



Full wwPDB NMR Structure Validation Report ⓘ

Mar 19, 2026 – 10:21 PM UTC

PDB ID : 2K39 / pdb_00002k39
Title : Recognition dynamics up to microseconds revealed from RDC derived ubiquitin ensemble in solution
Authors : Lange, O.F.; Lakomek, N.A.; Fares, C.; Schroder, G.; Walter, K.; Becker, S.; Meiler, J.; Grubmuller, H.; Griesinger, C.; de Groot, B.L.
Deposited on : 2008-04-25

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

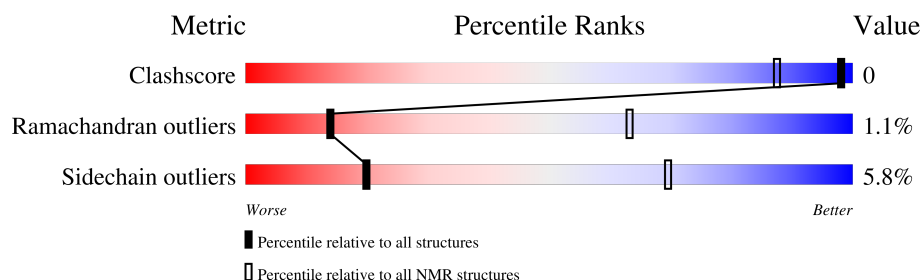
1 Overall quality at a glance

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	54% 39% 7%

2 Ensemble composition and analysis

This entry contains 116 models. Model 79 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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)	0.98	79

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

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

The models can be grouped into 5 clusters and 3 single-model clusters were found.

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

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.

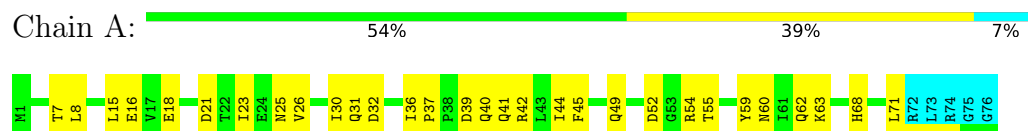
Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1231	378	629	105	118	1	

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

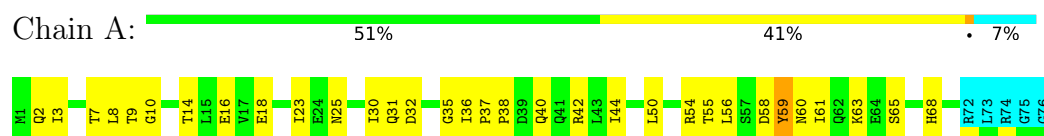


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

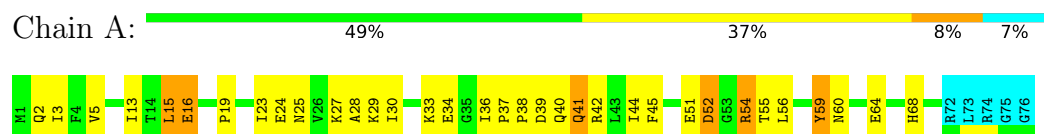
4.2.1 Score per residue for model 1

- Molecule 1: Ubiquitin



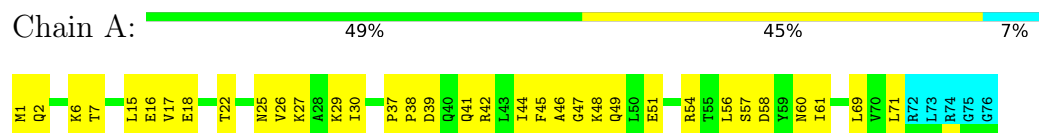
4.2.2 Score per residue for model 2

- Molecule 1: Ubiquitin



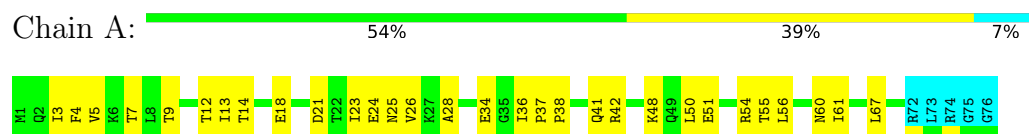
4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin



4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin



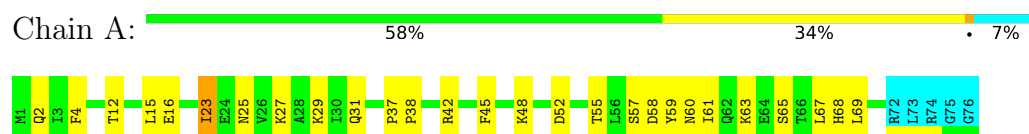
4.2.5 Score per residue for model 5

- Molecule 1: Ubiquitin



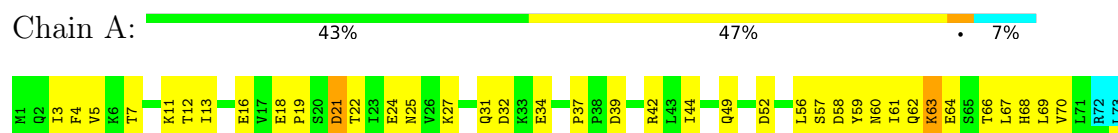
4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin



4.2.7 Score per residue for model 7

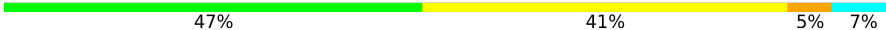
- Molecule 1: Ubiquitin



R74
G75
G76

4.2.8 Score per residue for model 8

- Molecule 1: Ubiquitin

Chain A: 



G75
G76

4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin

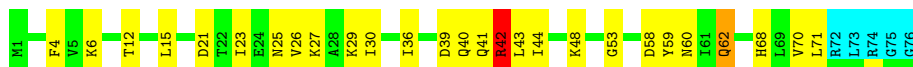
Chain A: 



4.2.10 Score per residue for model 10

- Molecule 1: Ubiquitin

Chain A: 



4.2.11 Score per residue for model 11

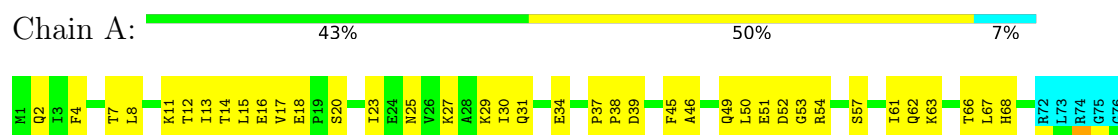
- Molecule 1: Ubiquitin

Chain A: 



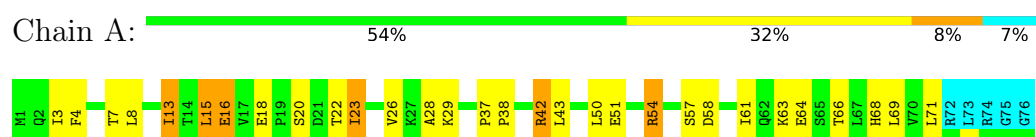
4.2.12 Score per residue for model 12

- Molecule 1: Ubiquitin



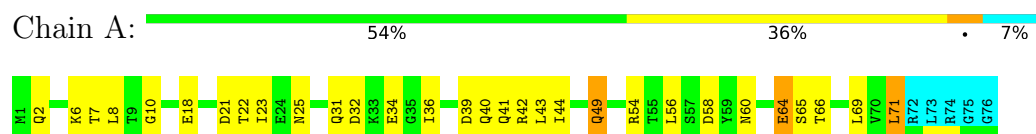
4.2.13 Score per residue for model 13

- Molecule 1: Ubiquitin



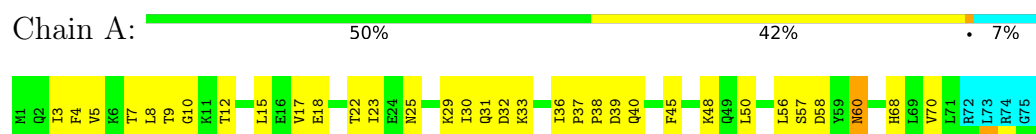
4.2.14 Score per residue for model 14

- Molecule 1: Ubiquitin



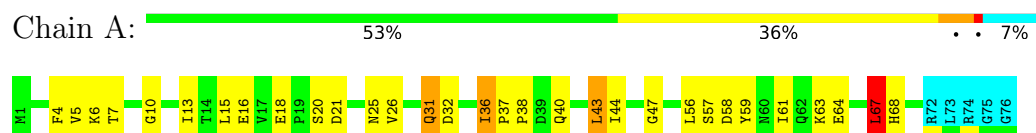
4.2.15 Score per residue for model 15

- Molecule 1: Ubiquitin



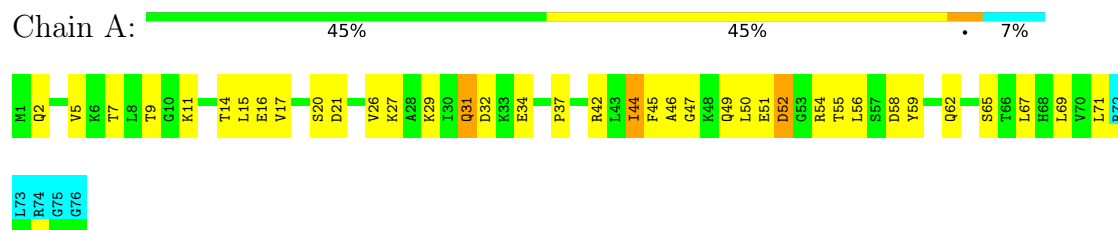
4.2.16 Score per residue for model 16

- Molecule 1: Ubiquitin



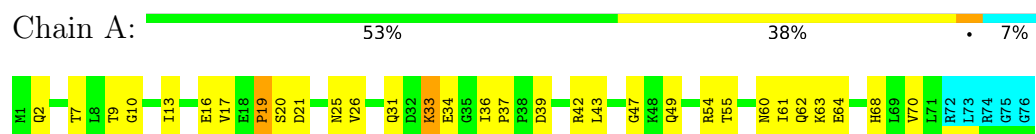
4.2.17 Score per residue for model 17

- Molecule 1: Ubiquitin



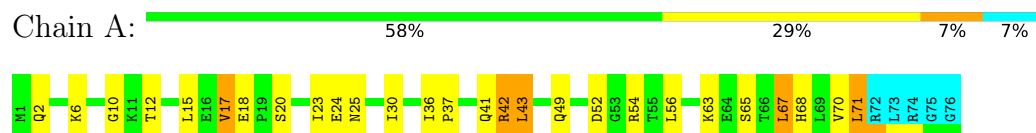
4.2.18 Score per residue for model 18

- Molecule 1: Ubiquitin



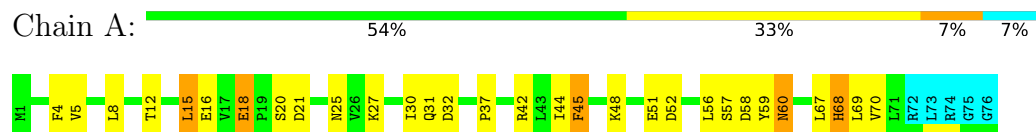
4.2.19 Score per residue for model 19

- 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

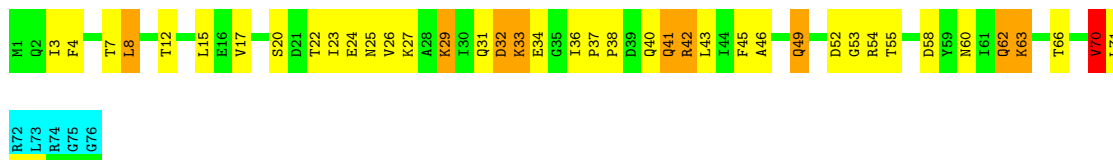




4.2.22 Score per residue for model 22

- Molecule 1: Ubiquitin

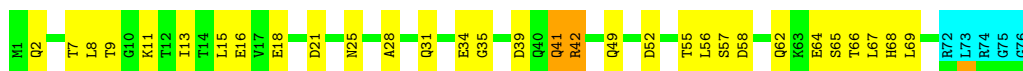
Chain A: 41% 39% 12% 7%



4.2.23 Score per residue for model 23

- Molecule 1: Ubiquitin

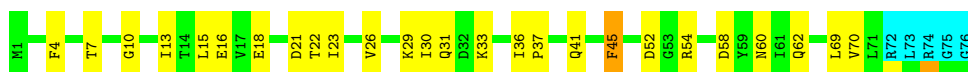
Chain A: 53% 38% 7%



4.2.24 Score per residue for model 24

- Molecule 1: Ubiquitin

Chain A: 59% 33% 7%



4.2.25 Score per residue for model 25

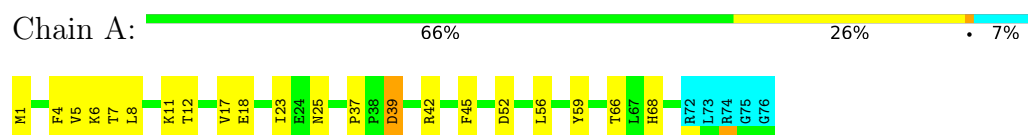
- Molecule 1: Ubiquitin

Chain A: 50% 39% 7%



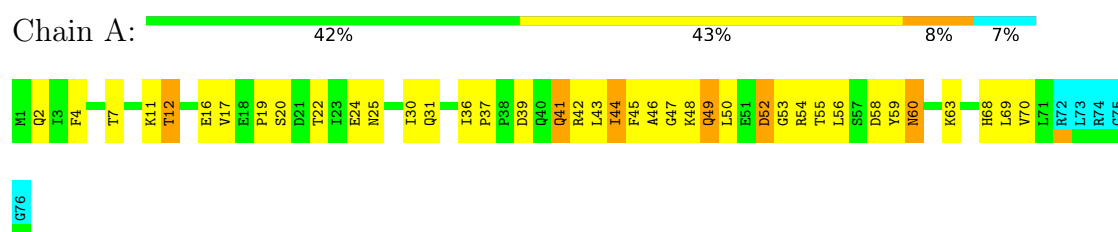
4.2.26 Score per residue for model 26

- Molecule 1: Ubiquitin



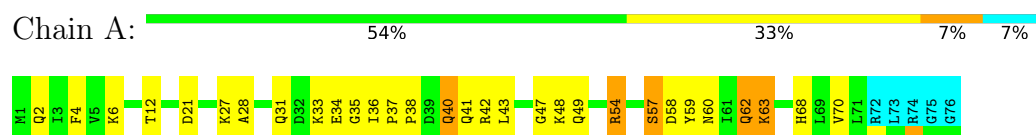
4.2.27 Score per residue for model 27

- Molecule 1: Ubiquitin



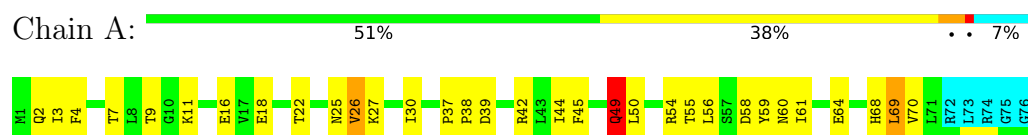
4.2.28 Score per residue for model 28

- Molecule 1: Ubiquitin



4.2.29 Score per residue for model 29

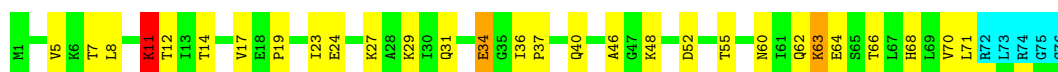
- Molecule 1: Ubiquitin



4.2.30 Score per residue for model 30

- Molecule 1: Ubiquitin





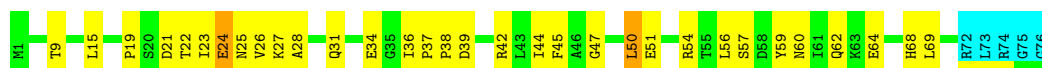
4.2.31 Score per residue for model 31

- 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





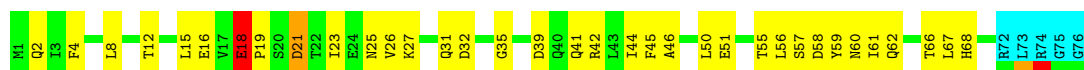
4.2.36 Score per residue for model 36

- 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



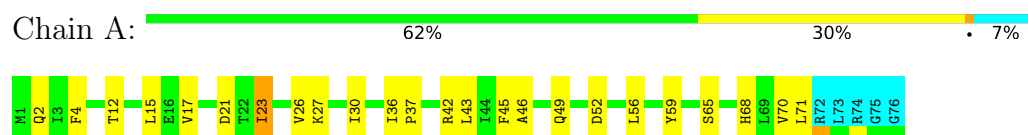
4.2.39 Score per residue for model 39

- Molecule 1: Ubiquitin



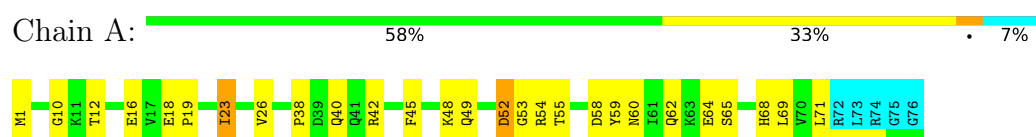
4.2.40 Score per residue for model 40

- Molecule 1: Ubiquitin



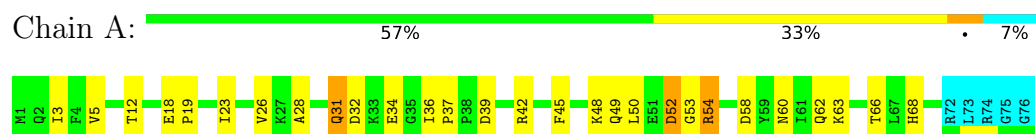
4.2.41 Score per residue for model 41

- Molecule 1: Ubiquitin



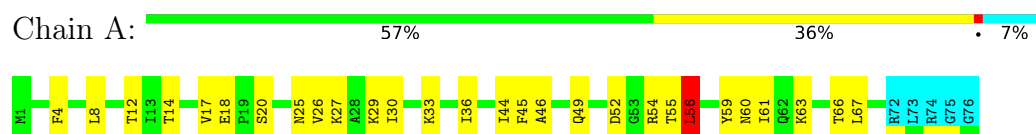
4.2.42 Score per residue for model 42

- Molecule 1: Ubiquitin



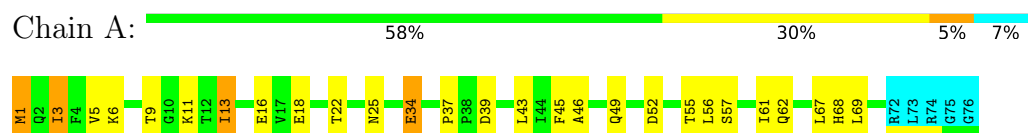
4.2.43 Score per residue for model 43

- Molecule 1: Ubiquitin



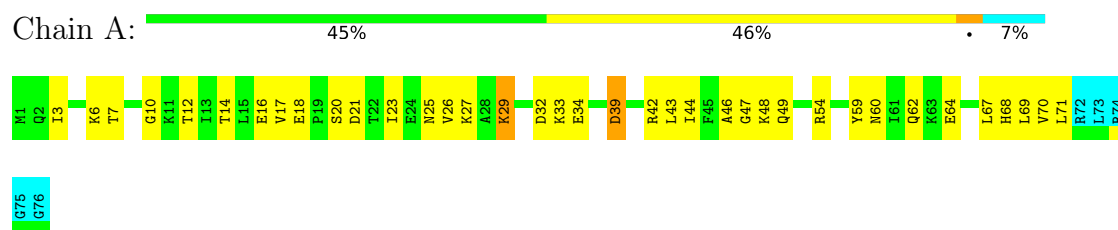
4.2.44 Score per residue for model 44

- Molecule 1: Ubiquitin



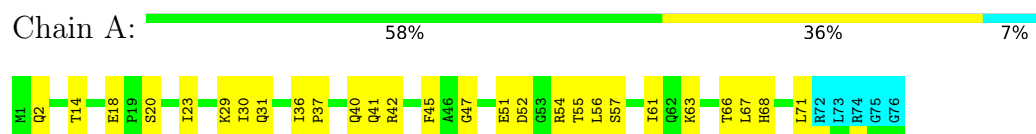
4.2.45 Score per residue for model 45

- Molecule 1: Ubiquitin



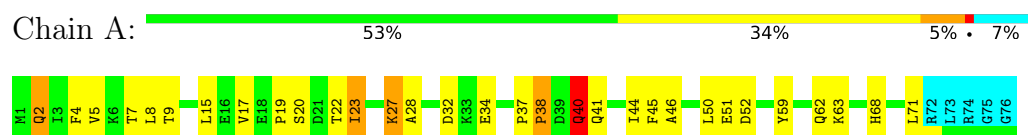
4.2.46 Score per residue for model 46

- Molecule 1: Ubiquitin



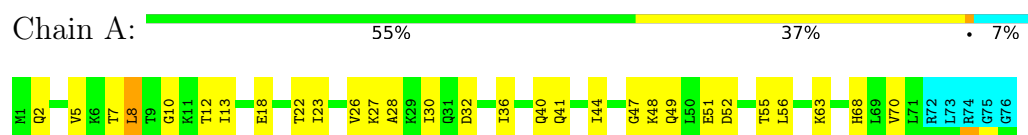
4.2.47 Score per residue for model 47

- Molecule 1: Ubiquitin



4.2.48 Score per residue for model 48

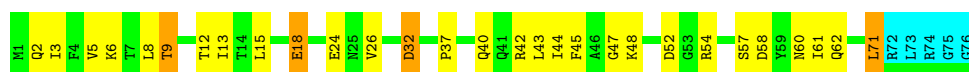
- Molecule 1: Ubiquitin



4.2.49 Score per residue for model 49

- Molecule 1: Ubiquitin

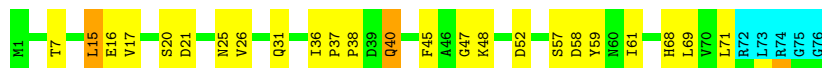




4.2.50 Score per residue for model 50

- Molecule 1: Ubiquitin

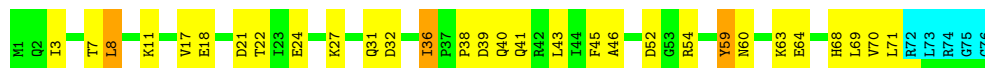
Chain A: 62% 29% 7%



4.2.51 Score per residue for model 51

- Molecule 1: Ubiquitin

Chain A: 54% 36% 7%



4.2.52 Score per residue for model 52

- Molecule 1: Ubiquitin

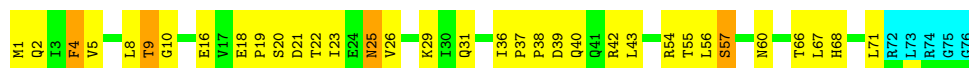
Chain A: 57% 33% 7%



4.2.53 Score per residue for model 53

- Molecule 1: Ubiquitin

Chain A: 49% 39% 5% 7%



4.2.54 Score per residue for model 54

- Molecule 1: Ubiquitin

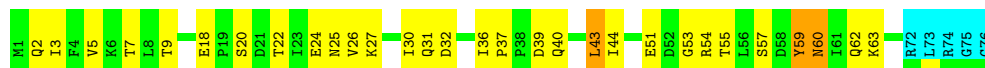
Chain A: 61% 33% 7%



4.2.55 Score per residue for model 55

- Molecule 1: Ubiquitin

Chain A: 54% 36% 7%



4.2.56 Score per residue for model 56

- Molecule 1: Ubiquitin

Chain A: 57% 33% 7%



4.2.57 Score per residue for model 57

- Molecule 1: Ubiquitin

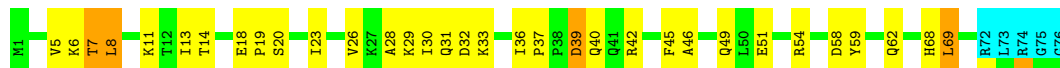
Chain A: 43% 45% 5% 7%



4.2.58 Score per residue for model 58

- Molecule 1: Ubiquitin

Chain A: 50% 38% 5% 7%



4.2.59 Score per residue for model 59

- Molecule 1: Ubiquitin

Chain A: 55% 37% 7%



4.2.60 Score per residue for model 60

- Molecule 1: Ubiquitin



4.2.61 Score per residue for model 61

- Molecule 1: Ubiquitin



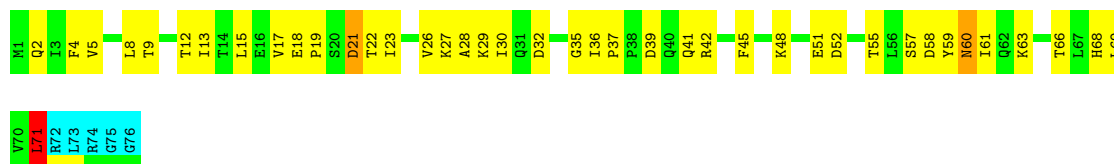
4.2.62 Score per residue for model 62

- Molecule 1: Ubiquitin



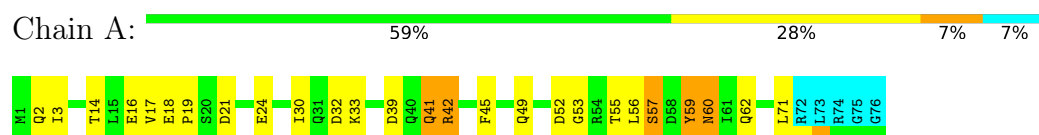
4.2.63 Score per residue for model 63

- Molecule 1: Ubiquitin



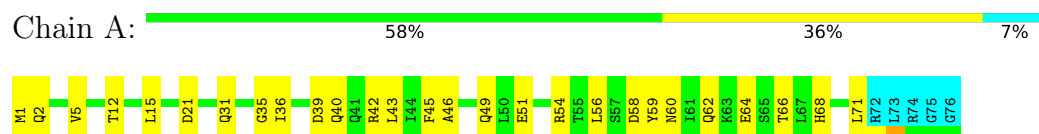
4.2.64 Score per residue for model 64

- Molecule 1: Ubiquitin



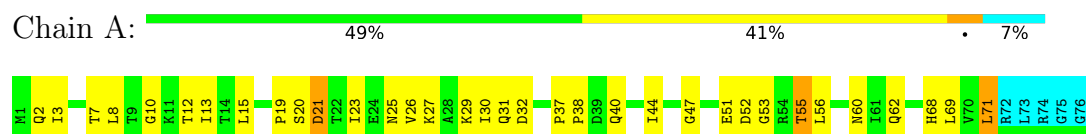
4.2.65 Score per residue for model 65

- Molecule 1: Ubiquitin



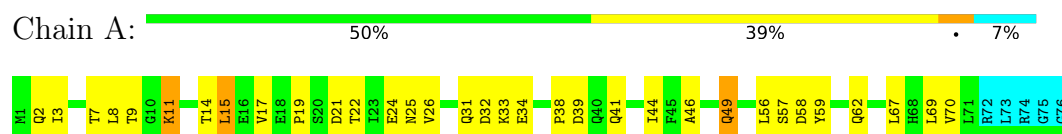
4.2.66 Score per residue for model 66

- Molecule 1: Ubiquitin



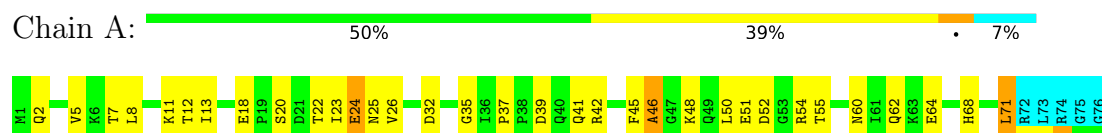
4.2.67 Score per residue for model 67

- Molecule 1: Ubiquitin



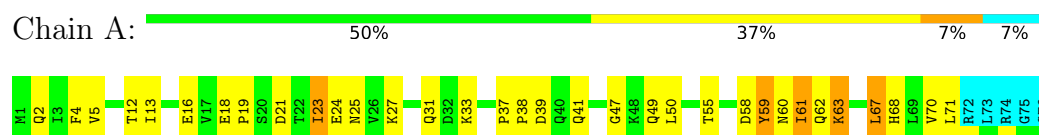
4.2.68 Score per residue for model 68

- Molecule 1: Ubiquitin



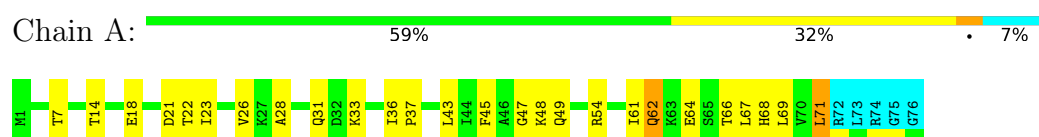
4.2.69 Score per residue for model 69

- Molecule 1: Ubiquitin



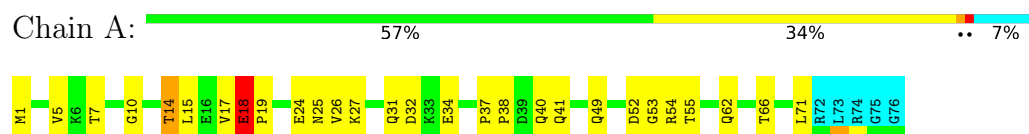
4.2.70 Score per residue for model 70

- Molecule 1: Ubiquitin



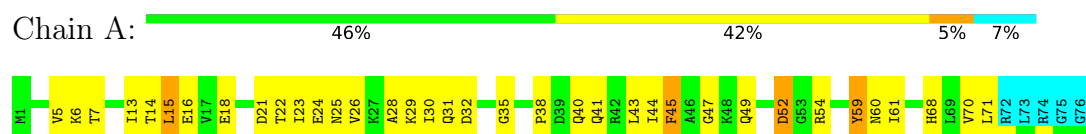
4.2.71 Score per residue for model 71

- Molecule 1: Ubiquitin



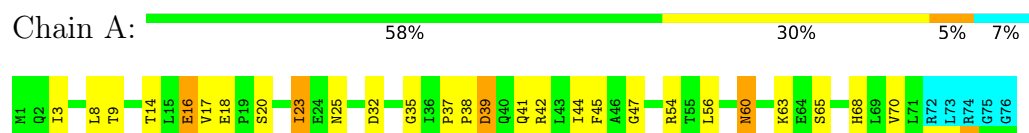
4.2.72 Score per residue for model 72

- Molecule 1: Ubiquitin



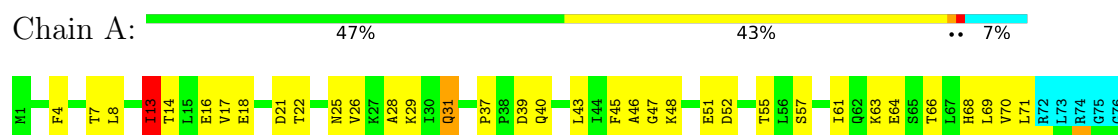
4.2.73 Score per residue for model 73

- Molecule 1: Ubiquitin



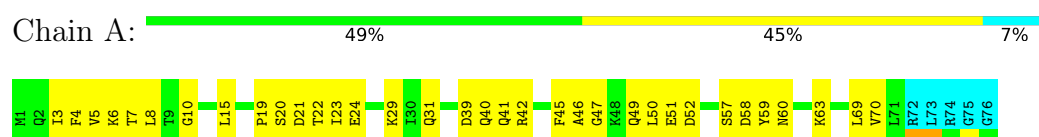
4.2.74 Score per residue for model 74

- Molecule 1: Ubiquitin



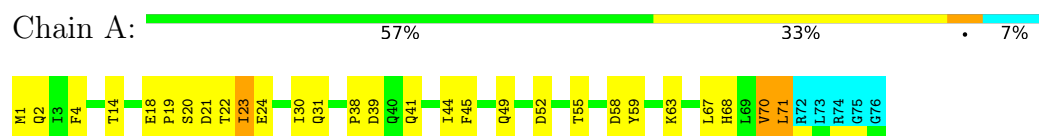
4.2.75 Score per residue for model 75

- Molecule 1: Ubiquitin



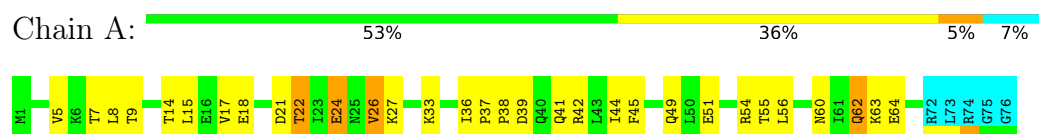
4.2.76 Score per residue for model 76

- Molecule 1: Ubiquitin



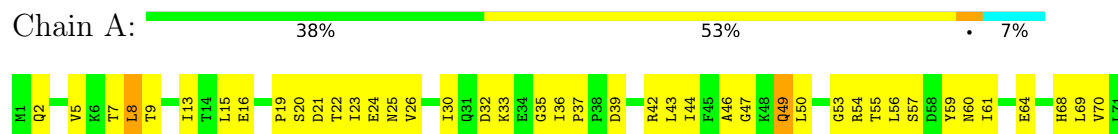
4.2.77 Score per residue for model 77

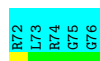
- Molecule 1: Ubiquitin



4.2.78 Score per residue for model 78

- Molecule 1: Ubiquitin





4.2.79 Score per residue for model 79 (medoid)

- Molecule 1: Ubiquitin

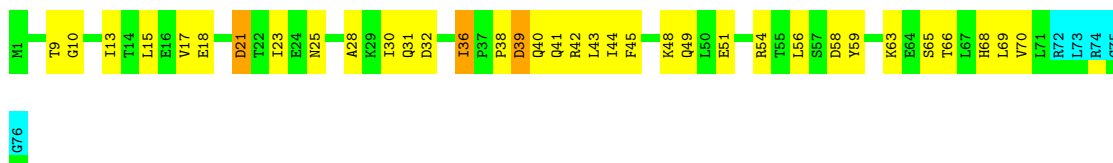
Chain A: 55% 37% • 7%



4.2.80 Score per residue for model 80

- Molecule 1: Ubiquitin

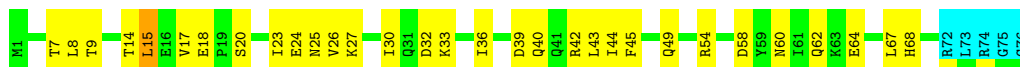
Chain A: 47% 42% • 7%



4.2.81 Score per residue for model 81

- Molecule 1: Ubiquitin

Chain A: 53% 39% • 7%



4.2.82 Score per residue for model 82

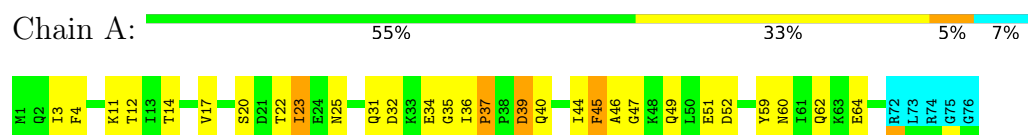
- Molecule 1: Ubiquitin

Chain A: 55% 36% • 7%



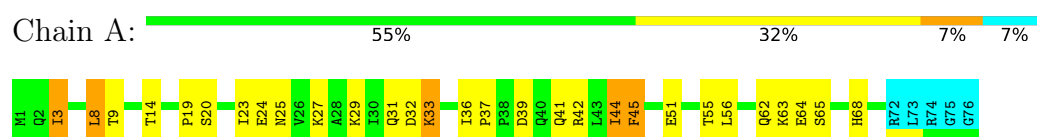
4.2.83 Score per residue for model 83

- Molecule 1: Ubiquitin



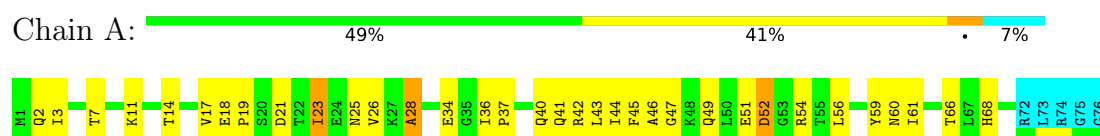
4.2.84 Score per residue for model 84

- Molecule 1: Ubiquitin



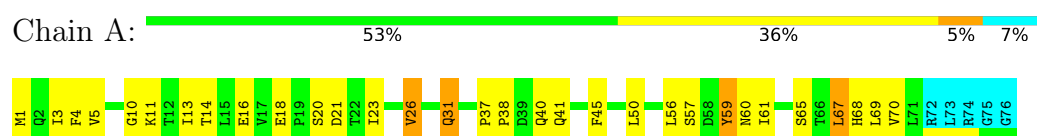
4.2.85 Score per residue for model 85

- Molecule 1: Ubiquitin



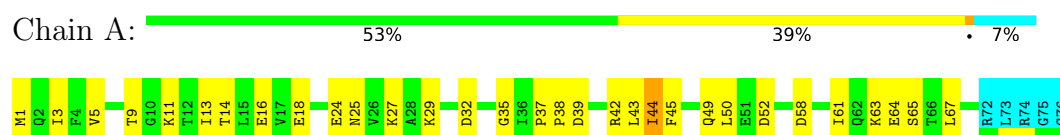
4.2.86 Score per residue for model 86

- Molecule 1: Ubiquitin



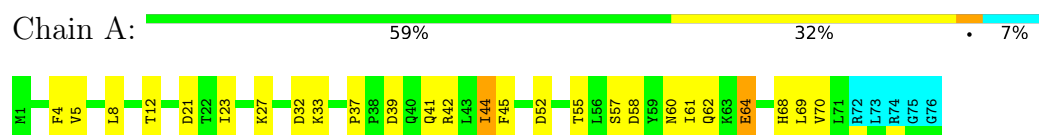
4.2.87 Score per residue for model 87

- Molecule 1: Ubiquitin



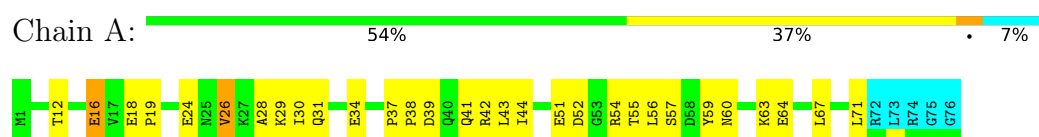
4.2.88 Score per residue for model 88

- Molecule 1: Ubiquitin



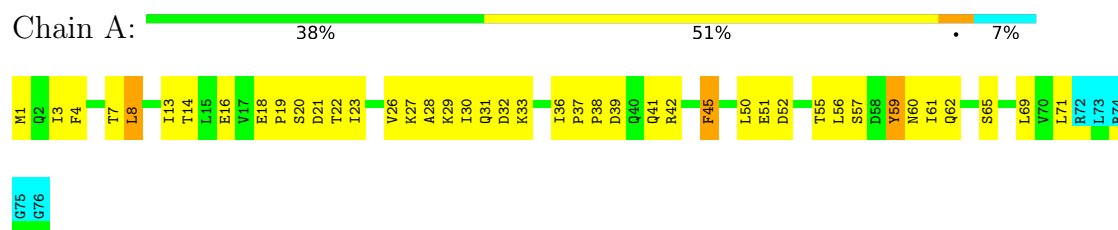
4.2.89 Score per residue for model 89

- Molecule 1: Ubiquitin



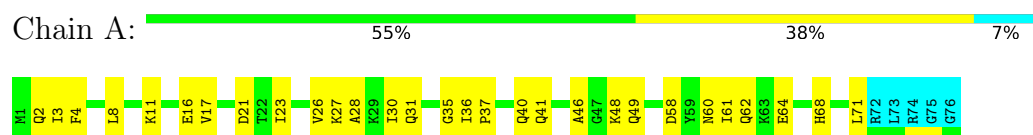
4.2.90 Score per residue for model 90

- Molecule 1: Ubiquitin



4.2.91 Score per residue for model 91

- Molecule 1: Ubiquitin



4.2.92 Score per residue for model 92

- Molecule 1: Ubiquitin





4.2.93 Score per residue for model 93

- Molecule 1: Ubiquitin



4.2.94 Score per residue for model 94

- Molecule 1: Ubiquitin



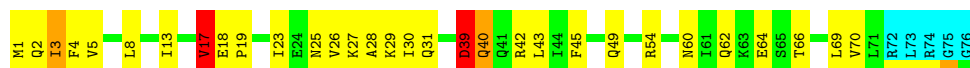
4.2.95 Score per residue for model 95

- Molecule 1: Ubiquitin



4.2.96 Score per residue for model 96

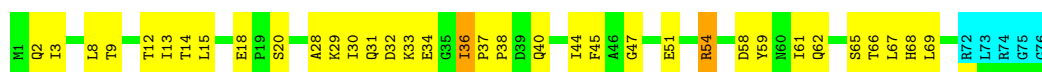
- Molecule 1: Ubiquitin



4.2.97 Score per residue for model 97

- Molecule 1: Ubiquitin





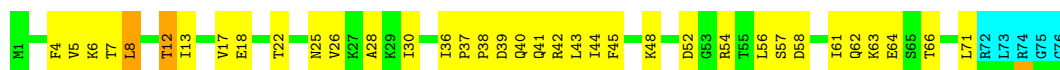
4.2.98 Score per residue for model 98

- Molecule 1: Ubiquitin



4.2.99 Score per residue for model 99

- Molecule 1: Ubiquitin



4.2.100 Score per residue for model 100

- Molecule 1: Ubiquitin



4.2.101 Score per residue for model 101

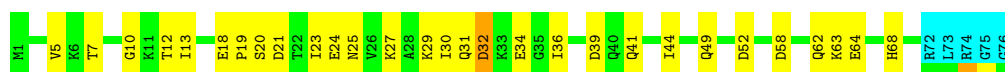
- Molecule 1: Ubiquitin



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



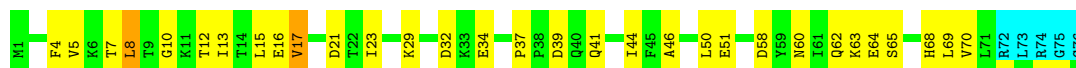
4.2.105 Score per residue for model 105

- Molecule 1: Ubiquitin



4.2.106 Score per residue for model 106

- Molecule 1: Ubiquitin



4.2.107 Score per residue for model 107

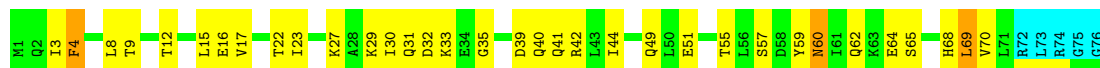
- Molecule 1: Ubiquitin





4.2.108 Score per residue for model 108

- Molecule 1: Ubiquitin



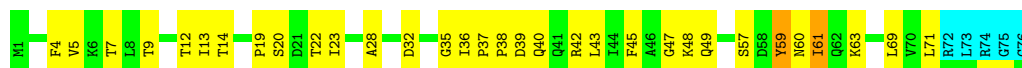
4.2.109 Score per residue for model 109

- Molecule 1: Ubiquitin



4.2.110 Score per residue for model 110

- Molecule 1: Ubiquitin



4.2.111 Score per residue for model 111

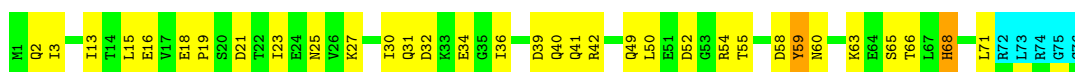
- Molecule 1: Ubiquitin



4.2.112 Score per residue for model 112

- Molecule 1: Ubiquitin





4.2.113 Score per residue for model 113

- Molecule 1: Ubiquitin

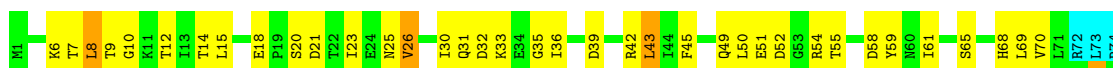
Chain A: 54% 39% 7%



4.2.114 Score per residue for model 114

- Molecule 1: Ubiquitin

Chain A: 45% 45% 7%



4.2.115 Score per residue for model 115

- Molecule 1: Ubiquitin

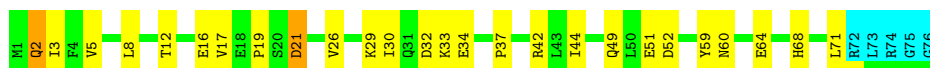
Chain A: 47% 43% 7%



4.2.116 Score per residue for model 116

- Molecule 1: Ubiquitin

Chain A: 59% 32% 7%



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing*.

Of the 1000 calculated structures, 116 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
GROMACS	refinement	

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.60±0.01	0±0/570 (0.0± 0.0%)	2.58±0.09	45±7/770 (5.9± 1.0%)
All	All	0.60	0/66120 (0.0%)	2.58	5237/89320 (5.9%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.2±1.0
All	All	0	143

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	17.35	112.24	103.22	57	24
1	A	39	ASP	CA-CB-CG	16.73	129.33	112.60	88	39
1	A	68	HIS	CA-CB-CG	13.41	127.21	113.80	30	24
1	A	52	ASP	CA-CB-CG	12.52	125.12	112.60	22	32
1	A	4	PHE	CA-CB-CG	12.45	126.25	113.80	101	28
1	A	18	GLU	CA-C-N	11.88	131.59	119.24	64	37
1	A	18	GLU	C-N-CA	11.88	131.59	119.24	64	37
1	A	37	PRO	O-C-N	11.83	126.71	121.15	109	10
1	A	36	ILE	CA-C-N	11.71	128.09	119.66	57	29
1	A	36	ILE	C-N-CA	11.71	128.09	119.66	57	29
1	A	45	PHE	CA-CB-CG	11.66	125.46	113.80	21	32
1	A	60	ASN	CA-CB-CG	11.59	124.19	112.60	68	29
1	A	56	LEU	CA-C-N	11.06	135.49	120.44	54	26
1	A	56	LEU	C-N-CA	11.06	135.49	120.44	54	26
1	A	37	PRO	CA-C-O	-10.94	112.08	120.73	74	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	64	GLU	CB-CA-C	10.74	120.46	109.83	109	11
1	A	26	VAL	CA-C-O	-10.73	108.55	120.46	11	14
1	A	25	ASN	CA-CB-CG	10.69	123.29	112.60	53	20
1	A	25	ASN	OD1-CG-ND2	-10.56	112.04	122.60	60	21
1	A	60	ASN	OD1-CG-ND2	-10.53	112.08	122.60	45	19
1	A	58	ASP	CA-CB-CG	10.49	123.09	112.60	113	33
1	A	31	GLN	CA-C-N	10.47	134.67	120.54	67	35
1	A	31	GLN	C-N-CA	10.47	134.67	120.54	67	35
1	A	10	GLY	CA-C-N	10.46	135.72	120.87	95	20
1	A	10	GLY	C-N-CA	10.46	135.72	120.87	95	20
1	A	35	GLY	CA-C-N	10.38	130.07	122.59	101	13
1	A	35	GLY	C-N-CA	10.38	130.07	122.59	101	13
1	A	21	ASP	CA-CB-CG	10.37	122.97	112.60	74	35
1	A	25	ASN	CA-C-N	10.35	133.80	120.56	101	24
1	A	25	ASN	C-N-CA	10.35	133.80	120.56	101	24
1	A	21	ASP	CA-C-N	10.32	135.52	120.87	45	11
1	A	21	ASP	C-N-CA	10.32	135.52	120.87	45	11
1	A	22	THR	CA-C-N	10.29	133.88	120.60	104	19
1	A	22	THR	C-N-CA	10.29	133.88	120.60	104	19
1	A	51	GLU	CA-C-N	10.28	137.54	121.19	77	38
1	A	51	GLU	C-N-CA	10.28	137.54	121.19	77	38
1	A	43	LEU	CB-CA-C	10.19	125.50	110.62	72	4
1	A	70	VAL	CB-CA-C	10.16	125.10	111.19	94	10
1	A	23	ILE	CA-C-N	10.14	134.27	120.38	1	35
1	A	23	ILE	C-N-CA	10.14	134.27	120.38	1	35
1	A	68	HIS	ND1-CE1-NE2	10.13	118.53	108.40	11	34
1	A	57	SER	CA-C-N	10.12	133.59	120.44	108	18
1	A	57	SER	C-N-CA	10.12	133.59	120.44	108	18
1	A	48	LYS	CA-C-N	10.11	135.11	120.95	15	15
1	A	48	LYS	C-N-CA	10.11	135.11	120.95	15	15
1	A	3	ILE	O-C-N	-9.98	112.29	122.97	79	6
1	A	70	VAL	O-C-N	-9.87	113.14	122.71	114	6
1	A	17	VAL	CA-CB-CG2	9.76	126.99	110.40	83	9
1	A	41	GLN	OE1-CD-NE2	-9.72	112.88	122.60	33	20
1	A	31	GLN	OE1-CD-NE2	-9.72	112.88	122.60	86	21
1	A	37	PRO	CA-C-N	9.63	131.88	119.84	33	46
1	A	37	PRO	C-N-CA	9.63	131.88	119.84	33	46
1	A	61	ILE	CB-CA-C	9.63	122.01	111.80	86	8
1	A	31	GLN	N-CA-C	9.59	122.62	111.11	97	11
1	A	42	ARG	NE-CZ-NH2	9.55	127.80	119.20	28	23
1	A	68	HIS	CB-CG-CD2	-9.55	118.78	131.20	27	11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	27	LYS	CA-C-N	9.53	133.06	120.28	6	31
1	A	27	LYS	C-N-CA	9.53	133.06	120.28	6	31
1	A	62	GLN	CA-C-N	9.52	136.41	121.56	10	29
1	A	62	GLN	C-N-CA	9.52	136.41	121.56	10	29
1	A	19	PRO	N-CA-CB	9.50	112.63	103.51	85	17
1	A	11	LYS	CA-C-N	9.47	135.15	122.84	36	10
1	A	11	LYS	C-N-CA	9.47	135.15	122.84	36	10
1	A	9	THR	CA-CB-OG1	9.46	123.80	109.60	47	7
1	A	23	ILE	CA-C-O	-9.45	110.34	120.64	106	14
1	A	60	ASN	CA-C-N	9.45	133.82	120.98	28	7
1	A	60	ASN	C-N-CA	9.45	133.82	120.98	28	7
1	A	2	GLN	CA-C-N	9.34	134.75	122.51	17	15
1	A	2	GLN	C-N-CA	9.34	134.75	122.51	17	15
1	A	22	THR	CB-CA-C	9.28	125.37	109.51	60	3
1	A	2	GLN	OE1-CD-NE2	-9.26	113.34	122.60	47	20
1	A	24	GLU	CA-C-N	9.24	132.66	120.28	5	16
1	A	24	GLU	C-N-CA	9.24	132.66	120.28	5	16
1	A	26	VAL	CA-C-N	9.19	133.34	120.29	114	30
1	A	26	VAL	C-N-CA	9.19	133.34	120.29	114	30
1	A	26	VAL	N-CA-C	-9.16	102.93	111.45	71	11
1	A	46	ALA	CA-C-N	9.16	136.23	122.86	17	7
1	A	46	ALA	C-N-CA	9.16	136.23	122.86	17	7
1	A	70	VAL	CA-C-O	9.14	130.10	120.51	114	4
1	A	40	GLN	CA-C-N	9.12	136.98	122.21	22	13
1	A	40	GLN	C-N-CA	9.12	136.98	122.21	22	13
1	A	37	PRO	N-CA-C	9.11	121.82	110.70	70	18
1	A	49	GLN	OE1-CD-NE2	-9.11	113.50	122.60	101	21
1	A	59	TYR	CA-C-N	9.06	138.84	121.54	58	29
1	A	59	TYR	C-N-CA	9.06	138.84	121.54	58	29
1	A	32	ASP	CA-CB-CG	9.03	121.63	112.60	56	33
1	A	30	ILE	CA-C-N	8.99	132.12	120.44	96	26
1	A	30	ILE	C-N-CA	8.99	132.12	120.44	96	26
1	A	12	THR	CA-CB-OG1	8.97	123.05	109.60	9	10
1	A	27	LYS	N-CA-C	8.92	122.12	111.33	35	7
1	A	10	GLY	O-C-N	8.91	132.58	122.42	92	6
1	A	7	THR	CA-CB-OG1	-8.90	96.25	109.60	48	20
1	A	47	GLY	CA-C-O	-8.88	112.28	119.83	66	7
1	A	55	THR	CA-C-N	8.88	131.98	120.44	61	32
1	A	55	THR	C-N-CA	8.88	131.98	120.44	61	32
1	A	71	LEU	CA-C-N	8.87	135.22	122.09	76	21
1	A	71	LEU	C-N-CA	8.87	135.22	122.09	76	21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	27	LYS	O-C-N	8.84	132.23	122.15	112	3
1	A	42	ARG	CD-NE-CZ	8.82	136.74	124.40	19	18
1	A	42	ARG	CA-C-N	8.81	134.14	122.42	37	11
1	A	42	ARG	C-N-CA	8.81	134.14	122.42	37	11
1	A	45	PHE	CA-C-N	8.81	138.36	121.54	65	23
1	A	45	PHE	C-N-CA	8.81	138.36	121.54	65	23
1	A	38	PRO	CA-C-N	8.80	135.42	120.72	71	21
1	A	38	PRO	C-N-CA	8.80	135.42	120.72	71	21
1	A	32	ASP	N-CA-C	8.80	120.87	111.28	38	13
1	A	17	VAL	CA-C-O	-8.78	113.29	121.72	3	11
1	A	5	VAL	CB-CA-C	8.76	124.11	110.28	116	14
1	A	12	THR	CA-C-N	8.74	132.21	120.50	42	16
1	A	12	THR	C-N-CA	8.74	132.21	120.50	42	16
1	A	62	GLN	OE1-CD-NE2	-8.73	113.87	122.60	30	19
1	A	65	SER	CA-C-O	-8.73	112.05	121.56	86	4
1	A	28	ALA	CA-C-O	-8.72	111.30	120.55	47	8
1	A	7	THR	O-C-N	-8.71	113.30	123.06	111	11
1	A	40	GLN	OE1-CD-NE2	-8.67	113.93	122.60	28	20
1	A	32	ASP	CA-C-N	8.66	131.70	120.44	14	11
1	A	32	ASP	C-N-CA	8.66	131.70	120.44	14	11
1	A	30	ILE	N-CA-CB	8.61	121.59	110.57	60	4
1	A	54	ARG	CD-NE-CZ	8.60	136.44	124.40	73	12
1	A	9	THR	CA-CB-CG2	8.57	125.07	110.50	104	8
1	A	12	THR	CA-CB-CG2	8.52	124.99	110.50	40	8
1	A	9	THR	CA-C-N	8.50	135.11	122.10	11	11
1	A	9	THR	C-N-CA	8.50	135.11	122.10	11	11
1	A	34	GLU	N-CA-C	8.50	124.85	113.97	33	5
1	A	14	THR	CB-CA-C	8.48	121.95	111.43	73	4
1	A	28	ALA	CA-C-N	8.47	131.63	120.28	48	16
1	A	28	ALA	C-N-CA	8.47	131.63	120.28	48	16
1	A	36	ILE	CA-C-O	-8.45	113.70	119.19	1	22
1	A	30	ILE	CA-C-O	-8.45	112.62	121.41	24	12
1	A	45	PHE	O-C-N	-8.43	111.99	123.12	101	3
1	A	16	GLU	CA-C-O	8.43	129.62	120.43	20	9
1	A	43	LEU	CA-C-N	8.40	134.67	122.99	70	18
1	A	43	LEU	C-N-CA	8.40	134.67	122.99	70	18
1	A	34	GLU	CA-C-O	8.40	128.90	119.41	85	9
1	A	36	ILE	O-C-N	8.39	128.87	121.57	48	7
1	A	22	THR	CA-CB-OG1	8.39	122.18	109.60	108	15
1	A	18	GLU	N-CA-CB	-8.38	100.17	109.72	94	6
1	A	50	LEU	CA-C-N	8.38	133.87	121.72	21	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	50	LEU	C-N-CA	8.38	133.87	121.72	21	13
1	A	41	GLN	CA-C-O	-8.37	111.26	120.38	24	10
1	A	58	ASP	N-CA-C	8.33	121.41	111.33	16	9
1	A	63	LYS	CA-C-N	8.32	134.50	122.35	7	15
1	A	63	LYS	C-N-CA	8.32	134.50	122.35	7	15
1	A	1	MET	CA-C-N	8.32	133.93	122.19	44	6
1	A	1	MET	C-N-CA	8.32	133.93	122.19	44	6
1	A	38	PRO	N-CA-CB	8.32	111.80	103.48	66	18
1	A	65	SER	CA-C-N	8.31	133.64	122.84	87	9
1	A	65	SER	C-N-CA	8.31	133.64	122.84	87	9
1	A	20	SER	CA-C-N	8.31	133.30	121.42	79	14
1	A	20	SER	C-N-CA	8.31	133.30	121.42	79	14
1	A	57	SER	N-CA-C	8.30	119.95	111.07	16	11
1	A	8	LEU	N-CA-C	8.30	121.37	111.33	15	10
1	A	29	LYS	CA-C-N	8.30	132.23	120.53	115	26
1	A	29	LYS	C-N-CA	8.30	132.23	120.53	115	26
1	A	59	TYR	CB-CA-C	-8.29	96.55	110.56	7	3
1	A	71	LEU	CB-CA-C	8.27	125.72	109.35	99	5
1	A	50	LEU	CA-C-O	-8.27	111.42	120.92	78	8
1	A	16	GLU	CA-C-N	8.26	134.41	122.69	45	20
1	A	16	GLU	C-N-CA	8.26	134.41	122.69	45	20
1	A	31	GLN	CG-CD-NE2	8.25	128.78	116.40	59	7
1	A	2	GLN	CA-C-O	-8.24	111.55	121.28	11	5
1	A	70	VAL	CA-C-N	8.23	134.57	123.05	80	16
1	A	70	VAL	C-N-CA	8.23	134.57	123.05	80	16
1	A	26	VAL	CA-CB-CG1	8.20	124.34	110.40	63	11
1	A	36	ILE	CB-CA-C	8.17	118.54	110.94	81	7
1	A	19	PRO	CA-C-N	8.14	135.67	122.65	67	12
1	A	19	PRO	C-N-CA	8.14	135.67	122.65	67	12
1	A	5	VAL	CA-C-O	-8.12	112.07	120.27	58	8
1	A	42	ARG	NH1-CZ-NH2	-8.12	108.75	119.30	10	9
1	A	31	GLN	O-C-N	-8.11	112.91	122.15	38	6
1	A	54	ARG	NE-CZ-NH2	-8.09	111.92	119.20	5	15
1	A	4	PHE	CA-C-N	8.09	133.86	123.10	108	12
1	A	4	PHE	C-N-CA	8.09	133.86	123.10	108	12
1	A	34	GLU	CB-CA-C	8.09	121.50	109.29	100	7
1	A	58	ASP	CA-C-O	8.06	129.29	119.38	28	5
1	A	33	LYS	N-CA-C	8.05	119.83	111.14	108	6
1	A	36	ILE	N-CA-CB	-8.05	101.62	110.23	65	7
1	A	2	GLN	N-CA-CB	-8.05	97.58	110.46	97	4
1	A	13	ILE	CA-CB-CG1	8.03	124.06	110.40	8	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	44	ILE	N-CA-CB	-8.03	100.33	111.25	20	4
1	A	39	ASP	CB-CA-C	8.03	123.65	110.81	73	2
1	A	68	HIS	ND1-CG-CD2	8.03	114.12	106.10	63	18
1	A	63	LYS	CA-C-O	-8.02	112.37	121.19	34	7
1	A	17	VAL	O-C-N	-8.01	114.67	122.12	99	10
1	A	55	THR	CA-CB-OG1	8.01	121.61	109.60	109	24
1	A	68	HIS	CA-C-N	8.01	134.76	123.07	74	14
1	A	68	HIS	C-N-CA	8.01	134.76	123.07	74	14
1	A	36	ILE	N-CA-C	8.00	115.51	108.63	103	2
1	A	27	LYS	N-CA-CB	8.00	121.85	109.94	61	2
1	A	26	VAL	CB-CA-C	7.98	122.91	112.14	91	4
1	A	30	ILE	O-C-N	-7.97	113.85	121.90	27	7
1	A	53	GLY	N-CA-C	-7.96	103.78	115.63	78	4
1	A	54	ARG	O-C-N	-7.92	112.91	122.65	58	8
1	A	46	ALA	CB-CA-C	7.88	126.10	110.42	9	5
1	A	47	GLY	CA-C-N	7.88	132.90	122.42	75	17
1	A	47	GLY	C-N-CA	7.88	132.90	122.42	75	17
1	A	49	GLN	N-CA-C	7.88	121.34	110.24	71	3
1	A	13	ILE	CB-CA-C	7.87	121.82	110.33	49	8
1	A	22	THR	N-CA-CB	-7.86	98.50	110.45	77	8
1	A	54	ARG	NE-CZ-NH1	-7.86	113.64	121.50	96	13
1	A	28	ALA	O-C-N	7.86	132.86	122.33	74	4
1	A	39	ASP	CA-C-N	7.85	134.56	122.23	107	9
1	A	39	ASP	C-N-CA	7.85	134.56	122.23	107	9
1	A	52	ASP	CA-C-O	7.84	129.27	120.80	6	10
1	A	42	ARG	NE-CZ-NH1	7.84	129.34	121.50	112	12
1	A	35	GLY	O-C-N	7.84	131.36	122.42	68	3
1	A	20	SER	CA-C-O	-7.84	108.85	119.12	115	6
1	A	27	LYS	CA-C-O	-7.83	112.52	120.90	9	9
1	A	8	LEU	CA-C-N	7.82	131.80	120.38	91	21
1	A	8	LEU	C-N-CA	7.82	131.80	120.38	91	21
1	A	17	VAL	CB-CA-C	7.81	122.84	110.82	51	4
1	A	33	LYS	CA-CB-CG	7.81	129.71	114.10	24	2
1	A	65	SER	O-C-N	7.79	132.39	122.81	35	6
1	A	66	THR	CA-C-N	7.79	133.74	123.00	11	9
1	A	66	THR	C-N-CA	7.79	133.74	123.00	11	9
1	A	58	ASP	CB-CA-C	-7.74	97.52	110.68	16	2
1	A	5	VAL	CA-C-N	7.74	132.74	122.30	62	5
1	A	5	VAL	C-N-CA	7.74	132.74	122.30	62	5
1	A	5	VAL	N-CA-C	-7.71	97.32	108.11	44	8
1	A	44	ILE	O-C-N	-7.70	114.48	123.03	48	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	13	ILE	O-C-N	-7.68	114.78	123.00	39	7
1	A	32	ASP	O-C-N	-7.68	113.39	122.15	88	6
1	A	40	GLN	N-CA-C	-7.68	103.91	113.28	110	5
1	A	49	GLN	CA-C-N	7.67	131.69	120.95	36	9
1	A	49	GLN	C-N-CA	7.67	131.69	120.95	36	9
1	A	33	LYS	N-CA-CB	-7.67	98.83	110.26	28	2
1	A	44	ILE	CA-CB-CG1	7.67	123.43	110.40	17	7
1	A	13	ILE	N-CA-C	-7.64	97.05	109.12	78	6
1	A	25	ASN	N-CA-C	7.63	119.59	111.28	44	11
1	A	39	ASP	N-CA-CB	-7.63	99.17	110.53	102	5
1	A	19	PRO	CB-CA-C	-7.62	101.03	111.85	75	6
1	A	16	GLU	CB-CG-CD	7.62	125.55	112.60	69	6
1	A	20	SER	N-CA-C	7.61	122.14	113.01	78	12
1	A	14	THR	CA-C-N	7.61	131.60	120.95	36	5
1	A	14	THR	C-N-CA	7.61	131.60	120.95	36	5
1	A	7	THR	CA-C-N	7.61	132.77	120.60	113	27
1	A	7	THR	C-N-CA	7.61	132.77	120.60	113	27
1	A	64	GLU	O-C-N	7.60	130.02	121.88	100	3
1	A	15	LEU	CA-C-N	7.57	132.32	121.50	57	22
1	A	15	LEU	C-N-CA	7.57	132.32	121.50	57	22
1	A	32	ASP	CB-CA-C	7.57	122.95	110.92	25	5
1	A	53	GLY	CA-C-O	-7.56	110.77	118.86	27	5
1	A	52	ASP	CB-CA-C	-7.56	99.18	110.67	72	3
1	A	35	GLY	CA-C-O	7.55	128.37	119.46	94	4
1	A	14	THR	N-CA-CB	-7.54	98.08	110.52	100	3
1	A	64	GLU	CA-C-N	7.53	131.41	120.71	81	16
1	A	64	GLU	C-N-CA	7.53	131.41	120.71	81	16
1	A	25	ASN	CA-C-O	-7.51	112.93	120.82	107	7
1	A	42	ARG	CB-CA-C	7.51	121.26	111.42	31	11
1	A	5	VAL	N-CA-CB	-7.50	102.61	111.83	21	9
1	A	55	THR	O-C-N	-7.47	114.57	122.94	92	9
1	A	53	GLY	CA-C-N	7.47	135.34	122.64	111	8
1	A	53	GLY	C-N-CA	7.47	135.34	122.64	111	8
1	A	21	ASP	N-CA-CB	7.47	120.95	109.97	39	5
1	A	53	GLY	O-C-N	7.46	130.93	122.42	104	5
1	A	39	ASP	N-CA-C	7.45	121.29	111.75	26	8
1	A	67	LEU	N-CA-C	-7.45	98.59	110.14	97	5
1	A	58	ASP	CA-C-N	7.44	135.13	122.26	91	5
1	A	58	ASP	C-N-CA	7.44	135.13	122.26	91	5
1	A	30	ILE	CB-CA-C	7.43	121.48	111.97	112	7
1	A	12	THR	O-C-N	-7.43	114.75	123.22	108	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	7	THR	N-CA-CB	-7.42	99.77	110.45	29	3
1	A	5	VAL	CA-CB-CG2	7.41	122.99	110.40	31	2
1	A	18	GLU	N-CA-C	-7.40	100.76	110.39	72	12
1	A	18	GLU	CA-C-O	-7.40	113.31	120.19	64	17
1	A	7	THR	CA-CB-CG2	7.38	123.04	110.50	34	8
1	A	15	LEU	N-CA-C	7.37	120.28	109.07	22	2
1	A	23	ILE	CA-CB-CG2	7.37	123.03	110.50	76	8
1	A	71	LEU	CA-C-O	-7.36	112.53	120.92	68	7
1	A	34	GLU	CA-C-N	7.35	134.31	122.25	83	6
1	A	34	GLU	C-N-CA	7.35	134.31	122.25	83	6
1	A	59	TYR	O-C-N	-7.34	113.53	122.34	114	5
1	A	61	ILE	CA-C-N	7.33	134.85	121.06	69	8
1	A	61	ILE	C-N-CA	7.33	134.85	121.06	69	8
1	A	57	SER	O-C-N	-7.33	113.79	122.15	64	4
1	A	3	ILE	CA-C-N	7.33	132.20	122.30	7	7
1	A	3	ILE	C-N-CA	7.33	132.20	122.30	7	7
1	A	60	ASN	N-CA-C	7.32	121.51	112.58	55	5
1	A	33	LYS	CA-C-O	-7.32	113.20	120.89	58	8
1	A	56	LEU	O-C-N	7.31	129.69	122.09	16	2
1	A	62	GLN	CA-C-O	-7.30	112.86	121.11	62	7
1	A	3	ILE	CA-CB-CG1	7.30	122.81	110.40	1	8
1	A	44	ILE	CB-CA-C	7.29	120.97	110.33	1	13
1	A	56	LEU	CB-CA-C	7.28	122.45	110.81	46	4
1	A	18	GLU	CB-CA-C	7.27	120.91	108.91	97	19
1	A	44	ILE	CA-CB-CG2	7.26	122.85	110.50	33	2
1	A	45	PHE	CB-CA-C	7.25	120.87	110.79	17	8
1	A	62	GLN	CG-CD-NE2	7.25	127.27	116.40	31	5
1	A	57	SER	CA-C-O	-7.24	112.81	120.63	7	5
1	A	63	LYS	N-CA-C	7.23	120.72	110.23	19	9
1	A	14	THR	CA-CB-OG1	7.22	120.43	109.60	52	13
1	A	14	THR	N-CA-C	-7.22	97.45	109.07	64	4
1	A	44	ILE	CA-C-N	7.21	132.90	122.44	80	21
1	A	44	ILE	C-N-CA	7.21	132.90	122.44	80	21
1	A	19	PRO	N-CD-CG	7.21	114.02	103.20	69	4
1	A	20	SER	N-CA-CB	-7.21	99.83	110.49	55	19
1	A	37	PRO	CB-CA-C	-7.20	102.13	110.92	99	13
1	A	42	ARG	CB-CG-CD	7.20	127.86	111.30	41	1
1	A	40	GLN	N-CA-CB	-7.19	99.85	110.49	1	9
1	A	51	GLU	CA-C-O	-7.19	112.55	120.38	36	4
1	A	10	GLY	CA-C-O	7.19	127.22	119.03	106	5
1	A	66	THR	CA-CB-CG2	7.17	122.69	110.50	42	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	13	ILE	CA-C-N	7.17	134.12	122.29	54	12
1	A	13	ILE	C-N-CA	7.17	134.12	122.29	54	12
1	A	69	LEU	N-CA-C	-7.17	96.73	108.41	32	2
1	A	63	LYS	CB-CA-C	7.14	118.59	109.80	55	8
1	A	26	VAL	O-C-N	7.13	129.07	121.94	99	12
1	A	6	LYS	CA-C-N	7.13	132.92	120.87	49	4
1	A	6	LYS	C-N-CA	7.13	132.92	120.87	49	4
1	A	66	THR	OG1-CB-CG2	-7.11	95.08	109.30	92	8
1	A	66	THR	CA-C-O	-7.11	112.75	120.36	13	8
1	A	44	ILE	N-CA-C	-7.09	98.27	108.48	97	6
1	A	11	LYS	CA-C-O	-7.08	113.84	121.56	87	5
1	A	7	THR	CA-C-O	-7.08	113.80	121.94	71	4
1	A	3	ILE	CB-CA-C	7.07	121.24	111.34	56	13
1	A	69	LEU	CA-C-N	7.07	132.77	122.94	90	24
1	A	69	LEU	C-N-CA	7.07	132.77	122.94	90	24
1	A	15	LEU	CA-C-O	-7.07	113.07	120.70	71	6
1	A	12	THR	OG1-CB-CG2	-7.07	95.16	109.30	65	6
1	A	22	THR	O-C-N	-7.07	114.64	122.84	83	3
1	A	29	LYS	O-C-N	-7.06	113.05	122.23	6	6
1	A	7	THR	OG1-CB-CG2	-7.05	95.19	109.30	93	1
1	A	22	THR	CA-C-O	-7.05	113.92	121.88	11	4
1	A	41	GLN	CA-C-N	7.04	132.99	121.86	94	12
1	A	41	GLN	C-N-CA	7.04	132.99	121.86	94	12
1	A	14	THR	CA-C-O	-7.02	113.07	120.58	57	7
1	A	67	LEU	CA-C-N	7.00	131.88	121.72	25	9
1	A	67	LEU	C-N-CA	7.00	131.88	121.72	25	9
1	A	44	ILE	CA-C-O	-7.00	113.08	120.57	106	6
1	A	12	THR	CA-C-O	7.00	129.07	121.16	48	10
1	A	68	HIS	CB-CA-C	6.99	123.19	109.35	109	3
1	A	34	GLU	N-CA-CB	-6.99	101.61	110.90	7	7
1	A	24	GLU	O-C-N	-6.97	114.06	122.22	71	2
1	A	48	LYS	N-CA-C	6.97	119.76	109.24	41	2
1	A	60	ASN	O-C-N	-6.97	114.62	122.91	53	2
1	A	37	PRO	N-CD-CG	6.95	113.63	103.20	66	9
1	A	7	THR	CB-CA-C	6.95	125.39	110.45	15	3
1	A	71	LEU	N-CA-C	6.93	120.02	110.24	63	8
1	A	4	PHE	CB-CA-C	-6.93	97.73	109.72	13	2
1	A	9	THR	N-CA-CB	-6.91	100.05	110.07	47	7
1	A	43	LEU	CA-C-O	-6.89	113.40	120.71	74	8
1	A	19	PRO	N-CA-C	6.88	123.10	113.53	76	7
1	A	13	ILE	CA-C-O	6.88	128.09	120.59	16	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	14	THR	CA-CB-CG2	6.87	122.18	110.50	92	5
1	A	37	PRO	CA-N-CD	-6.87	102.38	112.00	20	1
1	A	47	GLY	O-C-N	6.86	131.15	122.43	105	7
1	A	36	ILE	CA-CB-CG2	6.86	122.16	110.50	28	7
1	A	5	VAL	CA-CB-CG1	6.86	122.06	110.40	38	6
1	A	31	GLN	CB-CG-CD	6.86	124.25	112.60	46	7
1	A	40	GLN	CB-CG-CD	6.84	124.22	112.60	41	7
1	A	16	GLU	CB-CA-C	6.84	120.81	109.53	106	2
1	A	8	LEU	CA-C-O	6.82	126.55	119.05	100	7
1	A	52	ASP	N-CA-C	-6.81	96.56	108.20	48	8
1	A	45	PHE	N-CA-CB	-6.80	100.53	110.40	74	5
1	A	23	ILE	CA-CB-CG1	6.80	121.96	110.40	40	6
1	A	17	VAL	N-CA-C	6.80	119.95	108.86	60	4
1	A	69	LEU	N-CA-CB	-6.80	99.45	111.08	13	2
1	A	29	LYS	N-CA-C	6.79	118.69	111.28	17	13
1	A	25	ASN	O-C-N	-6.79	113.33	122.43	20	5
1	A	24	GLU	CA-C-O	-6.79	113.30	120.63	104	5
1	A	52	ASP	CA-C-N	6.79	132.24	123.08	76	7
1	A	52	ASP	C-N-CA	6.79	132.24	123.08	76	7
1	A	68	HIS	O-C-N	6.76	131.09	123.05	12	2
1	A	49	GLN	N-CA-CB	-6.76	100.78	110.44	103	7
1	A	46	ALA	CA-C-O	6.75	127.89	120.12	83	6
1	A	52	ASP	N-CA-CB	6.74	119.93	109.48	114	6
1	A	40	GLN	CB-CA-C	6.74	120.87	109.55	85	4
1	A	21	ASP	O-C-N	6.74	130.60	123.06	66	4
1	A	18	GLU	O-C-N	-6.72	115.15	121.20	70	6
1	A	61	ILE	N-CA-C	-6.72	100.90	109.30	74	3
1	A	17	VAL	N-CA-CB	-6.72	104.68	112.34	85	5
1	A	46	ALA	N-CA-C	6.71	121.42	113.23	91	8
1	A	51	GLU	CB-CG-CD	6.71	124.00	112.60	4	5
1	A	29	LYS	N-CA-CB	-6.69	100.00	110.30	46	2
1	A	6	LYS	CA-C-O	-6.68	114.28	121.56	45	7
1	A	68	HIS	CA-C-O	-6.67	113.22	120.36	60	6
1	A	69	LEU	CB-CA-C	6.67	120.81	110.14	78	5
1	A	62	GLN	O-C-N	-6.66	115.44	123.10	92	2
1	A	61	ILE	CA-CB-CG2	6.66	121.81	110.50	95	7
1	A	56	LEU	N-CA-C	6.66	119.14	111.02	21	7
1	A	6	LYS	N-CA-CB	-6.66	100.10	110.55	33	2
1	A	31	GLN	CB-CA-C	-6.65	99.54	110.85	67	1
1	A	38	PRO	N-CD-CG	6.64	113.16	103.20	51	9
1	A	23	ILE	O-C-N	-6.63	115.00	121.83	81	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	68	HIS	CE1-NE2-CD2	-6.63	102.37	109.00	16	12
1	A	23	ILE	N-CA-C	6.63	118.17	110.62	36	8
1	A	60	ASN	CB-CG-ND2	6.62	126.34	116.40	45	4
1	A	65	SER	N-CA-C	6.62	118.85	110.24	56	5
1	A	31	GLN	CA-C-O	-6.62	113.53	120.55	61	10
1	A	28	ALA	N-CA-C	6.60	119.30	111.71	54	7
1	A	50	LEU	O-C-N	-6.60	115.69	123.22	68	4
1	A	51	GLU	O-C-N	6.59	130.44	123.06	79	4
1	A	5	VAL	O-C-N	-6.58	116.27	123.18	88	6
1	A	11	LYS	CB-CA-C	-6.58	98.89	109.75	91	3
1	A	59	TYR	N-CA-CB	-6.58	100.89	110.70	103	2
1	A	48	LYS	CA-C-O	-6.57	113.21	120.70	54	3
1	A	48	LYS	CB-CA-C	6.57	121.58	109.70	63	6
1	A	68	HIS	N-CA-CB	-6.55	100.33	110.56	45	4
1	A	55	THR	CA-CB-CG2	6.54	121.62	110.50	114	9
1	A	21	ASP	CA-C-O	-6.53	114.44	121.56	102	2
1	A	70	VAL	CA-CB-CG1	6.53	121.51	110.40	28	7
1	A	52	ASP	O-C-N	6.53	130.39	122.75	99	4
1	A	45	PHE	N-CA-C	-6.53	97.14	108.69	104	3
1	A	4	PHE	O-C-N	-6.50	115.25	123.24	54	5
1	A	10	GLY	N-CA-C	-6.50	106.96	114.69	25	6
1	A	41	GLN	CB-CG-CD	6.49	123.63	112.60	23	3
1	A	45	PHE	CA-C-O	-6.49	113.20	120.66	47	6
1	A	16	GLU	N-CA-C	6.48	118.97	108.34	50	8
1	A	30	ILE	N-CA-C	6.48	117.26	110.72	107	8
1	A	1	MET	O-C-N	-6.47	112.64	123.00	76	2
1	A	13	ILE	N-CA-CB	6.47	118.90	111.39	7	6
1	A	58	ASP	N-CA-CB	6.47	119.84	110.20	35	3
1	A	21	ASP	N-CA-C	6.47	120.21	110.64	72	1
1	A	51	GLU	N-CA-CB	-6.46	99.87	110.41	66	3
1	A	54	ARG	NH1-CZ-NH2	-6.46	110.90	119.30	18	5
1	A	61	ILE	N-CA-CB	-6.46	103.49	110.53	113	13
1	A	55	THR	CA-C-O	-6.45	114.01	121.82	59	5
1	A	55	THR	CB-CA-C	6.44	121.10	109.83	74	3
1	A	31	GLN	CA-CB-CG	6.44	126.98	114.10	22	1
1	A	29	LYS	CA-C-O	6.42	127.37	120.24	6	7
1	A	27	LYS	CG-CD-CE	6.41	126.05	111.30	48	2
1	A	7	THR	N-CA-C	6.41	120.00	110.52	67	3
1	A	31	GLN	N-CA-CB	6.41	119.54	110.12	7	4
1	A	49	GLN	CB-CG-CD	-6.40	101.72	112.60	17	7
1	A	38	PRO	O-C-N	-6.40	114.00	122.64	113	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	12	THR	CB-CA-C	6.40	119.96	110.62	6	3
1	A	49	GLN	CA-CB-CG	-6.40	101.31	114.10	7	2
1	A	59	TYR	N-CA-C	-6.39	104.63	112.88	72	5
1	A	33	LYS	O-C-N	6.38	129.65	122.11	58	2
1	A	58	ASP	O-C-N	-6.37	114.89	122.15	27	3
1	A	2	GLN	O-C-N	-6.37	115.78	123.10	5	6
1	A	54	ARG	CB-CA-C	-6.36	99.31	109.80	35	1
1	A	57	SER	CA-CB-OG	6.36	123.82	111.10	53	5
1	A	17	VAL	CA-C-N	6.36	131.75	121.83	12	3
1	A	17	VAL	C-N-CA	6.36	131.75	121.83	12	3
1	A	32	ASP	CA-C-O	-6.35	112.92	120.10	48	6
1	A	26	VAL	N-CA-CB	6.34	117.55	110.51	31	2
1	A	2	GLN	CG-CD-NE2	6.34	125.91	116.40	91	6
1	A	34	GLU	CB-CG-CD	6.34	123.38	112.60	57	6
1	A	25	ASN	CB-CG-ND2	6.34	125.90	116.40	111	2
1	A	24	GLU	N-CA-C	6.33	118.18	111.28	77	7
1	A	2	GLN	CB-CA-C	-6.33	99.94	110.19	79	2
1	A	3	ILE	CA-C-O	-6.33	115.03	121.67	39	9
1	A	67	LEU	CA-C-O	-6.32	114.66	121.36	4	4
1	A	65	SER	CB-CA-C	-6.32	99.38	109.80	19	1
1	A	9	THR	O-C-N	-6.31	113.45	122.41	49	2
1	A	8	LEU	O-C-N	-6.31	114.03	122.43	13	2
1	A	39	ASP	CA-C-O	6.28	126.31	119.15	102	7
1	A	42	ARG	N-CA-CB	-6.28	101.29	110.84	46	2
1	A	34	GLU	O-C-N	-6.27	115.28	121.93	97	5
1	A	62	GLN	N-CA-CB	6.27	121.08	110.49	98	3
1	A	45	PHE	CB-CG-CD2	-6.25	110.07	120.70	2	1
1	A	60	ASN	CB-CA-C	6.25	122.86	110.42	64	4
1	A	69	LEU	CA-C-O	-6.25	113.61	120.24	44	4
1	A	68	HIS	CG-ND1-CE1	-6.25	98.68	109.30	63	5
1	A	62	GLN	CB-CG-CD	6.24	123.21	112.60	37	3
1	A	66	THR	N-CA-C	-6.24	97.52	108.20	22	3
1	A	16	GLU	CA-CB-CG	6.24	126.58	114.10	87	5
1	A	6	LYS	CB-CA-C	6.24	120.51	109.72	14	2
1	A	23	ILE	CB-CA-C	6.24	121.52	111.29	53	5
1	A	65	SER	CA-CB-OG	-6.22	98.66	111.10	6	2
1	A	40	GLN	CG-CD-NE2	6.22	125.73	116.40	98	1
1	A	42	ARG	CA-C-O	-6.21	113.85	121.06	62	6
1	A	49	GLN	CG-CD-NE2	6.21	125.72	116.40	65	3
1	A	3	ILE	N-CA-CB	-6.21	104.59	112.60	115	6
1	A	35	GLY	N-CA-C	6.21	123.60	115.47	9	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	36	ILE	CA-CB-CG1	6.19	120.93	110.40	14	9
1	A	41	GLN	CA-CB-CG	6.19	126.49	114.10	72	2
1	A	50	LEU	N-CA-CB	6.19	120.26	110.23	78	1
1	A	49	GLN	CA-C-O	-6.18	113.61	120.60	96	4
1	A	4	PHE	CD1-CE1-CZ	-6.18	108.88	120.00	27	1
1	A	28	ALA	N-CA-CB	-6.18	100.78	110.30	97	3
1	A	24	GLU	CB-CA-C	6.18	120.99	110.74	22	3
1	A	15	LEU	O-C-N	-6.17	115.75	123.27	108	5
1	A	30	ILE	CA-CB-CG1	6.16	120.87	110.40	36	2
1	A	64	GLU	N-CA-C	6.16	120.37	112.86	52	2
1	A	42	ARG	O-C-N	-6.16	115.85	123.36	89	4
1	A	3	ILE	CA-CB-CG2	6.15	120.95	110.50	96	3
1	A	62	GLN	N-CA-C	6.14	117.52	108.86	45	3
1	A	47	GLY	N-CA-C	-6.14	106.45	115.72	49	6
1	A	2	GLN	CA-CB-CG	6.13	126.37	114.10	92	4
1	A	54	ARG	CA-CB-CG	6.12	126.35	114.10	42	6
1	A	70	VAL	CA-CB-CG2	6.12	120.80	110.40	29	6
1	A	54	ARG	CA-C-N	6.10	133.23	122.67	58	2
1	A	54	ARG	C-N-CA	6.10	133.23	122.67	58	2
1	A	22	THR	CA-CB-CG2	6.08	120.83	110.50	76	9
1	A	54	ARG	N-CA-C	6.05	118.52	110.53	3	2
1	A	68	HIS	CB-CG-ND1	-6.05	113.62	122.70	116	2
1	A	14	THR	OG1-CB-CG2	-6.05	97.20	109.30	56	2
1	A	11	LYS	N-CA-CB	-6.04	101.09	109.97	68	4
1	A	71	LEU	O-C-N	6.04	130.10	123.27	65	5
1	A	64	GLU	CA-C-O	6.04	126.25	119.78	108	3
1	A	12	THR	N-CA-C	-6.04	100.45	110.17	22	2
1	A	12	THR	N-CA-CB	-6.04	101.99	111.05	28	2
1	A	22	THR	OG1-CB-CG2	-6.03	97.23	109.30	3	3
1	A	27	LYS	CB-CG-CD	6.01	125.13	111.30	28	1
1	A	18	GLU	CB-CG-CD	6.01	122.82	112.60	69	1
1	A	4	PHE	N-CA-C	-6.01	99.91	109.59	69	2
1	A	41	GLN	N-CA-C	6.01	118.74	109.07	24	3
1	A	24	GLU	CA-CB-CG	6.00	126.11	114.10	104	3
1	A	4	PHE	CG-CD1-CE1	5.99	130.88	120.70	27	1
1	A	16	GLU	N-CA-CB	-5.98	100.67	110.43	101	5
1	A	59	TYR	CB-CG-CD1	-5.97	111.85	120.80	62	1
1	A	20	SER	CB-CA-C	5.96	120.36	109.99	16	1
1	A	55	THR	N-CA-C	-5.96	101.71	110.52	27	5
1	A	50	LEU	CB-CA-C	5.95	119.18	109.90	98	5
1	A	8	LEU	CB-CA-C	5.93	120.29	110.81	66	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	11	LYS	N-CA-C	5.91	123.40	110.80	67	4
1	A	49	GLN	CB-CA-C	5.91	119.98	110.16	64	3
1	A	46	ALA	N-CA-CB	-5.91	103.25	112.41	82	5
1	A	20	SER	O-C-N	-5.91	115.08	122.35	90	5
1	A	30	ILE	CA-CB-CG2	5.90	120.53	110.50	33	4
1	A	68	HIS	N-CA-C	-5.90	100.09	109.76	74	3
1	A	41	GLN	CB-CA-C	5.89	121.34	109.38	54	3
1	A	61	ILE	O-C-N	-5.89	116.23	122.95	70	5
1	A	61	ILE	CA-C-O	5.89	128.50	121.02	72	2
1	A	16	GLU	O-C-N	-5.88	116.36	123.13	61	2
1	A	67	LEU	O-C-N	-5.88	116.34	123.10	67	3
1	A	66	THR	N-CA-CB	-5.85	100.91	110.21	85	2
1	A	19	PRO	CA-N-CD	-5.84	103.82	112.00	60	2
1	A	8	LEU	N-CA-CB	5.84	119.22	110.22	98	2
1	A	63	LYS	N-CA-CB	5.82	120.33	110.49	36	2
1	A	25	ASN	N-CA-CB	5.80	118.75	110.16	38	3
1	A	69	LEU	O-C-N	-5.79	116.41	123.30	110	6
1	A	46	ALA	O-C-N	5.79	130.29	122.59	60	1
1	A	21	ASP	CB-CA-C	-5.79	101.83	110.16	65	4
1	A	41	GLN	N-CA-CB	-5.79	100.98	110.41	73	5
1	A	49	GLN	O-C-N	-5.78	115.82	122.93	112	3
1	A	51	GLU	N-CA-C	5.78	118.62	109.96	68	2
1	A	27	LYS	CA-CB-CG	5.77	125.65	114.10	59	1
1	A	43	LEU	O-C-N	-5.77	115.51	123.12	80	2
1	A	26	VAL	CA-CB-CG2	5.76	120.18	110.40	48	3
1	A	54	ARG	CA-C-O	5.72	127.51	121.33	45	1
1	A	56	LEU	N-CA-CB	5.72	118.53	110.12	36	2
1	A	63	LYS	CG-CD-CE	5.72	124.46	111.30	55	2
1	A	56	LEU	CA-C-O	-5.71	114.49	120.55	100	4
1	A	24	GLU	N-CA-CB	-5.71	101.53	110.44	2	5
1	A	17	VAL	CA-CB-CG1	5.70	120.09	110.40	45	3
1	A	38	PRO	CB-CA-C	-5.69	103.23	112.62	41	1
1	A	55	THR	N-CA-CB	-5.68	102.00	111.20	107	4
1	A	40	GLN	CA-C-O	-5.68	112.47	118.77	36	4
1	A	61	ILE	CB-CG1-CD1	5.68	125.72	113.80	62	1
1	A	57	SER	N-CA-CB	-5.67	101.79	110.01	46	5
1	A	9	THR	OG1-CB-CG2	-5.67	97.96	109.30	34	2
1	A	9	THR	N-CA-C	5.66	119.67	112.87	111	2
1	A	60	ASN	N-CA-CB	-5.66	103.31	111.91	96	2
1	A	66	THR	CA-CB-OG1	-5.65	101.12	109.60	85	3
1	A	25	ASN	CB-CA-C	5.63	119.80	110.90	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	59	TYR	CA-C-O	5.63	126.30	119.38	95	3
1	A	4	PHE	CA-C-O	-5.63	114.64	121.28	82	2
1	A	22	THR	N-CA-C	5.63	117.96	110.53	103	1
1	A	48	LYS	N-CA-CB	-5.62	101.25	110.52	10	3
1	A	70	VAL	N-CA-CB	-5.62	103.61	111.25	75	2
1	A	63	LYS	CA-CB-CG	5.60	125.30	114.10	76	3
1	A	40	GLN	CA-CB-CG	5.60	125.30	114.10	51	1
1	A	28	ALA	CB-CA-C	-5.59	101.34	110.85	35	1
1	A	6	LYS	N-CA-C	5.58	118.20	108.76	26	1
1	A	50	LEU	N-CA-C	5.58	118.34	109.96	101	1
1	A	64	GLU	CA-CB-CG	5.57	125.24	114.10	14	1
1	A	15	LEU	CB-CA-C	-5.55	100.84	110.45	19	1
1	A	57	SER	CB-CA-C	5.54	119.99	110.79	74	2
1	A	51	GLU	CB-CA-C	5.53	118.56	110.26	75	1
1	A	38	PRO	CA-C-O	-5.53	111.27	119.00	95	2
1	A	39	ASP	O-C-N	5.52	128.49	122.20	26	2
1	A	15	LEU	N-CA-CB	-5.51	101.92	110.57	12	1
1	A	29	LYS	CA-CB-CG	-5.51	103.08	114.10	15	1
1	A	41	GLN	CG-CD-NE2	-5.48	108.18	116.40	64	3
1	A	42	ARG	N-CA-C	5.47	118.00	108.76	81	3
1	A	62	GLN	CA-CB-CG	5.47	125.03	114.10	111	2
1	A	71	LEU	N-CA-CB	-5.46	101.73	110.63	17	1
1	A	59	TYR	CD1-CG-CD2	5.45	126.27	118.10	82	1
1	A	18	GLU	CA-CB-CG	5.45	124.99	114.10	71	1
1	A	40	GLN	O-C-N	5.44	128.57	122.27	60	2
1	A	61	ILE	CA-CB-CG1	5.43	119.63	110.40	88	3
1	A	13	ILE	CB-CG1-CD1	5.42	125.19	113.80	38	1
1	A	4	PHE	N-CA-CB	-5.39	101.62	110.52	100	1
1	A	42	ARG	CA-CB-CG	5.34	124.79	114.10	38	1
1	A	3	ILE	N-CA-C	-5.34	101.01	108.80	112	2
1	A	13	ILE	CA-CB-CG2	5.33	119.56	110.50	72	3
1	A	11	LYS	O-C-N	-5.32	115.51	122.59	67	1
1	A	23	ILE	CB-CG1-CD1	5.31	124.94	113.80	11	1
1	A	50	LEU	CD1-CG-CD2	-5.30	99.14	110.80	87	1
1	A	6	LYS	O-C-N	-5.29	117.19	123.22	9	2
1	A	62	GLN	CG-CD-OE1	5.29	131.38	120.80	109	1
1	A	1	MET	CA-C-O	5.28	129.78	120.80	41	1
1	A	2	GLN	N-CA-C	5.27	118.41	109.76	25	1
1	A	19	PRO	O-C-N	-5.26	115.54	122.64	47	1
1	A	38	PRO	CA-N-CD	-5.26	104.64	112.00	82	2
1	A	14	THR	O-C-N	-5.24	117.35	123.27	97	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	67	LEU	N-CA-CB	5.24	119.23	110.85	23	2
1	A	33	LYS	CA-C-N	5.24	130.09	122.08	18	2
1	A	33	LYS	C-N-CA	5.24	130.09	122.08	18	2
1	A	1	MET	N-CA-CB	5.24	119.40	110.50	65	1
1	A	66	THR	CB-CA-C	5.22	119.68	109.35	80	1
1	A	65	SER	N-CA-CB	5.20	117.69	109.83	14	1
1	A	38	PRO	N-CA-C	5.20	120.60	113.84	80	1
1	A	9	THR	CA-C-O	-5.18	113.01	119.38	34	1
1	A	1	MET	CA-CB-CG	5.18	124.45	114.10	93	1
1	A	29	LYS	CB-CG-CD	5.17	123.19	111.30	97	1
1	A	24	GLU	CB-CG-CD	5.16	121.37	112.60	34	1
1	A	64	GLU	CB-CG-CD	5.15	121.36	112.60	45	1
1	A	48	LYS	O-C-N	5.14	129.69	123.01	54	1
1	A	6	LYS	CB-CG-CD	5.14	123.12	111.30	72	1
1	A	8	LEU	CD1-CG-CD2	-5.13	99.51	110.80	49	1
1	A	1	MET	CB-CA-C	5.11	119.81	110.10	3	1
1	A	41	GLN	O-C-N	-5.10	116.56	123.19	68	1
1	A	4	PHE	CB-CG-CD1	-5.09	112.04	120.70	37	1
1	A	54	ARG	N-CA-CB	-5.09	103.42	111.05	4	2
1	A	63	LYS	O-C-N	-5.08	115.92	122.77	102	1
1	A	19	PRO	CA-C-O	-5.07	111.84	119.55	41	1
1	A	33	LYS	CG-CD-CE	5.05	122.91	111.30	107	1
1	A	33	LYS	CB-CA-C	5.05	119.43	110.85	36	1
1	A	67	LEU	CB-CA-C	-5.05	100.88	109.51	105	1
1	A	51	GLU	CA-CB-CG	5.04	124.19	114.10	92	1
1	A	2	GLN	CB-CG-CD	5.04	121.16	112.60	64	1
1	A	64	GLU	N-CA-CB	-5.04	104.81	112.47	68	1
1	A	43	LEU	N-CA-CB	-5.03	101.86	110.16	57	1
1	A	68	HIS	CG-CD2-NE2	-5.02	102.18	107.20	9	1
1	A	20	SER	CA-CB-OG	5.01	121.13	111.10	46	1
1	A	70	VAL	N-CA-C	-5.00	102.28	108.89	74	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	59	TYR	Sidechain	35
1	A	42	ARG	Sidechain,Peptide,Mainchain	12
1	A	45	PHE	Sidechain	10
1	A	41	GLN	Peptide	8

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	9	THR	Peptide,Mainchain	8
1	A	4	PHE	Sidechain,Peptide	8
1	A	54	ARG	Sidechain	7
1	A	33	LYS	Peptide	4
1	A	17	VAL	Peptide	4
1	A	68	HIS	Sidechain	3
1	A	71	LEU	Peptide	3
1	A	51	GLU	Mainchain,Peptide	3
1	A	70	VAL	Peptide,Mainchain	3
1	A	62	GLN	Peptide,Mainchain	3
1	A	50	LEU	Peptide	2
1	A	11	LYS	Mainchain,Peptide	2
1	A	39	ASP	Sidechain,Mainchain	2
1	A	23	ILE	Mainchain	2
1	A	15	LEU	Mainchain	2
1	A	52	ASP	Mainchain	2
1	A	66	THR	Mainchain	1
1	A	25	ASN	Mainchain	1
1	A	22	THR	Peptide	1
1	A	13	ILE	Peptide	1
1	A	31	GLN	Mainchain	1
1	A	61	ILE	Peptide	1
1	A	43	LEU	Mainchain	1
1	A	21	ASP	Mainchain	1
1	A	2	GLN	Peptide	1
1	A	56	LEU	Mainchain	1
1	A	32	ASP	Mainchain	1
1	A	38	PRO	Mainchain	1
1	A	37	PRO	Mainchain	1
1	A	28	ALA	Mainchain	1
1	A	26	VAL	Mainchain	1
1	A	24	GLU	Mainchain	1
1	A	34	GLU	Peptide	1
1	A	30	ILE	Mainchain	1
1	A	47	GLY	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±1
All	All	65308	67976	67976	49

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:8:LEU:H	1:A:8:LEU:HD13	0.65	1.51	48	2
1:A:7:THR:HG22	1:A:69:LEU:HD12	0.55	1.79	58	1
1:A:8:LEU:HD23	1:A:8:LEU:H	0.55	1.61	99	1
1:A:8:LEU:CD1	1:A:8:LEU:H	0.53	2.17	61	1
1:A:30:ILE:CG2	1:A:36:ILE:HD12	0.52	2.35	97	1
1:A:1:MET:N	1:A:16:GLU:OE2	0.52	2.42	35	1
1:A:18:GLU:O	1:A:21:ASP:HB2	0.51	2.06	37	1
1:A:49:GLN:HE21	1:A:49:GLN:H	0.48	1.51	29	1
1:A:42:ARG:CZ	1:A:70:VAL:HG12	0.48	2.39	10	1
1:A:71:LEU:O	1:A:71:LEU:HD22	0.47	2.09	63	1
1:A:61:ILE:HD13	1:A:67:LEU:HD21	0.47	1.86	69	1
1:A:23:ILE:HG23	1:A:43:LEU:HD13	0.47	1.86	8	1
1:A:13:ILE:N	1:A:13:ILE:HD13	0.46	2.24	74	1
1:A:3:ILE:HD12	1:A:67:LEU:HD22	0.46	1.87	44	1
1:A:71:LEU:HD12	1:A:71:LEU:N	0.46	2.26	64	1
1:A:45:PHE:CG	1:A:46:ALA:N	0.45	2.84	22	1
1:A:27:LYS:HB3	1:A:38:PRO:HB3	0.44	1.90	2	1
1:A:21:ASP:O	1:A:55:THR:HA	0.44	2.13	66	1
1:A:17:VAL:HG21	1:A:56:LEU:CD1	0.44	2.42	77	1
1:A:4:PHE:CE1	1:A:14:THR:HG23	0.44	2.47	4	1
1:A:11:LYS:NZ	1:A:34:GLU:OE1	0.44	2.50	30	1
1:A:43:LEU:HD12	1:A:67:LEU:HD22	0.44	1.88	16	1
1:A:54:ARG:HB2	1:A:59:TYR:CE2	0.43	2.48	9	1
1:A:8:LEU:N	1:A:8:LEU:HD22	0.43	2.27	60	1
1:A:70:VAL:HG12	1:A:71:LEU:N	0.43	2.28	100	1
1:A:5:VAL:HG21	1:A:15:LEU:HD12	0.43	1.91	63	1
1:A:70:VAL:HG22	1:A:71:LEU:H	0.43	1.73	22	1
1:A:27:LYS:NZ	1:A:52:ASP:OD2	0.43	2.47	115	1
1:A:36:ILE:HD12	1:A:36:ILE:N	0.42	2.28	80	1
1:A:26:VAL:HG21	1:A:56:LEU:HD21	0.42	1.91	86	1
1:A:45:PHE:CE2	1:A:61:ILE:HG12	0.42	2.49	110	1
1:A:56:LEU:N	1:A:56:LEU:CD1	0.42	2.83	84	1
1:A:42:ARG:CZ	1:A:70:VAL:CG1	0.41	2.98	10	1
1:A:21:ASP:OD2	1:A:29:LYS:NZ	0.41	2.51	38	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:THR:O	1:A:33:LYS:NZ	0.41	2.51	79	1
1:A:56:LEU:C	1:A:56:LEU:HD23	0.41	2.41	27	1
1:A:11:LYS:NZ	1:A:34:GLU:OE2	0.41	2.47	44	1
1:A:67:LEU:N	1:A:67:LEU:HD12	0.41	2.30	12	1
1:A:21:ASP:OD1	1:A:25:ASN:ND2	0.41	2.50	39	1
1:A:16:GLU:H	1:A:16:GLU:CD	0.40	2.23	1	1
1:A:51:GLU:OE1	1:A:54:ARG:NE	0.40	2.53	5	1
1:A:56:LEU:HD22	1:A:56:LEU:H	0.40	1.75	43	1
1:A:23:ILE:HD12	1:A:50:LEU:HD13	0.40	1.93	47	1
1:A:27:LYS:NZ	1:A:38:PRO:O	0.40	2.49	47	1
1:A:23:ILE:HD12	1:A:54:ARG:O	0.40	2.16	2	1
1:A:43:LEU:HD22	1:A:50:LEU:HD22	0.40	1.92	8	1
1:A:3:ILE:O	1:A:14:THR:HA	0.40	2.16	90	1
1:A:22:THR:HA	1:A:54:ARG:O	0.40	2.16	77	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	70/76 (92%)	65±2 (93±3%)	4±2 (6±3%)	1±1 (1±1%)	14	63
All	All	8120/8816 (92%)	7542 (93%)	490 (6%)	88 (1%)	14	63

All 30 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	60	ASN	15
1	A	46	ALA	11
1	A	63	LYS	8
1	A	64	GLU	6
1	A	8	LEU	5
1	A	52	ASP	5
1	A	23	ILE	4
1	A	39	ASP	4

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Mol	Chain	Res	Type	Models (Total)
1	A	18	GLU	3
1	A	19	PRO	3
1	A	9	THR	2
1	A	24	GLU	2
1	A	38	PRO	2
1	A	62	GLN	2
1	A	17	VAL	1
1	A	35	GLY	1
1	A	32	ASP	1
1	A	70	VAL	1
1	A	45	PHE	1
1	A	65	SER	1
1	A	40	GLN	1
1	A	57	SER	1
1	A	56	LEU	1
1	A	11	LYS	1
1	A	49	GLN	1
1	A	16	GLU	1
1	A	26	VAL	1
1	A	27	LYS	1
1	A	10	GLY	1
1	A	68	HIS	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	65/68 (96%)	61±2 (94±3%)	4±2 (6±3%)	20 69
All	All	7540/7888 (96%)	7100 (94%)	440 (6%)	20 69

All 59 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	15	LEU	32
1	A	8	LEU	24
1	A	71	LEU	21

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Mol	Chain	Res	Type	Models (Total)
1	A	49	GLN	21
1	A	67	LEU	15
1	A	64	GLU	15
1	A	31	GLN	13
1	A	63	LYS	13
1	A	69	LEU	13
1	A	52	ASP	12
1	A	44	ILE	12
1	A	23	ILE	12
1	A	21	ASP	12
1	A	39	ASP	12
1	A	43	LEU	10
1	A	33	LYS	10
1	A	24	GLU	10
1	A	16	GLU	9
1	A	1	MET	9
1	A	54	ARG	8
1	A	60	ASN	8
1	A	2	GLN	8
1	A	9	THR	7
1	A	62	GLN	7
1	A	56	LEU	7
1	A	36	ILE	7
1	A	17	VAL	7
1	A	18	GLU	7
1	A	40	GLN	7
1	A	3	ILE	6
1	A	25	ASN	6
1	A	68	HIS	5
1	A	13	ILE	5
1	A	57	SER	5
1	A	32	ASP	5
1	A	70	VAL	5
1	A	14	THR	4
1	A	12	THR	4
1	A	42	ARG	4
1	A	59	TYR	4
1	A	48	LYS	3
1	A	5	VAL	3
1	A	29	LYS	3
1	A	41	GLN	3
1	A	26	VAL	3

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Mol	Chain	Res	Type	Models (Total)
1	A	50	LEU	3
1	A	20	SER	3
1	A	58	ASP	2
1	A	7	THR	2
1	A	11	LYS	2
1	A	66	THR	2
1	A	45	PHE	2
1	A	61	ILE	2
1	A	19	PRO	1
1	A	34	GLU	1
1	A	37	PRO	1
1	A	65	SER	1
1	A	30	ILE	1
1	A	4	PHE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no 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

No chemical shift data were provided