Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 07:20 PM EDT

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

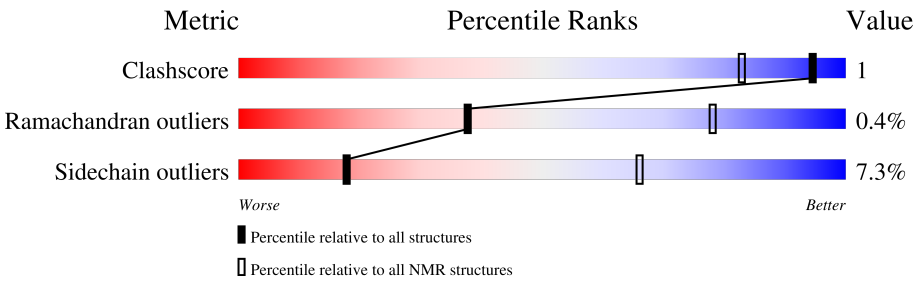
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 42%.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	76	72% 21% 7%

2 Ensemble composition and analysis (i)

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

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:1-A:71 (71)	0.61	210

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

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

The models can be grouped into 5 clusters. No single-model clusters were found.

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

4	57, 202
5	104, 248

3 Entry composition (i)

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

- Molecule 1 is a protein called Ubiquitin.

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

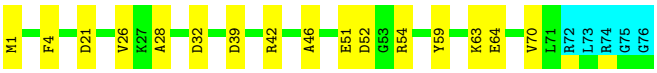
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Ubiquitin

Chain A: 72% 21% 7%



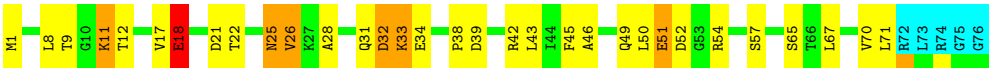
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Ubiquitin

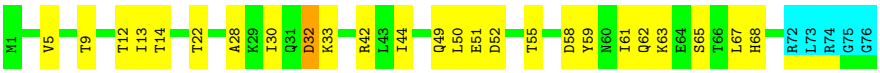
Chain A: 51% 33% 8% • 7%



4.2.2 Score per residue for model 2

• Molecule 1: Ubiquitin

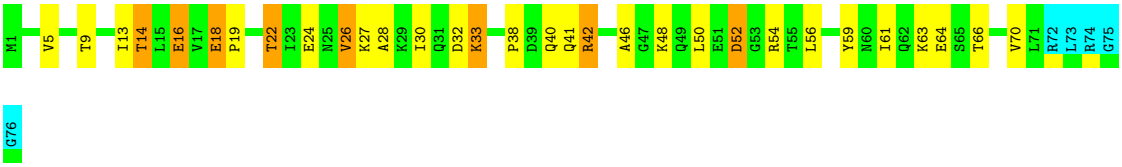
Chain A: 61% 32% • 7%



4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin

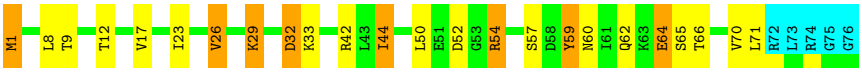
Chain A: 53% 30% 11% 7%



4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin

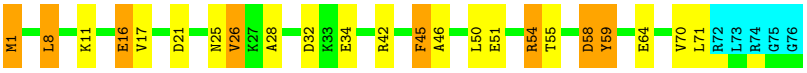
Chain A: 62% 21% 11% 7%



4.2.5 Score per residue for model 5

- Molecule 1: Ubiquitin

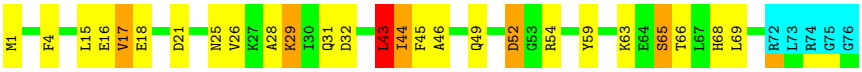
Chain A: 63% 20% 11% 7%



4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin

Chain A: 59% 26% 7% • 7%



4.2.7 Score per residue for model 7

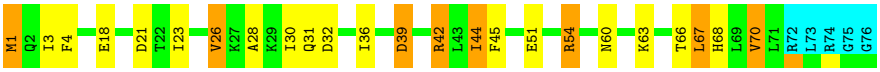
- Molecule 1: Ubiquitin

Chain A: 53% 33% 7% • 7%

4.2.8 Score per residue for model 8

- Molecule 1: Ubiquitin

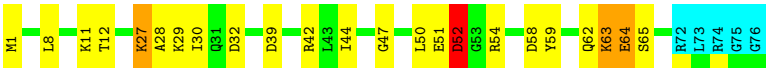
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin

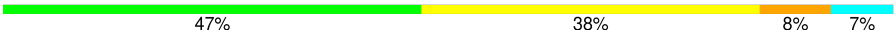
Chain A:

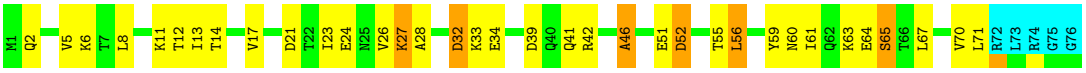


4.2.10 Score per residue for model 10

- Molecule 1: Ubiquitin

Chain A:





4.2.11 Score per residue for model 11

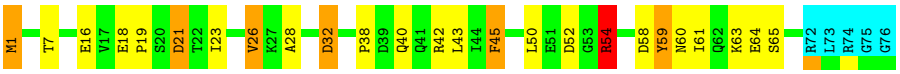
- Molecule 1: Ubiquitin

Chain A:

4.2.12 Score per residue for model 12

- Molecule 1: Ubiquitin

Chain A:



4.2.13 Score per residue for model 13

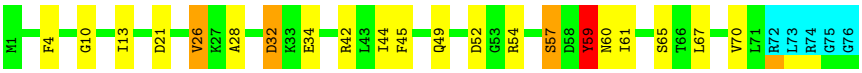
- Molecule 1: Ubiquitin

Chain A:

4.2.14 Score per residue for model 14

- Molecule 1: Ubiquitin

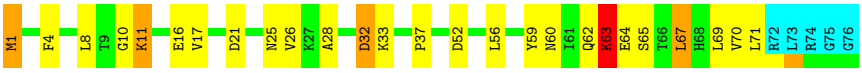
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: Ubiquitin

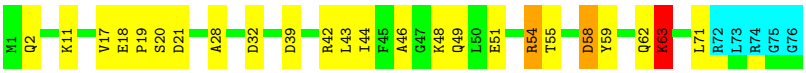
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: Ubiquitin

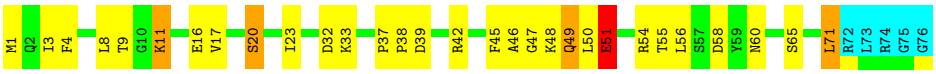
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: Ubiquitin

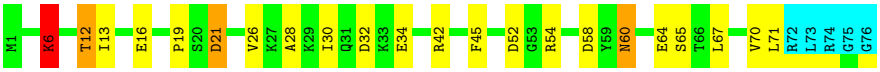
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: Ubiquitin

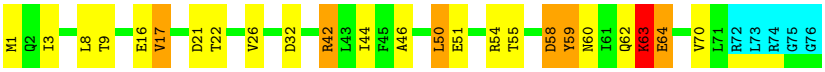
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Ubiquitin

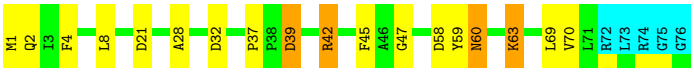
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Ubiquitin

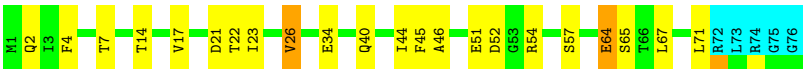
Chain A:



4.2.21 Score per residue for model 21

- Molecule 1: Ubiquitin

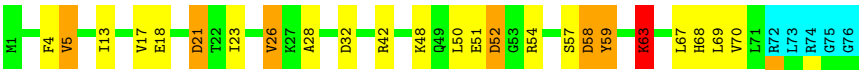
Chain A:



4.2.22 Score per residue for model 22

- Molecule 1: Ubiquitin

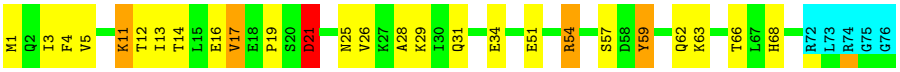
Chain A:



4.2.23 Score per residue for model 23

- Molecule 1: Ubiquitin

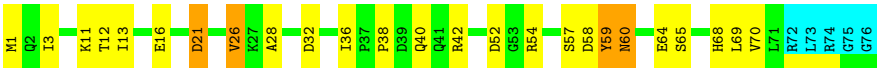
Chain A:



4.2.24 Score per residue for model 24

- Molecule 1: Ubiquitin

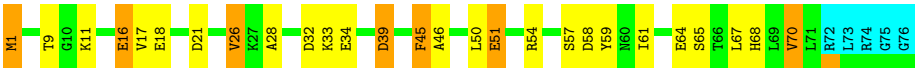
Chain A:



4.2.25 Score per residue for model 25

- Molecule 1: Ubiquitin

Chain A:



4.2.26 Score per residue for model 26

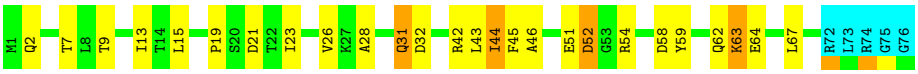
- Molecule 1: Ubiquitin

Chain A:

4.2.27 Score per residue for model 27

- Molecule 1: Ubiquitin

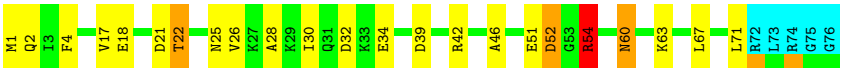
Chain A:



4.2.28 Score per residue for model 28

- Molecule 1: Ubiquitin

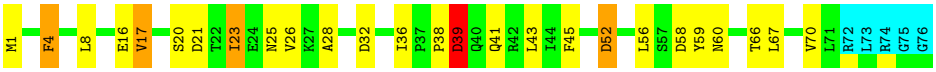
Chain A:



4.2.29 Score per residue for model 29

- Molecule 1: Ubiquitin

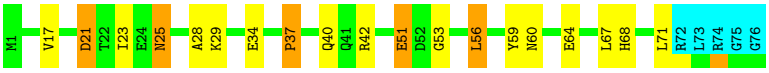
Chain A:



4.2.30 Score per residue for model 30

- Molecule 1: Ubiquitin

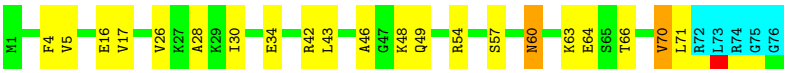
Chain A:



4.2.31 Score per residue for model 31

- Molecule 1: Ubiquitin

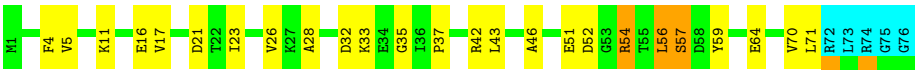
Chain A:



4.2.32 Score per residue for model 32

- Molecule 1: Ubiquitin

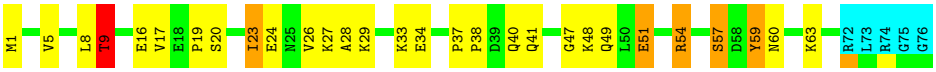
Chain A:



4.2.33 Score per residue for model 33

- Molecule 1: Ubiquitin

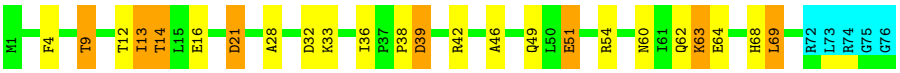
Chain A:



4.2.34 Score per residue for model 34

- Molecule 1: Ubiquitin

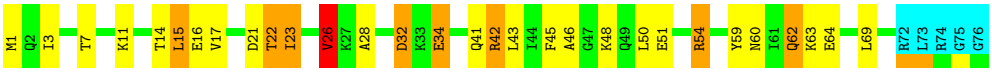
Chain A:



4.2.35 Score per residue for model 35

- Molecule 1: Ubiquitin

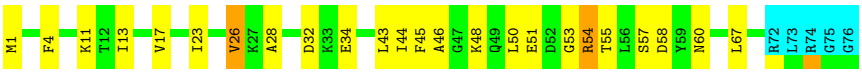
Chain A:



4.2.36 Score per residue for model 36

- Molecule 1: Ubiquitin

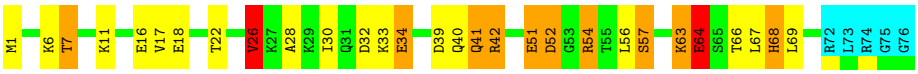
Chain A:



4.2.37 Score per residue for model 37

- Molecule 1: Ubiquitin

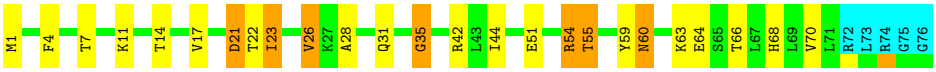
Chain A:



4.2.38 Score per residue for model 38

- Molecule 1: Ubiquitin

Chain A:



4.2.39 Score per residue for model 39

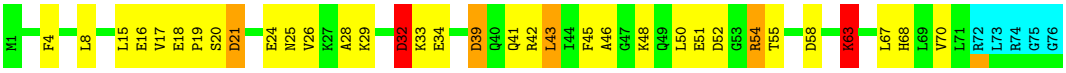
- Molecule 1: Ubiquitin

Chain A:

4.2.40 Score per residue for model 40

- Molecule 1: Ubiquitin

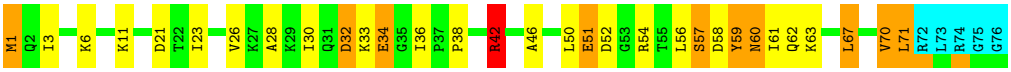
Chain A:



4.2.41 Score per residue for model 41

- Molecule 1: Ubiquitin

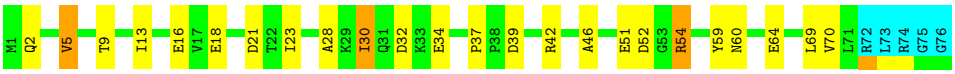
Chain A:



4.2.42 Score per residue for model 42

- Molecule 1: Ubiquitin

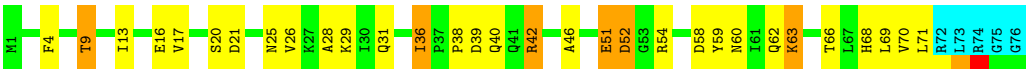
Chain A:



4.2.43 Score per residue for model 43

- Molecule 1: Ubiquitin

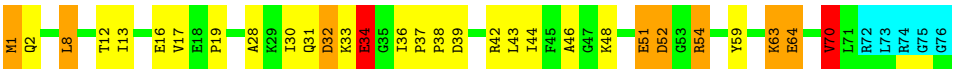
Chain A:



4.2.44 Score per residue for model 44

- Molecule 1: Ubiquitin

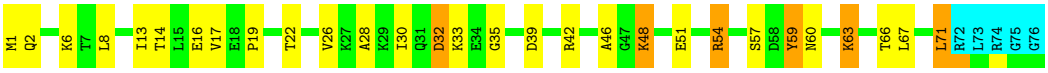
Chain A:



4.2.45 Score per residue for model 45

- Molecule 1: Ubiquitin

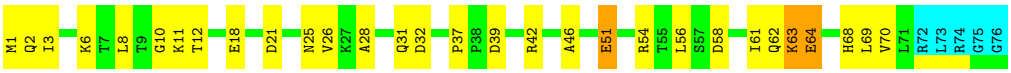
Chain A:



4.2.46 Score per residue for model 46

- Molecule 1: Ubiquitin

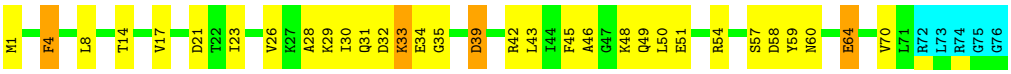
Chain A:



4.2.47 Score per residue for model 47

- Molecule 1: Ubiquitin

Chain A:



4.2.48 Score per residue for model 48

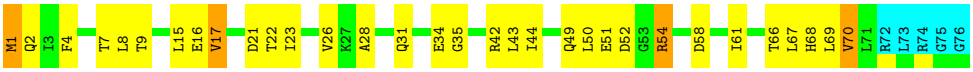
- Molecule 1: Ubiquitin

Chain A:

4.2.49 Score per residue for model 49

- Molecule 1: Ubiquitin

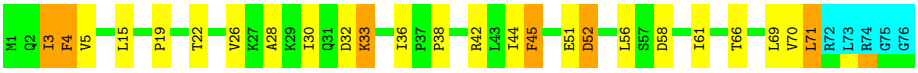
Chain A:



4.2.50 Score per residue for model 50

- Molecule 1: Ubiquitin

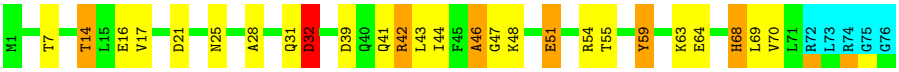
Chain A:



4.2.51 Score per residue for model 51

- Molecule 1: Ubiquitin

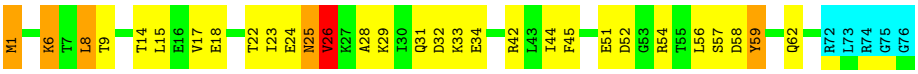
Chain A:



4.2.52 Score per residue for model 52

- Molecule 1: Ubiquitin

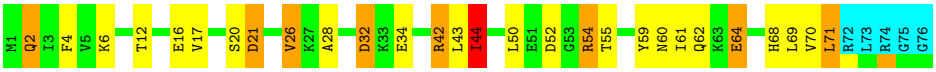
Chain A:



4.2.53 Score per residue for model 53

- Molecule 1: Ubiquitin

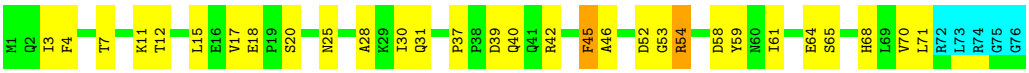
Chain A:



4.2.54 Score per residue for model 54

- Molecule 1: Ubiquitin

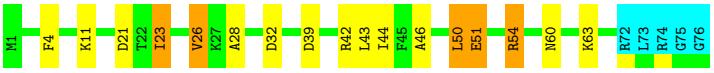
Chain A:



4.2.55 Score per residue for model 55

- Molecule 1: Ubiquitin

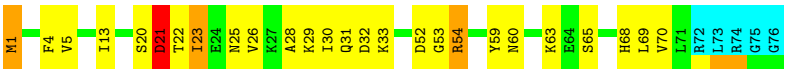
Chain A:



4.2.56 Score per residue for model 56

- Molecule 1: Ubiquitin

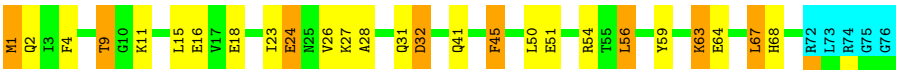
Chain A:



4.2.57 Score per residue for model 57

- Molecule 1: Ubiquitin

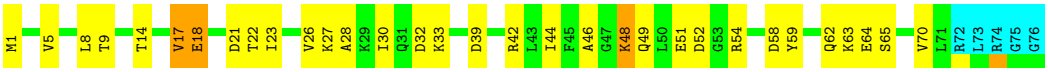
Chain A:



4.2.58 Score per residue for model 58

- Molecule 1: Ubiquitin

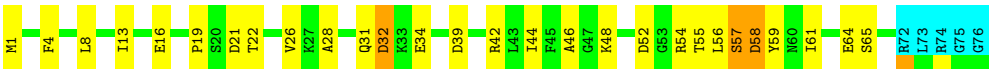
Chain A:



4.2.59 Score per residue for model 59

- Molecule 1: Ubiquitin

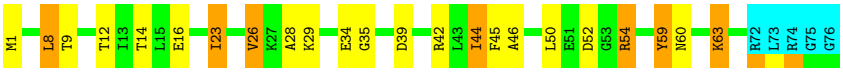
Chain A:



4.2.60 Score per residue for model 60

- Molecule 1: Ubiquitin

Chain A:



4.2.61 Score per residue for model 61

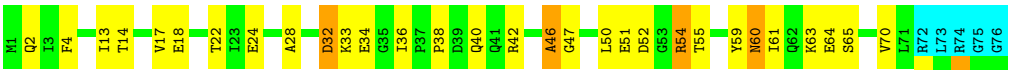
- Molecule 1: Ubiquitin

Chain A:

4.2.62 Score per residue for model 62

- Molecule 1: Ubiquitin

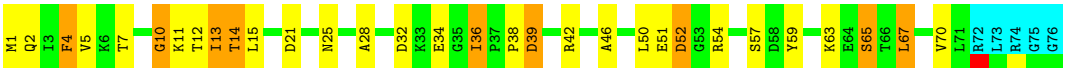
Chain A:



4.2.63 Score per residue for model 63

- Molecule 1: Ubiquitin

Chain A:



4.2.64 Score per residue for model 64

- Molecule 1: Ubiquitin

Chain A:

4.2.65 Score per residue for model 65

- Molecule 1: Ubiquitin

Chain A:

4.2.66 Score per residue for model 66

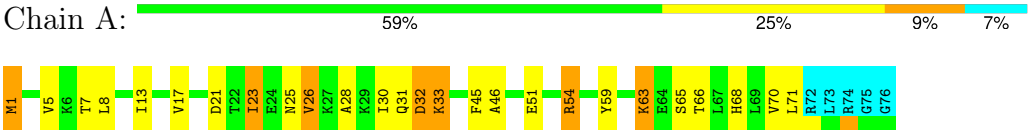
- Molecule 1: Ubiquitin

Chain A:

4.2.67 Score per residue for model 67

- Molecule 1: Ubiquitin

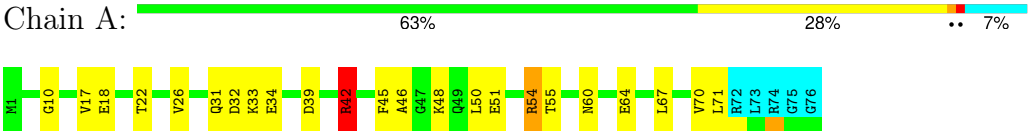
Chain A:



4.2.68 Score per residue for model 68

- Molecule 1: Ubiquitin

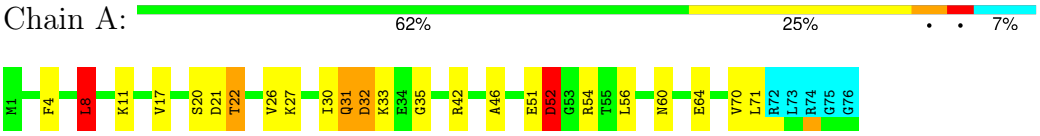
Chain A:



4.2.69 Score per residue for model 69

- Molecule 1: Ubiquitin

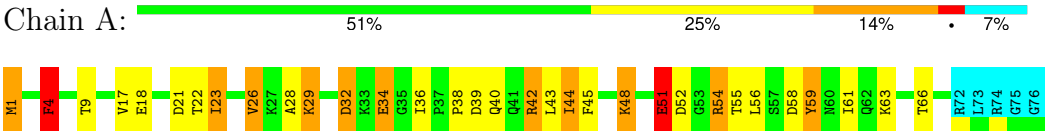
Chain A:



4.2.70 Score per residue for model 70

- Molecule 1: Ubiquitin

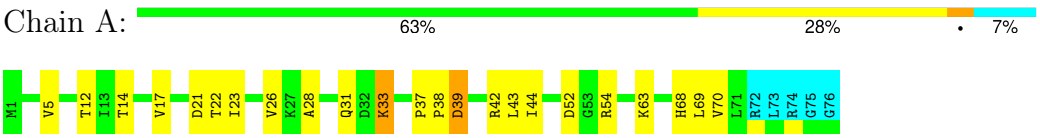
Chain A:



4.2.71 Score per residue for model 71

- Molecule 1: Ubiquitin

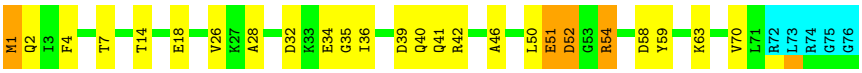
Chain A:



4.2.72 Score per residue for model 72

- Molecule 1: Ubiquitin

Chain A:



4.2.73 Score per residue for model 73

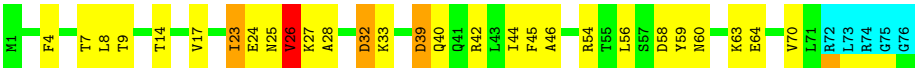
- Molecule 1: Ubiquitin

Chain A:

4.2.74 Score per residue for model 74

- Molecule 1: Ubiquitin

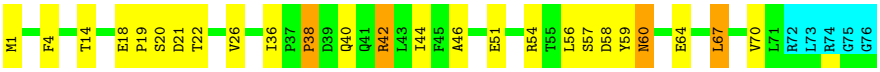
Chain A:



4.2.75 Score per residue for model 75

- Molecule 1: Ubiquitin

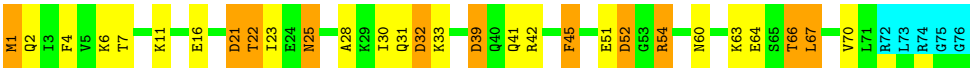
Chain A:



4.2.76 Score per residue for model 76

- Molecule 1: Ubiquitin

Chain A:



4.2.77 Score per residue for model 77

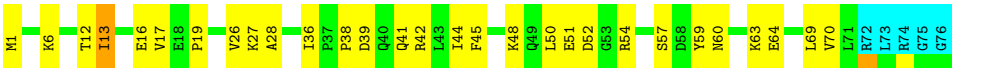
- Molecule 1: Ubiquitin

Chain A: 55% 28% 11% 7%

4.2.78 Score per residue for model 78

- Molecule 1: Ubiquitin

Chain A: 55% 37% • 7%



4.2.79 Score per residue for model 79

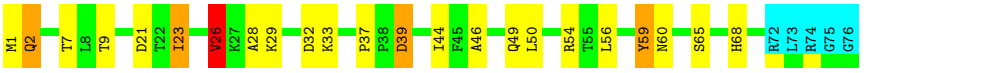
- Molecule 1: Ubiquitin

Chain A: 55% 29% 8% • 7%

4.2.80 Score per residue for model 80

- Molecule 1: Ubiquitin

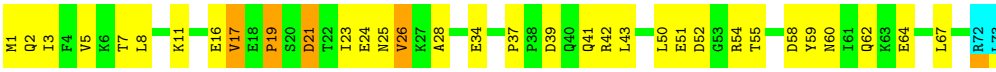
Chain A: 63% 24% 5% • 7%



4.2.81 Score per residue for model 81

- Molecule 1: Ubiquitin

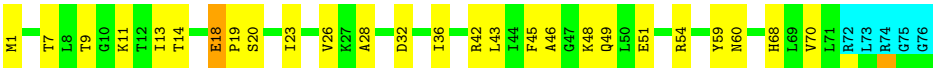
Chain A: 50% 38% 5% 7%



4.2.82 Score per residue for model 82

- Molecule 1: Ubiquitin

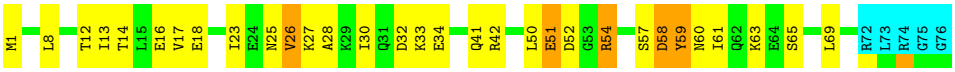
Chain A: 59% 33% • 7%



4.2.83 Score per residue for model 83

- Molecule 1: Ubiquitin

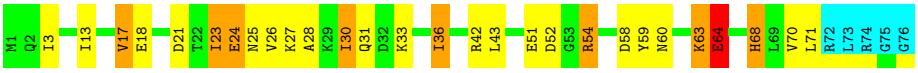
Chain A: 53% 34% 7% 7%



4.2.84 Score per residue for model 84

- Molecule 1: Ubiquitin

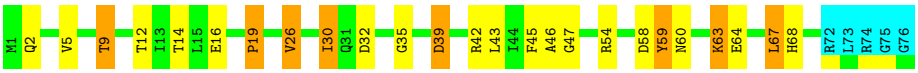
Chain A: 57% 25% 11% • 7%



4.2.85 Score per residue for model 85

- Molecule 1: Ubiquitin

Chain A: 61% 22% 11% 7%



4.2.86 Score per residue for model 86

- Molecule 1: Ubiquitin

Chain A: 66% 21% 5% • 7%

4.2.87 Score per residue for model 87

- Molecule 1: Ubiquitin

Chain A: 72% 20% • 7%

M1 F4 L8 P19 I23 V26 K27 A28 D32 K33 E34 Q40 Q41 R42 R54 T55 L56 Y59 V70 L71 R72 L73 R74 G75 G76

4.2.88 Score per residue for model 88

- Molecule 1: Ubiquitin

Chain A: 57% 33% • 7%

M1 F4 T9 G10 K11 T12 I13 T14 V17 E18 P19 V26 K27 A28 K29 I30 Q31 D32 K33 E34 P37 Q41 R42 L43 I44 F45 A46 G47 D52 G53 R54 T55 L56 S65 T66 L67 H68 L69 V70 L71 R72 L73 R74 G75 G76

4.2.89 Score per residue for model 89

- Molecule 1: Ubiquitin

Chain A: 54% 29% 11% 7%

M1 Q2 I3 F4 V5 L8 T9 T12 E16 V17 E18 D21 V26 K27 A28 K29 I30 Q31 D32 K33 E34 G35 I36 P37 P38 R42 L43 I44 F45 A46 Q49 D52 G53 R54 D58 H68 L69 V70 L71 R72 L73 R74 G75 G76

4.2.90 Score per residue for model 90

- Molecule 1: Ubiquitin

Chain A: 54% 28% 11% • 7%

M1 V5 K6 T7 L8 T14 L15 D21 T22 I23 E24 N25 V26 K27 A28 Q31 D32 K33 E34 G35 I36 R42 L43 I44 F45 A46 Q49 L50 E51 D52 G53 R54 Y59 N60 E64 H68 L69 V70 L71 R72 L73 R74 G75 G76

4.2.91 Score per residue for model 91

- Molecule 1: Ubiquitin

Chain A: 53% 34% • • 7%

M1 Q2 V5 T14 L15 E16 V17 E18 D21 V26 K27 A28 Q31 G35 I36 P37 P38 D39 Q40 Q41 R42 L43 I44 F45 K48 D52 D58 Y59 K63 E64 S65 T66 L69 V70 L71 R72 L73 R74 G75 G76

4.2.92 Score per residue for model 92

- Molecule 1: Ubiquitin

Chain A: 59% 28% 7% 7%

4.2.93 Score per residue for model 93

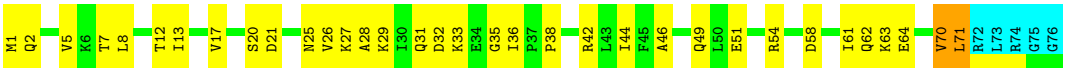
- Molecule 1: Ubiquitin

Chain A: 47% 38% 7% • 7%

4.2.94 Score per residue for model 94

- Molecule 1: Ubiquitin

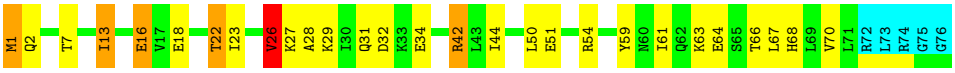
Chain A: 49% 42% • 7%



4.2.95 Score per residue for model 95

- Molecule 1: Ubiquitin

Chain A: 57% 29% 7% • 7%



4.2.96 Score per residue for model 96

- Molecule 1: Ubiquitin

Chain A: 59% 29% 5% 7%

4.2.97 Score per residue for model 97

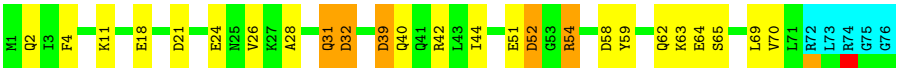
- Molecule 1: Ubiquitin

Chain A: 67% 24% • 7%

4.2.98 Score per residue for model 98

- Molecule 1: Ubiquitin

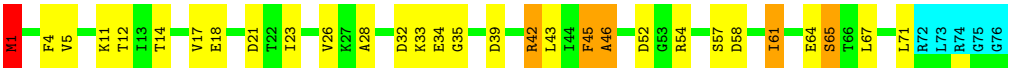
Chain A: 61% 26% 7% 7%



4.2.99 Score per residue for model 99

- Molecule 1: Ubiquitin

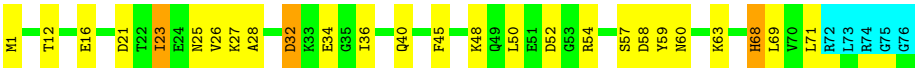
Chain A: 54% 32% 7% • 7%



4.2.100 Score per residue for model 100

- Molecule 1: Ubiquitin

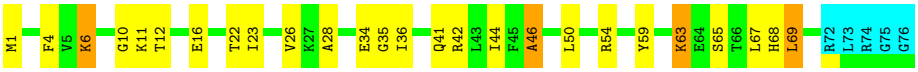
Chain A: 59% 30% • 7%



4.2.101 Score per residue for model 101

- Molecule 1: Ubiquitin

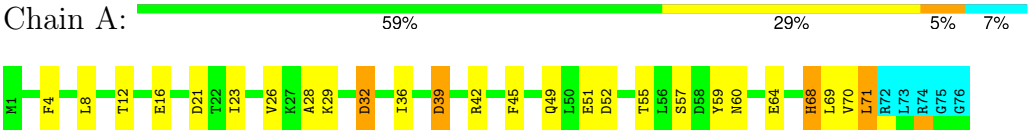
Chain A: 59% 29% 5% 7%



4.2.102 Score per residue for model 102

- Molecule 1: Ubiquitin

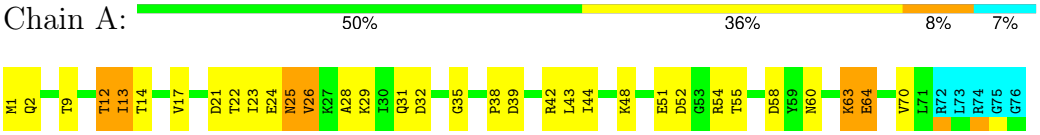
Chain A:



4.2.103 Score per residue for model 103

- Molecule 1: Ubiquitin

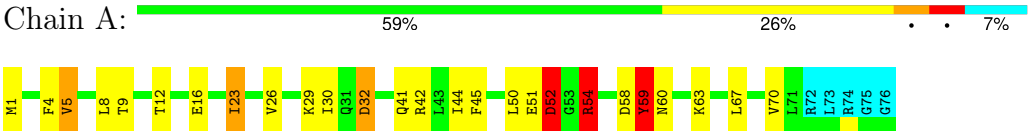
Chain A:



4.2.104 Score per residue for model 104

- Molecule 1: Ubiquitin

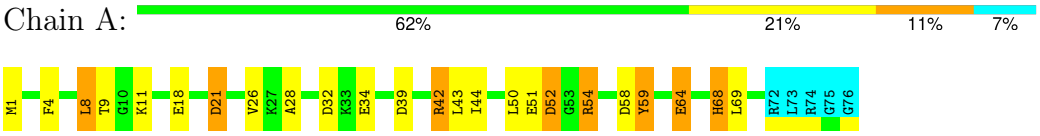
Chain A:



4.2.105 Score per residue for model 105

- Molecule 1: Ubiquitin

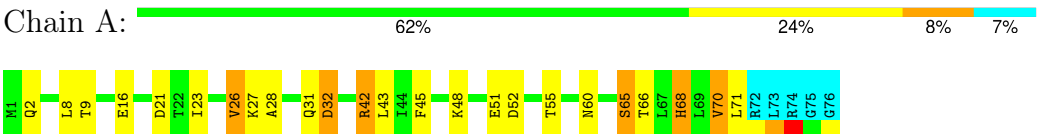
Chain A:



4.2.106 Score per residue for model 106

- Molecule 1: Ubiquitin

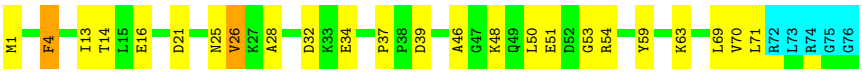
Chain A:



4.2.107 Score per residue for model 107

- Molecule 1: Ubiquitin

Chain A: 62% 29% • 7%



4.2.108 Score per residue for model 108

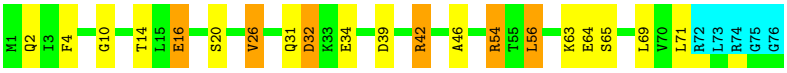
- Molecule 1: Ubiquitin

Chain A: 64% 22% 7% 7%

4.2.109 Score per residue for model 109

- Molecule 1: Ubiquitin

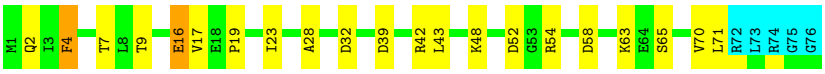
Chain A: 67% 18% 8% 7%



4.2.110 Score per residue for model 110

- Molecule 1: Ubiquitin

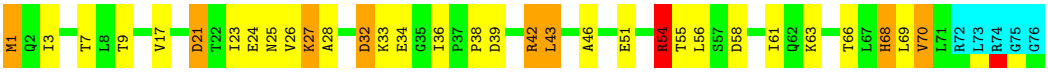
Chain A: 66% 25% • 7%



4.2.111 Score per residue for model 111

- Molecule 1: Ubiquitin

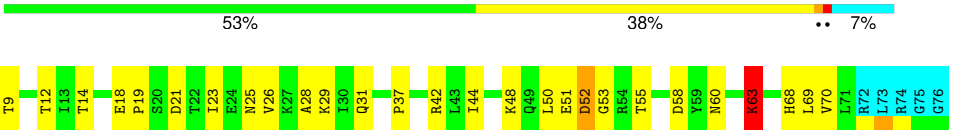
Chain A: 51% 30% 11% • 7%



4.2.112 Score per residue for model 112

- Molecule 1: Ubiquitin

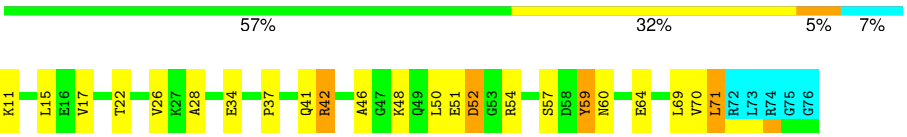
Chain A:



4.2.113 Score per residue for model 113

- Molecule 1: Ubiquitin

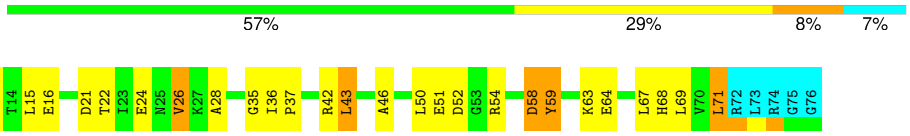
Chain A:



4.2.114 Score per residue for model 114

- Molecule 1: Ubiquitin

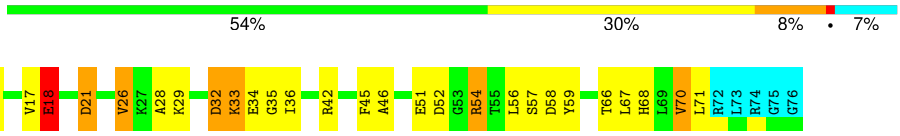
Chain A:



4.2.115 Score per residue for model 115

- Molecule 1: Ubiquitin

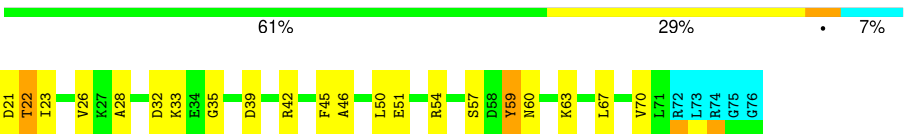
Chain A:



4.2.116 Score per residue for model 116

- Molecule 1: Ubiquitin

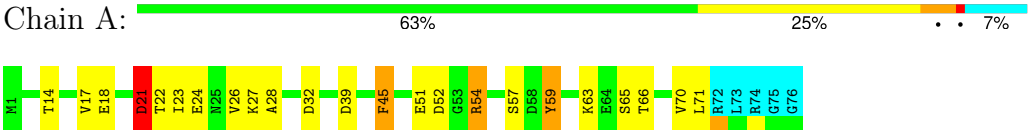
Chain A:



4.2.117 Score per residue for model 117

- Molecule 1: Ubiquitin

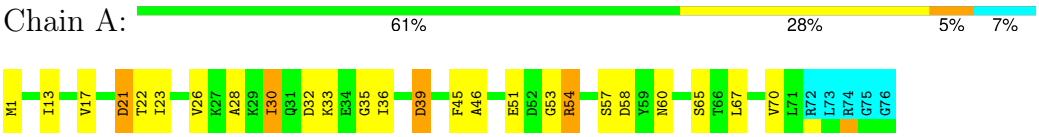
Chain A:



4.2.118 Score per residue for model 118

- Molecule 1: Ubiquitin

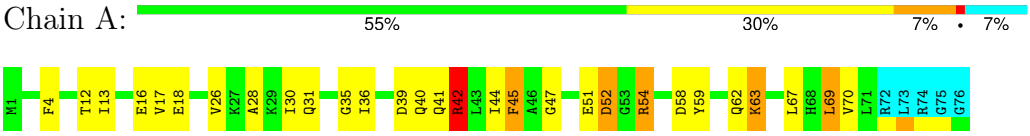
Chain A:



4.2.119 Score per residue for model 119

- Molecule 1: Ubiquitin

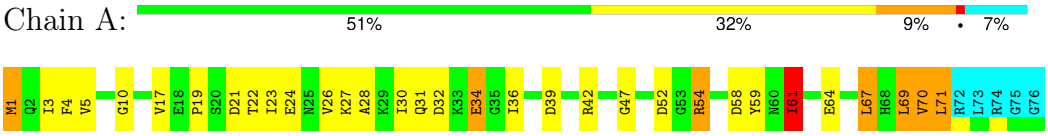
Chain A:



4.2.120 Score per residue for model 120

- Molecule 1: Ubiquitin

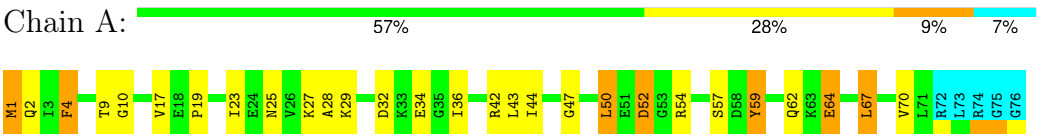
Chain A:



4.2.121 Score per residue for model 121

- Molecule 1: Ubiquitin

Chain A:



4.2.122 Score per residue for model 122

- Molecule 1: Ubiquitin

Chain A: 64% 26% • 7%

M1 V5 K6 T7 T12 P19 S20 D21 T22 V26 K27 A28 K29 I30 Q31 D32 G35 I36 D39 R42 F45 D52 G53 R54 T55 L56 S57 D58 I61 Q62 R72 L73 R74 G75 G76

4.2.123 Score per residue for model 123

- Molecule 1: Ubiquitin

Chain A: 53% 37% • • 7%

M1 Q2 I3 F4 L8 T9 L15 E16 V17 I23 V26 K27 A28 K29 I30 Q31 D32 K33 Q40 Q41 R42 L43 I44 F45 A46 G47 K48 Q49 G53 R54 T55 L56 S57 D58 Y59 K63 E64 S65 H68 R72 L73 R74 G75 G76

4.2.124 Score per residue for model 124

- Molecule 1: Ubiquitin

Chain A: 58% 26% 8% • 7%

M1 Q2 I3 F4 V5 K6 I13 E16 D21 T22 I23 V26 K27 A28 K29 I30 Q31 D32 G35 D39 R42 A46 G47 K48 Q49 L50 D58 Y59 N60 K63 E64 S65 T66 L67 V70 L71 R72 L73 R74 G75 G76

4.2.125 Score per residue for model 125

- Molecule 1: Ubiquitin

Chain A: 59% 29% • • 7%

M1 L8 T9 L15 E24 W25 V26 K27 A28 K29 I30 Q31 D32 K33 E34 R42 F45 A46 E51 D52 G53 R54 T55 L56 S57 D58 Y59 S65 T66 L67 H68 L69 V70 L71 R72 L73 R74 G75 G76

4.2.126 Score per residue for model 126

- Molecule 1: Ubiquitin

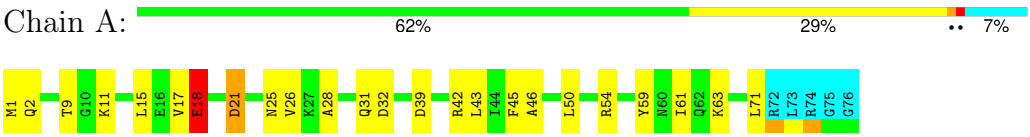
Chain A: 59% 32% •• 7%

M1 F4 L8 V17 E18 P19 S20 D21 T22 I23 A28 K29 I30 Q31 D32 K33 E34 D39 R42 L43 I44 F45 A46 G47 E51 T55 D58 Y59 N60 I61 Q62 K63 L69 V70 L71 R72 L73 R74 G75 G76

4.2.127 Score per residue for model 127

- Molecule 1: Ubiquitin

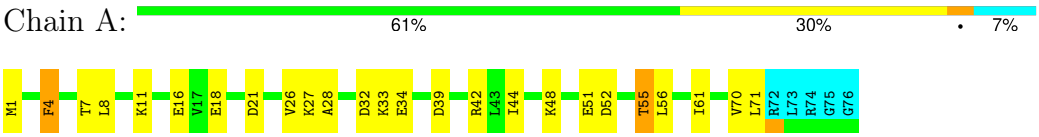
Chain A:



4.2.128 Score per residue for model 128

- Molecule 1: Ubiquitin

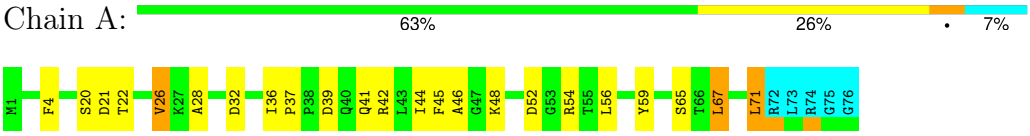
Chain A:



4.2.129 Score per residue for model 129

- Molecule 1: Ubiquitin

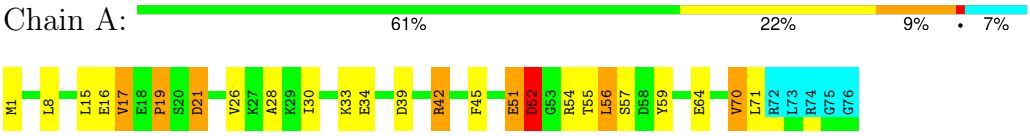
Chain A:



4.2.130 Score per residue for model 130

- Molecule 1: Ubiquitin

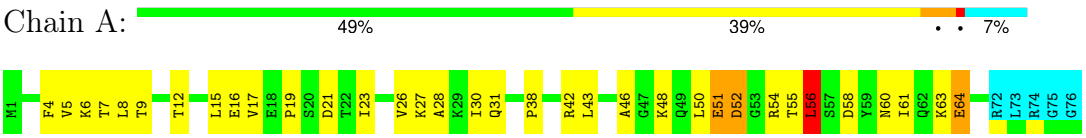
Chain A:



4.2.131 Score per residue for model 131

- Molecule 1: Ubiquitin

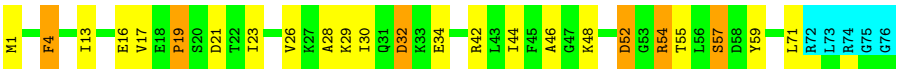
Chain A:



4.2.132 Score per residue for model 132

- Molecule 1: Ubiquitin

Chain A: 62% 24% 8% 7%



4.2.133 Score per residue for model 133

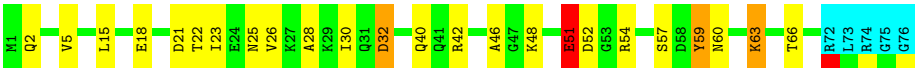
- Molecule 1: Ubiquitin

Chain A: 54% 29% 11% 7%

4.2.134 Score per residue for model 134

- Molecule 1: Ubiquitin

Chain A: 62% 26% • • 7%



4.2.135 Score per residue for model 135

- Molecule 1: Ubiquitin

Chain A: 64% 26% • 7%

4.2.136 Score per residue for model 136

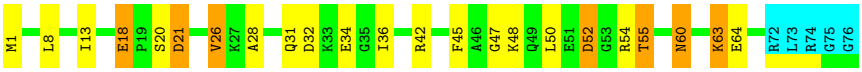
- Molecule 1: Ubiquitin

Chain A: 62% 28% • 7%

4.2.137 Score per residue for model 137

- Molecule 1: Ubiquitin

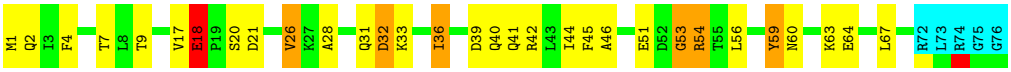
Chain A: 63% 21% 9% 7%



4.2.138 Score per residue for model 138

- Molecule 1: Ubiquitin

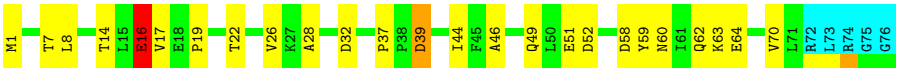
Chain A: 53% 32% 8% • 7%



4.2.139 Score per residue for model 139

- Molecule 1: Ubiquitin

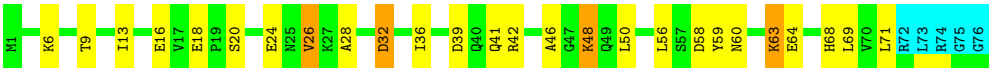
Chain A: 61% 30% •• 7%



4.2.140 Score per residue for model 140

- Molecule 1: Ubiquitin

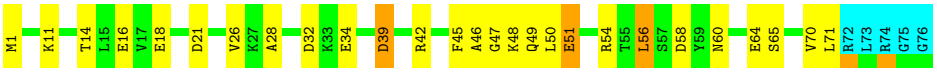
Chain A: 59% 29% 5% 7%



4.2.141 Score per residue for model 141

- Molecule 1: Ubiquitin

Chain A: 58% 32% • 7%



4.2.142 Score per residue for model 142

- Molecule 1: Ubiquitin

Chain A: 59% 30% • 7%

M1 F4 K11 L15 E18 P19 S20 D21 T22 V26 K27 A28 K33 E34 R42 L43 I44 F45 A46 E51 D52 G53 R54 T55 D58 Y59 N60 I61 E64 V70 L71 R72 L73 R74 G75 G76

4.2.143 Score per residue for model 143

- Molecule 1: Ubiquitin

Chain A: 55% 36% • 7%

M1 F4 K11 E16 V17 N25 V26 K27 A28 Q31 D32 K33 E34 P37 P38 R42 L43 I44 F45 A46 G47 K48 Q49 L50 E51 R54 Y59 N60 I61 E64 S65 T66 L67 V70 L71 R72 L73 R74 G75 G76

4.2.144 Score per residue for model 144

- Molecule 1: Ubiquitin

Chain A: 61% 28% 5% 7%

M1 Q2 I3 F4 V5 G10 I13 D21 T22 A28 K29 I30 K33 E34 P37 Q40 Q41 R42 L43 A46 G47 K48 E51 D52 G53 R54 D58 K63 L67 V70 L71 R72 L73 R74 G75 G76

4.2.145 Score per residue for model 145

- Molecule 1: Ubiquitin

Chain A: 66% 24% • • 7%

M1 V5 K6 P19 S20 D21 T22 I23 V26 K27 A28 E34 G35 D39 R42 E51 D52 G53 R54 D58 Y59 N60 I61 Q62 K63 E64 R72 L73 R74 G75 G76

4.2.146 Score per residue for model 146

- Molecule 1: Ubiquitin

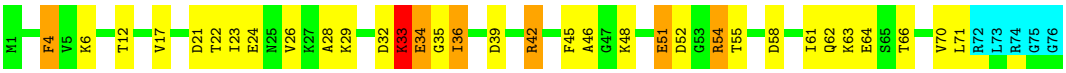
Chain A: 55% 29% 7% • 7%

M1 Q2 I3 F4 V5 K6 T9 V17 E18 I23 E24 N25 V26 K27 A28 D32 K33 E34 P37 Q41 R42 L43 A46 D52 G53 R54 T55 L56 S57 D58 Y59 K63 E64 S65 L69 V70 L71 R72 L73 R74 G75 G76

4.2.147 Score per residue for model 147

- Molecule 1: Ubiquitin

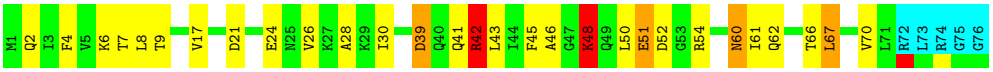
Chain A: 50% 34% 8% • 7%



4.2.148 Score per residue for model 148

- Molecule 1: Ubiquitin

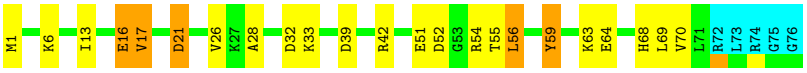
Chain A: 55% 30% 5% • 7%



4.2.149 Score per residue for model 149

- Molecule 1: Ubiquitin

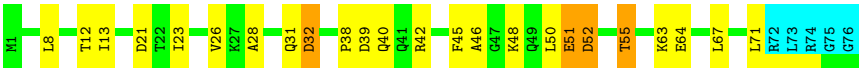
Chain A: 63% 24% 7% 7%



4.2.150 Score per residue for model 150

- Molecule 1: Ubiquitin

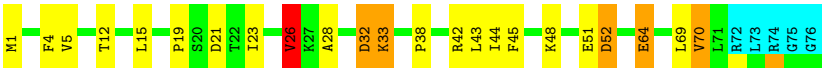
Chain A: 62% 26% 5% 7%



4.2.151 Score per residue for model 151

- Molecule 1: Ubiquitin

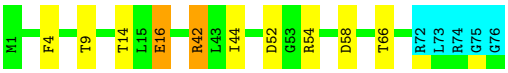
Chain A: 63% 22% 7% • 7%



4.2.152 Score per residue for model 152

- Molecule 1: Ubiquitin

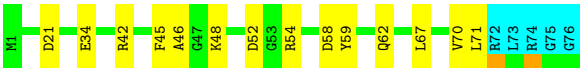
Chain A:



4.2.153 Score per residue for model 153

- Molecule 1: Ubiquitin

Chain A:



4.2.154 Score per residue for model 154

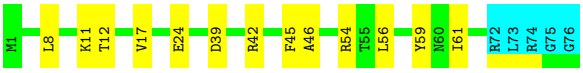
- Molecule 1: Ubiquitin

Chain A:

4.2.155 Score per residue for model 155

- Molecule 1: Ubiquitin

Chain A:



4.2.156 Score per residue for model 156

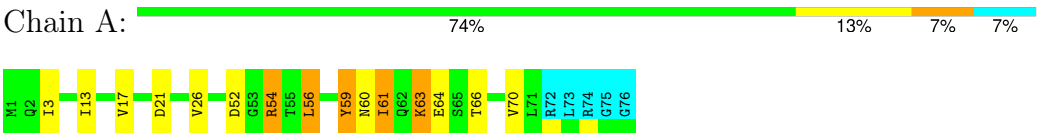
- Molecule 1: Ubiquitin

Chain A:

4.2.157 Score per residue for model 157

- Molecule 1: Ubiquitin

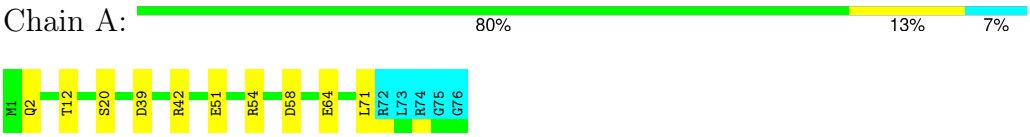
Chain A:



4.2.158 Score per residue for model 158

- Molecule 1: Ubiquitin

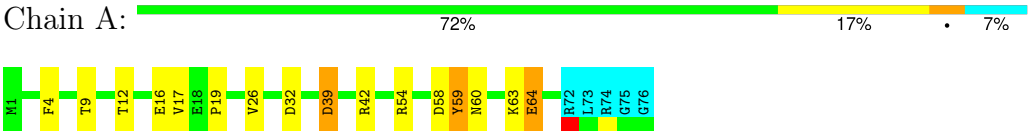
Chain A:



4.2.159 Score per residue for model 159

- Molecule 1: Ubiquitin

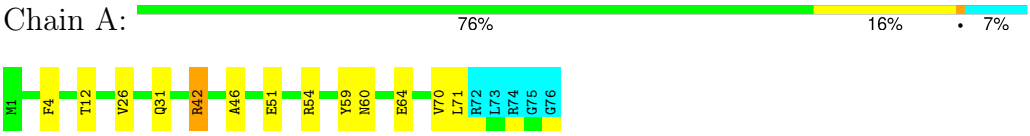
Chain A:



4.2.160 Score per residue for model 160

- Molecule 1: Ubiquitin

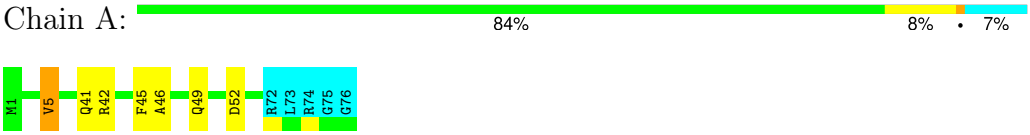
Chain A:



4.2.161 Score per residue for model 161

- Molecule 1: Ubiquitin

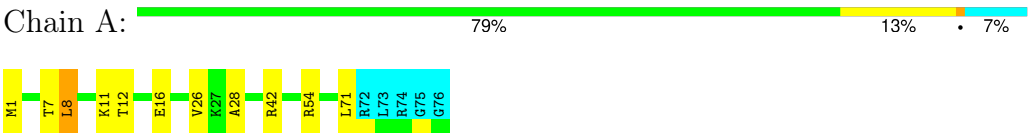
Chain A:



4.2.162 Score per residue for model 162

- Molecule 1: Ubiquitin

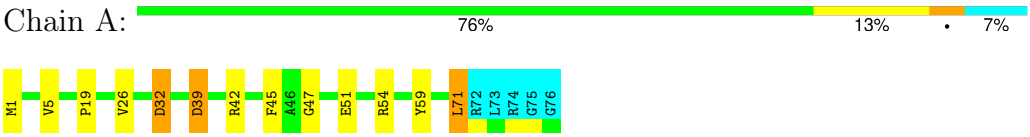
Chain A:



4.2.163 Score per residue for model 163

- Molecule 1: Ubiquitin

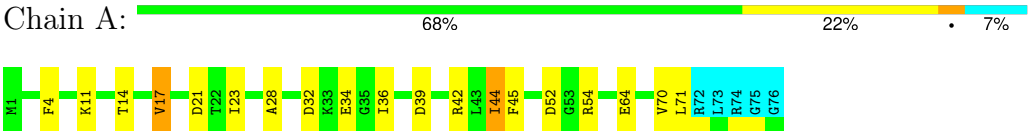
Chain A:



4.2.164 Score per residue for model 164

- Molecule 1: Ubiquitin

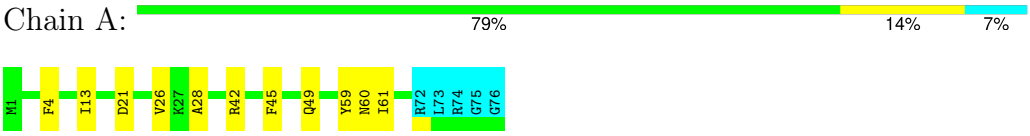
Chain A:



4.2.165 Score per residue for model 165

- Molecule 1: Ubiquitin

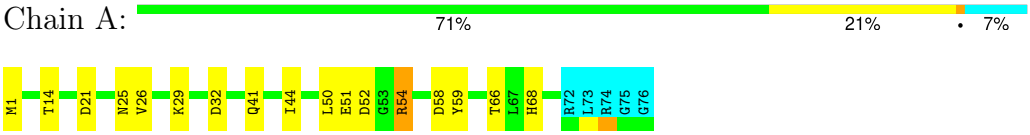
Chain A:



4.2.166 Score per residue for model 166

- Molecule 1: Ubiquitin

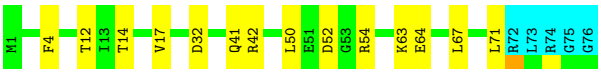
Chain A:



4.2.167 Score per residue for model 167

- Molecule 1: Ubiquitin

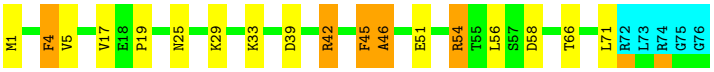
Chain A: 75% 18% 7%



4.2.168 Score per residue for model 168

- Molecule 1: Ubiquitin

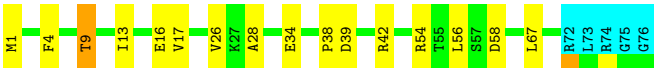
Chain A: 70% 17% 7% 7%



4.2.169 Score per residue for model 169

- Molecule 1: Ubiquitin

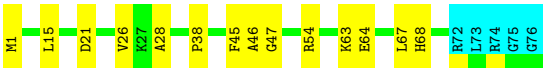
Chain A: 72% 20% • 7%



4.2.170 Score per residue for model 170

- Molecule 1: Ubiquitin

Chain A: 75% 18% 7%



4.2.171 Score per residue for model 171

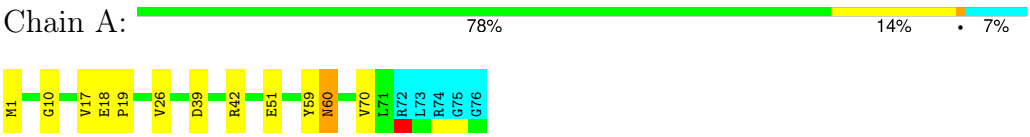
- Molecule 1: Ubiquitin

Chain A: 72% 21% 7%

4.2.172 Score per residue for model 172

- Molecule 1: Ubiquitin

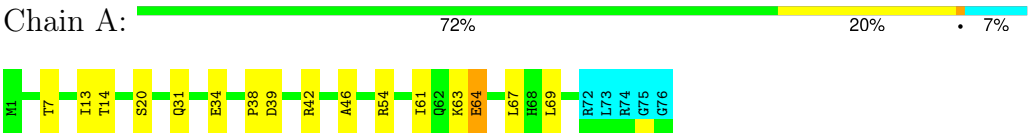
Chain A:



4.2.173 Score per residue for model 173

- Molecule 1: Ubiquitin

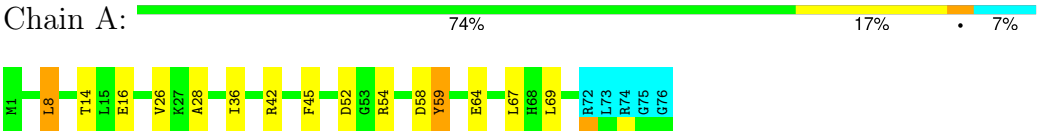
Chain A:



4.2.174 Score per residue for model 174

- Molecule 1: Ubiquitin

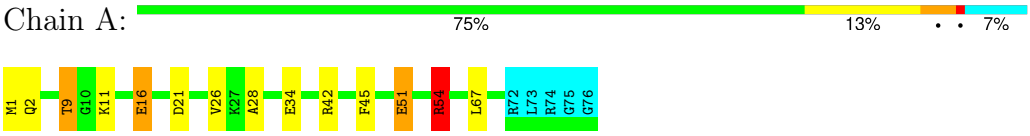
Chain A:



4.2.175 Score per residue for model 175

- Molecule 1: Ubiquitin

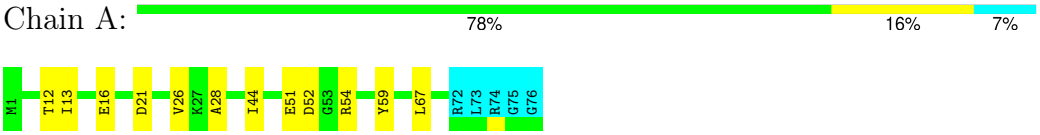
Chain A:



4.2.176 Score per residue for model 176

- Molecule 1: Ubiquitin

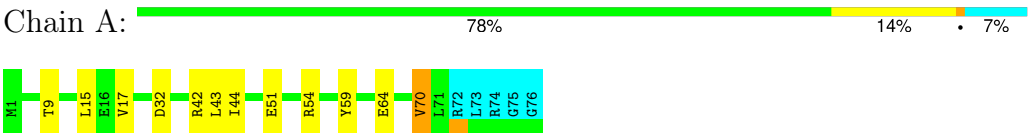
Chain A:



4.2.177 Score per residue for model 177

- Molecule 1: Ubiquitin

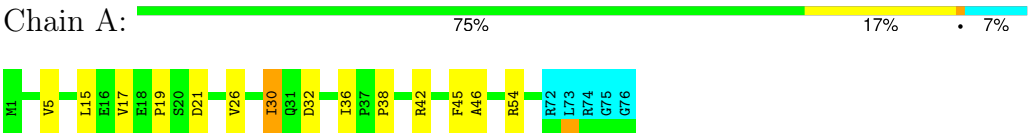
Chain A:



4.2.178 Score per residue for model 178

- Molecule 1: Ubiquitin

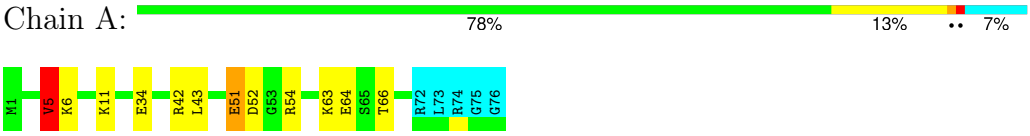
Chain A:



4.2.179 Score per residue for model 179

- Molecule 1: Ubiquitin

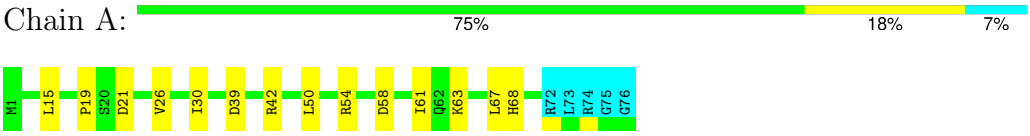
Chain A:



4.2.180 Score per residue for model 180

- Molecule 1: Ubiquitin

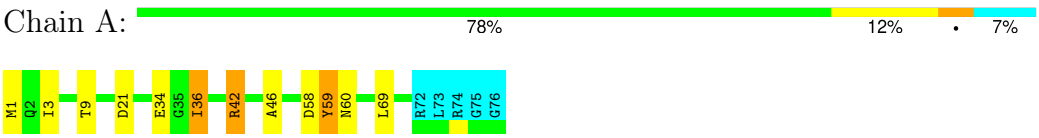
Chain A:



4.2.181 Score per residue for model 181

- Molecule 1: Ubiquitin

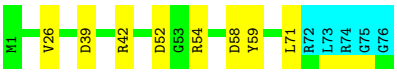
Chain A:



4.2.182 Score per residue for model 182

- Molecule 1: Ubiquitin

Chain A: 83% 11% 7%



4.2.183 Score per residue for model 183

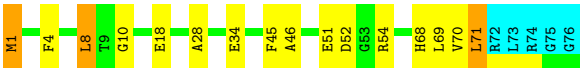
- Molecule 1: Ubiquitin

Chain A: 79% 12% • 7%

4.2.184 Score per residue for model 184

- Molecule 1: Ubiquitin

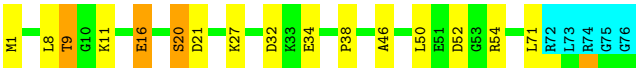
Chain A: 72% 17% • 7%



4.2.185 Score per residue for model 185

- Molecule 1: Ubiquitin

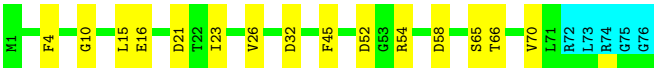
Chain A: 72% 17% • 7%



4.2.186 Score per residue for model 186

- Molecule 1: Ubiquitin

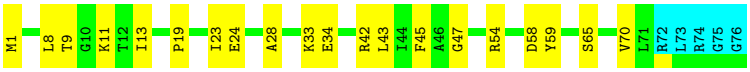
Chain A: 74% 20% 7%



4.2.187 Score per residue for model 187

- Molecule 1: Ubiquitin

Chain A:



4.2.188 Score per residue for model 188

- Molecule 1: Ubiquitin

Chain A:

4.2.189 Score per residue for model 189

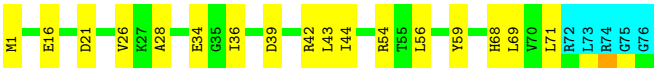
- Molecule 1: Ubiquitin

Chain A:

4.2.190 Score per residue for model 190

- Molecule 1: Ubiquitin

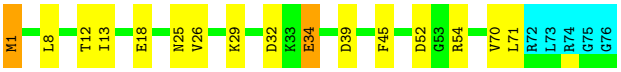
Chain A:



4.2.191 Score per residue for model 191

- Molecule 1: Ubiquitin

Chain A:



4.2.192 Score per residue for model 192

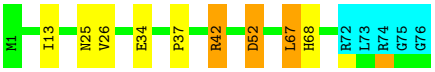
- Molecule 1: Ubiquitin

Chain A:

4.2.193 Score per residue for model 193

- Molecule 1: Ubiquitin

Chain A:



4.2.194 Score per residue for model 194

- Molecule 1: Ubiquitin

Chain A:

4.2.195 Score per residue for model 195

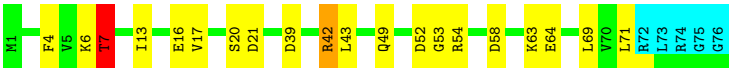
- Molecule 1: Ubiquitin

Chain A:

4.2.196 Score per residue for model 196

- Molecule 1: Ubiquitin

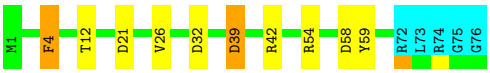
Chain A:



4.2.197 Score per residue for model 197

- Molecule 1: Ubiquitin

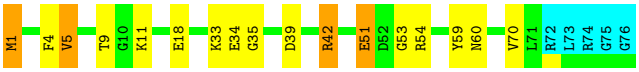
Chain A: 80% 11% • 7%



4.2.198 Score per residue for model 198

- Molecule 1: Ubiquitin

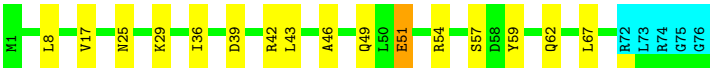
Chain A: 71% 17% 5% 7%



4.2.199 Score per residue for model 199

- Molecule 1: Ubiquitin

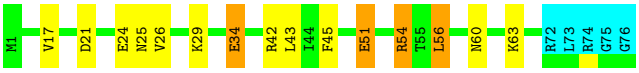
Chain A: 72% 20% • 7%



4.2.200 Score per residue for model 200

- Molecule 1: Ubiquitin

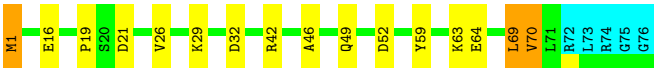
Chain A: 74% 14% 5% 7%



4.2.201 Score per residue for model 201

- Molecule 1: Ubiquitin

Chain A: 72% 17% • 7%



4.2.202 Score per residue for model 202

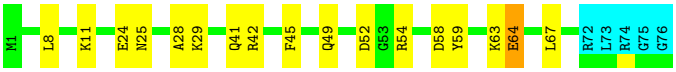
- Molecule 1: Ubiquitin

Chain A: 82% 11% • 7%

4.2.203 Score per residue for model 203

- Molecule 1: Ubiquitin

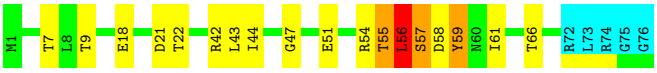
Chain A: 71% 21% • 7%



4.2.204 Score per residue for model 204

- Molecule 1: Ubiquitin

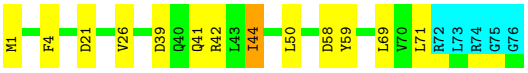
Chain A: 70% 18% • • 7%



4.2.205 Score per residue for model 205

- Molecule 1: Ubiquitin

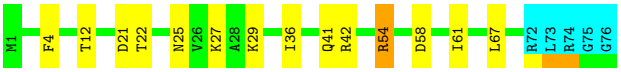
Chain A: 76% 16% • 7%



4.2.206 Score per residue for model 206

- Molecule 1: Ubiquitin

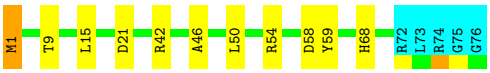
Chain A: 75% 17% • 7%



4.2.207 Score per residue for model 207

- Molecule 1: Ubiquitin

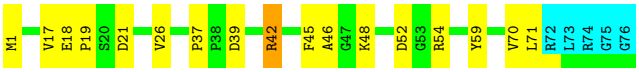
Chain A: 79% 13% • 7%



4.2.208 Score per residue for model 208

- Molecule 1: Ubiquitin

Chain A: 71% 21% • 7%



4.2.209 Score per residue for model 209

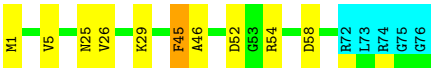
- Molecule 1: Ubiquitin

Chain A: 74% 20% 7%

4.2.210 Score per residue for model 210 (medoid)

- Molecule 1: Ubiquitin

Chain A: 80% 12% • 7%



4.2.211 Score per residue for model 211

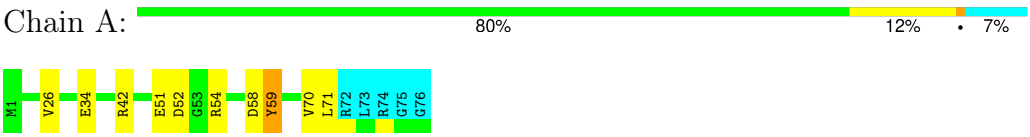
- Molecule 1: Ubiquitin

Chain A: 76% 12% 5% 7%

4.2.212 Score per residue for model 212

- Molecule 1: Ubiquitin

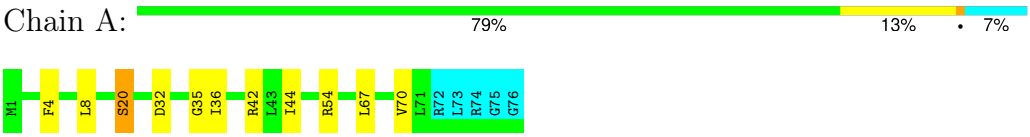
Chain A:



4.2.213 Score per residue for model 213

- Molecule 1: Ubiquitin

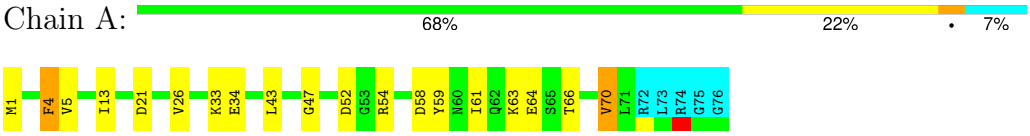
Chain A:



4.2.214 Score per residue for model 214

- Molecule 1: Ubiquitin

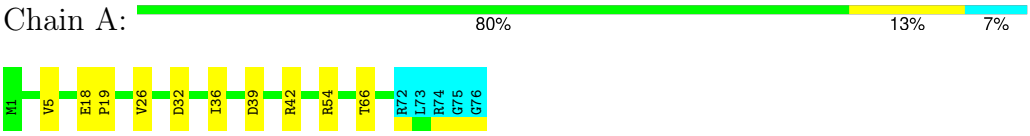
Chain A:



4.2.215 Score per residue for model 215

- Molecule 1: Ubiquitin

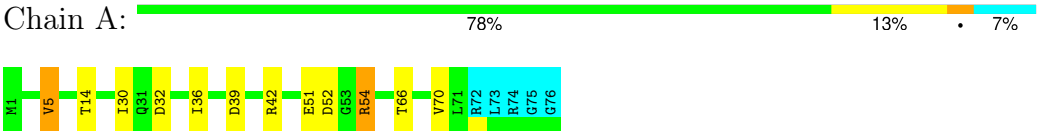
Chain A:



4.2.216 Score per residue for model 216

- Molecule 1: Ubiquitin

Chain A:



4.2.217 Score per residue for model 217

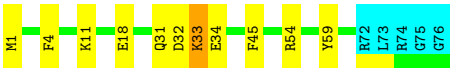
- Molecule 1: Ubiquitin

Chain A: 74% 20% 7%

4.2.218 Score per residue for model 218

- Molecule 1: Ubiquitin

Chain A: 79% 13% • 7%



4.2.219 Score per residue for model 219

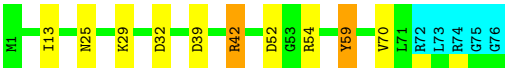
- Molecule 1: Ubiquitin

Chain A: 71% 20% • 7%

4.2.220 Score per residue for model 220

- Molecule 1: Ubiquitin

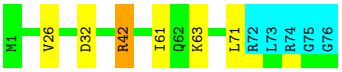
Chain A: 80% 11% • 7%



4.2.221 Score per residue for model 221

- Molecule 1: Ubiquitin

Chain A: 86% 7% • 7%



4.2.222 Score per residue for model 222

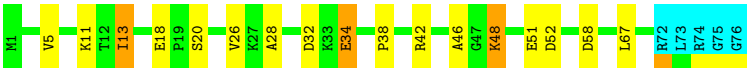
- Molecule 1: Ubiquitin

Chain A: 78% 16% 7%

4.2.223 Score per residue for model 223

- Molecule 1: Ubiquitin

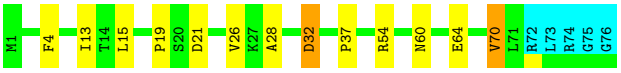
Chain A: 71% 18% • 7%



4.2.224 Score per residue for model 224

- Molecule 1: Ubiquitin

Chain A: 76% 14% • 7%



4.2.225 Score per residue for model 225

- Molecule 1: Ubiquitin

Chain A: 68% 24% • 7%

4.2.226 Score per residue for model 226

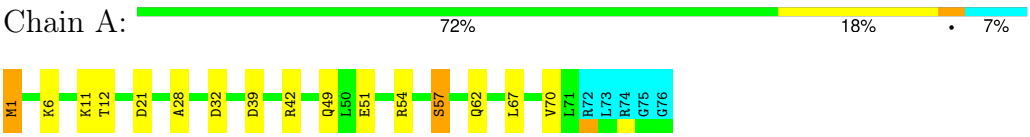
- Molecule 1: Ubiquitin

Chain A: 82% 11% • 7%

4.2.227 Score per residue for model 227

- Molecule 1: Ubiquitin

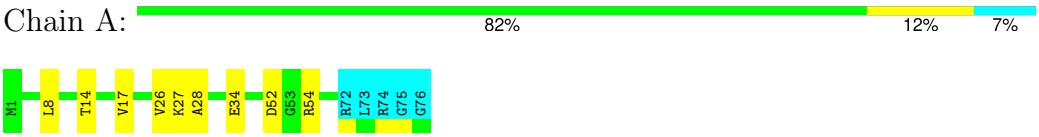
Chain A:



4.2.228 Score per residue for model 228

- Molecule 1: Ubiquitin

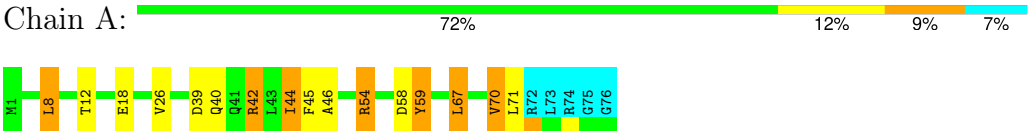
Chain A:



4.2.229 Score per residue for model 229

- Molecule 1: Ubiquitin

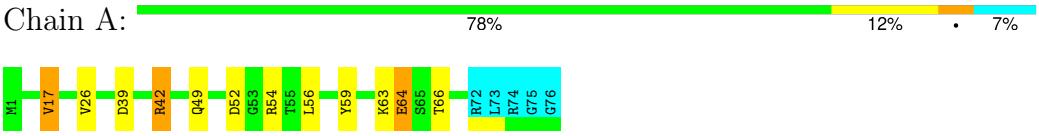
Chain A:



4.2.230 Score per residue for model 230

- Molecule 1: Ubiquitin

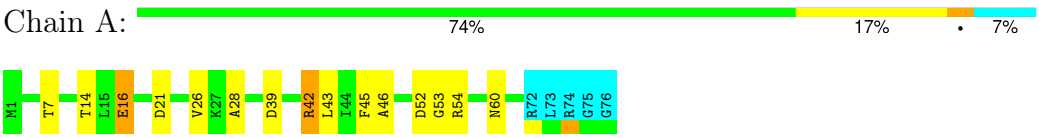
Chain A:



4.2.231 Score per residue for model 231

- Molecule 1: Ubiquitin

Chain A:



4.2.232 Score per residue for model 232

- Molecule 1: Ubiquitin

Chain A: 70% 22% • 7%

4.2.233 Score per residue for model 233

- Molecule 1: Ubiquitin

Chain A: 82% 12% 7%

4.2.234 Score per residue for model 234

- Molecule 1: Ubiquitin

Chain A: 74% 18% • 7%

4.2.235 Score per residue for model 235

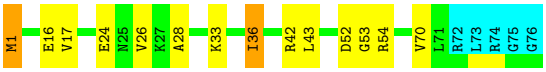
- Molecule 1: Ubiquitin

Chain A: 78% 16% 7%

4.2.236 Score per residue for model 236

- Molecule 1: Ubiquitin

Chain A: 75% 16% • 7%



4.2.237 Score per residue for model 237

- Molecule 1: Ubiquitin

Chain A: 79% 12% • 7%

4.2.238 Score per residue for model 238

- Molecule 1: Ubiquitin

Chain A: 67% 24% • 7%

4.2.239 Score per residue for model 239

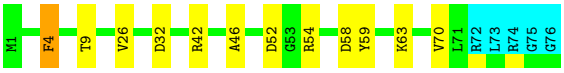
- Molecule 1: Ubiquitin

Chain A: 75% 18% 7%

4.2.240 Score per residue for model 240

- Molecule 1: Ubiquitin

Chain A: 78% 14% • 7%



4.2.241 Score per residue for model 241

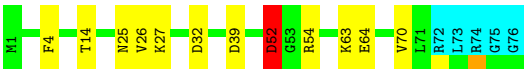
- Molecule 1: Ubiquitin

Chain A: 76% 13% • 7%

4.2.242 Score per residue for model 242

- Molecule 1: Ubiquitin

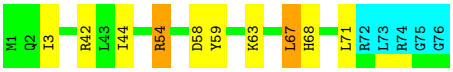
Chain A: 78% 14% • 7%



4.2.243 Score per residue for model 243

- Molecule 1: Ubiquitin

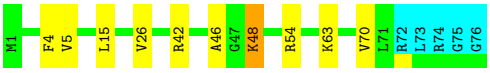
Chain A: 80% 11% • 7%



4.2.244 Score per residue for model 244

- Molecule 1: Ubiquitin

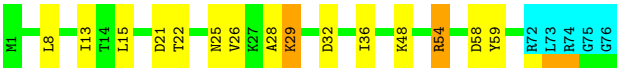
Chain A: 80% 12% • 7%



4.2.245 Score per residue for model 245

- Molecule 1: Ubiquitin

Chain A: 74% 17% • 7%



4.2.246 Score per residue for model 246

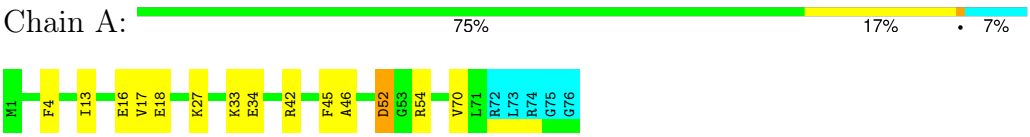
- Molecule 1: Ubiquitin

Chain A: 76% 13% • • 7%

4.2.247 Score per residue for model 247

- Molecule 1: Ubiquitin

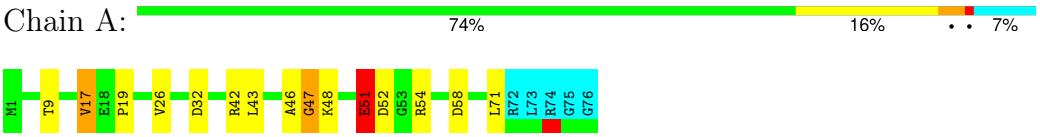
Chain A:



4.2.248 Score per residue for model 248

- Molecule 1: Ubiquitin

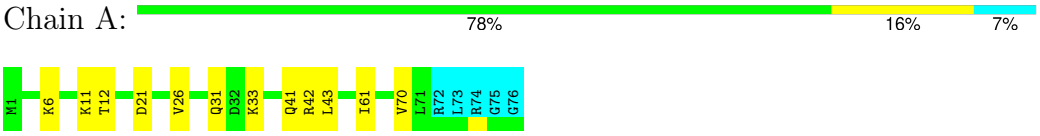
Chain A:



4.2.249 Score per residue for model 249

- Molecule 1: Ubiquitin

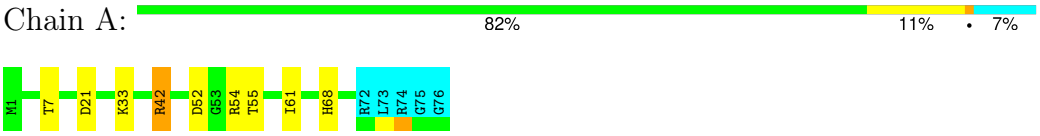
Chain A:



4.2.250 Score per residue for model 250

- Molecule 1: Ubiquitin

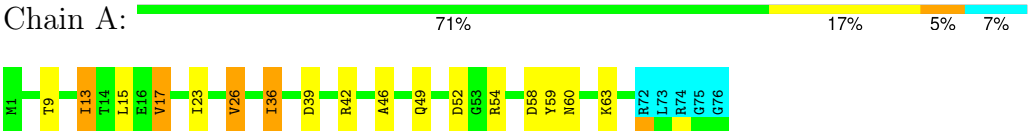
Chain A:



4.2.251 Score per residue for model 251

- Molecule 1: Ubiquitin

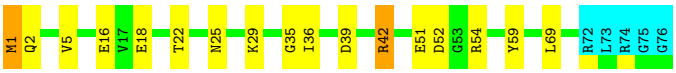
Chain A:



4.2.252 Score per residue for model 252

- Molecule 1: Ubiquitin

Chain A: 71% 20% • 7%



4.2.253 Score per residue for model 253

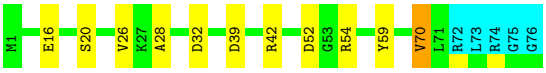
- Molecule 1: Ubiquitin

Chain A: 83% 7% • 7%

4.2.254 Score per residue for model 254

- Molecule 1: Ubiquitin

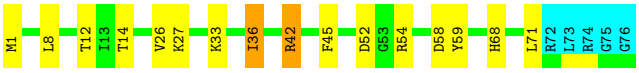
Chain A: 79% 13% • 7%



4.2.255 Score per residue for model 255

- Molecule 1: Ubiquitin

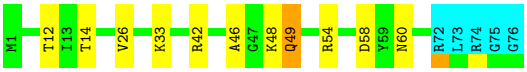
Chain A: 72% 18% • 7%



4.2.256 Score per residue for model 256

- Molecule 1: Ubiquitin

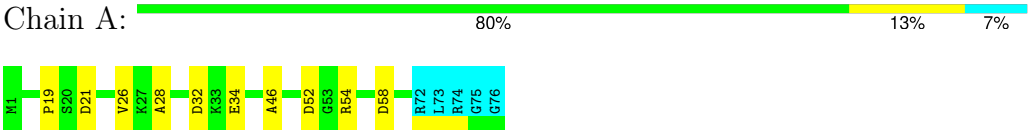
Chain A: 79% 13% • 7%



4.2.257 Score per residue for model 257

- Molecule 1: Ubiquitin

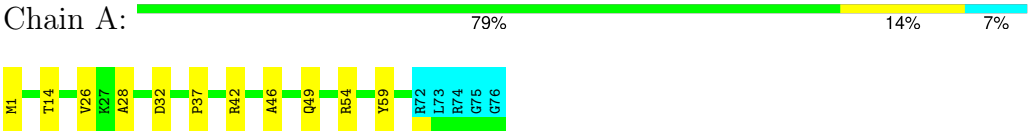
Chain A:



4.2.258 Score per residue for model 258

- Molecule 1: Ubiquitin

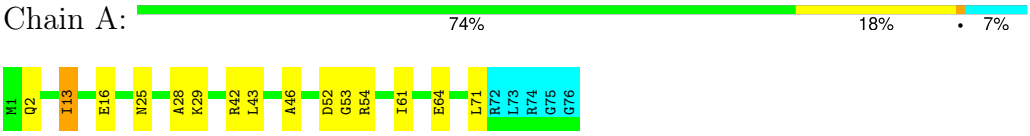
Chain A:



4.2.259 Score per residue for model 259

- Molecule 1: Ubiquitin

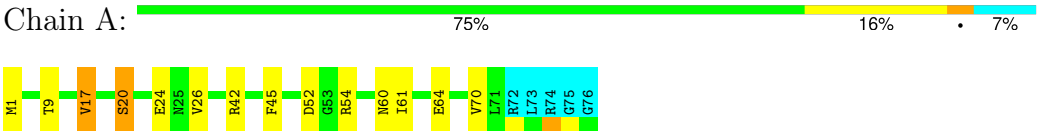
Chain A:



4.2.260 Score per residue for model 260

- Molecule 1: Ubiquitin

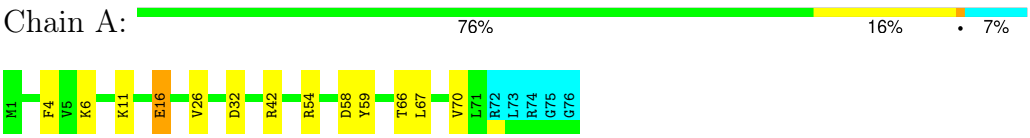
Chain A:



4.2.261 Score per residue for model 261

- Molecule 1: Ubiquitin

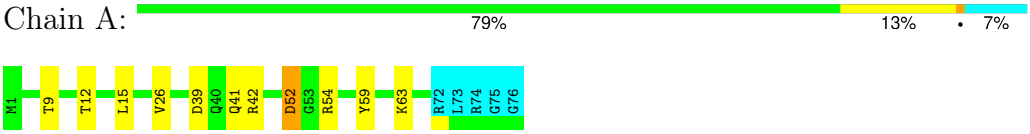
Chain A:



4.2.262 Score per residue for model 262

- Molecule 1: Ubiquitin

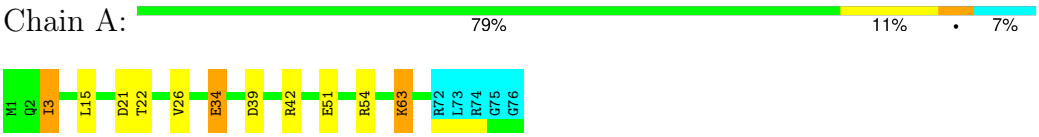
Chain A:



4.2.263 Score per residue for model 263

- Molecule 1: Ubiquitin

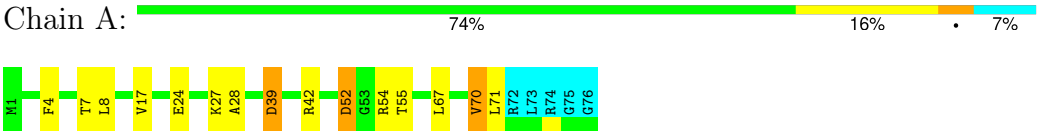
Chain A:



4.2.264 Score per residue for model 264

- Molecule 1: Ubiquitin

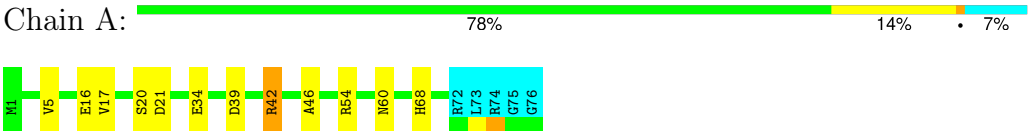
Chain A:



4.2.265 Score per residue for model 265

- Molecule 1: Ubiquitin

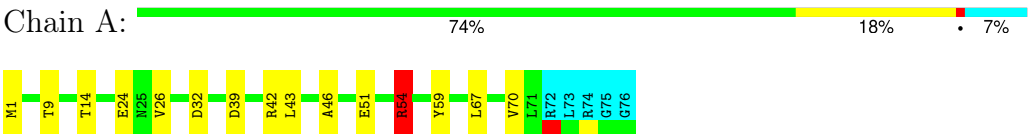
Chain A:



4.2.266 Score per residue for model 266

- Molecule 1: Ubiquitin

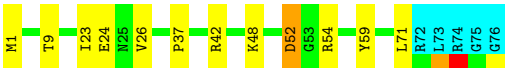
Chain A:



4.2.267 Score per residue for model 267

- Molecule 1: Ubiquitin

Chain A:



4.2.268 Score per residue for model 268

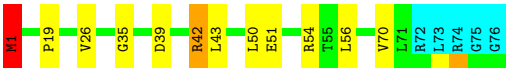
- Molecule 1: Ubiquitin

Chain A:

4.2.269 Score per residue for model 269

- Molecule 1: Ubiquitin

Chain A:



4.2.270 Score per residue for model 270

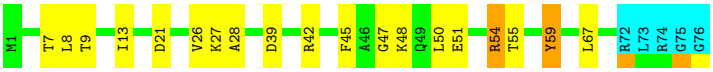
- Molecule 1: Ubiquitin

Chain A:

4.2.271 Score per residue for model 271

- Molecule 1: Ubiquitin

Chain A:



4.2.272 Score per residue for model 272

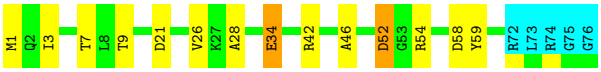
- Molecule 1: Ubiquitin

Chain A:

4.2.273 Score per residue for model 273

- Molecule 1: Ubiquitin

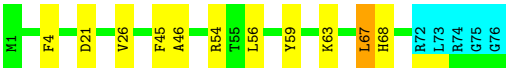
Chain A:



4.2.274 Score per residue for model 274

- Molecule 1: Ubiquitin

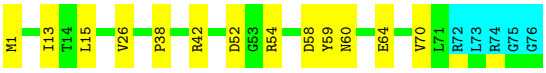
Chain A:



4.2.275 Score per residue for model 275

- Molecule 1: Ubiquitin

Chain A:



4.2.276 Score per residue for model 276

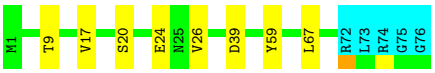
- Molecule 1: Ubiquitin

Chain A:

4.2.277 Score per residue for model 277

- Molecule 1: Ubiquitin

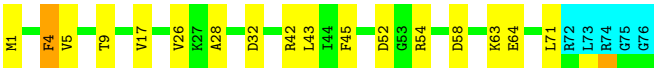
Chain A: 83% 11% 7%



4.2.278 Score per residue for model 278

- Molecule 1: Ubiquitin

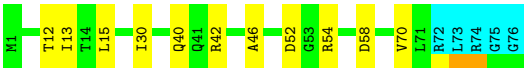
Chain A: 71% 21% • 7%



4.2.279 Score per residue for model 279

- Molecule 1: Ubiquitin

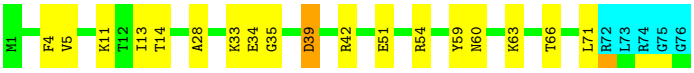
Chain A: 79% 14% 7%



4.2.280 Score per residue for model 280

- Molecule 1: Ubiquitin

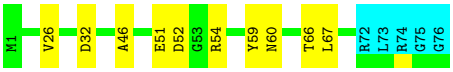
Chain A: 70% 22% • 7%



4.2.281 Score per residue for model 281

- Molecule 1: Ubiquitin

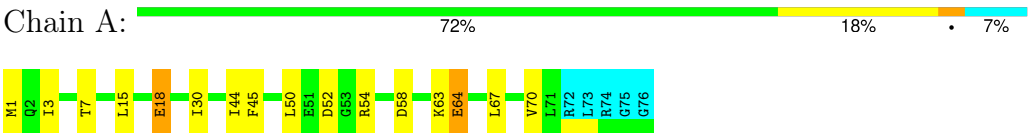
Chain A: 80% 13% 7%



4.2.282 Score per residue for model 282

- Molecule 1: Ubiquitin

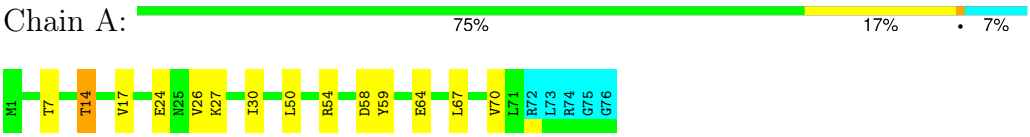
Chain A:



4.2.283 Score per residue for model 283

- Molecule 1: Ubiquitin

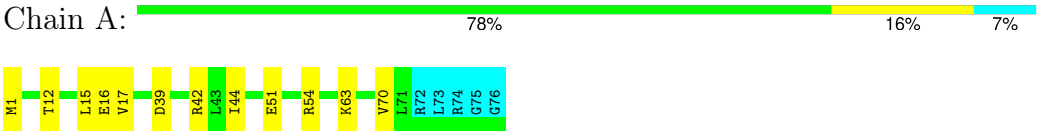
Chain A:



4.2.284 Score per residue for model 284

- Molecule 1: Ubiquitin

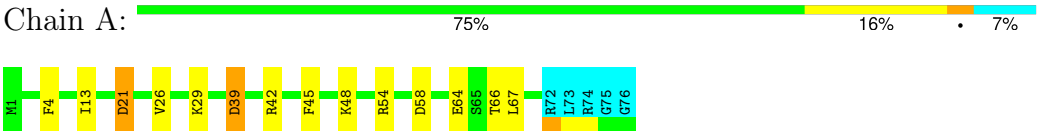
Chain A:



4.2.285 Score per residue for model 285

- Molecule 1: Ubiquitin

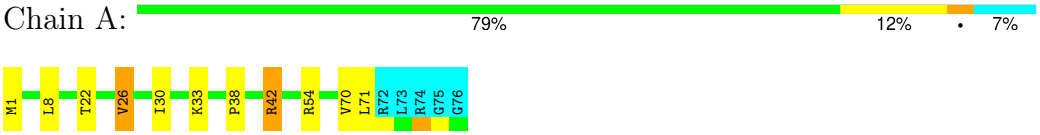
Chain A:



4.2.286 Score per residue for model 286

- Molecule 1: Ubiquitin

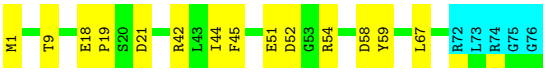
Chain A:



4.2.287 Score per residue for model 287

- Molecule 1: Ubiquitin

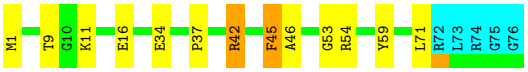
Chain A:



4.2.288 Score per residue for model 288

- Molecule 1: Ubiquitin

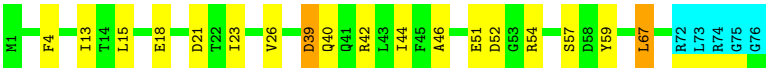
Chain A:



4.2.289 Score per residue for model 289

- Molecule 1: Ubiquitin

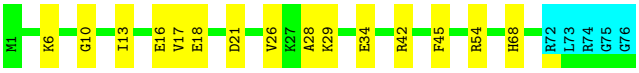
Chain A:



4.2.290 Score per residue for model 290

- Molecule 1: Ubiquitin

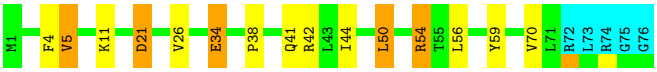
Chain A:



4.2.291 Score per residue for model 291

- Molecule 1: Ubiquitin

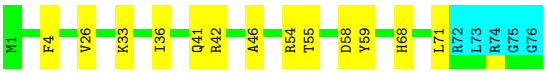
Chain A:



4.2.292 Score per residue for model 292

- Molecule 1: Ubiquitin

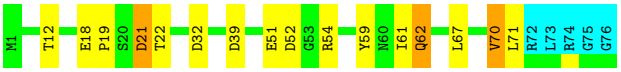
Chain A: 76% 17% 7%



4.2.293 Score per residue for model 293

- Molecule 1: Ubiquitin

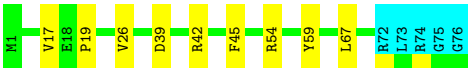
Chain A: 72% 17% • 7%



4.2.294 Score per residue for model 294

- Molecule 1: Ubiquitin

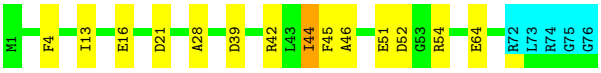
Chain A: 82% 12% 7%



4.2.295 Score per residue for model 295

- Molecule 1: Ubiquitin

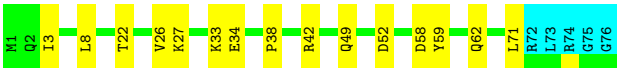
Chain A: 75% 17% • 7%



4.2.296 Score per residue for model 296

- Molecule 1: Ubiquitin

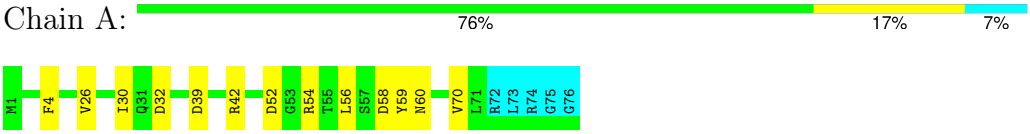
Chain A: 74% 20% 7%



4.2.297 Score per residue for model 297

- Molecule 1: Ubiquitin

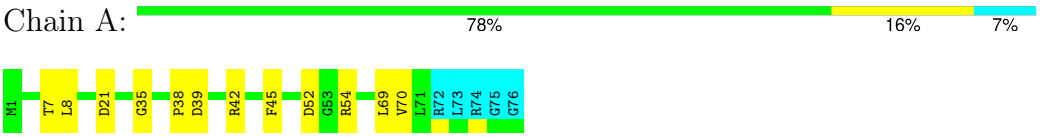
Chain A:



4.2.298 Score per residue for model 298

- Molecule 1: Ubiquitin

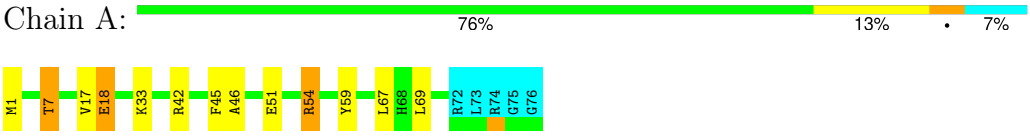
Chain A:



4.2.299 Score per residue for model 299

- Molecule 1: Ubiquitin

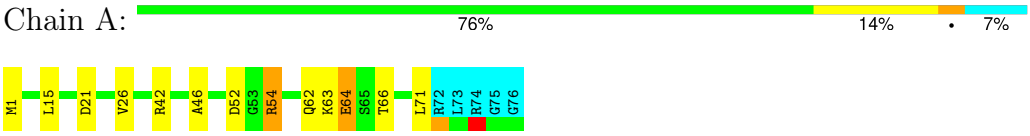
Chain A:



4.2.300 Score per residue for model 300

- Molecule 1: Ubiquitin

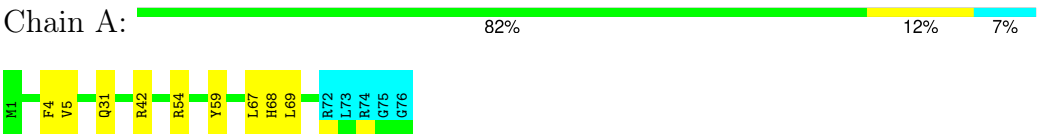
Chain A:



4.2.301 Score per residue for model 301

- Molecule 1: Ubiquitin

Chain A:



5 Refinement protocol and experimental data overview (i)

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

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

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

Software name	Classification	Version
GROMOS	geometry optimization	
GROMOS	refinement	

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

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

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.45±0.00	0±0/570 (0.0± 0.0%)	2.06±0.18	17±6/770 (2.2± 0.8%)
All	All	0.45	0/171570 (0.0%)	2.07	5172/231770 (2.2%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.9±2.1
All	All	0	877

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	54	ARG	NE-CZ-NH1	25.61	133.10	120.30	45	172
1	A	54	ARG	NE-CZ-NH2	-22.90	108.85	120.30	248	144
1	A	42	ARG	NE-CZ-NH1	19.67	130.14	120.30	89	144
1	A	42	ARG	NE-CZ-NH2	-19.16	110.72	120.30	1	140
1	A	59	TYR	CB-CG-CD2	-16.98	110.81	121.00	143	70
1	A	26	VAL	CA-CB-CG1	16.46	135.60	110.90	55	36
1	A	45	PHE	CB-CG-CD1	-16.14	109.50	120.80	288	40
1	A	21	ASP	CB-CG-OD1	16.09	132.78	118.30	274	102
1	A	32	ASP	CB-CG-OD2	-15.46	104.39	118.30	28	64
1	A	52	ASP	CB-CG-OD2	15.23	132.01	118.30	39	74
1	A	39	ASP	CB-CG-OD2	-14.82	104.97	118.30	92	46
1	A	54	ARG	NH1-CZ-NH2	-14.67	103.27	119.40	279	65
1	A	32	ASP	CB-CG-OD1	-14.54	105.21	118.30	51	78
1	A	59	TYR	CB-CG-CD1	-14.52	112.29	121.00	19	70
1	A	46	ALA	CB-CA-C	14.19	131.39	110.10	41	127

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	64	GLU	OE1-CD-OE2	-13.89	106.64	123.30	156	43
1	A	28	ALA	N-CA-CB	13.62	129.16	110.10	22	144
1	A	52	ASP	CB-CG-OD1	-13.45	106.19	118.30	3	63
1	A	70	VAL	CA-CB-CG2	12.51	129.66	110.90	118	40
1	A	17	VAL	CA-CB-CG1	12.42	129.53	110.90	51	54
1	A	26	VAL	CA-CB-CG2	12.34	129.40	110.90	151	105
1	A	4	PHE	CB-CG-CD2	12.30	129.41	120.80	34	57
1	A	39	ASP	CB-CG-OD1	12.08	129.18	118.30	173	48
1	A	14	THR	CA-CB-CG2	11.81	128.93	112.40	192	22
1	A	45	PHE	CB-CG-CD2	-11.66	112.64	120.80	5	55
1	A	58	ASP	CB-CG-OD1	11.58	128.72	118.30	153	62
1	A	42	ARG	NH1-CZ-NH2	-11.56	106.69	119.40	215	46
1	A	21	ASP	CB-CG-OD2	11.24	128.41	118.30	148	53
1	A	42	ARG	CD-NE-CZ	11.17	139.24	123.60	143	35
1	A	58	ASP	CB-CG-OD2	-11.01	108.40	118.30	223	58
1	A	69	LEU	CB-CG-CD1	10.98	129.67	111.00	98	9
1	A	26	VAL	CG1-CB-CG2	-10.88	93.49	110.90	232	137
1	A	16	GLU	OE1-CD-OE2	-10.83	110.30	123.30	51	32
1	A	4	PHE	CB-CG-CD1	10.66	128.26	120.80	48	39
1	A	17	VAL	CA-CB-CG2	10.54	126.70	110.90	130	29
1	A	34	GLU	OE1-CD-OE2	-10.26	110.99	123.30	291	61
1	A	1	MET	CA-CB-CG	10.03	130.34	113.30	103	48
1	A	54	ARG	CD-NE-CZ	9.81	137.34	123.60	267	57
1	A	17	VAL	CG1-CB-CG2	-9.81	95.20	110.90	209	30
1	A	15	LEU	CB-CG-CD2	9.80	127.67	111.00	142	16
1	A	67	LEU	CB-CG-CD2	-9.63	94.63	111.00	176	8
1	A	66	THR	CA-CB-CG2	9.63	125.88	112.40	232	36
1	A	7	THR	CA-CB-CG2	9.55	125.77	112.40	51	24
1	A	56	LEU	CA-CB-CG	9.52	137.21	115.30	204	2
1	A	70	VAL	CG1-CB-CG2	-9.51	95.68	110.90	72	68
1	A	19	PRO	N-CA-CB	9.39	114.57	103.30	27	38
1	A	51	GLU	OE1-CD-OE2	9.36	134.53	123.30	90	34
1	A	67	LEU	CB-CA-C	9.36	127.98	110.20	274	7
1	A	71	LEU	CB-CA-C	9.32	127.90	110.20	286	18
1	A	15	LEU	CB-CG-CD1	9.26	126.74	111.00	50	17
1	A	68	HIS	CB-CA-C	9.19	128.77	110.40	115	8
1	A	55	THR	CA-CB-CG2	9.17	125.24	112.40	276	16
1	A	69	LEU	CB-CG-CD2	9.17	126.58	111.00	205	22
1	A	28	ALA	CB-CA-C	8.86	123.39	110.10	73	43
1	A	48	LYS	O-C-N	8.79	136.76	122.70	141	3
1	A	67	LEU	CB-CG-CD1	8.72	125.82	111.00	176	16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	59	TYR	CG-CD2-CE2	-8.69	114.35	121.30	27	34
1	A	18	GLU	OE1-CD-OE2	-8.68	112.88	123.30	138	27
1	A	32	ASP	OD1-CG-OD2	8.63	139.70	123.30	4	6
1	A	12	THR	CA-CB-CG2	8.63	124.48	112.40	79	27
1	A	64	GLU	CG-CD-OE2	-8.56	101.17	118.30	75	11
1	A	38	PRO	N-CA-CB	8.47	113.46	103.30	91	15
1	A	2	GLN	N-CA-CB	8.46	125.83	110.60	211	3
1	A	59	TYR	CG-CD1-CE1	-8.44	114.55	121.30	86	10
1	A	67	LEU	O-C-N	-8.37	109.31	122.70	37	15
1	A	1	MET	CG-SD-CE	8.35	113.56	100.20	65	26
1	A	43	LEU	CB-CG-CD2	8.31	125.13	111.00	111	12
1	A	11	LYS	CA-CB-CG	8.25	131.55	113.40	81	9
1	A	14	THR	C-N-CA	8.22	142.25	121.70	99	4
1	A	8	LEU	CB-CG-CD2	8.14	124.83	111.00	74	22
1	A	16	GLU	CB-CA-C	8.13	126.66	110.40	247	15
1	A	33	LYS	CB-CG-CD	8.13	132.73	111.60	142	13
1	A	22	THR	CA-CB-OG1	8.09	125.99	109.00	293	4
1	A	57	SER	N-CA-CB	8.04	122.57	110.50	115	11
1	A	44	ILE	CA-CB-CG2	7.98	126.87	110.90	59	20
1	A	12	THR	CA-CB-OG1	7.98	125.76	109.00	249	9
1	A	51	GLU	O-C-N	7.95	135.42	122.70	34	3
1	A	9	THR	CA-CB-CG2	7.92	123.50	112.40	260	19
1	A	71	LEU	CB-CG-CD2	7.91	124.45	111.00	160	14
1	A	5	VAL	CA-CB-CG1	-7.90	99.05	110.90	120	5
1	A	67	LEU	CA-CB-CG	7.81	133.26	115.30	287	8
1	A	64	GLU	CG-CD-OE1	7.79	133.89	118.30	217	13
1	A	42	ARG	N-CA-CB	7.78	124.61	110.60	90	6
1	A	54	ARG	CB-CA-C	7.75	125.91	110.40	46	13
1	A	71	LEU	CB-CG-CD1	7.73	124.14	111.00	264	6
1	A	20	SER	N-CA-CB	-7.71	98.93	110.50	96	8
1	A	52	ASP	N-CA-CB	-7.71	96.72	110.60	298	18
1	A	35	GLY	O-C-N	-7.70	110.38	122.70	60	13
1	A	36	ILE	CA-CB-CG1	7.70	125.63	111.00	174	12
1	A	41	GLN	N-CA-CB	-7.70	96.75	110.60	37	2
1	A	29	LYS	CB-CG-CD	7.67	131.53	111.60	33	1
1	A	60	ASN	CB-CA-C	7.66	125.72	110.40	139	39
1	A	5	VAL	CG1-CB-CG2	-7.66	98.65	110.90	161	17
1	A	43	LEU	CB-CG-CD1	7.65	124.00	111.00	121	10
1	A	55	THR	N-CA-CB	7.64	124.81	110.30	130	6
1	A	21	ASP	OD1-CG-OD2	-7.56	108.94	123.30	148	18
1	A	34	GLU	N-CA-CB	-7.56	96.99	110.60	121	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	56	LEU	N-CA-CB	-7.54	95.31	110.40	59	1
1	A	42	ARG	CB-CA-C	7.52	125.45	110.40	102	19
1	A	48	LYS	N-CA-C	7.52	131.31	111.00	256	8
1	A	26	VAL	CB-CA-C	7.50	125.65	111.40	53	10
1	A	61	ILE	CB-CA-C	7.50	126.59	111.60	46	13
1	A	32	ASP	CA-CB-CG	7.49	129.89	113.40	115	6
1	A	55	THR	CA-CB-OG1	7.49	124.73	109.00	132	4
1	A	48	LYS	N-CA-CB	-7.49	97.12	110.60	267	15
1	A	1	MET	CB-CG-SD	7.44	134.72	112.40	103	1
1	A	48	LYS	CA-CB-CG	7.42	129.73	113.40	137	8
1	A	40	GLN	O-C-N	-7.40	110.86	122.70	100	11
1	A	13	ILE	CB-CA-C	7.40	126.39	111.60	78	8
1	A	16	GLU	CG-CD-OE1	-7.39	103.51	118.30	91	1
1	A	50	LEU	CB-CG-CD2	7.39	123.56	111.00	140	6
1	A	1	MET	CB-CA-C	7.39	125.18	110.40	72	3
1	A	57	SER	O-C-N	-7.37	110.91	122.70	122	8
1	A	13	ILE	CG1-CB-CG2	7.37	127.61	111.40	279	9
1	A	19	PRO	N-CD-CG	7.36	114.24	103.20	172	3
1	A	68	HIS	N-CA-CB	-7.34	97.39	110.60	243	12
1	A	56	LEU	CB-CG-CD1	-7.33	98.55	111.00	200	10
1	A	15	LEU	CB-CA-C	7.30	124.06	110.20	131	4
1	A	48	LYS	CB-CG-CD	7.29	130.55	111.60	148	5
1	A	41	GLN	CB-CA-C	-7.29	95.83	110.40	291	4
1	A	30	ILE	CA-CB-CG1	7.26	124.79	111.00	84	5
1	A	41	GLN	CA-CB-CG	7.22	129.29	113.40	29	5
1	A	49	GLN	CB-CA-C	7.21	124.83	110.40	154	8
1	A	46	ALA	N-CA-CB	-7.20	100.02	110.10	17	31
1	A	51	GLU	CB-CG-CD	-7.18	94.80	114.20	90	1
1	A	50	LEU	CB-CA-C	7.17	123.82	110.20	143	20
1	A	34	GLU	CA-CB-CG	7.17	129.17	113.40	113	14
1	A	45	PHE	N-CA-CB	-7.15	97.73	110.60	174	4
1	A	39	ASP	O-C-N	-7.15	111.26	122.70	280	5
1	A	51	GLU	CA-CB-CG	7.14	129.10	113.40	105	9
1	A	12	THR	OG1-CB-CG2	-7.12	93.62	110.00	10	10
1	A	1	MET	O-C-N	-7.12	111.31	122.70	1	3
1	A	58	ASP	CB-CA-C	7.11	124.63	110.40	204	7
1	A	54	ARG	O-C-N	-7.11	111.32	122.70	92	5
1	A	61	ILE	CG1-CB-CG2	-7.11	95.77	111.40	62	1
1	A	50	LEU	O-C-N	7.09	134.05	122.70	39	4
1	A	33	LYS	CD-CE-NZ	7.09	128.00	111.70	2	3
1	A	70	VAL	CB-CA-C	7.06	124.81	111.40	31	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	57	SER	CA-C-O	-7.04	105.33	120.10	93	3
1	A	8	LEU	CB-CG-CD1	7.01	122.91	111.00	1	14
1	A	31	GLN	CB-CA-C	6.99	124.38	110.40	69	2
1	A	64	GLU	CA-CB-CG	6.98	128.76	113.40	149	12
1	A	70	VAL	CA-CB-CG1	6.98	121.36	110.90	293	9
1	A	59	TYR	CD1-CG-CD2	6.97	125.56	117.90	86	7
1	A	50	LEU	CB-CG-CD1	6.96	122.84	111.00	17	32
1	A	46	ALA	C-N-CA	6.96	136.93	122.30	259	6
1	A	24	GLU	OE1-CD-OE2	-6.96	114.95	123.30	217	18
1	A	22	THR	CA-CB-CG2	-6.96	102.66	112.40	69	15
1	A	19	PRO	CA-N-CD	-6.95	101.78	111.50	248	6
1	A	43	LEU	CB-CA-C	6.90	123.32	110.20	236	9
1	A	56	LEU	CA-C-O	-6.90	105.61	120.10	130	4
1	A	61	ILE	CB-CG1-CD1	6.88	133.18	113.90	143	6
1	A	44	ILE	CA-CB-CG1	6.88	124.08	111.00	205	21
1	A	27	LYS	CA-CB-CG	6.88	128.54	113.40	84	3
1	A	11	LYS	N-CA-CB	-6.87	98.23	110.60	5	7
1	A	62	GLN	CB-CA-C	6.87	124.13	110.40	2	9
1	A	49	GLN	OE1-CD-NE2	-6.85	106.16	121.90	47	1
1	A	64	GLU	CB-CA-C	6.85	124.09	110.40	99	10
1	A	14	THR	OG1-CB-CG2	-6.84	94.26	110.00	51	13
1	A	42	ARG	CA-C-O	-6.84	105.72	120.10	146	1
1	A	65	SER	O-C-N	-6.83	111.78	122.70	4	8
1	A	9	THR	CA-CB-OG1	6.82	123.32	109.00	177	4
1	A	39	ASP	N-CA-CB	-6.82	98.32	110.60	140	15
1	A	25	ASN	CA-CB-CG	6.82	128.40	113.40	65	8
1	A	14	THR	CA-CB-OG1	6.81	123.31	109.00	242	3
1	A	11	LYS	CB-CG-CD	6.80	129.29	111.60	93	2
1	A	57	SER	CB-CA-C	-6.80	97.17	110.10	204	3
1	A	53	GLY	N-CA-C	6.79	130.09	113.10	54	5
1	A	22	THR	OG1-CB-CG2	-6.79	94.38	110.00	206	4
1	A	59	TYR	CD1-CE1-CZ	-6.79	113.69	119.80	149	14
1	A	16	GLU	CA-CB-CG	6.78	128.32	113.40	25	8
1	A	34	GLU	CG-CD-OE2	6.78	131.86	118.30	35	8
1	A	37	PRO	N-CA-CB	6.77	111.43	103.30	112	17
1	A	32	ASP	CB-CA-C	6.76	123.93	110.40	57	2
1	A	55	THR	O-C-N	-6.76	111.89	122.70	147	7
1	A	5	VAL	O-C-N	-6.74	111.91	122.70	63	10
1	A	63	LYS	N-CA-CB	-6.73	98.49	110.60	137	7
1	A	61	ILE	C-N-CA	6.71	138.47	121.70	59	2
1	A	56	LEU	C-N-CA	6.68	138.41	121.70	59	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	5	VAL	CA-CB-CG2	6.68	120.92	110.90	91	9
1	A	34	GLU	C-N-CA	6.67	136.32	122.30	42	3
1	A	13	ILE	CA-CB-CG1	6.67	123.67	111.00	34	13
1	A	31	GLN	CA-CB-CG	6.66	128.06	113.40	112	1
1	A	40	GLN	CB-CA-C	6.65	123.71	110.40	229	4
1	A	17	VAL	CB-CA-C	-6.65	98.77	111.40	283	10
1	A	32	ASP	N-CA-CB	-6.64	98.64	110.60	164	10
1	A	65	SER	C-N-CA	6.64	138.30	121.70	110	4
1	A	63	LYS	CA-CB-CG	6.63	127.99	113.40	101	8
1	A	6	LYS	CB-CA-C	6.61	123.62	110.40	66	8
1	A	59	TYR	N-CA-CB	-6.60	98.72	110.60	261	3
1	A	47	GLY	CA-C-O	-6.60	108.73	120.60	171	4
1	A	13	ILE	CA-CB-CG2	-6.58	97.74	110.90	133	2
1	A	52	ASP	CA-C-N	6.58	129.36	116.20	72	3
1	A	11	LYS	CB-CA-C	-6.58	97.24	110.40	227	7
1	A	56	LEU	CB-CA-C	6.57	122.69	110.20	131	9
1	A	62	GLN	N-CA-CB	-6.57	98.77	110.60	23	4
1	A	16	GLU	N-CA-CB	6.55	122.40	110.60	140	8
1	A	30	ILE	CG1-CB-CG2	-6.54	97.00	111.40	85	5
1	A	27	LYS	O-C-N	6.54	133.16	122.70	74	2
1	A	27	LYS	CB-CA-C	-6.53	97.34	110.40	131	5
1	A	39	ASP	OD1-CG-OD2	-6.51	110.93	123.30	128	4
1	A	23	ILE	O-C-N	-6.51	112.29	122.70	70	2
1	A	55	THR	CA-C-O	6.49	133.73	120.10	125	15
1	A	60	ASN	O-C-N	-6.49	112.32	122.70	148	3
1	A	29	LYS	O-C-N	-6.48	112.33	122.70	70	3
1	A	43	LEU	CA-CB-CG	-6.48	100.40	115.30	91	1
1	A	25	ASN	CB-CA-C	6.48	123.35	110.40	30	7
1	A	29	LYS	CB-CA-C	6.48	123.35	110.40	147	4
1	A	10	GLY	CA-C-O	-6.48	108.94	120.60	15	3
1	A	56	LEU	CB-CG-CD2	6.47	121.99	111.00	157	9
1	A	70	VAL	O-C-N	-6.45	112.38	122.70	54	6
1	A	53	GLY	C-N-CA	6.44	137.80	121.70	138	2
1	A	38	PRO	N-CD-CG	6.44	112.86	103.20	291	5
1	A	9	THR	OG1-CB-CG2	-6.42	95.23	110.00	60	5
1	A	49	GLN	N-CA-CB	-6.42	99.05	110.60	201	2
1	A	4	PHE	CG-CD2-CE2	-6.40	113.76	120.80	289	10
1	A	2	GLN	CB-CA-C	6.38	123.17	110.40	103	4
1	A	8	LEU	N-CA-CB	-6.36	97.67	110.40	90	4
1	A	8	LEU	CB-CA-C	6.36	122.28	110.20	130	7
1	A	4	PHE	N-CA-CB	-6.35	99.16	110.60	29	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	30	ILE	O-C-N	-6.34	112.55	122.70	42	7
1	A	27	LYS	N-CA-CB	-6.32	99.22	110.60	106	3
1	A	63	LYS	CG-CD-CE	6.29	130.78	111.90	60	1
1	A	23	ILE	CA-CB-CG1	6.29	122.96	111.00	83	2
1	A	3	ILE	CA-CB-CG1	6.29	122.96	111.00	136	7
1	A	26	VAL	O-C-N	-6.29	112.64	122.70	53	1
1	A	62	GLN	CA-C-O	6.28	133.28	120.10	35	2
1	A	44	ILE	CG1-CB-CG2	-6.27	97.61	111.40	36	6
1	A	34	GLU	O-C-N	-6.27	112.55	123.20	184	6
1	A	49	GLN	O-C-N	6.25	132.70	122.70	66	4
1	A	71	LEU	CA-CB-CG	6.25	129.68	115.30	45	4
1	A	46	ALA	CA-C-N	6.25	128.70	116.20	17	4
1	A	55	THR	C-N-CA	6.25	137.31	121.70	103	3
1	A	52	ASP	OD1-CG-OD2	-6.24	111.45	123.30	114	5
1	A	2	GLN	C-N-CA	6.23	137.28	121.70	81	19
1	A	58	ASP	C-N-CA	6.22	137.26	121.70	59	2
1	A	64	GLU	O-C-N	-6.22	112.74	122.70	4	7
1	A	61	ILE	CA-CB-CG2	6.22	123.33	110.90	131	1
1	A	3	ILE	N-CA-CB	6.21	125.09	110.80	112	3
1	A	66	THR	OG1-CB-CG2	-6.20	95.73	110.00	215	3
1	A	63	LYS	C-N-CA	6.20	137.19	121.70	27	13
1	A	23	ILE	CG1-CB-CG2	-6.20	97.77	111.40	55	2
1	A	69	LEU	N-CA-CB	-6.19	98.02	110.40	301	3
1	A	29	LYS	CA-CB-CG	6.19	127.02	113.40	4	3
1	A	62	GLN	CA-CB-CG	6.17	126.97	113.40	296	2
1	A	17	VAL	O-C-N	-6.16	112.84	122.70	103	3
1	A	20	SER	CB-CA-C	-6.14	98.43	110.10	185	2
1	A	2	GLN	CA-CB-CG	6.13	126.90	113.40	121	5
1	A	18	GLU	CG-CD-OE1	-6.12	106.05	118.30	98	3
1	A	61	ILE	N-CA-CB	6.11	124.86	110.80	95	2
1	A	59	TYR	CB-CA-C	6.10	122.61	110.40	113	7
1	A	61	ILE	N-CA-C	-6.10	94.54	111.00	12	1
1	A	51	GLU	C-N-CA	6.09	136.91	121.70	212	1
1	A	33	LYS	N-CA-CB	-6.08	99.65	110.60	147	4
1	A	42	ARG	C-N-CA	6.08	136.89	121.70	207	3
1	A	35	GLY	C-N-CA	6.06	136.86	121.70	45	7
1	A	48	LYS	CB-CA-C	6.05	122.50	110.40	144	3
1	A	45	PHE	CB-CA-C	6.04	122.48	110.40	298	1
1	A	34	GLU	CB-CA-C	-6.03	98.34	110.40	83	2
1	A	45	PHE	CD1-CG-CD2	6.02	126.12	118.30	229	2
1	A	42	ARG	CB-CG-CD	6.00	127.19	111.60	46	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	63	LYS	CB-CA-C	5.99	122.38	110.40	119	2
1	A	23	ILE	CB-CA-C	5.98	123.56	111.60	84	5
1	A	25	ASN	O-C-N	-5.98	113.14	122.70	46	4
1	A	54	ARG	CA-C-O	5.98	132.65	120.10	133	2
1	A	60	ASN	CB-CG-OD1	-5.97	109.66	121.60	134	3
1	A	12	THR	CA-C-O	-5.97	107.57	120.10	94	1
1	A	25	ASN	OD1-CG-ND2	-5.97	108.18	121.90	83	1
1	A	22	THR	O-C-N	-5.96	113.16	122.70	133	3
1	A	52	ASP	CA-CB-CG	5.95	126.50	113.40	125	5
1	A	51	GLU	CB-CA-C	5.94	122.28	110.40	51	6
1	A	27	LYS	CA-C-O	-5.94	107.63	120.10	39	8
1	A	6	LYS	N-CA-CB	-5.93	99.93	110.60	46	4
1	A	34	GLU	CG-CD-OE1	5.92	130.14	118.30	90	1
1	A	23	ILE	CB-CG1-CD1	5.92	130.46	113.90	64	2
1	A	12	THR	C-N-CA	5.91	136.48	121.70	102	1
1	A	14	THR	O-C-N	5.90	132.14	122.70	13	6
1	A	51	GLU	N-CA-CB	-5.90	99.98	110.60	130	6
1	A	67	LEU	C-N-CA	5.90	136.45	121.70	95	1
1	A	65	SER	N-CA-CB	5.89	119.34	110.50	18	5
1	A	33	LYS	O-C-N	-5.89	113.27	122.70	52	6
1	A	1	MET	N-CA-CB	-5.89	99.99	110.60	76	4
1	A	28	ALA	O-C-N	-5.88	113.29	122.70	245	3
1	A	53	GLY	O-C-N	-5.88	113.29	122.70	288	3
1	A	29	LYS	CA-C-O	5.88	132.44	120.10	80	1
1	A	61	ILE	CA-CB-CG1	5.88	122.17	111.00	293	7
1	A	60	ASN	N-CA-CB	5.87	121.17	110.60	224	2
1	A	43	LEU	CD1-CG-CD2	-5.87	92.89	110.50	196	2
1	A	34	GLU	N-CA-C	5.87	126.85	111.00	141	4
1	A	25	ASN	CA-C-N	5.87	130.11	117.20	111	4
1	A	34	GLU	CB-CG-CD	-5.86	98.37	114.20	109	1
1	A	57	SER	CA-C-N	5.86	130.09	117.20	21	4
1	A	59	TYR	O-C-N	-5.86	113.33	122.70	267	5
1	A	59	TYR	CA-CB-CG	5.85	124.52	113.40	261	4
1	A	58	ASP	N-CA-CB	-5.84	100.09	110.60	59	3
1	A	40	GLN	N-CA-CB	-5.83	100.10	110.60	92	2
1	A	14	THR	N-CA-CB	5.83	121.38	110.30	231	2
1	A	41	GLN	O-C-N	-5.83	113.38	122.70	104	3
1	A	33	LYS	CA-CB-CG	5.82	126.21	113.40	249	5
1	A	62	GLN	CG-CD-OE1	5.82	133.25	121.60	81	1
1	A	45	PHE	CG-CD1-CE1	-5.82	114.39	120.80	290	3
1	A	36	ILE	CB-CG1-CD1	5.82	130.20	113.90	63	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	47	GLY	C-N-CA	5.81	136.22	121.70	163	2
1	A	24	GLU	O-C-N	-5.81	113.41	122.70	40	4
1	A	39	ASP	CA-C-N	5.81	129.97	117.20	10	2
1	A	37	PRO	N-CD-CG	5.81	111.91	103.20	288	9
1	A	16	GLU	C-N-CA	5.80	136.20	121.70	5	6
1	A	4	PHE	O-C-N	-5.79	113.44	122.70	55	4
1	A	18	GLU	CG-CD-OE2	5.79	129.88	118.30	127	2
1	A	52	ASP	N-CA-C	5.79	126.63	111.00	121	5
1	A	68	HIS	CG-CD2-NE2	-5.78	98.22	109.20	301	1
1	A	59	TYR	CZ-CE2-CD2	-5.78	114.60	119.80	24	6
1	A	18	GLU	N-CA-CB	-5.77	100.21	110.60	252	2
1	A	51	GLU	CA-C-O	-5.76	108.00	120.10	10	1
1	A	52	ASP	CB-CA-C	5.76	121.92	110.40	268	7
1	A	71	LEU	C-N-CA	5.75	136.08	121.70	18	1
1	A	64	GLU	N-CA-C	5.75	126.51	111.00	27	3
1	A	49	GLN	CA-CB-CG	5.74	126.04	113.40	124	6
1	A	30	ILE	CB-CG1-CD1	5.74	129.98	113.90	45	9
1	A	54	ARG	CA-CB-CG	-5.74	100.77	113.40	39	4
1	A	71	LEU	N-CA-CB	5.74	121.88	110.40	120	3
1	A	18	GLU	CB-CA-C	5.73	121.86	110.40	299	3
1	A	27	LYS	C-N-CA	-5.72	107.39	121.70	74	1
1	A	50	LEU	N-CA-C	5.72	126.45	111.00	185	1
1	A	4	PHE	CZ-CE2-CD2	5.72	126.96	120.10	214	2
1	A	38	PRO	C-N-CA	5.71	135.98	121.70	103	4
1	A	58	ASP	CA-C-O	5.70	132.07	120.10	111	1
1	A	5	VAL	CB-CA-C	5.70	122.22	111.40	210	4
1	A	54	ARG	CG-CD-NE	5.70	123.76	111.80	244	2
1	A	30	ILE	CA-C-N	5.68	129.71	117.20	93	1
1	A	65	SER	CB-CA-C	-5.67	99.32	110.10	56	3
1	A	7	THR	OG1-CB-CG2	-5.67	96.95	110.00	196	3
1	A	33	LYS	C-N-CA	5.67	135.88	121.70	7	4
1	A	63	LYS	CA-C-O	5.66	131.98	120.10	28	1
1	A	31	GLN	N-CA-CB	-5.65	100.42	110.60	69	3
1	A	30	ILE	CA-CB-CG2	5.64	122.18	110.90	180	6
1	A	11	LYS	N-CA-C	5.64	126.23	111.00	1	1
1	A	62	GLN	O-C-N	-5.64	113.68	122.70	122	1
1	A	68	HIS	C-N-CA	5.64	135.79	121.70	171	1
1	A	54	ARG	N-CA-CB	-5.62	100.47	110.60	300	3
1	A	14	THR	N-CA-C	-5.62	95.81	111.00	141	3
1	A	62	GLN	CA-C-N	-5.62	104.83	117.20	148	3
1	A	71	LEU	CA-C-N	-5.62	104.83	117.20	248	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	70	VAL	C-N-CA	5.62	135.74	121.70	87	2
1	A	54	ARG	CB-CG-CD	5.61	126.18	111.60	18	3
1	A	44	ILE	CB-CA-C	5.61	122.81	111.60	112	3
1	A	1	MET	N-CA-C	-5.60	95.87	111.00	57	1
1	A	31	GLN	CA-C-N	5.60	129.52	117.20	301	2
1	A	64	GLU	N-CA-CB	5.60	120.68	110.60	84	5
1	A	46	ALA	O-C-N	-5.60	113.68	123.20	96	2
1	A	42	ARG	O-C-N	-5.59	113.76	122.70	20	2
1	A	35	GLY	CA-C-O	-5.59	110.54	120.60	72	3
1	A	20	SER	CA-C-N	5.58	129.48	117.20	138	6
1	A	2	GLN	OE1-CD-NE2	-5.58	109.06	121.90	76	2
1	A	58	ASP	O-C-N	-5.57	113.78	122.70	145	4
1	A	8	LEU	C-N-CA	5.57	135.62	121.70	33	1
1	A	19	PRO	CA-CB-CG	-5.56	93.43	104.00	132	2
1	A	17	VAL	CA-C-N	5.56	129.42	117.20	10	2
1	A	56	LEU	CA-C-N	5.55	129.41	117.20	276	1
1	A	63	LYS	CB-CG-CD	5.55	126.03	111.60	79	7
1	A	66	THR	CA-CB-OG1	5.55	120.65	109.00	285	3
1	A	68	HIS	CA-CB-CG	5.54	123.03	113.60	88	5
1	A	23	ILE	CA-C-N	5.54	129.38	117.20	70	1
1	A	58	ASP	CA-CB-CG	5.53	125.56	113.40	296	5
1	A	1	MET	CA-C-N	5.52	129.35	117.20	113	1
1	A	59	TYR	C-N-CA	5.52	135.51	121.70	254	3
1	A	66	THR	O-C-N	5.52	131.53	122.70	157	3
1	A	26	VAL	N-CA-CB	5.51	123.62	111.50	24	11
1	A	1	MET	CA-C-O	-5.50	108.54	120.10	113	1
1	A	45	PHE	CG-CD2-CE2	-5.50	114.75	120.80	165	3
1	A	44	ILE	O-C-N	-5.50	113.91	122.70	152	5
1	A	67	LEU	N-CA-CB	-5.49	99.41	110.40	135	1
1	A	44	ILE	C-N-CA	5.49	135.42	121.70	139	3
1	A	69	LEU	CD1-CG-CD2	-5.48	94.06	110.50	39	2
1	A	60	ASN	CA-CB-CG	-5.47	101.36	113.40	31	3
1	A	61	ILE	O-C-N	-5.46	113.96	122.70	237	8
1	A	4	PHE	CD1-CE1-CZ	-5.46	113.55	120.10	276	1
1	A	19	PRO	O-C-N	-5.45	113.97	122.70	209	1
1	A	45	PHE	O-C-N	5.45	131.42	122.70	247	2
1	A	3	ILE	CB-CG1-CD1	5.45	129.16	113.90	50	2
1	A	23	ILE	CA-CB-CG2	5.44	121.79	110.90	133	3
1	A	66	THR	CB-CA-C	-5.44	96.91	111.60	125	2
1	A	16	GLU	O-C-N	-5.44	114.00	122.70	95	1
1	A	60	ASN	CA-C-N	-5.44	105.24	117.20	113	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	21	ASP	N-CA-CB	-5.44	100.82	110.60	96	2
1	A	27	LYS	CB-CG-CD	5.43	125.72	111.60	120	1
1	A	4	PHE	N-CA-C	-5.43	96.35	111.00	168	1
1	A	58	ASP	OD1-CG-OD2	5.42	133.61	123.30	141	3
1	A	63	LYS	O-C-N	-5.42	114.03	122.70	10	1
1	A	21	ASP	CA-CB-CG	5.42	125.33	113.40	32	4
1	A	21	ASP	CB-CA-C	-5.42	99.56	110.40	19	4
1	A	25	ASN	CA-C-O	-5.42	108.72	120.10	52	1
1	A	18	GLU	CB-CG-CD	5.42	128.82	114.20	137	1
1	A	16	GLU	N-CA-C	-5.40	96.42	111.00	247	1
1	A	68	HIS	O-C-N	5.39	131.33	122.70	93	3
1	A	15	LEU	CA-C-N	-5.39	105.34	117.20	113	1
1	A	6	LYS	O-C-N	-5.39	114.08	122.70	45	1
1	A	50	LEU	CA-CB-CG	5.38	127.68	115.30	2	2
1	A	65	SER	CA-CB-OG	-5.38	96.67	111.20	25	1
1	A	47	GLY	O-C-N	-5.38	114.09	122.70	137	3
1	A	3	ILE	CA-CB-CG2	-5.37	100.16	110.90	23	2
1	A	52	ASP	O-C-N	-5.37	114.07	123.20	129	7
1	A	62	GLN	OE1-CD-NE2	-5.37	109.56	121.90	270	3
1	A	50	LEU	C-N-CA	5.37	135.11	121.70	167	3
1	A	18	GLU	CA-CB-CG	5.37	125.21	113.40	115	2
1	A	19	PRO	N-CA-C	5.36	126.04	112.10	130	2
1	A	9	THR	O-C-N	-5.36	114.08	123.20	185	2
1	A	11	LYS	C-N-CA	5.36	135.10	121.70	198	2
1	A	64	GLU	C-N-CA	5.36	135.10	121.70	130	1
1	A	2	GLN	CB-CG-CD	5.36	125.53	111.60	10	1
1	A	2	GLN	O-C-N	5.36	131.27	122.70	211	3
1	A	47	GLY	N-CA-C	5.34	126.46	113.10	209	1
1	A	13	ILE	O-C-N	5.34	131.25	122.70	107	2
1	A	69	LEU	C-N-CA	5.34	135.05	121.70	11	2
1	A	4	PHE	CD1-CG-CD2	5.34	125.24	118.30	171	1
1	A	10	GLY	N-CA-C	5.33	126.43	113.10	63	2
1	A	52	ASP	C-N-CA	5.33	133.49	122.30	259	2
1	A	37	PRO	CA-N-CD	-5.32	104.05	111.50	267	1
1	A	42	ARG	CG-CD-NE	5.32	122.97	111.80	294	1
1	A	16	GLU	CG-CD-OE2	-5.32	107.67	118.30	15	2
1	A	35	GLY	CA-C-N	5.32	128.89	117.20	32	2
1	A	29	LYS	CD-CE-NZ	-5.31	99.48	111.70	47	1
1	A	3	ILE	CG1-CB-CG2	5.30	123.06	111.40	111	1
1	A	44	ILE	N-CA-C	5.29	125.30	111.00	121	1
1	A	55	THR	OG1-CB-CG2	-5.29	97.83	110.00	102	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	9	THR	CA-C-N	5.28	126.77	116.20	185	1
1	A	66	THR	N-CA-CB	-5.28	100.27	110.30	23	1
1	A	68	HIS	CA-C-N	-5.28	105.59	117.20	51	3
1	A	64	GLU	CA-C-O	5.27	131.18	120.10	130	1
1	A	17	VAL	N-CA-CB	5.27	123.09	111.50	283	1
1	A	8	LEU	N-CA-C	5.26	125.20	111.00	9	1
1	A	24	GLU	N-CA-CB	-5.24	101.17	110.60	147	2
1	A	34	GLU	CA-C-O	5.23	131.09	120.10	100	1
1	A	49	GLN	CG-CD-NE2	5.22	129.24	116.70	102	1
1	A	36	ILE	CG1-CB-CG2	-5.22	99.92	111.40	171	1
1	A	7	THR	C-N-CA	5.22	134.75	121.70	162	1
1	A	7	THR	CA-CB-OG1	5.22	119.96	109.00	148	1
1	A	14	THR	CA-C-N	-5.20	105.76	117.20	7	2
1	A	30	ILE	C-N-CA	5.20	134.70	121.70	58	1
1	A	28	ALA	CA-C-N	5.19	128.63	117.20	6	2
1	A	70	VAL	N-CA-CB	-5.19	100.07	111.50	64	1
1	A	4	PHE	C-N-CA	5.19	134.68	121.70	274	1
1	A	20	SER	N-CA-C	5.19	125.00	111.00	129	1
1	A	40	GLN	C-N-CA	5.17	134.64	121.70	11	1
1	A	33	LYS	N-CA-C	5.17	124.97	111.00	111	1
1	A	36	ILE	CA-C-O	-5.17	109.23	120.10	252	2
1	A	13	ILE	N-CA-CB	5.17	122.69	110.80	271	1
1	A	66	THR	N-CA-C	5.16	124.94	111.00	91	1
1	A	51	GLU	CA-C-N	-5.16	105.86	117.20	34	1
1	A	8	LEU	O-C-N	-5.14	114.47	122.70	187	1
1	A	3	ILE	CA-C-O	5.14	130.90	120.10	183	2
1	A	3	ILE	CA-C-N	-5.13	105.91	117.20	54	1
1	A	36	ILE	N-CA-C	5.13	124.85	111.00	90	1
1	A	22	THR	N-CA-CB	5.13	120.05	110.30	129	1
1	A	17	VAL	N-CA-C	5.13	124.84	111.00	71	1
1	A	25	ASN	CB-CG-OD1	5.12	131.85	121.60	28	1
1	A	45	PHE	CD1-CE1-CZ	-5.12	113.95	120.10	184	1
1	A	2	GLN	CA-C-N	5.12	128.46	117.20	252	1
1	A	21	ASP	O-C-N	-5.11	114.52	122.70	47	1
1	A	5	VAL	CA-C-O	5.11	130.83	120.10	94	2
1	A	51	GLU	CG-CD-OE1	-5.11	108.08	118.30	90	1
1	A	67	LEU	CA-C-N	5.10	128.42	117.20	45	1
1	A	10	GLY	O-C-N	5.10	130.85	122.70	14	2
1	A	16	GLU	CA-C-O	5.10	130.81	120.10	107	1
1	A	33	LYS	CG-CD-CE	-5.09	96.61	111.90	50	1
1	A	20	SER	O-C-N	-5.08	114.57	122.70	54	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	58	ASP	CA-C-N	-5.08	106.03	117.20	7	1
1	A	40	GLN	OE1-CD-NE2	-5.08	110.22	121.90	279	1
1	A	71	LEU	O-C-N	-5.08	114.58	122.70	7	1
1	A	33	LYS	CB-CA-C	-5.08	100.25	110.40	15	2
1	A	40	GLN	CA-CB-CG	-5.06	102.26	113.40	21	1
1	A	9	THR	N-CA-C	5.06	124.67	111.00	34	1
1	A	7	THR	O-C-N	5.06	130.80	122.70	76	1
1	A	60	ASN	CA-C-O	5.06	130.73	120.10	64	1
1	A	50	LEU	N-CA-CB	-5.06	100.29	110.40	166	1
1	A	50	LEU	CA-C-O	-5.05	109.50	120.10	78	2
1	A	36	ILE	CB-CA-C	-5.05	101.51	111.60	77	1
1	A	48	LYS	CA-C-O	5.04	130.67	120.10	128	1
1	A	38	PRO	O-C-N	-5.03	114.65	122.70	75	1
1	A	38	PRO	CA-N-CD	-5.03	104.46	111.50	63	1
1	A	39	ASP	CA-C-O	-5.03	109.54	120.10	25	1
1	A	34	GLU	CA-C-N	5.01	126.23	116.20	181	2
1	A	8	LEU	CA-CB-CG	5.01	126.83	115.30	46	1
1	A	36	ILE	N-CA-CB	5.01	122.33	110.80	147	1
1	A	56	LEU	O-C-N	-5.01	114.68	122.70	202	1
1	A	65	SER	CA-C-O	-5.01	109.58	120.10	106	1
1	A	49	GLN	CA-C-N	-5.01	106.18	117.20	141	1
1	A	5	VAL	N-CA-C	-5.00	97.49	111.00	156	1

There are no chirality outliers.

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

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

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	47	GLY	Mainchain,Peptide	12
1	A	7	THR	Mainchain,Peptide	12
1	A	21	ASP	Mainchain,Sidechain	11
1	A	13	ILE	Mainchain,Peptide	11
1	A	34	GLU	Sidechain,Mainchain,Peptide	11
1	A	57	SER	Mainchain,Peptide	10
1	A	23	ILE	Mainchain	10
1	A	33	LYS	Peptide,Mainchain	10
1	A	50	LEU	Peptide,Mainchain	10
1	A	48	LYS	Mainchain,Peptide	9
1	A	56	LEU	Mainchain,Peptide	9
1	A	29	LYS	Peptide,Mainchain	9
1	A	26	VAL	Peptide,Mainchain	8
1	A	6	LYS	Mainchain,Peptide	8
1	A	10	GLY	Peptide,Mainchain	8
1	A	55	THR	Mainchain,Peptide	7
1	A	58	ASP	Sidechain,Mainchain	7
1	A	52	ASP	Mainchain,Sidechain	7
1	A	20	SER	Peptide,Mainchain	7
1	A	53	GLY	Peptide,Mainchain	7
1	A	24	GLU	Mainchain,Peptide	7
1	A	35	GLY	Mainchain,Peptide	7
1	A	39	ASP	Mainchain	7
1	A	46	ALA	Mainchain,Peptide	7
1	A	1	MET	Peptide,Mainchain	6
1	A	62	GLN	Peptide,Mainchain	6
1	A	37	PRO	Peptide	6
1	A	15	LEU	Peptide,Mainchain	6
1	A	40	GLN	Peptide,Mainchain,Sidechain	6
1	A	5	VAL	Mainchain	5
1	A	18	GLU	Mainchain,Peptide	5
1	A	44	ILE	Mainchain	5
1	A	16	GLU	Mainchain	5
1	A	28	ALA	Mainchain	5
1	A	38	PRO	Mainchain	4
1	A	25	ASN	Peptide,Mainchain	4
1	A	70	VAL	Peptide	4
1	A	31	GLN	Mainchain	4
1	A	61	ILE	Mainchain	4
1	A	12	THR	Peptide,Mainchain	3
1	A	60	ASN	Mainchain	3
1	A	43	LEU	Mainchain	3

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	9	THR	Peptide,Mainchain	3
1	A	14	THR	Peptide,Mainchain	3
1	A	69	LEU	Mainchain	2
1	A	36	ILE	Mainchain	2
1	A	3	ILE	Mainchain	2
1	A	32	ASP	Sidechain,Mainchain	2
1	A	2	GLN	Peptide	2
1	A	27	LYS	Mainchain	2
1	A	8	LEU	Mainchain	2
1	A	30	ILE	Mainchain	2
1	A	63	LYS	Mainchain	1
1	A	67	LEU	Mainchain	1
1	A	49	GLN	Mainchain	1

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	563	586	586	1±1
All	All	169463	176386	176386	378

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ILE:HA	1:A:26:VAL:HG23	0.73	1.59	151	9
1:A:7:THR:HG22	1:A:69:LEU:HD23	0.71	1.61	154	3
1:A:68:HIS:CG	1:A:69:LEU:H	0.71	2.03	49	8
1:A:63:LYS:HE2	1:A:64:GLU:OE2	0.69	1.87	173	4
1:A:23:ILE:HG23	1:A:43:LEU:HD13	0.68	1.66	90	1
1:A:63:LYS:NZ	1:A:64:GLU:OE1	0.67	2.26	44	15
1:A:63:LYS:HE2	1:A:64:GLU:OE1	0.67	1.89	300	4
1:A:63:LYS:NZ	1:A:64:GLU:OE2	0.63	2.31	233	7
1:A:48:LYS:HE2	1:A:59:TYR:CE1	0.62	2.29	45	2
1:A:18:GLU:OE1	1:A:19:PRO:HD2	0.62	1.94	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:HIS:CG	1:A:69:LEU:N	0.62	2.68	105	7
1:A:15:LEU:HD11	1:A:29:LYS:CB	0.62	2.23	40	1
1:A:5:VAL:HG21	1:A:30:ILE:HD11	0.62	1.70	64	14
1:A:7:THR:HG21	1:A:34:GLU:CD	0.60	2.16	273	1
1:A:48:LYS:HE2	1:A:49:GLN:O	0.58	1.99	58	1
1:A:11:LYS:NZ	1:A:34:GLU:OE1	0.55	2.39	128	5
1:A:16:GLU:O	1:A:29:LYS:HE3	0.55	2.02	132	1
1:A:45:PHE:HB2	1:A:67:LEU:HD23	0.55	1.77	27	1
1:A:48:LYS:CE	1:A:59:TYR:CE1	0.55	2.89	143	1
1:A:48:LYS:NZ	1:A:51:GLU:OE2	0.55	2.40	134	2
1:A:27:LYS:HE3	1:A:52:ASP:OD1	0.54	2.02	65	1
1:A:16:GLU:OE1	1:A:16:GLU:HA	0.54	2.02	60	2
1:A:8:LEU:HD11	1:A:71:LEU:HD21	0.54	1.80	162	1
1:A:6:LYS:HE2	1:A:10:GLY:O	0.54	2.03	290	1
1:A:48:LYS:NZ	1:A:51:GLU:OE1	0.53	2.41	148	2
1:A:17:VAL:HG21	1:A:56:LEU:HD21	0.53	1.80	276	1
1:A:32:ASP:OD1	1:A:33:LYS:NZ	0.53	2.42	151	3
1:A:41:GLN:HA	1:A:69:LEU:HD11	0.53	1.78	37	1
1:A:1:MET:HG2	1:A:18:GLU:OE1	0.53	2.03	115	1
1:A:25:ASN:OD1	1:A:29:LYS:HE3	0.53	2.04	200	17
1:A:70:VAL:HG12	1:A:71:LEU:H	0.53	1.64	84	3
1:A:1:MET:N	1:A:18:GLU:OE2	0.53	2.41	57	14
1:A:15:LEU:HD23	1:A:15:LEU:N	0.52	2.18	282	1
1:A:8:LEU:HD13	1:A:70:VAL:HG23	0.52	1.81	229	1
1:A:1:MET:N	1:A:16:GLU:OE2	0.52	2.42	5	2
1:A:69:LEU:O	1:A:69:LEU:HD23	0.52	2.05	146	1
1:A:18:GLU:OE1	1:A:18:GLU:HA	0.52	2.05	116	7
1:A:67:LEU:HD12	1:A:67:LEU:N	0.52	2.19	121	16
1:A:30:ILE:HB	1:A:41:GLN:HE22	0.52	1.64	3	1
1:A:43:LEU:HD12	1:A:43:LEU:N	0.51	2.19	188	3
1:A:8:LEU:HD13	1:A:70:VAL:HG13	0.51	1.82	29	1
1:A:71:LEU:CD1	1:A:71:LEU:N	0.51	2.74	50	1
1:A:24:GLU:CD	1:A:27:LYS:HE3	0.51	2.26	117	1
1:A:36:ILE:N	1:A:36:ILE:HD13	0.51	2.21	236	5
1:A:49:GLN:HE21	1:A:51:GLU:CD	0.50	2.09	17	1
1:A:22:THR:O	1:A:26:VAL:HG23	0.50	2.05	195	2
1:A:15:LEU:HD22	1:A:15:LEU:N	0.50	2.21	61	1
1:A:33:LYS:HA	1:A:33:LYS:HE3	0.50	1.81	1	1
1:A:11:LYS:NZ	1:A:34:GLU:OE2	0.50	2.39	79	8
1:A:24:GLU:OE1	1:A:27:LYS:CE	0.50	2.59	283	1
1:A:1:MET:HG2	1:A:17:VAL:O	0.49	2.07	260	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:VAL:HG12	1:A:29:LYS:NZ	0.49	2.22	23	1
1:A:63:LYS:HZ3	1:A:64:GLU:CD	0.49	2.10	66	1
1:A:7:THR:HG21	1:A:34:GLU:OE1	0.49	2.08	273	1
1:A:17:VAL:HG21	1:A:56:LEU:CD1	0.49	2.37	169	2
1:A:68:HIS:CD2	1:A:69:LEU:H	0.49	2.25	34	1
1:A:23:ILE:HA	1:A:26:VAL:HG12	0.49	1.85	21	1
1:A:50:LEU:HD22	1:A:59:TYR:CD1	0.49	2.43	22	1
1:A:23:ILE:N	1:A:23:ILE:HD13	0.48	2.23	135	3
1:A:43:LEU:HB3	1:A:50:LEU:HD12	0.48	1.86	40	1
1:A:50:LEU:HD22	1:A:59:TYR:CD2	0.48	2.43	61	5
1:A:25:ASN:OD1	1:A:29:LYS:CE	0.48	2.61	156	1
1:A:27:LYS:NZ	1:A:52:ASP:OD2	0.48	2.46	242	6
1:A:50:LEU:HD22	1:A:59:TYR:CG	0.48	2.44	19	3
1:A:15:LEU:HD11	1:A:29:LYS:HB3	0.48	1.84	40	1
1:A:16:GLU:N	1:A:16:GLU:CD	0.48	2.67	128	1
1:A:15:LEU:HD11	1:A:29:LYS:HB2	0.48	1.85	40	1
1:A:3:ILE:HG12	1:A:17:VAL:HG21	0.48	1.85	19	2
1:A:27:LYS:HZ2	1:A:52:ASP:CG	0.48	2.12	9	1
1:A:25:ASN:OD1	1:A:29:LYS:HE2	0.48	2.08	206	4
1:A:45:PHE:CD2	1:A:61:ILE:HD11	0.47	2.43	99	1
1:A:36:ILE:HD11	1:A:69:LEU:HD21	0.47	1.86	190	1
1:A:44:ILE:N	1:A:44:ILE:HD13	0.47	2.25	6	2
1:A:61:ILE:HD13	1:A:67:LEU:HD21	0.47	1.87	77	1
1:A:44:ILE:HD13	1:A:44:ILE:H	0.47	1.69	6	1
1:A:15:LEU:HD11	1:A:30:ILE:HG12	0.47	1.86	125	1
1:A:5:VAL:HG22	1:A:67:LEU:HB2	0.47	1.85	235	3
1:A:44:ILE:HA	1:A:48:LYS:O	0.47	2.09	123	2
1:A:8:LEU:HD22	1:A:71:LEU:H	0.47	1.69	184	1
1:A:27:LYS:HE3	1:A:41:GLN:HB2	0.47	1.86	57	1
1:A:8:LEU:HD23	1:A:8:LEU:H	0.47	1.70	203	1
1:A:17:VAL:HG12	1:A:21:ASP:OD2	0.46	2.10	6	1
1:A:63:LYS:CE	1:A:64:GLU:OE2	0.46	2.63	203	1
1:A:62:GLN:NE2	1:A:62:GLN:H	0.46	2.08	293	1
1:A:1:MET:N	1:A:16:GLU:OE1	0.46	2.46	132	3
1:A:39:ASP:OD2	1:A:40:GLN:NE2	0.46	2.49	289	1
1:A:56:LEU:HD22	1:A:61:ILE:HG21	0.46	1.86	3	1
1:A:54:ARG:NH1	1:A:58:ASP:OD1	0.46	2.49	12	1
1:A:48:LYS:NZ	1:A:59:TYR:HA	0.46	2.26	22	1
1:A:63:LYS:NZ	1:A:64:GLU:CD	0.46	2.69	66	1
1:A:45:PHE:CE2	1:A:61:ILE:HD13	0.46	2.45	147	1
1:A:8:LEU:O	1:A:8:LEU:HD23	0.46	2.10	234	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:LEU:CD1	1:A:67:LEU:N	0.46	2.79	144	1
1:A:16:GLU:H	1:A:16:GLU:CD	0.46	2.13	185	1
1:A:13:ILE:HG22	1:A:14:THR:N	0.45	2.25	3	1
1:A:61:ILE:HD13	1:A:67:LEU:HD11	0.45	1.87	14	1
1:A:32:ASP:OD2	1:A:33:LYS:NZ	0.45	2.48	147	4
1:A:12:THR:C	1:A:13:ILE:CG2	0.45	2.85	78	1
1:A:61:ILE:CD1	1:A:67:LEU:HD11	0.45	2.40	120	1
1:A:27:LYS:HE2	1:A:52:ASP:OD1	0.45	2.11	69	1
1:A:17:VAL:HG12	1:A:29:LYS:HZ2	0.45	1.72	23	1
1:A:43:LEU:HD23	1:A:68:HIS:O	0.45	2.12	84	1
1:A:1:MET:N	1:A:17:VAL:O	0.45	2.47	236	1
1:A:63:LYS:HD2	1:A:63:LYS:C	0.45	2.32	45	1
1:A:23:ILE:HG21	1:A:50:LEU:HB3	0.45	1.87	100	1
1:A:71:LEU:HD12	1:A:71:LEU:N	0.45	2.26	229	2
1:A:70:VAL:C	1:A:71:LEU:HD12	0.45	2.32	208	1
1:A:27:LYS:CE	1:A:38:PRO:O	0.45	2.64	111	1
1:A:31:GLN:HE21	1:A:32:ASP:N	0.45	2.10	98	1
1:A:63:LYS:HE3	1:A:64:GLU:OE2	0.45	2.12	242	1
1:A:13:ILE:HG12	1:A:34:GLU:HG3	0.45	1.88	191	1
1:A:50:LEU:HD23	1:A:59:TYR:CD2	0.44	2.46	116	1
1:A:59:TYR:O	1:A:60:ASN:C	0.44	2.54	157	1
1:A:47:GLY:C	1:A:48:LYS:HG3	0.44	2.33	248	1
1:A:45:PHE:CD2	1:A:61:ILE:HD13	0.44	2.46	64	1
1:A:68:HIS:N	1:A:68:HIS:CD2	0.44	2.79	106	1
1:A:25:ASN:OD1	1:A:29:LYS:NZ	0.44	2.51	112	1
1:A:21:ASP:OD2	1:A:29:LYS:NZ	0.44	2.50	285	2
1:A:11:LYS:HE2	1:A:34:GLU:OE2	0.44	2.11	64	1
1:A:7:THR:HG23	1:A:69:LEU:HD23	0.44	1.90	196	1
1:A:46:ALA:O	1:A:48:LYS:HE2	0.44	2.12	51	1
1:A:1:MET:N	1:A:18:GLU:OE1	0.44	2.51	58	1
1:A:27:LYS:NZ	1:A:52:ASP:OD1	0.44	2.50	78	2
1:A:54:ARG:HH11	1:A:54:ARG:HG3	0.44	1.72	90	1
1:A:54:ARG:HD2	1:A:59:TYR:CZ	0.44	2.47	104	1
1:A:23:ILE:O	1:A:26:VAL:HG23	0.44	2.12	146	1
1:A:5:VAL:HG21	1:A:30:ILE:CD1	0.44	2.42	77	1
1:A:67:LEU:N	1:A:67:LEU:CD1	0.44	2.80	283	2
1:A:23:ILE:HB	1:A:52:ASP:HA	0.44	1.89	267	2
1:A:71:LEU:N	1:A:71:LEU:HD12	0.44	2.28	50	1
1:A:32:ASP:OD1	1:A:33:LYS:HE2	0.44	2.13	123	1
1:A:63:LYS:HB2	1:A:64:GLU:OE2	0.44	2.13	9	1
1:A:23:ILE:HG13	1:A:50:LEU:HD13	0.43	1.89	36	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:GLN:HE21	1:A:51:GLU:HG2	0.43	1.71	199	1
1:A:32:ASP:OD2	1:A:33:LYS:CE	0.43	2.67	50	1
1:A:19:PRO:HA	1:A:56:LEU:HD22	0.43	1.90	131	1
1:A:27:LYS:HZ3	1:A:52:ASP:CG	0.43	2.17	264	1
1:A:63:LYS:O	1:A:63:LYS:HG3	0.43	2.14	234	1
1:A:16:GLU:OE1	1:A:33:LYS:NZ	0.43	2.52	3	1
1:A:43:LEU:HD22	1:A:67:LEU:HD23	0.43	1.91	36	1
1:A:3:ILE:HG12	1:A:17:VAL:CG2	0.43	2.43	84	1
1:A:24:GLU:HA	1:A:27:LYS:HE2	0.43	1.89	3	1
1:A:68:HIS:CD2	1:A:68:HIS:N	0.43	2.87	255	3
1:A:68:HIS:CD2	1:A:69:LEU:N	0.43	2.87	71	2
1:A:43:LEU:C	1:A:44:ILE:CG2	0.42	2.86	53	2
1:A:67:LEU:N	1:A:67:LEU:CD2	0.42	2.81	76	1
1:A:23:ILE:HG21	1:A:50:LEU:HB2	0.42	1.90	124	1
1:A:44:ILE:HG22	1:A:68:HIS:ND1	0.42	2.30	11	1
1:A:5:VAL:HG21	1:A:43:LEU:HD21	0.42	1.91	31	1
1:A:63:LYS:CE	1:A:64:GLU:OE1	0.42	2.67	57	1
1:A:1:MET:CA	1:A:16:GLU:OE1	0.42	2.68	130	1
1:A:48:LYS:HD3	1:A:48:LYS:C	0.42	2.34	93	1
1:A:27:LYS:CE	1:A:52:ASP:OD1	0.42	2.67	10	1
1:A:63:LYS:HD2	1:A:63:LYS:O	0.42	2.14	67	1
1:A:67:LEU:N	1:A:67:LEU:HD22	0.42	2.29	76	1
1:A:51:GLU:CD	1:A:54:ARG:HE	0.42	2.18	299	1
1:A:23:ILE:CD1	1:A:56:LEU:HD12	0.42	2.44	29	1
1:A:23:ILE:HD12	1:A:54:ARG:O	0.42	2.14	56	1
1:A:8:LEU:H	1:A:8:LEU:CD2	0.42	2.27	203	1
1:A:21:ASP:O	1:A:56:LEU:HD13	0.42	2.15	291	1
1:A:27:LYS:HE2	1:A:38:PRO:O	0.42	2.14	48	1
1:A:50:LEU:HD22	1:A:59:TYR:CE2	0.42	2.49	25	1
1:A:27:LYS:HE2	1:A:38:PRO:HB3	0.42	1.91	185	1
1:A:18:GLU:HB3	1:A:19:PRO:CD	0.41	2.44	39	1
1:A:27:LYS:HE3	1:A:41:GLN:CB	0.41	2.45	57	1
1:A:24:GLU:OE1	1:A:24:GLU:HA	0.41	2.15	125	1
1:A:45:PHE:C	1:A:47:GLY:N	0.41	2.72	85	1
1:A:23:ILE:HA	1:A:26:VAL:HG22	0.41	1.92	124	1
1:A:5:VAL:HB	1:A:13:ILE:HD12	0.41	1.91	223	1
1:A:6:LYS:CE	1:A:12:THR:OG1	0.41	2.68	18	1
1:A:51:GLU:OE1	1:A:54:ARG:NH2	0.41	2.52	200	2
1:A:18:GLU:O	1:A:21:ASP:HB2	0.41	2.16	293	1
1:A:50:LEU:CD2	1:A:59:TYR:CD1	0.41	3.04	95	1
1:A:11:LYS:HE3	1:A:34:GLU:OE2	0.41	2.14	142	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:ILE:HG22	1:A:49:GLN:HA	0.41	1.93	6	2
1:A:12:THR:C	1:A:13:ILE:HG13	0.41	2.36	7	1
1:A:54:ARG:HD3	1:A:58:ASP:OD2	0.41	2.16	115	2
1:A:18:GLU:OE1	1:A:19:PRO:HD3	0.41	2.16	287	1
1:A:22:THR:HA	1:A:55:THR:HA	0.41	1.91	70	1
1:A:12:THR:C	1:A:13:ILE:HD12	0.41	2.36	150	1
1:A:33:LYS:HA	1:A:33:LYS:NZ	0.41	2.31	67	1
1:A:54:ARG:N	1:A:54:ARG:HD3	0.41	2.30	98	1
1:A:71:LEU:HD22	1:A:71:LEU:N	0.41	2.31	136	1
1:A:44:ILE:HD13	1:A:49:GLN:HA	0.41	1.93	94	1
1:A:23:ILE:HG23	1:A:43:LEU:HD12	0.41	1.93	187	1
1:A:39:ASP:C	1:A:39:ASP:OD1	0.40	2.60	29	1
1:A:50:LEU:HD22	1:A:59:TYR:CE1	0.40	2.52	63	1
1:A:66:THR:C	1:A:67:LEU:HD22	0.40	2.37	76	1
1:A:1:MET:SD	1:A:1:MET:C	0.40	3.00	44	1
1:A:40:GLN:HA	1:A:40:GLN:NE2	0.40	2.31	123	1
1:A:11:LYS:HZ1	1:A:34:GLU:CD	0.40	2.19	25	1
1:A:49:GLN:HG2	1:A:49:GLN:O	0.40	2.16	256	1
1:A:18:GLU:HA	1:A:18:GLU:OE1	0.40	2.17	134	1
1:A:36:ILE:N	1:A:36:ILE:CD1	0.40	2.84	236	1
1:A:55:THR:O	1:A:58:ASP:HB2	0.40	2.17	253	1
1:A:62:GLN:O	1:A:63:LYS:C	0.40	2.60	16	1
1:A:1:MET:C	1:A:16:GLU:OE2	0.40	2.60	49	1
1:A:7:THR:CG2	1:A:13:ILE:HD12	0.40	2.46	67	1
1:A:37:PRO:HB2	1:A:38:PRO:HD2	0.40	1.92	71	1
1:A:27:LYS:HE2	1:A:41:GLN:HB2	0.40	1.93	206	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%)	67±2 (96±3%)	3±2 (4±2%)	0±1 (0±1%)	38	78
All	All	21070/22876 (92%)	20213 (96%)	777 (4%)	80 (0%)	38	78

All 26 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

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

6.3.2 Protein sidechains (i)

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

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

All 65 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	63	LYS	82
1	A	32	ASP	70
1	A	1	MET	67
1	A	52	ASP	64
1	A	9	THR	55
1	A	60	ASN	54
1	A	70	VAL	52
1	A	26	VAL	51
1	A	31	GLN	51
1	A	36	ILE	51
1	A	23	ILE	49
1	A	39	ASP	43
1	A	71	LEU	40
1	A	21	ASP	39
1	A	22	THR	39
1	A	67	LEU	39
1	A	13	ILE	37
1	A	16	GLU	31
1	A	43	LEU	29
1	A	33	LYS	28
1	A	8	LEU	27
1	A	56	LEU	25
1	A	64	GLU	23
1	A	69	LEU	23
1	A	18	GLU	22
1	A	57	SER	21
1	A	44	ILE	21
1	A	30	ILE	19
1	A	14	THR	18
1	A	49	GLN	17
1	A	54	ARG	17
1	A	20	SER	16
1	A	38	PRO	14
1	A	48	LYS	13
1	A	2	GLN	13
1	A	42	ARG	12
1	A	6	LYS	12
1	A	61	ILE	12
1	A	25	ASN	11
1	A	62	GLN	11
1	A	51	GLU	10
1	A	4	PHE	9
1	A	11	LYS	9

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Mol	Chain	Res	Type	Models (Total)
1	A	7	THR	9
1	A	12	THR	9
1	A	19	PRO	8
1	A	58	ASP	8
1	A	15	LEU	8
1	A	3	ILE	6
1	A	68	HIS	5
1	A	5	VAL	5
1	A	66	THR	4
1	A	65	SER	4
1	A	24	GLU	4
1	A	34	GLU	3
1	A	40	GLN	3
1	A	55	THR	2
1	A	41	GLN	2
1	A	29	LYS	2
1	A	17	VAL	2
1	A	50	LEU	2
1	A	27	LYS	1
1	A	59	TYR	1
1	A	37	PRO	1
1	A	45	PHE	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

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

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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

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

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	72	-0.22 ± 0.20	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	68	0.16 ± 0.26	None needed (< 0.5 ppm)
$^{13}C'$	72	-0.30 ± 0.12	None needed (< 0.5 ppm)
^{15}N	71	1.30 ± 0.22	Should be applied

7.1.3 Completeness of resonance assignments (i)

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

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

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

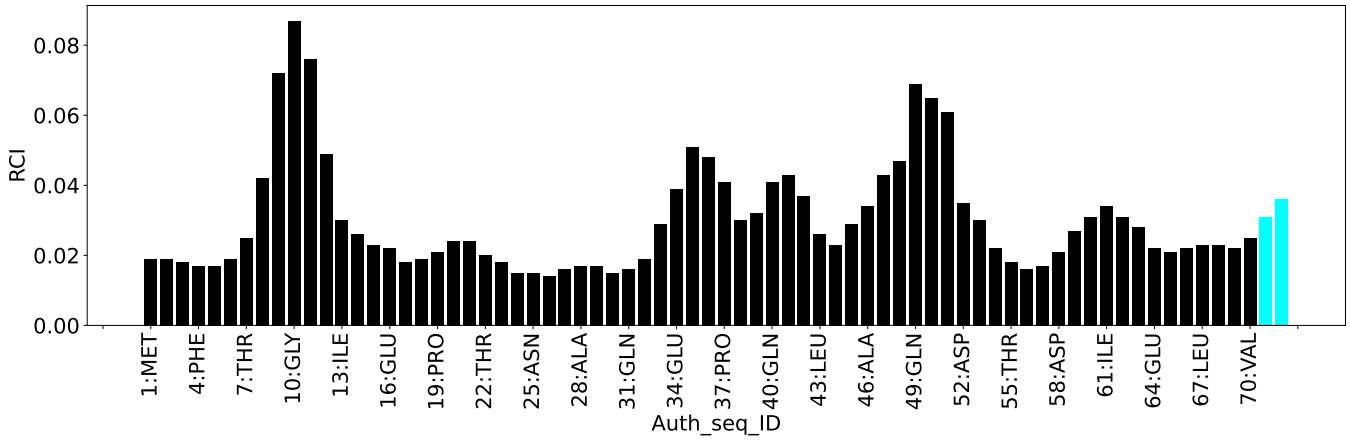
The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 39%, i.e. 423 atoms were assigned a chemical shift out of a possible 1071. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

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

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A: