



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 08:04 AM UTC

PDB ID : 2NR2 / pdb_00002nr2
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

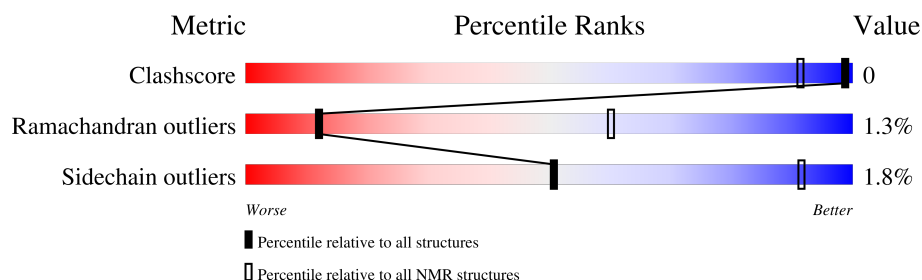
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	76	

2 Ensemble composition and analysis

This entry contains 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)	0.62	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.

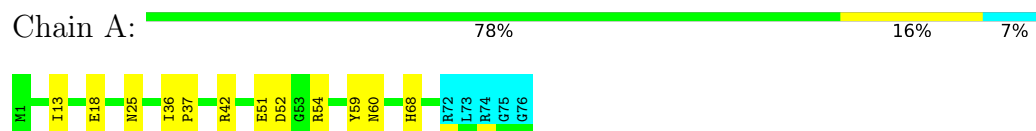
Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1231	378	629	105	118	1	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Ubiquitin

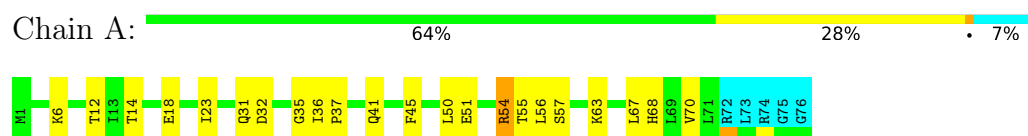


4.2 Scores per residue for each member of the ensemble

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

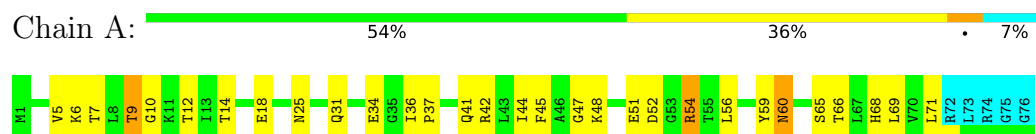
4.2.1 Score per residue for model 1

- Molecule 1: Ubiquitin



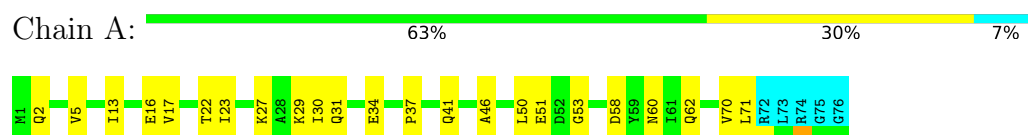
4.2.2 Score per residue for model 2

- Molecule 1: Ubiquitin



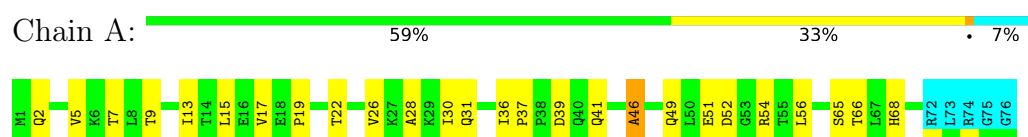
4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin



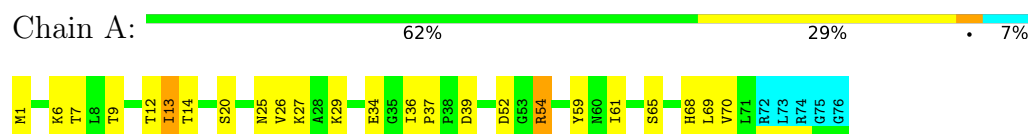
4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin



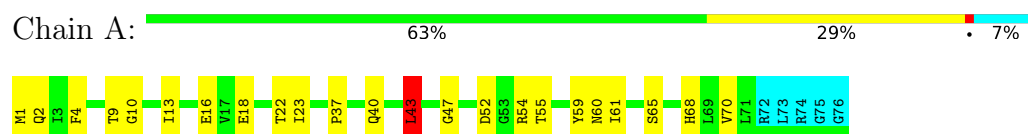
4.2.5 Score per residue for model 5

- Molecule 1: Ubiquitin



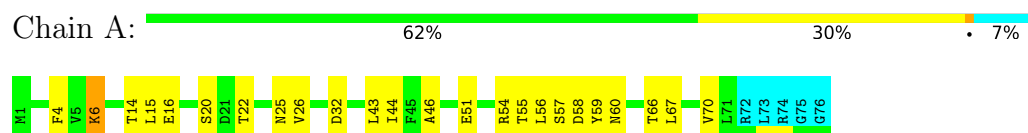
4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin



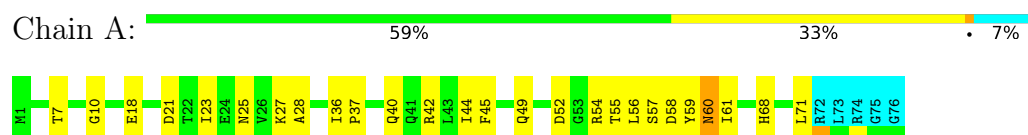
4.2.7 Score per residue for model 7

- Molecule 1: Ubiquitin



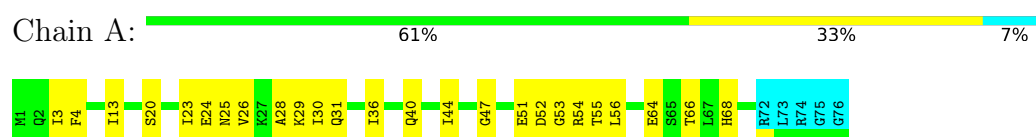
4.2.8 Score per residue for model 8

- Molecule 1: Ubiquitin



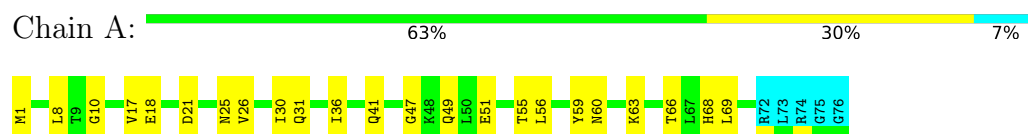
4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin



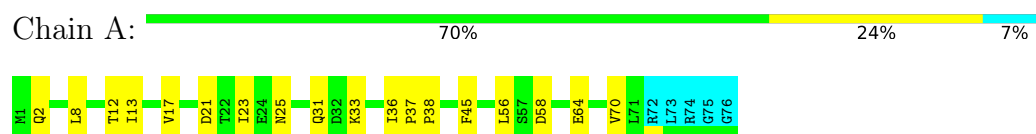
4.2.10 Score per residue for model 10

- Molecule 1: Ubiquitin



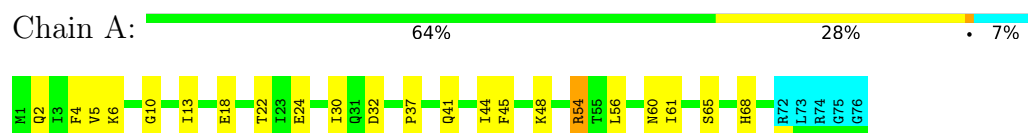
4.2.11 Score per residue for model 11

- Molecule 1: Ubiquitin



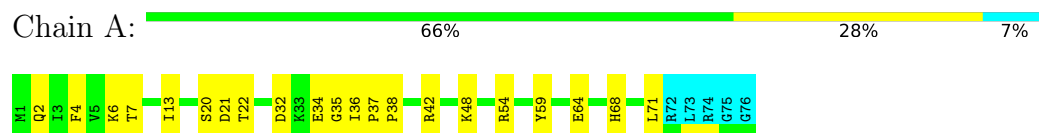
4.2.12 Score per residue for model 12

- Molecule 1: Ubiquitin



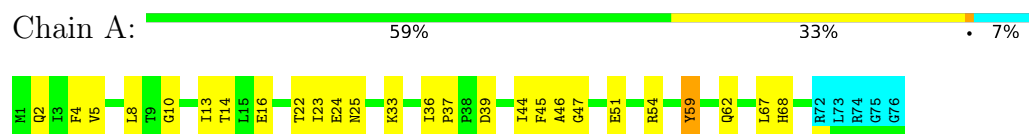
4.2.13 Score per residue for model 13

- Molecule 1: Ubiquitin



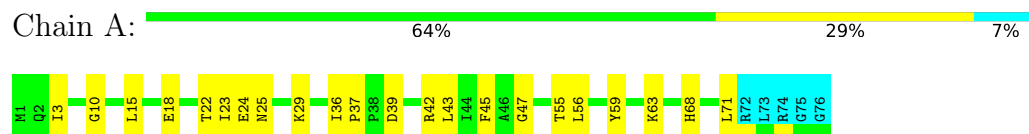
4.2.14 Score per residue for model 14

- Molecule 1: Ubiquitin



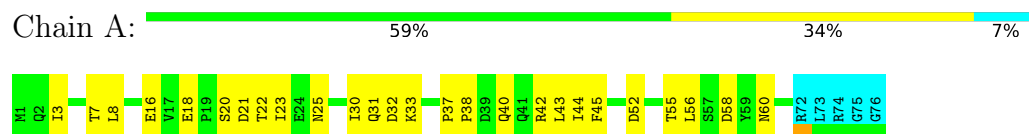
4.2.15 Score per residue for model 15

- Molecule 1: Ubiquitin



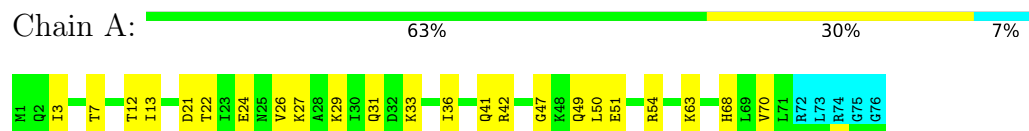
4.2.16 Score per residue for model 16

- Molecule 1: Ubiquitin



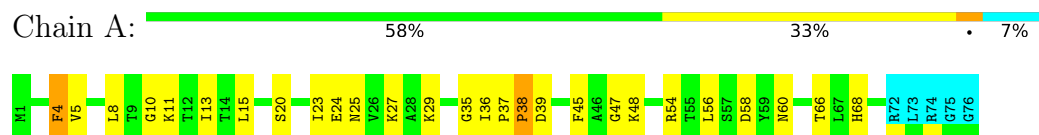
4.2.17 Score per residue for model 17

- Molecule 1: Ubiquitin



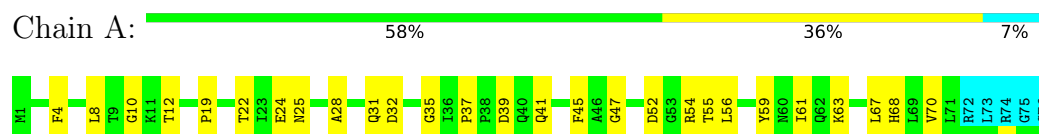
4.2.18 Score per residue for model 18

- Molecule 1: Ubiquitin



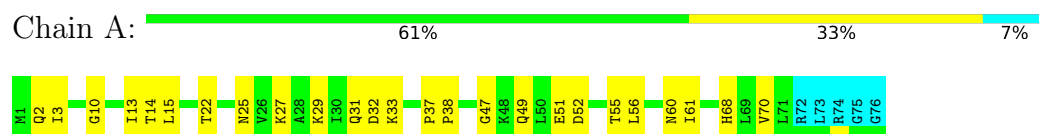
4.2.19 Score per residue for model 19

- Molecule 1: Ubiquitin



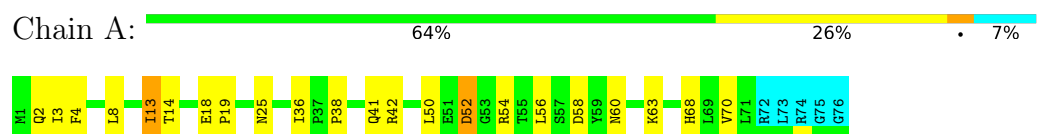
4.2.20 Score per residue for model 20

- Molecule 1: Ubiquitin



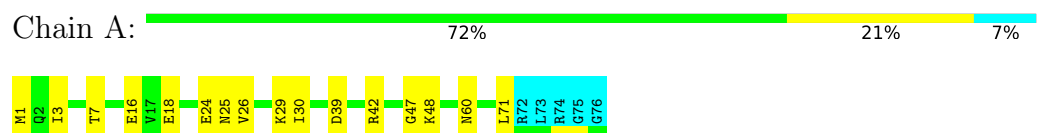
4.2.21 Score per residue for model 21

- Molecule 1: Ubiquitin



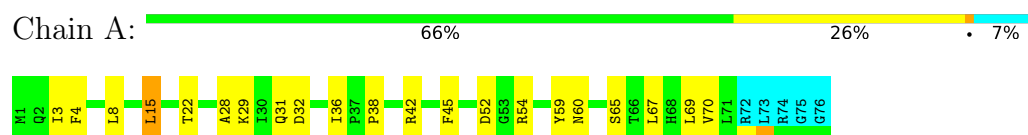
4.2.22 Score per residue for model 22

- Molecule 1: Ubiquitin



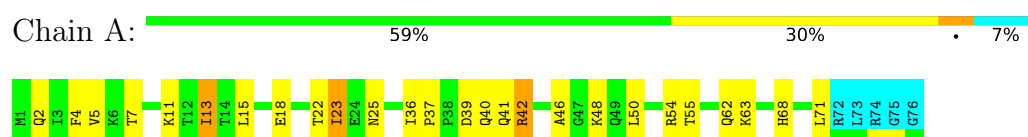
4.2.23 Score per residue for model 23

- Molecule 1: Ubiquitin



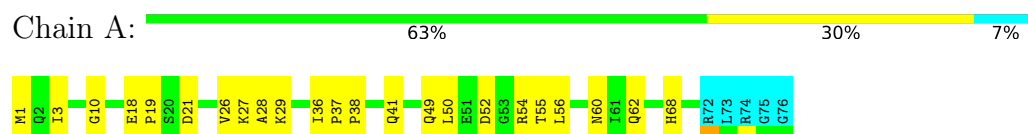
4.2.24 Score per residue for model 24

- Molecule 1: Ubiquitin



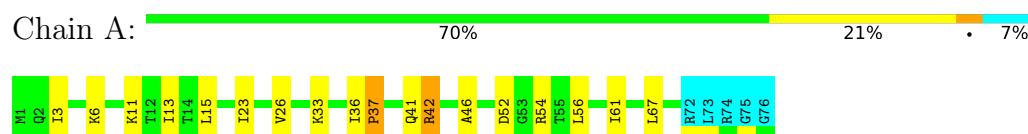
4.2.25 Score per residue for model 25

- Molecule 1: Ubiquitin



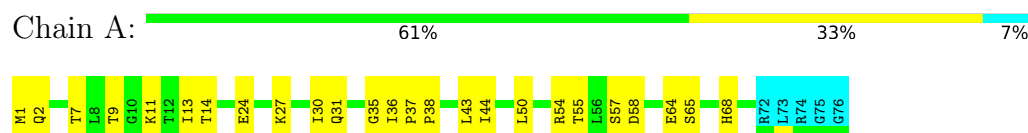
4.2.26 Score per residue for model 26

- Molecule 1: Ubiquitin



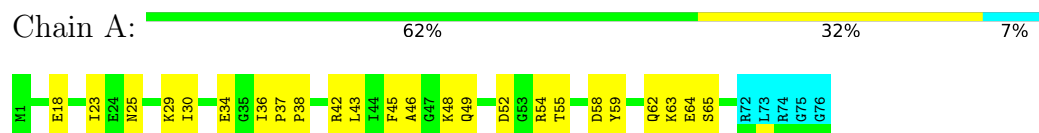
4.2.27 Score per residue for model 27

- Molecule 1: Ubiquitin



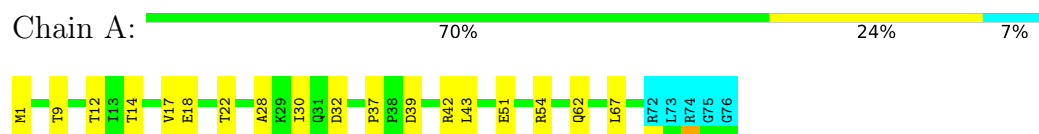
4.2.28 Score per residue for model 28

- Molecule 1: Ubiquitin



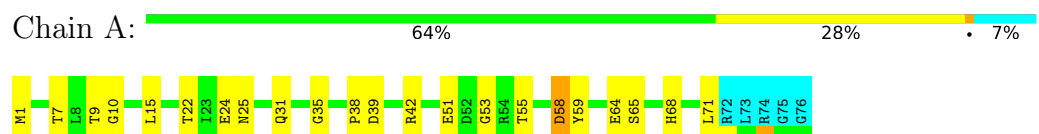
4.2.29 Score per residue for model 29

- Molecule 1: Ubiquitin



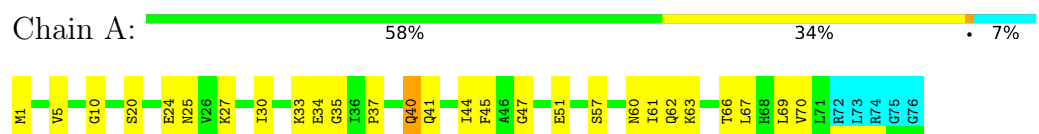
4.2.30 Score per residue for model 30

- Molecule 1: Ubiquitin



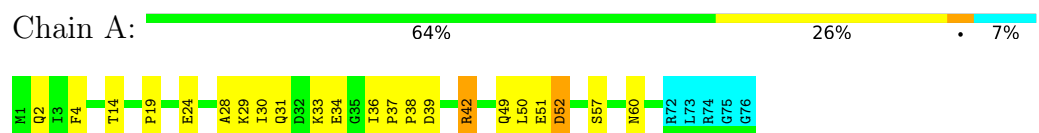
4.2.31 Score per residue for model 31

- Molecule 1: Ubiquitin



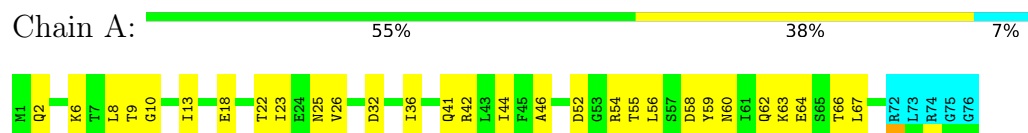
4.2.32 Score per residue for model 32

- Molecule 1: Ubiquitin



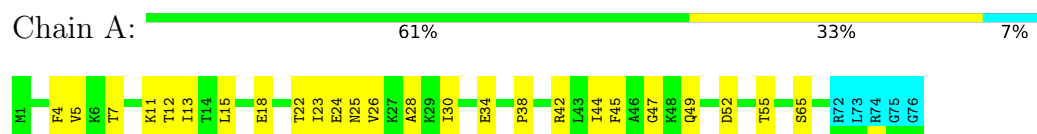
4.2.33 Score per residue for model 33

- Molecule 1: Ubiquitin



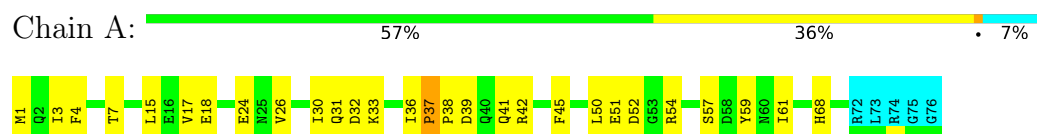
4.2.34 Score per residue for model 34

- Molecule 1: Ubiquitin



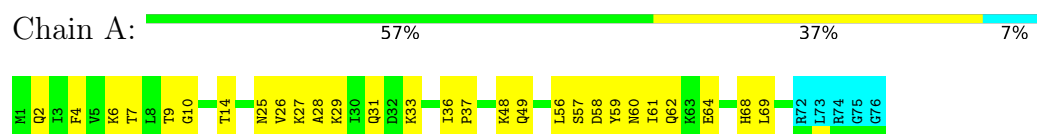
4.2.35 Score per residue for model 35

- Molecule 1: Ubiquitin



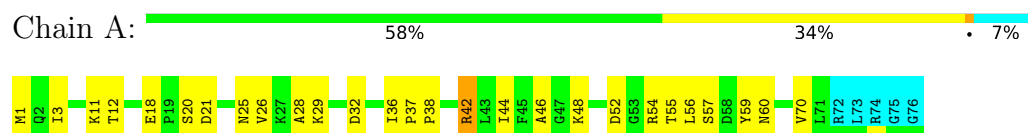
4.2.36 Score per residue for model 36

- Molecule 1: Ubiquitin



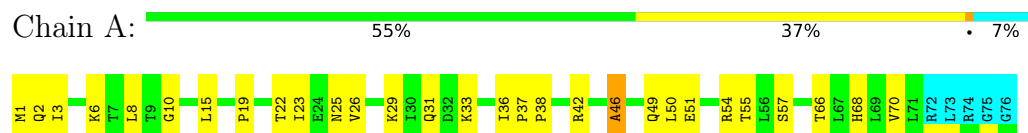
4.2.37 Score per residue for model 37

- Molecule 1: Ubiquitin



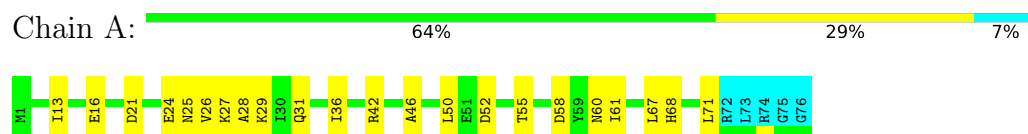
4.2.38 Score per residue for model 38

- Molecule 1: Ubiquitin



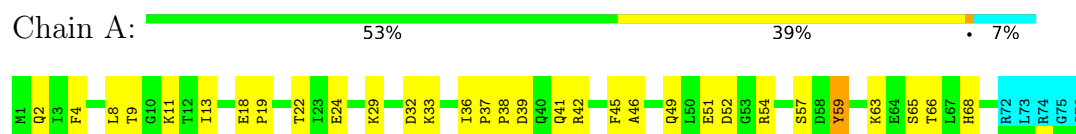
4.2.39 Score per residue for model 39

- Molecule 1: Ubiquitin



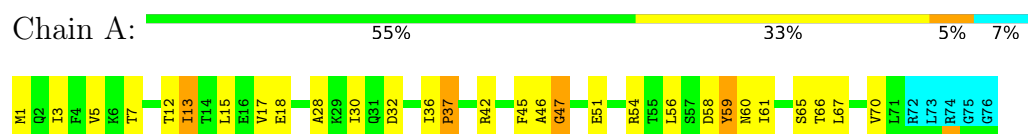
4.2.40 Score per residue for model 40

- Molecule 1: Ubiquitin



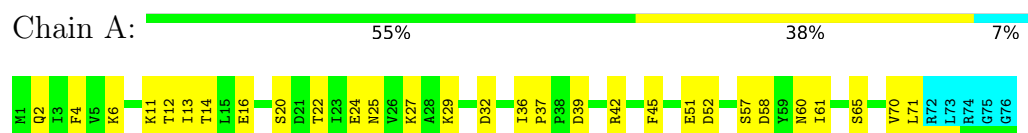
4.2.41 Score per residue for model 41

- Molecule 1: Ubiquitin



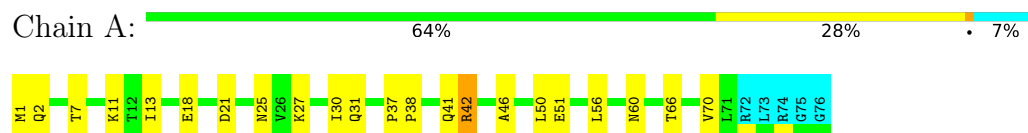
4.2.42 Score per residue for model 42

- Molecule 1: Ubiquitin



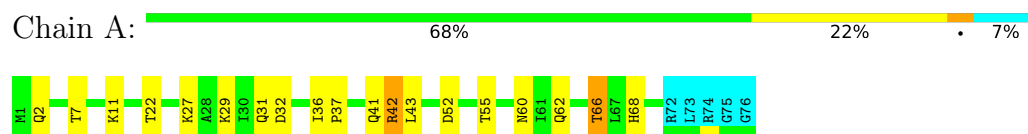
4.2.43 Score per residue for model 43

- Molecule 1: Ubiquitin



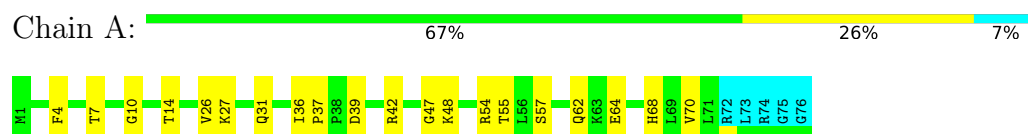
4.2.44 Score per residue for model 44

- Molecule 1: Ubiquitin



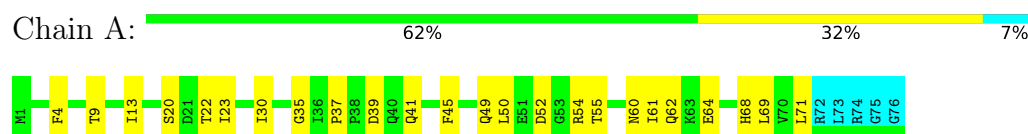
4.2.45 Score per residue for model 45

- Molecule 1: Ubiquitin



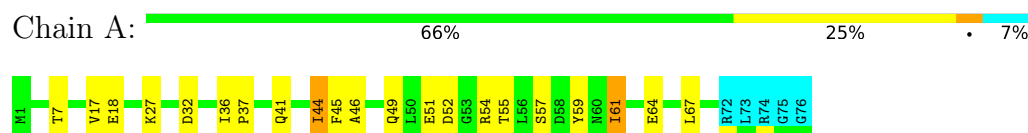
4.2.46 Score per residue for model 46

- Molecule 1: Ubiquitin



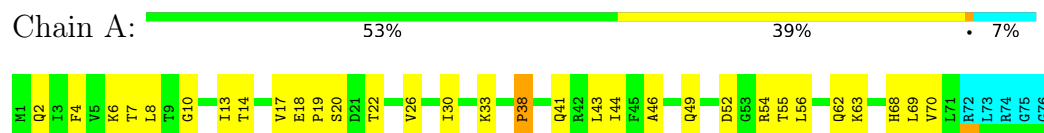
4.2.47 Score per residue for model 47

- Molecule 1: Ubiquitin



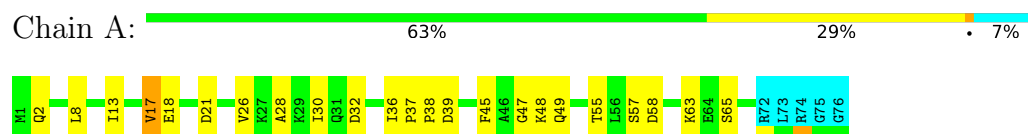
4.2.48 Score per residue for model 48

- Molecule 1: Ubiquitin



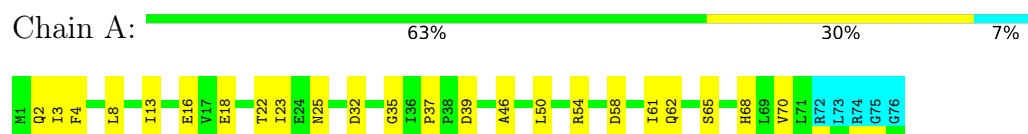
4.2.49 Score per residue for model 49

- Molecule 1: Ubiquitin



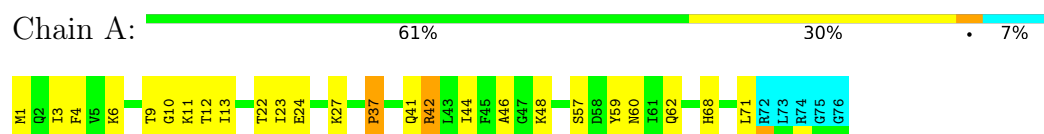
4.2.50 Score per residue for model 50

- Molecule 1: Ubiquitin



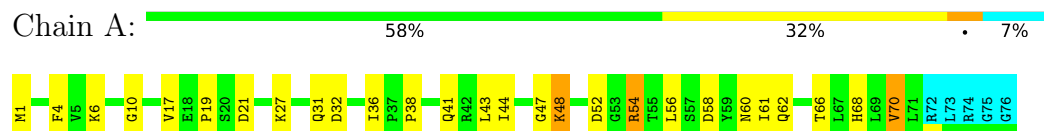
4.2.51 Score per residue for model 51

- Molecule 1: Ubiquitin



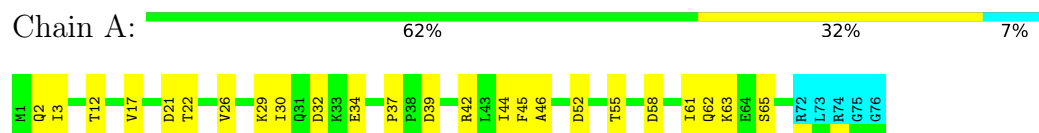
4.2.52 Score per residue for model 52

- Molecule 1: Ubiquitin



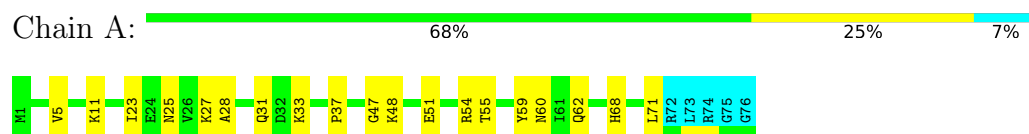
4.2.53 Score per residue for model 53

- Molecule 1: Ubiquitin



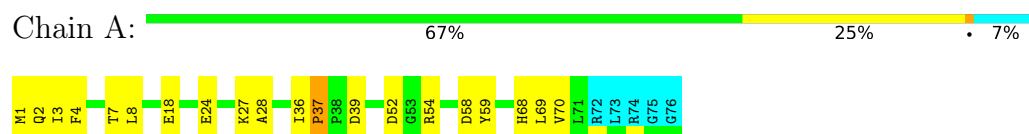
4.2.54 Score per residue for model 54

- Molecule 1: Ubiquitin



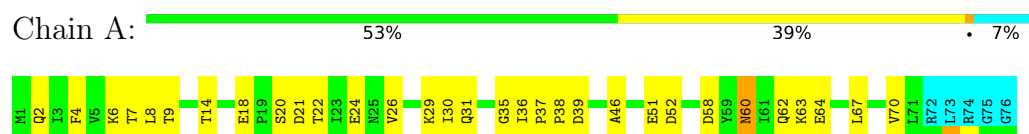
4.2.55 Score per residue for model 55

- Molecule 1: Ubiquitin



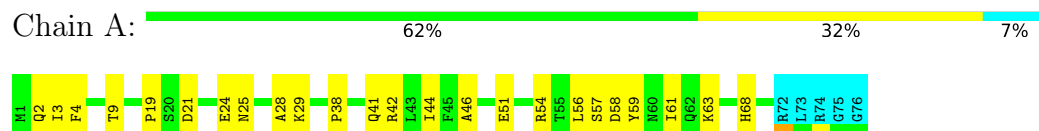
4.2.56 Score per residue for model 56

- Molecule 1: Ubiquitin



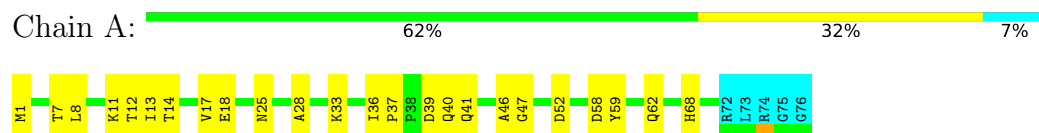
4.2.57 Score per residue for model 57

- Molecule 1: Ubiquitin



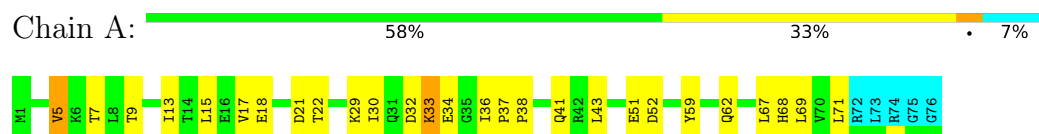
4.2.58 Score per residue for model 58

- Molecule 1: Ubiquitin



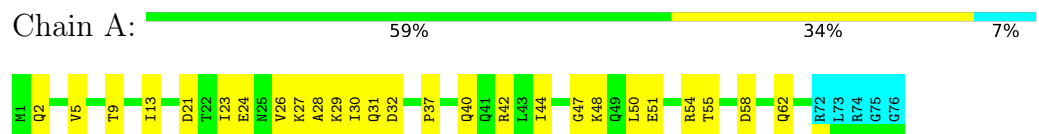
4.2.59 Score per residue for model 59

- Molecule 1: Ubiquitin



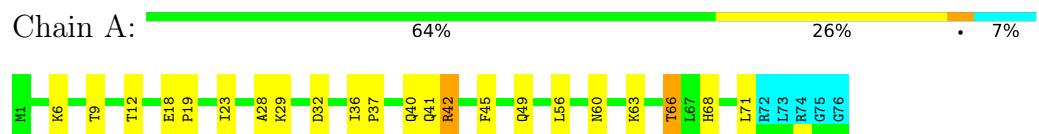
4.2.60 Score per residue for model 60

- Molecule 1: Ubiquitin



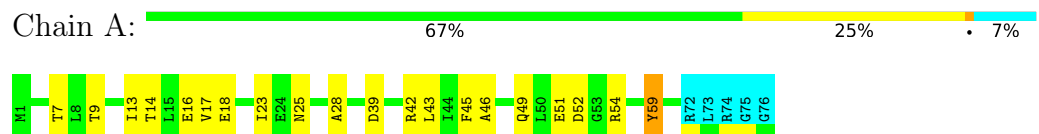
4.2.61 Score per residue for model 61

- Molecule 1: Ubiquitin



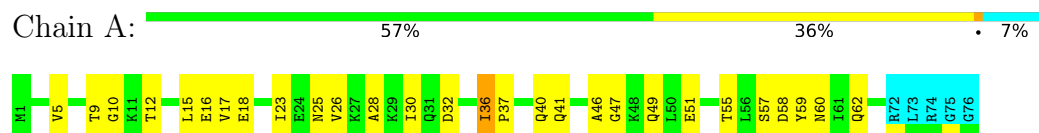
4.2.62 Score per residue for model 62

- Molecule 1: Ubiquitin



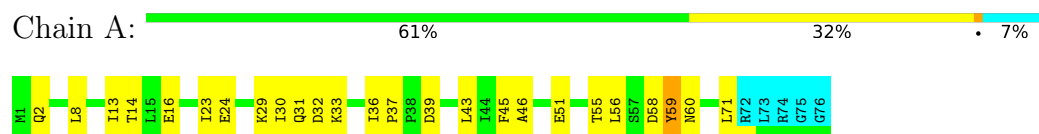
4.2.63 Score per residue for model 63

- Molecule 1: Ubiquitin



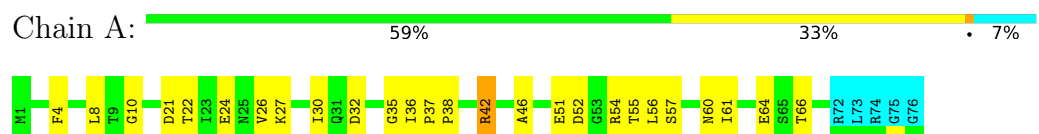
4.2.64 Score per residue for model 64

- Molecule 1: Ubiquitin



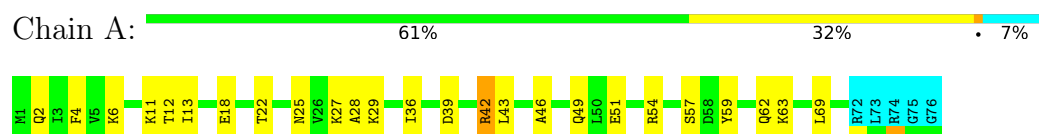
4.2.65 Score per residue for model 65

- Molecule 1: Ubiquitin



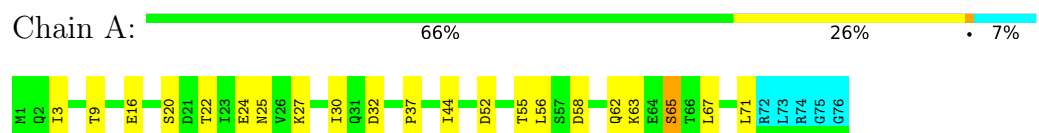
4.2.66 Score per residue for model 66

- Molecule 1: Ubiquitin



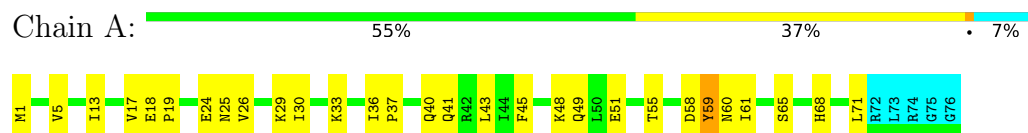
4.2.67 Score per residue for model 67

- Molecule 1: Ubiquitin



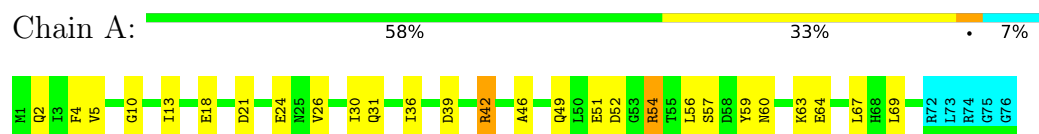
4.2.68 Score per residue for model 68

- Molecule 1: Ubiquitin



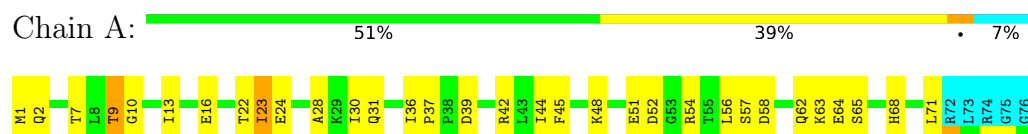
4.2.69 Score per residue for model 69

- Molecule 1: Ubiquitin



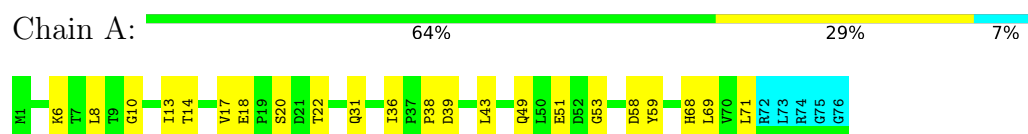
4.2.70 Score per residue for model 70

- Molecule 1: Ubiquitin



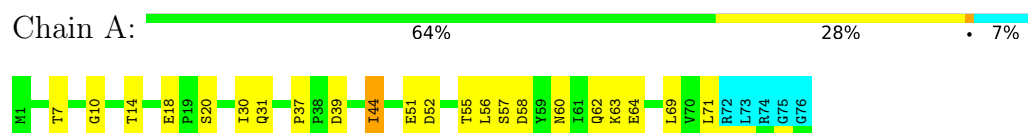
4.2.71 Score per residue for model 71

- Molecule 1: Ubiquitin



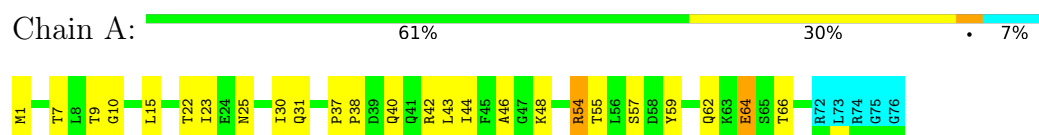
4.2.72 Score per residue for model 72

- Molecule 1: Ubiquitin



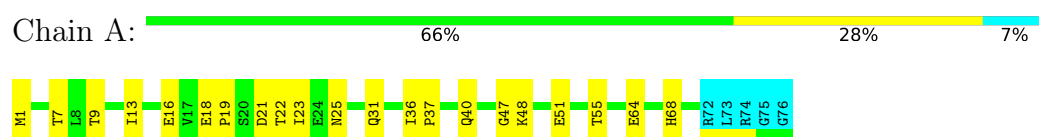
4.2.73 Score per residue for model 73

- Molecule 1: Ubiquitin



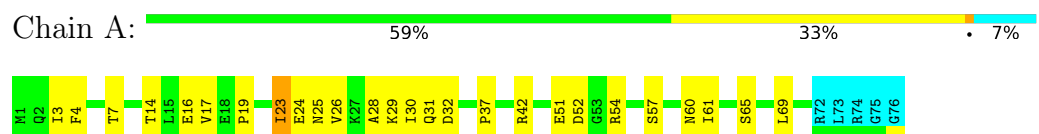
4.2.74 Score per residue for model 74

- Molecule 1: Ubiquitin



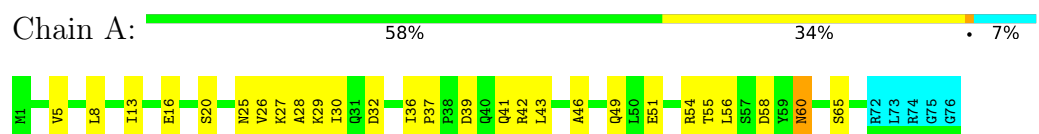
4.2.75 Score per residue for model 75

- Molecule 1: Ubiquitin



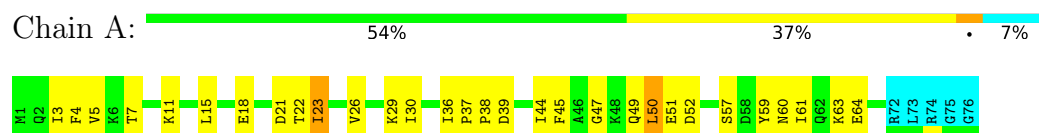
4.2.76 Score per residue for model 76

- Molecule 1: Ubiquitin



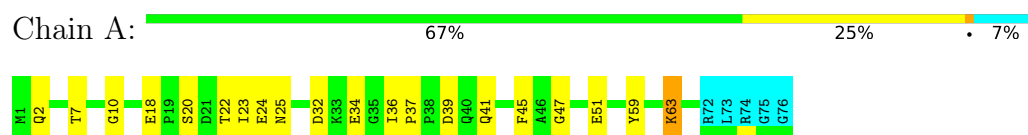
4.2.77 Score per residue for model 77

- Molecule 1: Ubiquitin



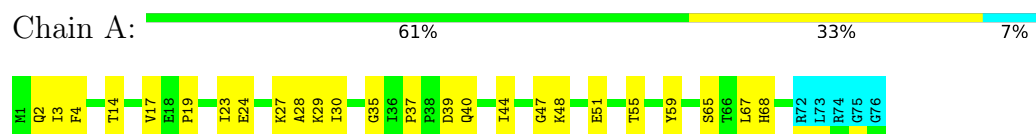
4.2.78 Score per residue for model 78

- Molecule 1: Ubiquitin



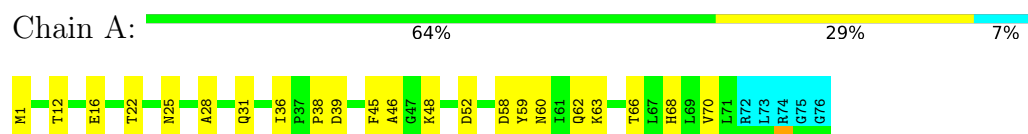
4.2.79 Score per residue for model 79

- Molecule 1: Ubiquitin



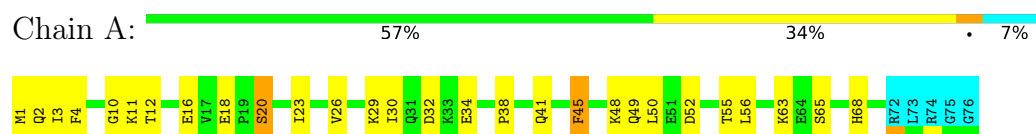
4.2.80 Score per residue for model 80

- Molecule 1: Ubiquitin



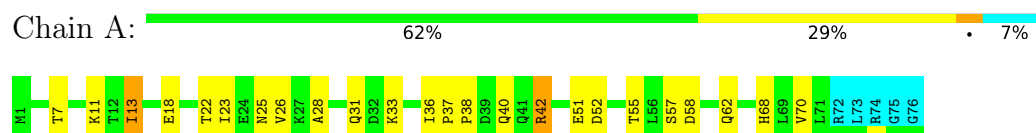
4.2.81 Score per residue for model 81

- Molecule 1: Ubiquitin



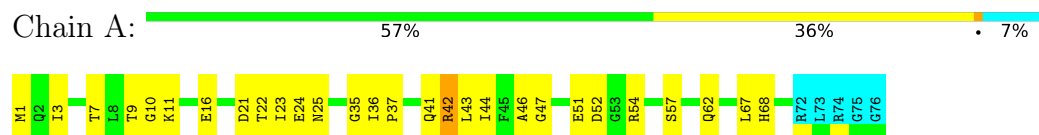
4.2.82 Score per residue for model 82

- Molecule 1: Ubiquitin



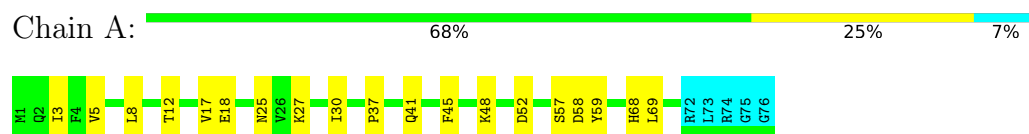
4.2.83 Score per residue for model 83

- Molecule 1: Ubiquitin



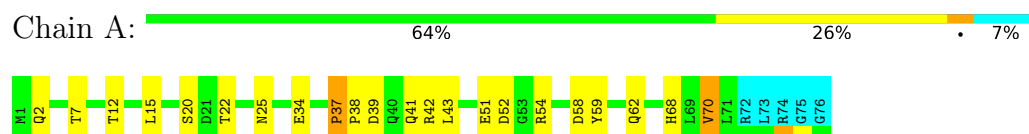
4.2.84 Score per residue for model 84

- Molecule 1: Ubiquitin



4.2.85 Score per residue for model 85

- Molecule 1: Ubiquitin



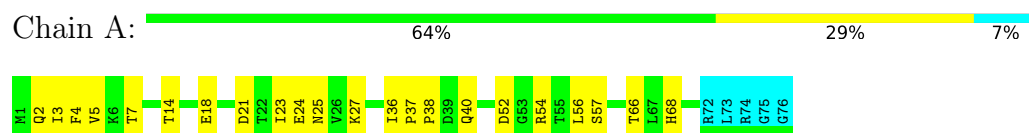
4.2.86 Score per residue for model 86

- Molecule 1: Ubiquitin



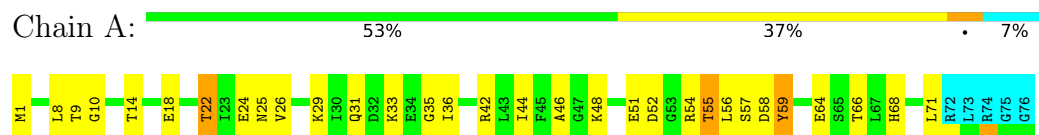
4.2.87 Score per residue for model 87

- Molecule 1: Ubiquitin



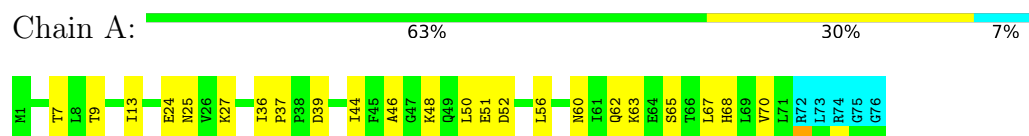
4.2.88 Score per residue for model 88

- Molecule 1: Ubiquitin



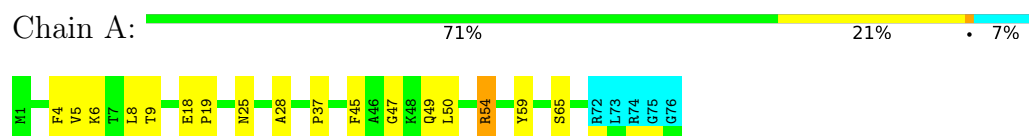
4.2.89 Score per residue for model 89

- Molecule 1: Ubiquitin



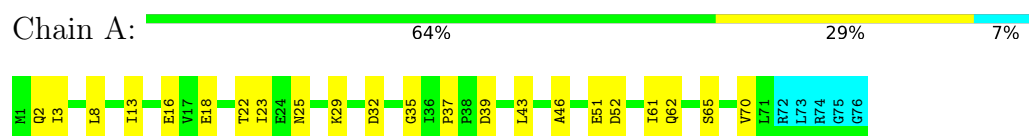
4.2.90 Score per residue for model 90

- Molecule 1: Ubiquitin



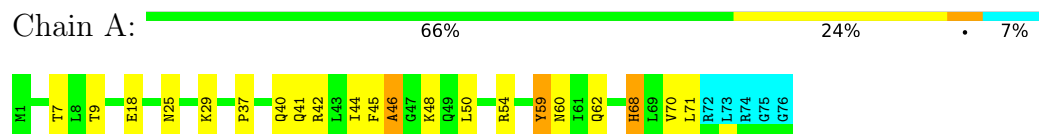
4.2.91 Score per residue for model 91

- Molecule 1: Ubiquitin



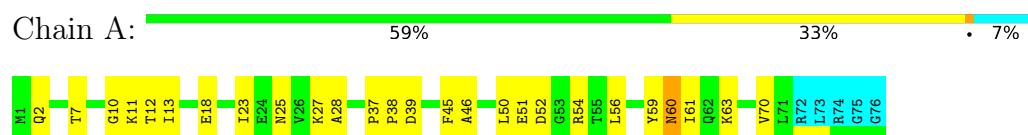
4.2.92 Score per residue for model 92

- Molecule 1: Ubiquitin



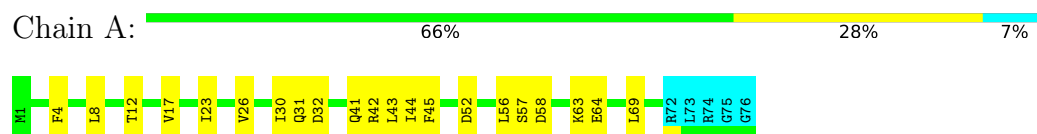
4.2.93 Score per residue for model 93

- Molecule 1: Ubiquitin



4.2.94 Score per residue for model 94

- Molecule 1: Ubiquitin



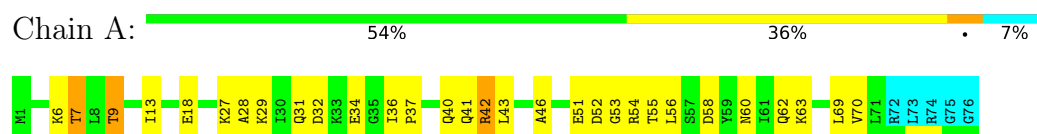
4.2.95 Score per residue for model 95

- Molecule 1: Ubiquitin



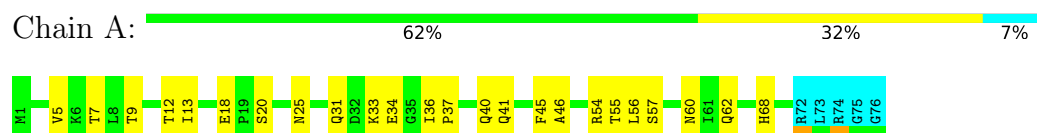
4.2.96 Score per residue for model 96

- Molecule 1: Ubiquitin



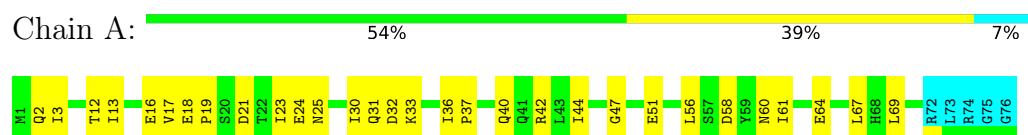
4.2.97 Score per residue for model 97

- Molecule 1: Ubiquitin



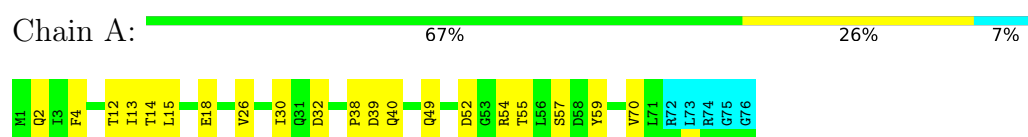
4.2.98 Score per residue for model 98

- Molecule 1: Ubiquitin



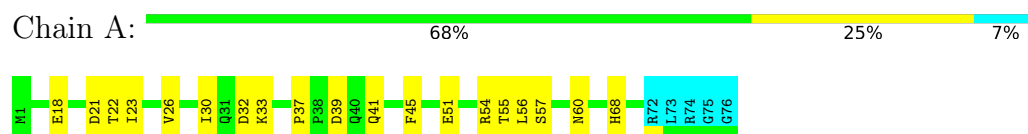
4.2.99 Score per residue for model 99

- Molecule 1: Ubiquitin



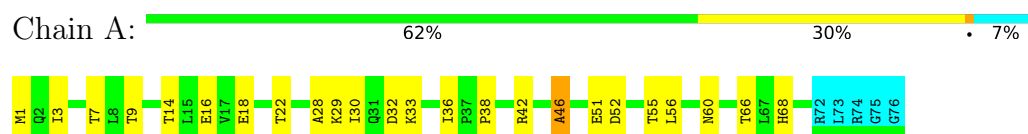
4.2.100 Score per residue for model 100 (medoid)

- Molecule 1: Ubiquitin



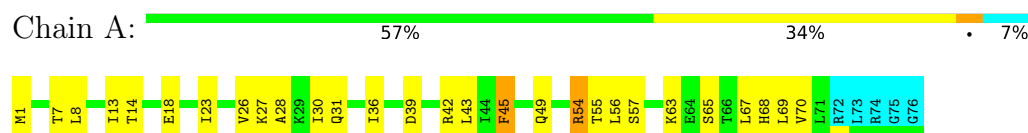
4.2.101 Score per residue for model 101

- Molecule 1: Ubiquitin



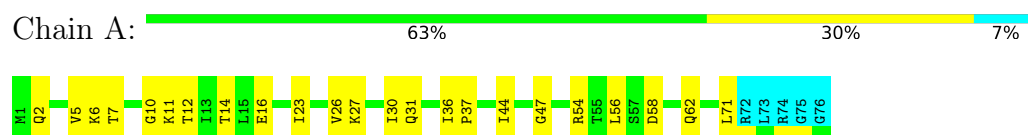
4.2.102 Score per residue for model 102

- Molecule 1: Ubiquitin



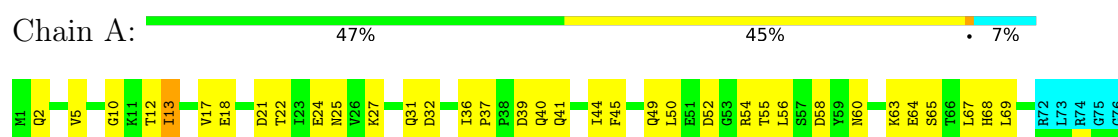
4.2.103 Score per residue for model 103

- Molecule 1: Ubiquitin



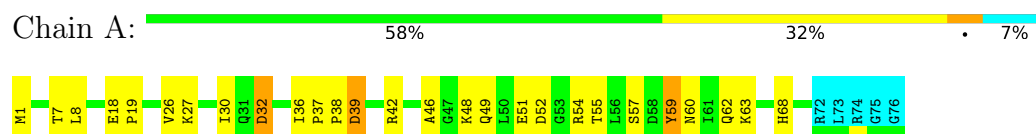
4.2.104 Score per residue for model 104

- Molecule 1: Ubiquitin



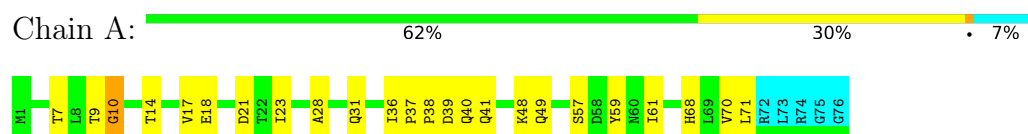
4.2.105 Score per residue for model 105

- Molecule 1: Ubiquitin



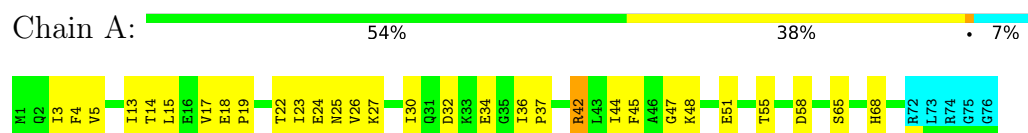
4.2.106 Score per residue for model 106

- Molecule 1: Ubiquitin



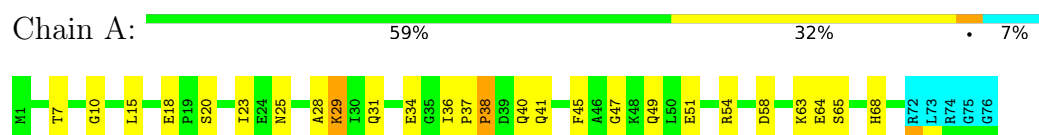
4.2.107 Score per residue for model 107

- Molecule 1: Ubiquitin



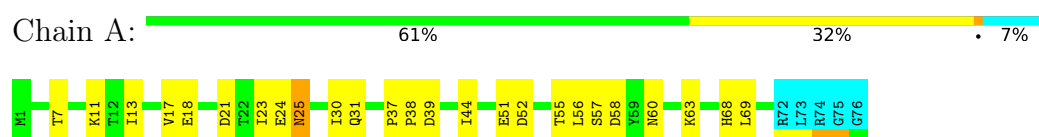
4.2.108 Score per residue for model 108

- Molecule 1: Ubiquitin



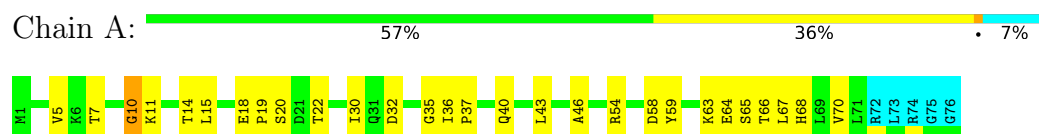
4.2.109 Score per residue for model 109

- Molecule 1: Ubiquitin



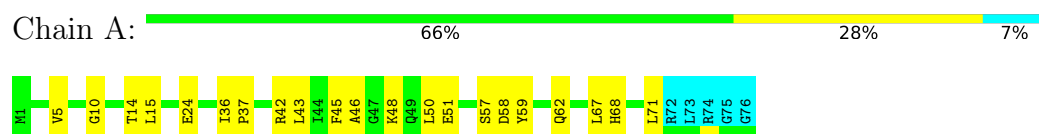
4.2.110 Score per residue for model 110

- Molecule 1: Ubiquitin



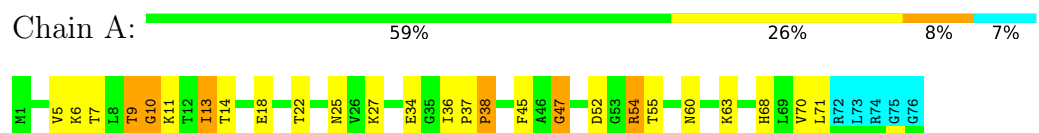
4.2.111 Score per residue for model 111

- Molecule 1: Ubiquitin



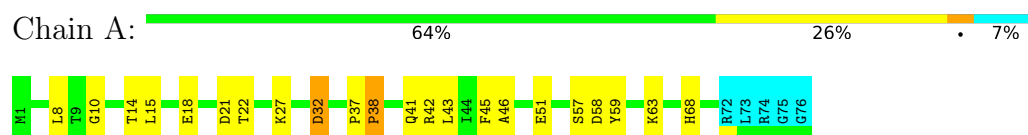
4.2.112 Score per residue for model 112

- Molecule 1: Ubiquitin



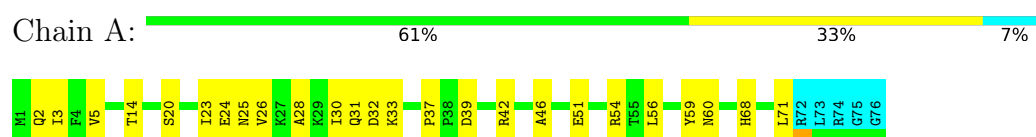
4.2.113 Score per residue for model 113

- Molecule 1: Ubiquitin



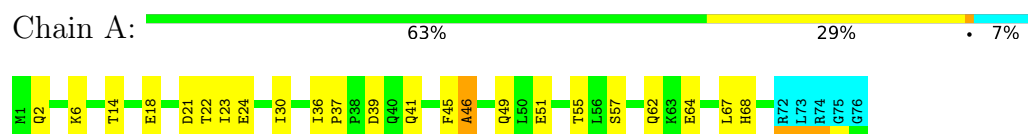
4.2.114 Score per residue for model 114

- Molecule 1: Ubiquitin



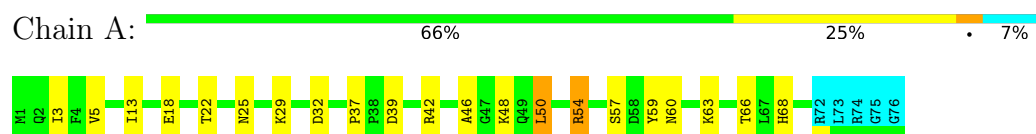
4.2.115 Score per residue for model 115

- Molecule 1: Ubiquitin



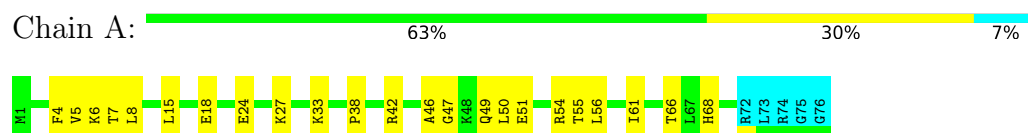
4.2.116 Score per residue for model 116

- Molecule 1: Ubiquitin



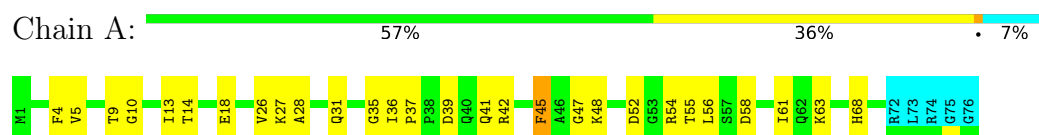
4.2.117 Score per residue for model 117

- Molecule 1: Ubiquitin



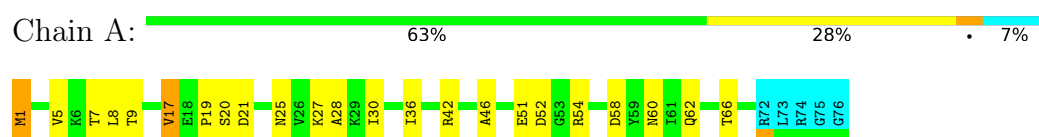
4.2.118 Score per residue for model 118

- Molecule 1: Ubiquitin



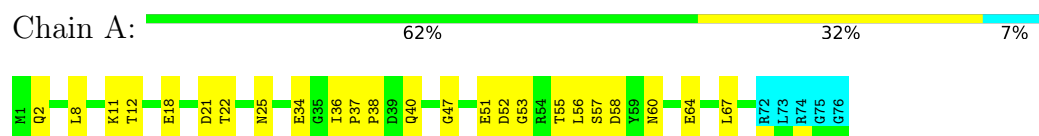
4.2.119 Score per residue for model 119

- Molecule 1: Ubiquitin



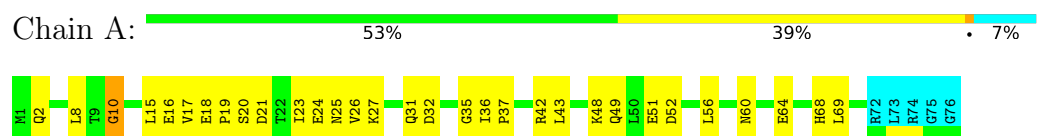
4.2.120 Score per residue for model 120

- Molecule 1: Ubiquitin



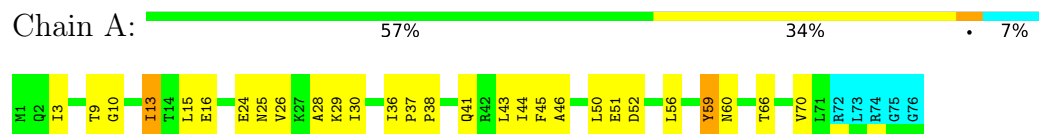
4.2.121 Score per residue for model 121

- Molecule 1: Ubiquitin



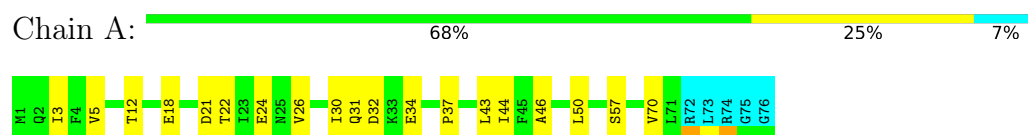
4.2.122 Score per residue for model 122

- Molecule 1: Ubiquitin



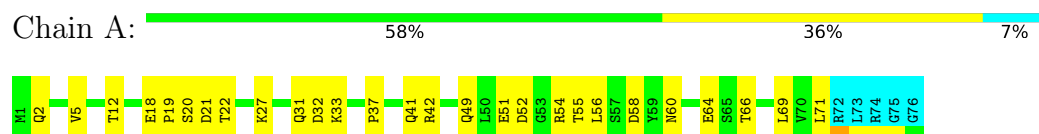
4.2.123 Score per residue for model 123

- Molecule 1: Ubiquitin



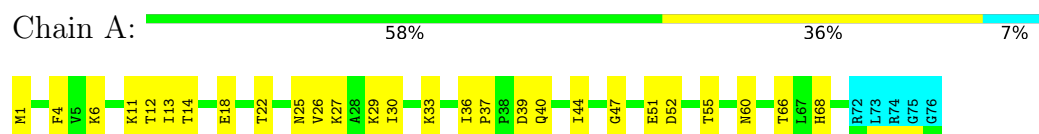
4.2.124 Score per residue for model 124

- Molecule 1: Ubiquitin



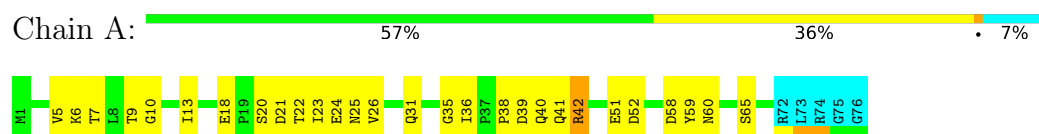
4.2.125 Score per residue for model 125

- Molecule 1: Ubiquitin



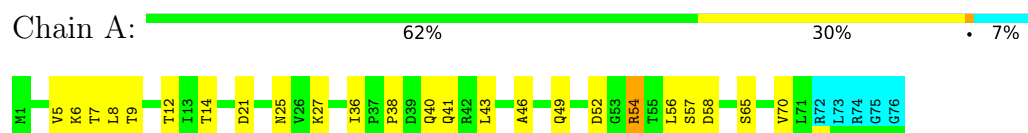
4.2.126 Score per residue for model 126

- Molecule 1: Ubiquitin



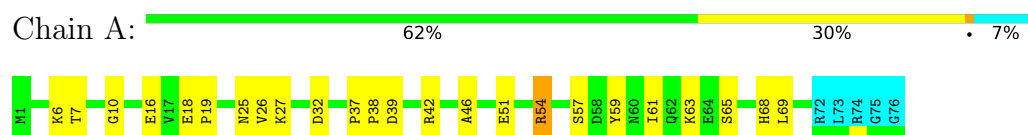
4.2.127 Score per residue for model 127

- Molecule 1: Ubiquitin



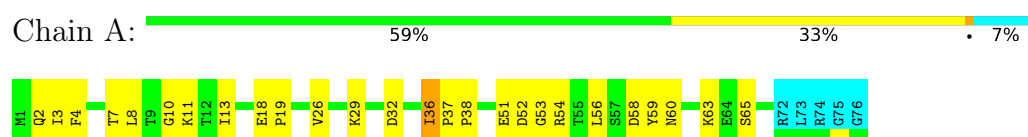
4.2.128 Score per residue for model 128

- Molecule 1: Ubiquitin



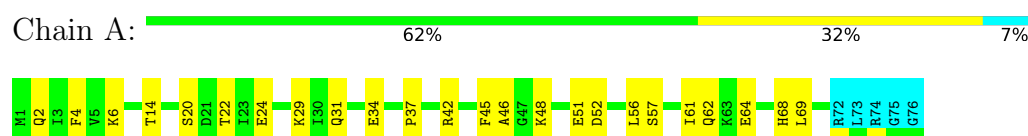
4.2.129 Score per residue for model 129

- Molecule 1: Ubiquitin



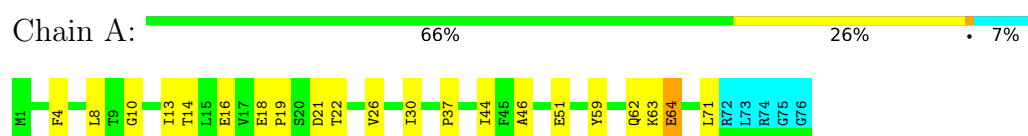
4.2.130 Score per residue for model 130

- Molecule 1: Ubiquitin



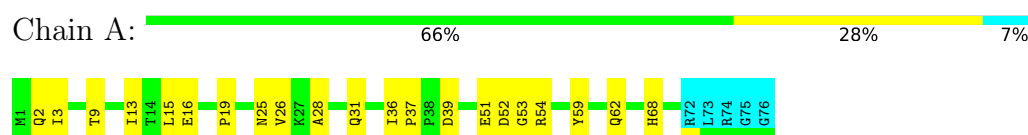
4.2.131 Score per residue for model 131

- Molecule 1: Ubiquitin



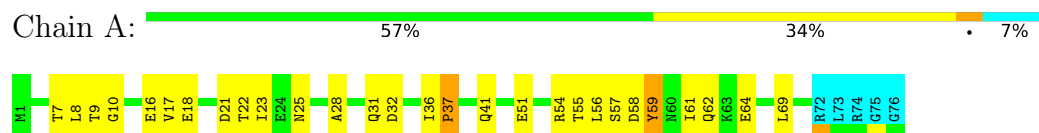
4.2.132 Score per residue for model 132

- Molecule 1: Ubiquitin



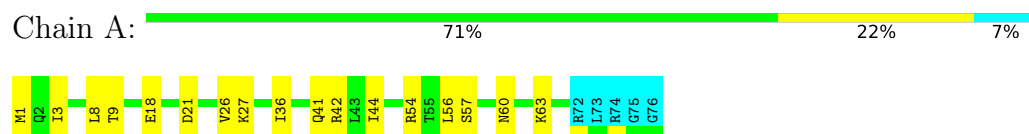
4.2.133 Score per residue for model 133

- Molecule 1: Ubiquitin



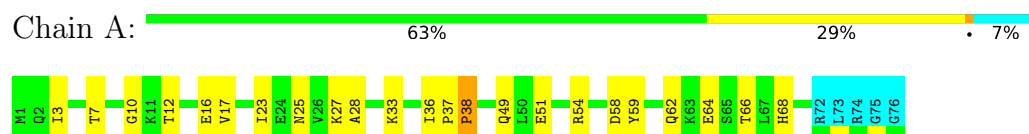
4.2.134 Score per residue for model 134

- Molecule 1: Ubiquitin



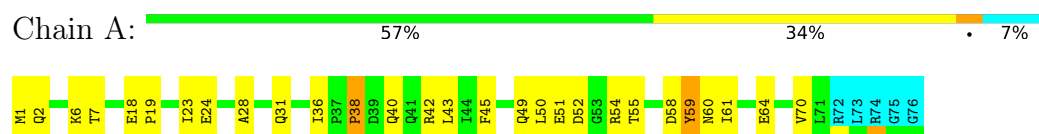
4.2.135 Score per residue for model 135

- Molecule 1: Ubiquitin



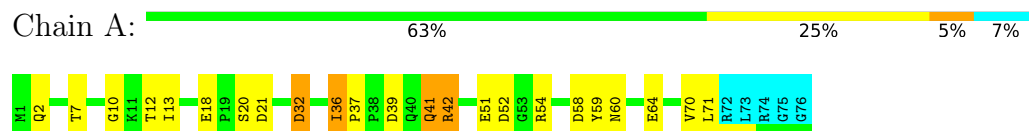
4.2.136 Score per residue for model 136

- Molecule 1: Ubiquitin



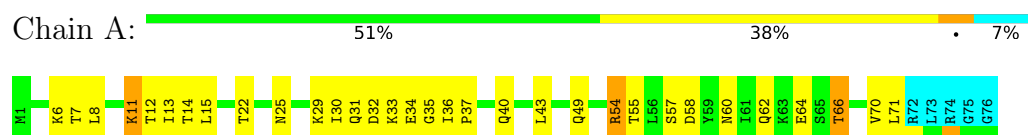
4.2.137 Score per residue for model 137

- Molecule 1: Ubiquitin



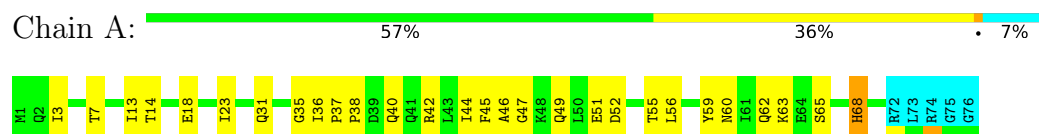
4.2.138 Score per residue for model 138

- Molecule 1: Ubiquitin



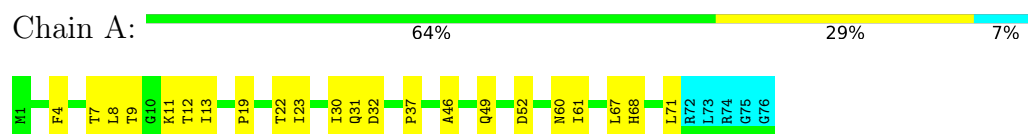
4.2.139 Score per residue for model 139

- Molecule 1: Ubiquitin



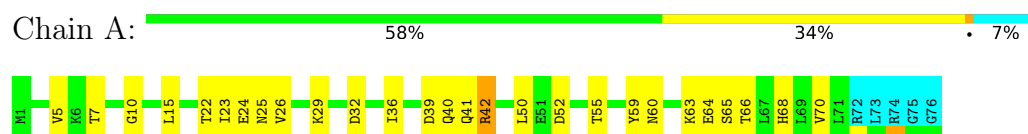
4.2.140 Score per residue for model 140

- Molecule 1: Ubiquitin



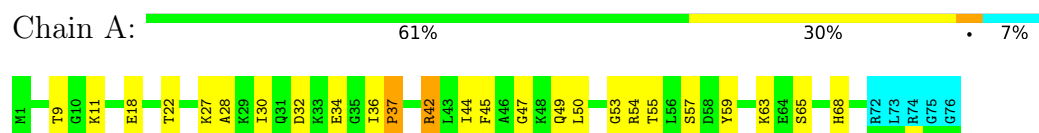
4.2.141 Score per residue for model 141

- Molecule 1: Ubiquitin



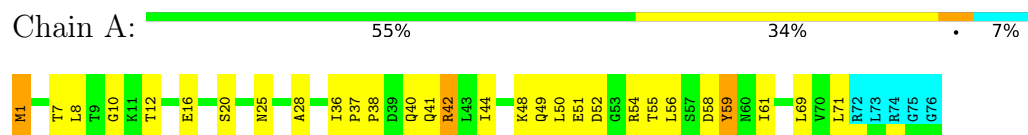
4.2.142 Score per residue for model 142

- Molecule 1: Ubiquitin



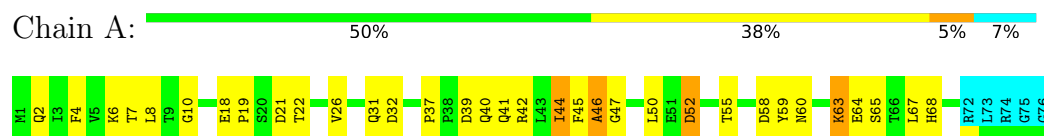
4.2.143 Score per residue for model 143

- Molecule 1: Ubiquitin



4.2.144 Score per residue for model 144

- Molecule 1: Ubiquitin



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.

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.46±0.01	0±0/570 (0.0± 0.1%)	2.40±0.08	34±6/770 (4.5± 0.8%)
All	All	1.46	17/82080 (0.0%)	2.40	4951/110880 (4.5%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	46	ALA	CA-C	-5.52	1.49	1.52	80	1
1	A	36	ILE	CA-CB	-5.30	1.50	1.54	97	16

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	CA-C-O	-17.88	106.61	120.73	43	47
1	A	37	PRO	O-C-N	-16.46	113.41	121.15	44	27
1	A	52	ASP	N-CA-C	14.84	127.46	111.28	95	56
1	A	68	HIS	CA-CB-CG	-14.83	98.97	113.80	17	30
1	A	51	GLU	CA-C-N	13.12	137.86	120.28	108	56
1	A	51	GLU	C-N-CA	13.12	137.86	120.28	108	56
1	A	36	ILE	CA-C-O	-12.59	111.70	119.51	56	40
1	A	60	ASN	CA-CB-CG	-11.90	100.70	112.60	10	33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	39	ASP	CA-CB-CG	-11.83	100.77	112.60	56	27
1	A	36	ILE	CA-C-N	11.72	128.22	119.66	120	34
1	A	36	ILE	C-N-CA	11.72	128.22	119.66	120	34
1	A	18	GLU	O-C-N	-11.54	111.54	121.35	117	42
1	A	63	LYS	N-CA-C	11.54	123.84	111.03	94	17
1	A	29	LYS	CA-C-N	11.32	135.20	120.60	88	17
1	A	29	LYS	C-N-CA	11.32	135.20	120.60	88	17
1	A	37	PRO	N-CA-C	11.31	124.50	110.70	92	41
1	A	35	GLY	CA-C-N	11.30	134.78	123.02	13	7
1	A	35	GLY	C-N-CA	11.30	134.78	123.02	13	7
1	A	22	THR	CA-C-N	11.26	134.74	120.56	71	15
1	A	22	THR	C-N-CA	11.26	134.74	120.56	71	15
1	A	70	VAL	O-C-N	-11.17	111.02	122.97	42	18
1	A	32	ASP	CA-CB-CG	11.07	123.67	112.60	113	22
1	A	37	PRO	N-CA-CB	11.06	113.81	103.08	2	20
1	A	18	GLU	CA-C-O	-10.77	108.29	120.46	104	31
1	A	4	PHE	CA-CB-CG	-10.57	103.23	113.80	65	28
1	A	7	THR	CA-C-N	10.52	134.79	120.38	24	28
1	A	7	THR	C-N-CA	10.52	134.79	120.38	24	28
1	A	25	ASN	CA-CB-CG	-10.51	102.09	112.60	112	19
1	A	23	ILE	CA-C-N	10.51	134.10	120.44	86	34
1	A	23	ILE	C-N-CA	10.51	134.10	120.44	86	34
1	A	56	LEU	CA-C-N	10.49	134.34	120.28	109	45
1	A	56	LEU	C-N-CA	10.49	134.34	120.28	109	45
1	A	41	GLN	OE1-CD-NE2	-10.35	112.25	122.60	127	12
1	A	36	ILE	O-C-N	-10.16	112.36	121.61	65	38
1	A	52	ASP	CA-CB-CG	10.08	122.68	112.60	21	22
1	A	13	ILE	N-CA-CB	9.97	121.59	110.72	91	25
1	A	33	LYS	N-CA-CB	9.97	124.89	110.13	95	5
1	A	55	THR	O-C-N	-9.92	111.54	122.85	81	13
1	A	8	LEU	O-C-N	9.92	133.89	122.19	19	8
1	A	54	ARG	NE-CZ-NH1	9.83	131.33	121.50	104	16
1	A	40	GLN	OE1-CD-NE2	-9.77	112.83	122.60	120	10
1	A	8	LEU	CA-C-N	9.60	133.32	120.65	88	17
1	A	8	LEU	C-N-CA	9.60	133.32	120.65	88	17
1	A	37	PRO	CA-C-N	9.60	129.35	119.56	14	35
1	A	37	PRO	C-N-CA	9.60	129.35	119.56	14	35
1	A	2	GLN	OE1-CD-NE2	-9.56	113.04	122.60	114	18
1	A	60	ASN	N-CA-C	9.41	124.29	112.24	96	11
1	A	39	ASP	CA-C-N	9.40	133.81	120.28	42	10
1	A	39	ASP	C-N-CA	9.40	133.81	120.28	42	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	43	LEU	CA-C-N	9.37	135.19	123.10	102	12
1	A	43	LEU	C-N-CA	9.37	135.19	123.10	102	12
1	A	31	GLN	CA-C-N	9.35	132.81	120.28	123	25
1	A	31	GLN	C-N-CA	9.35	132.81	120.28	123	25
1	A	63	LYS	CA-C-N	9.31	135.95	122.35	113	14
1	A	63	LYS	C-N-CA	9.31	135.95	122.35	113	14
1	A	46	ALA	CA-C-O	9.29	132.34	120.81	33	9
1	A	55	THR	CA-C-N	9.12	132.30	120.44	63	34
1	A	55	THR	C-N-CA	9.12	132.30	120.44	63	34
1	A	7	THR	O-C-N	-9.11	110.91	122.20	27	20
1	A	62	GLN	OE1-CD-NE2	-9.08	113.52	122.60	56	19
1	A	9	THR	CA-CB-OG1	9.04	123.16	109.60	112	14
1	A	59	TYR	CA-C-N	9.01	135.51	122.35	14	24
1	A	59	TYR	C-N-CA	9.01	135.51	122.35	14	24
1	A	58	ASP	N-CA-C	8.97	121.06	111.28	68	23
1	A	70	VAL	CA-C-O	8.95	129.97	120.48	45	9
1	A	37	PRO	CB-CA-C	-8.92	102.78	111.17	25	19
1	A	24	GLU	O-C-N	-8.90	111.81	122.22	15	11
1	A	32	ASP	N-CA-CB	-8.85	97.02	110.20	37	7
1	A	57	SER	N-CA-C	8.84	120.92	111.28	87	20
1	A	69	LEU	CA-C-N	8.84	134.07	122.93	23	11
1	A	69	LEU	C-N-CA	8.84	134.07	122.93	23	11
1	A	46	ALA	N-CA-CB	8.80	125.36	110.49	4	6
1	A	44	ILE	O-C-N	-8.78	113.69	123.18	9	19
1	A	25	ASN	CA-C-N	8.78	131.63	120.56	76	28
1	A	25	ASN	C-N-CA	8.78	131.63	120.56	76	28
1	A	58	ASP	CA-CB-CG	8.78	121.38	112.60	67	20
1	A	39	ASP	N-CA-C	8.77	121.79	111.71	118	10
1	A	38	PRO	CA-C-N	8.76	132.38	120.38	23	33
1	A	38	PRO	C-N-CA	8.76	132.38	120.38	23	33
1	A	57	SER	CA-C-N	8.73	132.85	120.28	97	32
1	A	57	SER	C-N-CA	8.73	132.85	120.28	97	32
1	A	52	ASP	O-C-N	-8.71	113.10	122.07	137	8
1	A	61	ILE	N-CA-CB	-8.70	101.24	110.72	75	8
1	A	27	LYS	CA-C-N	8.70	133.53	120.31	17	15
1	A	27	LYS	C-N-CA	8.70	133.53	120.31	17	15
1	A	27	LYS	N-CA-C	8.68	121.69	111.71	105	25
1	A	68	HIS	O-C-N	-8.66	113.34	123.22	140	8
1	A	28	ALA	CA-C-N	8.66	131.88	120.28	101	22
1	A	28	ALA	C-N-CA	8.66	131.88	120.28	101	22
1	A	49	GLN	OE1-CD-NE2	8.65	131.25	122.60	8	17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	9	THR	N-CA-C	8.64	120.38	110.97	86	13
1	A	7	THR	N-CA-C	8.62	121.65	110.53	102	9
1	A	33	LYS	N-CA-C	8.57	120.40	111.14	32	15
1	A	39	ASP	CA-C-O	-8.57	111.33	120.42	104	12
1	A	39	ASP	N-CA-CB	8.57	122.43	110.01	105	5
1	A	21	ASP	CA-CB-CG	8.56	121.17	112.60	77	17
1	A	4	PHE	O-C-N	-8.54	112.22	122.63	46	8
1	A	45	PHE	CA-CB-CG	8.45	122.25	113.80	80	14
1	A	66	THR	CA-C-N	8.44	132.85	120.87	10	6
1	A	66	THR	C-N-CA	8.44	132.85	120.87	10	6
1	A	33	LYS	CA-C-O	8.43	129.58	120.90	54	7
1	A	24	GLU	N-CA-C	8.41	121.51	111.33	67	24
1	A	68	HIS	CE1-NE2-CD2	-8.40	100.60	109.00	104	40
1	A	31	GLN	N-CA-C	8.40	121.27	111.02	64	15
1	A	1	MET	CG-SD-CE	-8.38	82.47	100.90	143	15
1	A	8	LEU	N-CA-CB	-8.36	97.89	110.01	119	7
1	A	28	ALA	O-C-N	-8.35	111.37	122.23	60	13
1	A	33	LYS	CA-C-N	8.35	133.32	121.71	138	2
1	A	33	LYS	C-N-CA	8.35	133.32	121.71	138	2
1	A	49	GLN	O-C-N	-8.33	113.55	123.13	86	12
1	A	8	LEU	CA-C-O	8.31	129.62	119.31	33	10
1	A	55	THR	N-CA-C	8.30	121.04	110.33	68	9
1	A	21	ASP	O-C-N	-8.29	113.59	122.96	119	12
1	A	50	LEU	CA-C-N	8.29	132.55	120.95	123	8
1	A	50	LEU	C-N-CA	8.29	132.55	120.95	123	8
1	A	41	GLN	N-CA-C	8.26	121.04	109.15	1	19
1	A	65	SER	O-C-N	-8.25	113.54	123.19	6	10
1	A	64	GLU	CA-C-N	8.24	133.73	122.77	47	11
1	A	64	GLU	C-N-CA	8.24	133.73	122.77	47	11
1	A	13	ILE	O-C-N	-8.22	114.75	123.14	112	11
1	A	44	ILE	CA-C-O	8.21	128.56	120.27	12	8
1	A	9	THR	CA-C-N	8.19	134.18	120.91	142	4
1	A	9	THR	C-N-CA	8.19	134.18	120.91	142	4
1	A	22	THR	N-CA-CB	8.19	121.96	110.17	51	23
1	A	18	GLU	CA-C-N	8.17	127.83	119.82	77	16
1	A	18	GLU	C-N-CA	8.17	127.83	119.82	77	16
1	A	30	ILE	O-C-N	-8.15	113.92	121.91	3	17
1	A	13	ILE	CB-CA-C	8.15	123.20	110.81	34	10
1	A	35	GLY	CA-C-O	8.14	128.14	118.86	19	8
1	A	19	PRO	CA-C-N	8.14	134.31	120.72	124	8
1	A	19	PRO	C-N-CA	8.14	134.31	120.72	124	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	51	GLU	O-C-N	-8.11	112.90	122.87	14	16
1	A	12	THR	N-CA-CB	8.10	122.91	109.94	137	10
1	A	7	THR	N-CA-CB	8.10	123.61	110.41	108	11
1	A	58	ASP	CB-CA-C	8.10	123.59	110.88	135	7
1	A	26	VAL	N-CA-C	8.08	118.18	110.42	63	16
1	A	12	THR	O-C-N	-8.05	114.04	123.22	42	12
1	A	28	ALA	CA-C-O	8.04	129.27	119.79	41	8
1	A	30	ILE	CA-C-N	8.03	131.04	120.28	140	30
1	A	30	ILE	C-N-CA	8.03	131.04	120.28	140	30
1	A	64	GLU	CA-C-O	8.03	130.94	120.98	108	4
1	A	39	ASP	CB-CA-C	8.03	123.59	110.90	102	2
1	A	2	GLN	N-CA-C	8.01	122.53	109.72	6	4
1	A	58	ASP	CA-C-O	7.99	129.02	120.55	98	15
1	A	17	VAL	O-C-N	-7.99	114.09	122.95	107	15
1	A	41	GLN	CA-C-O	7.97	129.35	120.43	31	6
1	A	15	LEU	O-C-N	-7.96	113.56	123.27	18	15
1	A	41	GLN	O-C-N	-7.93	114.01	123.13	31	10
1	A	42	ARG	O-C-N	-7.92	114.04	123.31	40	12
1	A	26	VAL	O-C-N	-7.92	113.87	121.87	123	13
1	A	68	HIS	ND1-CE1-NE2	7.92	116.32	108.40	61	23
1	A	24	GLU	CA-C-N	7.91	130.88	120.28	130	18
1	A	24	GLU	C-N-CA	7.91	130.88	120.28	130	18
1	A	6	LYS	O-C-N	-7.90	113.25	122.89	51	16
1	A	55	THR	CA-CB-OG1	7.89	121.43	109.60	34	10
1	A	33	LYS	O-C-N	-7.83	112.69	122.17	48	3
1	A	36	ILE	N-CA-C	7.82	117.28	108.05	27	9
1	A	2	GLN	CA-C-O	-7.82	112.63	121.39	144	10
1	A	54	ARG	O-C-N	-7.81	113.02	123.10	119	10
1	A	46	ALA	O-C-N	-7.80	112.90	122.11	63	1
1	A	9	THR	CA-C-O	7.79	128.97	119.31	57	8
1	A	58	ASP	O-C-N	7.79	130.13	122.03	113	12
1	A	32	ASP	N-CA-C	7.79	119.55	111.14	76	15
1	A	42	ARG	NE-CZ-NH2	7.76	126.19	119.20	126	17
1	A	66	THR	O-C-N	-7.76	114.12	123.27	44	6
1	A	54	ARG	N-CA-C	-7.74	97.61	109.14	136	7
1	A	59	TYR	N-CA-C	7.74	122.30	113.01	135	10
1	A	13	ILE	CA-C-O	7.74	128.85	120.57	39	4
1	A	69	LEU	CA-C-O	7.73	128.81	120.38	94	8
1	A	47	GLY	CA-C-N	7.73	133.53	122.09	103	5
1	A	47	GLY	C-N-CA	7.73	133.53	122.09	103	5
1	A	34	GLU	O-C-N	-7.72	113.85	122.34	59	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	29	LYS	O-C-N	-7.72	112.78	122.27	5	12
1	A	31	GLN	CA-C-O	7.70	128.82	119.97	123	5
1	A	52	ASP	CA-C-O	7.67	128.60	120.70	140	6
1	A	7	THR	CA-CB-OG1	7.65	121.08	109.60	59	14
1	A	59	TYR	O-C-N	-7.64	114.14	122.85	99	5
1	A	24	GLU	CB-CA-C	-7.62	98.63	110.81	89	4
1	A	30	ILE	N-CA-C	7.61	118.38	110.62	28	5
1	A	27	LYS	CA-C-O	7.59	128.72	119.38	127	7
1	A	25	ASN	OD1-CG-ND2	7.57	130.17	122.60	119	9
1	A	56	LEU	CA-C-O	7.56	128.44	120.42	36	10
1	A	22	THR	O-C-N	-7.56	113.35	122.65	82	12
1	A	28	ALA	N-CA-C	7.54	120.46	111.33	23	13
1	A	63	LYS	O-C-N	-7.54	113.08	122.20	96	5
1	A	70	VAL	N-CA-CB	7.52	120.94	111.46	123	7
1	A	5	VAL	O-C-N	-7.51	113.04	122.88	76	19
1	A	54	ARG	CD-NE-CZ	-7.51	113.89	124.40	70	5
1	A	48	LYS	CA-C-N	7.51	134.34	122.17	121	12
1	A	48	LYS	C-N-CA	7.51	134.34	122.17	121	12
1	A	12	THR	N-CA-C	7.50	120.73	109.25	84	5
1	A	60	ASN	CA-C-N	7.50	132.25	122.95	46	13
1	A	60	ASN	C-N-CA	7.50	132.25	122.95	46	13
1	A	44	ILE	N-CA-C	-7.50	97.29	108.46	142	5
1	A	12	THR	CA-C-O	7.49	128.33	120.54	58	9
1	A	36	ILE	N-CA-CB	7.49	120.44	111.23	71	4
1	A	51	GLU	N-CA-C	7.48	121.53	110.30	35	14
1	A	43	LEU	CA-C-O	-7.47	112.79	120.71	71	10
1	A	31	GLN	OE1-CD-NE2	-7.47	115.13	122.60	19	16
1	A	11	LYS	O-C-N	-7.47	113.83	123.02	138	7
1	A	48	LYS	N-CA-C	7.45	121.54	110.52	84	3
1	A	23	ILE	N-CA-C	-7.44	103.03	110.62	14	11
1	A	32	ASP	O-C-N	-7.44	114.41	122.07	114	8
1	A	21	ASP	N-CA-C	7.43	120.34	110.53	131	6
1	A	54	ARG	NE-CZ-NH2	-7.42	112.52	119.20	17	17
1	A	68	HIS	CG-CD2-NE2	7.41	114.61	107.20	87	31
1	A	11	LYS	N-CA-C	7.39	121.10	110.24	110	3
1	A	30	ILE	CA-CB-CG2	7.37	123.04	110.50	94	1
1	A	41	GLN	CB-CA-C	-7.37	98.41	109.90	143	8
1	A	11	LYS	CA-C-O	-7.36	112.66	121.05	66	7
1	A	3	ILE	O-C-N	-7.35	114.91	123.00	122	10
1	A	29	LYS	N-CA-C	7.35	119.29	111.28	125	13
1	A	62	GLN	CA-C-N	7.35	131.56	121.05	58	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	62	GLN	C-N-CA	7.35	131.56	121.05	58	15
1	A	46	ALA	N-CA-C	7.33	121.62	112.24	33	11
1	A	22	THR	CA-CB-OG1	7.31	120.57	109.60	16	11
1	A	71	LEU	CA-C-N	7.31	130.39	120.44	13	14
1	A	71	LEU	C-N-CA	7.31	130.39	120.44	13	14
1	A	61	ILE	N-CA-C	7.30	118.47	108.84	98	5
1	A	62	GLN	N-CA-C	7.29	119.99	110.43	50	4
1	A	38	PRO	CB-CA-C	-7.29	101.47	112.11	11	4
1	A	17	VAL	N-CA-C	-7.29	99.64	108.53	133	4
1	A	43	LEU	O-C-N	-7.28	114.92	123.22	27	5
1	A	23	ILE	O-C-N	-7.28	113.57	121.80	81	7
1	A	48	LYS	O-C-N	-7.28	114.92	123.22	118	12
1	A	10	GLY	CA-C-N	7.28	131.74	120.75	63	4
1	A	10	GLY	C-N-CA	7.28	131.74	120.75	63	4
1	A	56	LEU	O-C-N	7.26	129.81	122.12	64	6
1	A	16	GLU	CB-CG-CD	-7.25	100.28	112.60	62	6
1	A	50	LEU	N-CA-C	7.25	120.34	109.25	21	6
1	A	25	ASN	CA-C-O	-7.25	112.87	120.55	18	8
1	A	42	ARG	CB-CA-C	-7.23	98.33	110.19	114	3
1	A	32	ASP	CA-C-N	7.23	130.46	120.63	141	12
1	A	32	ASP	C-N-CA	7.23	130.46	120.63	141	12
1	A	26	VAL	CA-C-N	7.22	130.28	120.38	141	17
1	A	26	VAL	C-N-CA	7.22	130.28	120.38	141	17
1	A	27	LYS	O-C-N	-7.19	113.04	122.39	5	10
1	A	5	VAL	N-CA-C	7.19	118.17	108.11	104	3
1	A	70	VAL	N-CA-C	7.18	118.22	108.17	96	7
1	A	54	ARG	NH1-CZ-NH2	7.17	128.62	119.30	90	9
1	A	8	LEU	N-CA-C	7.16	119.95	111.71	10	10
1	A	30	ILE	CA-C-O	7.16	128.37	120.71	43	12
1	A	65	SER	CA-C-N	7.15	133.06	123.05	81	6
1	A	65	SER	C-N-CA	7.15	133.06	123.05	81	6
1	A	38	PRO	N-CA-CB	7.15	110.34	103.19	57	8
1	A	61	ILE	O-C-N	-7.14	114.88	122.67	143	7
1	A	68	HIS	CB-CG-CD2	-7.14	121.92	131.20	61	11
1	A	14	THR	N-CA-CB	7.14	121.56	110.21	36	13
1	A	12	THR	CA-C-N	7.13	132.91	122.99	94	5
1	A	12	THR	C-N-CA	7.13	132.91	122.99	94	5
1	A	67	LEU	O-C-N	-7.12	115.08	123.06	86	15
1	A	25	ASN	O-C-N	-7.12	113.51	122.27	107	8
1	A	65	SER	N-CA-CB	7.12	120.81	110.06	76	3
1	A	16	GLU	N-CA-C	7.12	121.64	107.62	22	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	69	LEU	N-CA-C	7.10	119.68	108.67	109	2
1	A	36	ILE	CB-CA-C	-7.08	104.35	110.94	133	4
1	A	48	LYS	CA-C-O	7.08	127.94	120.36	118	6
1	A	39	ASP	O-C-N	-7.08	114.61	122.12	14	7
1	A	5	VAL	CA-C-O	7.07	126.52	120.22	63	7
1	A	35	GLY	N-CA-C	-7.07	105.09	115.63	118	2
1	A	45	PHE	CA-C-N	7.06	135.03	121.54	14	9
1	A	45	PHE	C-N-CA	7.06	135.03	121.54	14	9
1	A	49	GLN	CB-CA-C	-7.06	99.49	110.78	47	7
1	A	54	ARG	CA-C-O	7.06	130.10	121.56	119	5
1	A	49	GLN	N-CA-C	7.04	121.51	110.32	17	7
1	A	15	LEU	CA-C-O	7.04	127.96	120.36	73	6
1	A	21	ASP	N-CA-CB	-7.04	100.04	110.17	106	3
1	A	45	PHE	N-CA-C	-7.03	95.64	107.80	94	7
1	A	65	SER	N-CA-C	7.03	120.92	110.52	75	8
1	A	27	LYS	N-CA-CB	7.02	120.55	110.16	31	5
1	A	14	THR	CA-C-O	-7.02	113.07	120.58	131	7
1	A	31	GLN	O-C-N	-7.02	114.51	122.09	16	7
1	A	12	THR	CB-CA-C	-7.01	98.51	110.22	37	5
1	A	71	LEU	O-C-N	-7.00	114.97	123.30	112	13
1	A	3	ILE	CA-CB-CG1	7.00	122.30	110.40	116	4
1	A	61	ILE	CA-C-O	7.00	128.86	120.74	106	8
1	A	61	ILE	CA-CB-CG2	6.99	122.38	110.50	130	1
1	A	27	LYS	CG-CD-CE	6.99	127.37	111.30	103	3
1	A	9	THR	N-CA-CB	6.98	121.10	110.28	101	7
1	A	29	LYS	CA-C-O	6.98	127.99	120.10	92	6
1	A	16	GLU	CA-C-O	6.97	128.41	120.54	128	8
1	A	25	ASN	N-CA-C	6.95	118.94	111.36	10	14
1	A	2	GLN	O-C-N	6.94	130.80	122.96	13	6
1	A	47	GLY	CA-C-O	-6.94	112.33	119.20	52	4
1	A	15	LEU	N-CA-C	6.93	120.97	109.95	122	5
1	A	50	LEU	CA-C-O	6.93	128.78	120.81	122	3
1	A	20	SER	N-CA-CB	-6.91	99.66	110.44	9	6
1	A	6	LYS	N-CA-C	6.89	119.64	108.34	127	5
1	A	6	LYS	CA-C-O	-6.87	113.43	120.71	138	7
1	A	26	VAL	CB-CA-C	-6.86	103.06	112.04	22	5
1	A	53	GLY	O-C-N	-6.86	113.78	122.70	71	4
1	A	10	GLY	O-C-N	-6.84	113.80	122.70	137	5
1	A	5	VAL	CA-C-N	6.83	131.63	121.72	123	4
1	A	5	VAL	C-N-CA	6.83	131.63	121.72	123	4
1	A	56	LEU	N-CA-C	6.82	119.55	111.71	25	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	49	GLN	CG-CD-OE1	6.81	134.43	120.80	48	4
1	A	41	GLN	CG-CD-NE2	6.81	126.61	116.40	35	1
1	A	50	LEU	O-C-N	-6.81	115.46	123.22	90	11
1	A	1	MET	CA-C-O	-6.80	109.23	120.80	6	3
1	A	23	ILE	CA-C-O	6.80	127.82	120.47	81	6
1	A	57	SER	CA-C-O	-6.80	113.34	120.55	8	3
1	A	42	ARG	NH1-CZ-NH2	-6.80	110.46	119.30	57	7
1	A	45	PHE	CB-CA-C	6.79	121.63	111.17	92	10
1	A	50	LEU	CB-CA-C	6.79	121.12	109.51	143	4
1	A	49	GLN	CG-CD-NE2	-6.79	106.22	116.40	48	5
1	A	45	PHE	O-C-N	-6.79	116.05	123.52	84	6
1	A	19	PRO	N-CA-CB	6.78	109.77	103.46	61	9
1	A	40	GLN	CA-C-O	6.78	127.77	119.97	141	6
1	A	34	GLU	CA-C-O	-6.76	113.27	120.71	138	5
1	A	30	ILE	N-CA-CB	6.74	120.69	110.58	103	3
1	A	4	PHE	CB-CA-C	-6.73	99.00	110.16	130	7
1	A	70	VAL	CA-C-N	-6.72	113.18	122.93	56	5
1	A	70	VAL	C-N-CA	-6.72	113.18	122.93	56	5
1	A	3	ILE	CA-C-N	-6.72	112.63	122.65	101	7
1	A	3	ILE	C-N-CA	-6.72	112.63	122.65	101	7
1	A	40	GLN	CA-C-N	6.71	131.46	121.72	68	7
1	A	40	GLN	C-N-CA	6.71	131.46	121.72	68	7
1	A	43	LEU	N-CA-C	6.71	119.67	108.73	94	2
1	A	52	ASP	CB-CA-C	-6.71	100.55	110.95	126	8
1	A	57	SER	N-CA-CB	6.68	119.94	110.12	88	5
1	A	67	LEU	CA-C-N	6.67	131.93	122.72	1	2
1	A	67	LEU	C-N-CA	6.67	131.93	122.72	1	2
1	A	60	ASN	OD1-CG-ND2	-6.67	115.93	122.60	39	10
1	A	41	GLN	CA-C-N	6.66	133.28	122.29	124	4
1	A	41	GLN	C-N-CA	6.66	133.28	122.29	124	4
1	A	31	GLN	CB-CG-CD	6.65	123.91	112.60	45	4
1	A	64	GLU	O-C-N	-6.65	113.69	122.47	108	6
1	A	16	GLU	CA-C-N	6.65	132.13	122.69	122	6
1	A	16	GLU	C-N-CA	6.65	132.13	122.69	122	6
1	A	62	GLN	O-C-N	-6.63	115.55	122.84	25	7
1	A	58	ASP	CA-C-N	6.62	130.05	120.38	8	1
1	A	58	ASP	C-N-CA	6.62	130.05	120.38	8	1
1	A	4	PHE	CA-C-O	6.62	127.72	120.71	107	2
1	A	17	VAL	CA-C-O	6.61	128.38	121.44	59	6
1	A	70	VAL	CB-CA-C	6.60	119.10	110.91	31	1
1	A	63	LYS	N-CA-CB	6.59	119.66	110.17	31	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	45	PHE	CA-C-O	6.59	127.76	120.31	84	4
1	A	58	ASP	N-CA-CB	-6.58	100.45	110.12	27	3
1	A	2	GLN	N-CA-CB	6.57	121.00	110.16	11	4
1	A	21	ASP	CA-C-O	6.57	128.51	121.16	120	5
1	A	48	LYS	CB-CA-C	-6.56	99.39	109.89	49	3
1	A	15	LEU	N-CA-CB	6.56	121.10	110.41	7	5
1	A	42	ARG	N-CA-CB	6.55	122.85	111.13	139	2
1	A	71	LEU	N-CA-C	6.55	119.61	109.07	114	4
1	A	63	LYS	CG-CD-CE	6.54	126.35	111.30	70	3
1	A	65	SER	CB-CA-C	-6.54	96.88	109.37	34	9
1	A	71	LEU	CA-C-O	6.54	127.46	120.46	46	6
1	A	61	ILE	CB-CA-C	6.54	119.65	111.15	77	4
1	A	59	TYR	CA-CB-CG	-6.52	102.16	113.90	69	5
1	A	40	GLN	N-CA-C	-6.51	105.47	113.41	79	8
1	A	60	ASN	CA-C-O	6.51	129.26	121.65	101	4
1	A	42	ARG	NE-CZ-NH1	6.51	128.01	121.50	101	7
1	A	3	ILE	CA-CB-CG2	-6.50	99.44	110.50	83	3
1	A	38	PRO	N-CA-C	-6.50	107.92	114.68	49	9
1	A	68	HIS	ND1-CG-CD2	-6.50	99.60	106.10	109	1
1	A	52	ASP	N-CA-CB	6.49	119.42	110.01	56	3
1	A	26	VAL	CA-C-O	-6.49	114.29	121.17	25	7
1	A	14	THR	O-C-N	-6.49	115.14	122.93	138	10
1	A	59	TYR	CB-CG-CD1	-6.48	111.07	120.80	62	4
1	A	60	ASN	CB-CA-C	-6.47	103.19	111.86	20	8
1	A	14	THR	CA-CB-CG2	6.46	121.48	110.50	118	3
1	A	17	VAL	N-CA-CB	6.46	119.70	112.34	98	3
1	A	40	GLN	CB-CG-CD	-6.46	101.62	112.60	106	4
1	A	22	THR	CA-C-O	-6.46	114.51	121.94	104	6
1	A	3	ILE	CA-C-O	-6.45	115.09	121.67	15	7
1	A	41	GLN	N-CA-CB	6.44	119.94	109.95	48	4
1	A	43	LEU	CB-CA-C	6.44	120.75	110.19	29	4
1	A	49	GLN	CA-C-O	6.43	128.38	121.05	49	4
1	A	60	ASN	O-C-N	6.43	131.02	122.41	18	3
1	A	64	GLU	N-CA-C	6.41	120.44	112.24	88	7
1	A	55	THR	N-CA-CB	6.40	120.18	110.45	44	16
1	A	2	GLN	CG-CD-NE2	6.39	125.99	116.40	136	4
1	A	68	HIS	CB-CA-C	6.39	120.76	110.16	70	3
1	A	62	GLN	CB-CA-C	-6.34	103.16	113.37	111	1
1	A	3	ILE	N-CA-CB	6.33	121.39	112.52	20	8
1	A	18	GLU	CB-CA-C	-6.33	99.74	108.86	93	3
1	A	57	SER	O-C-N	-6.33	115.41	122.12	102	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	42	ARG	CD-NE-CZ	-6.33	115.55	124.40	66	7
1	A	55	THR	CA-C-O	6.32	129.29	121.89	97	4
1	A	22	THR	CA-CB-CG2	-6.32	99.76	110.50	12	4
1	A	68	HIS	CA-C-O	6.31	127.33	120.58	132	7
1	A	69	LEU	CB-CA-C	6.31	120.41	110.19	95	2
1	A	25	ASN	N-CA-CB	-6.30	100.84	110.16	108	9
1	A	49	GLN	CB-CG-CD	6.28	123.27	112.60	127	3
1	A	40	GLN	N-CA-CB	6.28	119.75	110.53	98	2
1	A	41	GLN	CB-CG-CD	-6.27	101.94	112.60	81	8
1	A	34	GLU	CB-CA-C	-6.27	98.53	109.07	120	4
1	A	14	THR	CA-CB-OG1	6.27	119.00	109.60	95	5
1	A	2	GLN	CB-CG-CD	-6.27	101.95	112.60	20	2
1	A	62	GLN	CA-C-O	-6.26	114.02	121.60	59	4
1	A	5	VAL	N-CA-CB	6.26	119.79	111.90	84	7
1	A	49	GLN	CA-C-N	6.26	130.46	121.50	135	3
1	A	49	GLN	C-N-CA	6.26	130.46	121.50	135	3
1	A	66	THR	N-CA-CB	6.26	119.67	110.35	110	8
1	A	9	THR	CA-CB-CG2	-6.25	99.87	110.50	106	1
1	A	20	SER	CA-C-O	6.25	126.61	119.18	72	3
1	A	43	LEU	N-CA-CB	6.22	120.57	110.43	111	7
1	A	68	HIS	CB-CG-ND1	6.22	132.03	122.70	44	5
1	A	15	LEU	CA-C-N	6.22	131.26	121.99	117	4
1	A	15	LEU	C-N-CA	6.22	131.26	121.99	117	4
1	A	69	LEU	O-C-N	-6.22	115.93	123.27	72	3
1	A	16	GLU	N-CA-CB	6.21	120.56	110.43	14	3
1	A	71	LEU	CB-CA-C	6.21	120.47	109.72	59	4
1	A	17	VAL	CA-CB-CG1	6.21	120.96	110.40	29	1
1	A	44	ILE	N-CA-CB	6.21	119.29	111.46	103	1
1	A	42	ARG	CA-C-O	6.19	126.80	120.24	45	4
1	A	68	HIS	CA-C-N	6.17	130.89	122.19	40	7
1	A	68	HIS	C-N-CA	6.17	130.89	122.19	40	7
1	A	45	PHE	N-CA-CB	-6.17	101.28	110.90	118	5
1	A	55	THR	CA-CB-CG2	6.17	120.99	110.50	67	1
1	A	54	ARG	CG-CD-NE	-6.15	98.46	112.00	45	6
1	A	19	PRO	N-CA-C	-6.15	106.66	114.35	128	9
1	A	29	LYS	N-CA-CB	-6.14	101.05	110.20	122	4
1	A	26	VAL	CA-CB-CG2	-6.14	99.96	110.40	69	3
1	A	65	SER	CA-C-O	-6.14	114.47	121.72	102	4
1	A	61	ILE	CA-C-N	6.12	131.96	121.86	5	2
1	A	61	ILE	C-N-CA	6.12	131.96	121.86	5	2
1	A	9	THR	O-C-N	-6.12	114.77	122.17	6	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	47	GLY	O-C-N	6.11	130.16	122.39	118	5
1	A	24	GLU	CB-CG-CD	-6.10	102.22	112.60	42	2
1	A	25	ASN	CB-CA-C	-6.10	100.48	110.85	143	5
1	A	46	ALA	CB-CA-C	6.10	122.56	110.42	115	7
1	A	44	ILE	CA-CB-CG2	6.09	120.86	110.50	98	2
1	A	31	GLN	N-CA-CB	6.08	119.17	110.16	69	4
1	A	44	ILE	CA-CB-CG1	6.08	120.73	110.40	70	6
1	A	19	PRO	O-C-N	-6.07	114.05	122.30	48	1
1	A	24	GLU	CA-C-O	6.07	127.18	120.63	57	5
1	A	7	THR	CA-C-O	6.06	128.98	121.89	34	4
1	A	14	THR	CB-CA-C	-6.05	101.10	110.78	45	2
1	A	67	LEU	CA-C-O	6.04	128.42	121.47	14	3
1	A	25	ASN	CB-CG-ND2	6.04	125.45	116.40	90	1
1	A	37	PRO	N-CD-CG	6.04	112.25	103.20	53	1
1	A	34	GLU	CB-CG-CD	6.03	122.86	112.60	96	2
1	A	26	VAL	N-CA-CB	6.03	117.60	110.55	65	6
1	A	51	GLU	CB-CG-CD	6.03	122.85	112.60	136	6
1	A	59	TYR	CA-C-O	-6.03	112.51	119.56	133	5
1	A	49	GLN	N-CA-CB	-6.03	100.57	110.52	117	3
1	A	35	GLY	O-C-N	-6.03	115.80	122.55	110	5
1	A	23	ILE	CB-CG1-CD1	6.03	126.45	113.80	87	2
1	A	66	THR	CA-C-O	6.02	126.81	120.54	41	6
1	A	46	ALA	CA-C-N	6.02	129.68	123.30	65	2
1	A	46	ALA	C-N-CA	6.02	129.68	123.30	65	2
1	A	23	ILE	CA-CB-CG2	6.00	120.71	110.50	82	4
1	A	13	ILE	N-CA-C	6.00	116.76	108.84	69	6
1	A	2	GLN	CA-C-N	6.00	131.57	122.92	32	3
1	A	2	GLN	C-N-CA	6.00	131.57	122.92	32	3
1	A	67	LEU	N-CA-C	-5.99	100.79	110.32	26	7
1	A	51	GLU	CA-C-O	5.99	127.52	120.69	101	3
1	A	4	PHE	CA-C-N	5.99	131.25	123.10	99	2
1	A	4	PHE	C-N-CA	5.99	131.25	123.10	99	2
1	A	22	THR	N-CA-C	5.99	117.77	110.41	140	8
1	A	63	LYS	CA-C-O	5.99	128.02	121.02	96	8
1	A	34	GLU	N-CA-CB	-5.98	103.05	111.00	53	3
1	A	6	LYS	N-CA-CB	-5.97	100.56	110.23	61	5
1	A	11	LYS	CA-C-N	-5.96	113.08	121.72	142	4
1	A	11	LYS	C-N-CA	-5.96	113.08	121.72	142	4
1	A	6	LYS	CB-CA-C	-5.96	99.47	109.48	128	1
1	A	1	MET	O-C-N	-5.96	113.47	123.00	83	4
1	A	14	THR	OG1-CB-CG2	-5.94	97.42	109.30	99	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	20	SER	CA-C-N	-5.93	113.31	122.09	48	8
1	A	20	SER	C-N-CA	-5.93	113.31	122.09	48	8
1	A	63	LYS	CB-CA-C	5.93	118.30	110.06	116	1
1	A	69	LEU	N-CA-CB	-5.93	100.76	110.42	95	2
1	A	38	PRO	O-C-N	5.92	130.18	122.24	135	5
1	A	3	ILE	N-CA-C	-5.92	99.21	108.86	132	3
1	A	18	GLU	N-CA-CB	5.91	117.19	110.03	35	1
1	A	64	GLU	CB-CA-C	5.91	119.67	111.63	47	5
1	A	32	ASP	CA-C-O	5.91	127.20	121.00	75	7
1	A	20	SER	N-CA-C	5.91	120.33	113.18	13	5
1	A	13	ILE	CA-C-N	5.90	132.50	123.23	96	3
1	A	13	ILE	C-N-CA	5.90	132.50	123.23	96	3
1	A	19	PRO	CB-CA-C	-5.89	102.55	111.44	140	4
1	A	54	ARG	CA-C-N	5.87	132.10	122.07	124	2
1	A	54	ARG	C-N-CA	5.87	132.10	122.07	124	2
1	A	26	VAL	CA-CB-CG1	5.84	120.33	110.40	95	2
1	A	33	LYS	CB-CA-C	-5.80	101.96	110.95	26	1
1	A	66	THR	N-CA-C	5.80	118.12	109.25	138	5
1	A	20	SER	CB-CA-C	-5.79	99.59	110.01	31	3
1	A	64	GLU	N-CA-CB	5.78	120.25	110.49	135	4
1	A	67	LEU	CB-CA-C	5.78	119.94	109.83	95	3
1	A	48	LYS	N-CA-CB	5.77	119.27	109.87	79	4
1	A	40	GLN	O-C-N	-5.76	114.74	122.23	74	3
1	A	40	GLN	CA-CB-CG	-5.75	102.60	114.10	136	2
1	A	44	ILE	CB-CA-C	-5.72	102.31	110.83	7	3
1	A	40	GLN	CG-CD-OE1	5.72	132.24	120.80	138	2
1	A	60	ASN	N-CA-CB	5.72	119.80	111.62	6	3
1	A	1	MET	CA-CB-CG	5.72	125.53	114.10	25	1
1	A	42	ARG	N-CA-C	-5.70	99.13	108.76	43	1
1	A	23	ILE	CB-CA-C	5.67	120.05	112.22	15	2
1	A	20	SER	O-C-N	-5.67	114.63	122.46	18	2
1	A	34	GLU	N-CA-C	-5.67	106.04	113.12	13	4
1	A	16	GLU	CB-CA-C	5.66	119.09	109.80	80	1
1	A	6	LYS	CG-CD-CE	5.66	124.31	111.30	66	4
1	A	28	ALA	CB-CA-C	-5.65	101.24	110.85	133	1
1	A	62	GLN	CB-CG-CD	-5.65	103.00	112.60	70	2
1	A	30	ILE	CA-CB-CG1	5.65	120.00	110.40	123	1
1	A	1	MET	CA-C-N	5.64	128.85	120.95	10	2
1	A	1	MET	C-N-CA	5.64	128.85	120.95	10	2
1	A	13	ILE	CA-CB-CG2	-5.63	100.92	110.50	82	3
1	A	30	ILE	CB-CA-C	5.62	119.73	112.14	12	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	23	ILE	CA-CB-CG1	5.62	119.95	110.40	1	2
1	A	11	LYS	CG-CD-CE	5.61	124.20	111.30	54	2
1	A	68	HIS	N-CA-CB	-5.61	101.30	110.21	118	1
1	A	60	ASN	CB-CG-ND2	5.60	124.80	116.40	139	2
1	A	12	THR	CA-CB-CG2	5.59	120.00	110.50	137	1
1	A	48	LYS	CG-CD-CE	5.56	124.08	111.30	52	1
1	A	66	THR	CB-CA-C	-5.56	101.18	110.19	122	1
1	A	4	PHE	N-CA-CB	-5.54	102.22	111.20	13	1
1	A	61	ILE	CB-CG1-CD1	5.54	125.44	113.80	52	1
1	A	42	ARG	CA-CB-CG	5.52	125.14	114.10	22	1
1	A	68	HIS	N-CA-C	5.52	117.30	108.41	118	3
1	A	66	THR	CA-CB-OG1	5.52	117.88	109.60	52	1
1	A	24	GLU	N-CA-CB	-5.50	101.74	109.94	87	3
1	A	55	THR	OG1-CB-CG2	-5.50	98.31	109.30	133	2
1	A	51	GLU	CB-CA-C	5.49	118.79	109.84	137	2
1	A	31	GLN	CG-CD-OE1	5.49	131.78	120.80	4	1
1	A	5	VAL	CB-CA-C	5.49	118.67	111.53	24	3
1	A	61	ILE	CA-CB-CG1	-5.49	101.08	110.40	20	2
1	A	4	PHE	N-CA-C	-5.48	99.58	108.52	6	1
1	A	59	TYR	CB-CA-C	-5.48	101.29	110.56	137	1
1	A	2	GLN	CB-CA-C	5.48	119.56	110.74	121	4
1	A	57	SER	CB-CA-C	-5.48	100.15	110.67	45	1
1	A	42	ARG	CG-CD-NE	-5.46	100.00	112.00	76	3
1	A	42	ARG	CA-C-N	5.45	130.01	122.77	76	2
1	A	42	ARG	C-N-CA	5.45	130.01	122.77	76	2
1	A	51	GLU	N-CA-CB	5.42	118.25	110.06	121	3
1	A	29	LYS	CB-CA-C	-5.39	100.32	110.67	75	2
1	A	14	THR	N-CA-C	5.38	117.01	108.67	21	4
1	A	9	THR	OG1-CB-CG2	-5.38	98.54	109.30	73	2
1	A	56	LEU	CB-CA-C	-5.38	101.71	110.85	61	1
1	A	12	THR	OG1-CB-CG2	-5.37	98.56	109.30	2	4
1	A	18	GLU	CB-CG-CD	5.36	121.72	112.60	108	2
1	A	18	GLU	N-CA-C	-5.36	101.90	110.10	120	5
1	A	33	LYS	CG-CD-CE	5.34	123.58	111.30	36	1
1	A	62	GLN	CG-CD-OE1	-5.33	110.13	120.80	24	1
1	A	16	GLU	O-C-N	-5.33	117.25	123.27	42	3
1	A	53	GLY	N-CA-C	5.31	120.51	114.67	3	1
1	A	3	ILE	CB-CA-C	-5.30	103.26	110.90	16	2
1	A	32	ASP	CB-CA-C	5.30	120.40	110.70	37	1
1	A	11	LYS	N-CA-CB	5.30	119.27	110.63	40	2
1	A	56	LEU	N-CA-CB	-5.30	102.38	110.33	87	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	36	ILE	CA-CB-CG1	5.29	119.39	110.40	80	2
1	A	6	LYS	CB-CG-CD	5.29	123.47	111.30	2	1
1	A	7	THR	CA-CB-CG2	-5.29	101.51	110.50	141	3
1	A	16	GLU	CA-CB-CG	-5.28	103.54	114.10	6	1
1	A	50	LEU	N-CA-CB	5.27	118.12	109.95	1	1
1	A	38	PRO	N-CD-CG	5.26	111.10	103.20	128	1
1	A	70	VAL	CA-CB-CG1	5.26	119.33	110.40	91	1
1	A	9	THR	CB-CA-C	5.25	119.61	110.79	36	1
1	A	47	GLY	N-CA-C	-5.25	108.44	114.69	117	1
1	A	65	SER	CA-CB-OG	5.23	121.57	111.10	2	1
1	A	45	PHE	CB-CG-CD1	5.23	129.60	120.70	8	1
1	A	10	GLY	CA-C-O	5.23	124.18	118.95	12	1
1	A	13	ILE	CA-CB-CG1	5.23	119.29	110.40	118	2
1	A	41	GLN	CG-CD-OE1	5.22	131.25	120.80	127	1
1	A	17	VAL	CB-CA-C	-5.21	101.09	110.48	3	3
1	A	66	THR	OG1-CB-CG2	-5.21	98.89	109.30	38	1
1	A	63	LYS	CA-CB-CG	5.20	124.51	114.10	78	1
1	A	54	ARG	CB-CA-C	-5.18	100.50	110.24	112	2
1	A	31	GLN	CG-CD-NE2	-5.14	108.69	116.40	9	1
1	A	31	GLN	CB-CA-C	-5.13	102.27	110.79	36	2
1	A	52	ASP	CA-C-N	5.12	131.46	121.41	46	1
1	A	52	ASP	C-N-CA	5.12	131.46	121.41	46	1
1	A	66	THR	CA-CB-CG2	5.12	119.21	110.50	4	1
1	A	31	GLN	CA-CB-CG	5.12	124.33	114.10	2	1
1	A	1	MET	N-CA-CB	5.10	119.17	110.50	43	4
1	A	53	GLY	CA-C-N	5.08	132.12	123.03	120	1
1	A	53	GLY	C-N-CA	5.08	132.12	123.03	120	1
1	A	11	LYS	CA-CB-CG	5.08	124.25	114.10	18	1
1	A	12	THR	CA-CB-OG1	5.05	117.18	109.60	84	1
1	A	18	GLU	CG-CD-OE1	5.04	129.99	118.40	47	1
1	A	5	VAL	CA-CB-CG1	5.04	118.97	110.40	123	1
1	A	17	VAL	CA-CB-CG2	-5.04	101.84	110.40	48	1
1	A	15	LEU	CB-CA-C	-5.03	101.03	109.48	85	1
1	A	62	GLN	N-CA-CB	-5.02	103.29	110.87	130	1
1	A	27	LYS	CB-CA-C	-5.01	99.74	110.32	112	1
1	A	22	THR	CB-CA-C	-5.00	101.08	109.83	126	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	66	THR	Mainchain	1
1	A	19	PRO	Mainchain	1
1	A	12	THR	Mainchain	1
1	A	35	GLY	Mainchain	1
1	A	5	VAL	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	83212	23

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:15:LEU:HD22	1:A:29:LYS:HB3	0.47	1.84	20	1
1:A:7:THR:HG22	1:A:69:LEU:HD23	0.47	1.85	96	2
1:A:56:LEU:HD23	1:A:61:ILE:HD12	0.47	1.86	93	1
1:A:45:PHE:C	1:A:47:GLY:H	0.45	2.19	107	1
1:A:42:ARG:HB2	1:A:70:VAL:HG23	0.44	1.88	141	1
1:A:56:LEU:CD2	1:A:61:ILE:HD12	0.43	2.43	93	1
1:A:36:ILE:HG22	1:A:41:GLN:HG3	0.43	1.90	137	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:13:ILE:HD12	1:A:33:LYS:CE	0.41	2.46	59	1
1:A:23:ILE:O	1:A:23:ILE:HG22	0.41	2.15	139	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:54:ARG:HH21	1:A:58:ASP:CG	0.40	2.24	50	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	70/76 (92%)	65±2 (93±3%)	4±2 (5±3%)	1±1 (1±1%)	12	60
All	All	10080/10944 (92%)	9407 (93%)	546 (5%)	127 (1%)	12	60

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
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 ⓘ

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%)	63±3 (98±5%)	1±1 (2±1%)	51	91
All	All	9311/9792 (95%)	9141 (98%)	170 (2%)	51	91

All 52 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	13	ILE	21
1	A	1	MET	9
1	A	38	PRO	9
1	A	37	PRO	9
1	A	9	THR	7
1	A	44	ILE	7
1	A	52	ASP	6
1	A	70	VAL	5
1	A	20	SER	5
1	A	32	ASP	5
1	A	65	SER	5
1	A	2	GLN	5
1	A	64	GLU	4
1	A	50	LEU	3
1	A	21	ASP	3
1	A	39	ASP	3
1	A	29	LYS	3
1	A	17	VAL	3
1	A	23	ILE	3
1	A	60	ASN	3
1	A	69	LEU	3
1	A	11	LYS	3
1	A	68	HIS	3
1	A	56	LEU	2
1	A	51	GLU	2
1	A	48	LYS	2
1	A	67	LEU	2
1	A	3	ILE	2
1	A	54	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	16	GLU	2
1	A	66	THR	2
1	A	5	VAL	2
1	A	36	ILE	2
1	A	71	LEU	2
1	A	22	THR	2
1	A	26	VAL	2
1	A	18	GLU	2
1	A	12	THR	1
1	A	43	LEU	1
1	A	6	LYS	1
1	A	15	LEU	1
1	A	63	LYS	1
1	A	58	ASP	1
1	A	40	GLN	1
1	A	57	SER	1
1	A	49	GLN	1
1	A	31	GLN	1
1	A	7	THR	1
1	A	8	LEU	1
1	A	61	ILE	1
1	A	19	PRO	1
1	A	25	ASN	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 oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided