



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 03:28 PM UTC

PDB ID : 6V5D / pdb_00006v5d
BMRB ID : 30693
Title : EROS3 RDC and NOE Derived Ubiquitin Ensemble
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Deposited on : 2019-12-04

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

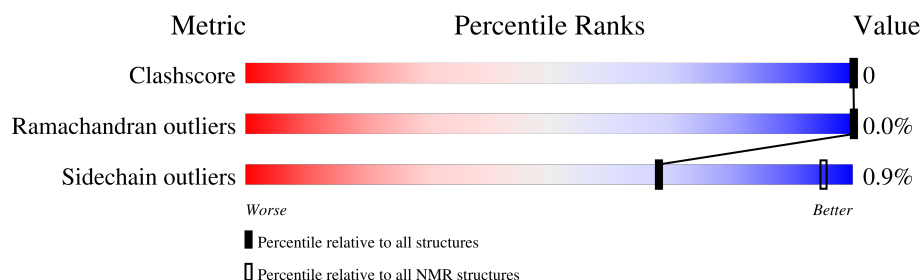
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 94%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	76	 87% 13%

2 Ensemble composition and analysis

This entry contains 176 models. Model 33 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *first structure*.

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:6, A:11-A:70 (66)	0.58	33

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 14 clusters and 10 single-model clusters were found.

Cluster number	Models
1	2, 3, 5, 6, 7, 9, 10, 13, 14, 16, 17, 18, 19, 22, 23, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 38, 39, 40, 41, 42, 43, 45, 46, 48, 49, 50, 52, 53, 54, 55, 56, 57, 58, 59, 62, 63, 68, 72, 73, 76, 77, 79, 85, 86, 87, 88, 89, 91, 95, 96, 97, 98, 104, 105, 106, 107, 109, 113, 114, 115, 116, 117, 119, 120, 121, 123, 124, 126, 127, 129, 132, 133, 135, 136, 137, 142, 143, 145, 146, 147, 150, 151, 153, 154, 157, 158, 159, 164, 166, 167, 168, 169, 171, 174, 175, 176
2	1, 12, 20, 21, 35, 65, 69, 71, 74, 93, 101, 103, 118, 131, 139, 141, 148, 149, 156, 163, 165, 170
3	11, 80, 83, 94, 100, 110, 152
4	8, 36, 67, 102, 162
5	31, 60, 66, 172
6	81, 112, 134, 161
7	92, 125, 140
8	64, 82, 128
9	90, 144
10	70, 130
11	99, 138
12	47, 108
13	61, 84
14	75, 111
Single-model clusters	4; 15; 37; 44; 51; 78; 122; 155; 160; 173

3 Entry composition [i](#)

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

- Molecule 1 is a protein called Ubiquitin.

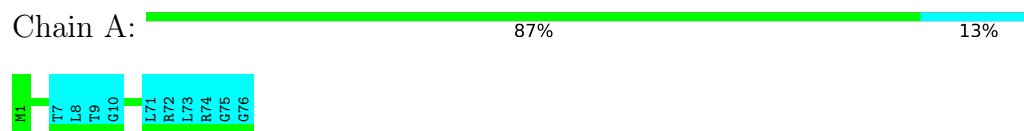
Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1231	378	629	105	118	1	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Ubiquitin

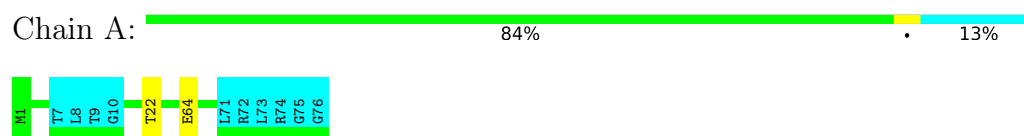


4.2 Scores per residue for each member of the ensemble

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

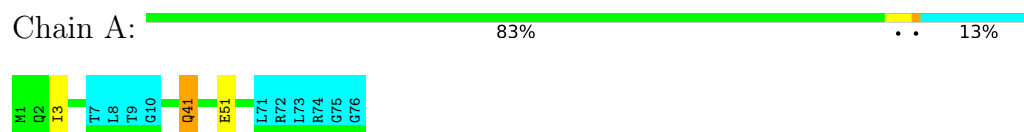
4.2.1 Score per residue for model 1

- Molecule 1: Ubiquitin



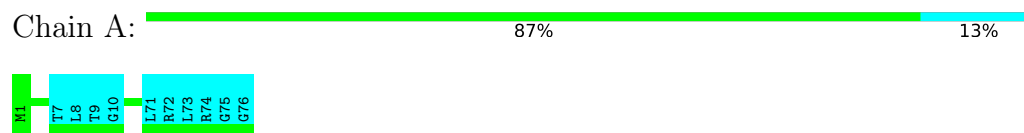
4.2.2 Score per residue for model 2

- Molecule 1: Ubiquitin



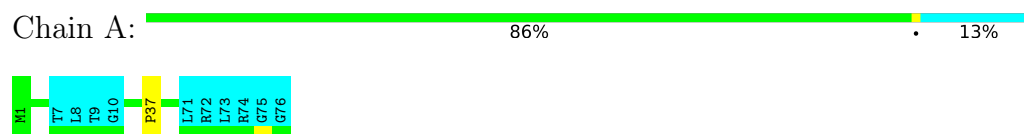
4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin



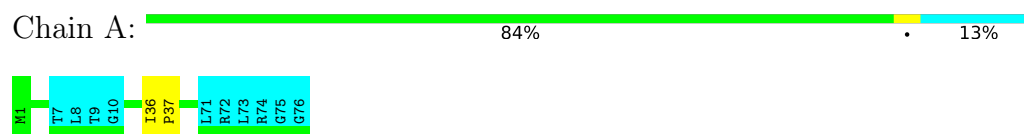
4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin



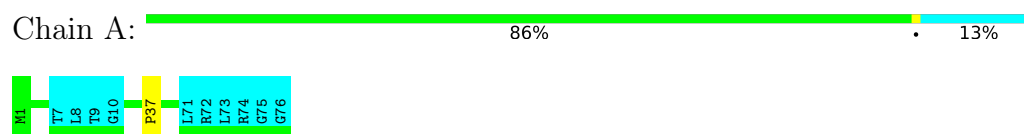
4.2.5 Score per residue for model 5

- Molecule 1: Ubiquitin



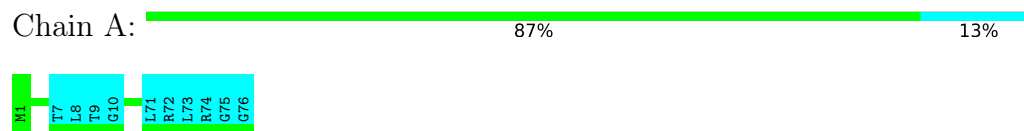
4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin



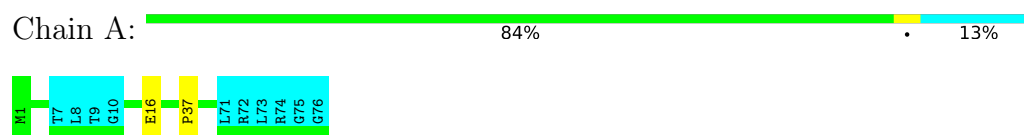
4.2.7 Score per residue for model 7

- Molecule 1: Ubiquitin



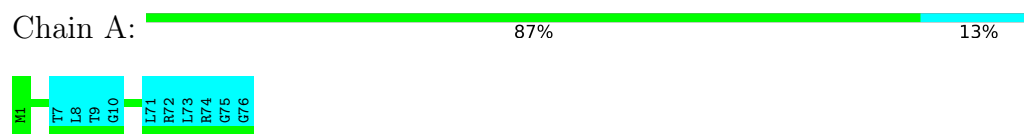
4.2.8 Score per residue for model 8

- Molecule 1: Ubiquitin



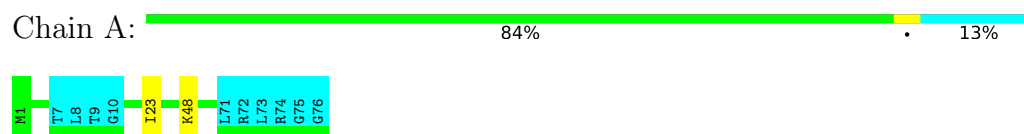
4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin



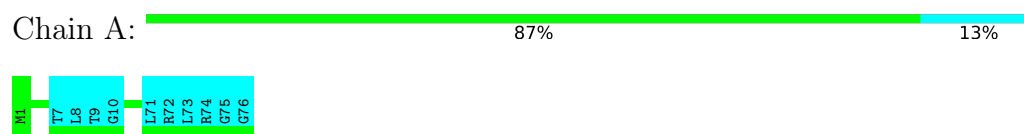
4.2.10 Score per residue for model 10

- Molecule 1: Ubiquitin



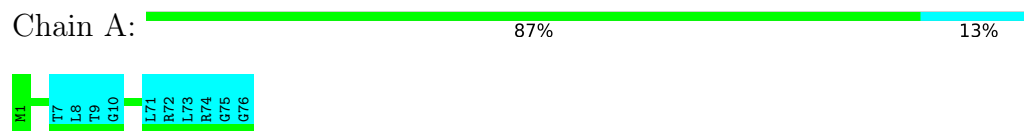
4.2.11 Score per residue for model 11

- Molecule 1: Ubiquitin



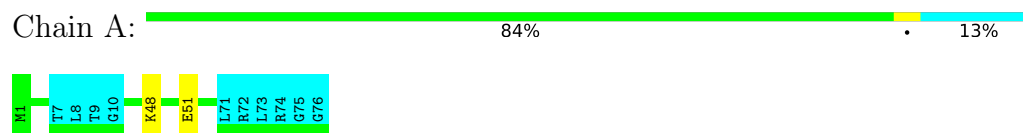
4.2.12 Score per residue for model 12

- Molecule 1: Ubiquitin



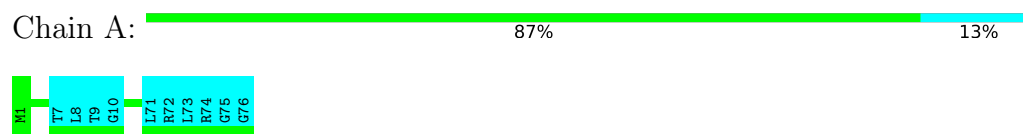
4.2.13 Score per residue for model 13

- Molecule 1: Ubiquitin



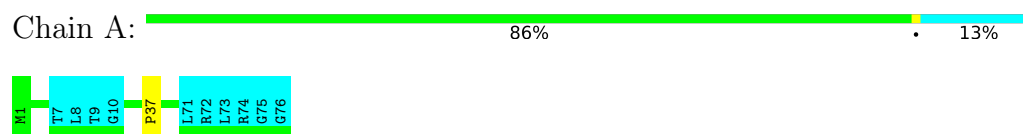
4.2.14 Score per residue for model 14

- Molecule 1: Ubiquitin



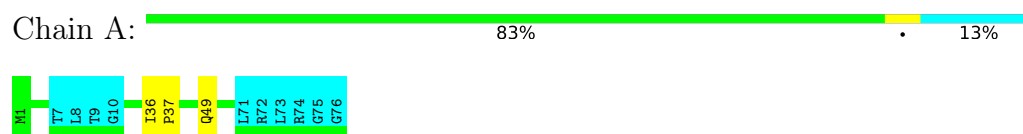
4.2.15 Score per residue for model 15

- Molecule 1: Ubiquitin



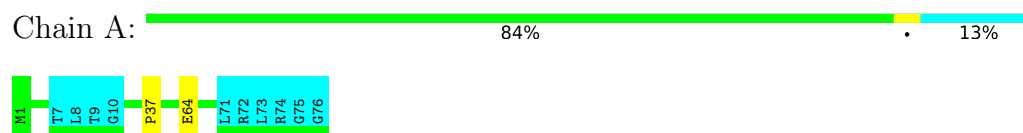
4.2.16 Score per residue for model 16

- Molecule 1: Ubiquitin



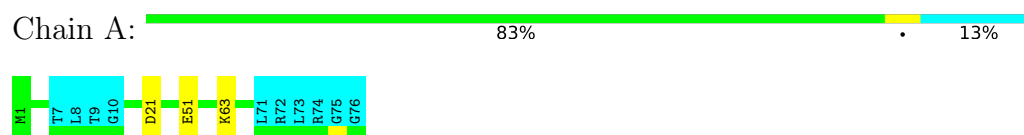
4.2.17 Score per residue for model 17

- Molecule 1: Ubiquitin



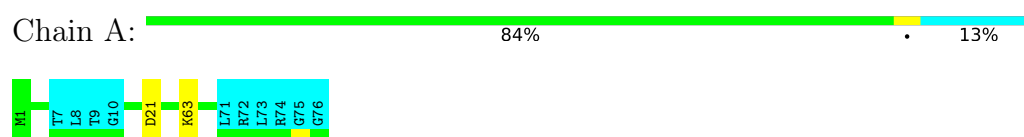
4.2.18 Score per residue for model 18

- Molecule 1: Ubiquitin



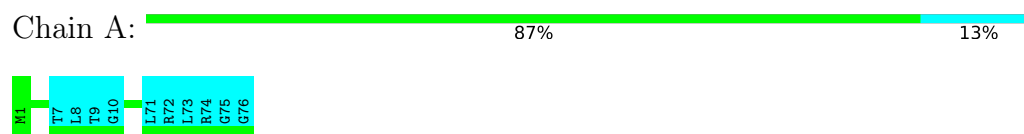
4.2.19 Score per residue for model 19

- Molecule 1: Ubiquitin



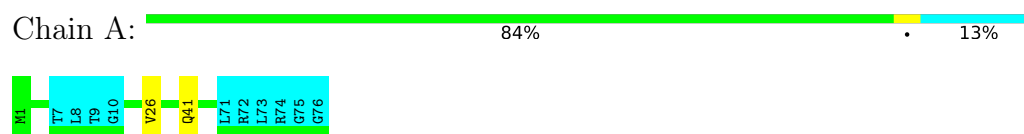
4.2.20 Score per residue for model 20

- Molecule 1: Ubiquitin



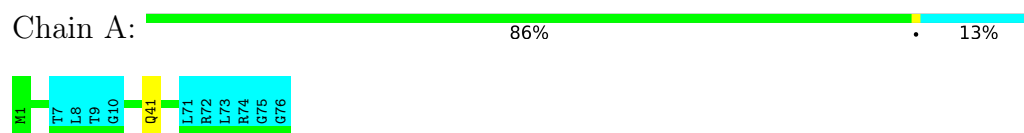
4.2.21 Score per residue for model 21

- Molecule 1: Ubiquitin



4.2.22 Score per residue for model 22

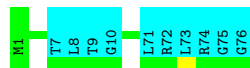
- Molecule 1: Ubiquitin



4.2.23 Score per residue for model 23

- Molecule 1: Ubiquitin

Chain A:  87% 13%



4.2.24 Score per residue for model 24

- Molecule 1: Ubiquitin

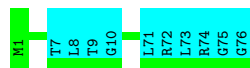
Chain A:  84% 13%



4.2.25 Score per residue for model 25

- Molecule 1: Ubiquitin

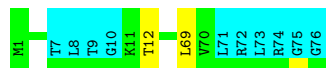
Chain A:  87% 13%



4.2.26 Score per residue for model 26

- Molecule 1: Ubiquitin

Chain A:  84% 13%



4.2.27 Score per residue for model 27

- Molecule 1: Ubiquitin

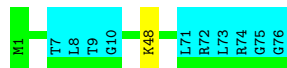
Chain A:  84% 13%



4.2.28 Score per residue for model 28

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.29 Score per residue for model 29

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.30 Score per residue for model 30

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.31 Score per residue for model 31

- Molecule 1: Ubiquitin

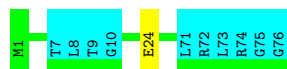
Chain A:  87% 13%



4.2.32 Score per residue for model 32

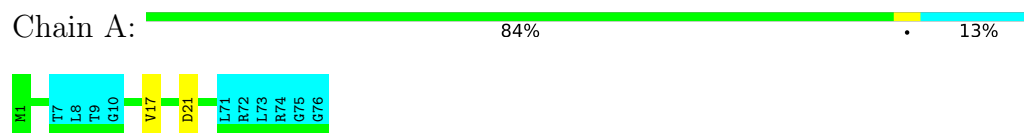
- Molecule 1: Ubiquitin

Chain A:  86% 13%



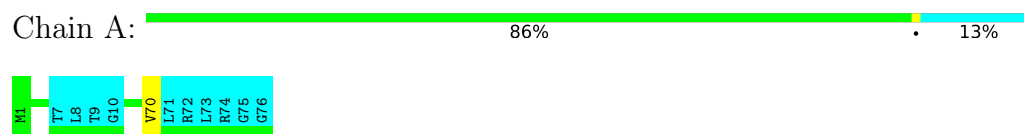
4.2.33 Score per residue for model 33 (medoid)

- Molecule 1: Ubiquitin



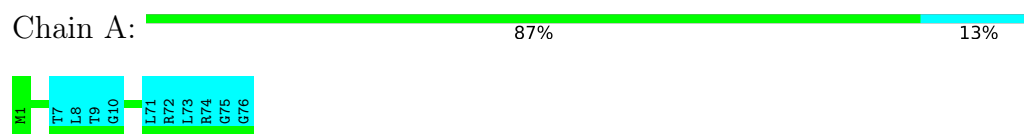
4.2.34 Score per residue for model 34

- Molecule 1: Ubiquitin



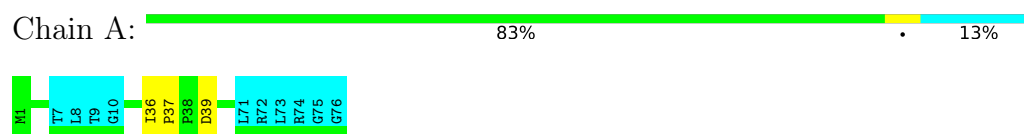
4.2.35 Score per residue for model 35

- Molecule 1: Ubiquitin



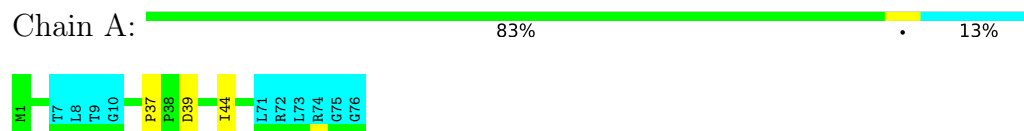
4.2.36 Score per residue for model 36

- Molecule 1: Ubiquitin



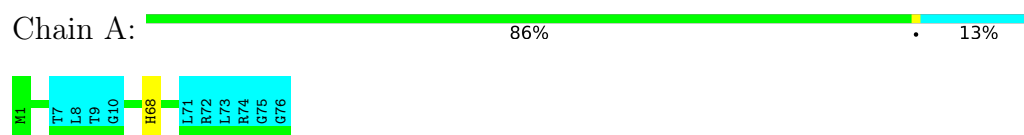
4.2.37 Score per residue for model 37

- Molecule 1: Ubiquitin



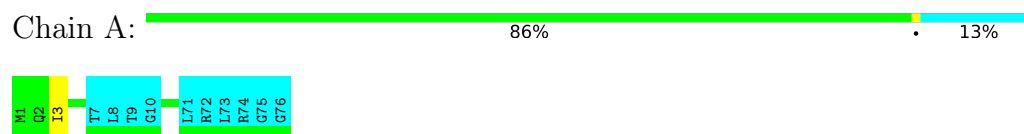
4.2.38 Score per residue for model 38

- Molecule 1: Ubiquitin



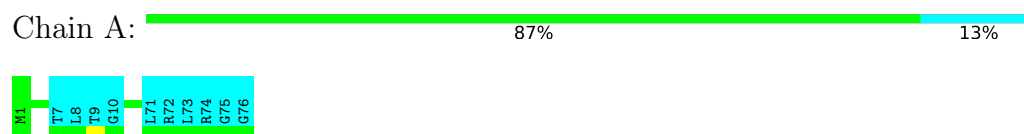
4.2.39 Score per residue for model 39

- Molecule 1: Ubiquitin



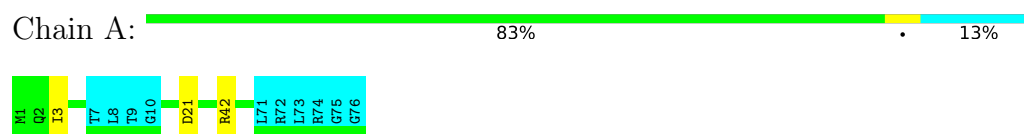
4.2.40 Score per residue for model 40

- Molecule 1: Ubiquitin



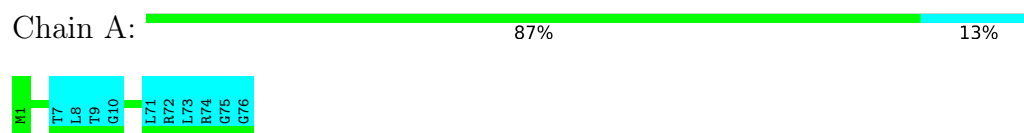
4.2.41 Score per residue for model 41

- 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

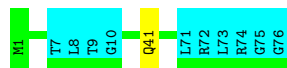
Chain A:  86% 13%



4.2.44 Score per residue for model 44

- Molecule 1: Ubiquitin

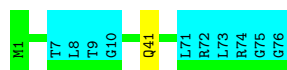
Chain A:  86% 13%



4.2.45 Score per residue for model 45

- Molecule 1: Ubiquitin

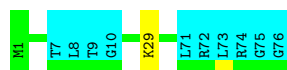
Chain A:  86% 13%



4.2.46 Score per residue for model 46

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.47 Score per residue for model 47

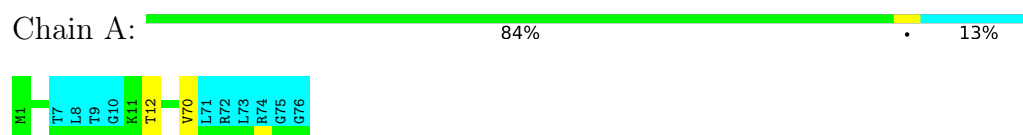
- Molecule 1: Ubiquitin

Chain A:  86% 13%



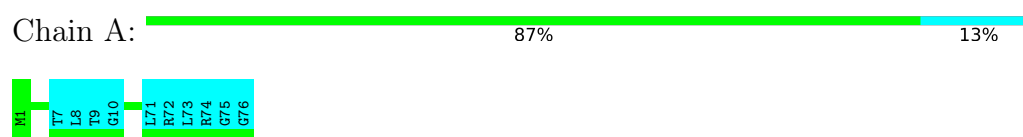
4.2.48 Score per residue for model 48

- Molecule 1: Ubiquitin



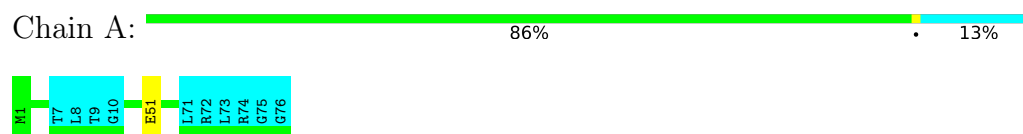
4.2.49 Score per residue for model 49

- Molecule 1: Ubiquitin



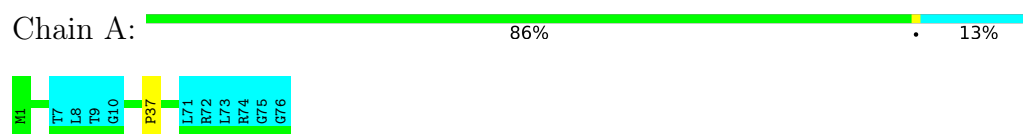
4.2.50 Score per residue for model 50

- Molecule 1: Ubiquitin



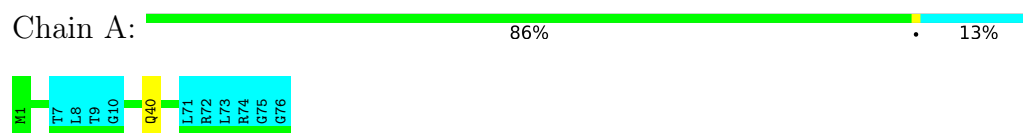
4.2.51 Score per residue for model 51

- Molecule 1: Ubiquitin



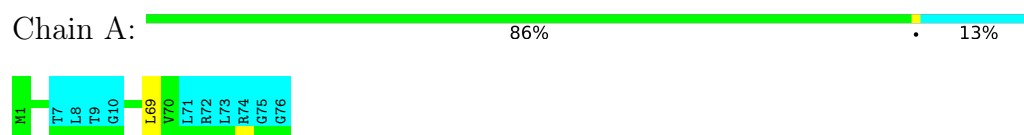
4.2.52 Score per residue for model 52

- Molecule 1: Ubiquitin



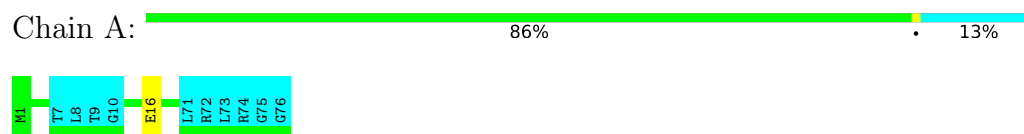
4.2.53 Score per residue for model 53

- Molecule 1: Ubiquitin



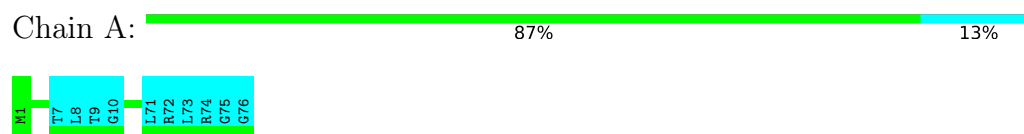
4.2.54 Score per residue for model 54

- Molecule 1: Ubiquitin



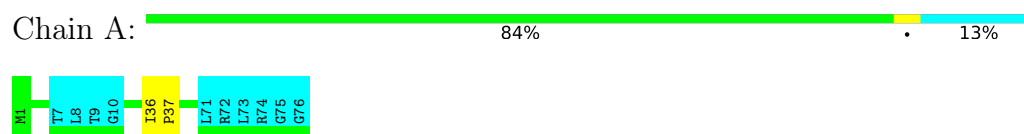
4.2.55 Score per residue for model 55

- Molecule 1: Ubiquitin



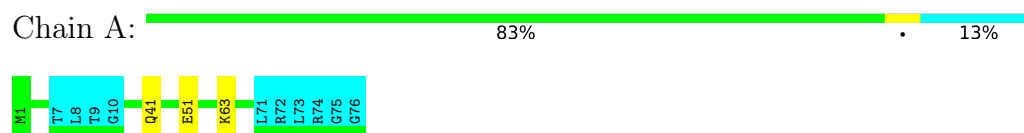
4.2.56 Score per residue for model 56

- Molecule 1: Ubiquitin



4.2.57 Score per residue for model 57

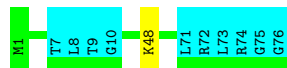
- Molecule 1: Ubiquitin



4.2.58 Score per residue for model 58

- Molecule 1: Ubiquitin

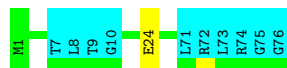
Chain A:  86% 13%



4.2.59 Score per residue for model 59

- Molecule 1: Ubiquitin

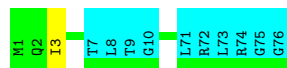
Chain A:  86% 13%



4.2.60 Score per residue for model 60

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.61 Score per residue for model 61

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.62 Score per residue for model 62

- Molecule 1: Ubiquitin

Chain A:  87% 13%



4.2.63 Score per residue for model 63

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.64 Score per residue for model 64

- Molecule 1: Ubiquitin

Chain A:  83% 13%



4.2.65 Score per residue for model 65

- Molecule 1: Ubiquitin

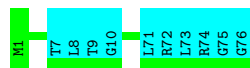
Chain A:  86% 13%



4.2.66 Score per residue for model 66

- Molecule 1: Ubiquitin

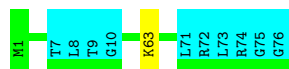
Chain A:  87% 13%



4.2.67 Score per residue for model 67

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.68 Score per residue for model 68

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.69 Score per residue for model 69

- Molecule 1: Ubiquitin

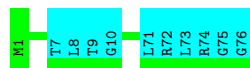
Chain A:  86% 13%



4.2.70 Score per residue for model 70

- Molecule 1: Ubiquitin

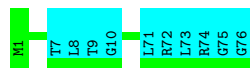
Chain A:  87% 13%



4.2.71 Score per residue for model 71

- Molecule 1: Ubiquitin

Chain A:  87% 13%



4.2.72 Score per residue for model 72

- Molecule 1: Ubiquitin

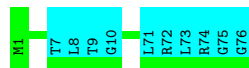
Chain A:  84% 13%



4.2.73 Score per residue for model 73

- Molecule 1: Ubiquitin

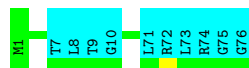
Chain A:  87% 13%



4.2.74 Score per residue for model 74

- Molecule 1: Ubiquitin

Chain A:  87% 13%



4.2.75 Score per residue for model 75

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.76 Score per residue for model 76

- Molecule 1: Ubiquitin

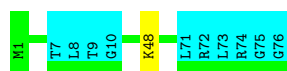
Chain A:  84% 13%



4.2.77 Score per residue for model 77

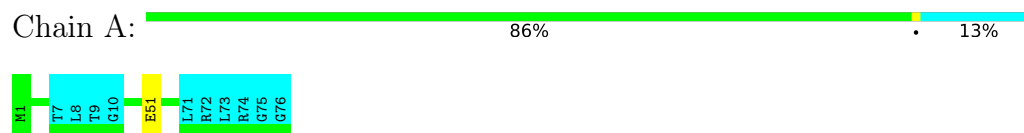
- Molecule 1: Ubiquitin

Chain A:  86% 13%



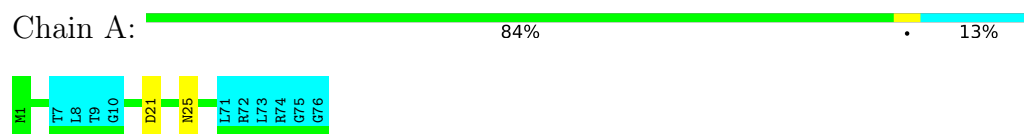
4.2.78 Score per residue for model 78

- Molecule 1: Ubiquitin



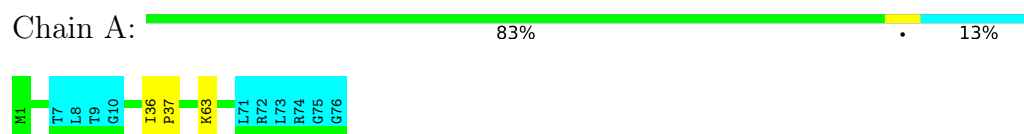
4.2.79 Score per residue for model 79

- Molecule 1: Ubiquitin



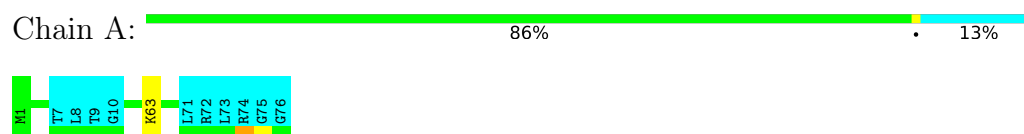
4.2.80 Score per residue for model 80

- Molecule 1: Ubiquitin



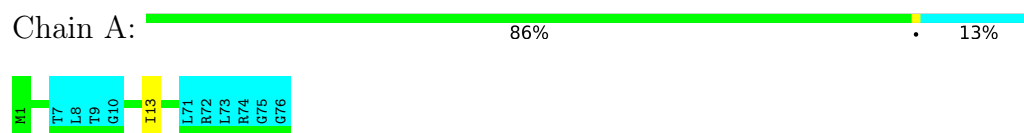
4.2.81 Score per residue for model 81

- Molecule 1: Ubiquitin



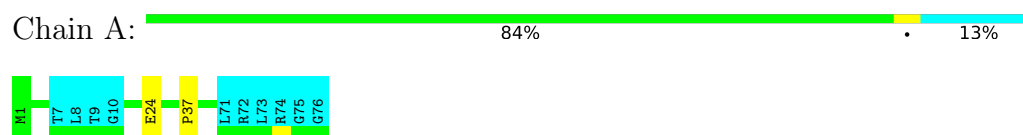
4.2.82 Score per residue for model 82

- Molecule 1: Ubiquitin



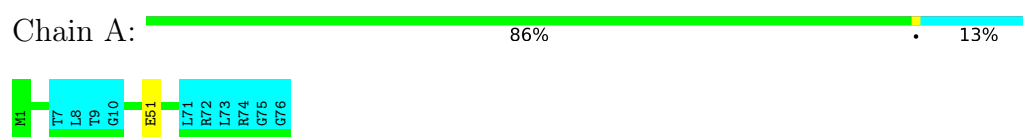
4.2.83 Score per residue for model 83

- Molecule 1: Ubiquitin



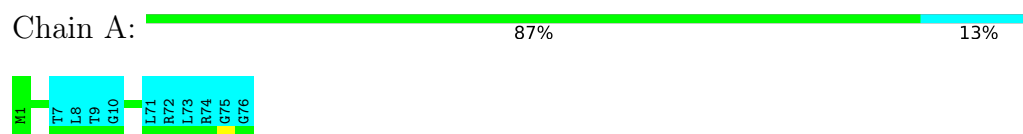
4.2.84 Score per residue for model 84

- Molecule 1: Ubiquitin



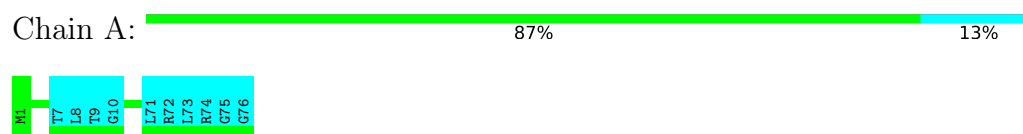
4.2.85 Score per residue for model 85

- Molecule 1: Ubiquitin



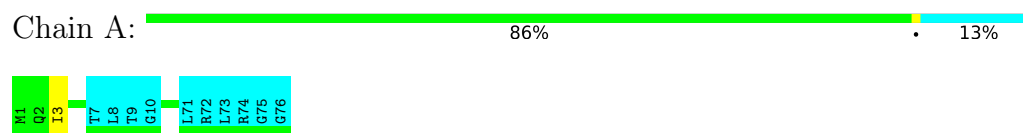
4.2.86 Score per residue for model 86

- 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

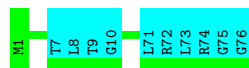
Chain A:  86% 13%



4.2.89 Score per residue for model 89

- Molecule 1: Ubiquitin

Chain A:  87% 13%



4.2.90 Score per residue for model 90

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.91 Score per residue for model 91

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.92 Score per residue for model 92

- Molecule 1: Ubiquitin

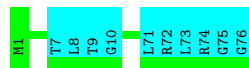
Chain A:  86% 13%



4.2.93 Score per residue for model 93

- Molecule 1: Ubiquitin

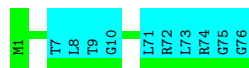
Chain A:  87% 13%



4.2.94 Score per residue for model 94

- Molecule 1: Ubiquitin

Chain A:  87% 13%



4.2.95 Score per residue for model 95

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.96 Score per residue for model 96

- Molecule 1: Ubiquitin

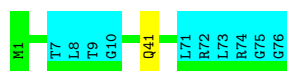
Chain A:  86% 13%



4.2.97 Score per residue for model 97

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.98 Score per residue for model 98

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.99 Score per residue for model 99

- Molecule 1: Ubiquitin

Chain A:  83% 13%



4.2.100 Score per residue for model 100

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.101 Score per residue for model 101

- Molecule 1: Ubiquitin

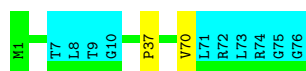
Chain A:  86% 13%



4.2.102 Score per residue for model 102

- Molecule 1: Ubiquitin

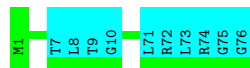
Chain A:  84% 13%



4.2.103 Score per residue for model 103

- Molecule 1: Ubiquitin

Chain A:  87% 13%



4.2.104 Score per residue for model 104

- Molecule 1: Ubiquitin

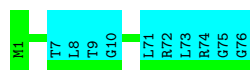
Chain A:  86% 13%



4.2.105 Score per residue for model 105

- Molecule 1: Ubiquitin

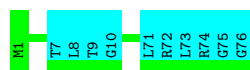
Chain A:  87% 13%



4.2.106 Score per residue for model 106

- Molecule 1: Ubiquitin

Chain A:  87% 13%



4.2.107 Score per residue for model 107

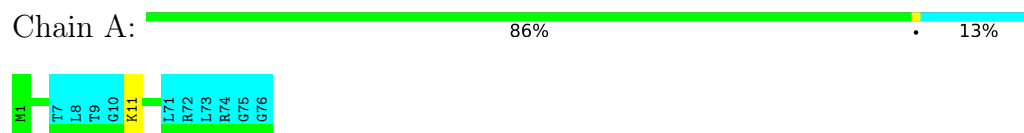
- Molecule 1: Ubiquitin

Chain A:  86% 13%



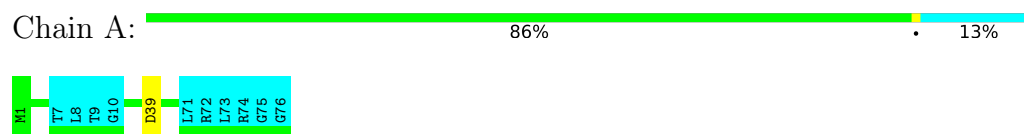
4.2.108 Score per residue for model 108

- Molecule 1: Ubiquitin



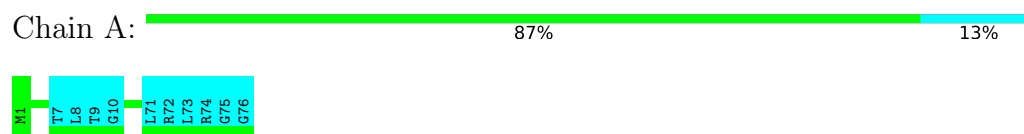
4.2.109 Score per residue for model 109

- Molecule 1: Ubiquitin



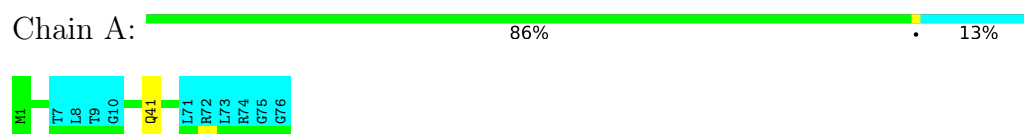
4.2.110 Score per residue for model 110

- Molecule 1: Ubiquitin



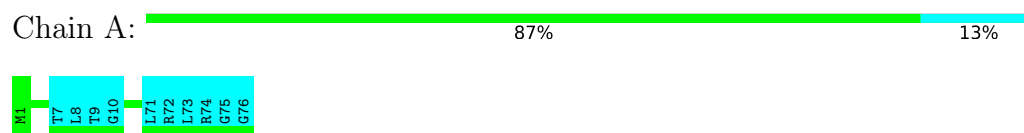
4.2.111 Score per residue for model 111

- 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

Chain A:  86% 13%



4.2.114 Score per residue for model 114

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.115 Score per residue for model 115

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.116 Score per residue for model 116

- Molecule 1: Ubiquitin

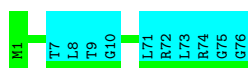
Chain A:  86% 13%



4.2.117 Score per residue for model 117

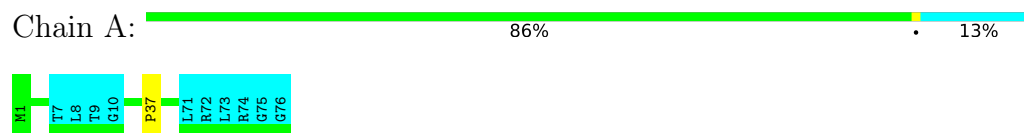
- Molecule 1: Ubiquitin

Chain A:  87% 13%



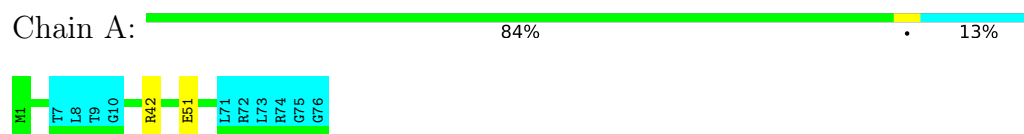
4.2.118 Score per residue for model 118

- Molecule 1: Ubiquitin



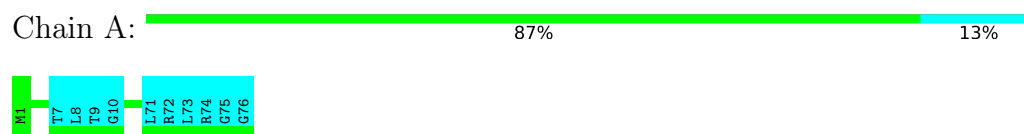
4.2.119 Score per residue for model 119

- Molecule 1: Ubiquitin



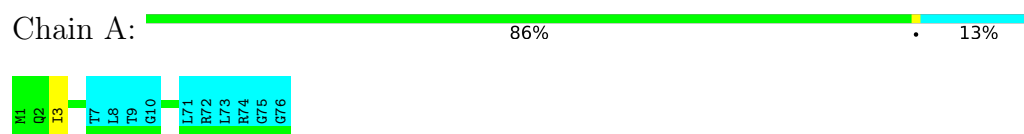
4.2.120 Score per residue for model 120

- Molecule 1: Ubiquitin



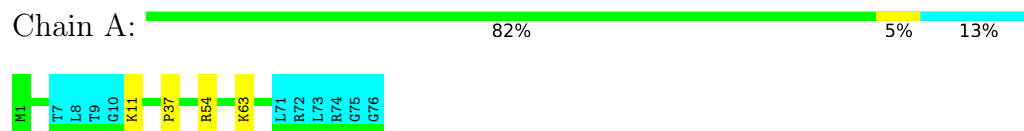
4.2.121 Score per residue for model 121

- 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

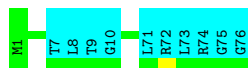
Chain A:  86% 13%



4.2.124 Score per residue for model 124

- Molecule 1: Ubiquitin

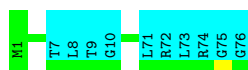
Chain A:  87% 13%



4.2.125 Score per residue for model 125

- Molecule 1: Ubiquitin

Chain A:  87% 13%



4.2.126 Score per residue for model 126

- Molecule 1: Ubiquitin

Chain A:  84% 13%



4.2.127 Score per residue for model 127

- Molecule 1: Ubiquitin

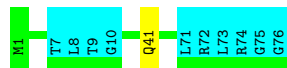
Chain A:  84% 13%



4.2.128 Score per residue for model 128

- Molecule 1: Ubiquitin

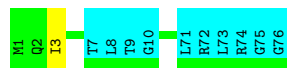
Chain A:  86% 13%



4.2.129 Score per residue for model 129

- Molecule 1: Ubiquitin

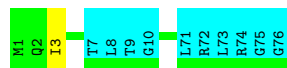
Chain A:  86% 13%



4.2.130 Score per residue for model 130

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.131 Score per residue for model 131

- Molecule 1: Ubiquitin

Chain A:  84% 13%



4.2.132 Score per residue for model 132

- Molecule 1: Ubiquitin

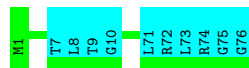
Chain A:  86% 13%



4.2.133 Score per residue for model 133

- Molecule 1: Ubiquitin

Chain A:  87% 13%



4.2.134 Score per residue for model 134

- Molecule 1: Ubiquitin

Chain A:  84% 13%



4.2.135 Score per residue for model 135

- Molecule 1: Ubiquitin

Chain A:  83% 13%



4.2.136 Score per residue for model 136

- Molecule 1: Ubiquitin

Chain A:  87% 13%



4.2.137 Score per residue for model 137

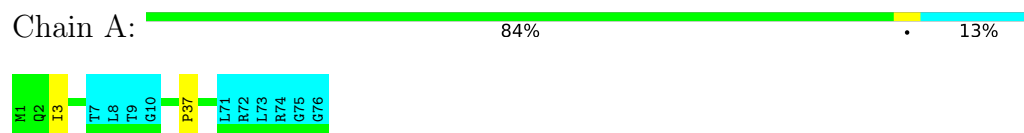
- Molecule 1: Ubiquitin

Chain A:  87% 13%



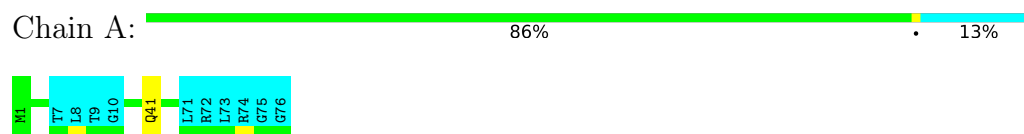
4.2.138 Score per residue for model 138

- Molecule 1: Ubiquitin



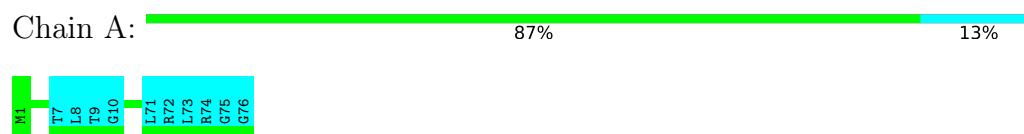
4.2.139 Score per residue for model 139

- Molecule 1: Ubiquitin



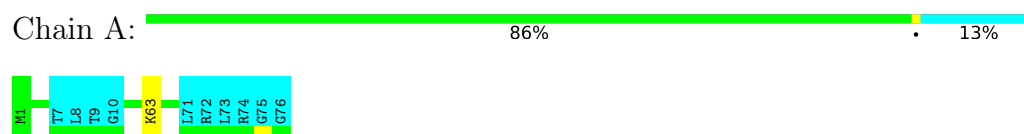
4.2.140 Score per residue for model 140

- Molecule 1: Ubiquitin



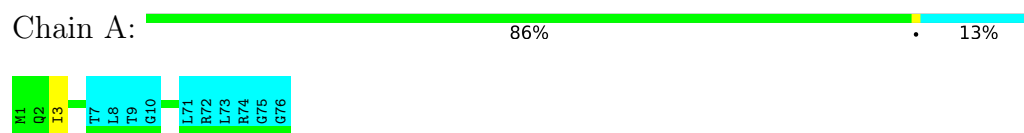
4.2.141 Score per residue for model 141

- 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

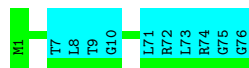
Chain A:  86% 13%



4.2.144 Score per residue for model 144

- Molecule 1: Ubiquitin

Chain A:  87% 13%



4.2.145 Score per residue for model 145

- Molecule 1: Ubiquitin

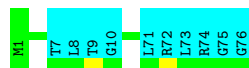
Chain A:  86% 13%



4.2.146 Score per residue for model 146

- Molecule 1: Ubiquitin

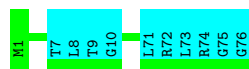
Chain A:  87% 13%



4.2.147 Score per residue for model 147

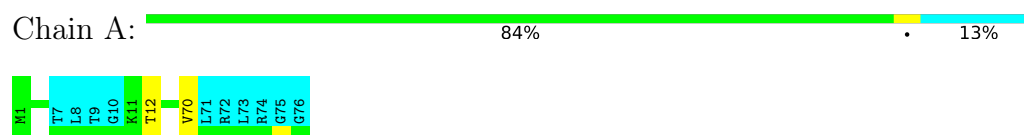
- Molecule 1: Ubiquitin

Chain A:  87% 13%



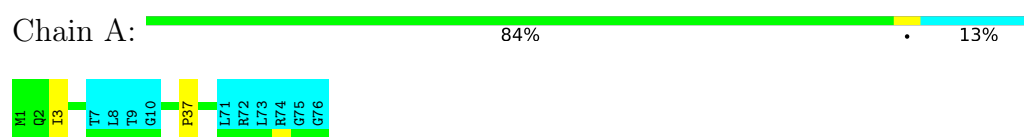
4.2.148 Score per residue for model 148

- Molecule 1: Ubiquitin



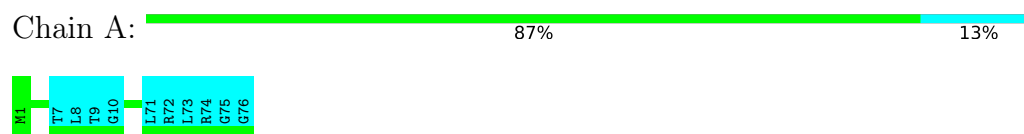
4.2.149 Score per residue for model 149

- Molecule 1: Ubiquitin



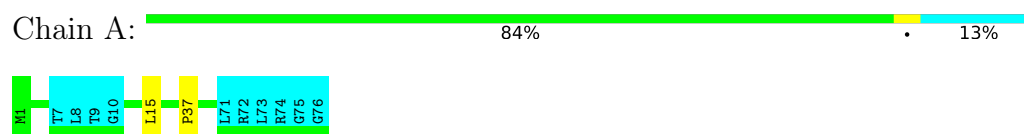
4.2.150 Score per residue for model 150

- Molecule 1: Ubiquitin



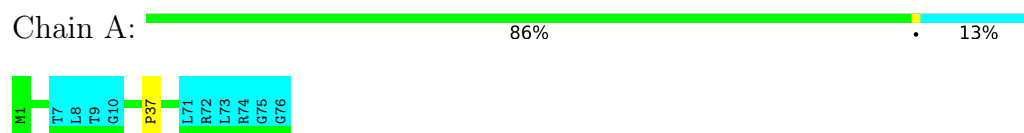
4.2.151 Score per residue for model 151

- Molecule 1: Ubiquitin



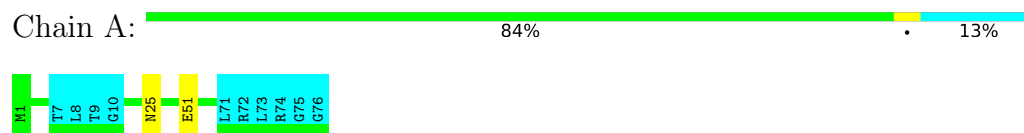
4.2.152 Score per residue for model 152

- Molecule 1: Ubiquitin



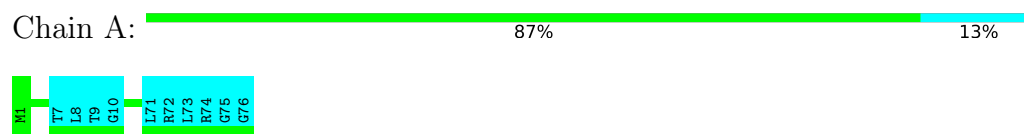
4.2.153 Score per residue for model 153

- Molecule 1: Ubiquitin



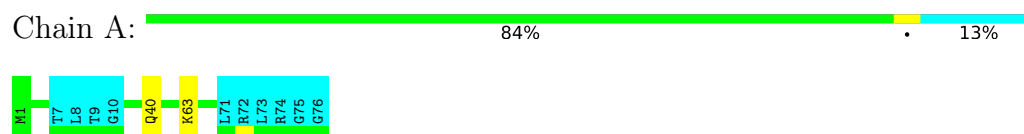
4.2.154 Score per residue for model 154

- Molecule 1: Ubiquitin



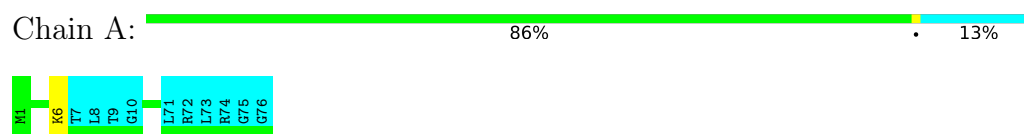
4.2.155 Score per residue for model 155

- Molecule 1: Ubiquitin



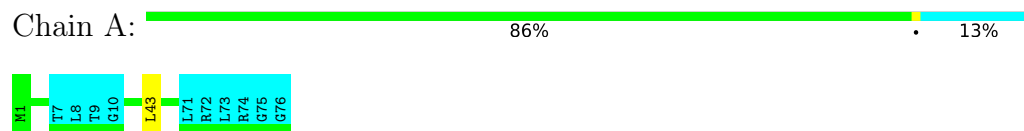
4.2.156 Score per residue for model 156

- Molecule 1: Ubiquitin



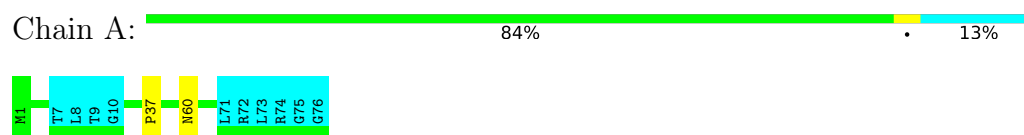
4.2.157 Score per residue for model 157

- Molecule 1: Ubiquitin



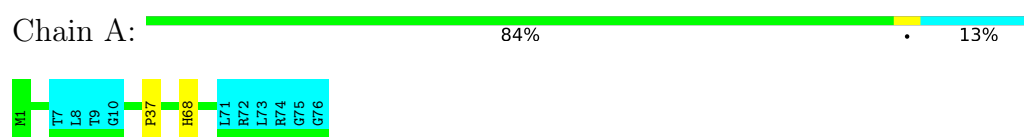
4.2.158 Score per residue for model 158

- Molecule 1: Ubiquitin



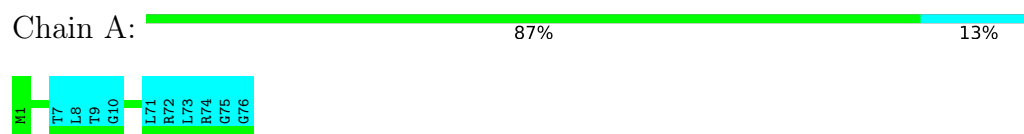
4.2.159 Score per residue for model 159

- Molecule 1: Ubiquitin



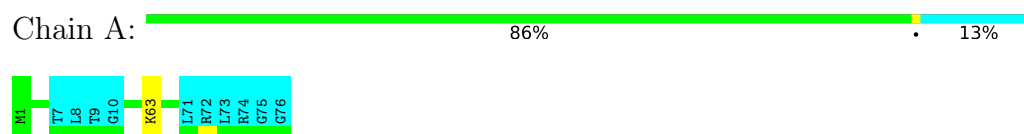
4.2.160 Score per residue for model 160

- Molecule 1: Ubiquitin



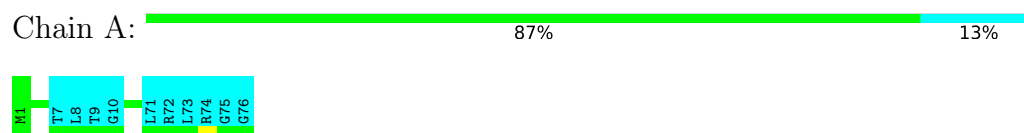
4.2.161 Score per residue for model 161

- Molecule 1: Ubiquitin



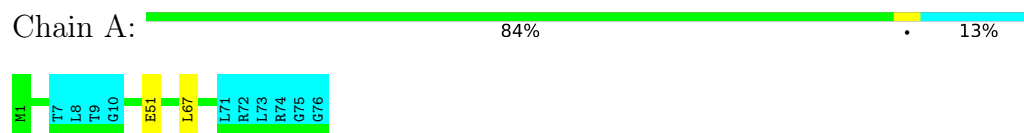
4.2.162 Score per residue for model 162

- Molecule 1: Ubiquitin



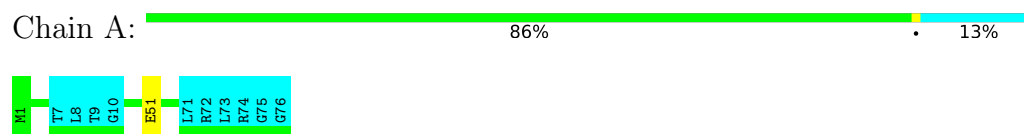
4.2.163 Score per residue for model 163

- Molecule 1: Ubiquitin



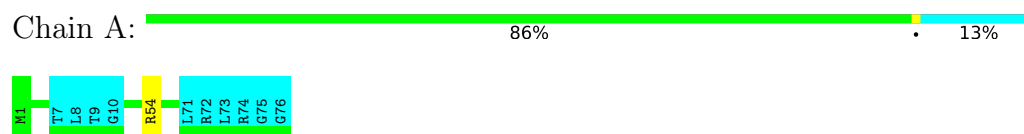
4.2.164 Score per residue for model 164

- Molecule 1: Ubiquitin



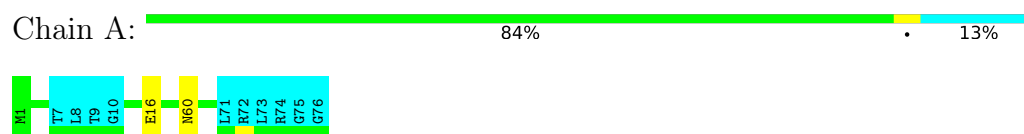
4.2.165 Score per residue for model 165

- Molecule 1: Ubiquitin



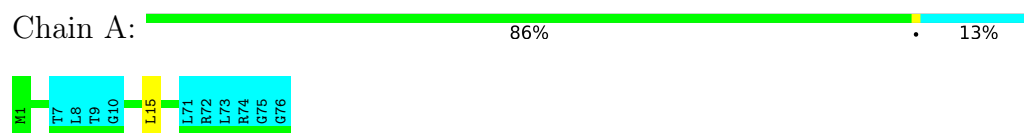
4.2.166 Score per residue for model 166

- Molecule 1: Ubiquitin



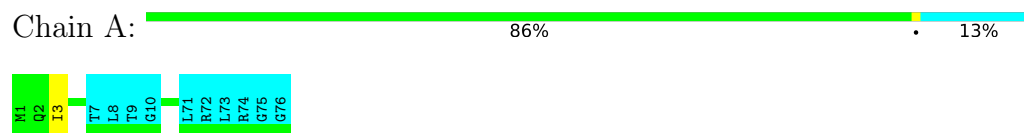
4.2.167 Score per residue for model 167

- Molecule 1: Ubiquitin



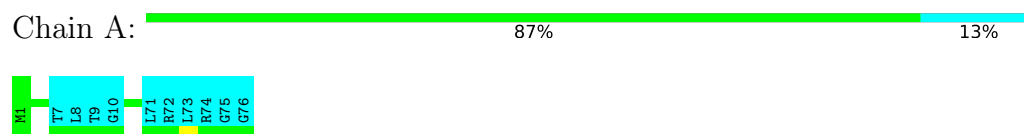
4.2.168 Score per residue for model 168

- Molecule 1: Ubiquitin



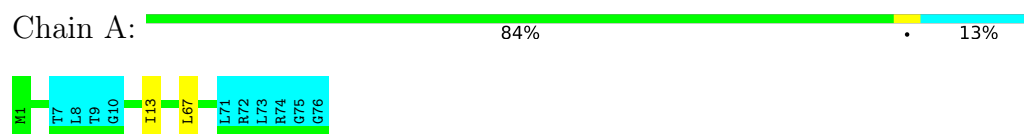
4.2.169 Score per residue for model 169

- Molecule 1: Ubiquitin



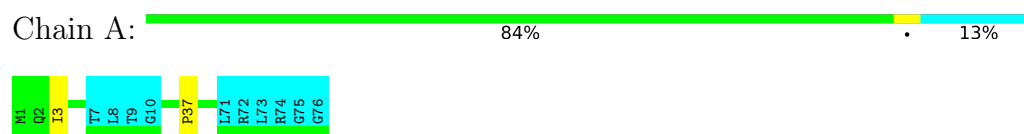
4.2.170 Score per residue for model 170

- Molecule 1: Ubiquitin



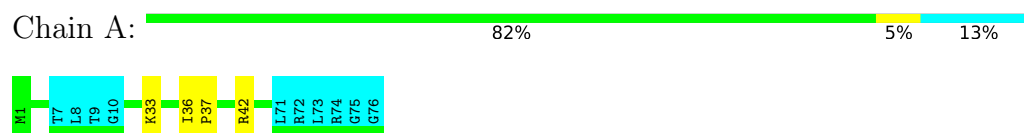
4.2.171 Score per residue for model 171

- Molecule 1: Ubiquitin



4.2.172 Score per residue for model 172

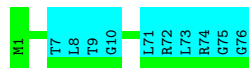
- Molecule 1: Ubiquitin



4.2.173 Score per residue for model 173

- Molecule 1: Ubiquitin

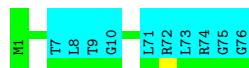
Chain A:  87% 13%



4.2.174 Score per residue for model 174

- Molecule 1: Ubiquitin

Chain A:  87% 13%



4.2.175 Score per residue for model 175

- Molecule 1: Ubiquitin

Chain A:  86% 13%



4.2.176 Score per residue for model 176

- Molecule 1: Ubiquitin

Chain A:  84% 13%



5 Refinement protocol and experimental data overview

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

Of the 800 calculated structures, 176 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
GROMACS	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	997
Number of shifts mapped to atoms	997
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.56±0.01	0±0/536 (0.0± 0.0%)	1.33±0.04	1±1/723 (0.1± 0.1%)
All	All	0.56	0/94336 (0.0%)	1.33	106/127248 (0.1%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
All	All	0	12

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	37	PRO	N-CA-CB	6.94	107.08	103.19	118	34
1	A	36	ILE	CA-C-N	6.93	124.72	119.66	80	8
1	A	36	ILE	C-N-CA	6.93	124.72	119.66	80	8
1	A	51	GLU	CA-C-N	6.03	129.18	120.38	99	13
1	A	51	GLU	C-N-CA	6.03	129.18	120.38	99	13
1	A	63	LYS	CA-C-N	5.75	132.06	121.70	122	1
1	A	63	LYS	C-N-CA	5.75	132.06	121.70	122	1
1	A	37	PRO	N-CA-C	5.64	115.88	110.47	172	3
1	A	39	ASP	CA-CB-CG	5.46	118.06	112.60	37	1
1	A	68	HIS	CB-CG-CD2	-5.29	124.33	131.20	176	3
1	A	37	PRO	CA-C-N	5.20	125.50	119.47	171	4
1	A	37	PRO	C-N-CA	5.20	125.50	119.47	171	4
1	A	41	GLN	OE1-CD-NE2	-5.19	117.41	122.60	2	8
1	A	40	GLN	OE1-CD-NE2	-5.10	117.50	122.60	52	1
1	A	60	ASN	CA-CB-CG	5.10	117.70	112.60	166	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	25	ASN	CA-CB-CG	5.05	117.65	112.60	153	1
1	A	49	GLN	OE1-CD-NE2	-5.04	117.56	122.60	16	1
1	A	52	ASP	CA-CB-CG	5.04	117.64	112.60	95	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	41	GLN	Peptide	6
1	A	54	ARG	Sidechain	3
1	A	42	ARG	Sidechain	2
1	A	17	VAL	Peptide	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
All	All	93104	96272	96272	-

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 -.

There are no clashes.

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	65/76 (86%)	64±1 (99±1%)	0±1 (1±1%)	0±0 (0±0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	11440/13376 (86%)	11349 (99%)	88 (1%)	3 (0%)	100	100

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	63	LYS	3

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	61/68 (90%)	60±1 (99±1%)	1±1 (1±1%)	68	95
All	All	10736/11968 (90%)	10635 (99%)	101 (1%)	68	95

All 32 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	3	ILE	16
1	A	15	LEU	9
1	A	63	LYS	8
1	A	48	LYS	6
1	A	21	ASP	5
1	A	24	GLU	5
1	A	16	GLU	4
1	A	12	THR	4
1	A	70	VAL	4
1	A	64	GLU	3
1	A	69	LEU	3
1	A	39	ASP	3
1	A	42	ARG	3
1	A	11	LYS	3
1	A	22	THR	2
1	A	26	VAL	2
1	A	29	LYS	2
1	A	13	ILE	2
1	A	51	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	43	LEU	2
1	A	67	LEU	2
1	A	23	ILE	1
1	A	44	ILE	1
1	A	25	ASN	1
1	A	50	LEU	1
1	A	20	SER	1
1	A	14	THR	1
1	A	54	ARG	1
1	A	40	GLN	1
1	A	6	LYS	1
1	A	60	ASN	1
1	A	33	LYS	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 94% for the well-defined parts and 93% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `ubi_chemical_shifts.str`

7.1.1 Bookkeeping

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	997
Number of shifts mapped to atoms	997
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	76	-0.25 ± 0.24	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	70	0.16 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	76	-0.31 ± 0.12	None needed (< 0.5 ppm)
^{15}N	75	0.80 ± 0.37	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 872 atoms were assigned a chemical shift out of a possible 931. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	325/327 (99%)	131/132 (99%)	132/132 (100%)	62/63 (98%)
Sidechain	521/568 (92%)	353/366 (96%)	160/181 (88%)	8/21 (38%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	26/36 (72%)	16/18 (89%)	10/17 (59%)	0/1 (0%)
Overall	872/931 (94%)	500/516 (97%)	302/330 (92%)	70/85 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 994 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	378/380 (99%)	154/155 (99%)	152/152 (100%)	72/73 (99%)
Sidechain	590/655 (90%)	400/423 (95%)	182/205 (89%)	8/27 (30%)
Aromatic	26/36 (72%)	16/18 (89%)	10/17 (59%)	0/1 (0%)
Overall	994/1071 (93%)	570/596 (96%)	344/374 (92%)	80/101 (79%)

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:

