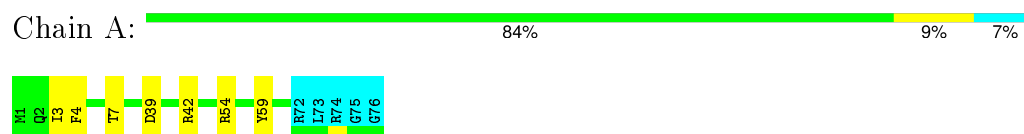
4.2.133 Score per residue for model 133

- Molecule 1: Ubiquitin



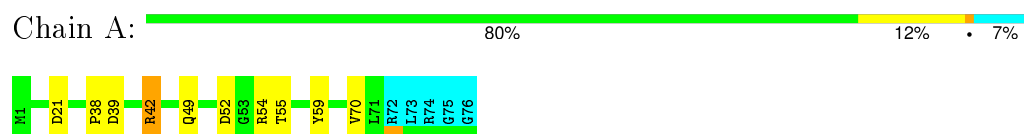
4.2.134 Score per residue for model 134

- Molecule 1: Ubiquitin



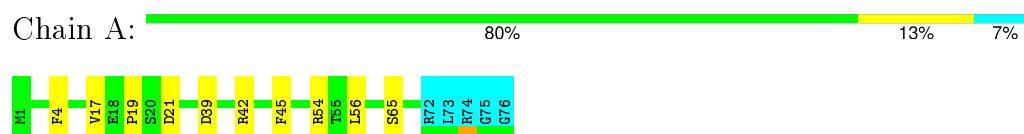
4.2.135 Score per residue for model 135

- Molecule 1: Ubiquitin



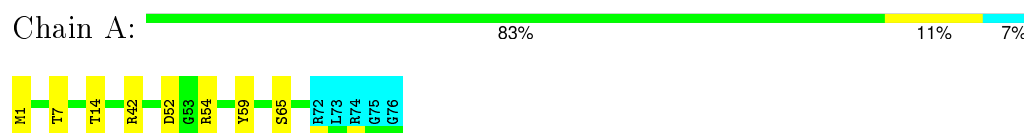
4.2.136 Score per residue for model 136

- Molecule 1: Ubiquitin



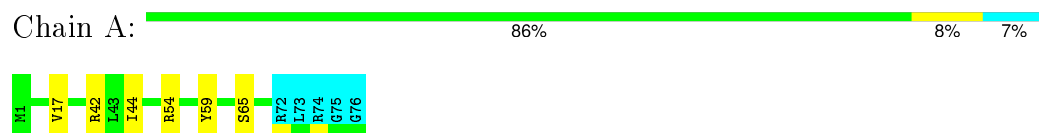
4.2.137 Score per residue for model 137

- Molecule 1: Ubiquitin



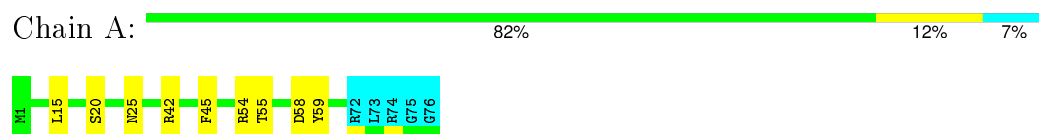
4.2.138 Score per residue for model 138

- Molecule 1: Ubiquitin



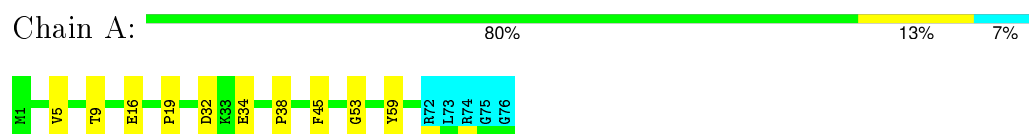
4.2.139 Score per residue for model 139

- Molecule 1: Ubiquitin



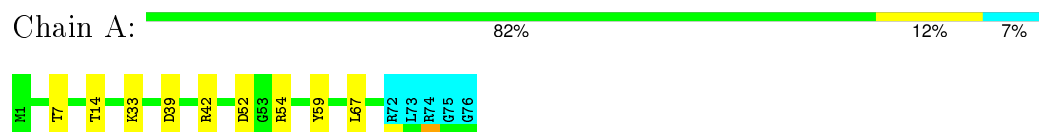
4.2.140 Score per residue for model 140

- Molecule 1: Ubiquitin



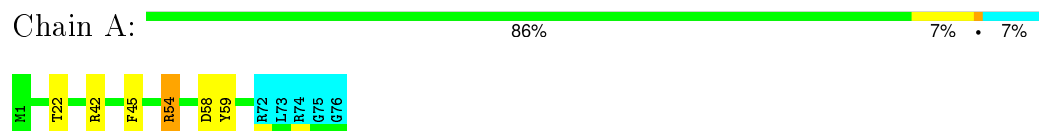
4.2.141 Score per residue for model 141

- Molecule 1: Ubiquitin



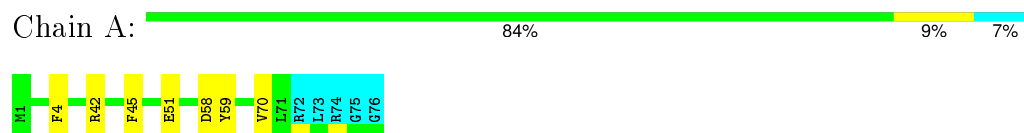
4.2.142 Score per residue for model 142

- Molecule 1: Ubiquitin



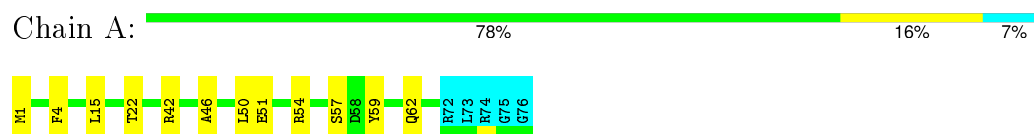
4.2.143 Score per residue for model 143

- Molecule 1: Ubiquitin



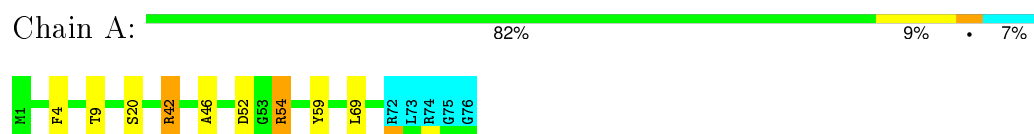
4.2.144 Score per residue for model 144

- Molecule 1: Ubiquitin



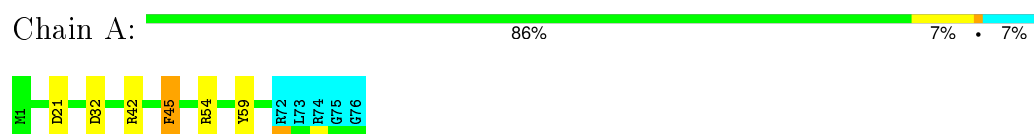
4.2.145 Score per residue for model 145

- Molecule 1: Ubiquitin



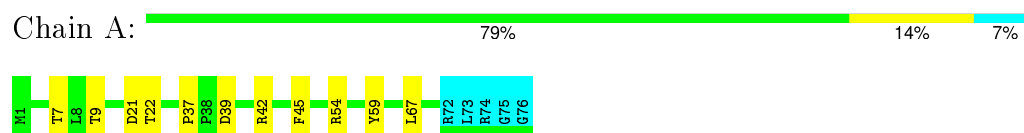
4.2.146 Score per residue for model 146

- 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

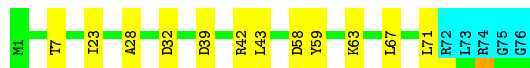
Chain A:  88% . . 7%



4.2.149 Score per residue for model 149


- Molecule 1: Ubiquitin

Chain A:  78% 16% 7%



4.2.150 Score per residue for model 150


- Molecule 1: Ubiquitin

Chain A:  88% . . 7%



4.2.151 Score per residue for model 151


- Molecule 1: Ubiquitin

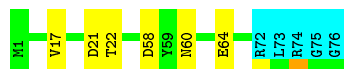
Chain A:  88% 5% 7%



4.2.152 Score per residue for model 152

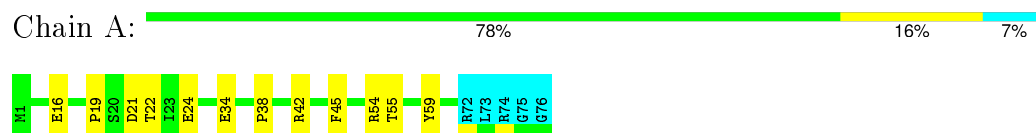
- Molecule 1: Ubiquitin

Chain A:  86% 8% 7%



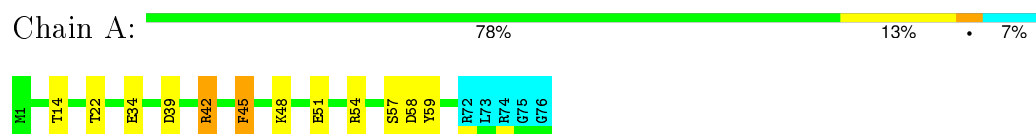
4.2.153 Score per residue for model 153

- Molecule 1: Ubiquitin



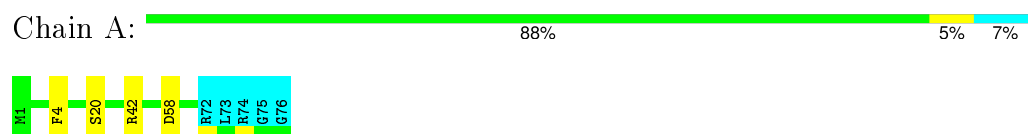
4.2.154 Score per residue for model 154

- Molecule 1: Ubiquitin



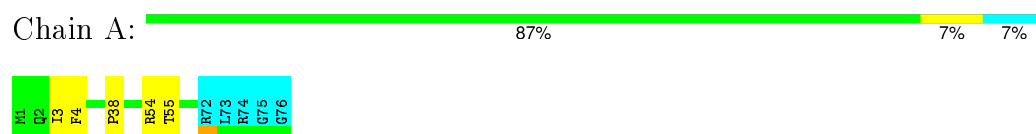
4.2.155 Score per residue for model 155

- Molecule 1: Ubiquitin



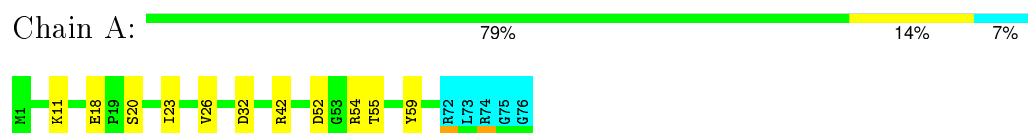
4.2.156 Score per residue for model 156

- Molecule 1: Ubiquitin



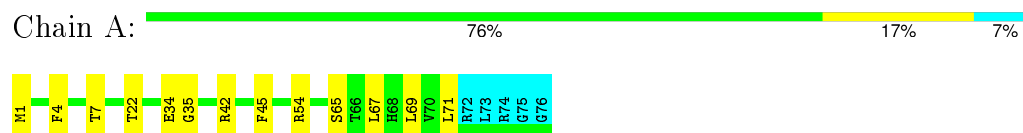
4.2.157 Score per residue for model 157

- Molecule 1: Ubiquitin



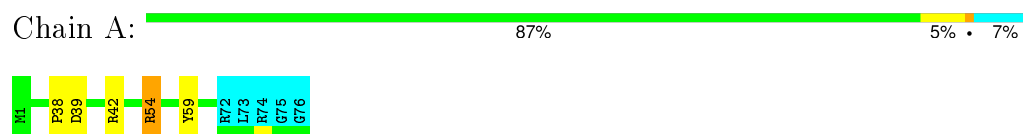
4.2.158 Score per residue for model 158

- Molecule 1: Ubiquitin



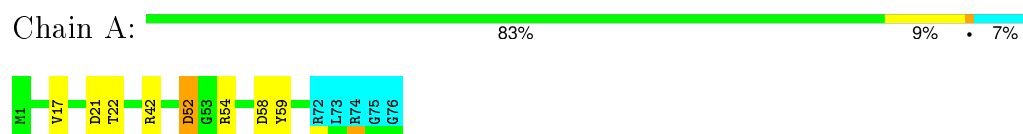
4.2.159 Score per residue for model 159

- Molecule 1: Ubiquitin



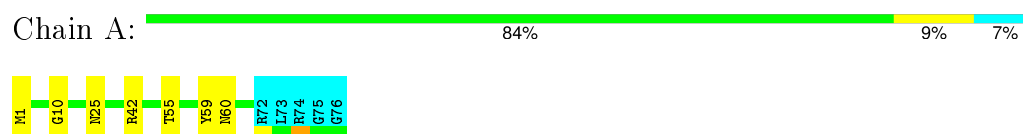
4.2.160 Score per residue for model 160

- Molecule 1: Ubiquitin



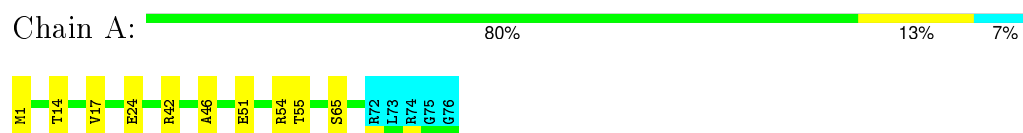
4.2.161 Score per residue for model 161

- Molecule 1: Ubiquitin



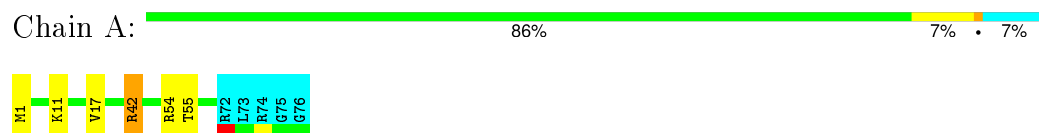
4.2.162 Score per residue for model 162

- Molecule 1: Ubiquitin



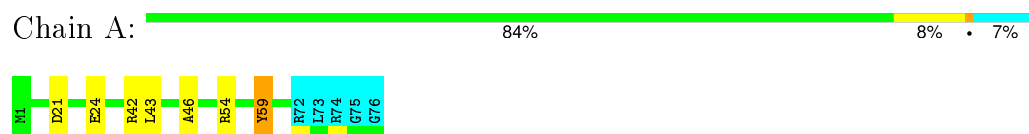
4.2.163 Score per residue for model 163

- Molecule 1: Ubiquitin



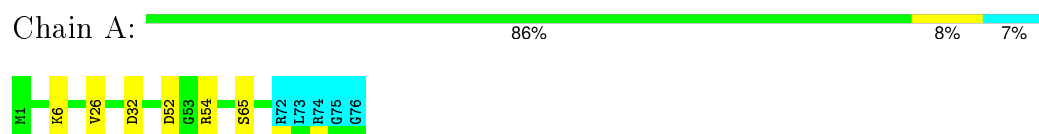
4.2.164 Score per residue for model 164

- Molecule 1: Ubiquitin



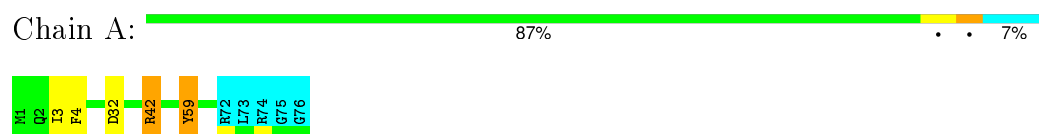
4.2.165 Score per residue for model 165

- Molecule 1: Ubiquitin



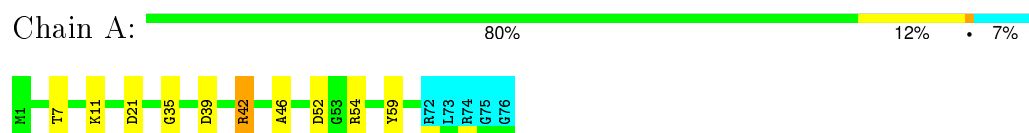
4.2.166 Score per residue for model 166

- Molecule 1: Ubiquitin



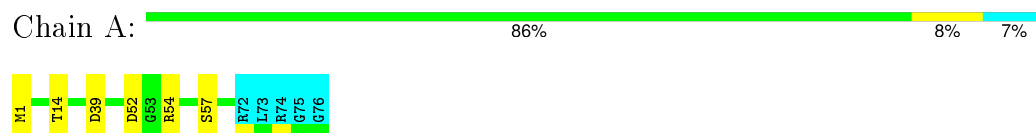
4.2.167 Score per residue for model 167

- Molecule 1: Ubiquitin



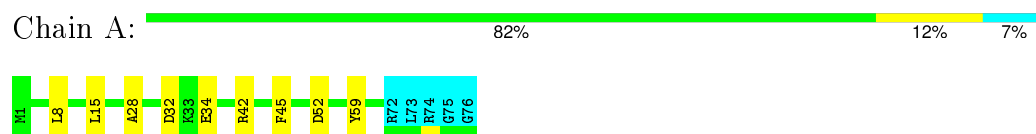
4.2.168 Score per residue for model 168

- Molecule 1: Ubiquitin



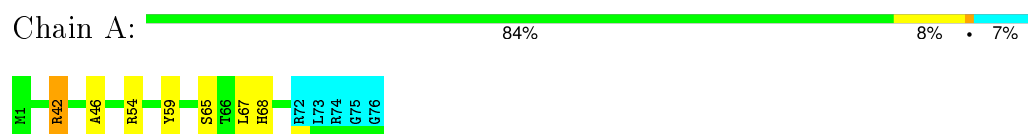
4.2.169 Score per residue for model 169

- Molecule 1: Ubiquitin



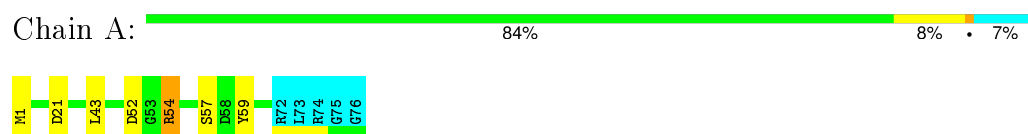
4.2.170 Score per residue for model 170

- Molecule 1: Ubiquitin



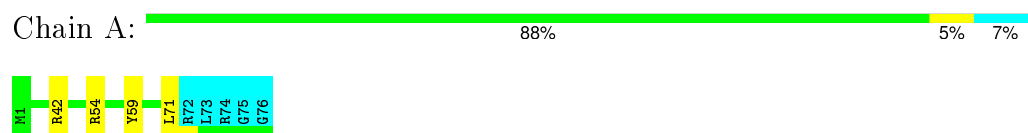
4.2.171 Score per residue for model 171

- Molecule 1: Ubiquitin



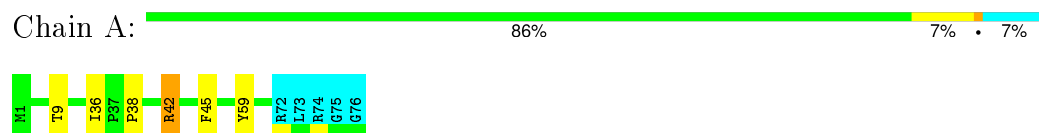
4.2.172 Score per residue for model 172

- Molecule 1: Ubiquitin



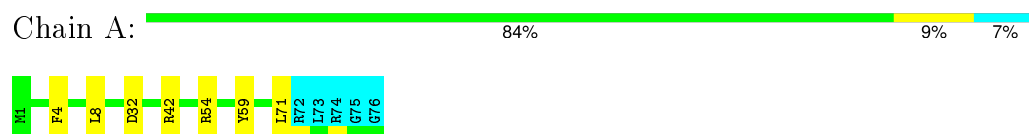
4.2.173 Score per residue for model 173

- Molecule 1: Ubiquitin



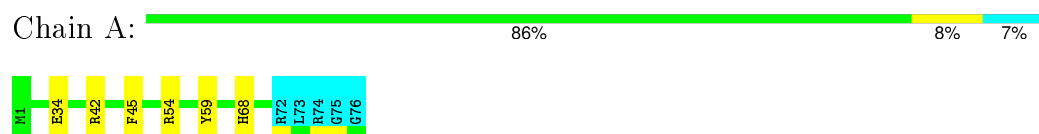
4.2.174 Score per residue for model 174

- Molecule 1: Ubiquitin



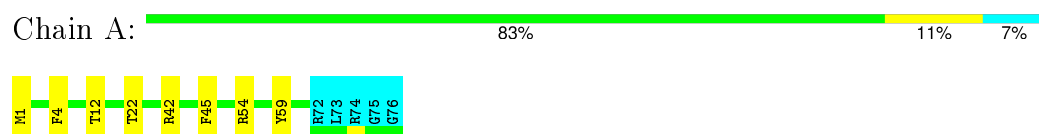
4.2.175 Score per residue for model 175

- Molecule 1: Ubiquitin



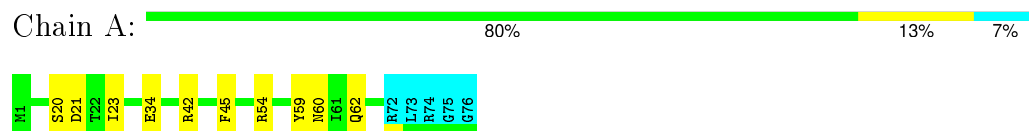
4.2.176 Score per residue for model 176

- Molecule 1: Ubiquitin



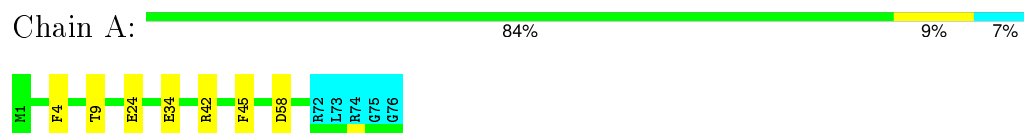
4.2.177 Score per residue for model 177

- Molecule 1: Ubiquitin



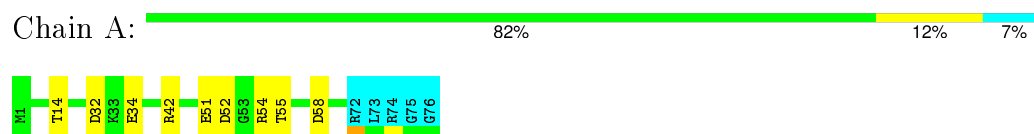
4.2.178 Score per residue for model 178

- Molecule 1: Ubiquitin



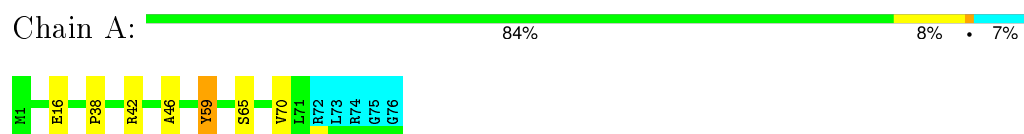
4.2.179 Score per residue for model 179

- Molecule 1: Ubiquitin



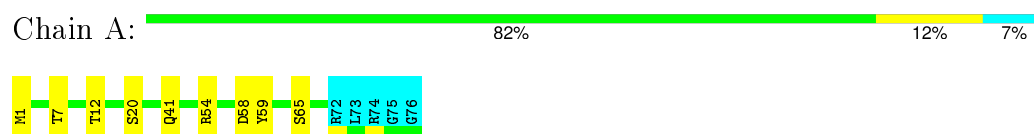
4.2.180 Score per residue for model 180

- Molecule 1: Ubiquitin



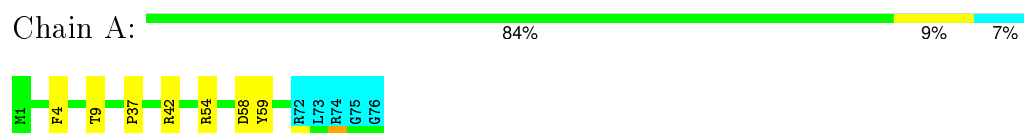
4.2.181 Score per residue for model 181

- Molecule 1: Ubiquitin



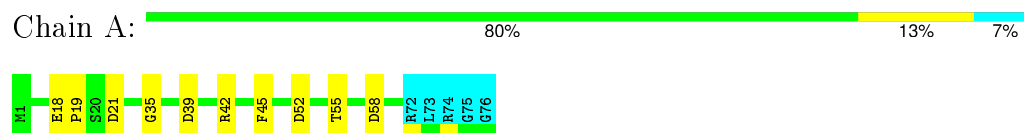
4.2.182 Score per residue for model 182

- Molecule 1: Ubiquitin



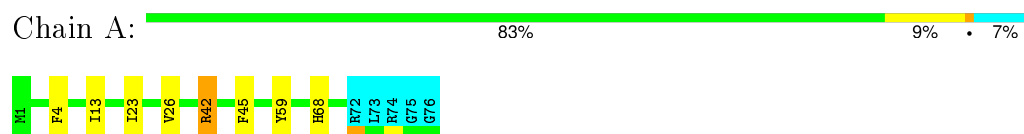
4.2.183 Score per residue for model 183

- Molecule 1: Ubiquitin



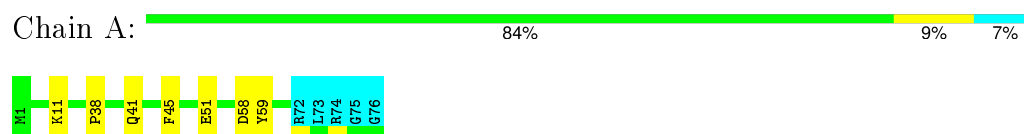
4.2.184 Score per residue for model 184

- Molecule 1: Ubiquitin



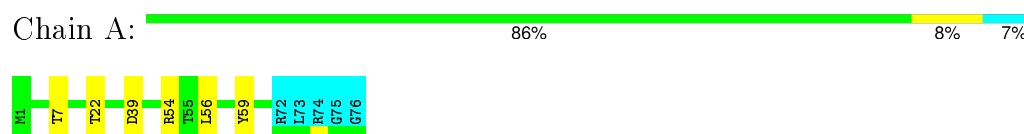
4.2.185 Score per residue for model 185

- Molecule 1: Ubiquitin



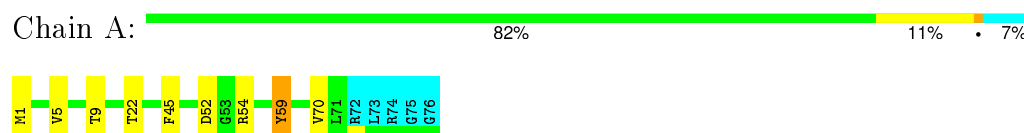
4.2.186 Score per residue for model 186

- Molecule 1: Ubiquitin



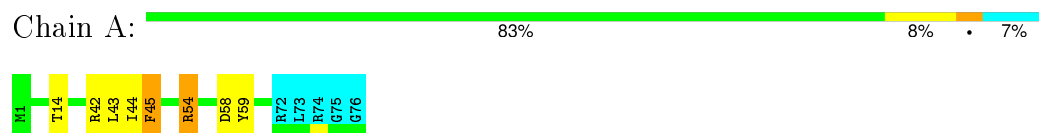
4.2.187 Score per residue for model 187

- Molecule 1: Ubiquitin



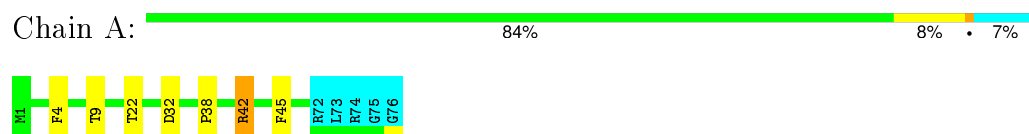
4.2.188 Score per residue for model 188

- Molecule 1: Ubiquitin



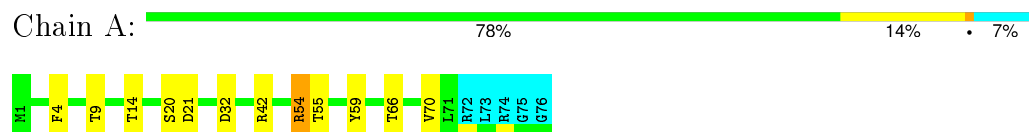
4.2.189 Score per residue for model 189

- Molecule 1: Ubiquitin



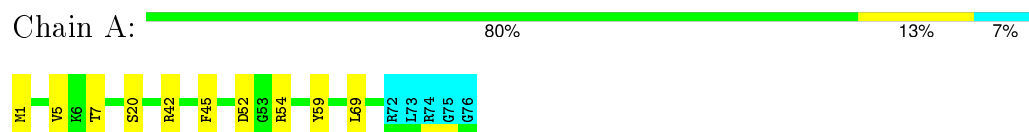
4.2.190 Score per residue for model 190

- Molecule 1: Ubiquitin



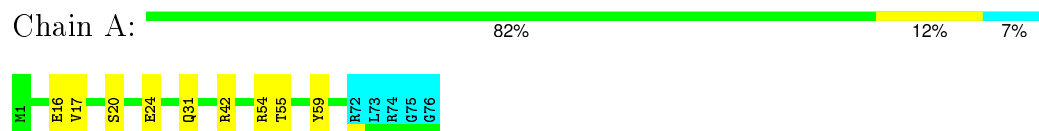
4.2.191 Score per residue for model 191

- Molecule 1: Ubiquitin



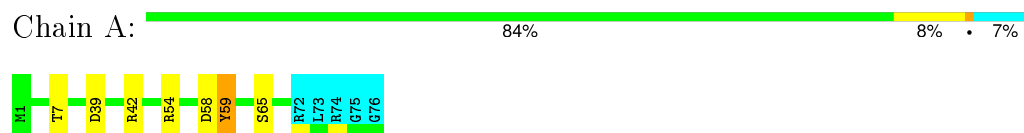
4.2.192 Score per residue for model 192

- Molecule 1: Ubiquitin



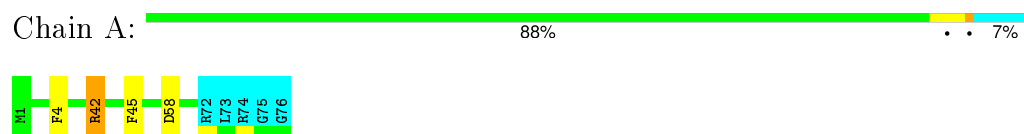
4.2.193 Score per residue for model 193

- Molecule 1: Ubiquitin



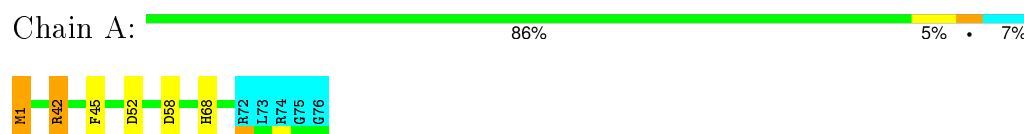
4.2.194 Score per residue for model 194

- Molecule 1: Ubiquitin



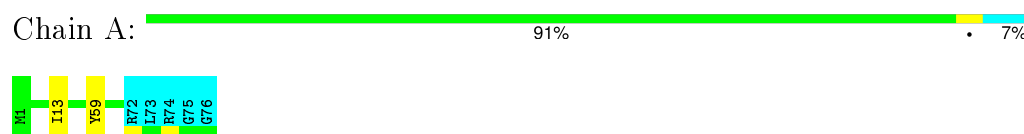
4.2.195 Score per residue for model 195

- Molecule 1: Ubiquitin



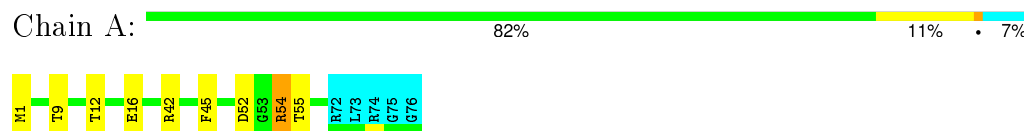
4.2.196 Score per residue for model 196

- Molecule 1: Ubiquitin



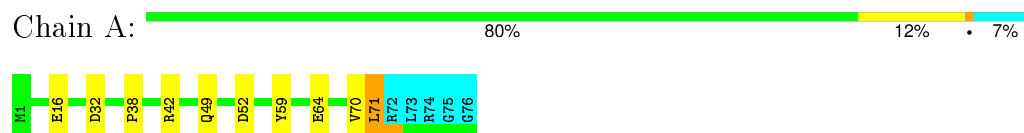
4.2.197 Score per residue for model 197

- Molecule 1: Ubiquitin



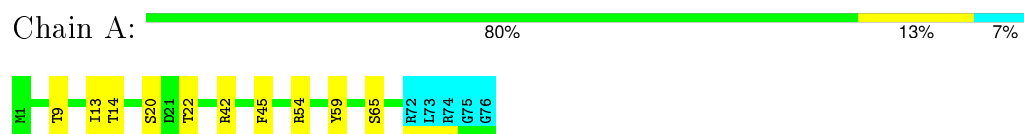
4.2.198 Score per residue for model 198

- Molecule 1: Ubiquitin



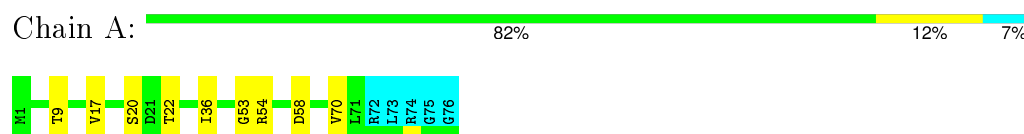
4.2.199 Score per residue for model 199

- Molecule 1: Ubiquitin



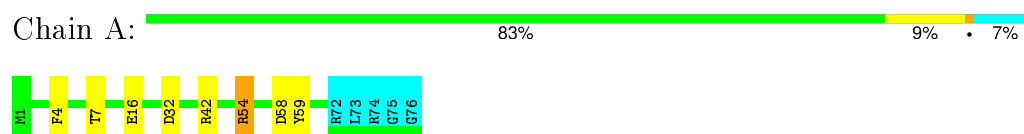
4.2.200 Score per residue for model 200

- Molecule 1: Ubiquitin



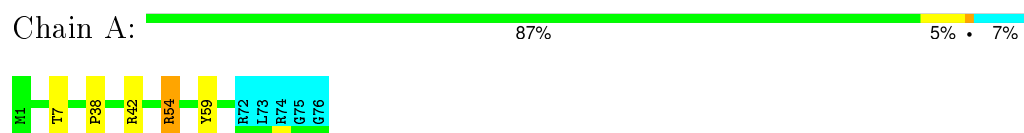
4.2.201 Score per residue for model 201

- Molecule 1: Ubiquitin



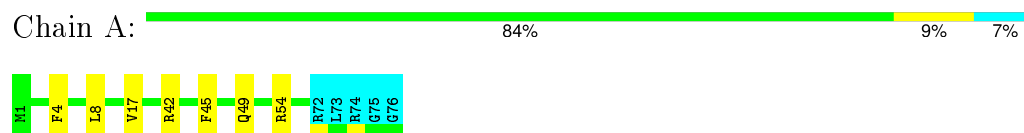
4.2.202 Score per residue for model 202

- Molecule 1: Ubiquitin



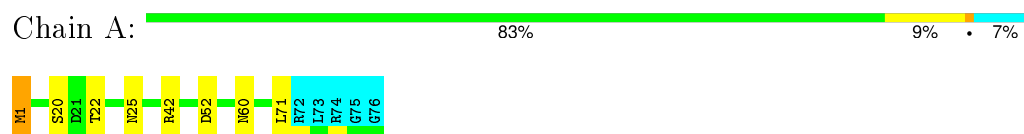
4.2.203 Score per residue for model 203

- Molecule 1: Ubiquitin



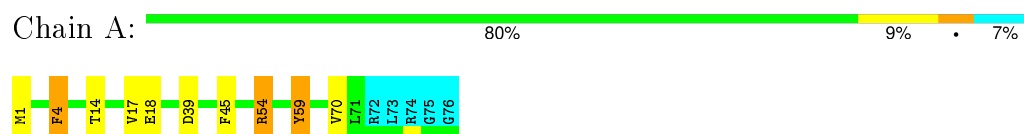
4.2.204 Score per residue for model 204

- Molecule 1: Ubiquitin



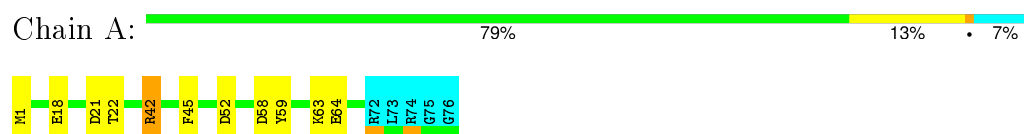
4.2.205 Score per residue for model 205

- Molecule 1: Ubiquitin



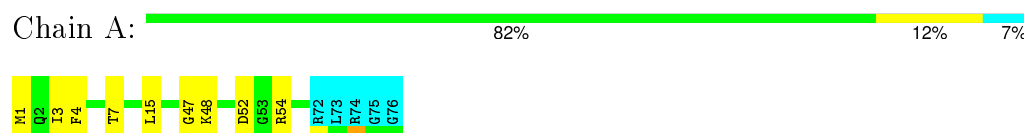
4.2.206 Score per residue for model 206

- Molecule 1: Ubiquitin




4.2.207 Score per residue for model 207

- Molecule 1: Ubiquitin



4.2.208 Score per residue for model 208

- Molecule 1: Ubiquitin

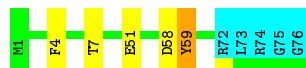
Chain A:  86% 7% • 7%



4.2.209 Score per residue for model 209


- Molecule 1: Ubiquitin

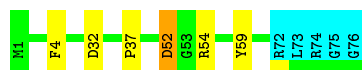
Chain A:  87% 5% • 7%



4.2.210 Score per residue for model 210


- Molecule 1: Ubiquitin

Chain A:  86% 7% • 7%



4.2.211 Score per residue for model 211


- Molecule 1: Ubiquitin

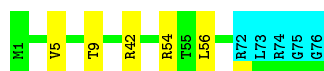
Chain A:  89% • 7%



4.2.212 Score per residue for model 212

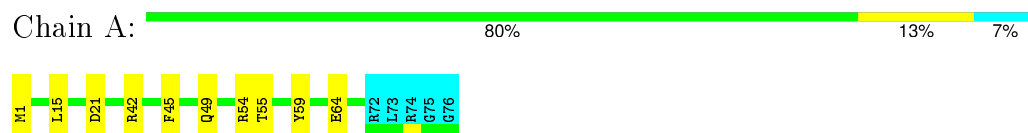
- Molecule 1: Ubiquitin

Chain A:  87% 7% 7%



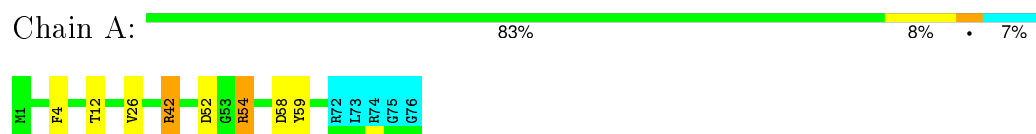
4.2.213 Score per residue for model 213

- Molecule 1: Ubiquitin



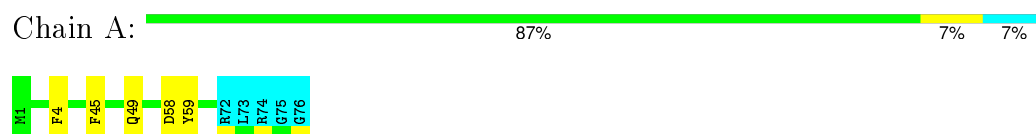
4.2.214 Score per residue for model 214

- Molecule 1: Ubiquitin



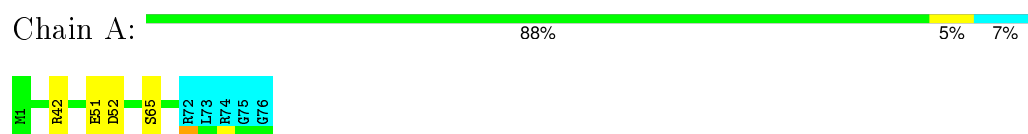
4.2.215 Score per residue for model 215

- Molecule 1: Ubiquitin



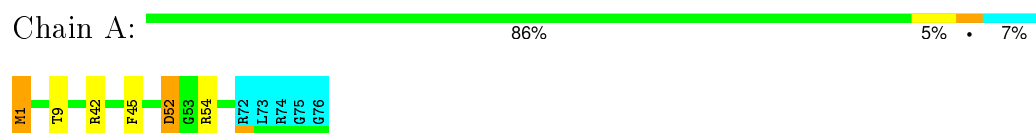
4.2.216 Score per residue for model 216

- Molecule 1: Ubiquitin



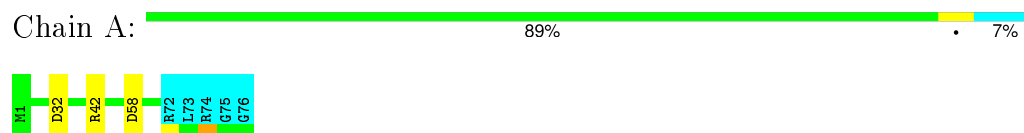
4.2.217 Score per residue for model 217

- Molecule 1: Ubiquitin



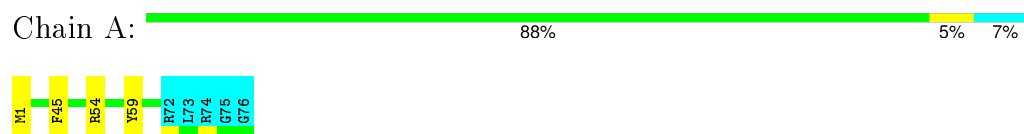
4.2.218 Score per residue for model 218

- Molecule 1: Ubiquitin



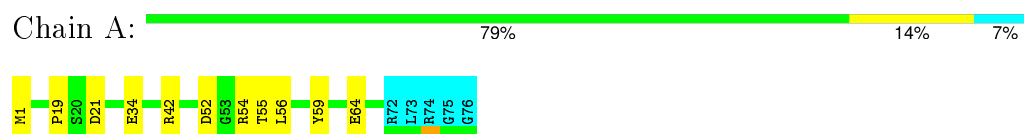
4.2.219 Score per residue for model 219

- Molecule 1: Ubiquitin



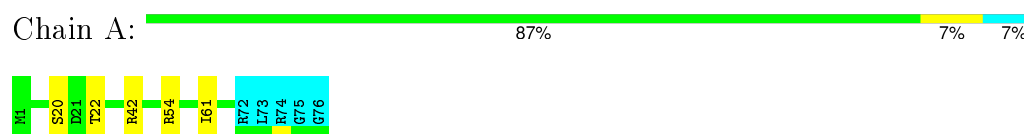
4.2.220 Score per residue for model 220

- Molecule 1: Ubiquitin



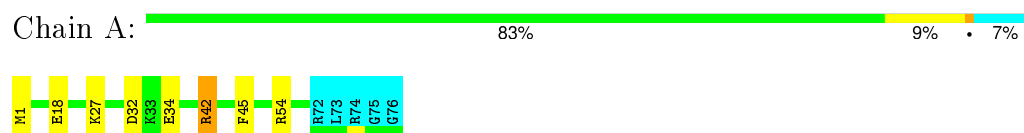
4.2.221 Score per residue for model 221

- Molecule 1: Ubiquitin



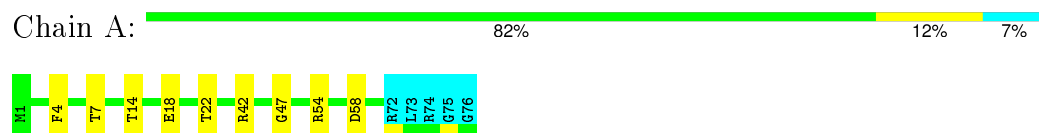
4.2.222 Score per residue for model 222

- Molecule 1: Ubiquitin



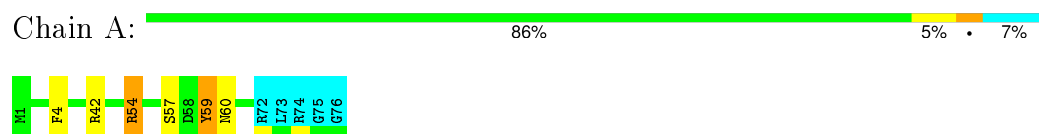
4.2.223 Score per residue for model 223

- Molecule 1: Ubiquitin



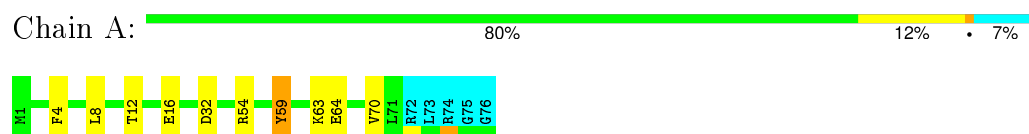
4.2.224 Score per residue for model 224

- Molecule 1: Ubiquitin



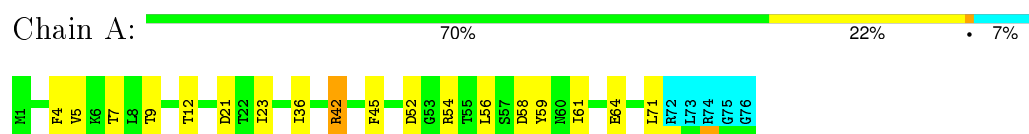
4.2.225 Score per residue for model 225

- Molecule 1: Ubiquitin



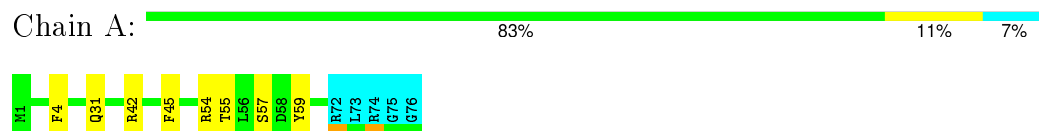
4.2.226 Score per residue for model 226

- Molecule 1: Ubiquitin



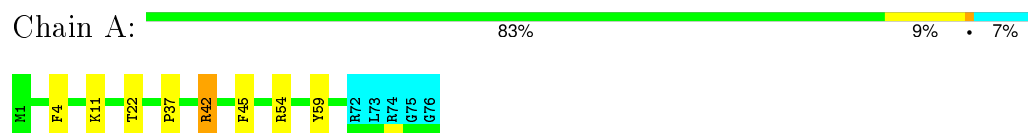
4.2.227 Score per residue for model 227

- Molecule 1: Ubiquitin



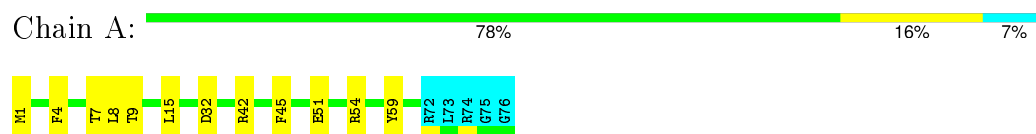
4.2.228 Score per residue for model 228

- Molecule 1: Ubiquitin



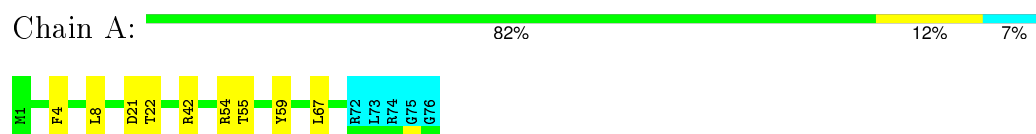
4.2.229 Score per residue for model 229

- Molecule 1: Ubiquitin



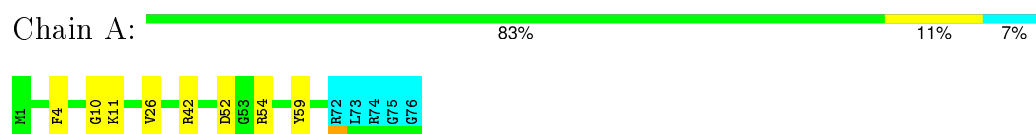
4.2.230 Score per residue for model 230

- Molecule 1: Ubiquitin



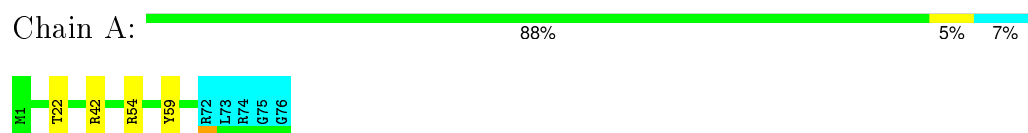
4.2.231 Score per residue for model 231

- Molecule 1: Ubiquitin



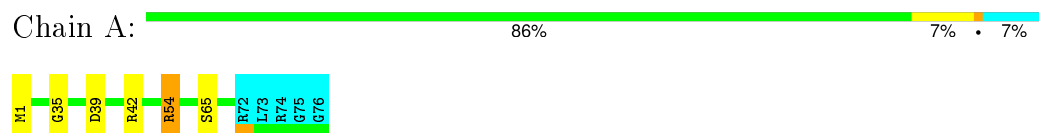
4.2.232 Score per residue for model 232

- Molecule 1: Ubiquitin



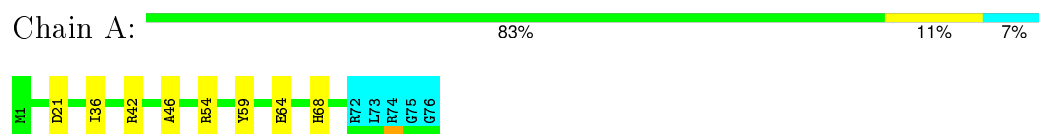
4.2.233 Score per residue for model 233

- Molecule 1: Ubiquitin



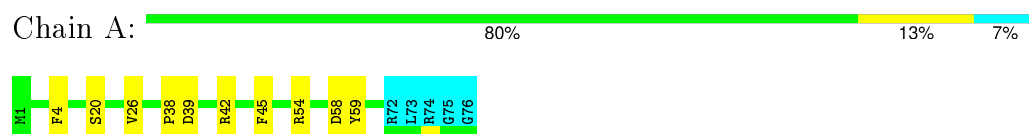
4.2.234 Score per residue for model 234

- Molecule 1: Ubiquitin



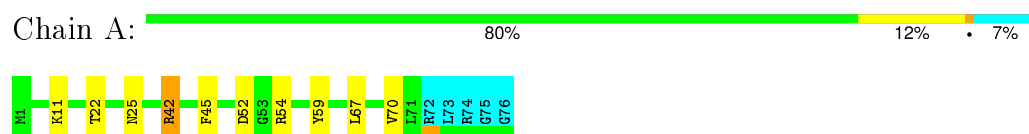
4.2.235 Score per residue for model 235

- Molecule 1: Ubiquitin



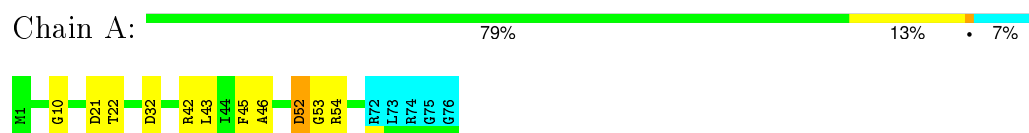
4.2.236 Score per residue for model 236

- Molecule 1: Ubiquitin



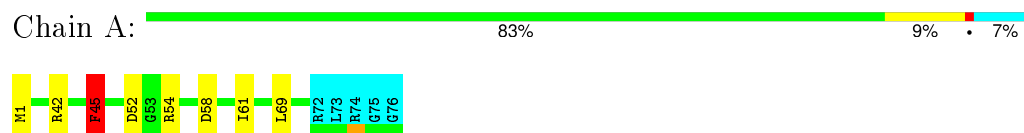
4.2.237 Score per residue for model 237

- Molecule 1: Ubiquitin



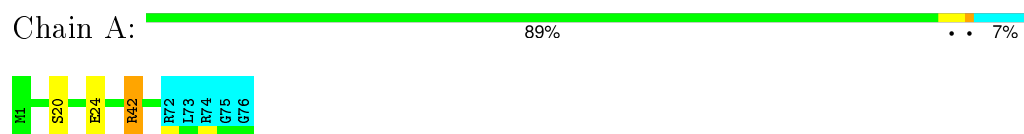
4.2.238 Score per residue for model 238

- Molecule 1: Ubiquitin



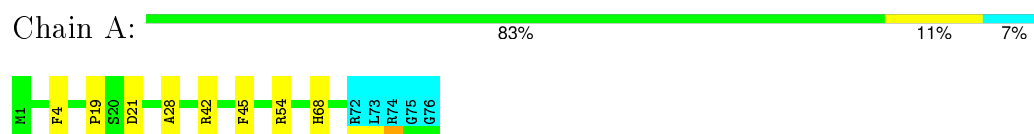
4.2.239 Score per residue for model 239

- Molecule 1: Ubiquitin



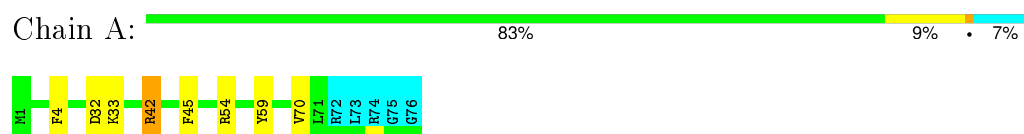
4.2.240 Score per residue for model 240

- Molecule 1: Ubiquitin



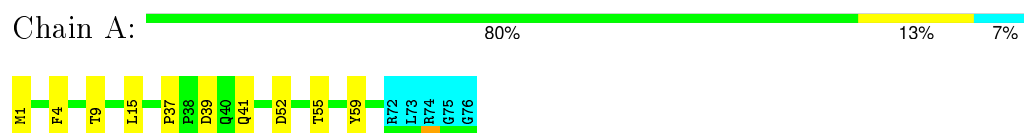
4.2.241 Score per residue for model 241

- Molecule 1: Ubiquitin



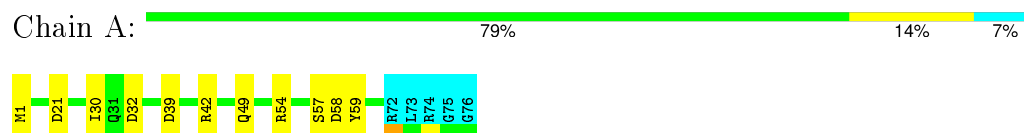
4.2.242 Score per residue for model 242

- Molecule 1: Ubiquitin



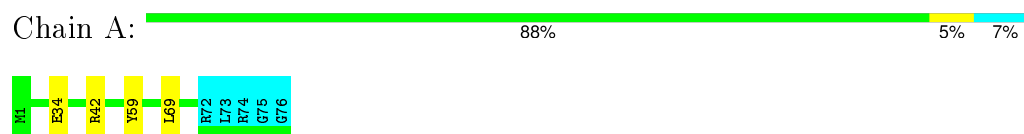
4.2.243 Score per residue for model 243

- Molecule 1: Ubiquitin



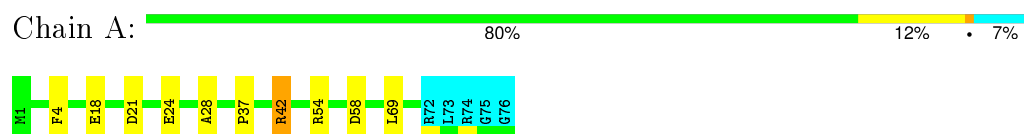
4.2.244 Score per residue for model 244

- Molecule 1: Ubiquitin



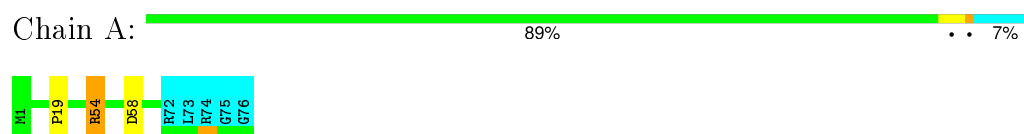
4.2.245 Score per residue for model 245

- Molecule 1: Ubiquitin



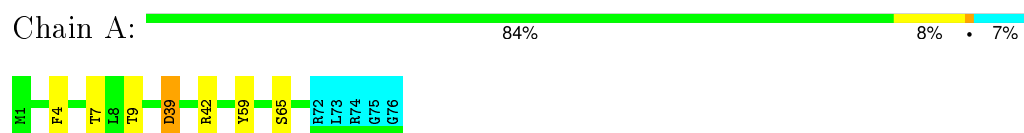
4.2.246 Score per residue for model 246

- Molecule 1: Ubiquitin



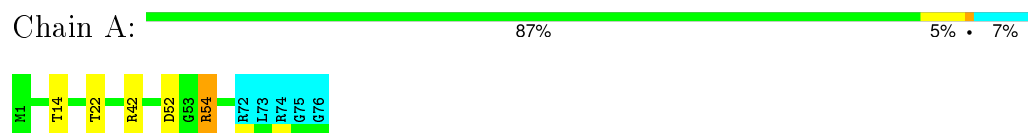
4.2.247 Score per residue for model 247

- Molecule 1: Ubiquitin



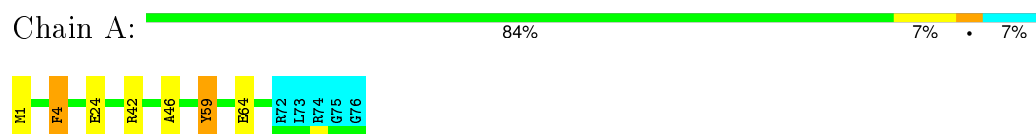
4.2.248 Score per residue for model 248

- Molecule 1: Ubiquitin



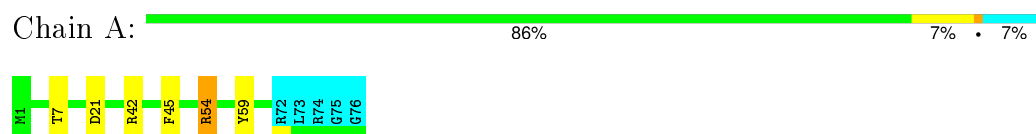
4.2.249 Score per residue for model 249

- Molecule 1: Ubiquitin



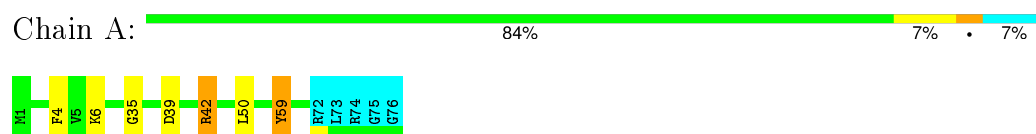
4.2.250 Score per residue for model 250

- Molecule 1: Ubiquitin



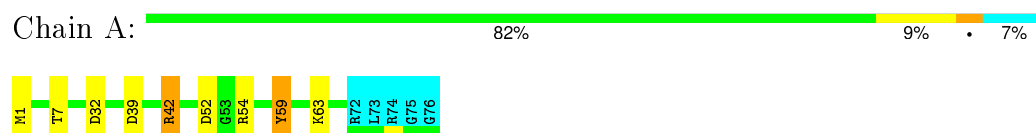
4.2.251 Score per residue for model 251

- Molecule 1: Ubiquitin



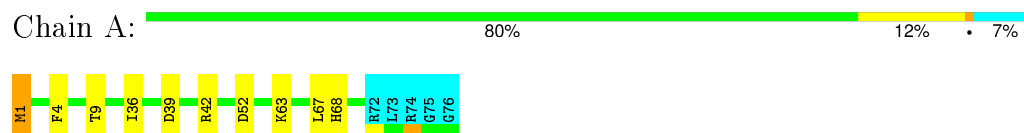
4.2.252 Score per residue for model 252

- Molecule 1: Ubiquitin



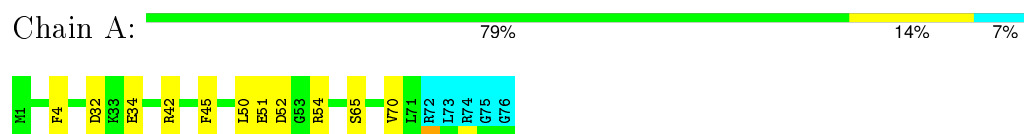
4.2.253 Score per residue for model 253

- Molecule 1: Ubiquitin



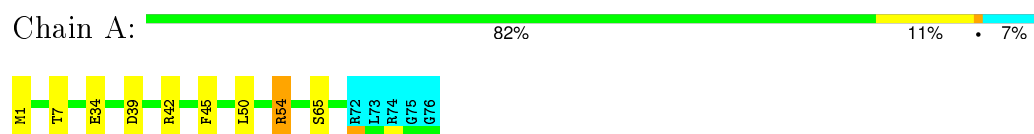
4.2.254 Score per residue for model 254

- Molecule 1: Ubiquitin



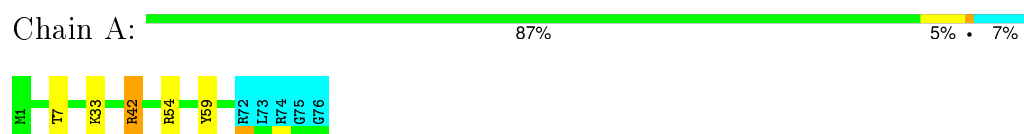
4.2.255 Score per residue for model 255

- Molecule 1: Ubiquitin



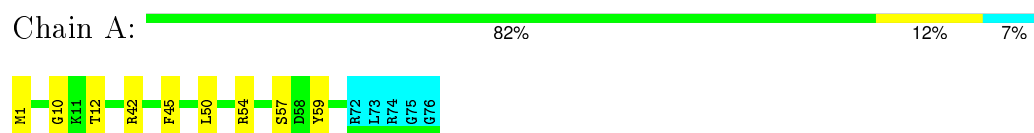
4.2.256 Score per residue for model 256

- Molecule 1: Ubiquitin



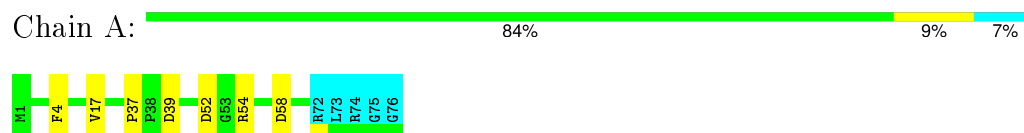
4.2.257 Score per residue for model 257

- Molecule 1: Ubiquitin



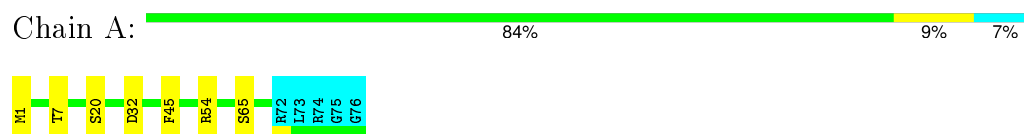
4.2.258 Score per residue for model 258

- Molecule 1: Ubiquitin



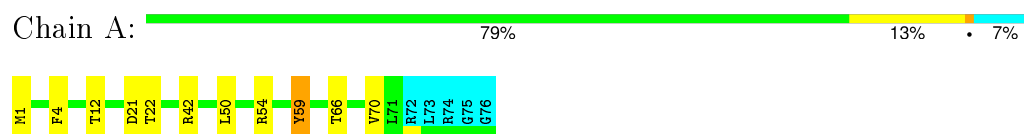
4.2.259 Score per residue for model 259

- Molecule 1: Ubiquitin



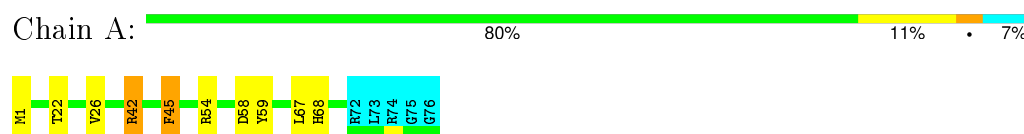
4.2.260 Score per residue for model 260

- Molecule 1: Ubiquitin



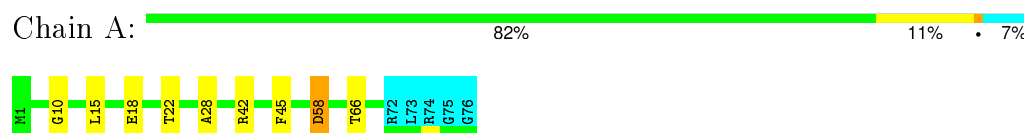
4.2.261 Score per residue for model 261

- Molecule 1: Ubiquitin



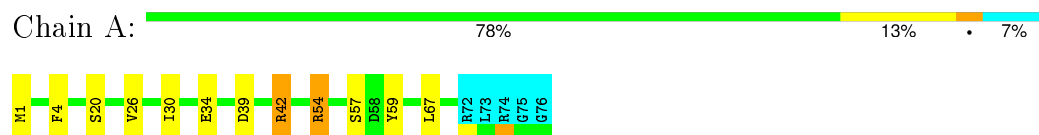
4.2.262 Score per residue for model 262

- Molecule 1: Ubiquitin



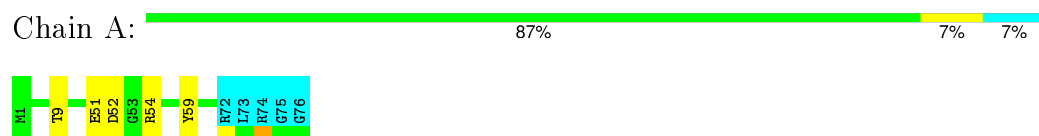
4.2.263 Score per residue for model 263

- Molecule 1: Ubiquitin



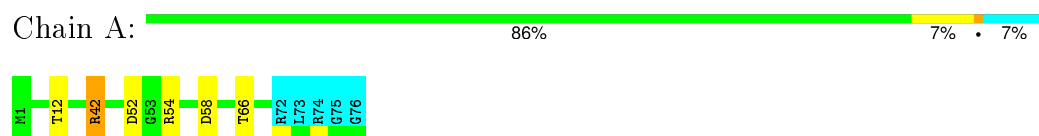
4.2.264 Score per residue for model 264

- Molecule 1: Ubiquitin



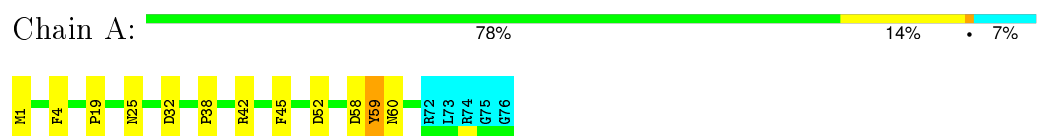
4.2.265 Score per residue for model 265

- Molecule 1: Ubiquitin



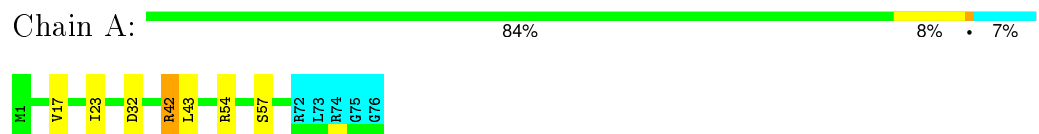
4.2.266 Score per residue for model 266

- Molecule 1: Ubiquitin



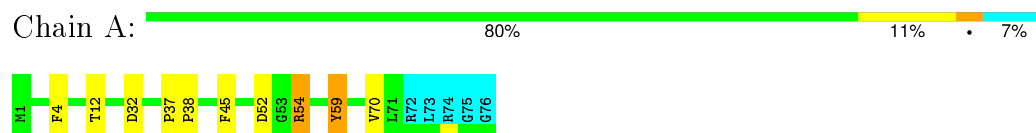
4.2.267 Score per residue for model 267

- Molecule 1: Ubiquitin



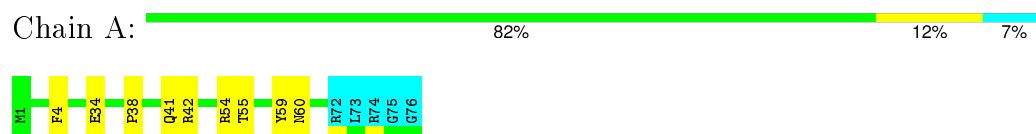
4.2.268 Score per residue for model 268

- Molecule 1: Ubiquitin



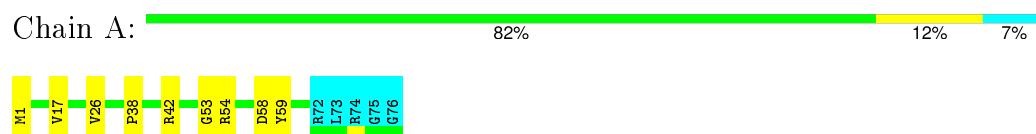
4.2.269 Score per residue for model 269

- Molecule 1: Ubiquitin



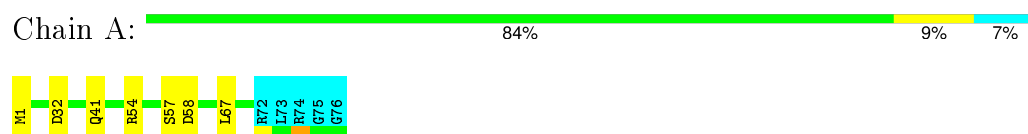
4.2.270 Score per residue for model 270

- Molecule 1: Ubiquitin



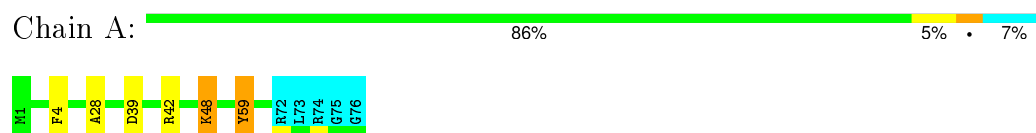
4.2.271 Score per residue for model 271

- Molecule 1: Ubiquitin



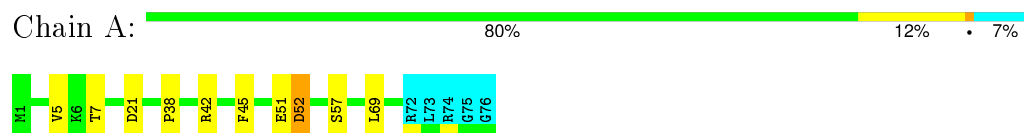
4.2.272 Score per residue for model 272

- Molecule 1: Ubiquitin



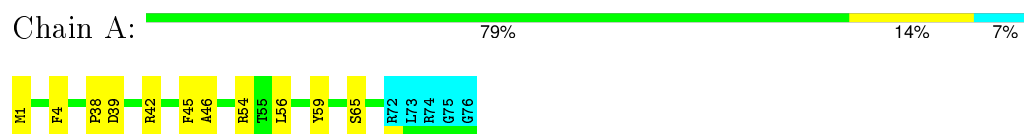
4.2.273 Score per residue for model 273

- Molecule 1: Ubiquitin



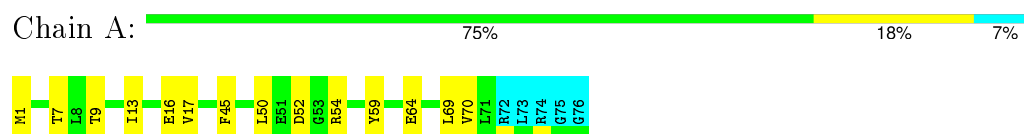
4.2.274 Score per residue for model 274

- Molecule 1: Ubiquitin



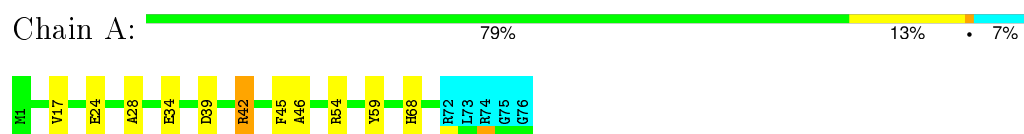
4.2.275 Score per residue for model 275

- Molecule 1: Ubiquitin



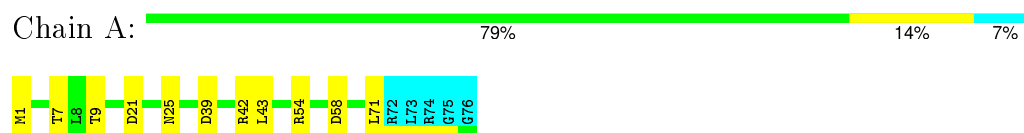
4.2.276 Score per residue for model 276

- Molecule 1: Ubiquitin



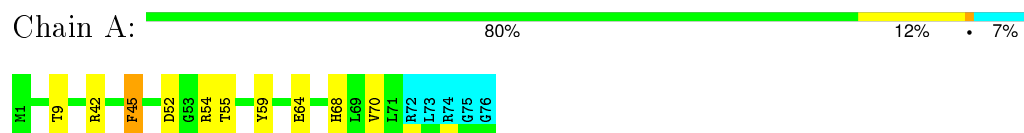
4.2.277 Score per residue for model 277

- Molecule 1: Ubiquitin



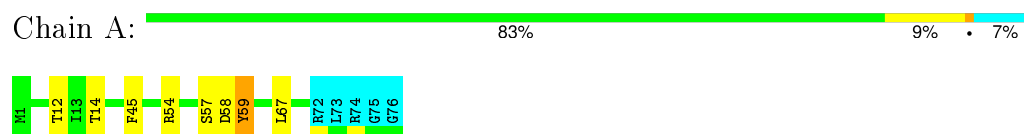
4.2.278 Score per residue for model 278

- Molecule 1: Ubiquitin



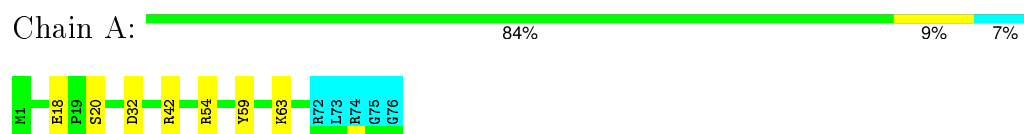
4.2.279 Score per residue for model 279

- Molecule 1: Ubiquitin



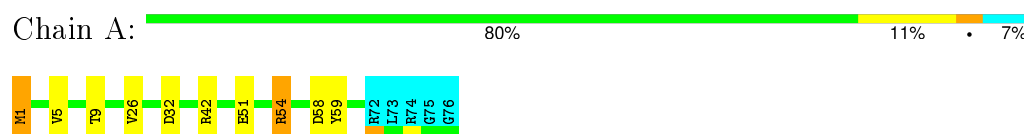
4.2.280 Score per residue for model 280

- Molecule 1: Ubiquitin



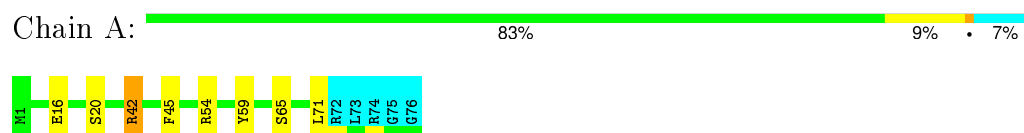
4.2.281 Score per residue for model 281

- Molecule 1: Ubiquitin



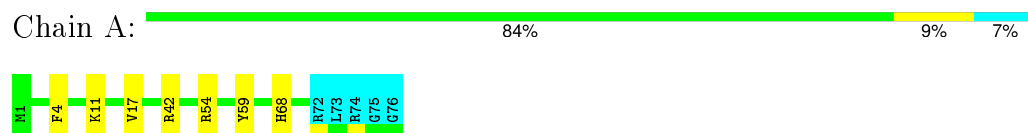
4.2.282 Score per residue for model 282

- Molecule 1: Ubiquitin



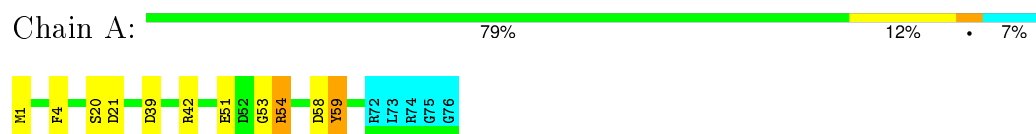
4.2.283 Score per residue for model 283

- Molecule 1: Ubiquitin



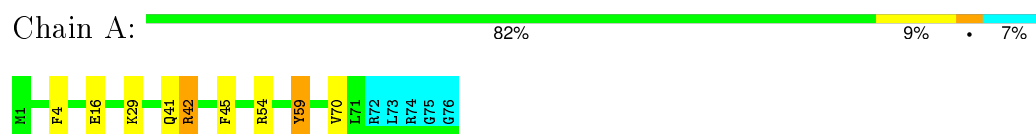
4.2.284 Score per residue for model 284

- Molecule 1: Ubiquitin



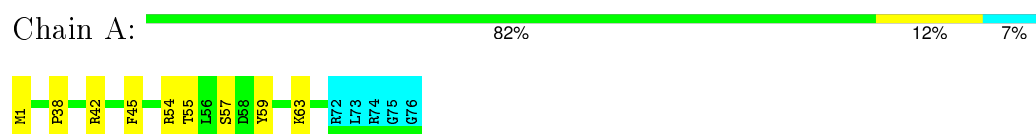
4.2.285 Score per residue for model 285

- Molecule 1: Ubiquitin



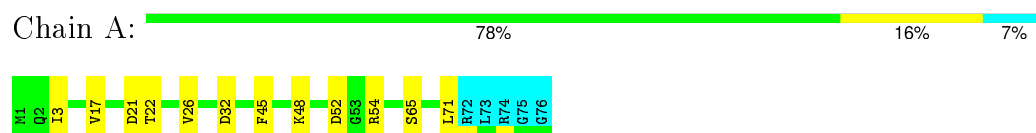
4.2.286 Score per residue for model 286

- Molecule 1: Ubiquitin



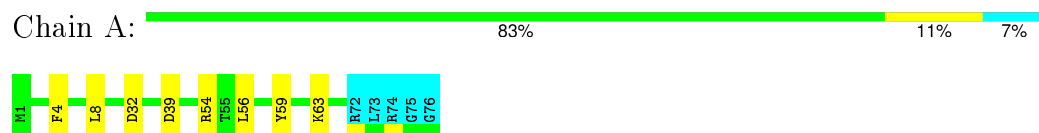
4.2.287 Score per residue for model 287

- Molecule 1: Ubiquitin



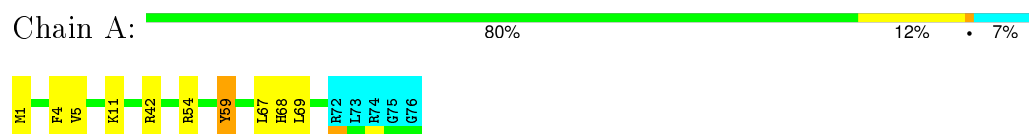
4.2.288 Score per residue for model 288

- Molecule 1: Ubiquitin



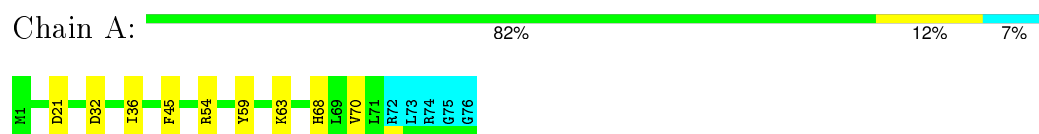
4.2.289 Score per residue for model 289

- Molecule 1: Ubiquitin



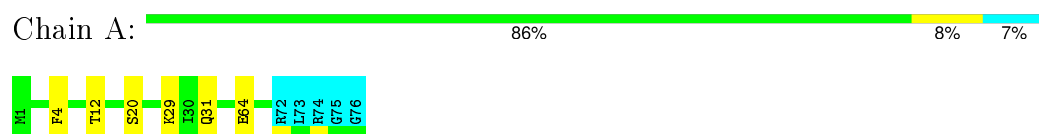
4.2.290 Score per residue for model 290

- Molecule 1: Ubiquitin



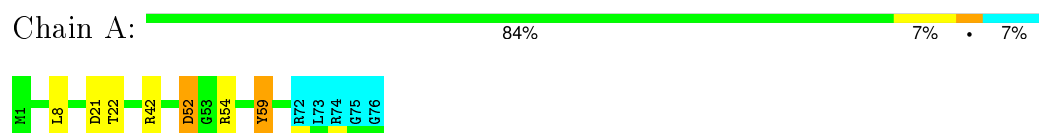
4.2.291 Score per residue for model 291

- Molecule 1: Ubiquitin



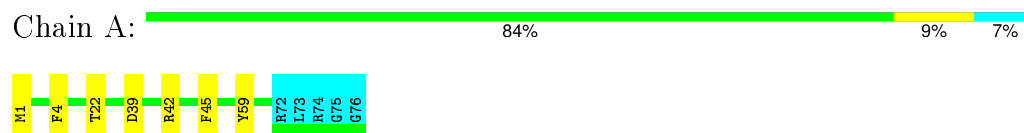
4.2.292 Score per residue for model 292

- Molecule 1: Ubiquitin



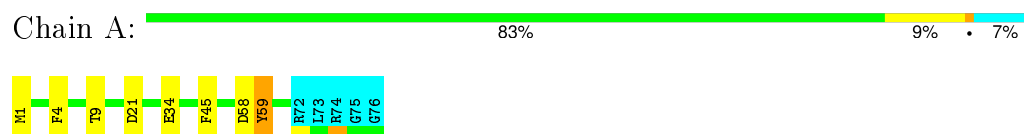
4.2.293 Score per residue for model 293

- Molecule 1: Ubiquitin



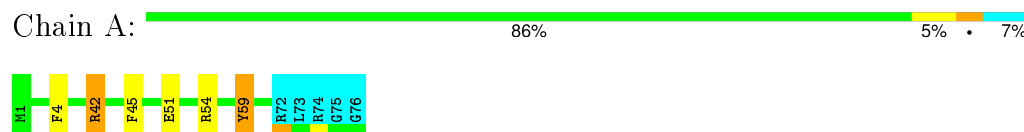
4.2.294 Score per residue for model 294

- Molecule 1: Ubiquitin



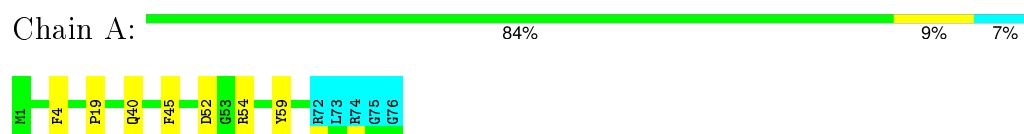
4.2.295 Score per residue for model 295

- Molecule 1: Ubiquitin



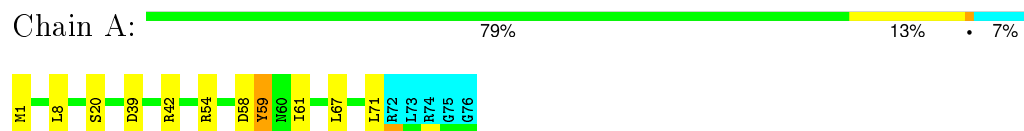
4.2.296 Score per residue for model 296

- Molecule 1: Ubiquitin



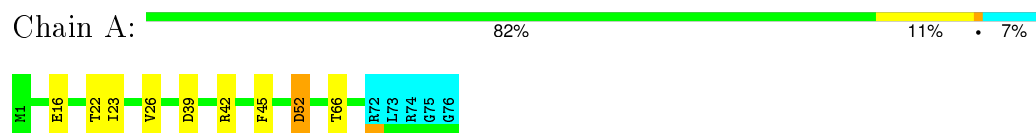
4.2.297 Score per residue for model 297

- Molecule 1: Ubiquitin



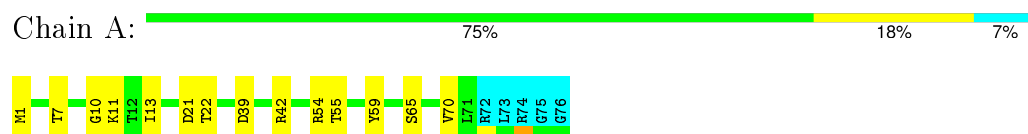
4.2.298 Score per residue for model 298

- Molecule 1: Ubiquitin



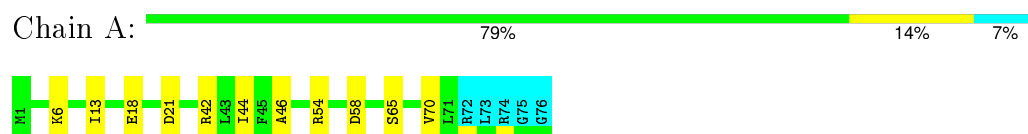
4.2.299 Score per residue for model 299

- Molecule 1: Ubiquitin



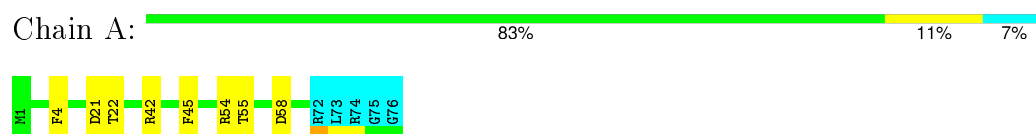
4.2.300 Score per residue for model 300

- Molecule 1: Ubiquitin



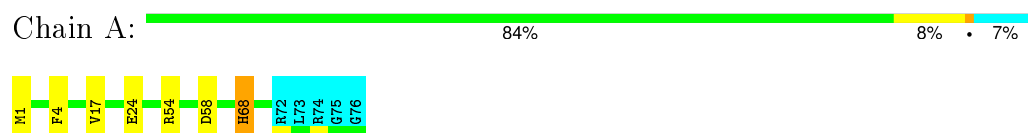
4.2.301 Score per residue for model 301

- Molecule 1: Ubiquitin



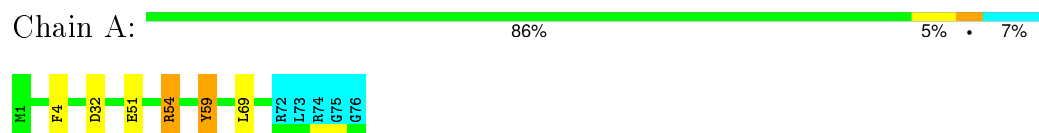
4.2.302 Score per residue for model 302

- Molecule 1: Ubiquitin



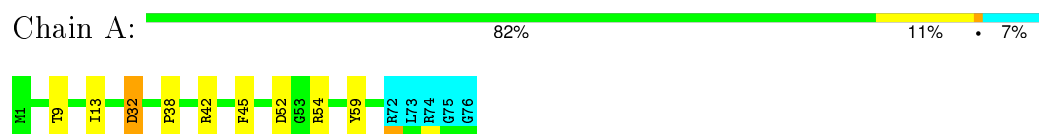
4.2.303 Score per residue for model 303

- Molecule 1: Ubiquitin



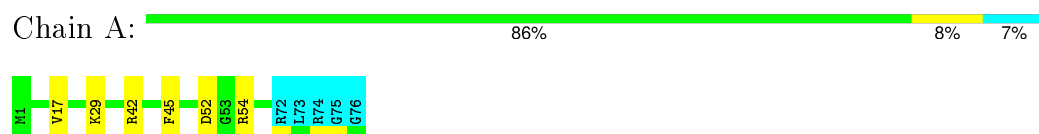
4.2.304 Score per residue for model 304

- Molecule 1: Ubiquitin



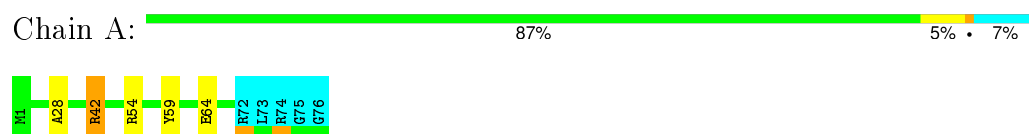
4.2.305 Score per residue for model 305

- Molecule 1: Ubiquitin



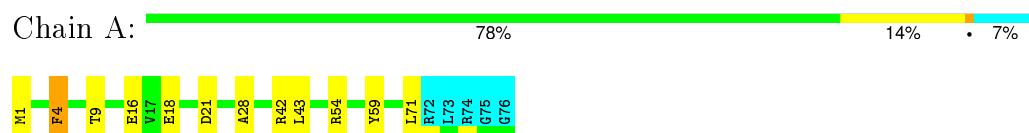
4.2.306 Score per residue for model 306

- 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

Chain A:  89% .. 7%



4.2.309 Score per residue for model 309


- Molecule 1: Ubiquitin

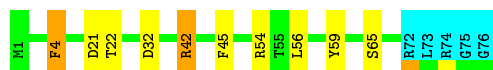
Chain A:  80% 13% 7%



4.2.310 Score per residue for model 310


- Molecule 1: Ubiquitin

Chain A:  80% 11% 7%



4.2.311 Score per residue for model 311

- Molecule 1: Ubiquitin

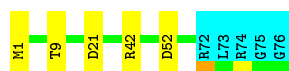
Chain A:  79% 12% 7%



4.2.312 Score per residue for model 312

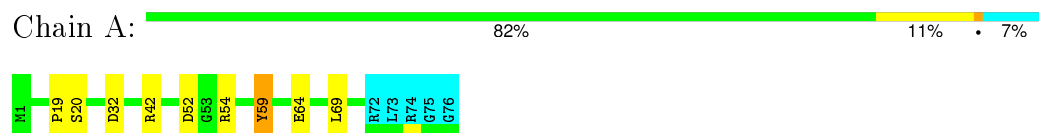
- Molecule 1: Ubiquitin

Chain A:  87% 7% 7%



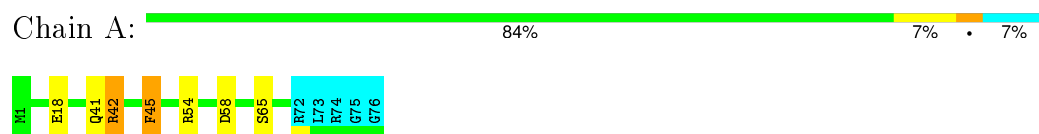
4.2.313 Score per residue for model 313

- Molecule 1: Ubiquitin



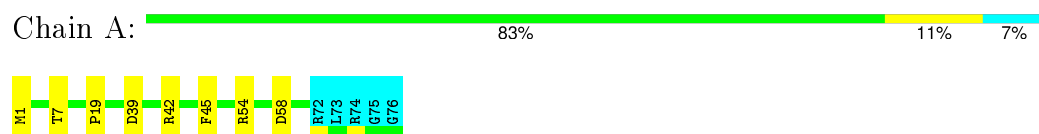
4.2.314 Score per residue for model 314

- Molecule 1: Ubiquitin



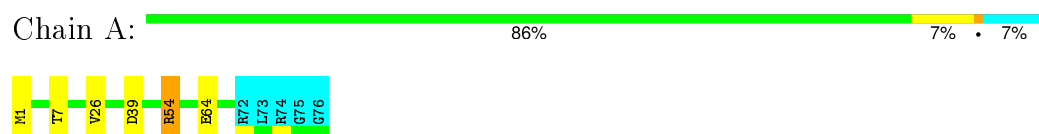
4.2.315 Score per residue for model 315

- Molecule 1: Ubiquitin



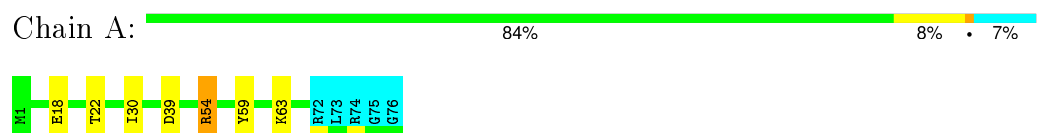
4.2.316 Score per residue for model 316

- Molecule 1: Ubiquitin



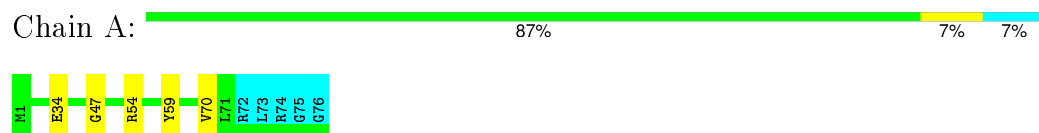
4.2.317 Score per residue for model 317

- Molecule 1: Ubiquitin



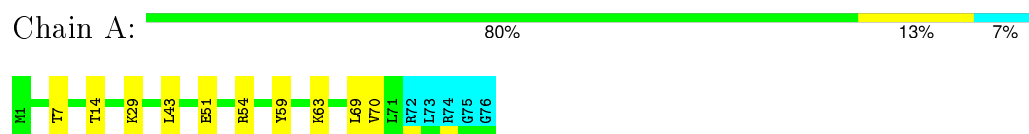
4.2.318 Score per residue for model 318

- Molecule 1: Ubiquitin



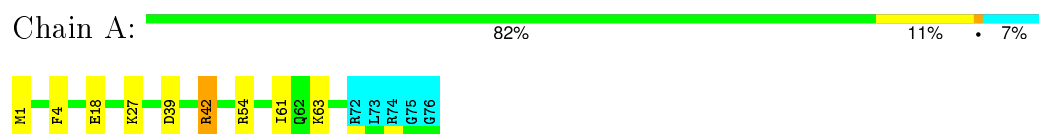
4.2.319 Score per residue for model 319

- Molecule 1: Ubiquitin



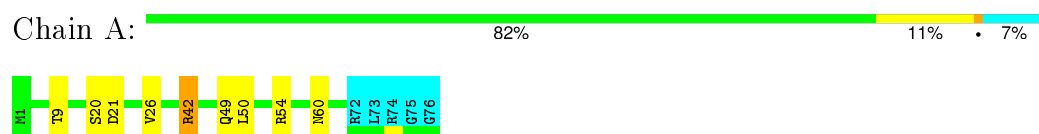
4.2.320 Score per residue for model 320

- Molecule 1: Ubiquitin



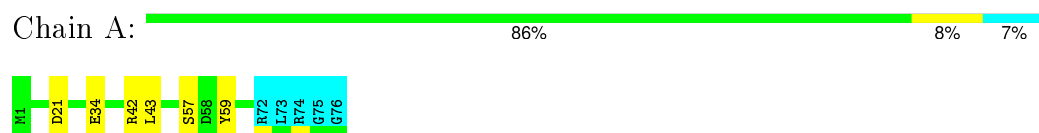
4.2.321 Score per residue for model 321

- Molecule 1: Ubiquitin



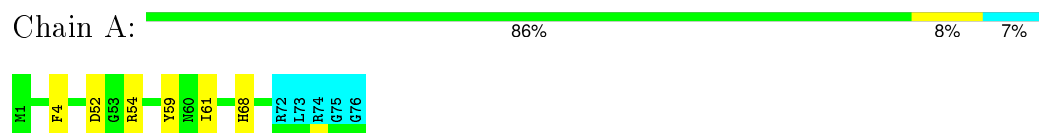
4.2.322 Score per residue for model 322

- Molecule 1: Ubiquitin



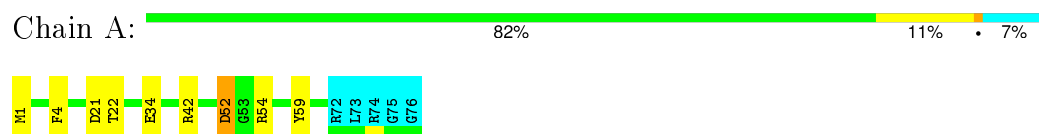
4.2.323 Score per residue for model 323

- Molecule 1: Ubiquitin



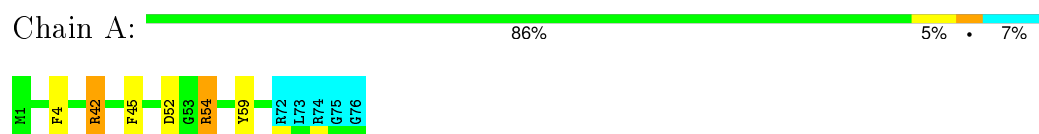
4.2.324 Score per residue for model 324

- Molecule 1: Ubiquitin



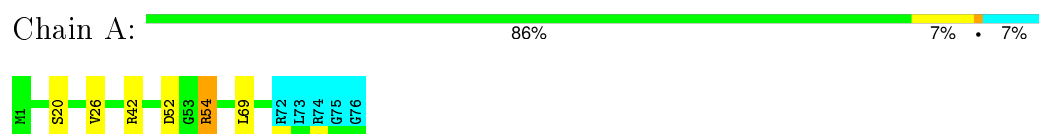
4.2.325 Score per residue for model 325

- Molecule 1: Ubiquitin



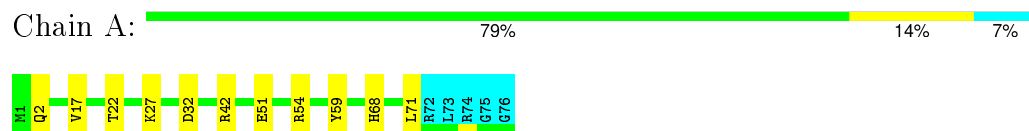
4.2.326 Score per residue for model 326

- 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

Chain A:  88% • • 7%



4.2.329 Score per residue for model 329


- Molecule 1: Ubiquitin

Chain A:  84% 8% • 7%



4.2.330 Score per residue for model 330


- Molecule 1: Ubiquitin

Chain A:  86% 8% 7%



4.2.331 Score per residue for model 331

- Molecule 1: Ubiquitin

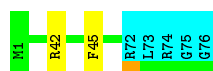
Chain A:  84% 7% • 7%



4.2.332 Score per residue for model 332

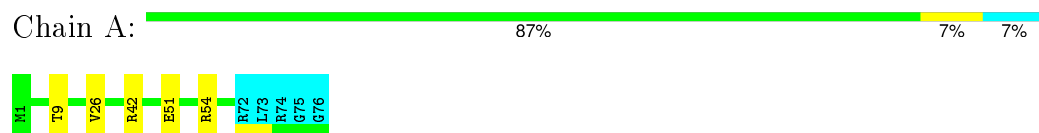
- Molecule 1: Ubiquitin

Chain A:  91% • 7%



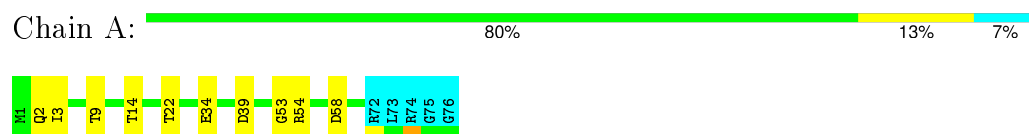
4.2.333 Score per residue for model 333

- Molecule 1: Ubiquitin



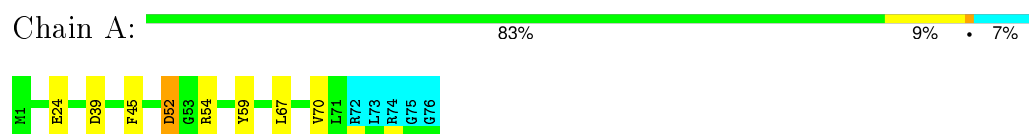
4.2.334 Score per residue for model 334

- Molecule 1: Ubiquitin



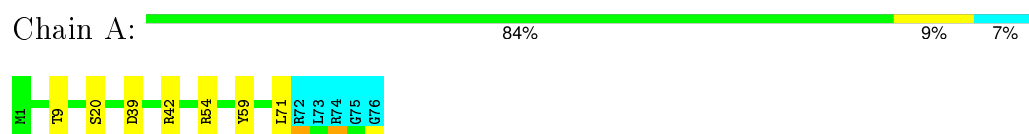
4.2.335 Score per residue for model 335

- Molecule 1: Ubiquitin



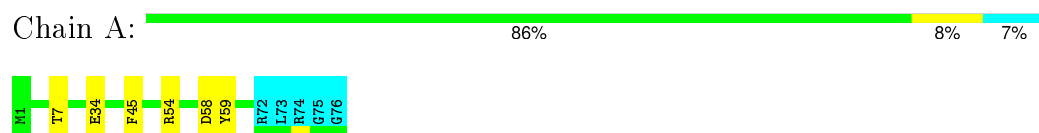
4.2.336 Score per residue for model 336

- Molecule 1: Ubiquitin



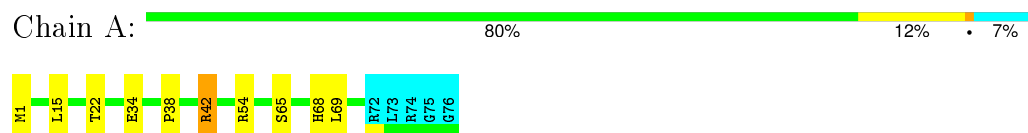
4.2.337 Score per residue for model 337

- Molecule 1: Ubiquitin



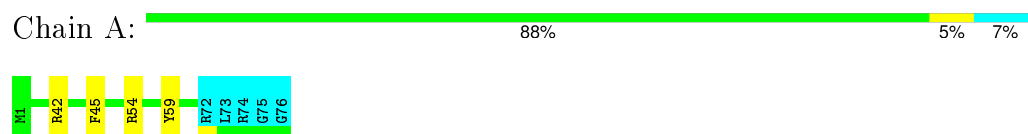
4.2.338 Score per residue for model 338

- Molecule 1: Ubiquitin



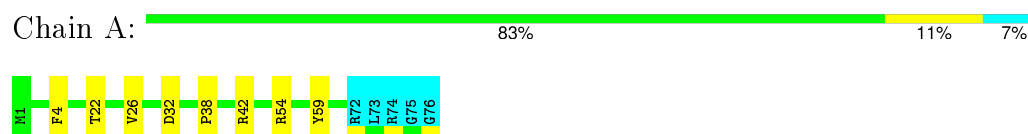
4.2.339 Score per residue for model 339

- Molecule 1: Ubiquitin



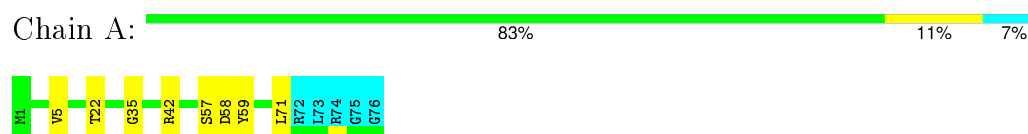
4.2.340 Score per residue for model 340

- Molecule 1: Ubiquitin



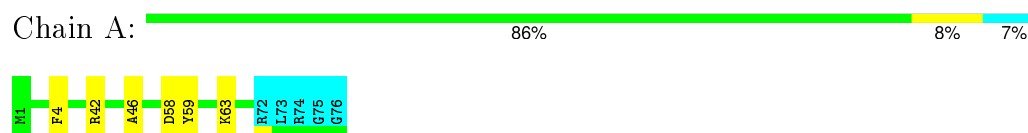
4.2.341 Score per residue for model 341

- Molecule 1: Ubiquitin



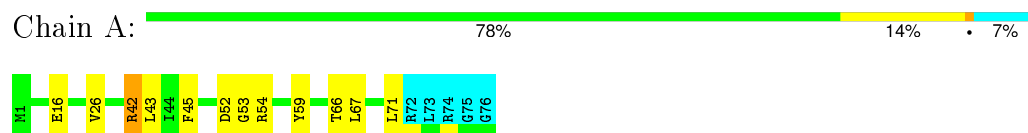
4.2.342 Score per residue for model 342

- Molecule 1: Ubiquitin



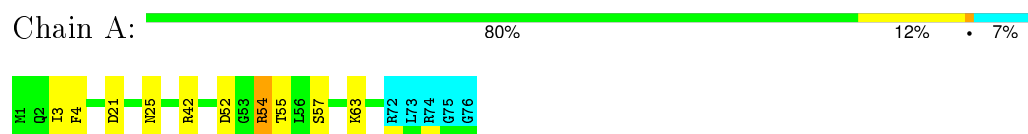
4.2.343 Score per residue for model 343

- Molecule 1: Ubiquitin



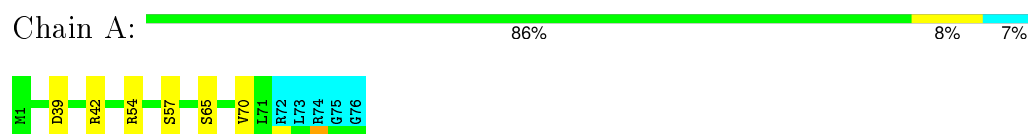
4.2.344 Score per residue for model 344

- Molecule 1: Ubiquitin



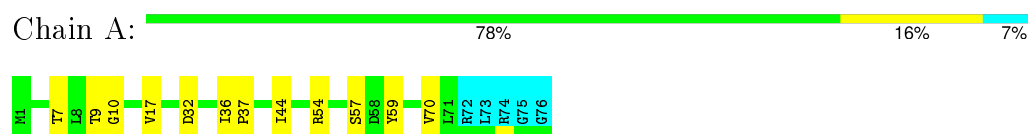
4.2.345 Score per residue for model 345

- Molecule 1: Ubiquitin



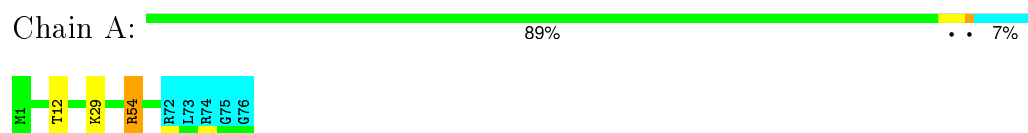
4.2.346 Score per residue for model 346

- Molecule 1: Ubiquitin



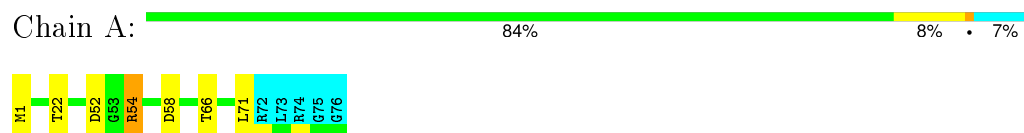
4.2.347 Score per residue for model 347

- Molecule 1: Ubiquitin



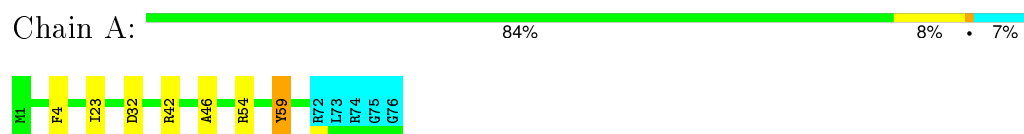
4.2.348 Score per residue for model 348

- Molecule 1: Ubiquitin



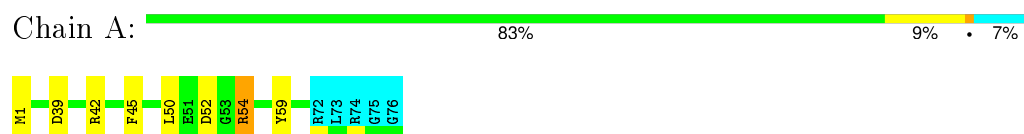
4.2.349 Score per residue for model 349

- Molecule 1: Ubiquitin



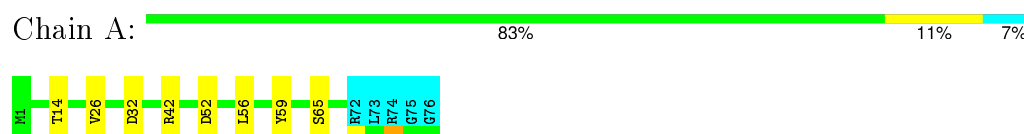
4.2.350 Score per residue for model 350

- Molecule 1: Ubiquitin



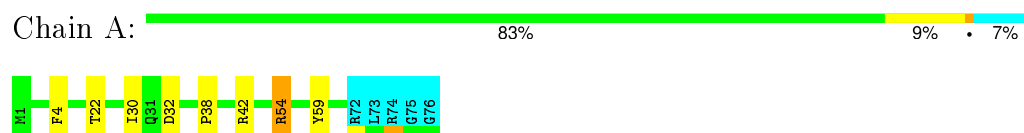
4.2.351 Score per residue for model 351

- 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

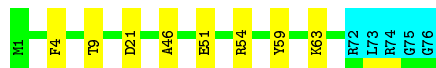
Chain A:  84% 9% 7%



4.2.354 Score per residue for model 354


- Molecule 1: Ubiquitin

Chain A:  83% 11% 7%



4.2.355 Score per residue for model 355


- Molecule 1: Ubiquitin

Chain A:  86% 7% 7%



4.2.356 Score per residue for model 356


- Molecule 1: Ubiquitin

Chain A:  86% 8% 7%



4.2.357 Score per residue for model 357

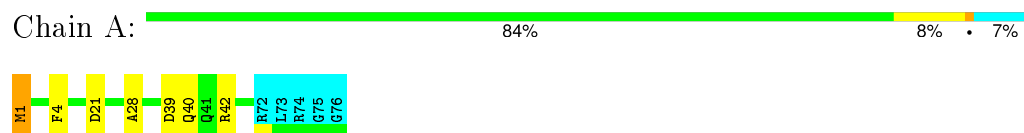
- Molecule 1: Ubiquitin

Chain A:  84% 9% 7%



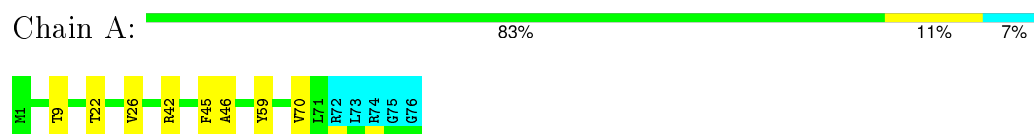
4.2.358 Score per residue for model 358

- Molecule 1: Ubiquitin



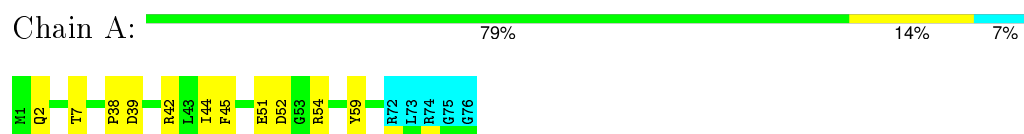
4.2.359 Score per residue for model 359

- Molecule 1: Ubiquitin



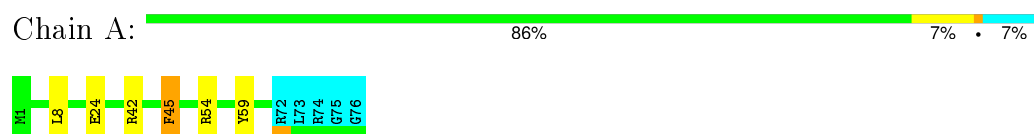
4.2.360 Score per residue for model 360

- Molecule 1: Ubiquitin



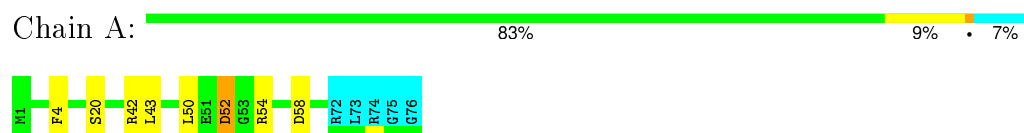
4.2.361 Score per residue for model 361

- Molecule 1: Ubiquitin



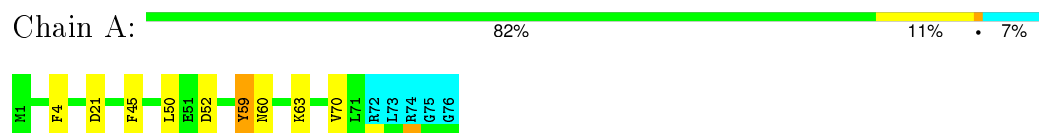
4.2.362 Score per residue for model 362

- Molecule 1: Ubiquitin



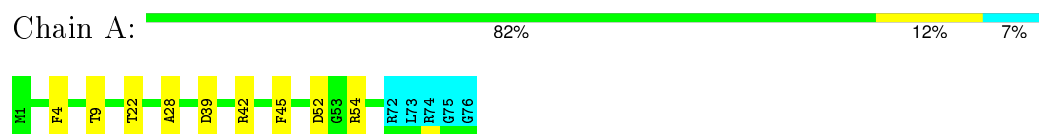
4.2.363 Score per residue for model 363

- Molecule 1: Ubiquitin



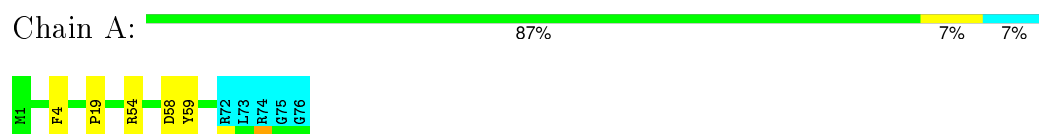
4.2.364 Score per residue for model 364

- Molecule 1: Ubiquitin



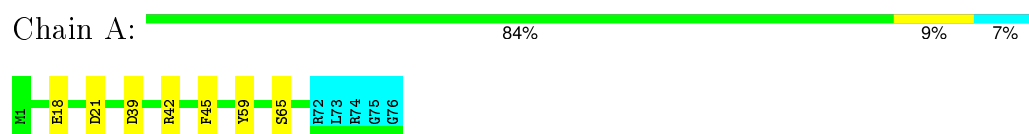
4.2.365 Score per residue for model 365

- Molecule 1: Ubiquitin



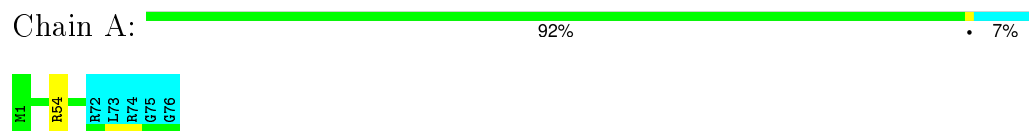
4.2.366 Score per residue for model 366

- 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

Chain A:  86% 7% 7%



4.2.369 Score per residue for model 369


- Molecule 1: Ubiquitin

Chain A:  82% 12% 7%



4.2.370 Score per residue for model 370


- Molecule 1: Ubiquitin

Chain A:  86% 7% 7%



4.2.371 Score per residue for model 371


- Molecule 1: Ubiquitin

Chain A:  86% 5% 7%



4.2.372 Score per residue for model 372

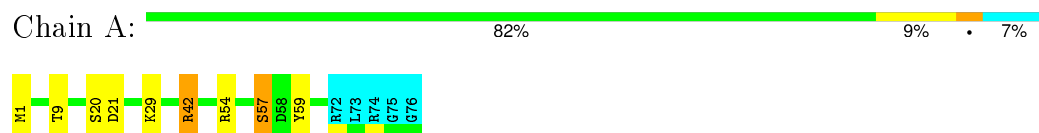
- Molecule 1: Ubiquitin

Chain A:  83% 11% 7%



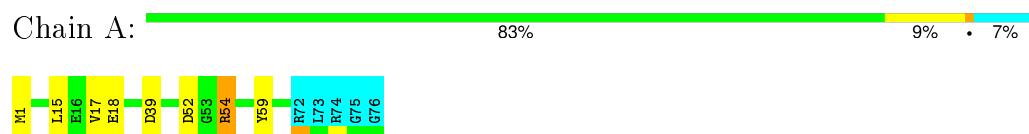
4.2.373 Score per residue for model 373

- Molecule 1: Ubiquitin



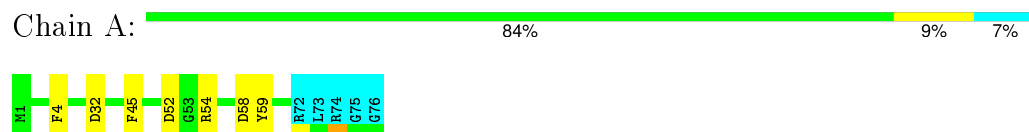
4.2.374 Score per residue for model 374

- Molecule 1: Ubiquitin



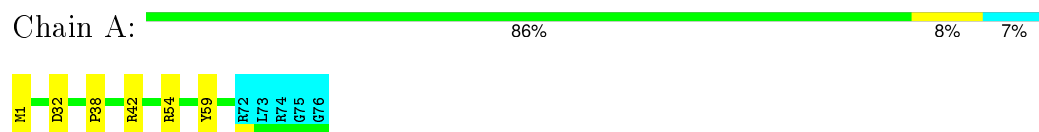
4.2.375 Score per residue for model 375

- Molecule 1: Ubiquitin



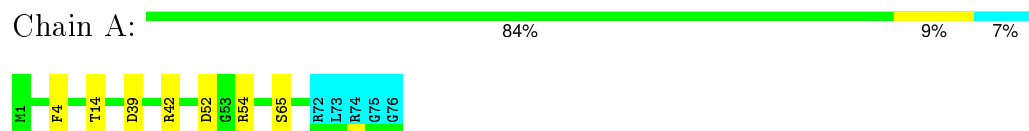
4.2.376 Score per residue for model 376

- Molecule 1: Ubiquitin



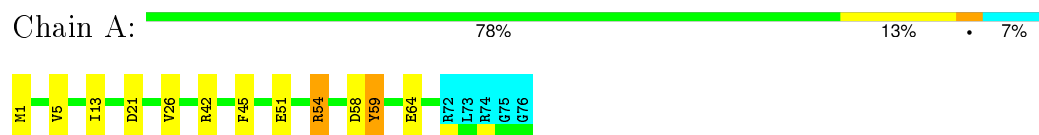
4.2.377 Score per residue for model 377

- Molecule 1: Ubiquitin



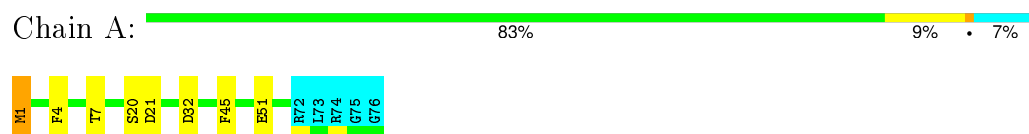
4.2.378 Score per residue for model 378

- Molecule 1: Ubiquitin



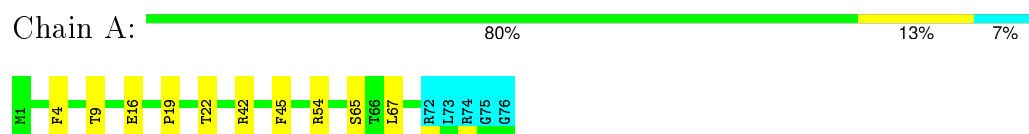
4.2.379 Score per residue for model 379

- Molecule 1: Ubiquitin



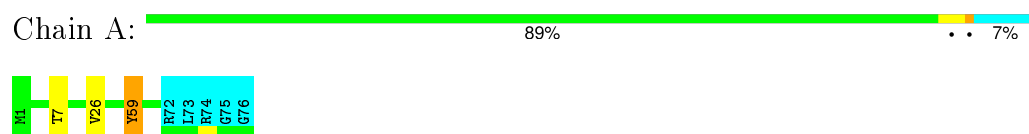
4.2.380 Score per residue for model 380

- Molecule 1: Ubiquitin



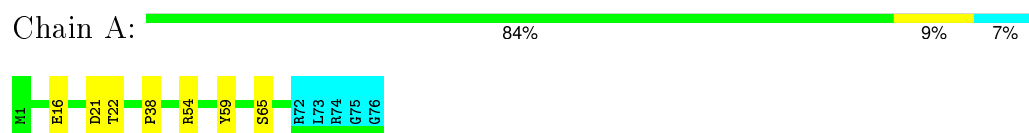
4.2.381 Score per residue for model 381

- Molecule 1: Ubiquitin



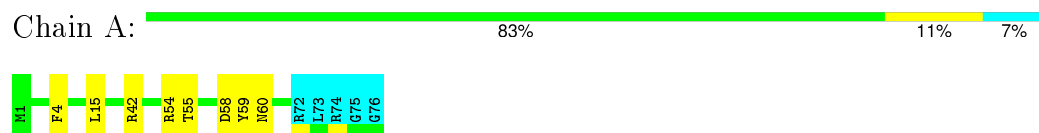
4.2.382 Score per residue for model 382

- Molecule 1: Ubiquitin



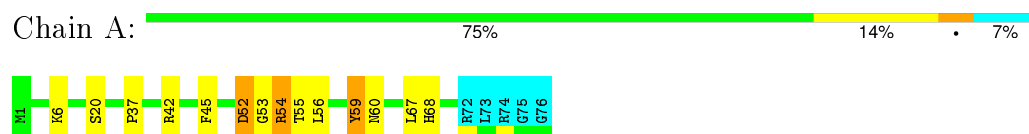
4.2.383 Score per residue for model 383

- Molecule 1: Ubiquitin



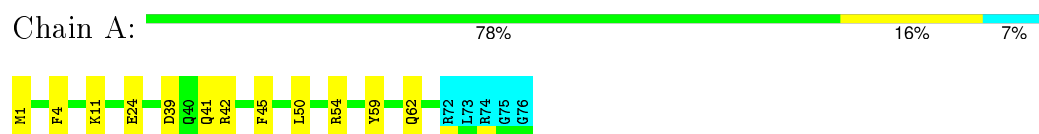
4.2.384 Score per residue for model 384

- Molecule 1: Ubiquitin



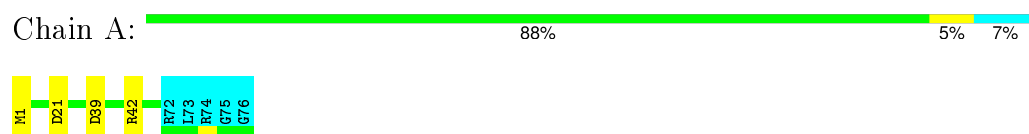
4.2.385 Score per residue for model 385

- Molecule 1: Ubiquitin



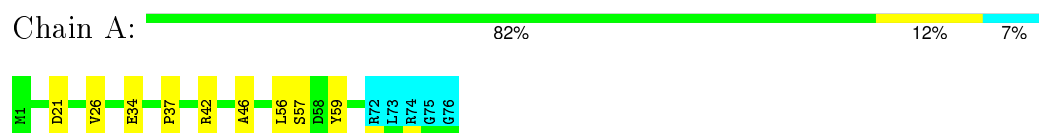
4.2.386 Score per residue for model 386

- Molecule 1: Ubiquitin



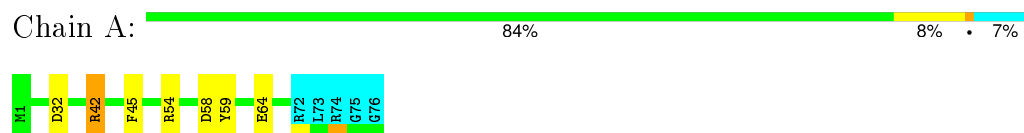
4.2.387 Score per residue for model 387

- Molecule 1: Ubiquitin



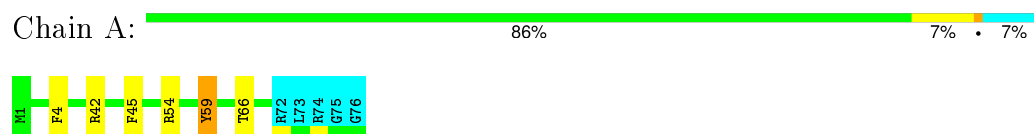
4.2.388 Score per residue for model 388

- Molecule 1: Ubiquitin



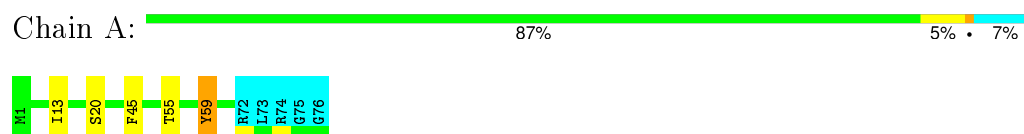
4.2.389 Score per residue for model 389

- Molecule 1: Ubiquitin



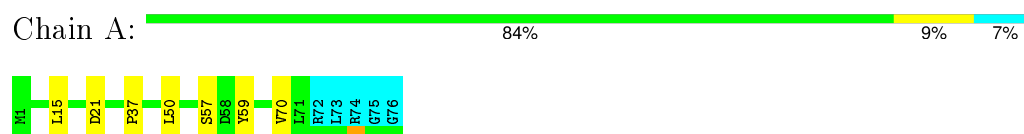
4.2.390 Score per residue for model 390

- Molecule 1: Ubiquitin



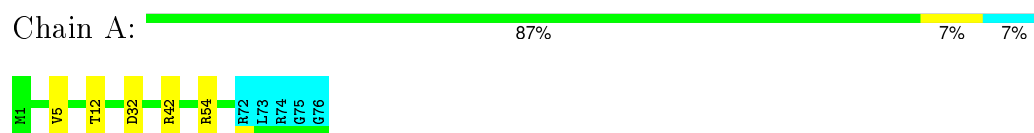
4.2.391 Score per residue for model 391

- Molecule 1: Ubiquitin




4.2.392 Score per residue for model 392

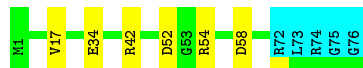
- Molecule 1: Ubiquitin



4.2.393 Score per residue for model 393


- Molecule 1: Ubiquitin

Chain A:  86% 8% 7%



4.2.394 Score per residue for model 394


- Molecule 1: Ubiquitin

Chain A:  86% 7% 7%



4.2.395 Score per residue for model 395


- Molecule 1: Ubiquitin

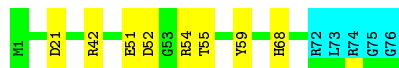
Chain A:  80% 13% 7%



4.2.396 Score per residue for model 396


- Molecule 1: Ubiquitin

Chain A:  83% 11% 7%



4.2.397 Score per residue for model 397

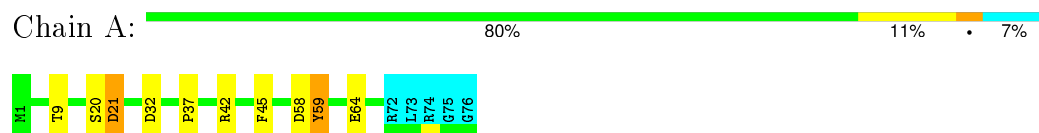
- Molecule 1: Ubiquitin

Chain A:  87% 7% 7%



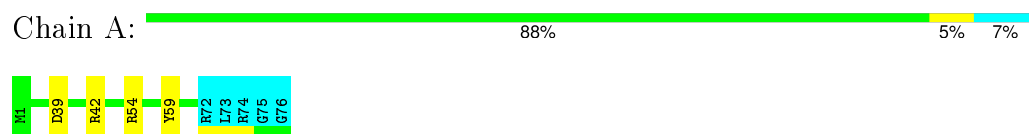
4.2.398 Score per residue for model 398

- Molecule 1: Ubiquitin



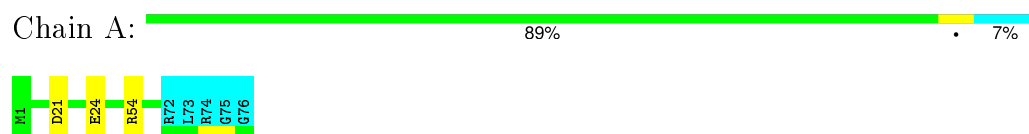
4.2.399 Score per residue for model 399

- Molecule 1: Ubiquitin



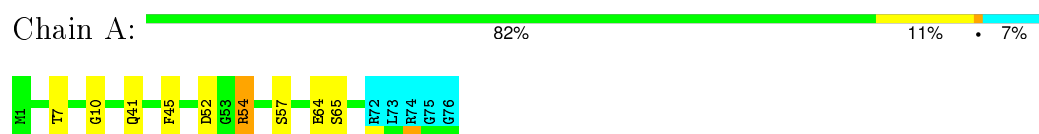
4.2.400 Score per residue for model 400

- Molecule 1: Ubiquitin



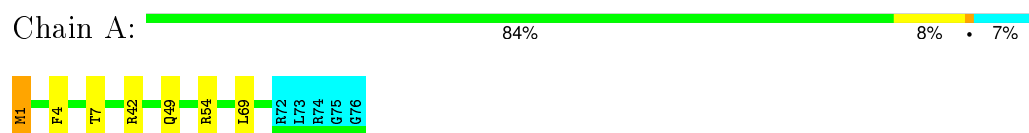
4.2.401 Score per residue for model 401

- Molecule 1: Ubiquitin



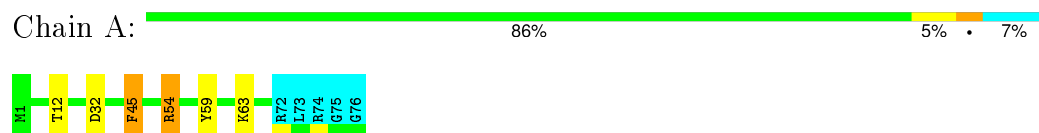
4.2.402 Score per residue for model 402

- Molecule 1: Ubiquitin



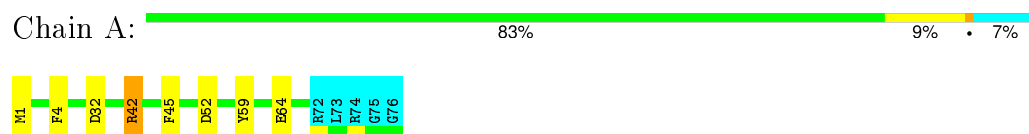
4.2.403 Score per residue for model 403

- Molecule 1: Ubiquitin



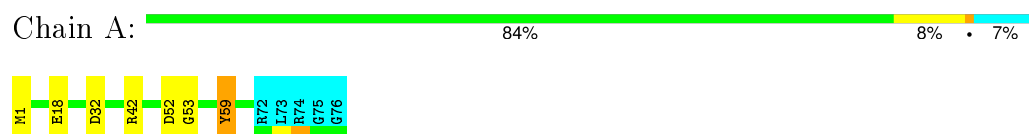
4.2.404 Score per residue for model 404

- Molecule 1: Ubiquitin



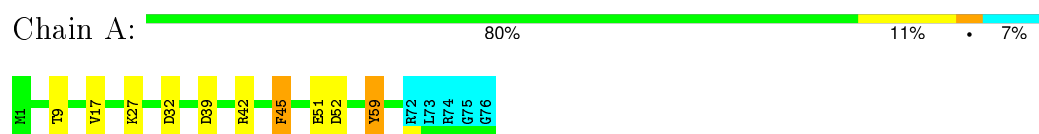
4.2.405 Score per residue for model 405

- Molecule 1: Ubiquitin



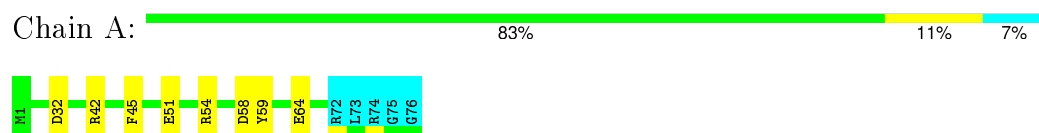
4.2.406 Score per residue for model 406

- Molecule 1: Ubiquitin



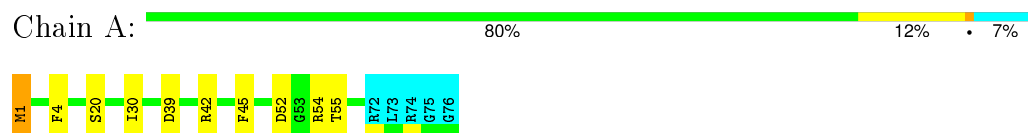
4.2.407 Score per residue for model 407

- Molecule 1: Ubiquitin



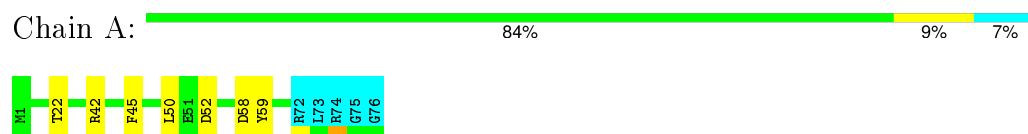
4.2.408 Score per residue for model 408

- Molecule 1: Ubiquitin



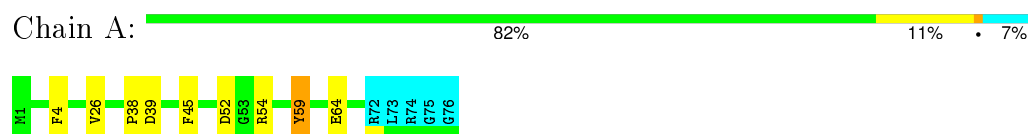
4.2.409 Score per residue for model 409

- Molecule 1: Ubiquitin



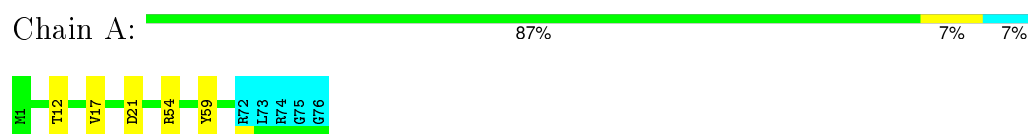
4.2.410 Score per residue for model 410

- Molecule 1: Ubiquitin



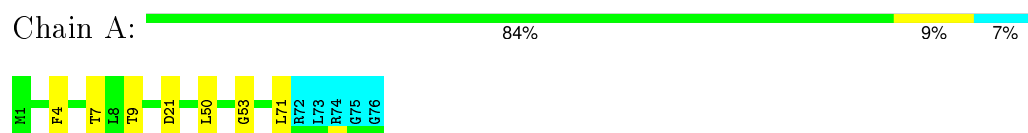
4.2.411 Score per residue for model 411

- Molecule 1: Ubiquitin



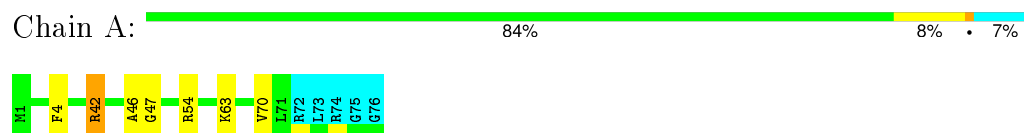
4.2.412 Score per residue for model 412

- Molecule 1: Ubiquitin



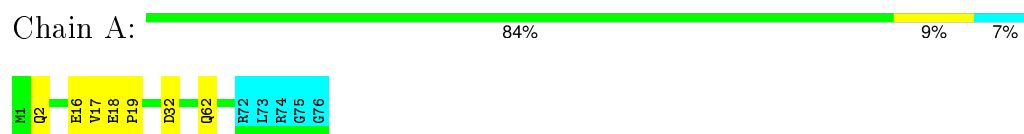
4.2.413 Score per residue for model 413

- Molecule 1: Ubiquitin



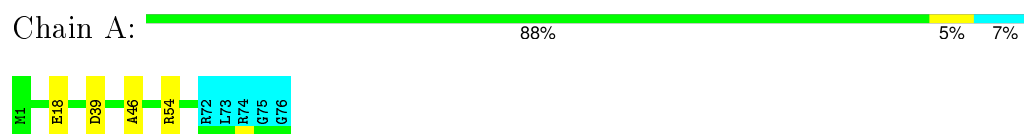
4.2.414 Score per residue for model 414

- Molecule 1: Ubiquitin



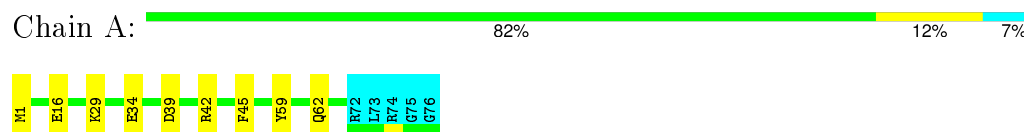
4.2.415 Score per residue for model 415

- Molecule 1: Ubiquitin



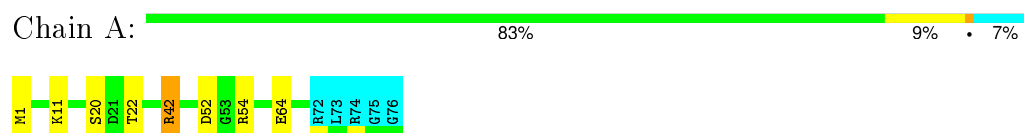
4.2.416 Score per residue for model 416

- Molecule 1: Ubiquitin



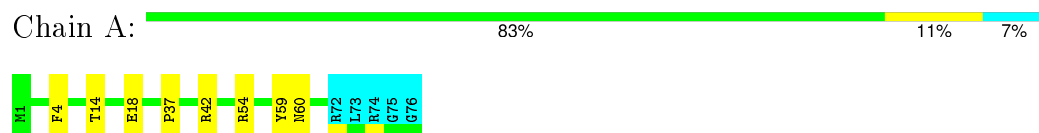
4.2.417 Score per residue for model 417

- Molecule 1: Ubiquitin



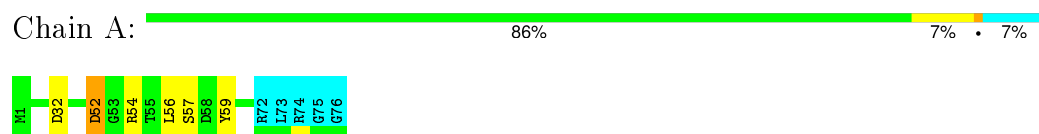
4.2.418 Score per residue for model 418

- Molecule 1: Ubiquitin



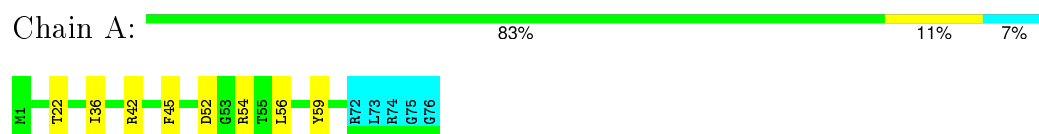
4.2.419 Score per residue for model 419

- Molecule 1: Ubiquitin



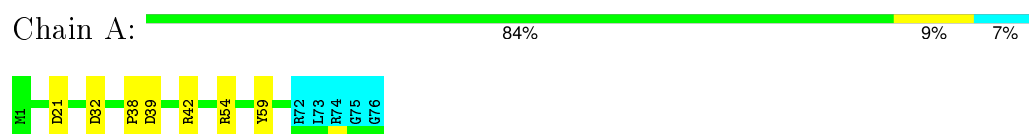
4.2.420 Score per residue for model 420

- Molecule 1: Ubiquitin



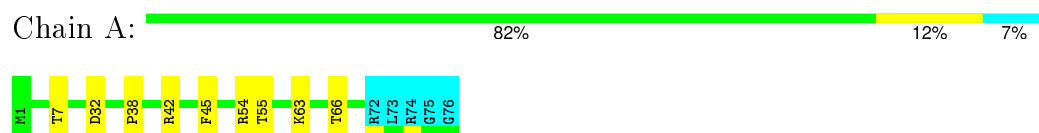
4.2.421 Score per residue for model 421

- Molecule 1: Ubiquitin



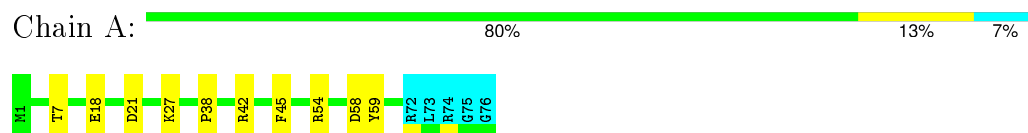
4.2.422 Score per residue for model 422

- Molecule 1: Ubiquitin



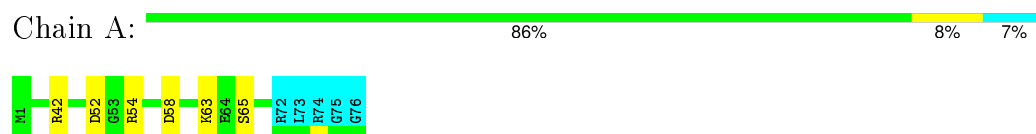
4.2.423 Score per residue for model 423

- Molecule 1: Ubiquitin



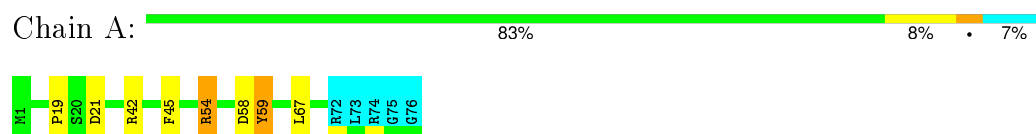
4.2.424 Score per residue for model 424

- Molecule 1: Ubiquitin



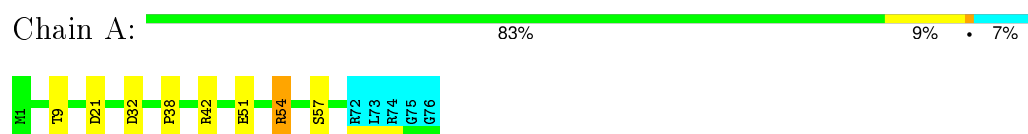
4.2.425 Score per residue for model 425

- Molecule 1: Ubiquitin



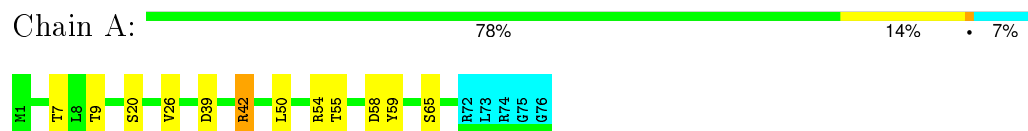
4.2.426 Score per residue for model 426

- Molecule 1: Ubiquitin



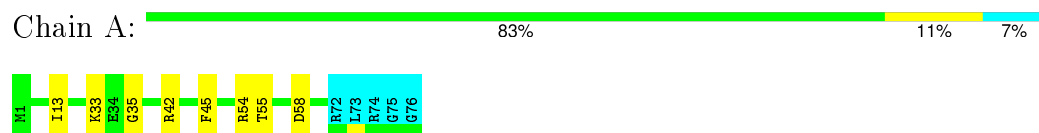
4.2.427 Score per residue for model 427

- Molecule 1: Ubiquitin



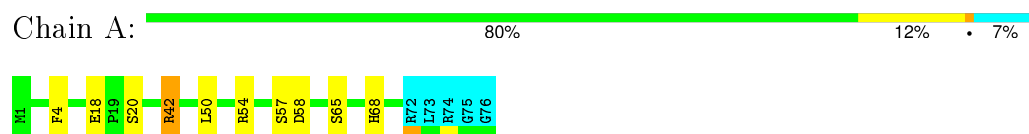
4.2.428 Score per residue for model 428

- Molecule 1: Ubiquitin



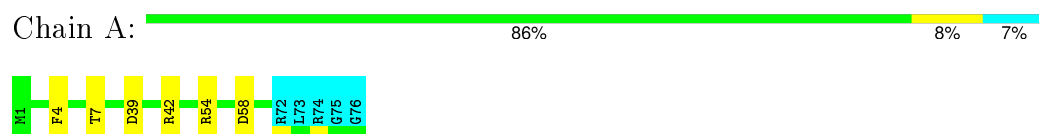
4.2.429 Score per residue for model 429

- Molecule 1: Ubiquitin



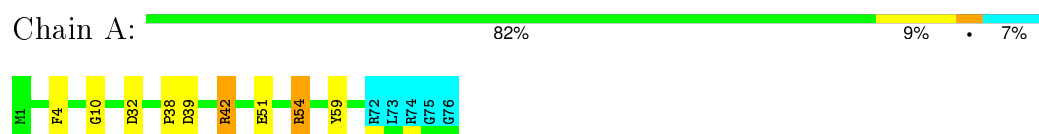
4.2.430 Score per residue for model 430

- Molecule 1: Ubiquitin



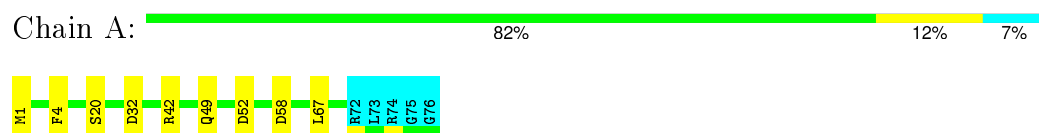
4.2.431 Score per residue for model 431

- Molecule 1: Ubiquitin



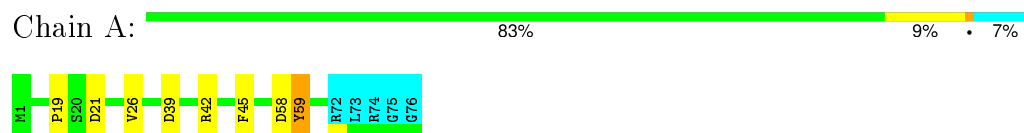
4.2.432 Score per residue for model 432

- Molecule 1: Ubiquitin



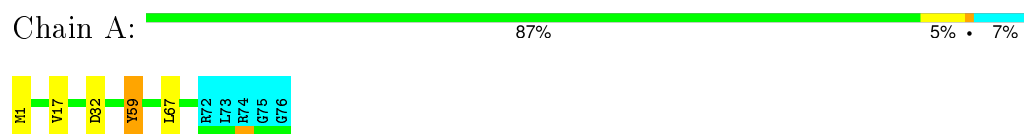
4.2.433 Score per residue for model 433

- Molecule 1: Ubiquitin



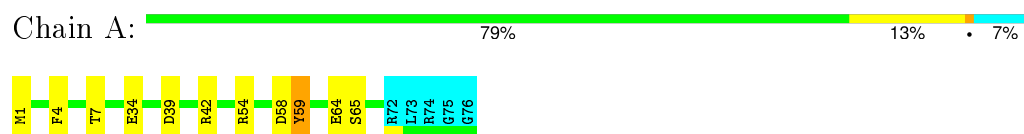
4.2.434 Score per residue for model 434

- Molecule 1: Ubiquitin



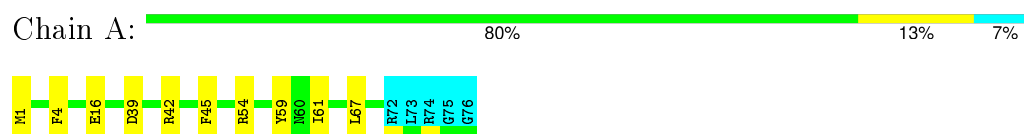
4.2.435 Score per residue for model 435

- Molecule 1: Ubiquitin



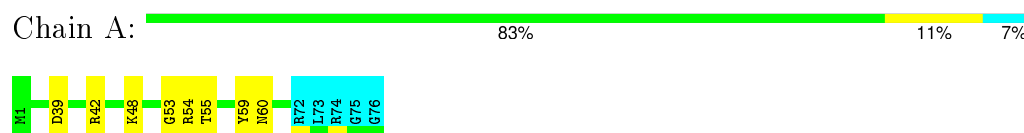
4.2.436 Score per residue for model 436

- Molecule 1: Ubiquitin



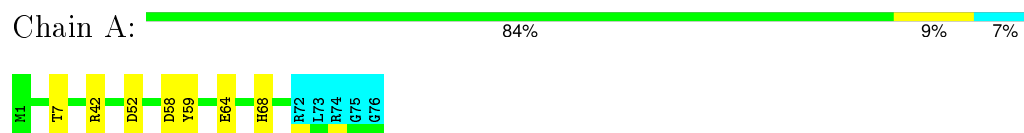
4.2.437 Score per residue for model 437

- Molecule 1: Ubiquitin



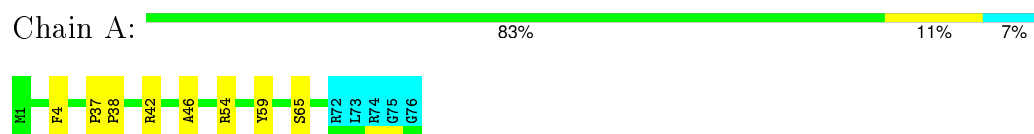
4.2.438 Score per residue for model 438

- Molecule 1: Ubiquitin



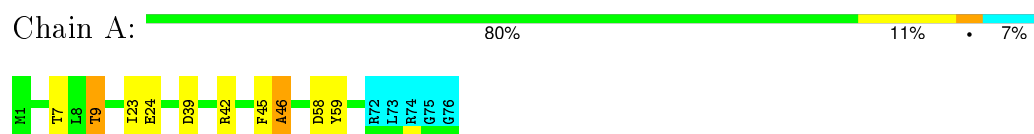
4.2.439 Score per residue for model 439

- Molecule 1: Ubiquitin



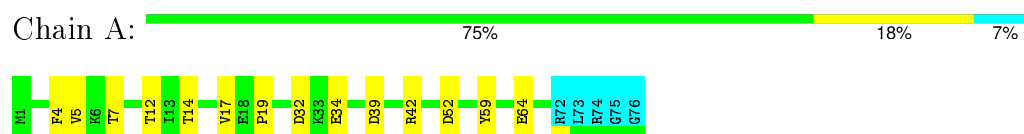
4.2.440 Score per residue for model 440

- Molecule 1: Ubiquitin



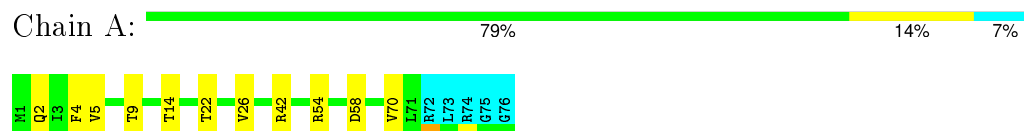
4.2.441 Score per residue for model 441

- Molecule 1: Ubiquitin



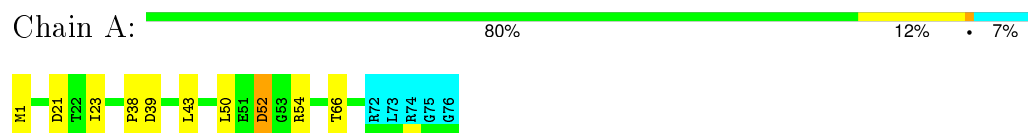
4.2.442 Score per residue for model 442

- Molecule 1: Ubiquitin



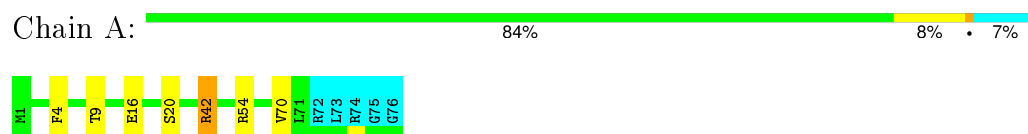
4.2.443 Score per residue for model 443

- Molecule 1: Ubiquitin



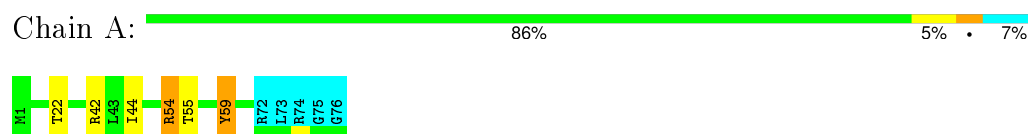
4.2.444 Score per residue for model 444

- Molecule 1: Ubiquitin



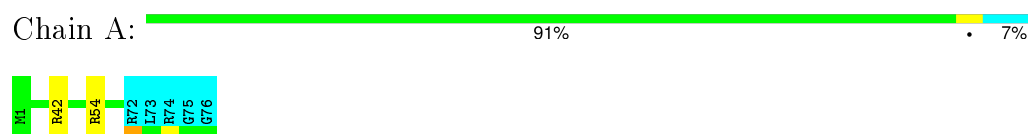
4.2.445 Score per residue for model 445

- Molecule 1: Ubiquitin



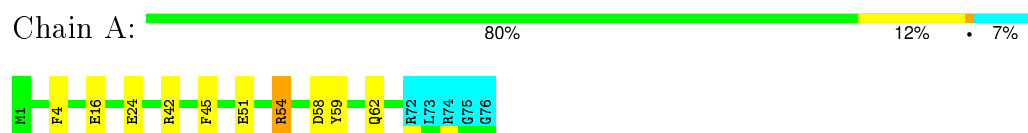
4.2.446 Score per residue for model 446

- Molecule 1: Ubiquitin



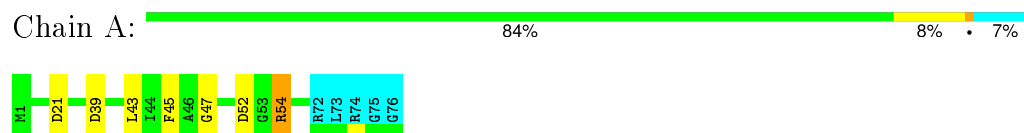
4.2.447 Score per residue for model 447

- Molecule 1: Ubiquitin



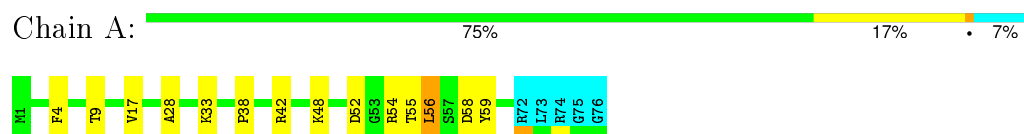
4.2.448 Score per residue for model 448

- Molecule 1: Ubiquitin



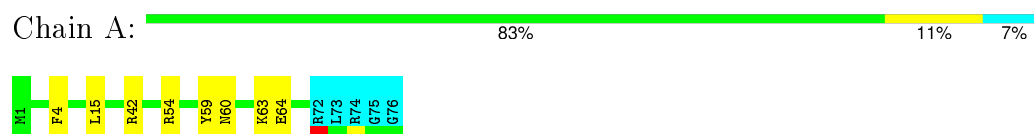
4.2.449 Score per residue for model 449

- Molecule 1: Ubiquitin



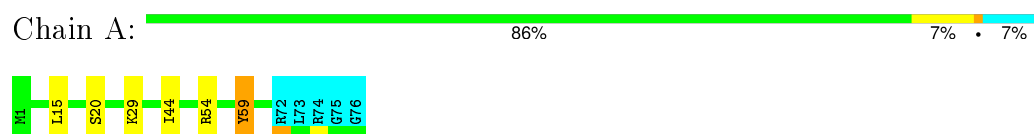
4.2.450 Score per residue for model 450

- Molecule 1: Ubiquitin



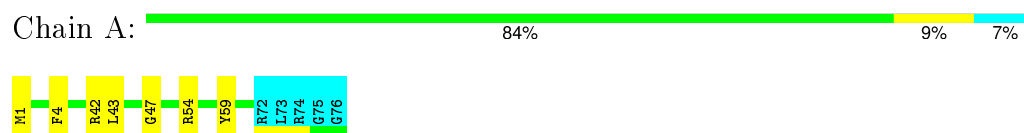
4.2.451 Score per residue for model 451

- Molecule 1: Ubiquitin




4.2.452 Score per residue for model 452

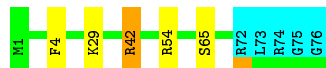
- Molecule 1: Ubiquitin



4.2.453 Score per residue for model 453


- Molecule 1: Ubiquitin

Chain A:  87% 5% • 7%



4.2.454 Score per residue for model 454


- Molecule 1: Ubiquitin

Chain A:  82% 12% 7%



4.2.455 Score per residue for model 455


- Molecule 1: Ubiquitin

Chain A:  86% 8% 7%



4.2.456 Score per residue for model 456


- Molecule 1: Ubiquitin

Chain A:  82% 12% 7%



4.2.457 Score per residue for model 457

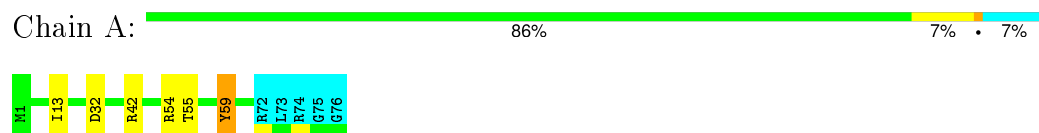
- Molecule 1: Ubiquitin

Chain A:  86% 7% • 7%



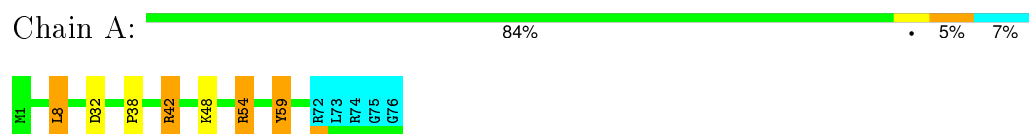
4.2.458 Score per residue for model 458

- Molecule 1: Ubiquitin



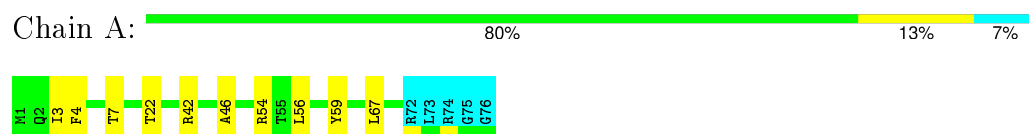
4.2.459 Score per residue for model 459

- Molecule 1: Ubiquitin



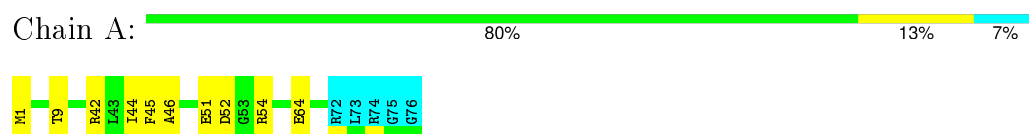
4.2.460 Score per residue for model 460

- Molecule 1: Ubiquitin



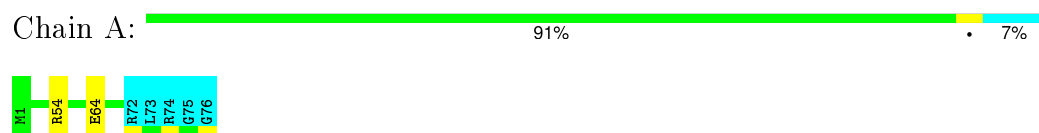
4.2.461 Score per residue for model 461

- Molecule 1: Ubiquitin



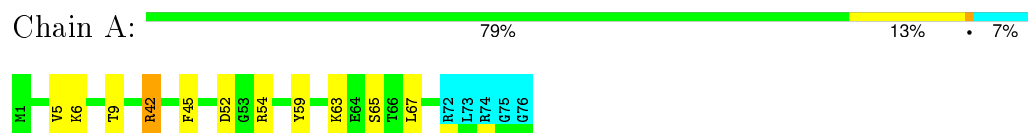
4.2.462 Score per residue for model 462

- Molecule 1: Ubiquitin



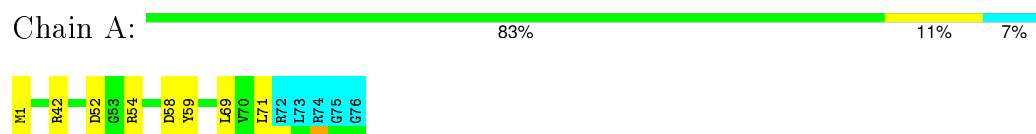
4.2.463 Score per residue for model 463

- Molecule 1: Ubiquitin



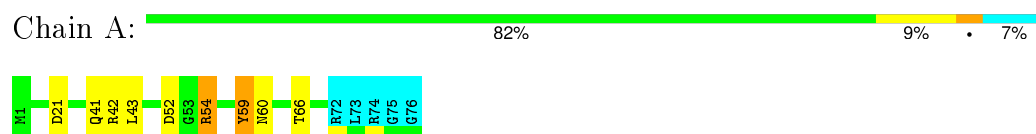
4.2.464 Score per residue for model 464

- Molecule 1: Ubiquitin



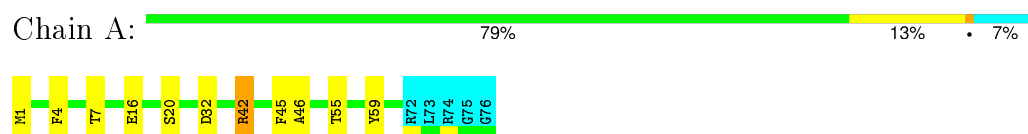
4.2.465 Score per residue for model 465

- Molecule 1: Ubiquitin



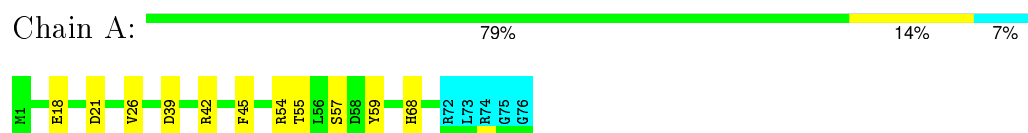
4.2.466 Score per residue for model 466

- Molecule 1: Ubiquitin



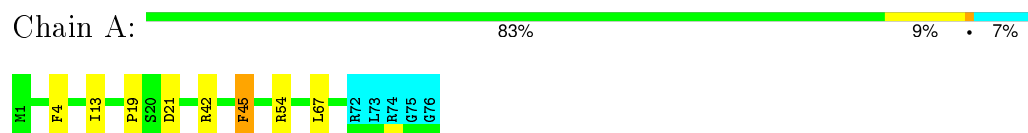
4.2.467 Score per residue for model 467

- Molecule 1: Ubiquitin



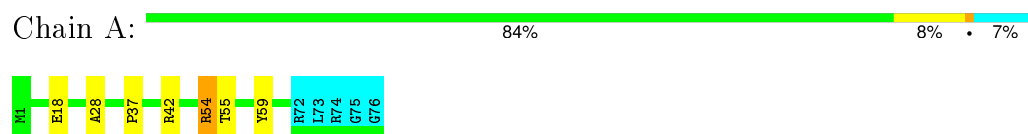
4.2.468 Score per residue for model 468

- Molecule 1: Ubiquitin



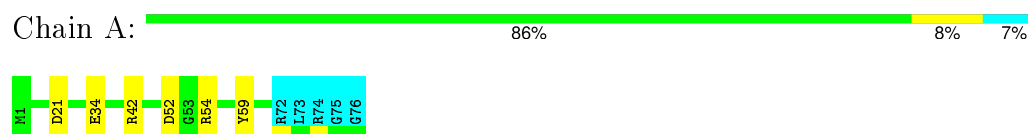
4.2.469 Score per residue for model 469

- Molecule 1: Ubiquitin



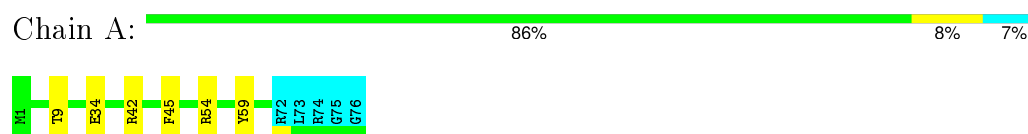
4.2.470 Score per residue for model 470

- Molecule 1: Ubiquitin



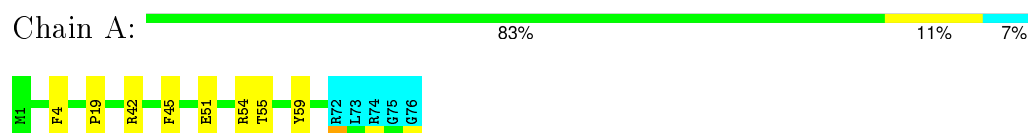
4.2.471 Score per residue for model 471

- Molecule 1: Ubiquitin



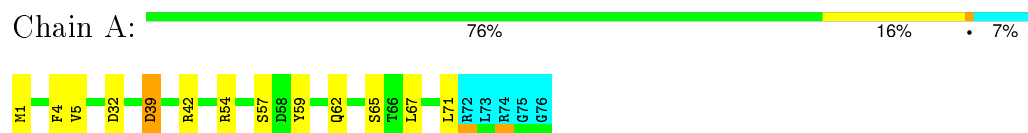
4.2.472 Score per residue for model 472

- Molecule 1: Ubiquitin



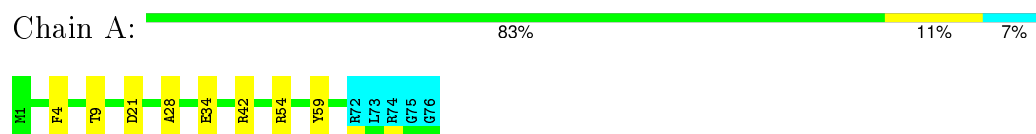
4.2.473 Score per residue for model 473

- Molecule 1: Ubiquitin



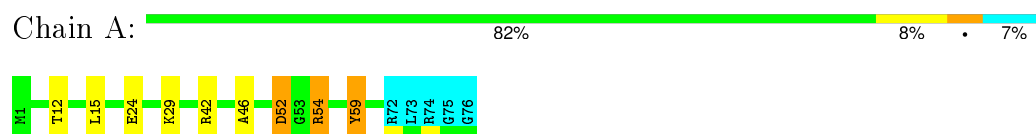
4.2.474 Score per residue for model 474

- Molecule 1: Ubiquitin



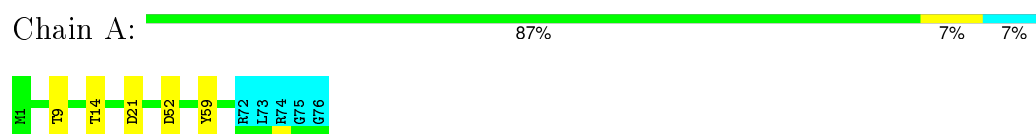
4.2.475 Score per residue for model 475

- Molecule 1: Ubiquitin



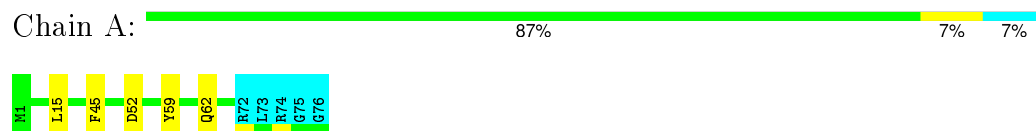
4.2.476 Score per residue for model 476

- Molecule 1: Ubiquitin



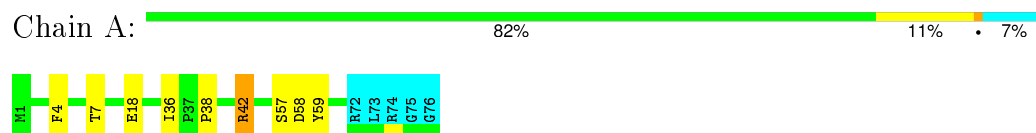
4.2.477 Score per residue for model 477

- Molecule 1: Ubiquitin



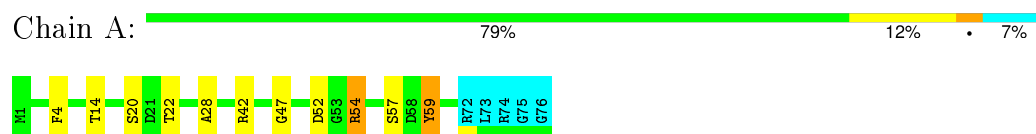
4.2.478 Score per residue for model 478

- Molecule 1: Ubiquitin



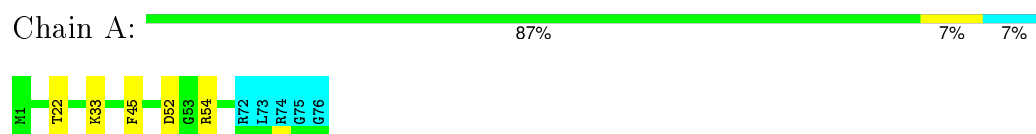
4.2.479 Score per residue for model 479

- Molecule 1: Ubiquitin



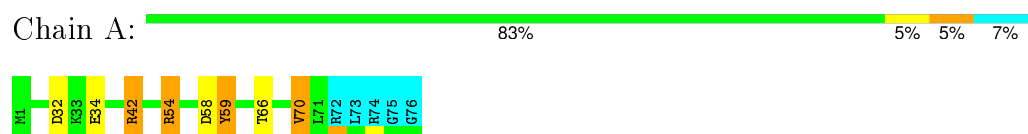
4.2.480 Score per residue for model 480

- Molecule 1: Ubiquitin



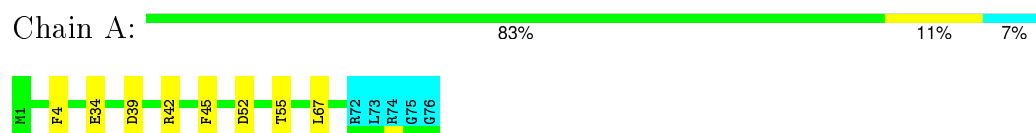
4.2.481 Score per residue for model 481

- Molecule 1: Ubiquitin



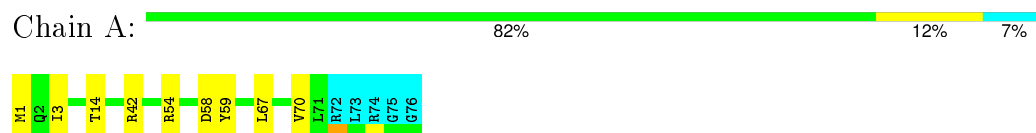
4.2.482 Score per residue for model 482

- Molecule 1: Ubiquitin



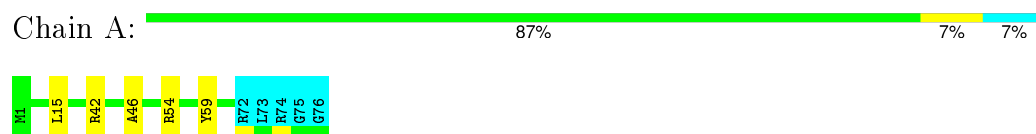
4.2.483 Score per residue for model 483

- Molecule 1: Ubiquitin



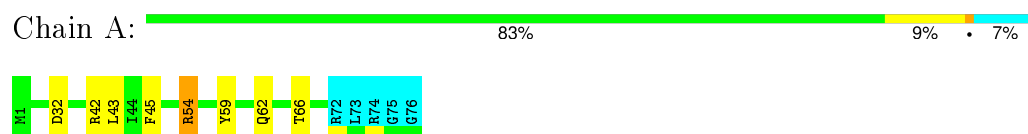
4.2.484 Score per residue for model 484

- Molecule 1: Ubiquitin



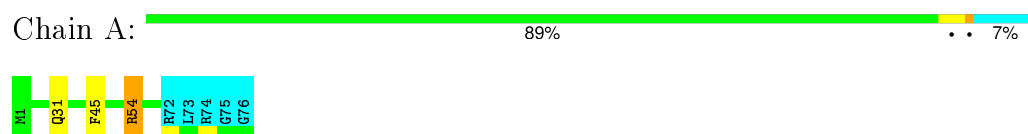
4.2.485 Score per residue for model 485

- Molecule 1: Ubiquitin



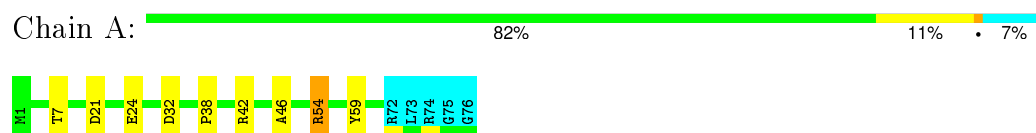
4.2.486 Score per residue for model 486

- Molecule 1: Ubiquitin



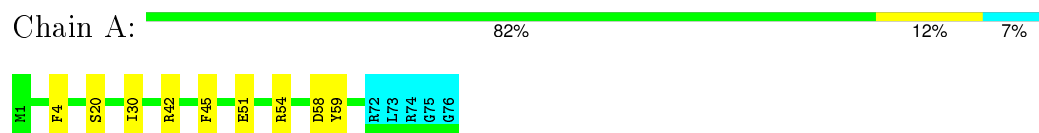
4.2.487 Score per residue for model 487

- Molecule 1: Ubiquitin



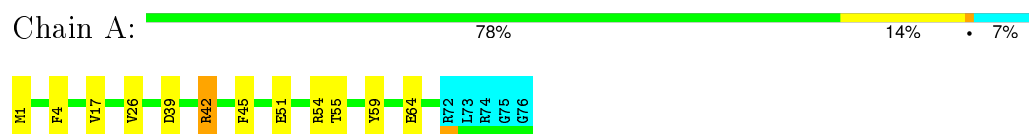
4.2.488 Score per residue for model 488

- Molecule 1: Ubiquitin



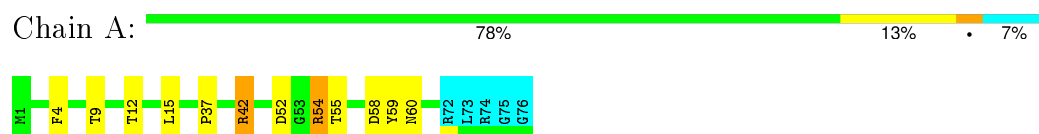
4.2.489 Score per residue for model 489

- Molecule 1: Ubiquitin



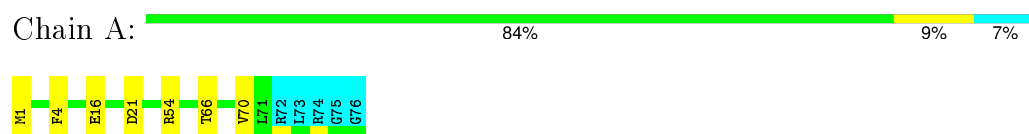
4.2.490 Score per residue for model 490

- Molecule 1: Ubiquitin



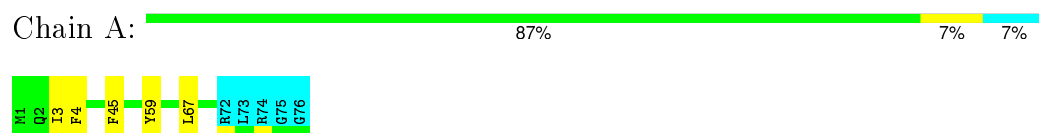
4.2.491 Score per residue for model 491

- Molecule 1: Ubiquitin



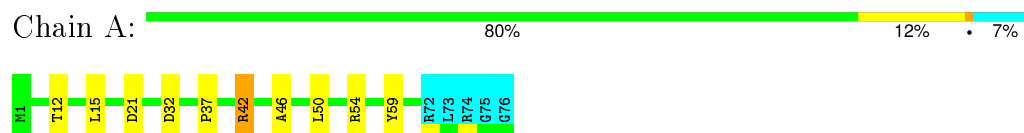
4.2.492 Score per residue for model 492

- Molecule 1: Ubiquitin



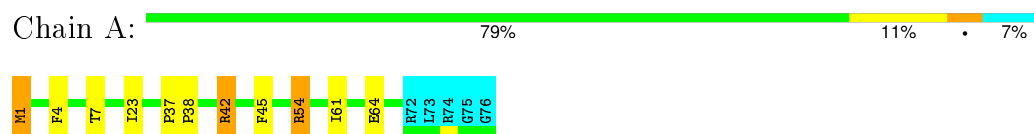
4.2.493 Score per residue for model 493

- Molecule 1: Ubiquitin



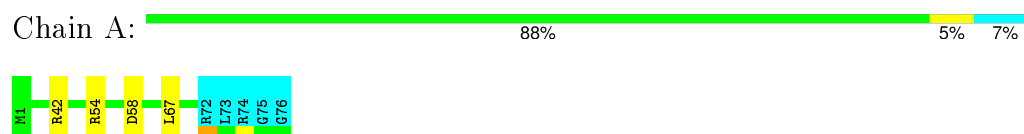
4.2.494 Score per residue for model 494

- Molecule 1: Ubiquitin



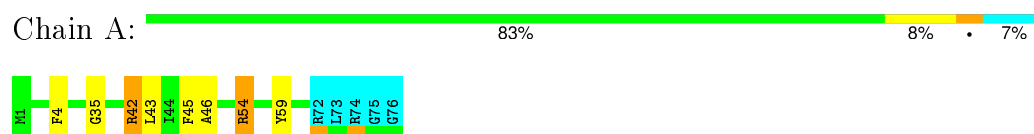
4.2.495 Score per residue for model 495

- Molecule 1: Ubiquitin



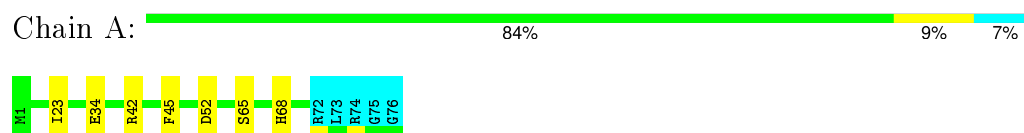
4.2.496 Score per residue for model 496

- Molecule 1: Ubiquitin



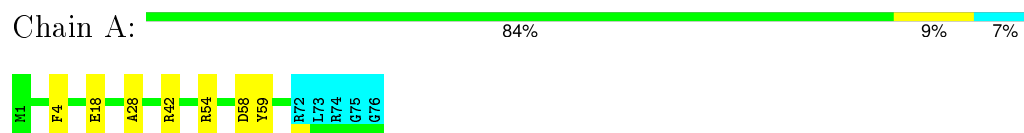
4.2.497 Score per residue for model 497

- Molecule 1: Ubiquitin



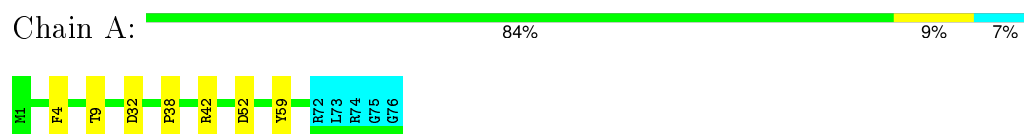
4.2.498 Score per residue for model 498

- Molecule 1: Ubiquitin



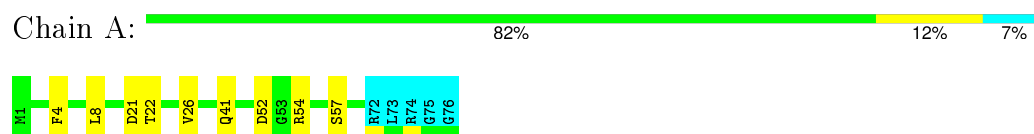
4.2.499 Score per residue for model 499

- Molecule 1: Ubiquitin



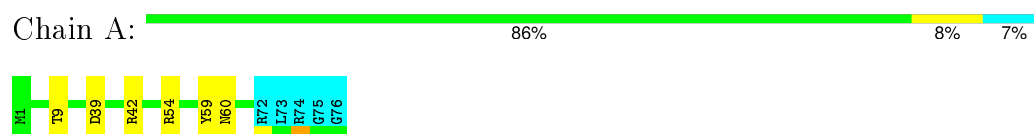
4.2.500 Score per residue for model 500

- Molecule 1: Ubiquitin



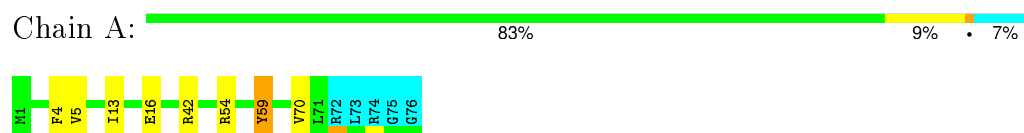
4.2.501 Score per residue for model 501

- Molecule 1: Ubiquitin



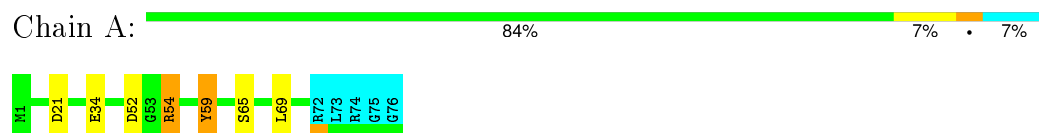
4.2.502 Score per residue for model 502

- Molecule 1: Ubiquitin



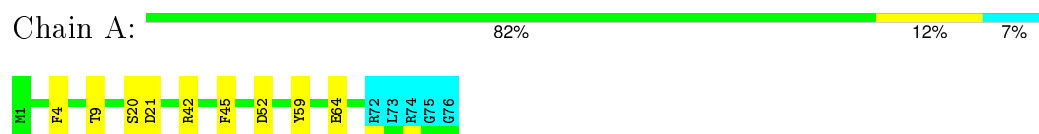
4.2.503 Score per residue for model 503

- Molecule 1: Ubiquitin



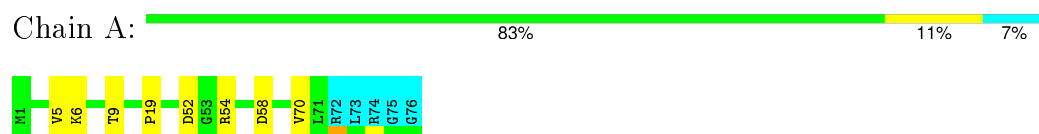
4.2.504 Score per residue for model 504

- Molecule 1: Ubiquitin



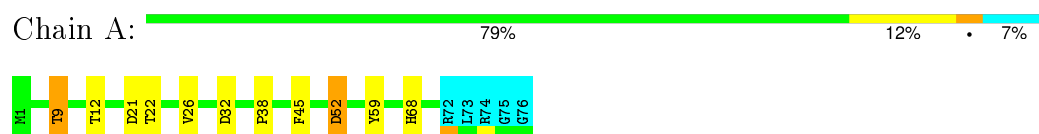
4.2.505 Score per residue for model 505

- Molecule 1: Ubiquitin



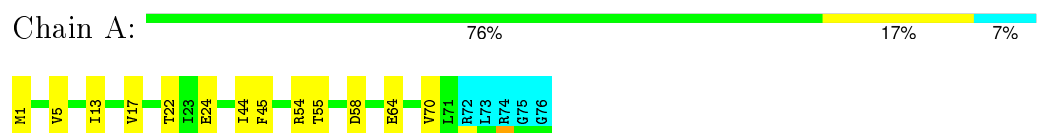
4.2.506 Score per residue for model 506

- Molecule 1: Ubiquitin



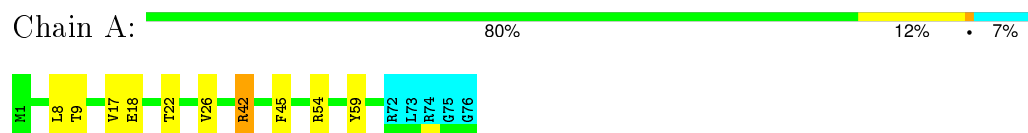
4.2.507 Score per residue for model 507

- Molecule 1: Ubiquitin



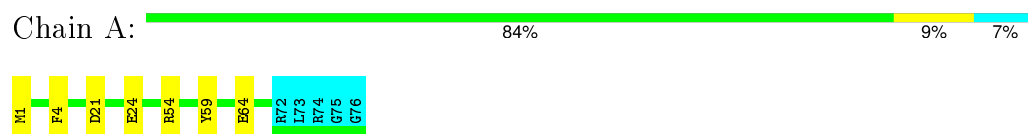
4.2.508 Score per residue for model 508

- Molecule 1: Ubiquitin



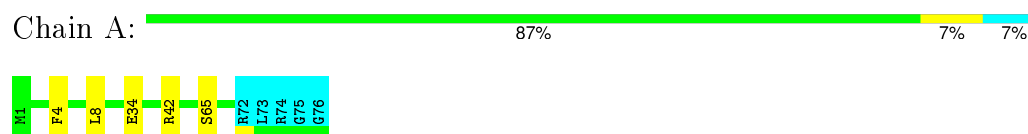
4.2.509 Score per residue for model 509

- Molecule 1: Ubiquitin



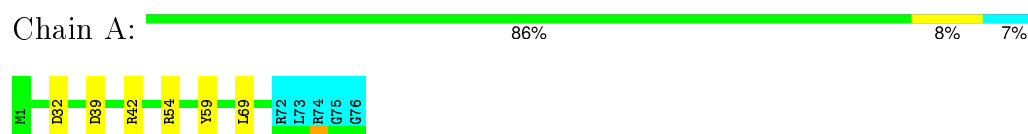
4.2.510 Score per residue for model 510

- Molecule 1: Ubiquitin



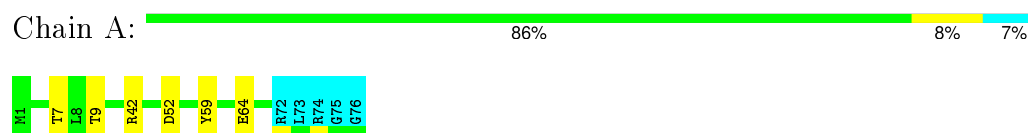
4.2.511 Score per residue for model 511

- Molecule 1: Ubiquitin



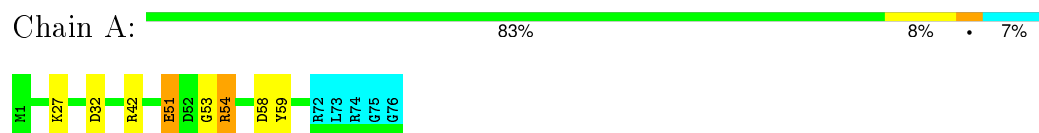
4.2.512 Score per residue for model 512

- Molecule 1: Ubiquitin



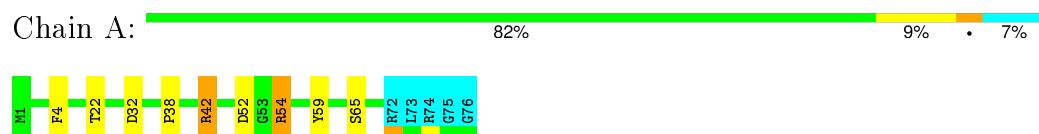
4.2.513 Score per residue for model 513

- Molecule 1: Ubiquitin



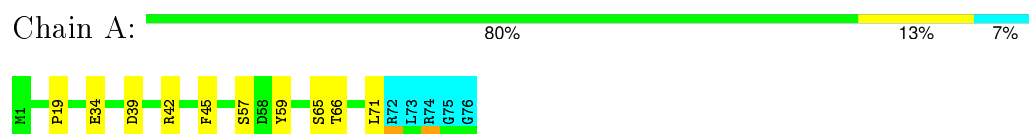
4.2.514 Score per residue for model 514

- Molecule 1: Ubiquitin



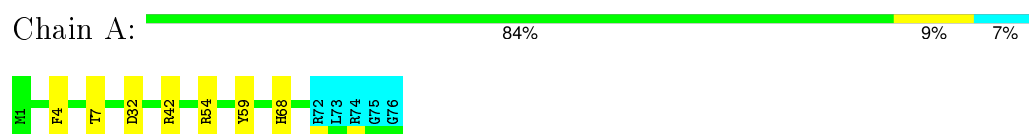
4.2.515 Score per residue for model 515

- Molecule 1: Ubiquitin



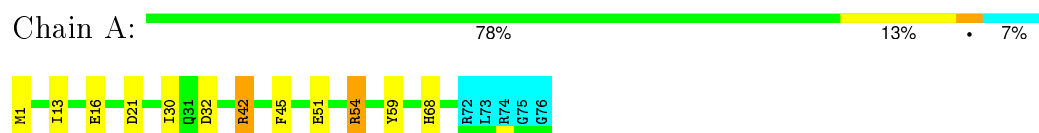
4.2.516 Score per residue for model 516

- Molecule 1: Ubiquitin



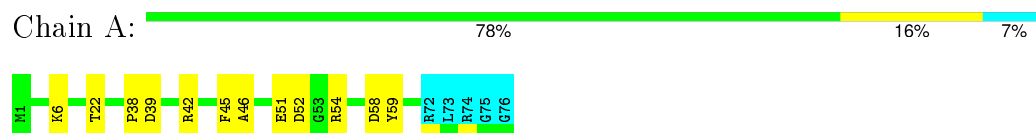
4.2.517 Score per residue for model 517

- Molecule 1: Ubiquitin



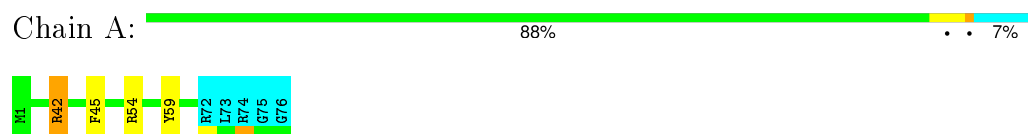
4.2.518 Score per residue for model 518

- Molecule 1: Ubiquitin



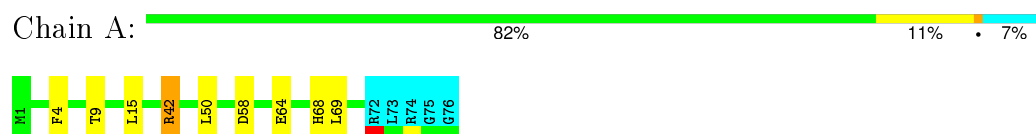
4.2.519 Score per residue for model 519

- Molecule 1: Ubiquitin



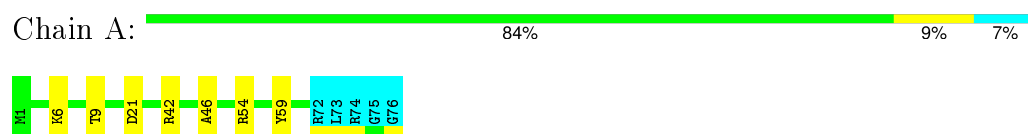
4.2.520 Score per residue for model 520

- Molecule 1: Ubiquitin



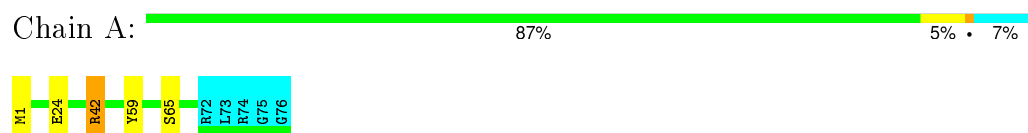
4.2.521 Score per residue for model 521

- Molecule 1: Ubiquitin



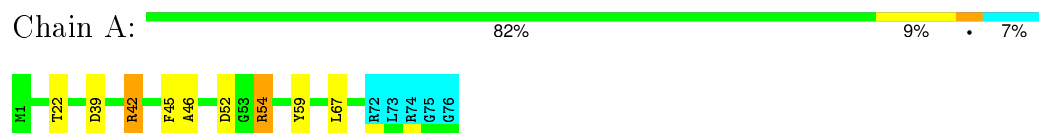
4.2.522 Score per residue for model 522

- Molecule 1: Ubiquitin



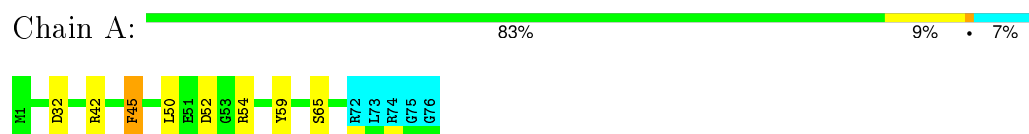
4.2.523 Score per residue for model 523

- Molecule 1: Ubiquitin



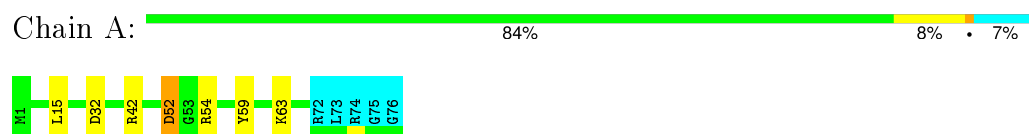
4.2.524 Score per residue for model 524

- Molecule 1: Ubiquitin



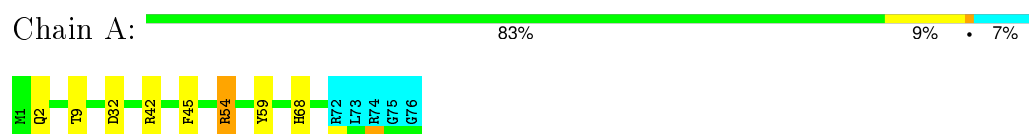
4.2.525 Score per residue for model 525

- Molecule 1: Ubiquitin



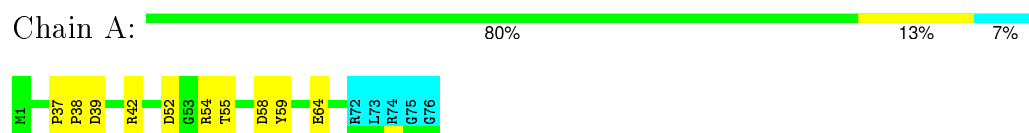
4.2.526 Score per residue for model 526

- Molecule 1: Ubiquitin



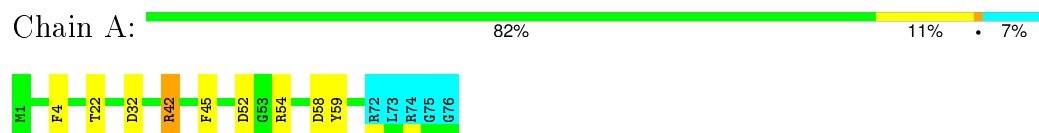
4.2.527 Score per residue for model 527

- Molecule 1: Ubiquitin



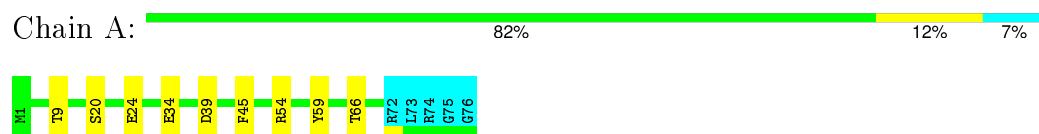
4.2.528 Score per residue for model 528

- Molecule 1: Ubiquitin



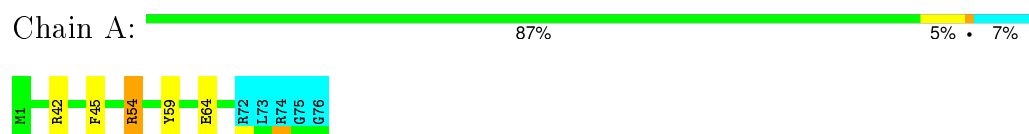
4.2.529 Score per residue for model 529

- Molecule 1: Ubiquitin



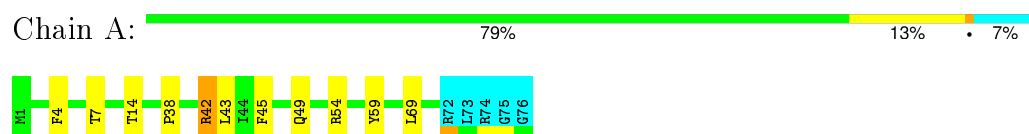
4.2.530 Score per residue for model 530

- Molecule 1: Ubiquitin



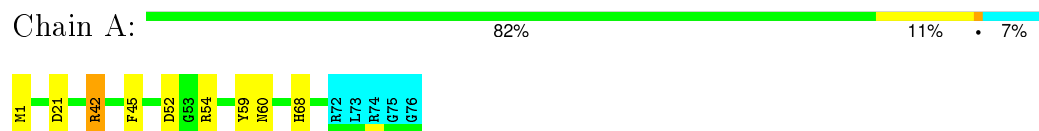
4.2.531 Score per residue for model 531

- Molecule 1: Ubiquitin



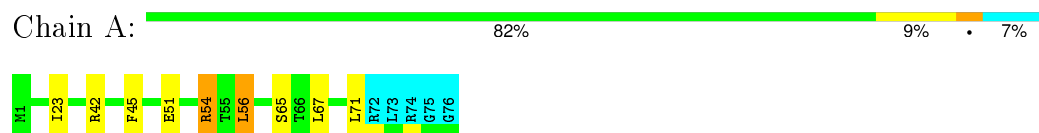
4.2.532 Score per residue for model 532

- Molecule 1: Ubiquitin



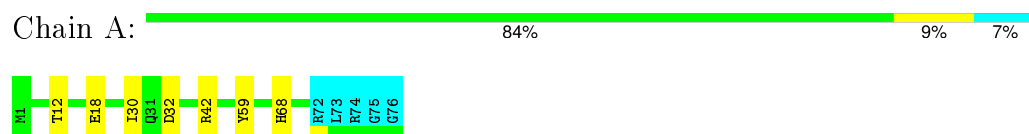
4.2.533 Score per residue for model 533

- Molecule 1: Ubiquitin



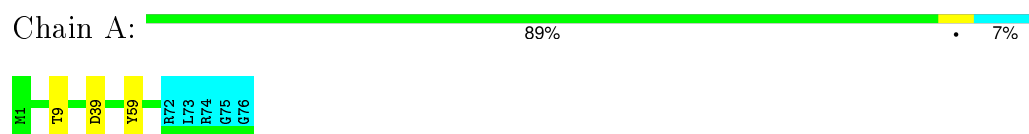
4.2.534 Score per residue for model 534

- Molecule 1: Ubiquitin



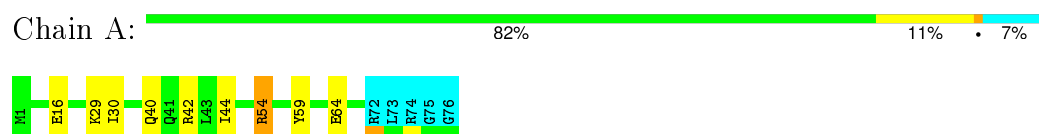
4.2.535 Score per residue for model 535

- Molecule 1: Ubiquitin



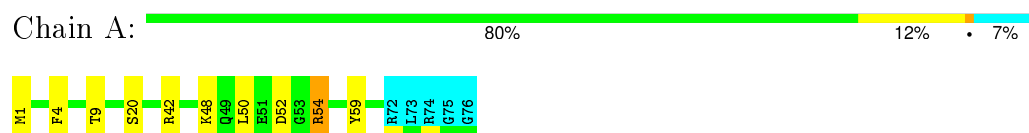
4.2.536 Score per residue for model 536

- Molecule 1: Ubiquitin



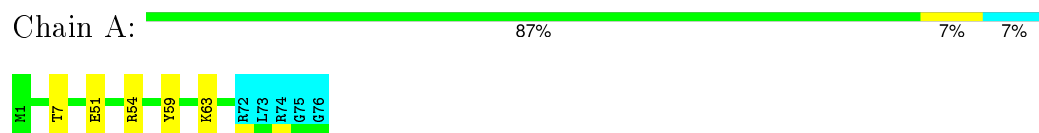
4.2.537 Score per residue for model 537

- Molecule 1: Ubiquitin



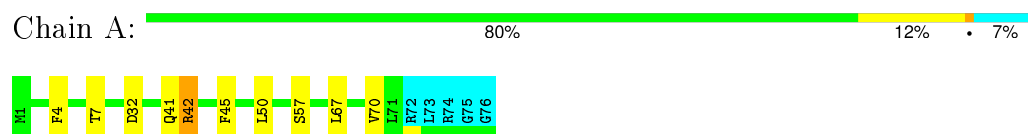
4.2.538 Score per residue for model 538

- Molecule 1: Ubiquitin



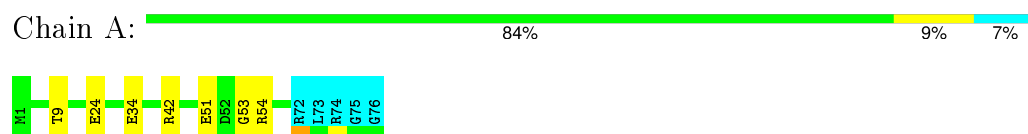
4.2.539 Score per residue for model 539

- Molecule 1: Ubiquitin



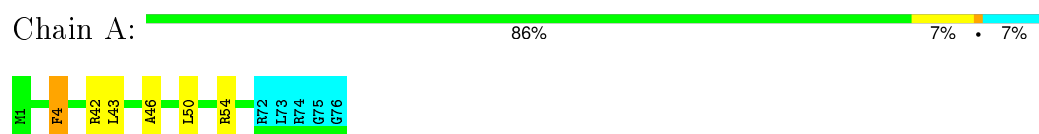
4.2.540 Score per residue for model 540

- Molecule 1: Ubiquitin



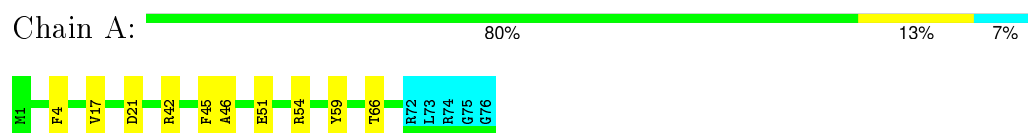
4.2.541 Score per residue for model 541

- Molecule 1: Ubiquitin



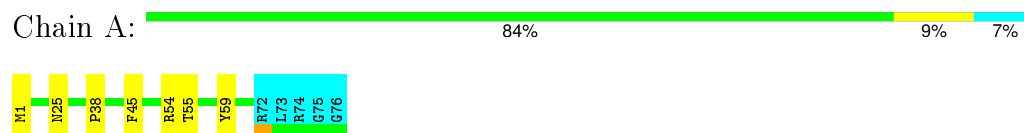
4.2.542 Score per residue for model 542

- Molecule 1: Ubiquitin



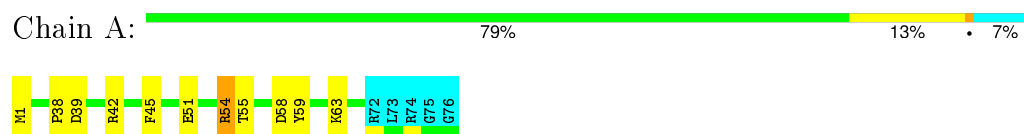
4.2.543 Score per residue for model 543

- Molecule 1: Ubiquitin



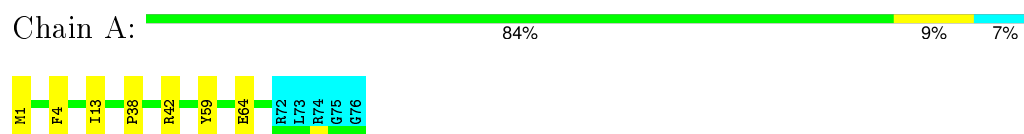
4.2.544 Score per residue for model 544

- Molecule 1: Ubiquitin



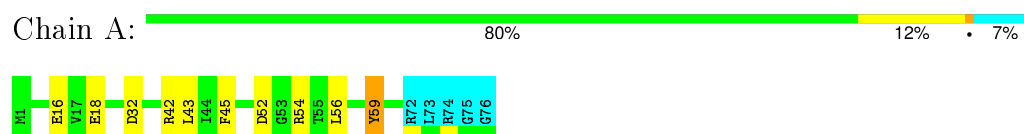
4.2.545 Score per residue for model 545

- Molecule 1: Ubiquitin



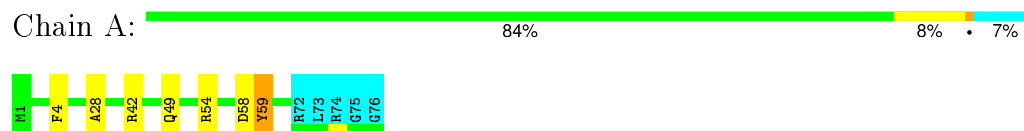
4.2.546 Score per residue for model 546

- Molecule 1: Ubiquitin



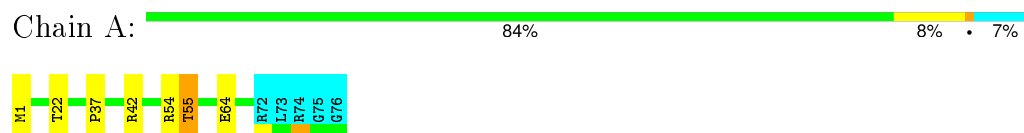
4.2.547 Score per residue for model 547

- Molecule 1: Ubiquitin



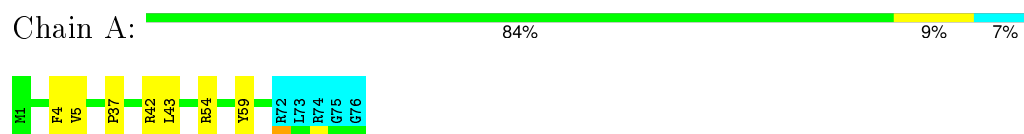
4.2.548 Score per residue for model 548

- Molecule 1: Ubiquitin



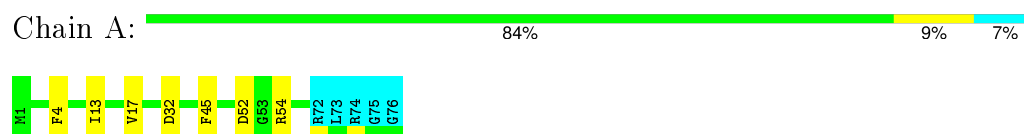
4.2.549 Score per residue for model 549

- Molecule 1: Ubiquitin



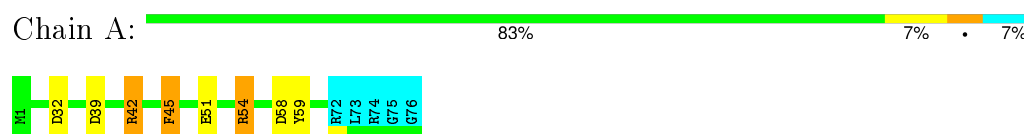
4.2.550 Score per residue for model 550

- Molecule 1: Ubiquitin



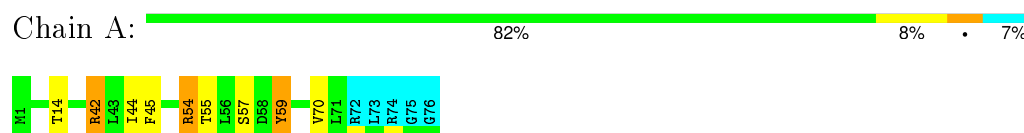
4.2.551 Score per residue for model 551

- Molecule 1: Ubiquitin



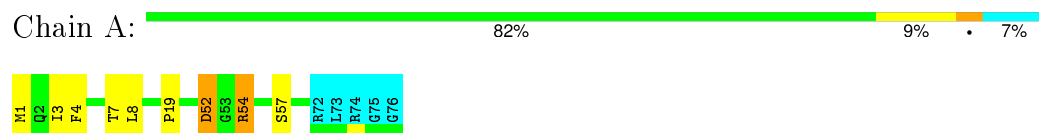
4.2.552 Score per residue for model 552

- Molecule 1: Ubiquitin



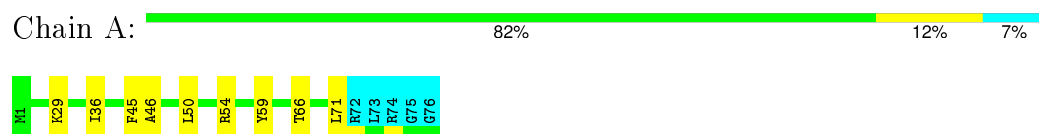
4.2.553 Score per residue for model 553

- Molecule 1: Ubiquitin



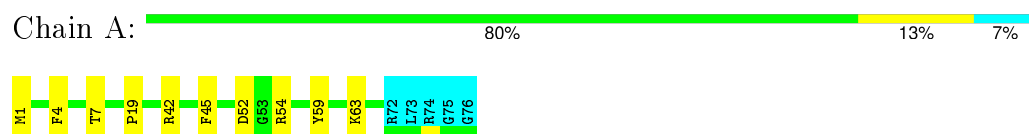
4.2.554 Score per residue for model 554

- Molecule 1: Ubiquitin



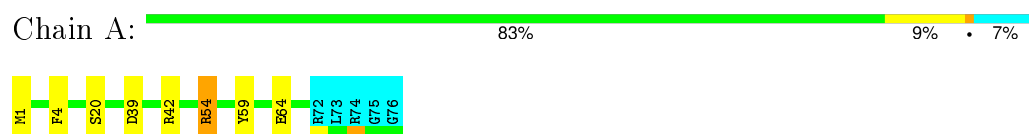
4.2.555 Score per residue for model 555

- Molecule 1: Ubiquitin



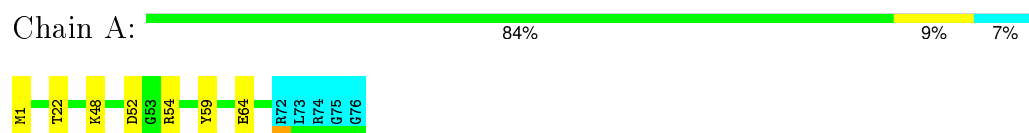
4.2.556 Score per residue for model 556

- Molecule 1: Ubiquitin



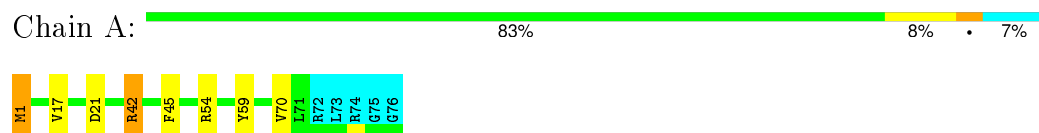
4.2.557 Score per residue for model 557

- Molecule 1: Ubiquitin



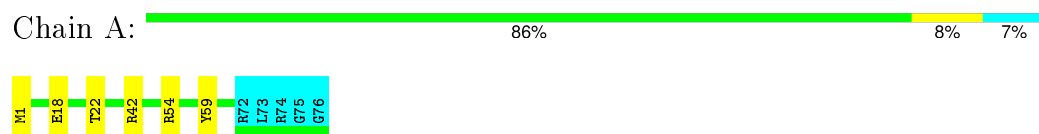
4.2.558 Score per residue for model 558

- Molecule 1: Ubiquitin



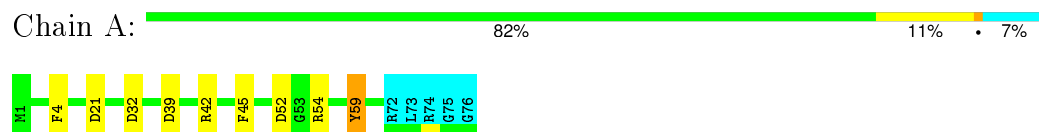
4.2.559 Score per residue for model 559

- Molecule 1: Ubiquitin



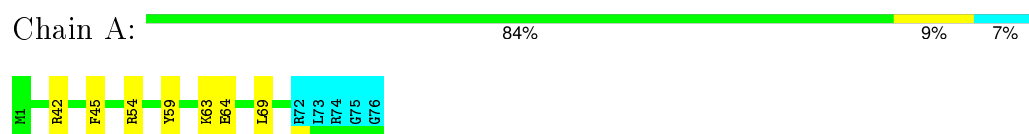
4.2.560 Score per residue for model 560

- Molecule 1: Ubiquitin



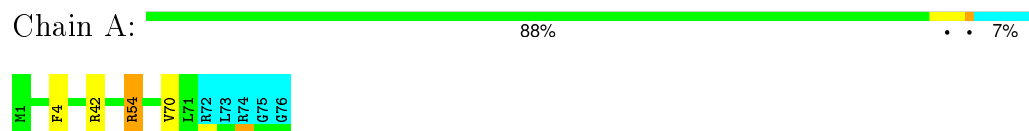
4.2.561 Score per residue for model 561

- Molecule 1: Ubiquitin



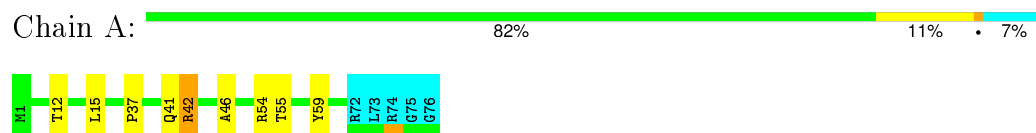
4.2.562 Score per residue for model 562

- Molecule 1: Ubiquitin



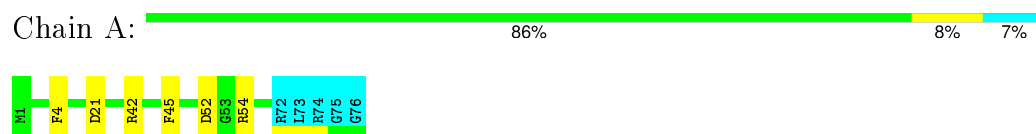
4.2.563 Score per residue for model 563

- Molecule 1: Ubiquitin



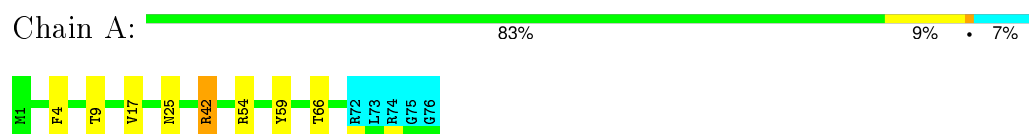
4.2.564 Score per residue for model 564

- Molecule 1: Ubiquitin



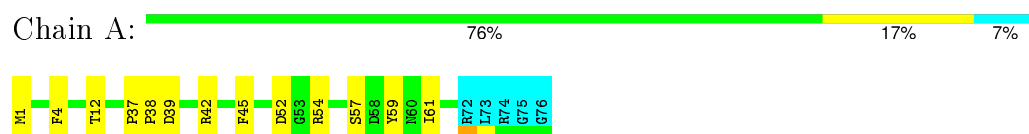
4.2.565 Score per residue for model 565

- Molecule 1: Ubiquitin



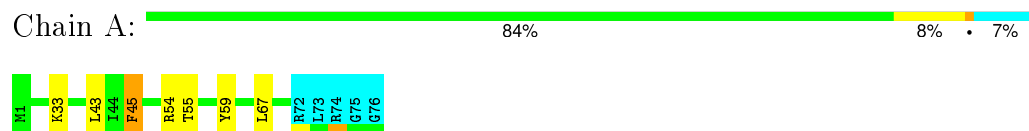
4.2.566 Score per residue for model 566

- Molecule 1: Ubiquitin



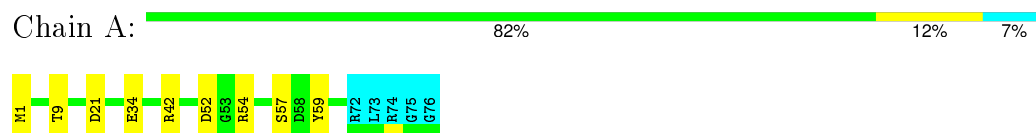
4.2.567 Score per residue for model 567

- Molecule 1: Ubiquitin



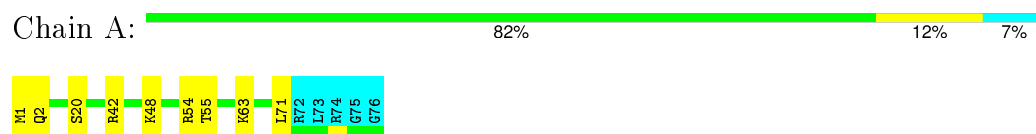
4.2.568 Score per residue for model 568

- Molecule 1: Ubiquitin



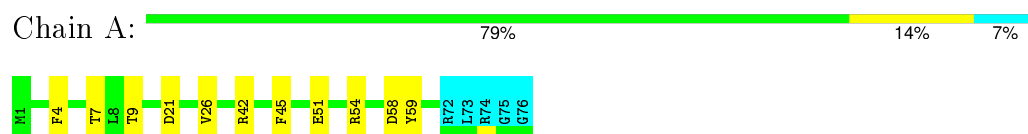
4.2.569 Score per residue for model 569

- Molecule 1: Ubiquitin



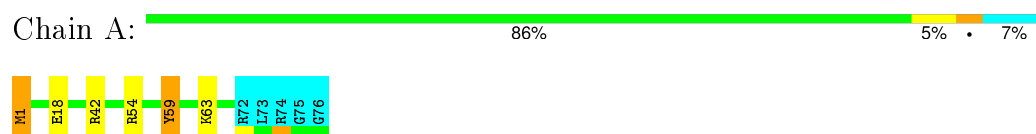
4.2.570 Score per residue for model 570

- Molecule 1: Ubiquitin



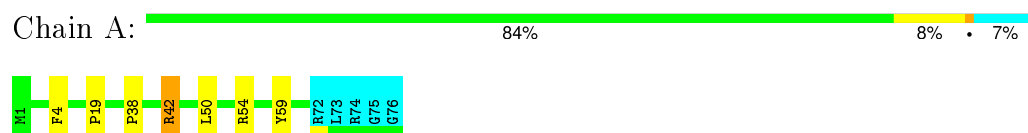
4.2.571 Score per residue for model 571

- Molecule 1: Ubiquitin



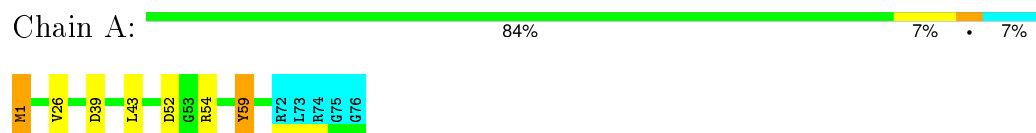
4.2.572 Score per residue for model 572

- Molecule 1: Ubiquitin



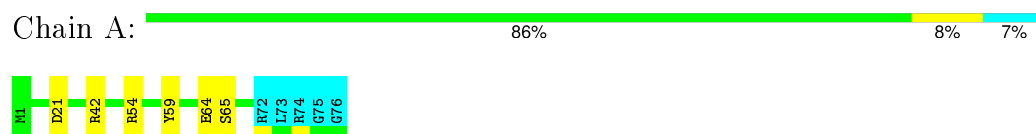
4.2.573 Score per residue for model 573

- Molecule 1: Ubiquitin



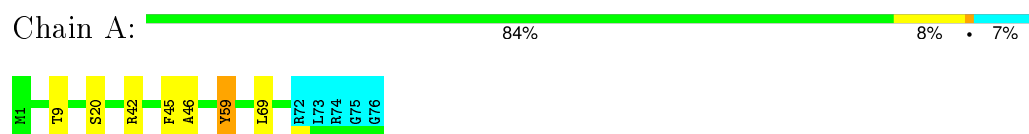
4.2.574 Score per residue for model 574

- Molecule 1: Ubiquitin



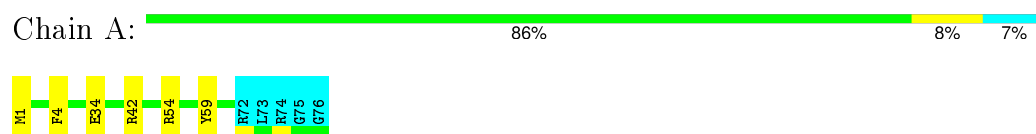
4.2.575 Score per residue for model 575

- Molecule 1: Ubiquitin



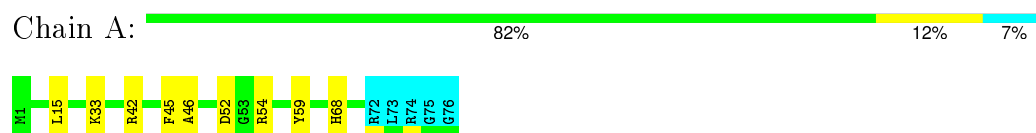
4.2.576 Score per residue for model 576

- Molecule 1: Ubiquitin



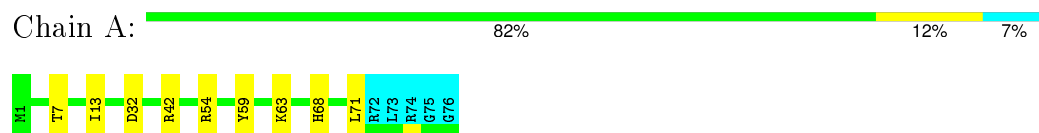
4.2.577 Score per residue for model 577

- Molecule 1: Ubiquitin



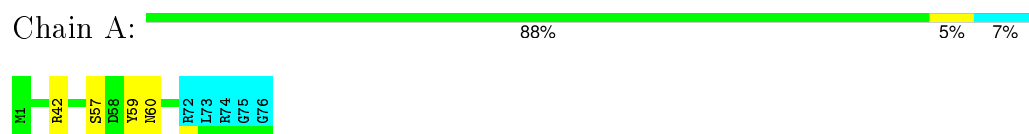
4.2.578 Score per residue for model 578

- Molecule 1: Ubiquitin



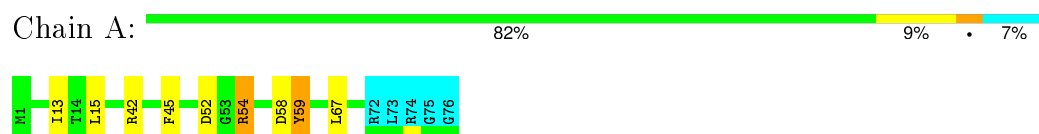
4.2.579 Score per residue for model 579

- Molecule 1: Ubiquitin



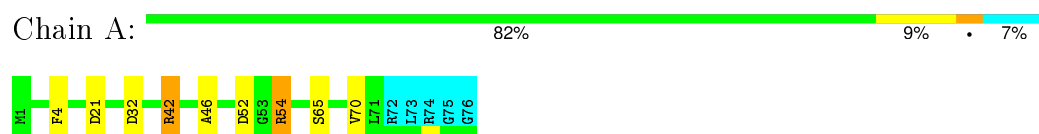
4.2.580 Score per residue for model 580

- Molecule 1: Ubiquitin



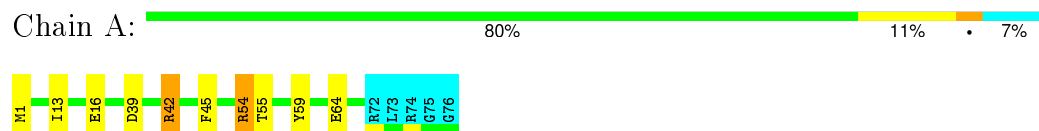
4.2.581 Score per residue for model 581

- Molecule 1: Ubiquitin



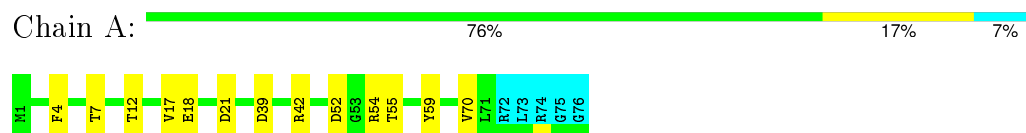
4.2.582 Score per residue for model 582

- Molecule 1: Ubiquitin



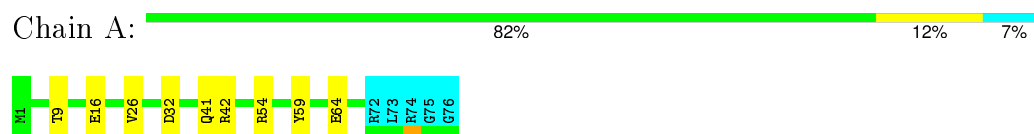
4.2.583 Score per residue for model 583

- Molecule 1: Ubiquitin



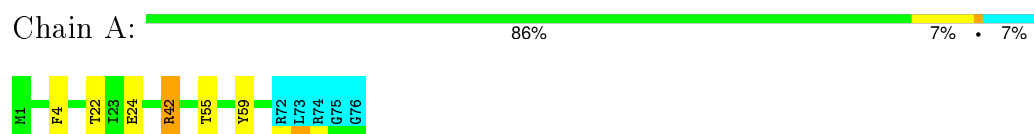
4.2.584 Score per residue for model 584

- Molecule 1: Ubiquitin



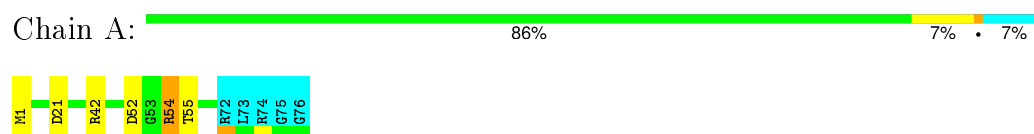
4.2.585 Score per residue for model 585

- Molecule 1: Ubiquitin



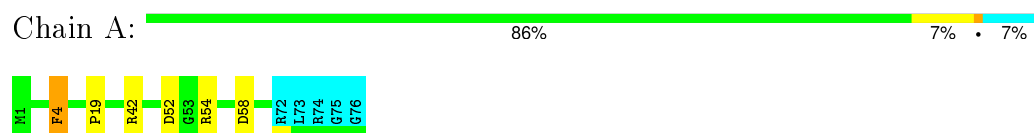
4.2.586 Score per residue for model 586

- Molecule 1: Ubiquitin



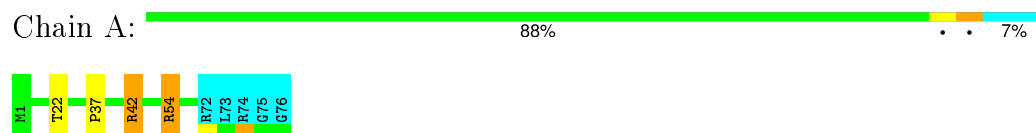
4.2.587 Score per residue for model 587

- Molecule 1: Ubiquitin



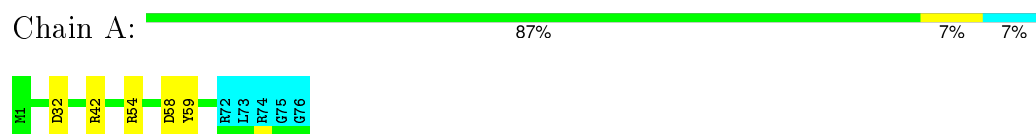
4.2.588 Score per residue for model 588

- Molecule 1: Ubiquitin



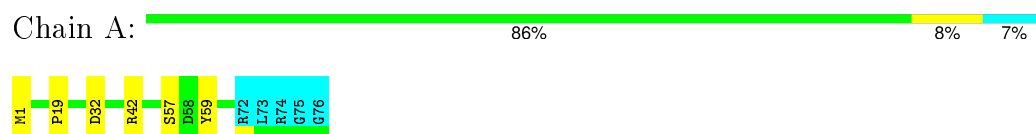
4.2.589 Score per residue for model 589

- Molecule 1: Ubiquitin



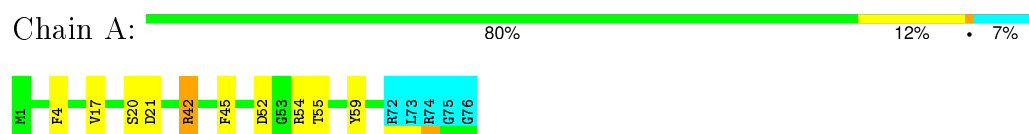
4.2.590 Score per residue for model 590

- Molecule 1: Ubiquitin



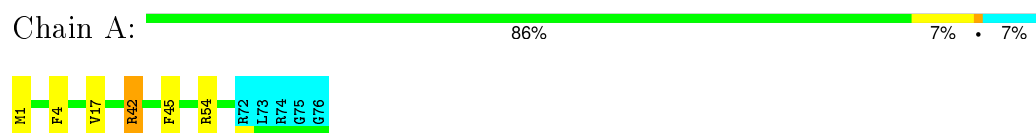
4.2.591 Score per residue for model 591

- 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

Chain A:  79% 13% • 7%



4.2.594 Score per residue for model 594


- Molecule 1: Ubiquitin

Chain A:  87% 7% 7%



4.2.595 Score per residue for model 595


- Molecule 1: Ubiquitin

Chain A:  86% 8% 7%



4.2.596 Score per residue for model 596


- Molecule 1: Ubiquitin

Chain A:  86% 8% 7%



4.2.597 Score per residue for model 597


- Molecule 1: Ubiquitin

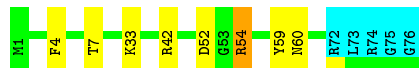
Chain A:  87% 5% • 7%



4.2.598 Score per residue for model 598


- Molecule 1: Ubiquitin

Chain A:  83% 9% 7%



4.2.599 Score per residue for model 599


- Molecule 1: Ubiquitin

Chain A:  84% 9% 7%



4.2.600 Score per residue for model 600


- Molecule 1: Ubiquitin

Chain A:  83% 11% 7%



4.2.601 Score per residue for model 601


- Molecule 1: Ubiquitin

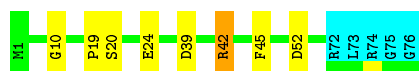
Chain A:  84% 8% 7%



4.2.602 Score per residue for model 602

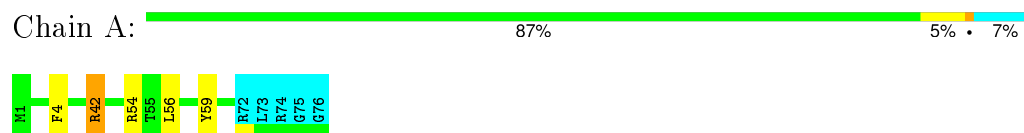
- Molecule 1: Ubiquitin

Chain A:  83% 9% 7%



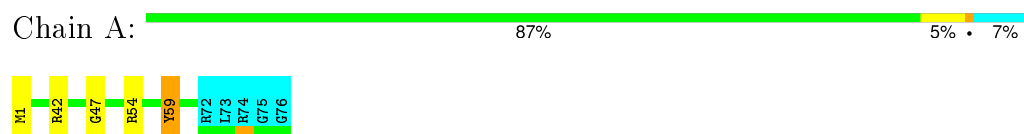
4.2.603 Score per residue for model 603

- Molecule 1: Ubiquitin



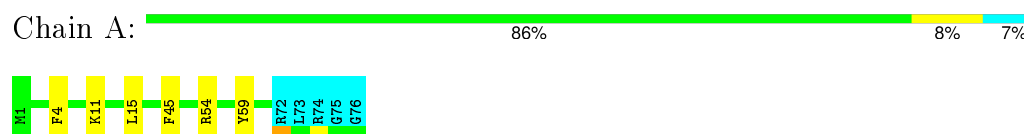
4.2.604 Score per residue for model 604

- Molecule 1: Ubiquitin



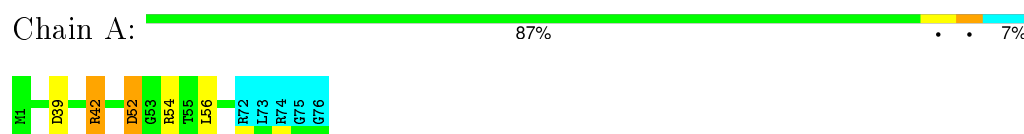
4.2.605 Score per residue for model 605

- Molecule 1: Ubiquitin



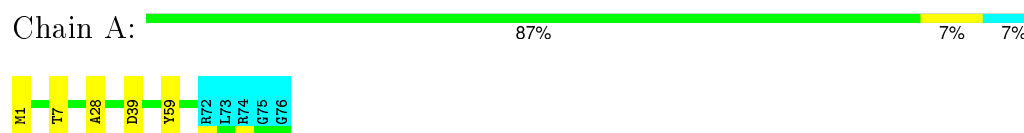
4.2.606 Score per residue for model 606

- Molecule 1: Ubiquitin



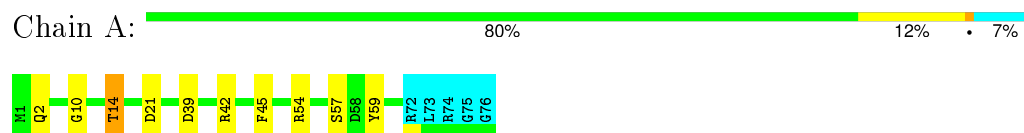
4.2.607 Score per residue for model 607

- Molecule 1: Ubiquitin



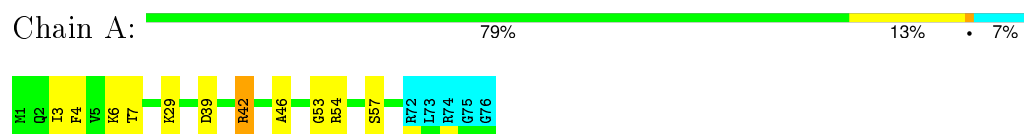
4.2.608 Score per residue for model 608

- Molecule 1: Ubiquitin



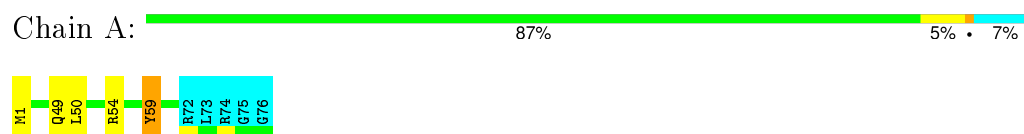
4.2.609 Score per residue for model 609

- Molecule 1: Ubiquitin



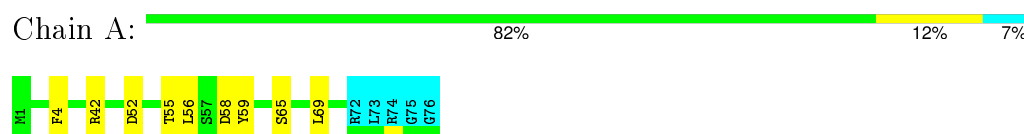
4.2.610 Score per residue for model 610

- Molecule 1: Ubiquitin



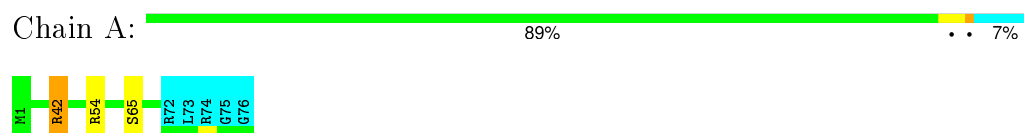
4.2.611 Score per residue for model 611

- Molecule 1: Ubiquitin



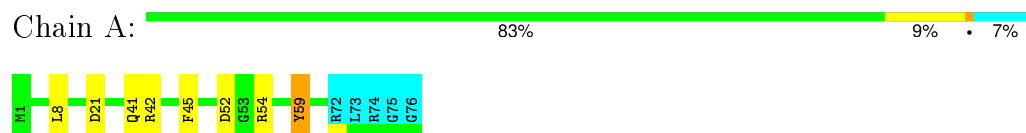
4.2.612 Score per residue for model 612

- Molecule 1: Ubiquitin



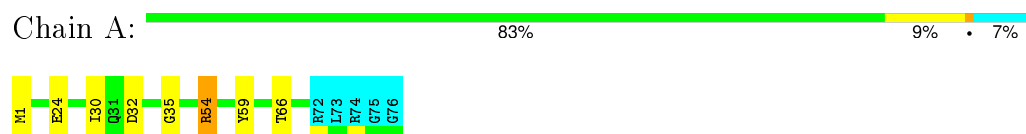
4.2.613 Score per residue for model 613

- Molecule 1: Ubiquitin



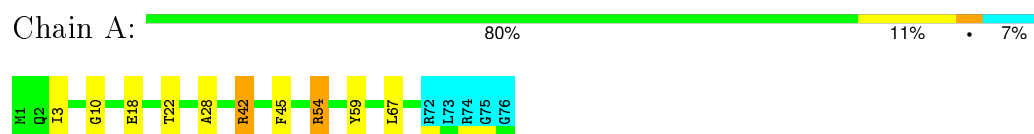
4.2.614 Score per residue for model 614

- Molecule 1: Ubiquitin



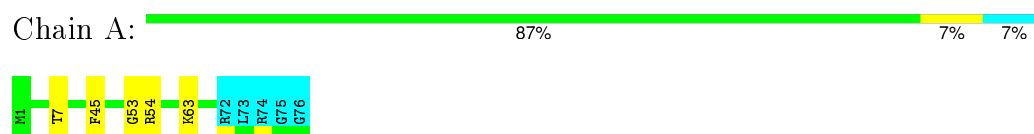
4.2.615 Score per residue for model 615

- Molecule 1: Ubiquitin



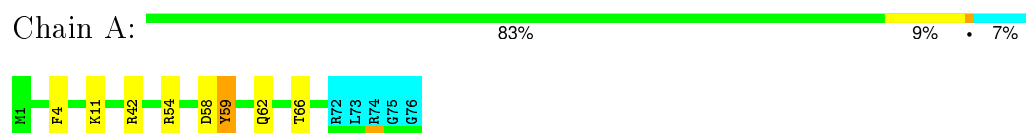
4.2.616 Score per residue for model 616

- Molecule 1: Ubiquitin



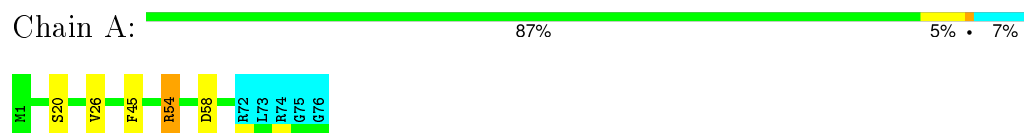
4.2.617 Score per residue for model 617

- Molecule 1: Ubiquitin



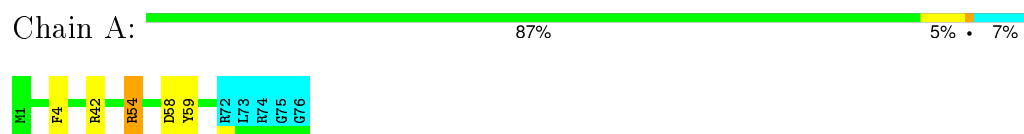
4.2.618 Score per residue for model 618

- Molecule 1: Ubiquitin



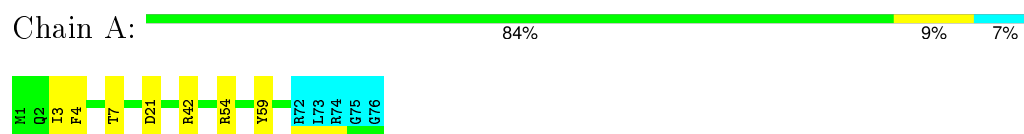
4.2.619 Score per residue for model 619

- Molecule 1: Ubiquitin



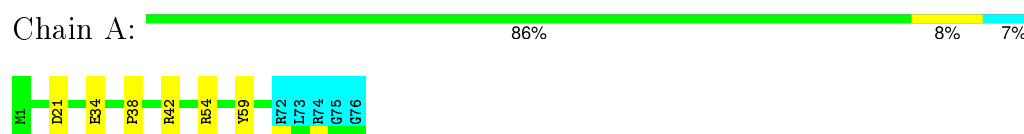
4.2.620 Score per residue for model 620

- Molecule 1: Ubiquitin



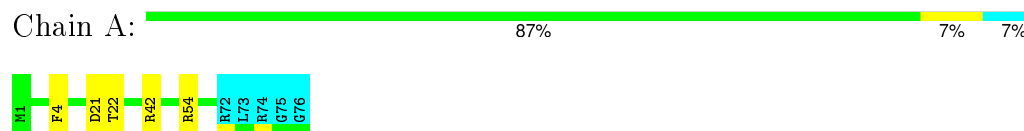
4.2.621 Score per residue for model 621

- Molecule 1: Ubiquitin




4.2.622 Score per residue for model 622

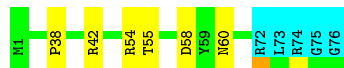
- Molecule 1: Ubiquitin



4.2.623 Score per residue for model 623


- Molecule 1: Ubiquitin

Chain A:  86% 8% 7%



4.2.624 Score per residue for model 624


- Molecule 1: Ubiquitin

Chain A:  82% 11% 7%



4.2.625 Score per residue for model 625


- Molecule 1: Ubiquitin

Chain A:  82% 12% 7%



4.2.626 Score per residue for model 626


- Molecule 1: Ubiquitin

Chain A:  83% 11% 7%



4.2.627 Score per residue for model 627

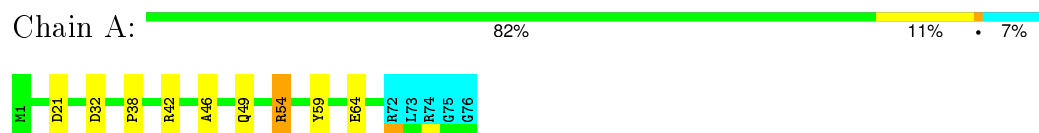
- Molecule 1: Ubiquitin

Chain A:  79% 14% 7%



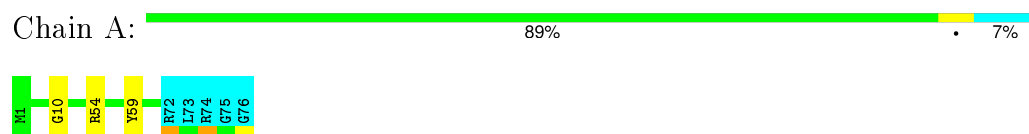
4.2.628 Score per residue for model 628

- Molecule 1: Ubiquitin



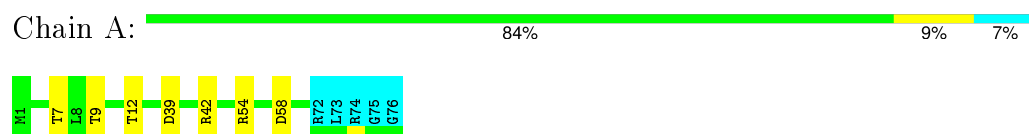
4.2.629 Score per residue for model 629

- Molecule 1: Ubiquitin



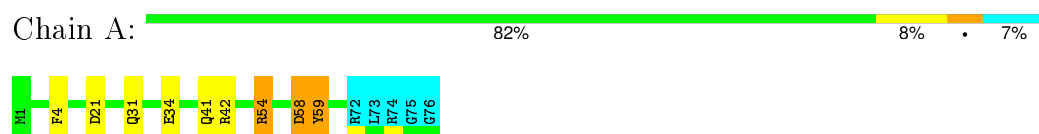
4.2.630 Score per residue for model 630

- Molecule 1: Ubiquitin



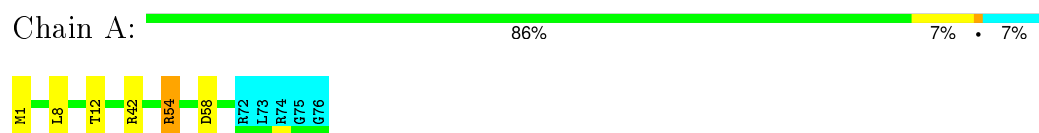
4.2.631 Score per residue for model 631

- Molecule 1: Ubiquitin



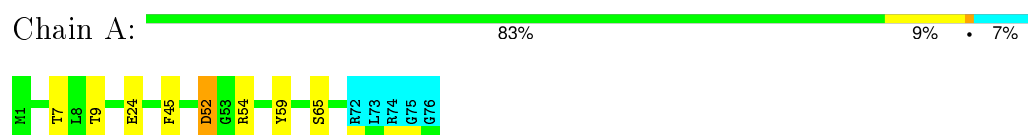
4.2.632 Score per residue for model 632

- Molecule 1: Ubiquitin



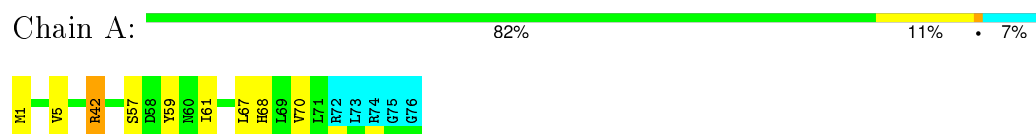
4.2.633 Score per residue for model 633

- Molecule 1: Ubiquitin



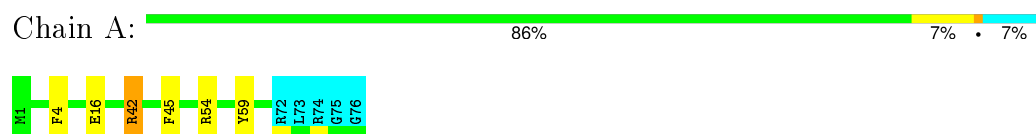
4.2.634 Score per residue for model 634

- Molecule 1: Ubiquitin



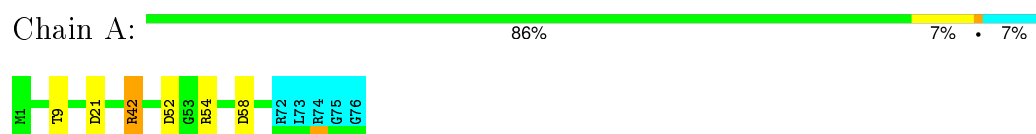
4.2.635 Score per residue for model 635

- Molecule 1: Ubiquitin



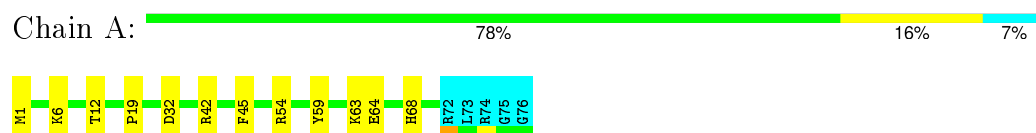
4.2.636 Score per residue for model 636

- 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

Chain A:  89% • 7%



4.2.639 Score per residue for model 639


- Molecule 1: Ubiquitin

Chain A:  83% • 9% • 7%



4.2.640 Score per residue for model 640

- Molecule 1: Ubiquitin

Chain A:  80% • 13% • 7%



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

6 Model quality

6.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|--------------------|-------------|--------------------|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 1.37±0.05 | 1±1/570 (0.2±0.2%) | 1.70±0.07 | 7±3/770 (0.9±0.3%) |
| All | All | 1.37 | 655/364800 (0.2%) | 1.70 | 4559/492800 (0.9%) |

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 | 16 | GLU | CG-CD | 10.83 | 1.68 | 1.51 | 414 | 10 |
| 1 | A | 57 | SER | CA-CB | 8.60 | 1.65 | 1.52 | 590 | 32 |
| 1 | A | 65 | SER | CB-OG | 8.10 | 1.52 | 1.42 | 439 | 4 |
| 1 | A | 59 | TYR | CG-CD1 | 8.06 | 1.49 | 1.39 | 151 | 21 |
| 1 | A | 42 | ARG | CD-NE | 8.01 | 1.60 | 1.46 | 551 | 27 |
| 1 | A | 41 | GLN | CA-CB | 7.99 | 1.71 | 1.53 | 584 | 1 |
| 1 | A | 18 | GLU | CB-CG | 7.96 | 1.67 | 1.52 | 115 | 12 |
| 1 | A | 64 | GLU | CB-CG | 7.90 | 1.67 | 1.52 | 407 | 8 |
| 1 | A | 4 | PHE | CG-CD1 | 7.80 | 1.50 | 1.38 | 389 | 9 |
| 1 | A | 4 | PHE | CE1-CZ | 7.80 | 1.52 | 1.37 | 379 | 4 |
| 1 | A | 20 | SER | CA-CB | 7.48 | 1.64 | 1.52 | 90 | 36 |
| 1 | A | 65 | SER | CA-CB | 7.44 | 1.64 | 1.52 | 581 | 28 |
| 1 | A | 17 | VAL | CB-CG1 | 7.38 | 1.68 | 1.52 | 414 | 1 |
| 1 | A | 54 | ARG | CD-NE | 7.17 | 1.58 | 1.46 | 130 | 31 |
| 1 | A | 59 | TYR | CG-CD2 | 7.02 | 1.48 | 1.39 | 479 | 28 |
| 1 | A | 17 | VAL | N-CA | 7.00 | 1.60 | 1.46 | 414 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 45 | PHE | CG-CD2 | 6.99 | 1.49 | 1.38 | 123 | 12 |
| 1 | A | 24 | GLU | CD-OE2 | 6.98 | 1.33 | 1.25 | 640 | 6 |
| 1 | A | 51 | GLU | CD-OE2 | 6.96 | 1.33 | 1.25 | 513 | 6 |
| 1 | A | 64 | GLU | CD-OE2 | 6.94 | 1.33 | 1.25 | 54 | 11 |
| 1 | A | 24 | GLU | CG-CD | -6.92 | 1.41 | 1.51 | 633 | 9 |
| 1 | A | 4 | PHE | CG-CD2 | 6.89 | 1.49 | 1.38 | 592 | 10 |
| 1 | A | 59 | TYR | CE2-CZ | 6.87 | 1.47 | 1.38 | 127 | 20 |
| 1 | A | 45 | PHE | CB-CG | 6.87 | 1.63 | 1.51 | 371 | 4 |
| 1 | A | 18 | GLU | CD-OE1 | 6.87 | 1.33 | 1.25 | 624 | 7 |
| 1 | A | 70 | VAL | CB-CG1 | 6.85 | 1.67 | 1.52 | 190 | 2 |
| 1 | A | 59 | TYR | CE1-CZ | 6.85 | 1.47 | 1.38 | 624 | 14 |
| 1 | A | 16 | GLU | CD-OE2 | -6.82 | 1.18 | 1.25 | 414 | 9 |
| 1 | A | 59 | TYR | CZ-OH | 6.79 | 1.49 | 1.37 | 213 | 13 |
| 1 | A | 59 | TYR | CD1-CE1 | 6.76 | 1.49 | 1.39 | 187 | 4 |
| 1 | A | 47 | GLY | CA-C | -6.76 | 1.41 | 1.51 | 207 | 7 |
| 1 | A | 59 | TYR | CB-CG | -6.72 | 1.41 | 1.51 | 516 | 10 |
| 1 | A | 59 | TYR | CD2-CE2 | 6.67 | 1.49 | 1.39 | 608 | 9 |
| 1 | A | 35 | GLY | CA-C | -6.67 | 1.41 | 1.51 | 496 | 6 |
| 1 | A | 18 | GLU | CG-CD | -6.66 | 1.42 | 1.51 | 206 | 7 |
| 1 | A | 64 | GLU | CG-CD | -6.65 | 1.42 | 1.51 | 574 | 8 |
| 1 | A | 20 | SER | CB-OG | 6.62 | 1.50 | 1.42 | 432 | 4 |
| 1 | A | 34 | GLU | CB-CG | 6.61 | 1.64 | 1.52 | 497 | 6 |
| 1 | A | 34 | GLU | CD-OE1 | 6.58 | 1.32 | 1.25 | 13 | 3 |
| 1 | A | 45 | PHE | CE2-CZ | 6.55 | 1.49 | 1.37 | 139 | 4 |
| 1 | A | 53 | GLY | CA-C | 6.54 | 1.62 | 1.51 | 609 | 11 |
| 1 | A | 1 | MET | N-CA | 6.53 | 1.59 | 1.46 | 307 | 6 |
| 1 | A | 34 | GLU | CD-OE2 | -6.51 | 1.18 | 1.25 | 294 | 7 |
| 1 | A | 16 | GLU | CB-CG | 6.42 | 1.64 | 1.52 | 546 | 9 |
| 1 | A | 42 | ARG | NE-CZ | 6.36 | 1.41 | 1.33 | 470 | 7 |
| 1 | A | 37 | PRO | N-CD | -6.32 | 1.39 | 1.47 | 418 | 4 |
| 1 | A | 24 | GLU | CD-OE1 | 6.30 | 1.32 | 1.25 | 394 | 4 |
| 1 | A | 41 | GLN | N-CA | -6.29 | 1.33 | 1.46 | 613 | 1 |
| 1 | A | 51 | GLU | CB-CG | 6.27 | 1.64 | 1.52 | 542 | 6 |
| 1 | A | 59 | TYR | CA-CB | 6.22 | 1.67 | 1.53 | 27 | 1 |
| 1 | A | 19 | PRO | N-CD | -6.20 | 1.39 | 1.47 | 555 | 7 |
| 1 | A | 53 | GLY | N-CA | 6.13 | 1.55 | 1.46 | 237 | 3 |
| 1 | A | 45 | PHE | CG-CD1 | 6.07 | 1.47 | 1.38 | 25 | 7 |
| 1 | A | 20 | SER | N-CA | -6.06 | 1.34 | 1.46 | 204 | 1 |
| 1 | A | 49 | GLN | CA-CB | 6.01 | 1.67 | 1.53 | 321 | 1 |
| 1 | A | 35 | GLY | N-CA | 5.99 | 1.55 | 1.46 | 428 | 3 |
| 1 | A | 64 | GLU | CD-OE1 | 5.96 | 1.32 | 1.25 | 45 | 5 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 56 | LEU | CA-CB | 5.93 | 1.67 | 1.53 | 186 | 1 |
| 1 | A | 9 | THR | C-N | 5.84 | 1.43 | 1.33 | 355 | 2 |
| 1 | A | 18 | GLU | C-N | -5.81 | 1.23 | 1.34 | 418 | 1 |
| 1 | A | 57 | SER | CB-OG | 5.81 | 1.49 | 1.42 | 429 | 6 |
| 1 | A | 58 | ASP | CA-CB | 5.79 | 1.66 | 1.53 | 300 | 1 |
| 1 | A | 54 | ARG | CZ-NH1 | -5.79 | 1.25 | 1.33 | 278 | 1 |
| 1 | A | 16 | GLU | CD-OE1 | -5.76 | 1.19 | 1.25 | 74 | 5 |
| 1 | A | 24 | GLU | CB-CG | 5.75 | 1.63 | 1.52 | 529 | 7 |
| 1 | A | 47 | GLY | N-CA | 5.73 | 1.54 | 1.46 | 46 | 1 |
| 1 | A | 50 | LEU | N-CA | -5.69 | 1.34 | 1.46 | 520 | 1 |
| 1 | A | 37 | PRO | CA-C | -5.65 | 1.41 | 1.52 | 120 | 1 |
| 1 | A | 67 | LEU | N-CA | -5.63 | 1.35 | 1.46 | 62 | 1 |
| 1 | A | 51 | GLU | CG-CD | -5.60 | 1.43 | 1.51 | 154 | 9 |
| 1 | A | 45 | PHE | CA-CB | 5.60 | 1.66 | 1.53 | 187 | 1 |
| 1 | A | 18 | GLU | CD-OE2 | 5.56 | 1.31 | 1.25 | 314 | 3 |
| 1 | A | 46 | ALA | CA-CB | 5.55 | 1.64 | 1.52 | 496 | 2 |
| 1 | A | 4 | PHE | CE2-CZ | 5.54 | 1.47 | 1.37 | 547 | 2 |
| 1 | A | 10 | GLY | CA-C | -5.52 | 1.43 | 1.51 | 36 | 6 |
| 1 | A | 54 | ARG | NE-CZ | 5.51 | 1.40 | 1.33 | 316 | 2 |
| 1 | A | 49 | GLN | N-CA | -5.51 | 1.35 | 1.46 | 432 | 1 |
| 1 | A | 4 | PHE | CB-CG | -5.50 | 1.42 | 1.51 | 432 | 3 |
| 1 | A | 38 | PRO | N-CD | 5.49 | 1.55 | 1.47 | 45 | 8 |
| 1 | A | 18 | GLU | CA-CB | 5.47 | 1.66 | 1.53 | 366 | 1 |
| 1 | A | 10 | GLY | N-CA | -5.47 | 1.37 | 1.46 | 608 | 3 |
| 1 | A | 68 | HIS | CB-CG | -5.44 | 1.40 | 1.50 | 234 | 4 |
| 1 | A | 15 | LEU | N-CA | -5.43 | 1.35 | 1.46 | 262 | 1 |
| 1 | A | 45 | PHE | CE1-CZ | 5.41 | 1.47 | 1.37 | 169 | 3 |
| 1 | A | 5 | VAL | CB-CG2 | 5.41 | 1.64 | 1.52 | 505 | 1 |
| 1 | A | 62 | GLN | CA-CB | 5.40 | 1.65 | 1.53 | 416 | 1 |
| 1 | A | 34 | GLU | CG-CD | 5.38 | 1.60 | 1.51 | 337 | 8 |
| 1 | A | 52 | ASP | C-N | 5.38 | 1.42 | 1.33 | 633 | 5 |
| 1 | A | 69 | LEU | CA-CB | 5.38 | 1.66 | 1.53 | 73 | 2 |
| 1 | A | 42 | ARG | CZ-NH1 | 5.38 | 1.40 | 1.33 | 234 | 1 |
| 1 | A | 20 | SER | C-N | 5.36 | 1.46 | 1.34 | 297 | 1 |
| 1 | A | 64 | GLU | N-CA | -5.34 | 1.35 | 1.46 | 504 | 1 |
| 1 | A | 46 | ALA | C-N | 5.32 | 1.42 | 1.33 | 521 | 3 |
| 1 | A | 51 | GLU | CD-OE1 | -5.31 | 1.19 | 1.25 | 627 | 3 |
| 1 | A | 5 | VAL | CA-CB | -5.30 | 1.43 | 1.54 | 311 | 1 |
| 1 | A | 54 | ARG | N-CA | -5.29 | 1.35 | 1.46 | 470 | 1 |
| 1 | A | 63 | LYS | CB-CG | 5.26 | 1.66 | 1.52 | 538 | 1 |
| 1 | A | 22 | THR | N-CA | 5.26 | 1.56 | 1.46 | 223 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 11 | LYS | CD-CE | 5.25 | 1.64 | 1.51 | 228 | 1 |
| 1 | A | 29 | LYS | CD-CE | 5.25 | 1.64 | 1.51 | 347 | 1 |
| 1 | A | 42 | ARG | CZ-NH2 | -5.22 | 1.26 | 1.33 | 4 | 2 |
| 1 | A | 1 | MET | CA-CB | 5.21 | 1.65 | 1.53 | 548 | 1 |
| 1 | A | 31 | GLN | CB-CG | 5.20 | 1.66 | 1.52 | 57 | 1 |
| 1 | A | 26 | VAL | CA-CB | -5.19 | 1.43 | 1.54 | 165 | 1 |
| 1 | A | 19 | PRO | N-CA | -5.19 | 1.38 | 1.47 | 380 | 1 |
| 1 | A | 34 | GLU | C-N | 5.18 | 1.42 | 1.33 | 57 | 2 |
| 1 | A | 8 | LEU | CA-CB | 5.17 | 1.65 | 1.53 | 118 | 1 |
| 1 | A | 16 | GLU | CA-CB | 5.16 | 1.65 | 1.53 | 197 | 1 |
| 1 | A | 50 | LEU | C-N | 5.15 | 1.45 | 1.34 | 362 | 1 |
| 1 | A | 2 | GLN | CG-CD | 5.14 | 1.62 | 1.51 | 414 | 1 |
| 1 | A | 4 | PHE | N-CA | -5.12 | 1.36 | 1.46 | 308 | 1 |
| 1 | A | 17 | VAL | CB-CG2 | 5.10 | 1.63 | 1.52 | 258 | 1 |
| 1 | A | 17 | VAL | CA-CB | -5.04 | 1.44 | 1.54 | 583 | 1 |
| 1 | A | 25 | ASN | N-CA | -5.02 | 1.36 | 1.46 | 344 | 1 |
| 1 | A | 6 | LYS | CD-CE | 5.02 | 1.63 | 1.51 | 463 | 1 |
| 1 | A | 38 | PRO | CA-CB | 5.02 | 1.63 | 1.53 | 356 | 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 | 42 | ARG | NE-CZ-NH1 | 20.09 | 130.34 | 120.30 | 239 | 326 |
| 1 | A | 54 | ARG | NE-CZ-NH2 | -19.78 | 110.41 | 120.30 | 32 | 305 |
| 1 | A | 54 | ARG | NE-CZ-NH1 | 18.53 | 129.57 | 120.30 | 428 | 336 |
| 1 | A | 42 | ARG | NE-CZ-NH2 | -18.11 | 111.24 | 120.30 | 544 | 235 |
| 1 | A | 59 | TYR | CB-CG-CD1 | -16.69 | 110.98 | 121.00 | 595 | 178 |
| 1 | A | 59 | TYR | CB-CG-CD2 | 16.69 | 131.01 | 121.00 | 595 | 172 |
| 1 | A | 4 | PHE | CB-CG-CD1 | -14.48 | 110.67 | 120.80 | 549 | 125 |
| 1 | A | 45 | PHE | CB-CG-CD2 | -13.51 | 111.35 | 120.80 | 257 | 147 |
| 1 | A | 4 | PHE | CB-CG-CD2 | 12.90 | 129.83 | 120.80 | 79 | 127 |
| 1 | A | 21 | ASP | CB-CG-OD2 | -12.00 | 107.50 | 118.30 | 177 | 62 |
| 1 | A | 45 | PHE | CB-CG-CD1 | 11.23 | 128.66 | 120.80 | 129 | 141 |
| 1 | A | 58 | ASP | CB-CG-OD1 | 11.19 | 128.37 | 118.30 | 281 | 73 |
| 1 | A | 32 | ASP | CB-CG-OD1 | 10.90 | 128.11 | 118.30 | 327 | 74 |
| 1 | A | 21 | ASP | CB-CG-OD1 | 10.87 | 128.08 | 118.30 | 586 | 74 |
| 1 | A | 32 | ASP | CB-CG-OD2 | 10.62 | 127.86 | 118.30 | 5 | 58 |
| 1 | A | 39 | ASP | CB-CG-OD1 | 10.49 | 127.74 | 118.30 | 5 | 62 |
| 1 | A | 58 | ASP | CB-CG-OD2 | -10.41 | 108.93 | 118.30 | 28 | 89 |
| 1 | A | 52 | ASP | CB-CG-OD1 | -10.18 | 109.14 | 118.30 | 195 | 78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|--------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 52 | ASP | CB-CG-OD2 | -10.01 | 109.30 | 118.30 | 237 | 64 |
| 1 | A | 39 | ASP | CB-CG-OD2 | 9.80 | 127.12 | 118.30 | 334 | 58 |
| 1 | A | 1 | MET | CG-SD-CE | -9.62 | 84.80 | 100.20 | 28 | 128 |
| 1 | A | 59 | TYR | CG-CD2-CE2 | -9.46 | 113.73 | 121.30 | 295 | 55 |
| 1 | A | 7 | THR | CA-CB-CG2 | -9.37 | 99.28 | 112.40 | 250 | 51 |
| 1 | A | 9 | THR | CA-CB-CG2 | -9.12 | 99.63 | 112.40 | 101 | 93 |
| 1 | A | 54 | ARG | NH1-CZ-NH2 | -9.06 | 109.43 | 119.40 | 424 | 27 |
| 1 | A | 59 | TYR | CZ-CE2-CD2 | 8.45 | 127.41 | 119.80 | 133 | 23 |
| 1 | A | 55 | THR | CA-CB-CG2 | -8.44 | 100.58 | 112.40 | 220 | 34 |
| 1 | A | 22 | THR | CA-CB-CG2 | -8.23 | 100.87 | 112.40 | 334 | 39 |
| 1 | A | 59 | TYR | CD1-CE1-CZ | -8.10 | 112.51 | 119.80 | 66 | 15 |
| 1 | A | 54 | ARG | CD-NE-CZ | 8.04 | 134.85 | 123.60 | 321 | 9 |
| 1 | A | 69 | LEU | CB-CG-CD1 | 7.85 | 124.35 | 111.00 | 503 | 14 |
| 1 | A | 57 | SER | N-CA-CB | 7.85 | 122.28 | 110.50 | 227 | 10 |
| 1 | A | 59 | TYR | CG-CD1-CE1 | -7.81 | 115.05 | 121.30 | 375 | 38 |
| 1 | A | 14 | THR | CA-CB-CG2 | -7.74 | 101.57 | 112.40 | 137 | 22 |
| 1 | A | 16 | GLU | OE1-CD-OE2 | 7.52 | 132.33 | 123.30 | 414 | 8 |
| 1 | A | 20 | SER | N-CA-CB | 7.52 | 121.78 | 110.50 | 379 | 8 |
| 1 | A | 12 | THR | CA-CB-CG2 | -7.49 | 101.92 | 112.40 | 566 | 22 |
| 1 | A | 42 | ARG | NH1-CZ-NH2 | -7.47 | 111.18 | 119.40 | 468 | 32 |
| 1 | A | 22 | THR | N-CA-CB | 7.46 | 124.47 | 110.30 | 352 | 42 |
| 1 | A | 65 | SER | N-CA-CB | 7.32 | 121.47 | 110.50 | 427 | 19 |
| 1 | A | 64 | GLU | OE1-CD-OE2 | -7.24 | 114.62 | 123.30 | 29 | 11 |
| 1 | A | 24 | GLU | OE1-CD-OE2 | -7.17 | 114.69 | 123.30 | 372 | 9 |
| 1 | A | 40 | GLN | CG-CD-OE1 | 7.10 | 135.80 | 121.60 | 369 | 1 |
| 1 | A | 51 | GLU | OE1-CD-OE2 | -7.04 | 114.85 | 123.30 | 396 | 18 |
| 1 | A | 41 | GLN | CB-CA-C | -7.04 | 96.32 | 110.40 | 631 | 8 |
| 1 | A | 27 | LYS | O-C-N | -6.99 | 111.52 | 122.70 | 100 | 8 |
| 1 | A | 28 | ALA | N-CA-CB | 6.99 | 119.88 | 110.10 | 240 | 13 |
| 1 | A | 43 | LEU | CB-CG-CD1 | -6.98 | 99.13 | 111.00 | 34 | 4 |
| 1 | A | 14 | THR | N-CA-CB | 6.98 | 123.55 | 110.30 | 190 | 6 |
| 1 | A | 14 | THR | O-C-N | -6.96 | 111.56 | 122.70 | 248 | 1 |
| 1 | A | 60 | ASN | N-CA-CB | 6.91 | 123.04 | 110.60 | 501 | 14 |
| 1 | A | 34 | GLU | O-C-N | -6.90 | 111.47 | 123.20 | 503 | 6 |
| 1 | A | 1 | MET | O-C-N | -6.88 | 111.70 | 122.70 | 378 | 3 |
| 1 | A | 34 | GLU | OE1-CD-OE2 | -6.85 | 115.08 | 123.30 | 318 | 23 |
| 1 | A | 30 | ILE | O-C-N | -6.81 | 111.81 | 122.70 | 317 | 12 |
| 1 | A | 46 | ALA | CB-CA-C | 6.79 | 120.29 | 110.10 | 300 | 24 |
| 1 | A | 15 | LEU | CB-CG-CD2 | 6.78 | 122.53 | 111.00 | 580 | 11 |
| 1 | A | 23 | ILE | O-C-N | -6.76 | 111.89 | 122.70 | 177 | 9 |
| 1 | A | 55 | THR | N-CA-CB | 6.76 | 123.14 | 110.30 | 139 | 28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 48 | LYS | CB-CA-C | -6.74 | 96.93 | 110.40 | 537 | 3 |
| 1 | A | 15 | LEU | CB-CG-CD1 | 6.72 | 122.43 | 111.00 | 525 | 8 |
| 1 | A | 42 | ARG | CD-NE-CZ | -6.68 | 114.25 | 123.60 | 236 | 12 |
| 1 | A | 25 | ASN | O-C-N | -6.65 | 112.06 | 122.70 | 20 | 3 |
| 1 | A | 41 | GLN | N-CA-CB | -6.64 | 98.65 | 110.60 | 356 | 1 |
| 1 | A | 18 | GLU | OE1-CD-OE2 | -6.64 | 115.33 | 123.30 | 262 | 8 |
| 1 | A | 45 | PHE | CG-CD2-CE2 | -6.63 | 113.51 | 120.80 | 406 | 4 |
| 1 | A | 5 | VAL | CG1-CB-CG2 | -6.62 | 100.30 | 110.90 | 125 | 7 |
| 1 | A | 8 | LEU | CB-CA-C | -6.61 | 97.64 | 110.20 | 632 | 3 |
| 1 | A | 5 | VAL | CA-CB-CG2 | -6.60 | 101.00 | 110.90 | 634 | 12 |
| 1 | A | 68 | HIS | CA-CB-CG | -6.60 | 102.39 | 113.60 | 534 | 9 |
| 1 | A | 71 | LEU | CB-CA-C | 6.54 | 122.63 | 110.20 | 473 | 6 |
| 1 | A | 20 | SER | CB-CA-C | -6.50 | 97.75 | 110.10 | 427 | 9 |
| 1 | A | 49 | GLN | O-C-N | -6.50 | 112.31 | 122.70 | 135 | 3 |
| 1 | A | 56 | LEU | CB-CG-CD1 | 6.49 | 122.04 | 111.00 | 449 | 7 |
| 1 | A | 43 | LEU | CB-CG-CD2 | 6.49 | 122.03 | 111.00 | 452 | 13 |
| 1 | A | 52 | ASP | N-CA-CB | -6.49 | 98.93 | 110.60 | 226 | 2 |
| 1 | A | 26 | VAL | CA-CB-CG2 | -6.43 | 101.26 | 110.90 | 270 | 24 |
| 1 | A | 10 | GLY | O-C-N | -6.42 | 112.44 | 122.70 | 401 | 5 |
| 1 | A | 58 | ASP | CB-CA-C | -6.41 | 97.59 | 110.40 | 623 | 6 |
| 1 | A | 39 | ASP | O-C-N | -6.40 | 112.46 | 122.70 | 299 | 5 |
| 1 | A | 4 | PHE | O-C-N | -6.40 | 112.46 | 122.70 | 478 | 2 |
| 1 | A | 19 | PRO | N-CD-CG | 6.39 | 112.78 | 103.20 | 1 | 3 |
| 1 | A | 70 | VAL | CA-CB-CG2 | 6.37 | 120.46 | 110.90 | 299 | 11 |
| 1 | A | 65 | SER | CB-CA-C | -6.37 | 97.99 | 110.10 | 233 | 13 |
| 1 | A | 66 | THR | N-CA-CB | 6.33 | 122.33 | 110.30 | 260 | 13 |
| 1 | A | 67 | LEU | CB-CG-CD2 | 6.33 | 121.75 | 111.00 | 473 | 13 |
| 1 | A | 54 | ARG | O-C-N | -6.32 | 112.59 | 122.70 | 186 | 5 |
| 1 | A | 69 | LEU | CB-CG-CD2 | 6.30 | 121.72 | 111.00 | 561 | 7 |
| 1 | A | 64 | GLU | CB-CA-C | 6.30 | 122.99 | 110.40 | 494 | 5 |
| 1 | A | 45 | PHE | CG-CD1-CE1 | 6.29 | 127.72 | 120.80 | 310 | 5 |
| 1 | A | 70 | VAL | CA-CB-CG1 | -6.29 | 101.47 | 110.90 | 413 | 12 |
| 1 | A | 64 | GLU | N-CA-CB | 6.27 | 121.89 | 110.60 | 7 | 9 |
| 1 | A | 1 | MET | CB-CA-C | 6.26 | 122.92 | 110.40 | 217 | 1 |
| 1 | A | 45 | PHE | CD1-CG-CD2 | 6.26 | 126.43 | 118.30 | 406 | 3 |
| 1 | A | 59 | TYR | O-C-N | -6.25 | 112.70 | 122.70 | 173 | 2 |
| 1 | A | 42 | ARG | CG-CD-NE | -6.25 | 98.67 | 111.80 | 579 | 18 |
| 1 | A | 46 | ALA | N-CA-CB | 6.24 | 118.84 | 110.10 | 170 | 12 |
| 1 | A | 68 | HIS | N-CA-CB | 6.22 | 121.80 | 110.60 | 639 | 2 |
| 1 | A | 52 | ASP | O-C-N | -6.22 | 112.62 | 123.20 | 35 | 5 |
| 1 | A | 7 | THR | O-C-N | -6.22 | 112.75 | 122.70 | 440 | 5 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 59 | TYR | CB-CA-C | -6.22 | 97.96 | 110.40 | 626 | 3 |
| 1 | A | 28 | ALA | CB-CA-C | -6.21 | 100.78 | 110.10 | 449 | 13 |
| 1 | A | 42 | ARG | CB-CA-C | 6.20 | 122.80 | 110.40 | 128 | 1 |
| 1 | A | 33 | LYS | O-C-N | -6.20 | 112.78 | 122.70 | 480 | 2 |
| 1 | A | 67 | LEU | O-C-N | -6.20 | 112.79 | 122.70 | 425 | 7 |
| 1 | A | 1 | MET | CA-CB-CG | 6.19 | 123.82 | 113.30 | 386 | 11 |
| 1 | A | 70 | VAL | O-C-N | -6.19 | 112.80 | 122.70 | 9 | 7 |
| 1 | A | 40 | GLN | N-CA-CB | -6.17 | 99.48 | 110.60 | 296 | 1 |
| 1 | A | 9 | THR | O-C-N | -6.17 | 112.71 | 123.20 | 217 | 4 |
| 1 | A | 36 | ILE | CG1-CB-CG2 | -6.17 | 97.84 | 111.40 | 290 | 1 |
| 1 | A | 26 | VAL | CG1-CB-CG2 | -6.16 | 101.04 | 110.90 | 184 | 10 |
| 1 | A | 59 | TYR | CD1-CG-CD2 | 6.16 | 124.68 | 117.90 | 164 | 5 |
| 1 | A | 45 | PHE | O-C-N | -6.16 | 112.85 | 122.70 | 447 | 4 |
| 1 | A | 5 | VAL | CA-CB-CG1 | -6.16 | 101.66 | 110.90 | 140 | 5 |
| 1 | A | 50 | LEU | O-C-N | -6.13 | 112.89 | 122.70 | 255 | 4 |
| 1 | A | 70 | VAL | CG1-CB-CG2 | -6.13 | 101.09 | 110.90 | 3 | 7 |
| 1 | A | 34 | GLU | CB-CA-C | -6.12 | 98.16 | 110.40 | 255 | 1 |
| 1 | A | 26 | VAL | O-C-N | -6.12 | 112.91 | 122.70 | 298 | 6 |
| 1 | A | 51 | GLU | C-N-CA | 6.10 | 136.96 | 121.70 | 360 | 12 |
| 1 | A | 71 | LEU | CB-CG-CD1 | -6.10 | 100.63 | 111.00 | 307 | 4 |
| 1 | A | 50 | LEU | CB-CG-CD2 | 6.10 | 121.36 | 111.00 | 493 | 8 |
| 1 | A | 19 | PRO | O-C-N | -6.09 | 112.95 | 122.70 | 296 | 2 |
| 1 | A | 46 | ALA | C-N-CA | 6.09 | 135.08 | 122.30 | 577 | 4 |
| 1 | A | 13 | ILE | O-C-N | -6.08 | 112.97 | 122.70 | 517 | 1 |
| 1 | A | 6 | LYS | O-C-N | -6.07 | 112.98 | 122.70 | 165 | 2 |
| 1 | A | 1 | MET | N-CA-CB | -6.07 | 99.67 | 110.60 | 586 | 4 |
| 1 | A | 54 | ARG | CG-CD-NE | -6.07 | 99.05 | 111.80 | 186 | 19 |
| 1 | A | 7 | THR | N-CA-CB | 6.07 | 121.83 | 110.30 | 379 | 12 |
| 1 | A | 18 | GLU | N-CA-CB | 6.07 | 121.52 | 110.60 | 374 | 2 |
| 1 | A | 26 | VAL | CA-CB-CG1 | 6.07 | 120.00 | 110.90 | 467 | 3 |
| 1 | A | 43 | LEU | N-CA-CB | 6.06 | 122.52 | 110.40 | 549 | 5 |
| 1 | A | 61 | ILE | O-C-N | -6.05 | 113.01 | 122.70 | 62 | 2 |
| 1 | A | 61 | ILE | CB-CA-C | 6.05 | 123.71 | 111.60 | 221 | 1 |
| 1 | A | 2 | GLN | CB-CA-C | -6.05 | 98.29 | 110.40 | 360 | 1 |
| 1 | A | 17 | VAL | CA-CB-CG1 | -6.05 | 101.83 | 110.90 | 591 | 5 |
| 1 | A | 31 | GLN | N-CA-CB | 6.04 | 121.47 | 110.60 | 631 | 1 |
| 1 | A | 39 | ASP | CB-CA-C | -6.04 | 98.33 | 110.40 | 448 | 3 |
| 1 | A | 5 | VAL | O-C-N | -6.03 | 113.05 | 122.70 | 442 | 1 |
| 1 | A | 38 | PRO | N-CA-CB | 6.03 | 110.53 | 103.30 | 506 | 7 |
| 1 | A | 8 | LEU | CB-CG-CD2 | 6.02 | 121.23 | 111.00 | 459 | 3 |
| 1 | A | 58 | ASP | O-C-N | -6.01 | 113.08 | 122.70 | 124 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 45 | PHE | CZ-CE2-CD2 | 6.01 | 127.31 | 120.10 | 482 | 2 |
| 1 | A | 17 | VAL | CB-CA-C | -5.99 | 100.02 | 111.40 | 104 | 10 |
| 1 | A | 45 | PHE | CB-CA-C | 5.98 | 122.36 | 110.40 | 219 | 3 |
| 1 | A | 2 | GLN | N-CA-CB | -5.97 | 99.85 | 110.60 | 327 | 2 |
| 1 | A | 67 | LEU | CB-CG-CD1 | -5.96 | 100.88 | 111.00 | 151 | 5 |
| 1 | A | 64 | GLU | O-C-N | -5.95 | 113.18 | 122.70 | 450 | 5 |
| 1 | A | 18 | GLU | O-C-N | -5.94 | 109.81 | 121.10 | 157 | 2 |
| 1 | A | 48 | LYS | N-CA-CB | 5.93 | 121.28 | 110.60 | 207 | 1 |
| 1 | A | 7 | THR | CA-CB-OG1 | 5.93 | 121.46 | 109.00 | 609 | 1 |
| 1 | A | 66 | THR | CA-CB-CG2 | -5.92 | 104.11 | 112.40 | 49 | 13 |
| 1 | A | 3 | ILE | N-CA-CB | 5.92 | 124.42 | 110.80 | 334 | 7 |
| 1 | A | 56 | LEU | CB-CG-CD2 | 5.92 | 121.06 | 111.00 | 136 | 9 |
| 1 | A | 57 | SER | O-C-N | -5.92 | 113.23 | 122.70 | 279 | 2 |
| 1 | A | 36 | ILE | CB-CA-C | -5.91 | 99.77 | 111.60 | 200 | 5 |
| 1 | A | 15 | LEU | O-C-N | -5.91 | 113.25 | 122.70 | 169 | 2 |
| 1 | A | 12 | THR | N-CA-CB | 5.90 | 121.51 | 110.30 | 225 | 12 |
| 1 | A | 8 | LEU | CB-CG-CD1 | 5.89 | 121.02 | 111.00 | 68 | 4 |
| 1 | A | 42 | ARG | O-C-N | -5.87 | 113.30 | 122.70 | 626 | 3 |
| 1 | A | 54 | ARG | N-CA-CB | 5.87 | 121.17 | 110.60 | 615 | 1 |
| 1 | A | 54 | ARG | CA-CB-CG | 5.87 | 126.31 | 113.40 | 61 | 1 |
| 1 | A | 55 | THR | O-C-N | -5.86 | 113.32 | 122.70 | 586 | 5 |
| 1 | A | 29 | LYS | O-C-N | -5.86 | 113.33 | 122.70 | 554 | 3 |
| 1 | A | 50 | LEU | N-CA-CB | 5.86 | 122.12 | 110.40 | 350 | 2 |
| 1 | A | 67 | LEU | CB-CA-C | -5.84 | 99.11 | 110.20 | 523 | 3 |
| 1 | A | 60 | ASN | O-C-N | -5.83 | 113.37 | 122.70 | 353 | 4 |
| 1 | A | 38 | PRO | N-CD-CG | 5.83 | 111.95 | 103.20 | 376 | 5 |
| 1 | A | 62 | GLN | N-CA-CB | -5.83 | 100.11 | 110.60 | 617 | 2 |
| 1 | A | 27 | LYS | CD-CE-NZ | -5.82 | 98.31 | 111.70 | 513 | 1 |
| 1 | A | 34 | GLU | CA-C-N | 5.81 | 127.81 | 116.20 | 179 | 1 |
| 1 | A | 49 | GLN | CG-CD-OE1 | -5.80 | 110.00 | 121.60 | 93 | 2 |
| 1 | A | 8 | LEU | O-C-N | -5.80 | 113.42 | 122.70 | 292 | 3 |
| 1 | A | 70 | VAL | N-CA-CB | 5.80 | 124.26 | 111.50 | 225 | 2 |
| 1 | A | 39 | ASP | CA-CB-CG | -5.79 | 100.66 | 113.40 | 154 | 2 |
| 1 | A | 15 | LEU | CB-CA-C | -5.78 | 99.22 | 110.20 | 338 | 2 |
| 1 | A | 22 | THR | OG1-CB-CG2 | -5.76 | 96.76 | 110.00 | 301 | 1 |
| 1 | A | 48 | LYS | CD-CE-NZ | -5.75 | 98.47 | 111.70 | 449 | 2 |
| 1 | A | 3 | ILE | CA-CB-CG2 | -5.75 | 99.40 | 110.90 | 156 | 2 |
| 1 | A | 60 | ASN | C-N-CA | 5.75 | 136.07 | 121.70 | 579 | 1 |
| 1 | A | 51 | GLU | O-C-N | -5.74 | 113.51 | 122.70 | 551 | 2 |
| 1 | A | 59 | TYR | CA-CB-CG | -5.73 | 102.51 | 113.40 | 10 | 8 |
| 1 | A | 20 | SER | O-C-N | -5.73 | 113.53 | 122.70 | 155 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 32 | ASP | CB-CA-C | 5.72 | 121.85 | 110.40 | 76 | 2 |
| 1 | A | 47 | GLY | O-C-N | -5.72 | 113.55 | 122.70 | 318 | 1 |
| 1 | A | 49 | GLN | N-CA-CB | 5.71 | 120.88 | 110.60 | 243 | 3 |
| 1 | A | 45 | PHE | N-CA-CB | -5.71 | 100.33 | 110.60 | 104 | 1 |
| 1 | A | 4 | PHE | CB-CA-C | -5.70 | 98.99 | 110.40 | 190 | 2 |
| 1 | A | 36 | ILE | CA-CB-CG1 | 5.70 | 121.84 | 111.00 | 346 | 1 |
| 1 | A | 55 | THR | CA-CB-OG1 | 5.68 | 120.92 | 109.00 | 163 | 2 |
| 1 | A | 44 | ILE | CB-CA-C | -5.67 | 100.26 | 111.60 | 138 | 2 |
| 1 | A | 21 | ASP | O-C-N | -5.66 | 113.64 | 122.70 | 378 | 3 |
| 1 | A | 39 | ASP | N-CA-CB | -5.65 | 100.42 | 110.60 | 298 | 3 |
| 1 | A | 17 | VAL | O-C-N | -5.64 | 113.67 | 122.70 | 163 | 3 |
| 1 | A | 63 | LYS | O-C-N | -5.64 | 113.68 | 122.70 | 555 | 1 |
| 1 | A | 51 | GLU | N-CA-CB | 5.63 | 120.73 | 110.60 | 295 | 1 |
| 1 | A | 40 | GLN | O-C-N | -5.63 | 113.69 | 122.70 | 358 | 3 |
| 1 | A | 66 | THR | O-C-N | -5.62 | 113.70 | 122.70 | 190 | 3 |
| 1 | A | 44 | ILE | O-C-N | -5.62 | 113.71 | 122.70 | 536 | 2 |
| 1 | A | 24 | GLU | O-C-N | -5.61 | 113.72 | 122.70 | 509 | 4 |
| 1 | A | 15 | LEU | N-CA-CB | 5.61 | 121.62 | 110.40 | 520 | 3 |
| 1 | A | 71 | LEU | CB-CG-CD2 | -5.61 | 101.46 | 111.00 | 287 | 5 |
| 1 | A | 62 | GLN | O-C-N | -5.61 | 113.72 | 122.70 | 477 | 1 |
| 1 | A | 25 | ASN | N-CA-CB | 5.60 | 120.68 | 110.60 | 624 | 4 |
| 1 | A | 66 | THR | CA-CB-OG1 | 5.60 | 120.76 | 109.00 | 481 | 2 |
| 1 | A | 68 | HIS | O-C-N | -5.60 | 113.75 | 122.70 | 125 | 2 |
| 1 | A | 32 | ASP | N-CA-CB | -5.59 | 100.53 | 110.60 | 140 | 6 |
| 1 | A | 41 | GLN | CA-CB-CG | -5.59 | 101.09 | 113.40 | 271 | 4 |
| 1 | A | 7 | THR | C-N-CA | 5.59 | 135.67 | 121.70 | 127 | 2 |
| 1 | A | 60 | ASN | CB-CG-OD1 | 5.59 | 132.77 | 121.60 | 437 | 1 |
| 1 | A | 50 | LEU | CB-CG-CD1 | 5.58 | 120.49 | 111.00 | 409 | 1 |
| 1 | A | 45 | PHE | CD1-CE1-CZ | -5.57 | 113.42 | 120.10 | 199 | 1 |
| 1 | A | 62 | GLN | CB-CA-C | 5.55 | 121.50 | 110.40 | 144 | 1 |
| 1 | A | 67 | LEU | N-CA-CB | 5.54 | 121.48 | 110.40 | 434 | 1 |
| 1 | A | 71 | LEU | O-C-N | -5.54 | 113.84 | 122.70 | 357 | 2 |
| 1 | A | 49 | GLN | CB-CA-C | 5.53 | 121.47 | 110.40 | 82 | 2 |
| 1 | A | 42 | ARG | N-CA-CB | 5.53 | 120.56 | 110.60 | 479 | 4 |
| 1 | A | 17 | VAL | CA-CB-CG2 | 5.53 | 119.19 | 110.90 | 302 | 2 |
| 1 | A | 34 | GLU | N-CA-CB | -5.52 | 100.66 | 110.60 | 576 | 2 |
| 1 | A | 62 | GLN | CG-CD-OE1 | 5.52 | 132.63 | 121.60 | 118 | 1 |
| 1 | A | 41 | GLN | O-C-N | -5.51 | 113.88 | 122.70 | 314 | 2 |
| 1 | A | 9 | THR | N-CA-CB | 5.50 | 120.76 | 110.30 | 85 | 3 |
| 1 | A | 61 | ILE | C-N-CA | 5.50 | 135.46 | 121.70 | 494 | 2 |
| 1 | A | 25 | ASN | CB-CA-C | -5.50 | 99.39 | 110.40 | 236 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 13 | ILE | N-CA-CB | 5.49 | 123.43 | 110.80 | 507 | 1 |
| 1 | A | 48 | LYS | CA-CB-CG | 5.49 | 125.47 | 113.40 | 457 | 2 |
| 1 | A | 54 | ARG | CB-CA-C | -5.48 | 99.43 | 110.40 | 171 | 1 |
| 1 | A | 61 | ILE | CA-CB-CG2 | -5.48 | 99.93 | 110.90 | 566 | 2 |
| 1 | A | 18 | GLU | CB-CA-C | -5.48 | 99.44 | 110.40 | 106 | 2 |
| 1 | A | 53 | GLY | O-C-N | -5.48 | 113.94 | 122.70 | 343 | 1 |
| 1 | A | 4 | PHE | CD1-CE1-CZ | 5.45 | 126.64 | 120.10 | 207 | 2 |
| 1 | A | 63 | LYS | CB-CA-C | -5.45 | 99.49 | 110.40 | 413 | 1 |
| 1 | A | 60 | ASN | CA-CB-CG | -5.45 | 101.41 | 113.40 | 623 | 2 |
| 1 | A | 43 | LEU | CB-CA-C | -5.45 | 99.84 | 110.20 | 485 | 2 |
| 1 | A | 52 | ASP | CA-CB-CG | -5.43 | 101.45 | 113.40 | 61 | 4 |
| 1 | A | 37 | PRO | N-CA-CB | 5.43 | 109.81 | 103.30 | 387 | 4 |
| 1 | A | 14 | THR | OG1-CB-CG2 | -5.43 | 97.52 | 110.00 | 223 | 1 |
| 1 | A | 5 | VAL | CB-CA-C | -5.42 | 101.09 | 111.40 | 102 | 2 |
| 1 | A | 69 | LEU | O-C-N | -5.42 | 114.03 | 122.70 | 158 | 1 |
| 1 | A | 9 | THR | CB-CA-C | -5.42 | 96.96 | 111.60 | 294 | 1 |
| 1 | A | 11 | LYS | O-C-N | -5.42 | 114.03 | 122.70 | 236 | 2 |
| 1 | A | 51 | GLU | CB-CA-C | -5.42 | 99.57 | 110.40 | 461 | 1 |
| 1 | A | 11 | LYS | N-CA-CB | 5.41 | 120.34 | 110.60 | 185 | 2 |
| 1 | A | 9 | THR | OG1-CB-CG2 | -5.41 | 97.56 | 110.00 | 57 | 2 |
| 1 | A | 29 | LYS | CB-CA-C | -5.41 | 99.58 | 110.40 | 285 | 1 |
| 1 | A | 9 | THR | C-N-CA | 5.40 | 133.65 | 122.30 | 449 | 1 |
| 1 | A | 4 | PHE | N-CA-CB | 5.40 | 120.32 | 110.60 | 591 | 3 |
| 1 | A | 35 | GLY | O-C-N | -5.40 | 114.06 | 122.70 | 251 | 3 |
| 1 | A | 16 | GLU | O-C-N | -5.40 | 114.07 | 122.70 | 502 | 1 |
| 1 | A | 17 | VAL | CG1-CB-CG2 | -5.38 | 102.30 | 110.90 | 66 | 4 |
| 1 | A | 22 | THR | O-C-N | -5.37 | 114.10 | 122.70 | 298 | 5 |
| 1 | A | 33 | LYS | N-CA-CB | -5.37 | 100.93 | 110.60 | 256 | 1 |
| 1 | A | 3 | ILE | CB-CA-C | -5.37 | 100.85 | 111.60 | 609 | 1 |
| 1 | A | 68 | HIS | CB-CA-C | -5.37 | 99.66 | 110.40 | 240 | 3 |
| 1 | A | 46 | ALA | O-C-N | -5.36 | 114.08 | 123.20 | 628 | 4 |
| 1 | A | 4 | PHE | CG-CD1-CE1 | -5.36 | 114.90 | 120.80 | 531 | 3 |
| 1 | A | 52 | ASP | N-CA-C | 5.36 | 125.46 | 111.00 | 160 | 3 |
| 1 | A | 58 | ASP | CA-CB-CG | -5.36 | 101.62 | 113.40 | 429 | 1 |
| 1 | A | 13 | ILE | CB-CA-C | -5.35 | 100.90 | 111.60 | 468 | 2 |
| 1 | A | 58 | ASP | N-CA-CB | 5.35 | 120.23 | 110.60 | 427 | 2 |
| 1 | A | 6 | LYS | N-CA-CB | 5.34 | 120.21 | 110.60 | 89 | 3 |
| 1 | A | 13 | ILE | CA-CB-CG2 | -5.33 | 100.23 | 110.90 | 304 | 2 |
| 1 | A | 6 | LYS | CA-CB-CG | -5.31 | 101.71 | 113.40 | 518 | 2 |
| 1 | A | 53 | GLY | C-N-CA | 5.30 | 134.95 | 121.70 | 412 | 1 |
| 1 | A | 9 | THR | CA-CB-OG1 | 5.30 | 120.13 | 109.00 | 126 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 50 | LEU | CB-CA-C | -5.28 | 100.17 | 110.20 | 53 | 1 |
| 1 | A | 4 | PHE | CG-CD2-CE2 | -5.28 | 115.00 | 120.80 | 320 | 2 |
| 1 | A | 47 | GLY | CA-C-O | -5.26 | 111.13 | 120.60 | 604 | 1 |
| 1 | A | 4 | PHE | CZ-CE2-CD2 | 5.26 | 126.41 | 120.10 | 145 | 3 |
| 1 | A | 36 | ILE | CA-C-N | 5.24 | 131.76 | 117.10 | 173 | 1 |
| 1 | A | 32 | ASP | O-C-N | -5.22 | 114.35 | 122.70 | 267 | 2 |
| 1 | A | 59 | TYR | C-N-CA | 5.22 | 134.75 | 121.70 | 176 | 1 |
| 1 | A | 33 | LYS | CB-CA-C | -5.22 | 99.97 | 110.40 | 598 | 2 |
| 1 | A | 36 | ILE | CA-CB-CG2 | -5.21 | 100.47 | 110.90 | 253 | 1 |
| 1 | A | 66 | THR | N-CA-C | -5.21 | 96.93 | 111.00 | 542 | 1 |
| 1 | A | 71 | LEU | C-N-CA | 5.21 | 134.72 | 121.70 | 172 | 1 |
| 1 | A | 55 | THR | CA-C-O | 5.21 | 131.03 | 120.10 | 162 | 2 |
| 1 | A | 22 | THR | CA-CB-OG1 | 5.19 | 119.91 | 109.00 | 91 | 2 |
| 1 | A | 37 | PRO | O-C-N | 5.17 | 130.93 | 121.10 | 549 | 1 |
| 1 | A | 24 | GLU | N-CA-CB | -5.17 | 101.29 | 110.60 | 33 | 1 |
| 1 | A | 4 | PHE | N-CA-C | -5.17 | 97.05 | 111.00 | 61 | 1 |
| 1 | A | 42 | ARG | CA-CB-CG | 5.16 | 124.76 | 113.40 | 217 | 1 |
| 1 | A | 69 | LEU | CB-CA-C | 5.16 | 120.01 | 110.20 | 313 | 1 |
| 1 | A | 44 | ILE | N-CA-CB | 5.16 | 122.67 | 110.80 | 461 | 1 |
| 1 | A | 25 | ASN | CA-CB-CG | -5.16 | 102.05 | 113.40 | 565 | 1 |
| 1 | A | 27 | LYS | N-CA-CB | 5.16 | 119.88 | 110.60 | 369 | 2 |
| 1 | A | 60 | ASN | CB-CA-C | 5.15 | 120.69 | 110.40 | 17 | 2 |
| 1 | A | 56 | LEU | O-C-N | -5.14 | 114.47 | 122.70 | 603 | 1 |
| 1 | A | 16 | GLU | CG-CD-OE1 | -5.14 | 108.02 | 118.30 | 635 | 1 |
| 1 | A | 45 | PHE | C-N-CA | 5.13 | 134.53 | 121.70 | 63 | 1 |
| 1 | A | 24 | GLU | CG-CD-OE1 | 5.13 | 128.56 | 118.30 | 331 | 1 |
| 1 | A | 44 | ILE | CG1-CB-CG2 | -5.13 | 100.12 | 111.40 | 360 | 1 |
| 1 | A | 13 | ILE | CG1-CB-CG2 | -5.12 | 100.13 | 111.40 | 275 | 1 |
| 1 | A | 16 | GLU | CA-CB-CG | 5.12 | 124.66 | 113.40 | 54 | 1 |
| 1 | A | 24 | GLU | CB-CA-C | 5.12 | 120.64 | 110.40 | 361 | 1 |
| 1 | A | 36 | ILE | O-C-N | -5.10 | 111.41 | 121.10 | 9 | 1 |
| 1 | A | 21 | ASP | CB-CA-C | -5.09 | 100.21 | 110.40 | 301 | 1 |
| 1 | A | 19 | PRO | N-CA-CB | 5.09 | 109.41 | 103.30 | 433 | 1 |
| 1 | A | 39 | ASP | N-CA-C | 5.09 | 124.74 | 111.00 | 308 | 1 |
| 1 | A | 33 | LYS | CB-CG-CD | 5.09 | 124.82 | 111.60 | 600 | 1 |
| 1 | A | 35 | GLY | N-CA-C | 5.08 | 125.81 | 113.10 | 593 | 1 |
| 1 | A | 31 | GLN | O-C-N | -5.08 | 114.57 | 122.70 | 486 | 2 |
| 1 | A | 52 | ASP | CB-CA-C | -5.06 | 100.29 | 110.40 | 118 | 1 |
| 1 | A | 65 | SER | O-C-N | -5.06 | 114.61 | 122.70 | 515 | 1 |
| 1 | A | 3 | ILE | O-C-N | -5.06 | 114.61 | 122.70 | 620 | 1 |
| 1 | A | 52 | ASP | OD1-CG-OD2 | -5.05 | 113.70 | 123.30 | 326 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 3 | ILE | CA-CB-CG1 | 5.05 | 120.60 | 111.00 | 615 | 1 |
| 1 | A | 3 | ILE | N-CA-C | -5.03 | 97.42 | 111.00 | 309 | 2 |
| 1 | A | 63 | LYS | CB-CG-CD | 5.02 | 124.65 | 111.60 | 342 | 1 |
| 1 | A | 64 | GLU | CB-CG-CD | -5.01 | 100.67 | 114.20 | 316 | 1 |
| 1 | A | 37 | PRO | N-CD-CG | 5.01 | 110.72 | 103.20 | 527 | 1 |
| 1 | A | 2 | GLN | O-C-N | -5.00 | 114.69 | 122.70 | 596 | 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 | 51 | GLU | Peptide | 6 |
| 1 | A | 9 | THR | Peptide | 6 |
| 1 | A | 41 | GLN | Peptide | 3 |
| 1 | A | 17 | VAL | Peptide | 3 |
| 1 | A | 20 | SER | Peptide,Mainchain | 2 |
| 1 | A | 49 | GLN | Peptide | 1 |
| 1 | A | 33 | LYS | Peptide | 1 |
| 1 | A | 32 | ASP | Mainchain | 1 |
| 1 | A | 16 | GLU | Peptide | 1 |
| 1 | A | 61 | ILE | Peptide | 1 |
| 1 | A | 71 | LEU | Peptide | 1 |
| 1 | A | 8 | LEU | Peptide | 1 |
| 1 | A | 37 | PRO | Peptide | 1 |
| 1 | A | 34 | GLU | 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 |
| All | All | 360320 | 375040 | 375040 | 61 |

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: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: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:51:GLU:CD | 1:A:54:ARG:HE | 0.47 | 2.12 | 544 | 1 |
| 1:A:23:ILE:HB | 1:A:52:ASP:HA | 0.47 | 1.87 | 497 | 1 |
| 1:A:50:LEU:HD22 | 1:A:59:TYR:CD2 | 0.47 | 2.45 | 251 | 3 |
| 1:A:15:LEU:HD21 | 1:A:30:ILE:HG13 | 0.47 | 1.86 | 13 | 1 |
| 1:A:44:ILE:HD12 | 1:A:70:VAL:HG21 | 0.46 | 1.87 | 507 | 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:43:LEU:HD21 | 1:A:67:LEU:HD23 | 0.45 | 1.88 | 567 | 1 |
| 1:A:45:PHE:HB3 | 1:A:50:LEU:HD21 | 0.45 | 1.89 | 524 | 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:54:ARG:HH11 | 1:A:58:ASP:CG | 0.43 | 2.16 | 371 | 1 |
| 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:69:LEU:HD23 | 1:A:69:LEU:C | 0.42 | 2.35 | 238 | 1 |
| 1:A:50:LEU:HD11 | 1:A:67:LEU:HD22 | 0.42 | 1.91 | 539 | 1 |
| 1:A:13:ILE:HD12 | 1:A:33:LYS:HG2 | 0.41 | 1.92 | 428 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 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: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:36:ILE:H | 1:A:36:ILE:HD12 | 0.41 | 1.76 | 46 | 1 |
| 1:A:45:PHE:HB2 | 1:A:67:LEU:HD22 | 0.40 | 1.92 | 261 | 1 |
| 1:A:43:LEU:C | 1:A:44:ILE:HD12 | 0.40 | 2.37 | 188 | 1 |

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|----------------|------------|------------|-------------|----|
| 1 | A | 70/76 (92%) | 63±19 (90±26%) | 1±1 (2±2%) | 0±0 (0±1%) | 56 | 85 |
| All | All | 41230/48640 (85%) | 40226 (98%) | 899 (2%) | 105 (0%) | 50 | 83 |

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 | 26 |
| 1 | A | 52 | ASP | 15 |
| 1 | A | 11 | LYS | 11 |
| 1 | A | 37 | PRO | 10 |
| 1 | A | 50 | LEU | 10 |
| 1 | A | 7 | THR | 9 |
| 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 |
| 1 | A | 10 | GLY | 1 |
| 1 | A | 65 | SER | 1 |
| 1 | A | 45 | PHE | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 8 | LEU | 1 |
| 1 | A | 70 | VAL | 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%) | 81 | 97 |
| All | All | 41600/43520 (96%) | 41130 (99%) | 470 (1%) | 81 | 97 |

All 50 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 | 52 | ASP | 57 |
| 1 | A | 38 | PRO | 49 |
| 1 | A | 1 | MET | 39 |
| 1 | A | 19 | PRO | 21 |
| 1 | A | 17 | VAL | 19 |
| 1 | A | 39 | ASP | 16 |
| 1 | A | 37 | PRO | 16 |
| 1 | A | 70 | VAL | 16 |
| 1 | A | 65 | SER | 13 |
| 1 | A | 71 | LEU | 13 |
| 1 | A | 67 | LEU | 12 |
| 1 | A | 13 | ILE | 12 |
| 1 | A | 63 | LYS | 11 |
| 1 | A | 59 | TYR | 10 |
| 1 | A | 48 | LYS | 10 |
| 1 | A | 2 | GLN | 9 |
| 1 | A | 20 | SER | 9 |
| 1 | A | 49 | GLN | 8 |
| 1 | A | 68 | HIS | 8 |
| 1 | A | 7 | THR | 8 |
| 1 | A | 8 | LEU | 8 |
| 1 | A | 14 | THR | 8 |
| 1 | A | 29 | LYS | 7 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 11 | LYS | 7 |
| 1 | A | 21 | ASP | 6 |
| 1 | A | 57 | SER | 6 |
| 1 | A | 62 | GLN | 6 |
| 1 | A | 32 | ASP | 5 |
| 1 | A | 45 | PHE | 4 |
| 1 | A | 12 | THR | 4 |
| 1 | A | 9 | THR | 4 |
| 1 | A | 42 | ARG | 4 |
| 1 | A | 60 | ASN | 4 |
| 1 | A | 58 | ASP | 4 |
| 1 | A | 69 | LEU | 4 |
| 1 | A | 33 | LYS | 4 |
| 1 | A | 23 | ILE | 3 |
| 1 | A | 31 | GLN | 3 |
| 1 | A | 36 | ILE | 3 |
| 1 | A | 15 | LEU | 3 |
| 1 | A | 56 | LEU | 3 |
| 1 | A | 6 | LYS | 2 |
| 1 | A | 25 | ASN | 2 |
| 1 | A | 50 | LEU | 2 |
| 1 | A | 44 | ILE | 2 |
| 1 | A | 54 | ARG | 2 |
| 1 | A | 64 | GLU | 1 |
| 1 | A | 40 | GLN | 1 |
| 1 | A | 18 | GLU | 1 |
| 1 | A | 41 | GLN | 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 ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided