



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 07:19 AM BST

PDB ID : 2NR2  
Title : The MUMO (minimal under-restraining minimal over-restraining) method for the determination of native states ensembles of proteins  
Authors : Richter, B.; Gsponer, J.; Varnai, P.; Salvatella, X.; Vendruscolo, M.  
Deposited on : 2006-11-01

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

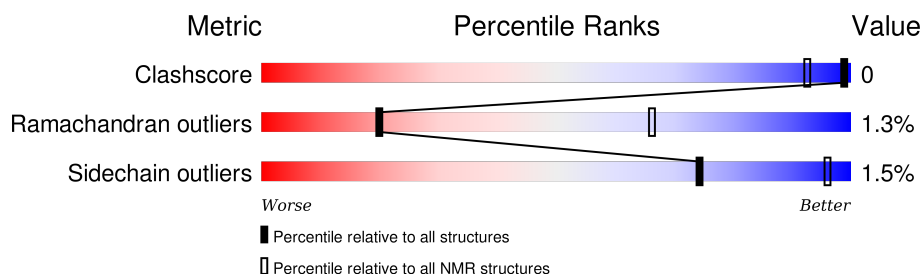
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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

Mol	Chain	Length	Quality of chain
1	A	76	 88% 5% 7%

## 2 Ensemble composition and analysis

This entry contains 144 models. Model 100 is the overall representative, medoid model (most similar to other models).

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)	0.36	100

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 18 clusters and 14 single-model clusters were found.

Cluster number	Models
1	1, 2, 6, 11, 13, 18, 22, 26, 27, 33, 37, 39, 41, 43, 45, 47, 56, 57, 58, 61, 87, 90, 102, 108, 110, 112, 115, 120, 125, 128, 133, 139, 140, 143
2	3, 7, 9, 10, 20, 25, 29, 31, 46, 49, 53, 60, 64, 71, 82, 83, 89, 114, 117, 118, 122, 134, 135, 136, 137, 141
3	8, 16, 35, 36, 54, 65, 66, 72, 84, 86, 103, 104, 105, 106, 124
4	23, 24, 42, 55, 91, 101, 107, 109, 119, 132
5	5, 30, 67, 69, 85, 88, 113, 131
6	4, 19, 21, 77, 111, 129
7	28, 32, 48, 70, 100, 130
8	50, 93, 98
9	15, 51, 127
10	17, 76, 78
11	14, 138
12	40, 44
13	73, 80
14	81, 96
15	68, 121
16	34, 94
17	52, 92
18	59, 142
Single-model clusters	12; 38; 62; 63; 74; 75; 79; 95; 97; 99; 116; 123; 126; 144

### 3 Entry composition [i](#)

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

- Molecule 1 is a protein called Ubiquitin.

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

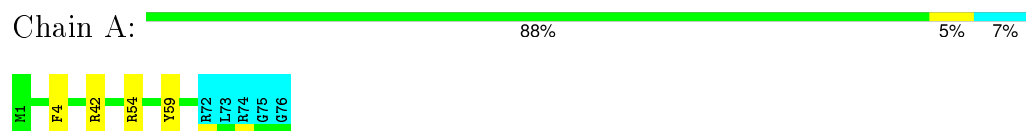


## 4 Residue-property plots [i](#)

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

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

- Molecule 1: Ubiquitin

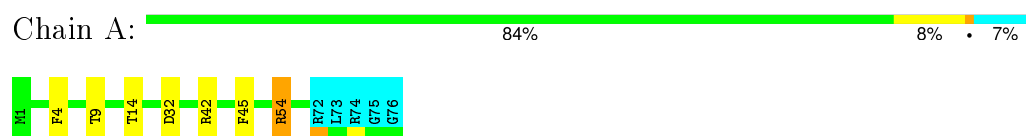


### 4.2 Scores per residue for each member of the ensemble

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

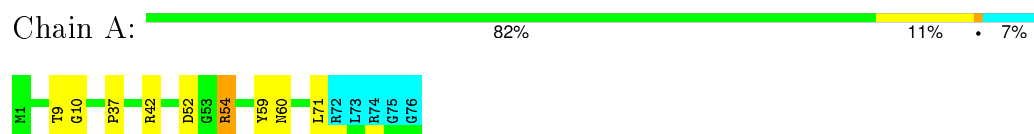
#### 4.2.1 Score per residue for model 1

- Molecule 1: Ubiquitin



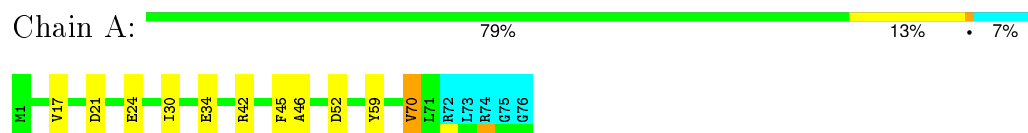
#### 4.2.2 Score per residue for model 2

- Molecule 1: Ubiquitin



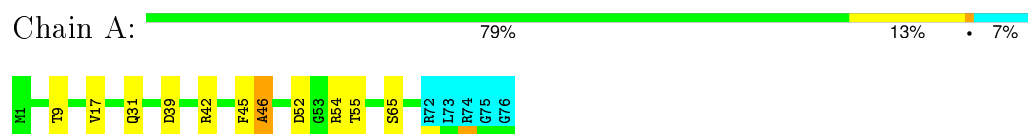
### 4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin



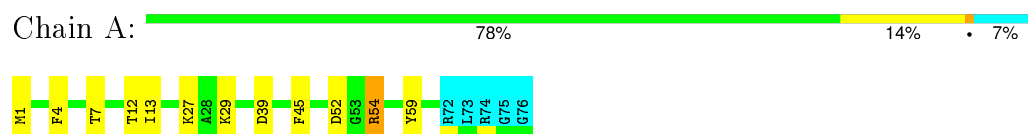
### 4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin



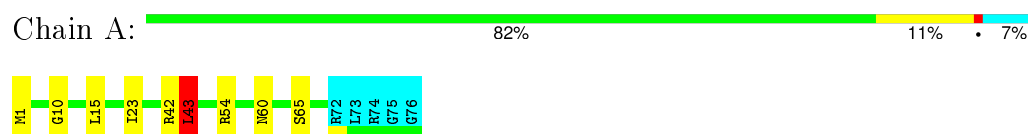
### 4.2.5 Score per residue for model 5

- Molecule 1: Ubiquitin



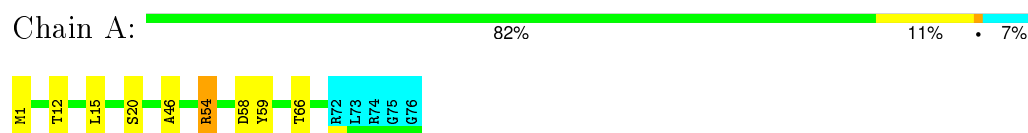
### 4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin



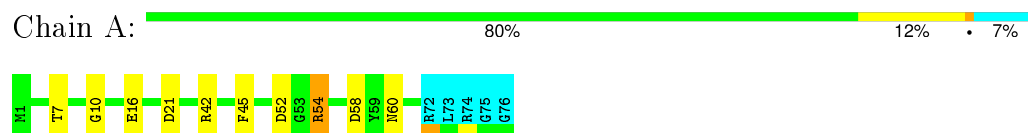
### 4.2.7 Score per residue for model 7

- Molecule 1: Ubiquitin



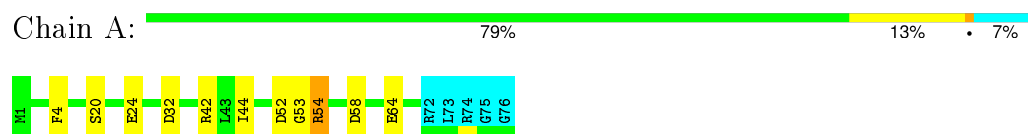
### 4.2.8 Score per residue for model 8

- Molecule 1: Ubiquitin



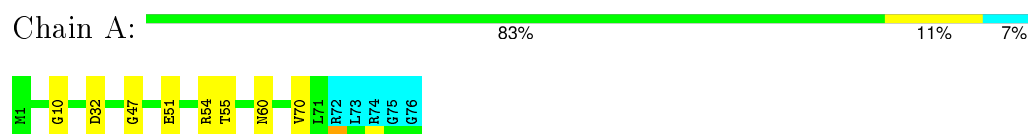
### 4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin



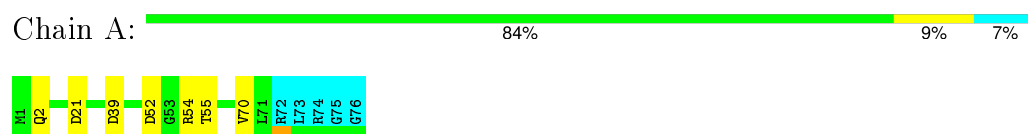
### 4.2.10 Score per residue for model 10

- Molecule 1: Ubiquitin



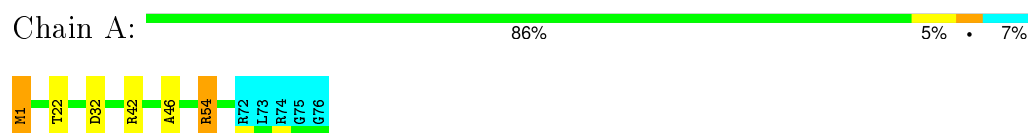
### 4.2.11 Score per residue for model 11

- Molecule 1: Ubiquitin



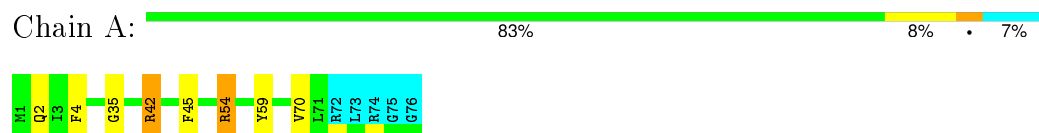
### 4.2.12 Score per residue for model 12

- Molecule 1: Ubiquitin



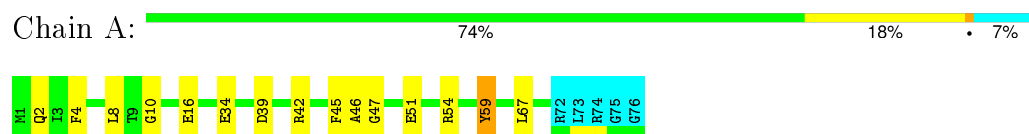
#### 4.2.13 Score per residue for model 13

- Molecule 1: Ubiquitin



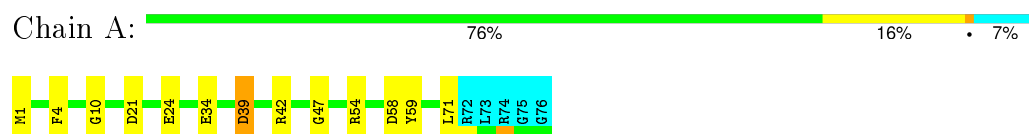
#### 4.2.14 Score per residue for model 14

- Molecule 1: Ubiquitin



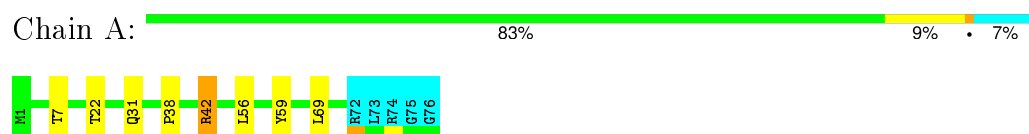
#### 4.2.15 Score per residue for model 15

- Molecule 1: Ubiquitin



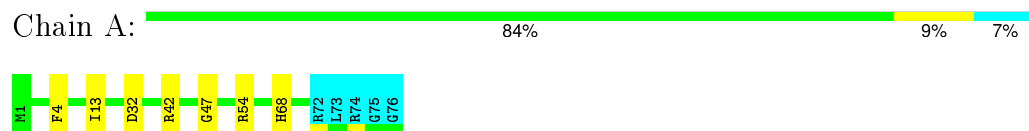
#### 4.2.16 Score per residue for model 16

- Molecule 1: Ubiquitin



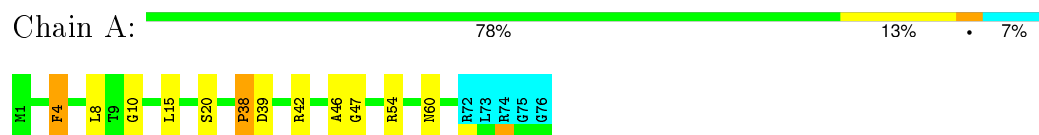
#### 4.2.17 Score per residue for model 17

- Molecule 1: Ubiquitin



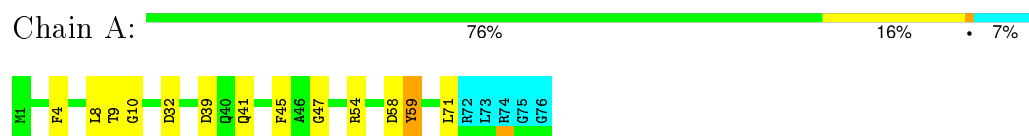
#### 4.2.18 Score per residue for model 18

- Molecule 1: Ubiquitin



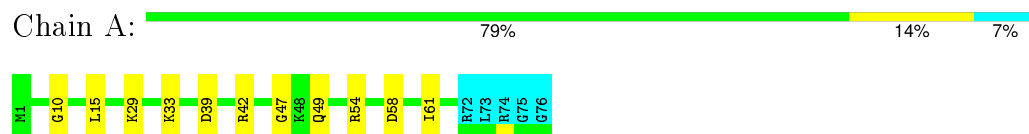
#### 4.2.19 Score per residue for model 19

- Molecule 1: Ubiquitin



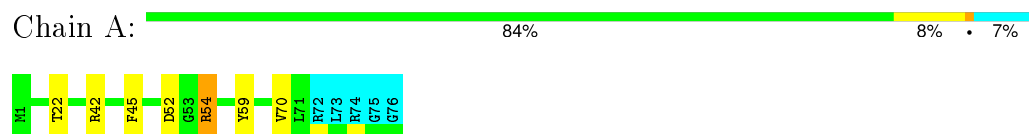
#### 4.2.20 Score per residue for model 20

- Molecule 1: Ubiquitin



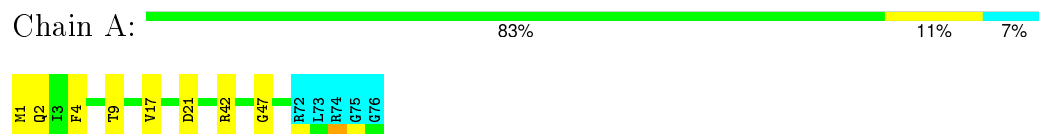
#### 4.2.21 Score per residue for model 21

- Molecule 1: Ubiquitin



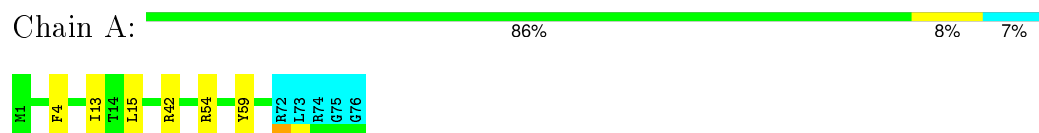
#### 4.2.22 Score per residue for model 22

- Molecule 1: Ubiquitin



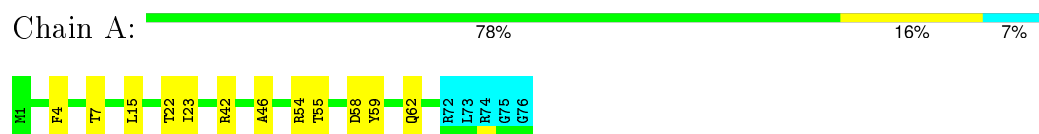
#### 4.2.23 Score per residue for model 23

- Molecule 1: Ubiquitin



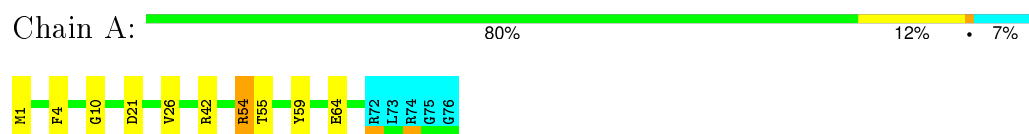
#### 4.2.24 Score per residue for model 24

- Molecule 1: Ubiquitin



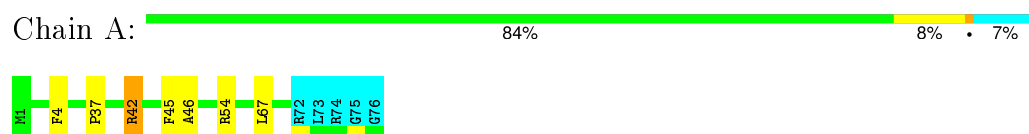
#### 4.2.25 Score per residue for model 25

- Molecule 1: Ubiquitin



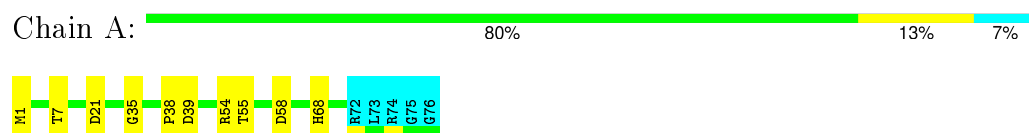
#### 4.2.26 Score per residue for model 26

- Molecule 1: Ubiquitin



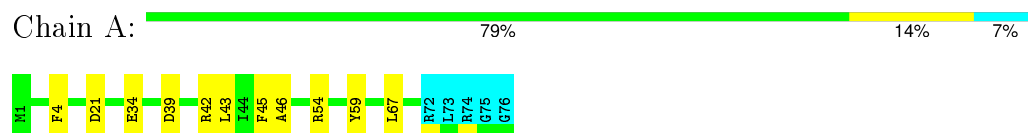
#### 4.2.27 Score per residue for model 27

- Molecule 1: Ubiquitin



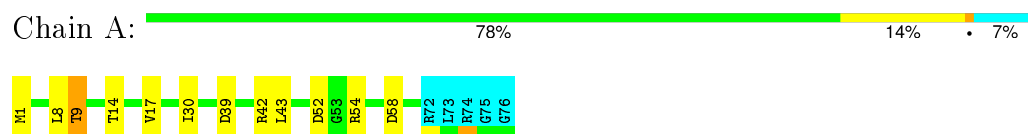
#### 4.2.28 Score per residue for model 28

- Molecule 1: Ubiquitin



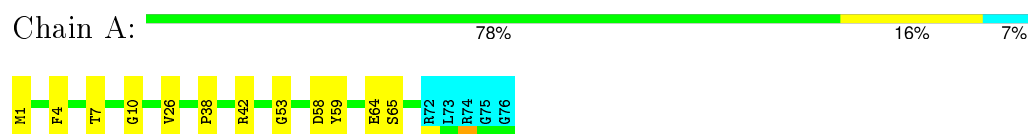
#### 4.2.29 Score per residue for model 29

- Molecule 1: Ubiquitin



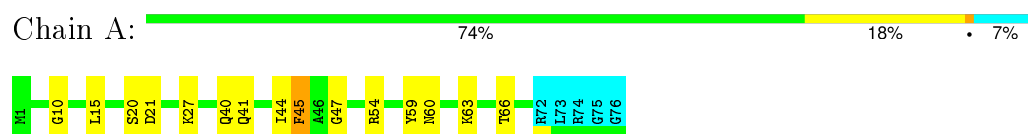
#### 4.2.30 Score per residue for model 30

- Molecule 1: Ubiquitin



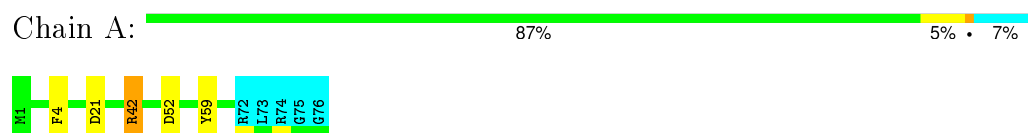
#### 4.2.31 Score per residue for model 31

- Molecule 1: Ubiquitin



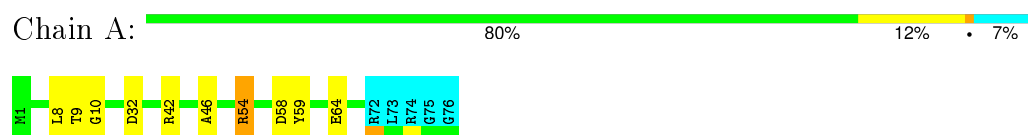
#### 4.2.32 Score per residue for model 32

- Molecule 1: Ubiquitin



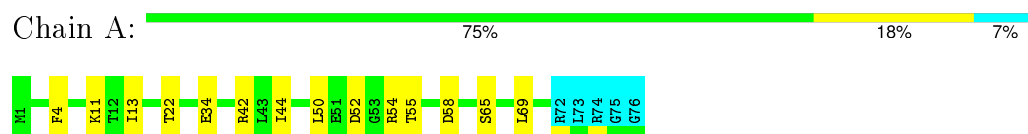
### 4.2.33 Score per residue for model 33

- Molecule 1: Ubiquitin



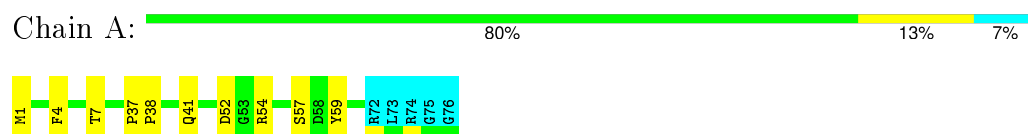
### 4.2.34 Score per residue for model 34

- Molecule 1: Ubiquitin



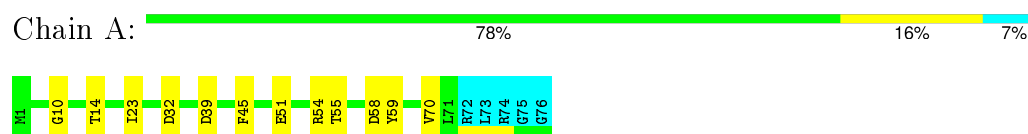
### 4.2.35 Score per residue for model 35

- Molecule 1: Ubiquitin



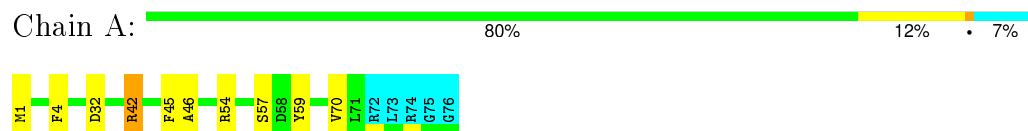
### 4.2.36 Score per residue for model 36

- Molecule 1: Ubiquitin



### 4.2.37 Score per residue for model 37

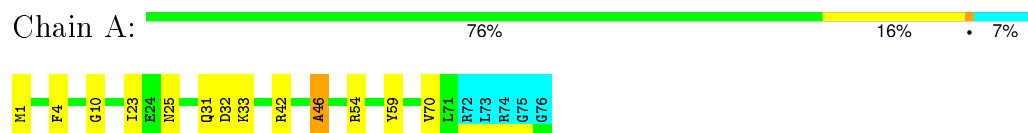
- Molecule 1: Ubiquitin





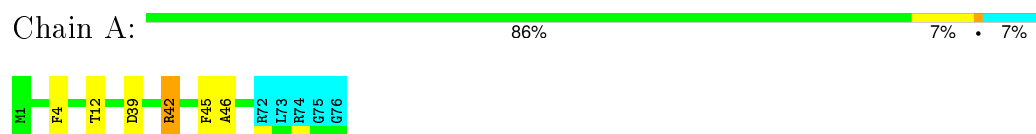
#### 4.2.38 Score per residue for model 38

- Molecule 1: Ubiquitin



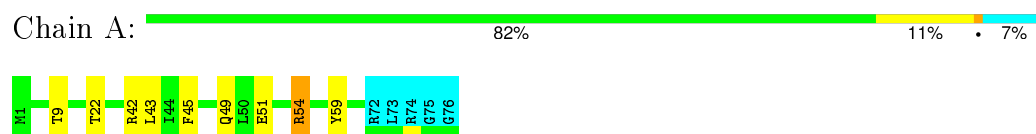
#### 4.2.39 Score per residue for model 39

- Molecule 1: Ubiquitin



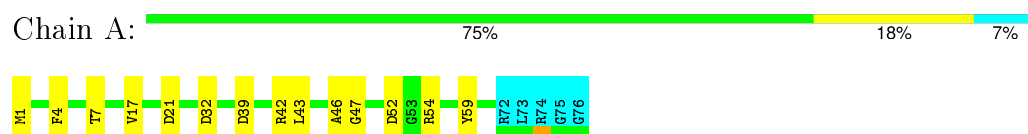
#### 4.2.40 Score per residue for model 40

- Molecule 1: Ubiquitin



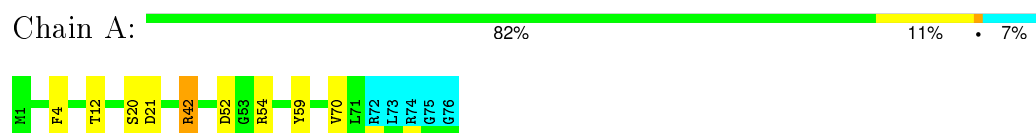
#### 4.2.41 Score per residue for model 41

- Molecule 1: Ubiquitin



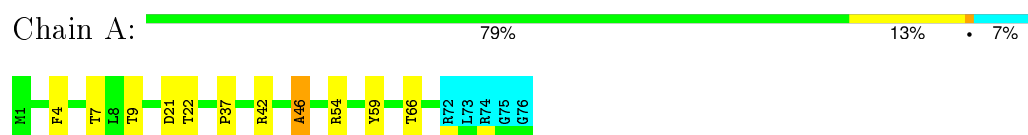
#### 4.2.42 Score per residue for model 42

- Molecule 1: Ubiquitin



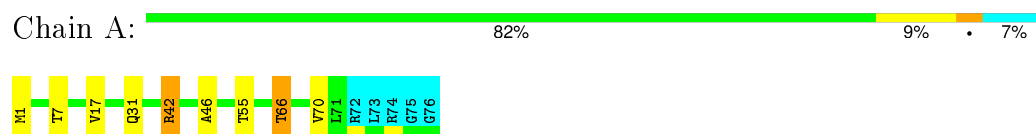
#### 4.2.43 Score per residue for model 43

- Molecule 1: Ubiquitin



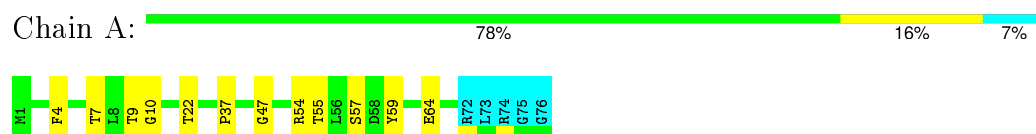
#### 4.2.44 Score per residue for model 44

- Molecule 1: Ubiquitin



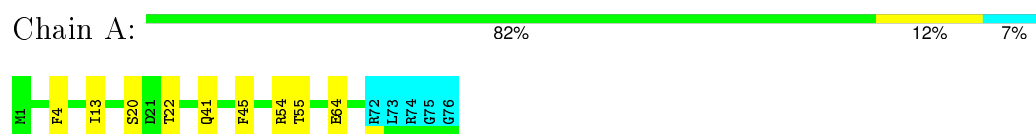
#### 4.2.45 Score per residue for model 45

- Molecule 1: Ubiquitin



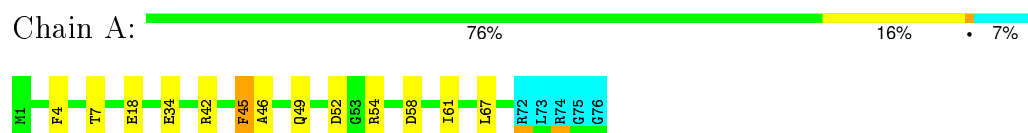
#### 4.2.46 Score per residue for model 46

- Molecule 1: Ubiquitin



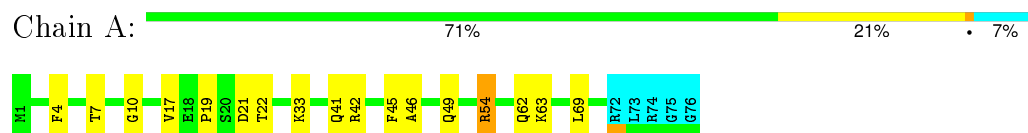
#### 4.2.47 Score per residue for model 47

- Molecule 1: Ubiquitin



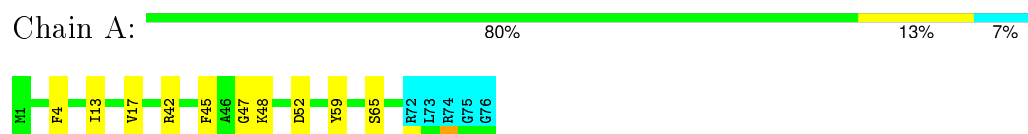
#### 4.2.48 Score per residue for model 48

- Molecule 1: Ubiquitin



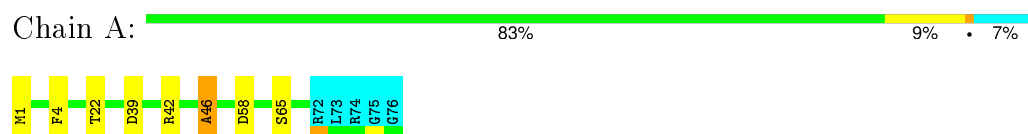
#### 4.2.49 Score per residue for model 49

- Molecule 1: Ubiquitin



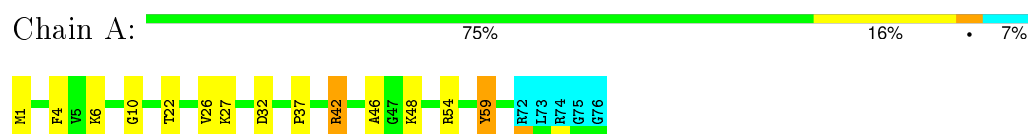
#### 4.2.50 Score per residue for model 50

- Molecule 1: Ubiquitin



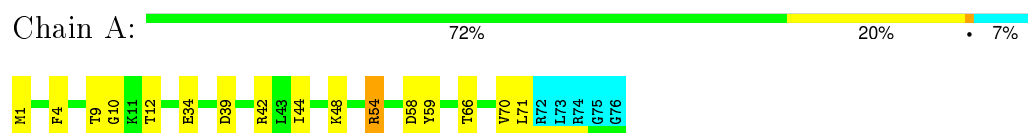
#### 4.2.51 Score per residue for model 51

- Molecule 1: Ubiquitin



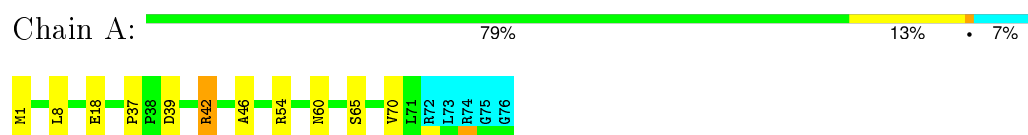
#### 4.2.52 Score per residue for model 52

- Molecule 1: Ubiquitin



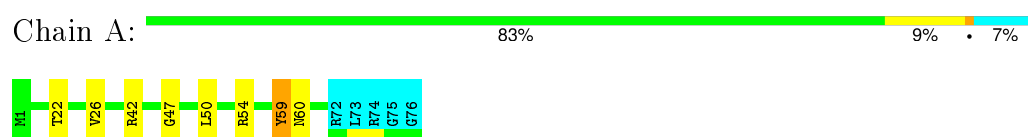
#### 4.2.53 Score per residue for model 53

- Molecule 1: Ubiquitin



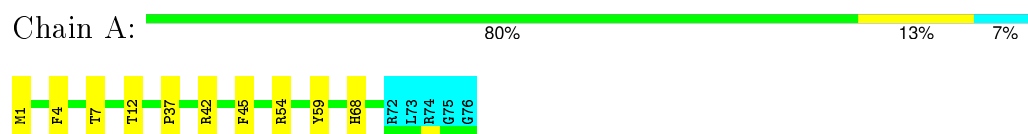
#### 4.2.54 Score per residue for model 54

- Molecule 1: Ubiquitin



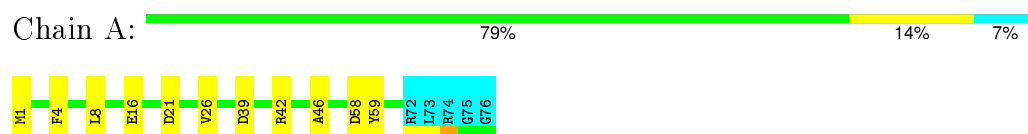
#### 4.2.55 Score per residue for model 55

- Molecule 1: Ubiquitin



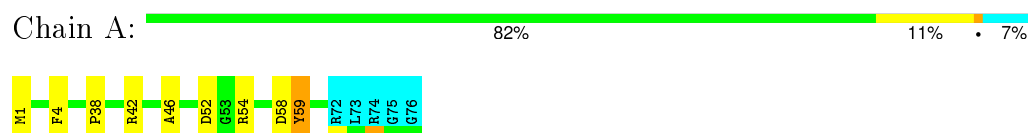
#### 4.2.56 Score per residue for model 56

- Molecule 1: Ubiquitin



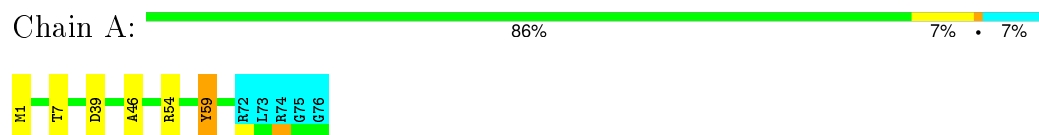
#### 4.2.57 Score per residue for model 57

- Molecule 1: Ubiquitin



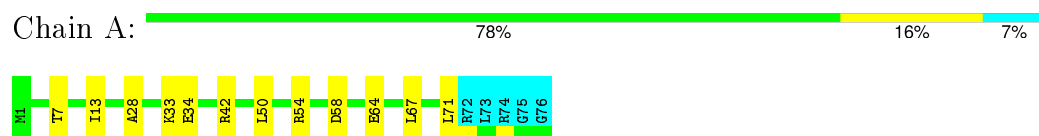
#### 4.2.58 Score per residue for model 58

- Molecule 1: Ubiquitin



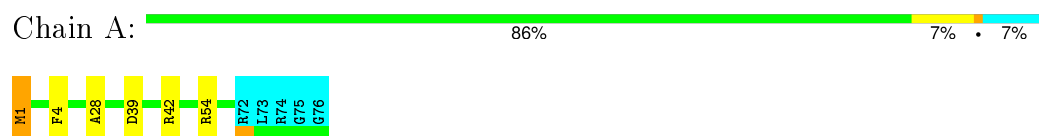
#### 4.2.59 Score per residue for model 59

- Molecule 1: Ubiquitin



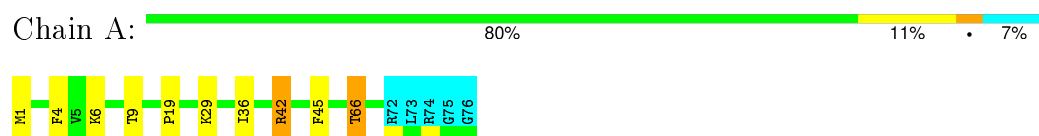
#### 4.2.60 Score per residue for model 60

- Molecule 1: Ubiquitin



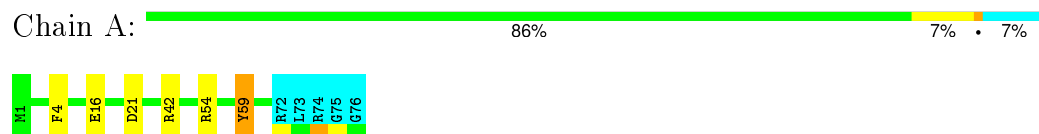
#### 4.2.61 Score per residue for model 61

- Molecule 1: Ubiquitin




#### 4.2.62 Score per residue for model 62

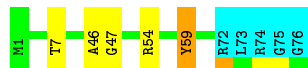
- Molecule 1: Ubiquitin



#### 4.2.63 Score per residue for model 63


- Molecule 1: Ubiquitin

Chain A:  87% 5% 7%



#### 4.2.64 Score per residue for model 64


- Molecule 1: Ubiquitin

Chain A:  84% 9% 7%



#### 4.2.65 Score per residue for model 65


- Molecule 1: Ubiquitin

Chain A:  86% 7% 7%



#### 4.2.66 Score per residue for model 66

- Molecule 1: Ubiquitin

Chain A:  79% 13% 7%



#### 4.2.67 Score per residue for model 67

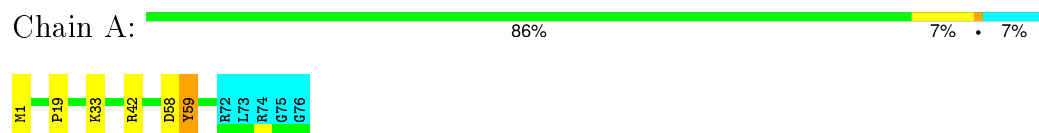
- Molecule 1: Ubiquitin

Chain A:  78% 16% 7%



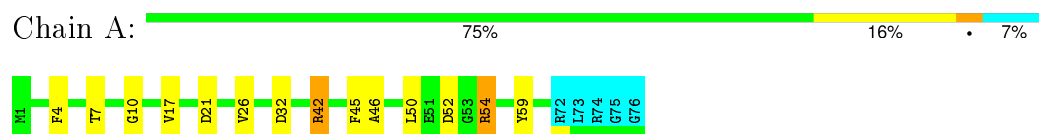
#### 4.2.68 Score per residue for model 68

- Molecule 1: Ubiquitin



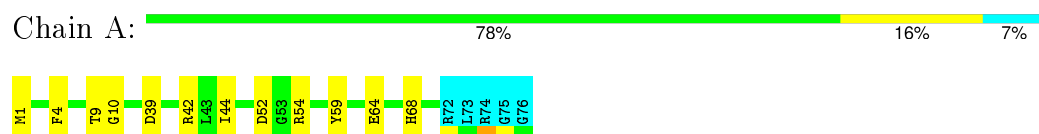
#### 4.2.69 Score per residue for model 69

- Molecule 1: Ubiquitin



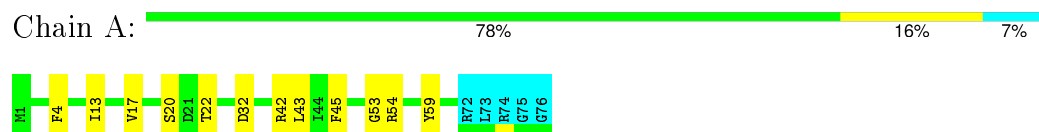
#### 4.2.70 Score per residue for model 70

- Molecule 1: Ubiquitin



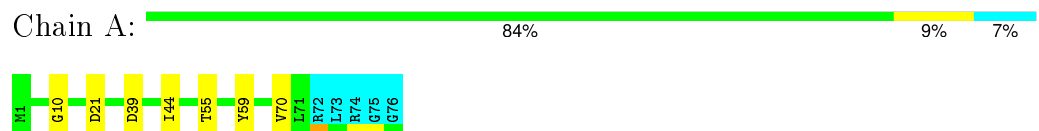
#### 4.2.71 Score per residue for model 71

- Molecule 1: Ubiquitin



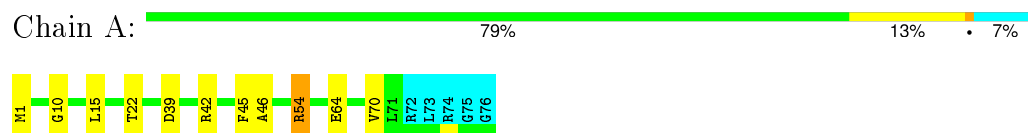
#### 4.2.72 Score per residue for model 72

- Molecule 1: Ubiquitin



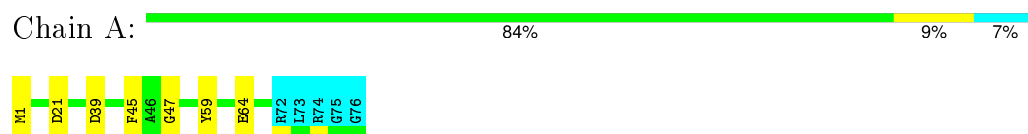
#### 4.2.73 Score per residue for model 73

- Molecule 1: Ubiquitin



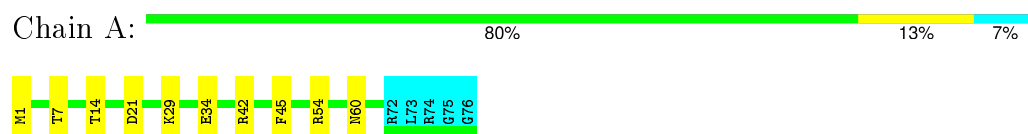
#### 4.2.74 Score per residue for model 74

- Molecule 1: Ubiquitin



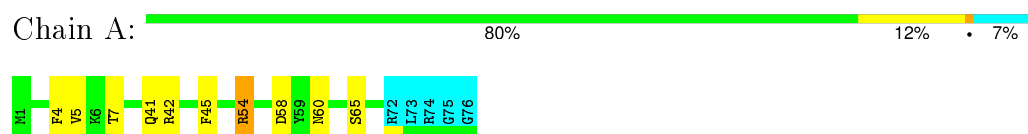
#### 4.2.75 Score per residue for model 75

- Molecule 1: Ubiquitin



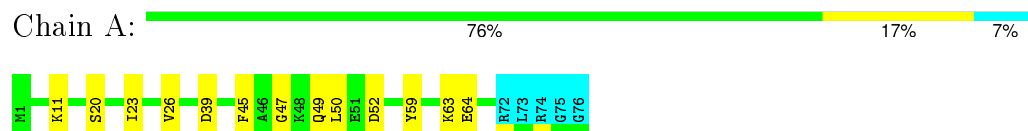
#### 4.2.76 Score per residue for model 76

- Molecule 1: Ubiquitin



#### 4.2.77 Score per residue for model 77

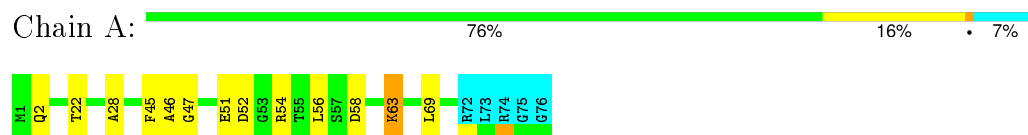
- Molecule 1: Ubiquitin





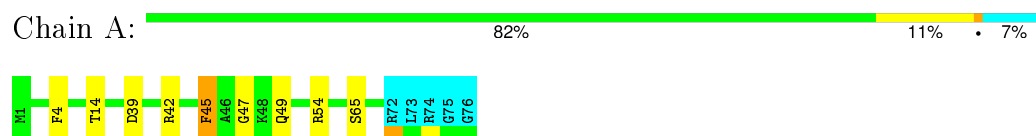
#### 4.2.78 Score per residue for model 78

- Molecule 1: Ubiquitin



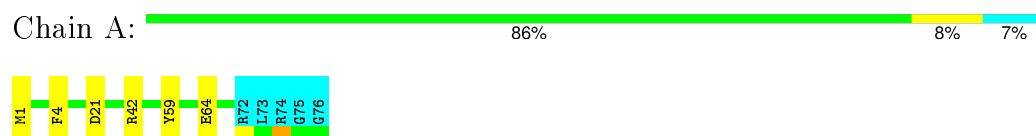
#### 4.2.79 Score per residue for model 79

- Molecule 1: Ubiquitin



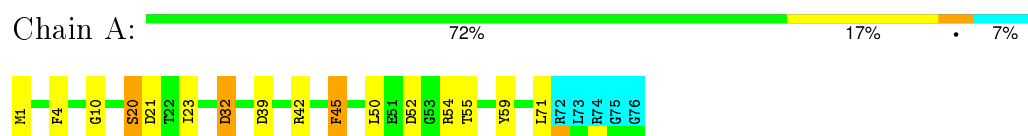
#### 4.2.80 Score per residue for model 80

- Molecule 1: Ubiquitin



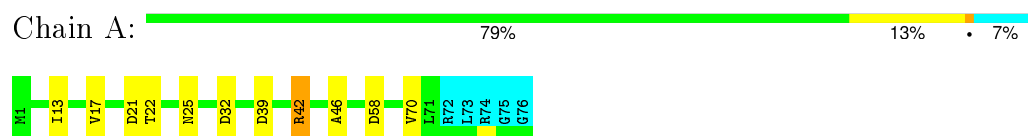
#### 4.2.81 Score per residue for model 81

- Molecule 1: Ubiquitin



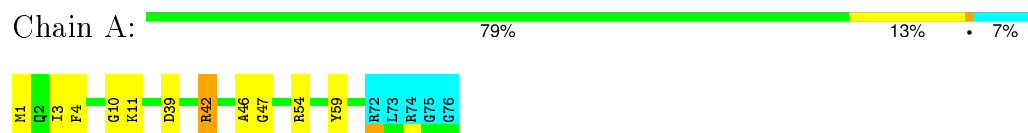
#### 4.2.82 Score per residue for model 82

- Molecule 1: Ubiquitin



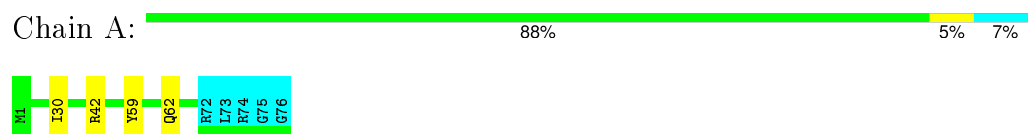
#### 4.2.83 Score per residue for model 83

- Molecule 1: Ubiquitin



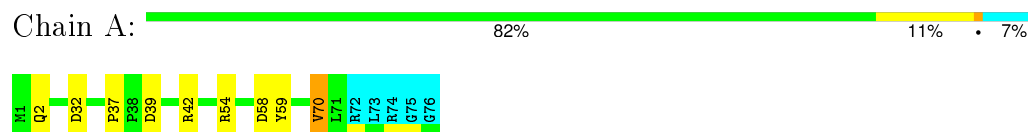
#### 4.2.84 Score per residue for model 84

- Molecule 1: Ubiquitin



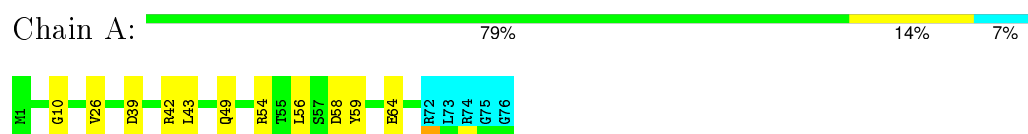
#### 4.2.85 Score per residue for model 85

- Molecule 1: Ubiquitin



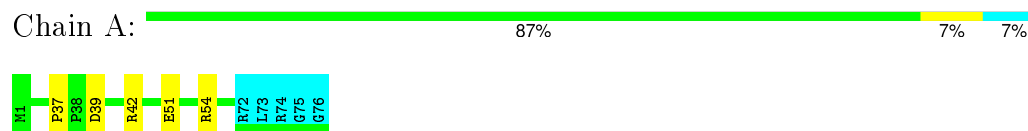
#### 4.2.86 Score per residue for model 86

- Molecule 1: Ubiquitin



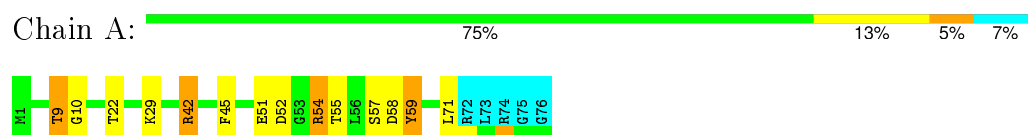
#### 4.2.87 Score per residue for model 87

- Molecule 1: Ubiquitin



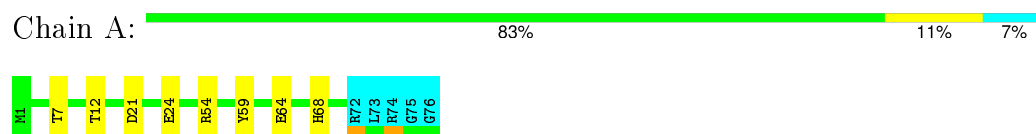
#### 4.2.88 Score per residue for model 88

- Molecule 1: Ubiquitin



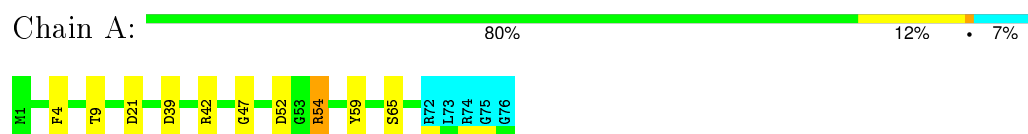
#### 4.2.89 Score per residue for model 89

- Molecule 1: Ubiquitin



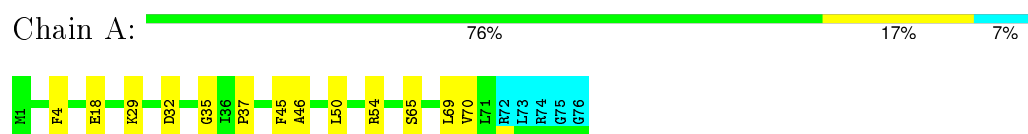
#### 4.2.90 Score per residue for model 90

- Molecule 1: Ubiquitin



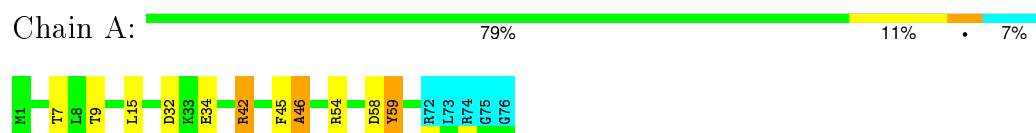
#### 4.2.91 Score per residue for model 91

- Molecule 1: Ubiquitin



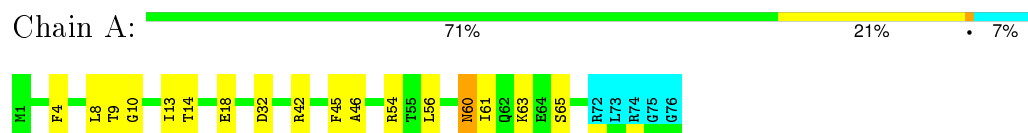
#### 4.2.92 Score per residue for model 92

- Molecule 1: Ubiquitin



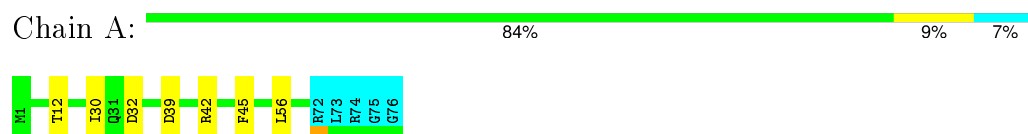
#### 4.2.93 Score per residue for model 93

- Molecule 1: Ubiquitin



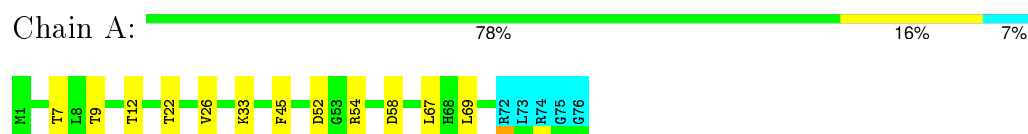
#### 4.2.94 Score per residue for model 94

- Molecule 1: Ubiquitin



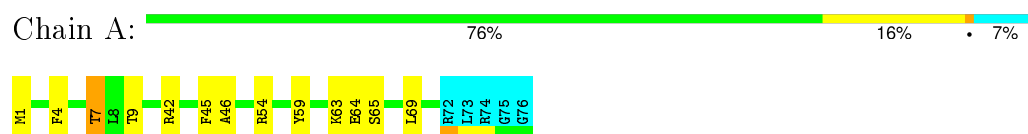
#### 4.2.95 Score per residue for model 95

- Molecule 1: Ubiquitin



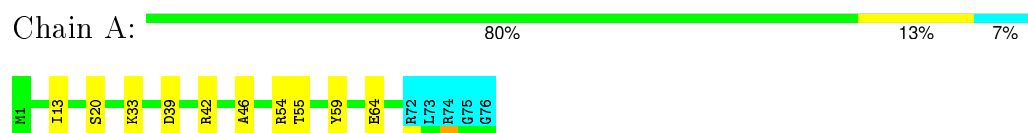
#### 4.2.96 Score per residue for model 96

- Molecule 1: Ubiquitin



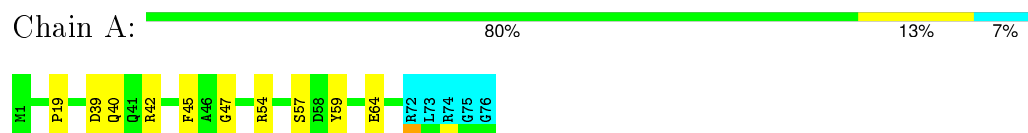
#### 4.2.97 Score per residue for model 97

- Molecule 1: Ubiquitin



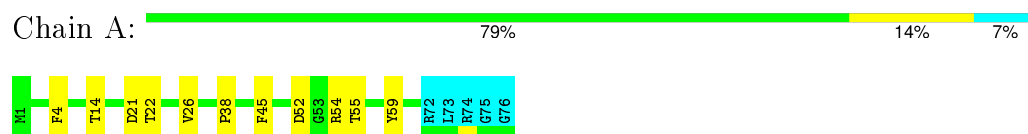
#### 4.2.98 Score per residue for model 98

- Molecule 1: Ubiquitin



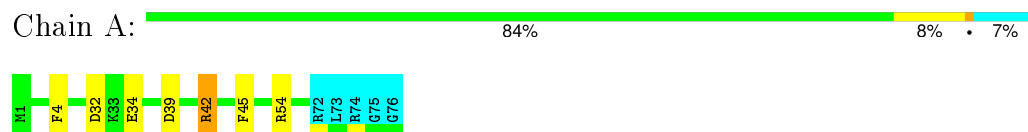
#### 4.2.99 Score per residue for model 99

- Molecule 1: Ubiquitin



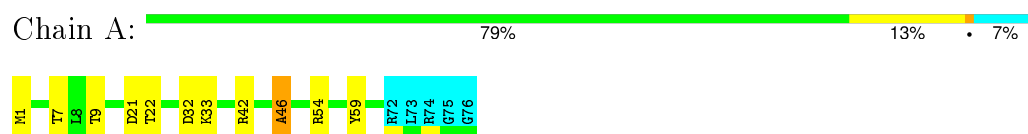
#### 4.2.100 Score per residue for model 100 (medoid)

- Molecule 1: Ubiquitin



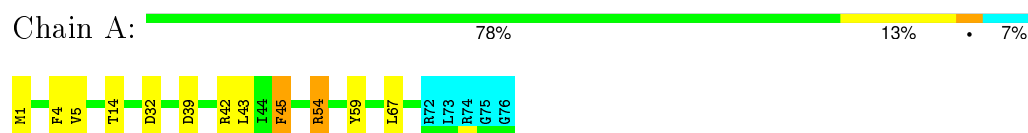
#### 4.2.101 Score per residue for model 101

- Molecule 1: Ubiquitin



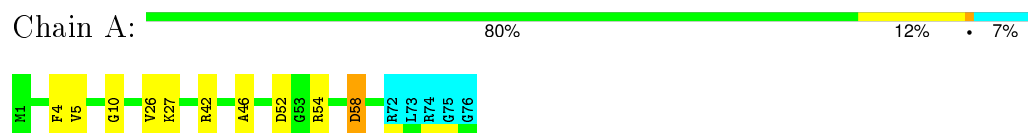
#### 4.2.102 Score per residue for model 102

- Molecule 1: Ubiquitin



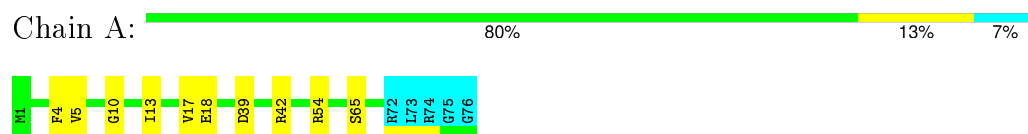
### 4.2.103 Score per residue for model 103

- Molecule 1: Ubiquitin



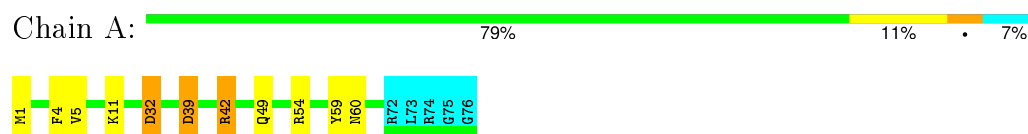
### 4.2.104 Score per residue for model 104

- Molecule 1: Ubiquitin



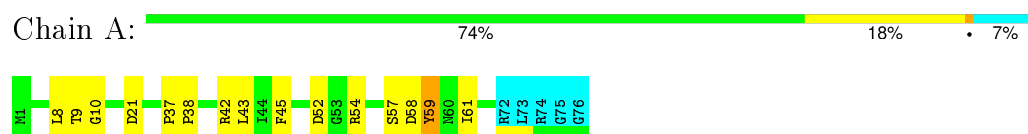
### 4.2.105 Score per residue for model 105

- Molecule 1: Ubiquitin



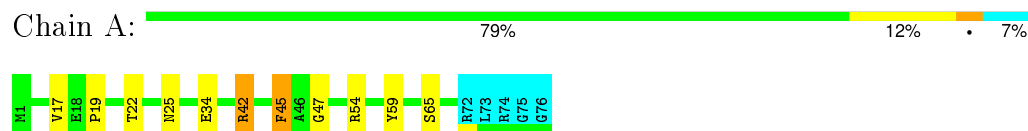
### 4.2.106 Score per residue for model 106

- Molecule 1: Ubiquitin



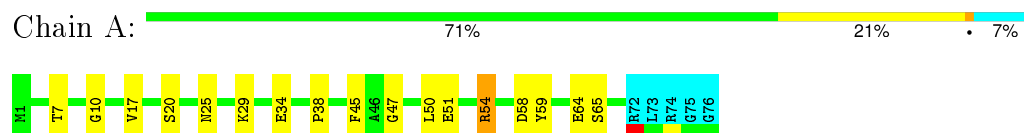
### 4.2.107 Score per residue for model 107

- Molecule 1: Ubiquitin



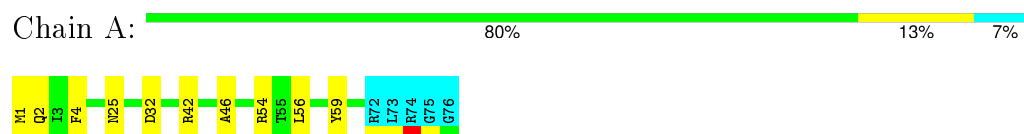
#### 4.2.108 Score per residue for model 108

- Molecule 1: Ubiquitin



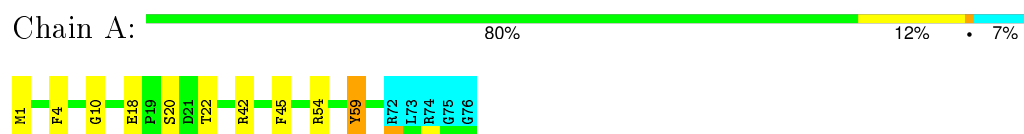
#### 4.2.109 Score per residue for model 109

- Molecule 1: Ubiquitin



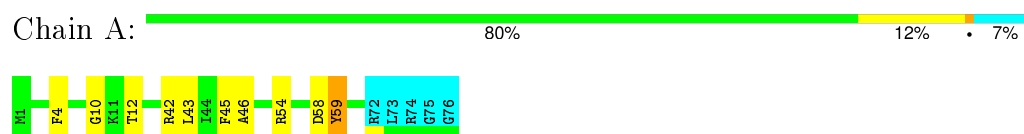
#### 4.2.110 Score per residue for model 110

- Molecule 1: Ubiquitin



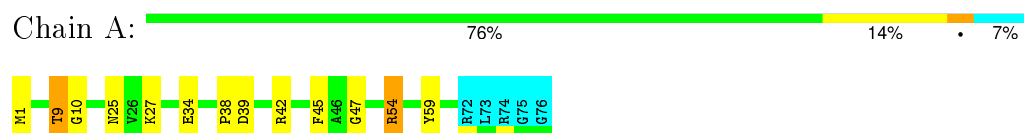
#### 4.2.111 Score per residue for model 111

- Molecule 1: Ubiquitin



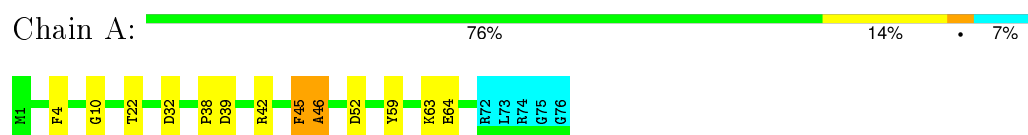
#### 4.2.112 Score per residue for model 112

- Molecule 1: Ubiquitin



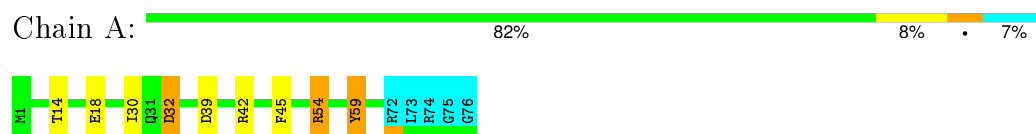
#### 4.2.113 Score per residue for model 113

- Molecule 1: Ubiquitin



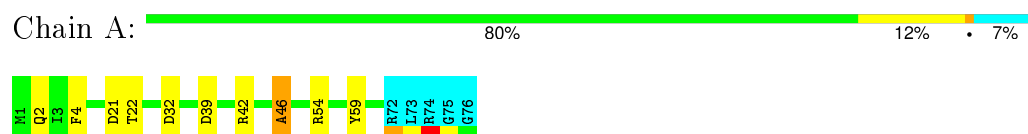
#### 4.2.114 Score per residue for model 114

- Molecule 1: Ubiquitin



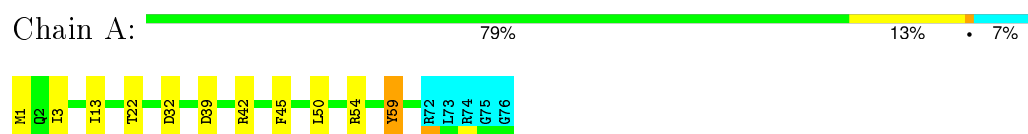
#### 4.2.115 Score per residue for model 115

- Molecule 1: Ubiquitin



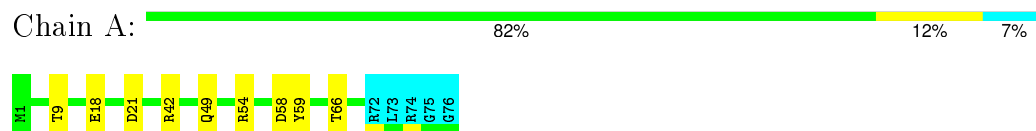
#### 4.2.116 Score per residue for model 116

- Molecule 1: Ubiquitin



#### 4.2.117 Score per residue for model 117

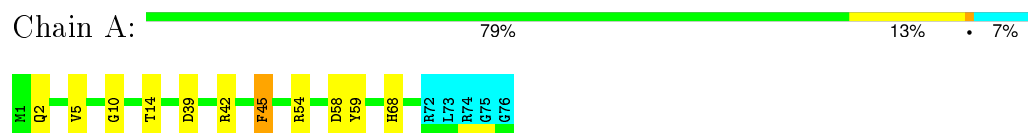
- Molecule 1: Ubiquitin





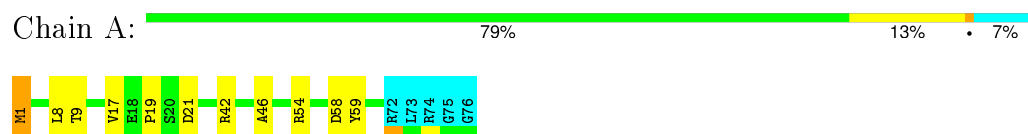
#### 4.2.118 Score per residue for model 118

- Molecule 1: Ubiquitin



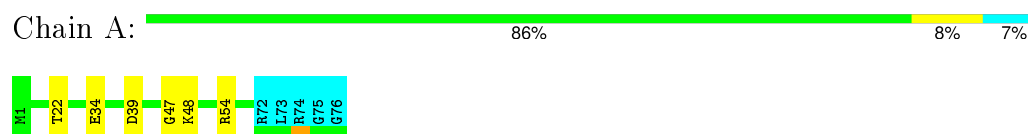
#### 4.2.119 Score per residue for model 119

- Molecule 1: Ubiquitin



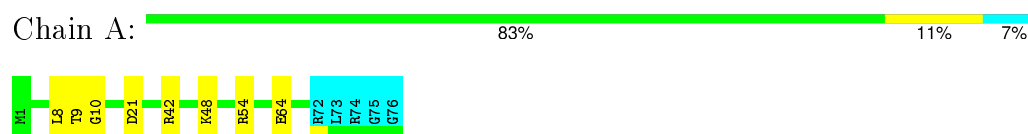
#### 4.2.120 Score per residue for model 120

- Molecule 1: Ubiquitin



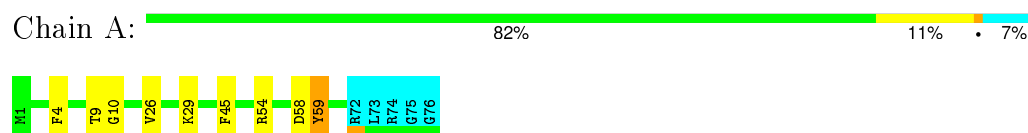
#### 4.2.121 Score per residue for model 121

- Molecule 1: Ubiquitin



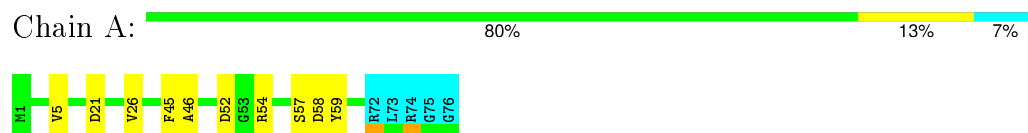
#### 4.2.122 Score per residue for model 122

- Molecule 1: Ubiquitin



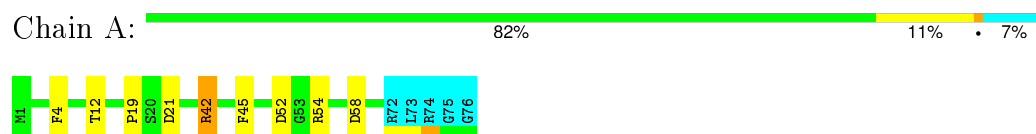
#### 4.2.123 Score per residue for model 123

- Molecule 1: Ubiquitin



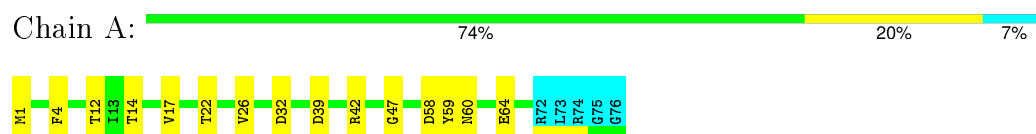
#### 4.2.124 Score per residue for model 124

- Molecule 1: Ubiquitin



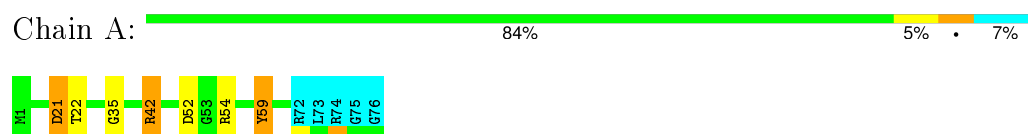
#### 4.2.125 Score per residue for model 125

- Molecule 1: Ubiquitin



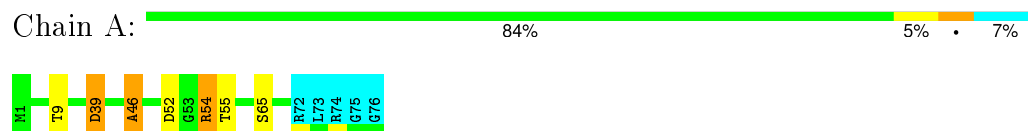
#### 4.2.126 Score per residue for model 126

- Molecule 1: Ubiquitin



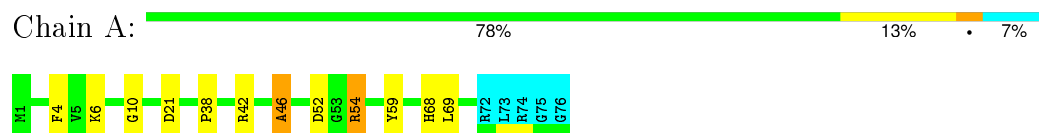
#### 4.2.127 Score per residue for model 127

- Molecule 1: Ubiquitin



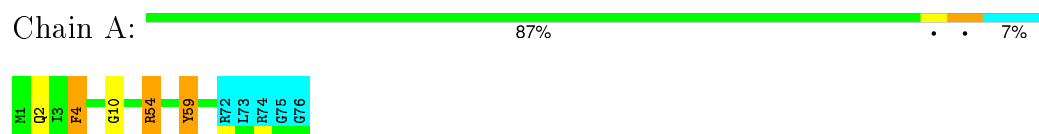
#### 4.2.128 Score per residue for model 128

- Molecule 1: Ubiquitin



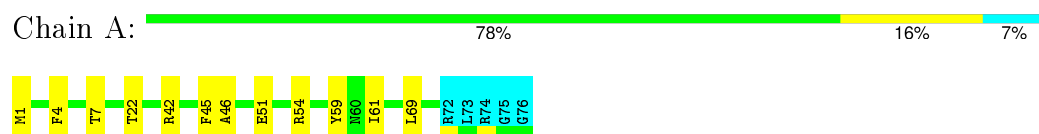
#### 4.2.129 Score per residue for model 129

- Molecule 1: Ubiquitin



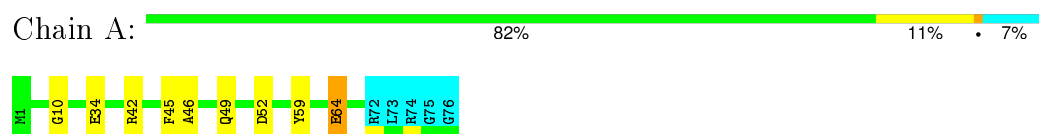
#### 4.2.130 Score per residue for model 130

- Molecule 1: Ubiquitin



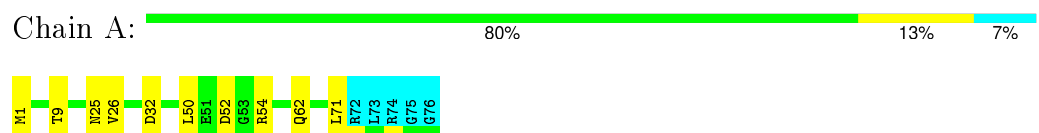
#### 4.2.131 Score per residue for model 131

- Molecule 1: Ubiquitin



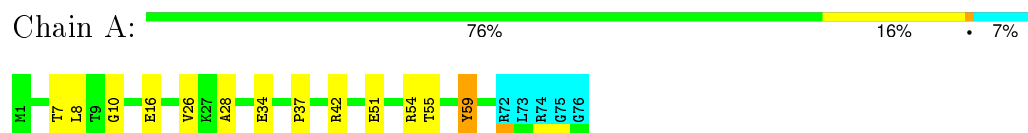
#### 4.2.132 Score per residue for model 132

- Molecule 1: Ubiquitin



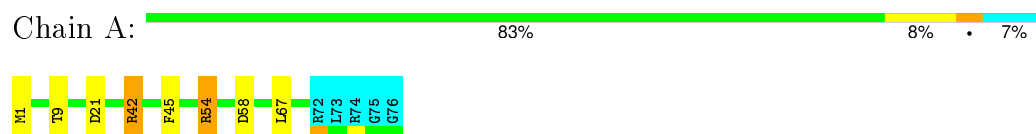
### 4.2.133 Score per residue for model 133

- Molecule 1: Ubiquitin



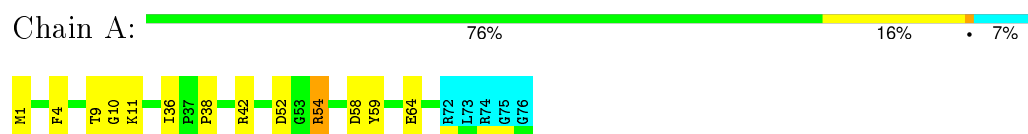
### 4.2.134 Score per residue for model 134

- Molecule 1: Ubiquitin



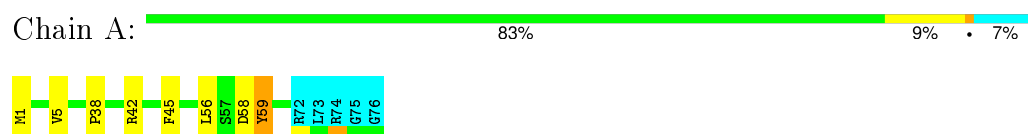
### 4.2.135 Score per residue for model 135

- Molecule 1: Ubiquitin



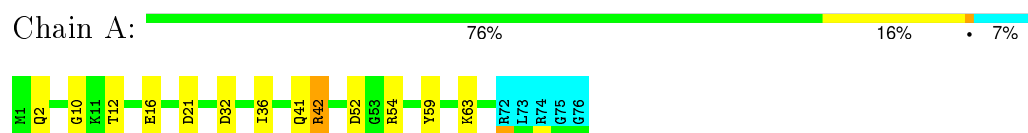
### 4.2.136 Score per residue for model 136

- Molecule 1: Ubiquitin



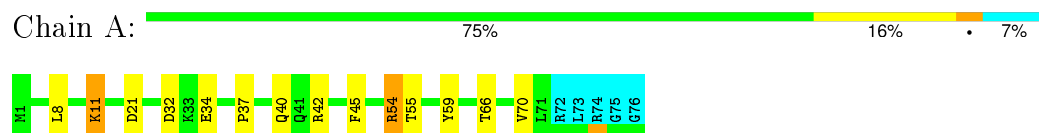
### 4.2.137 Score per residue for model 137

- Molecule 1: Ubiquitin



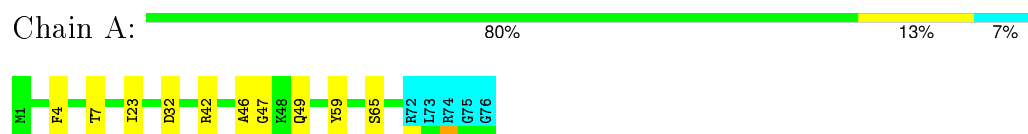
## 4.2.138 Score per residue for model 138

- Molecule 1: Ubiquitin



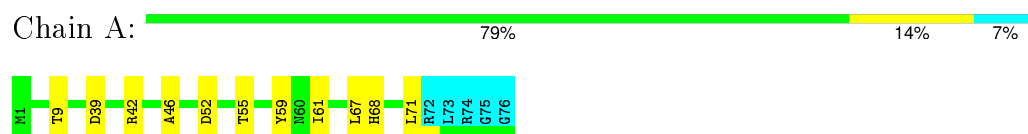
## 4.2.139 Score per residue for model 139

- Molecule 1: Ubiquitin



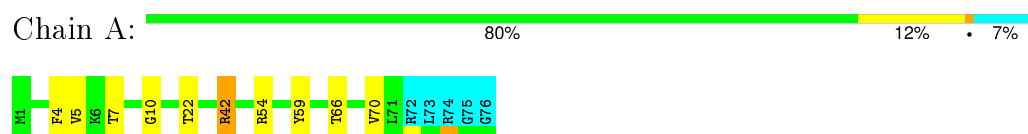
## 4.2.140 Score per residue for model 140

- Molecule 1: Ubiquitin



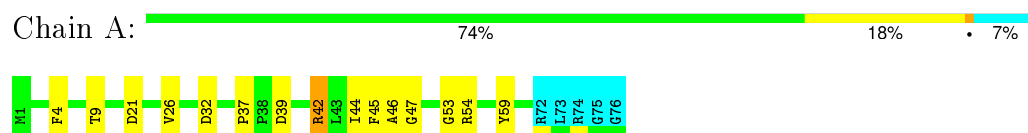
## 4.2.141 Score per residue for model 141

- Molecule 1: Ubiquitin




## 4.2.142 Score per residue for model 142

- Molecule 1: Ubiquitin



#### 4.2.143 Score per residue for model 143


- Molecule 1: Ubiquitin

Chain A:  79% 11% • 7%



#### 4.2.144 Score per residue for model 144

- Molecule 1: Ubiquitin

Chain A:  80% 12% • 7%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *MUMO (minimal under-restraining minimal over-restraining) refinement using previously published NOE distance restraints and order parameter restraints as inputs to ensemble-averaged simulated annealing.*

Of the 144 calculated structures, 144 were deposited, based on the following criterion: *all calculated structures submitted.*

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

Software name	Classification	Version
CHARMM	refinement	c30

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality 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	0.96±0.00	0±0/570 (0.0±0.0%)	1.85±0.07	10±3/770 (1.3±0.4%)
All	All	0.96	0/82080 (0.0%)	1.86	1464/110880 (1.3%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.9±0.9
All	All	0	134

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	54	ARG	NE-CZ-NH1	22.06	131.33	120.30	104	76
1	A	59	TYR	CB-CG-CD1	-16.54	111.07	121.00	62	46
1	A	54	ARG	NE-CZ-NH2	-15.56	112.52	120.30	17	65
1	A	42	ARG	NE-CZ-NH1	15.41	128.01	120.30	101	60
1	A	42	ARG	NE-CZ-NH2	-14.16	113.22	120.30	136	61
1	A	58	ASP	CB-CG-OD1	12.87	129.88	118.30	29	24
1	A	45	PHE	CB-CG-CD1	12.57	129.60	120.80	8	34
1	A	4	PHE	CB-CG-CD2	-12.22	112.25	120.80	129	43
1	A	59	TYR	CB-CG-CD2	-12.09	113.74	121.00	114	41
1	A	45	PHE	CB-CG-CD2	-11.59	112.68	120.80	88	37
1	A	58	ASP	CB-CG-OD2	-11.42	108.02	118.30	50	25
1	A	1	MET	CG-SD-CE	-11.08	82.47	100.20	143	31
1	A	46	ALA	N-CA-CB	10.90	125.36	110.10	4	11
1	A	4	PHE	CB-CG-CD1	10.57	128.20	120.80	46	44
1	A	21	ASP	CB-CG-OD1	10.31	127.58	118.30	137	18

*Continued on next page...*



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	52	ASP	CB-CG-OD1	9.42	126.77	118.30	49	15
1	A	21	ASP	CB-CG-OD2	-9.39	109.85	118.30	31	29
1	A	39	ASP	CB-CG-OD2	-9.08	110.13	118.30	4	29
1	A	22	THR	CA-CB-CG2	-9.03	99.76	112.40	12	17
1	A	9	THR	CA-CB-CG2	-8.95	99.87	112.40	106	22
1	A	37	PRO	N-CA-CB	8.76	113.81	103.30	2	3
1	A	39	ASP	CB-CG-OD1	8.72	126.15	118.30	120	25
1	A	68	HIS	CA-CB-CG	-8.61	98.97	113.60	17	4
1	A	34	GLU	OE1-CD-OE2	-8.46	113.15	123.30	138	10
1	A	54	ARG	NH1-CZ-NH2	8.38	128.62	119.40	90	15
1	A	46	ALA	CB-CA-C	8.30	122.56	110.10	115	16
1	A	42	ARG	NH1-CZ-NH2	-8.13	110.46	119.40	57	20
1	A	59	TYR	CZ-CE2-CD2	-8.09	112.52	119.80	42	11
1	A	32	ASP	CB-CG-OD2	8.04	125.54	118.30	144	23
1	A	33	LYS	N-CA-CB	7.94	124.89	110.60	95	3
1	A	7	THR	CA-CB-CG2	-7.78	101.51	112.40	141	10
1	A	59	TYR	CG-CD1-CE1	-7.76	115.09	121.30	99	10
1	A	32	ASP	N-CA-CB	-7.55	97.02	110.60	37	2
1	A	59	TYR	CG-CD2-CE2	-7.48	115.31	121.30	72	21
1	A	59	TYR	CD1-CE1-CZ	-7.47	113.08	119.80	31	4
1	A	43	LEU	CB-CG-CD2	7.41	123.59	111.00	6	4
1	A	4	PHE	CG-CD1-CE1	-7.40	112.66	120.80	18	2
1	A	7	THR	O-C-N	-7.37	110.91	122.70	27	8
1	A	52	ASP	CB-CG-OD2	-7.34	111.69	118.30	42	16
1	A	70	VAL	O-C-N	-7.30	111.02	122.70	42	2
1	A	26	VAL	CA-CB-CG2	-7.29	99.96	110.90	69	6
1	A	69	LEU	CB-CG-CD1	7.29	123.39	111.00	34	5
1	A	45	PHE	CZ-CE2-CD2	-7.27	111.38	120.10	113	1
1	A	20	SER	N-CA-CB	-7.23	99.66	110.50	9	7
1	A	12	THR	CA-CB-CG2	-7.21	102.31	112.40	89	9
1	A	1	MET	CA-CB-CG	7.20	125.53	113.30	25	5
1	A	54	ARG	CD-NE-CZ	7.16	133.63	123.60	28	7
1	A	32	ASP	CB-CG-OD1	-7.13	111.88	118.30	38	16
1	A	28	ALA	O-C-N	-7.08	111.37	122.70	60	1
1	A	50	LEU	CB-CG-CD1	-7.07	98.99	111.00	59	4
1	A	51	GLU	OE1-CD-OE2	-7.06	114.83	123.30	10	6
1	A	7	THR	N-CA-CB	7.01	123.61	110.30	108	7
1	A	8	LEU	O-C-N	7.00	133.89	122.70	19	4
1	A	55	THR	O-C-N	-6.97	111.54	122.70	81	4
1	A	65	SER	CB-CA-C	-6.96	96.88	110.10	34	8
1	A	55	THR	CA-CB-CG2	-6.93	102.69	112.40	11	10

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	65	SER	N-CA-CB	6.87	120.81	110.50	76	5
1	A	24	GLU	O-C-N	-6.81	111.81	122.70	15	2
1	A	42	ARG	N-CA-CB	6.81	122.85	110.60	139	2
1	A	9	THR	CA-CB-OG1	6.74	123.16	109.00	112	2
1	A	64	GLU	OE1-CD-OE2	-6.73	115.23	123.30	96	6
1	A	17	VAL	CA-CB-CG1	6.71	120.96	110.90	29	3
1	A	59	TYR	CD1-CG-CD2	6.70	125.27	117.90	3	5
1	A	26	VAL	CG1-CB-CG2	-6.69	100.19	110.90	103	9
1	A	12	THR	N-CA-CB	6.63	122.91	110.30	137	3
1	A	58	ASP	CB-CA-C	6.59	123.59	110.40	135	3
1	A	39	ASP	CB-CA-C	6.59	123.59	110.40	102	1
1	A	8	LEU	CB-CG-CD1	-6.58	99.81	111.00	29	4
1	A	39	ASP	N-CA-CB	6.57	122.43	110.60	105	2
1	A	4	PHE	O-C-N	-6.55	112.22	122.70	46	2
1	A	14	THR	CA-CB-CG2	6.49	121.48	112.40	118	4
1	A	67	LEU	CB-CG-CD2	6.49	122.03	111.00	66	4
1	A	51	GLU	C-N-CA	6.46	137.86	121.70	108	2
1	A	50	LEU	CB-CG-CD2	6.45	121.97	111.00	69	4
1	A	18	GLU	OE1-CD-OE2	-6.42	115.59	123.30	114	4
1	A	49	GLN	CG-CD-OE1	6.41	134.43	121.60	48	3
1	A	67	LEU	CB-CG-CD1	-6.37	100.17	111.00	134	2
1	A	17	VAL	CG1-CB-CG2	-6.36	100.73	110.90	22	3
1	A	54	ARG	CG-CD-NE	-6.35	98.46	111.80	45	8
1	A	57	SER	N-CA-CB	6.29	119.94	110.50	88	5
1	A	26	VAL	CA-CB-CG1	6.29	120.33	110.90	95	4
1	A	8	LEU	N-CA-CB	-6.26	97.89	110.40	119	2
1	A	33	LYS	O-C-N	-6.25	112.69	122.70	48	1
1	A	9	THR	C-N-CA	6.25	135.42	122.30	134	4
1	A	45	PHE	CB-CA-C	6.24	122.88	110.40	78	4
1	A	70	VAL	CG1-CB-CG2	-6.22	100.94	110.90	73	6
1	A	71	LEU	CB-CG-CD1	6.21	121.56	111.00	132	4
1	A	29	LYS	O-C-N	-6.20	112.78	122.70	5	3
1	A	56	LEU	CB-CG-CD2	-6.18	100.50	111.00	94	3
1	A	4	PHE	CG-CD2-CE2	-6.15	114.04	120.80	56	1
1	A	22	THR	N-CA-CB	6.14	121.96	110.30	51	8
1	A	51	GLU	O-C-N	-6.13	112.90	122.70	14	2
1	A	15	LEU	CB-CG-CD2	6.11	121.38	111.00	92	2
1	A	52	ASP	N-CA-C	6.09	127.46	111.00	95	2
1	A	24	GLU	OE1-CD-OE2	-6.07	116.02	123.30	64	2
1	A	30	ILE	CA-CB-CG2	6.07	123.04	110.90	94	1
1	A	46	ALA	O-C-N	-6.06	112.90	123.20	63	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	54	ARG	O-C-N	-6.05	113.02	122.70	119	3
1	A	17	VAL	CA-CB-CG2	-6.04	101.84	110.90	48	2
1	A	27	LYS	O-C-N	-6.04	113.04	122.70	5	2
1	A	5	VAL	O-C-N	-6.04	113.04	122.70	76	1
1	A	42	ARG	CB-CA-C	-6.04	98.33	110.40	114	1
1	A	37	PRO	N-CD-CG	6.04	112.25	103.20	53	1
1	A	63	LYS	O-C-N	-6.01	113.08	122.70	96	1
1	A	41	GLN	CB-CA-C	-6.00	98.41	110.40	143	3
1	A	21	ASP	O-C-N	-5.99	113.12	122.70	115	3
1	A	5	VAL	CG1-CB-CG2	-5.95	101.37	110.90	103	4
1	A	3	ILE	CA-CB-CG1	5.95	122.30	111.00	116	1
1	A	52	ASP	O-C-N	-5.94	113.10	123.20	137	3
1	A	34	GLU	CB-CA-C	-5.93	98.53	110.40	120	2
1	A	14	THR	N-CA-CB	5.93	121.56	110.30	36	5
1	A	55	THR	CA-CB-OG1	5.92	121.43	109.00	34	4
1	A	59	TYR	CA-CB-CG	-5.92	102.16	113.40	69	3
1	A	70	VAL	CA-CB-CG1	-5.91	102.03	110.90	37	6
1	A	38	PRO	N-CA-CB	5.91	110.39	103.30	27	4
1	A	6	LYS	O-C-N	-5.91	113.25	122.70	51	1
1	A	28	ALA	CB-CA-C	-5.91	101.24	110.10	133	2
1	A	24	GLU	CB-CA-C	-5.89	98.63	110.40	89	1
1	A	21	ASP	N-CA-CB	-5.87	100.04	110.60	106	1
1	A	65	SER	O-C-N	-5.85	113.34	122.70	53	2
1	A	68	HIS	O-C-N	-5.85	113.34	122.70	140	1
1	A	18	GLU	CG-CD-OE1	5.85	129.99	118.30	47	1
1	A	22	THR	O-C-N	-5.84	113.35	122.70	82	2
1	A	46	ALA	CA-C-O	5.83	132.34	120.10	33	1
1	A	59	TYR	O-C-N	-5.83	113.38	122.70	55	3
1	A	13	ILE	CB-CA-C	5.80	123.20	111.60	34	2
1	A	62	GLN	O-C-N	-5.79	113.44	122.70	132	1
1	A	2	GLN	N-CA-CB	5.78	121.00	110.60	11	2
1	A	60	ASN	CA-CB-CG	-5.77	100.70	113.40	10	2
1	A	58	ASP	O-C-N	-5.77	113.47	122.70	95	3
1	A	1	MET	O-C-N	-5.77	113.47	122.70	83	4
1	A	42	ARG	CD-NE-CZ	-5.75	115.55	123.60	66	7
1	A	7	THR	CA-CB-OG1	5.75	121.08	109.00	59	3
1	A	50	LEU	CB-CA-C	5.75	121.12	110.20	143	1
1	A	25	ASN	O-C-N	-5.74	113.51	122.70	107	3
1	A	39	ASP	CA-CB-CG	-5.74	100.77	113.40	56	1
1	A	61	ILE	CA-CB-CG2	5.74	122.38	110.90	130	1
1	A	62	GLN	CG-CD-OE1	-5.73	110.13	121.60	24	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	36	ILE	CA-C-N	5.73	133.15	117.10	66	1
1	A	3	ILE	CA-CB-CG2	-5.73	99.44	110.90	83	1
1	A	49	GLN	O-C-N	-5.72	113.55	122.70	86	2
1	A	15	LEU	O-C-N	-5.71	113.56	122.70	18	2
1	A	8	LEU	CB-CG-CD2	5.71	120.70	111.00	33	1
1	A	23	ILE	O-C-N	-5.70	113.57	122.70	81	2
1	A	4	PHE	CB-CA-C	-5.70	99.00	110.40	130	1
1	A	71	LEU	CB-CG-CD2	5.70	120.69	111.00	52	2
1	A	5	VAL	CA-CB-CG2	-5.70	102.35	110.90	102	2
1	A	63	LYS	C-N-CA	5.70	135.95	121.70	113	1
1	A	45	PHE	N-CA-C	-5.69	95.64	111.00	94	1
1	A	9	THR	N-CA-CB	5.68	121.10	110.30	101	1
1	A	37	PRO	CA-C-O	-5.66	106.61	120.20	43	1
1	A	30	ILE	O-C-N	-5.65	113.66	122.70	29	4
1	A	58	ASP	N-CA-CB	-5.64	100.45	110.60	27	1
1	A	44	ILE	O-C-N	-5.63	113.69	122.70	9	1
1	A	64	GLU	O-C-N	-5.63	113.69	122.70	108	5
1	A	70	VAL	CA-CB-CG2	-5.63	102.46	110.90	44	1
1	A	18	GLU	CA-C-O	-5.62	108.29	120.10	104	1
1	A	42	ARG	CG-CD-NE	-5.62	100.00	111.80	76	4
1	A	6	LYS	N-CA-CB	-5.58	100.56	110.60	61	1
1	A	53	GLY	O-C-N	-5.57	113.78	122.70	71	1
1	A	49	GLN	N-CA-CB	-5.57	100.57	110.60	117	2
1	A	10	GLY	O-C-N	-5.56	113.80	122.70	137	1
1	A	43	LEU	CB-CA-C	5.55	120.75	110.20	29	1
1	A	66	THR	CA-CB-CG2	-5.55	104.62	112.40	52	2
1	A	11	LYS	O-C-N	-5.54	113.83	122.70	138	1
1	A	16	GLU	N-CA-CB	5.53	120.56	110.60	14	1
1	A	20	SER	CB-CA-C	-5.53	99.59	110.10	31	1
1	A	27	LYS	N-CA-CB	5.53	120.55	110.60	31	1
1	A	59	TYR	C-N-CA	5.52	135.51	121.70	14	1
1	A	16	GLU	OE1-CD-OE2	-5.52	116.68	123.30	56	2
1	A	26	VAL	O-C-N	-5.52	113.87	122.70	123	1
1	A	22	THR	CA-CB-OG1	5.51	120.57	109.00	16	3
1	A	48	LYS	CB-CA-C	-5.50	99.39	110.40	49	1
1	A	34	GLU	O-C-N	-5.50	113.85	123.20	59	4
1	A	4	PHE	CD1-CE1-CZ	5.50	126.70	120.10	80	1
1	A	14	THR	OG1-CB-CG2	-5.47	97.42	110.00	99	2
1	A	6	LYS	CB-CA-C	-5.47	99.47	110.40	128	1
1	A	49	GLN	CB-CA-C	-5.46	99.49	110.40	47	1
1	A	55	THR	N-CA-CB	5.45	120.66	110.30	24	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	66	THR	O-C-N	-5.45	113.99	122.70	31	4
1	A	32	ASP	O-C-N	-5.44	114.00	122.70	91	2
1	A	41	GLN	O-C-N	-5.43	114.01	122.70	31	2
1	A	17	VAL	CB-CA-C	-5.42	101.09	111.40	3	1
1	A	25	ASN	N-CA-CB	-5.42	100.84	110.60	108	2
1	A	42	ARG	O-C-N	-5.41	114.04	122.70	40	3
1	A	12	THR	O-C-N	-5.41	114.04	122.70	42	1
1	A	19	PRO	O-C-N	-5.41	114.05	122.70	48	1
1	A	71	LEU	CB-CA-C	5.41	120.47	110.20	59	2
1	A	4	PHE	CD1-CG-CD2	5.41	125.33	118.30	122	1
1	A	29	LYS	C-N-CA	5.40	135.20	121.70	88	1
1	A	43	LEU	C-N-CA	5.39	135.19	121.70	102	2
1	A	19	PRO	N-CA-CB	5.39	109.77	103.30	61	3
1	A	61	ILE	O-C-N	-5.39	114.08	122.70	106	1
1	A	17	VAL	O-C-N	-5.38	114.09	122.70	107	4
1	A	5	VAL	CA-CB-CG1	5.38	118.97	110.90	123	1
1	A	69	LEU	CB-CA-C	5.37	120.41	110.20	95	1
1	A	36	ILE	O-C-N	-5.37	110.89	121.10	61	1
1	A	64	GLU	N-CA-CB	5.36	120.25	110.60	135	4
1	A	67	LEU	CB-CA-C	-5.35	100.03	110.20	14	2
1	A	15	LEU	N-CA-CB	5.35	121.10	110.40	7	2
1	A	15	LEU	CB-CG-CD1	-5.34	101.92	111.00	31	2
1	A	42	ARG	CA-CB-CG	5.34	125.14	113.40	22	1
1	A	45	PHE	C-N-CA	5.33	135.03	121.70	14	2
1	A	64	GLU	CB-CA-C	5.33	121.06	110.40	70	2
1	A	18	GLU	CB-CA-C	-5.33	99.74	110.40	93	1
1	A	27	LYS	CB-CA-C	-5.33	99.74	110.40	112	1
1	A	40	GLN	CG-CD-OE1	5.32	132.24	121.60	138	1
1	A	29	LYS	N-CA-CB	-5.31	101.05	110.60	122	1
1	A	45	PHE	CD1-CE1-CZ	5.30	126.46	120.10	79	1
1	A	25	ASN	CB-CA-C	-5.29	99.83	110.40	132	1
1	A	13	ILE	N-CA-CB	5.27	122.93	110.80	23	1
1	A	66	THR	N-CA-CB	5.26	120.30	110.30	43	2
1	A	38	PRO	N-CD-CG	5.26	111.10	103.20	128	1
1	A	43	LEU	CB-CG-CD1	-5.26	102.06	111.00	86	2
1	A	23	ILE	CG1-CB-CG2	5.25	122.96	111.40	36	1
1	A	18	GLU	CA-C-N	5.25	131.79	117.10	110	1
1	A	35	GLY	C-N-CA	5.24	134.79	121.70	91	2
1	A	7	THR	C-N-CA	5.24	134.79	121.70	24	2
1	A	57	SER	CB-CA-C	-5.24	100.15	110.10	45	1
1	A	61	ILE	CA-CB-CG1	-5.22	101.08	111.00	20	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	34	GLU	N-CA-CB	-5.22	101.20	110.60	3	1
1	A	22	THR	C-N-CA	5.22	134.74	121.70	71	1
1	A	38	PRO	O-C-N	-5.20	114.38	122.70	18	1
1	A	45	PHE	N-CA-CB	5.20	119.96	110.60	130	4
1	A	60	ASN	O-C-N	5.20	131.02	122.70	18	1
1	A	8	LEU	CA-CB-CG	-5.20	103.34	115.30	53	1
1	A	52	ASP	CB-CA-C	-5.20	100.00	110.40	95	1
1	A	62	GLN	CB-CA-C	5.19	120.79	110.40	84	1
1	A	41	GLN	N-CA-CB	5.19	119.94	110.60	48	2
1	A	60	ASN	CB-CG-OD1	-5.18	111.23	121.60	53	3
1	A	44	ILE	CA-CB-CG1	-5.18	101.15	111.00	31	4
1	A	68	HIS	CB-CA-C	5.18	120.76	110.40	70	1
1	A	1	MET	CA-C-O	-5.18	109.23	120.10	6	1
1	A	68	HIS	N-CA-CB	-5.17	101.30	110.60	118	1
1	A	64	GLU	CA-C-O	5.16	130.94	120.10	108	1
1	A	16	GLU	CB-CG-CD	-5.16	100.28	114.20	62	1
1	A	27	LYS	CG-CD-CE	5.16	127.37	111.90	103	1
1	A	25	ASN	CA-CB-CG	-5.14	102.09	113.40	112	1
1	A	16	GLU	CG-CD-OE1	5.12	128.54	118.30	8	1
1	A	31	GLN	O-C-N	-5.12	114.51	122.70	16	1
1	A	60	ASN	N-CA-CB	5.11	119.80	110.60	6	1
1	A	31	GLN	CG-CD-OE1	5.09	131.78	121.60	4	1
1	A	43	LEU	N-CA-CB	5.09	120.57	110.40	111	1
1	A	40	GLN	N-CA-CB	5.08	119.75	110.60	98	1
1	A	55	THR	OG1-CB-CG2	-5.08	98.31	110.00	133	1
1	A	44	ILE	N-CA-C	-5.08	97.29	111.00	142	1
1	A	67	LEU	CA-CB-CG	5.07	126.95	115.30	59	1
1	A	2	GLN	O-C-N	5.06	130.80	122.70	13	1
1	A	62	GLN	C-N-CA	5.06	134.35	121.70	48	1
1	A	13	ILE	O-C-N	-5.06	114.60	122.70	71	1
1	A	56	LEU	O-C-N	-5.06	114.61	122.70	86	1
1	A	48	LYS	O-C-N	-5.06	114.61	122.70	51	1
1	A	27	LYS	CD-CE-NZ	-5.06	100.07	111.70	67	1
1	A	56	LEU	C-N-CA	5.06	134.34	121.70	109	1
1	A	39	ASP	O-C-N	-5.05	114.61	122.70	14	2
1	A	48	LYS	C-N-CA	5.05	134.34	121.70	121	1
1	A	16	GLU	CG-CD-OE2	5.05	128.41	118.30	133	1
1	A	36	ILE	CG1-CB-CG2	-5.05	100.28	111.40	135	1
1	A	63	LYS	CA-CB-CG	5.05	124.51	113.40	78	1
1	A	37	PRO	CA-C-N	5.05	131.24	117.10	91	1
1	A	20	SER	O-C-N	-5.04	114.63	122.70	18	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	19	PRO	C-N-CA	5.04	134.31	121.70	124	1
1	A	29	LYS	CB-CA-C	-5.04	100.32	110.40	75	1
1	A	63	LYS	N-CA-CB	5.03	119.66	110.60	31	1
1	A	18	GLU	O-C-N	-5.03	111.54	121.10	117	1
1	A	28	ALA	N-CA-CB	-5.01	103.09	110.10	59	1
1	A	51	GLU	CB-CA-C	-5.01	100.39	110.40	133	1
1	A	32	ASP	CB-CA-C	5.00	120.40	110.40	37	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	42	ARG	Sidechain	40
1	A	54	ARG	Sidechain	39
1	A	59	TYR	Sidechain	36
1	A	45	PHE	Sidechain	7
1	A	4	PHE	Sidechain	6
1	A	23	ILE	Mainchain	1
1	A	5	VAL	Mainchain	1
1	A	35	GLY	Mainchain	1
1	A	66	THR	Mainchain	1
1	A	19	PRO	Mainchain	1
1	A	12	THR	Mainchain	1

## 6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	563	586	586	0±0
All	All	81072	84384	84384	22

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

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ILE:HD13	1:A:50:LEU:HB3	0.67	1.66	77	1
1:A:22:THR:O	1:A:26:VAL:HG23	0.54	2.02	125	1
1:A:61:ILE:HD13	1:A:67:LEU:HD21	0.54	1.80	140	1
1:A:45:PHE:HB2	1:A:50:LEU:HD21	0.51	1.83	81	1
1:A:7:THR:HG22	1:A:69:LEU:HD23	0.47	1.85	96	2
1:A:15:LEU:HD22	1:A:29:LYS:HB3	0.47	1.84	20	1
1:A:56:LEU:HD23	1:A:61:ILE:HD12	0.47	1.86	93	1
1:A:42:ARG:HB2	1:A:70:VAL:HG23	0.44	1.88	141	1
1:A:36:ILE:HG22	1:A:41:GLN:HG3	0.43	1.90	137	1
1:A:56:LEU:CD2	1:A:61:ILE:HD12	0.43	2.43	93	1
1:A:3:ILE:HG22	1:A:65:SER:H	0.42	1.73	67	1
1:A:37:PRO:HA	1:A:38:PRO:HD3	0.42	1.79	35	1
1:A:44:ILE:HD12	1:A:70:VAL:HG21	0.41	1.92	52	1
1:A:11:LYS:NZ	1:A:34:GLU:OE1	0.41	2.49	34	1
1:A:45:PHE:CE2	1:A:61:ILE:HG12	0.41	2.51	47	1
1:A:22:THR:HA	1:A:55:THR:HA	0.41	1.93	88	1
1:A:23:ILE:O	1:A:23:ILE:HG22	0.41	2.15	139	1
1:A:13:ILE:HD12	1:A:33:LYS:CE	0.41	2.46	59	1
1:A:23:ILE:CG2	1:A:43:LEU:HD23	0.41	2.46	6	1
1:A:50:LEU:HD22	1:A:59:TYR:CG	0.40	2.51	116	1
1:A:45:PHE:C	1:A:47:GLY:H	0.40	2.19	107	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	70/76 (92%)	65±2 (93±3%)	4±2 (5±3%)	1±1 (1±1%)	20	66
All	All	10080/10944 (92%)	9407 (93%)	546 (5%)	127 (1%)	20	66

All 10 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	10	GLY	48
1	A	46	ALA	32

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	47	GLY	27
1	A	60	ASN	5
1	A	63	LYS	5
1	A	53	GLY	3
1	A	33	LYS	3
1	A	64	GLU	2
1	A	35	GLY	1
1	A	9	THR	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%)	64±1 (98±2%)	1±1 (2±2%)	74	96
All	All	9360/9792 (96%)	9215 (98%)	145 (2%)	74	96

All 43 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	1	MET	16
1	A	52	ASP	11
1	A	2	GLN	9
1	A	38	PRO	8
1	A	13	ILE	8
1	A	37	PRO	8
1	A	9	THR	7
1	A	39	ASP	6
1	A	32	ASP	6
1	A	11	LYS	5
1	A	65	SER	5
1	A	64	GLU	5
1	A	70	VAL	4
1	A	20	SER	4
1	A	21	ASP	3
1	A	49	GLN	3
1	A	17	VAL	3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	31	GLN	3
1	A	60	ASN	2
1	A	48	LYS	2
1	A	66	THR	2
1	A	69	LEU	2
1	A	54	ARG	2
1	A	58	ASP	2
1	A	40	GLN	1
1	A	5	VAL	1
1	A	68	HIS	1
1	A	25	ASN	1
1	A	29	LYS	1
1	A	57	SER	1
1	A	16	GLU	1
1	A	8	LEU	1
1	A	71	LEU	1
1	A	56	LEU	1
1	A	63	LYS	1
1	A	43	LEU	1
1	A	45	PHE	1
1	A	62	GLN	1
1	A	19	PRO	1
1	A	15	LEU	1
1	A	7	THR	1
1	A	22	THR	1
1	A	42	ARG	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided