



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 12:13 AM UTC

PDB ID : 1XQQ / pdb_00001xqq
Title : Simultaneous determination of protein structure and dynamics
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Deposited on : 2004-10-13

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

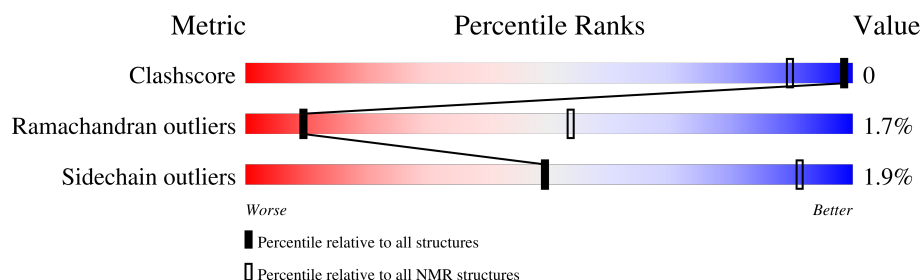
1 Overall quality at a glance

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	76% 17% 7%

2 Ensemble composition and analysis

This entry contains 128 models. Model 11 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)	0.71	11

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 9 clusters and 5 single-model clusters were found.

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

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.

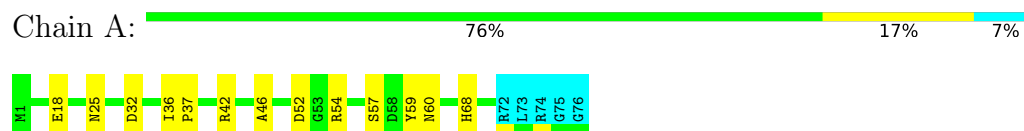
Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1231	378	629	105	118	1	

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

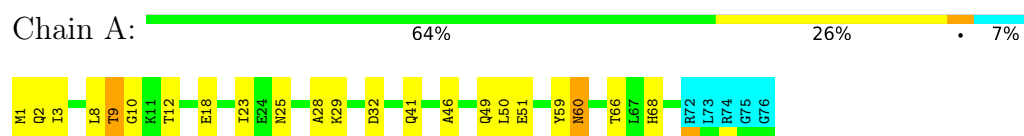


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

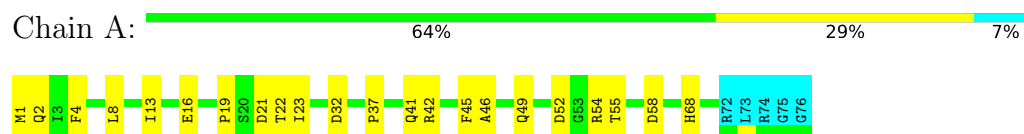
4.2.1 Score per residue for model 1

- Molecule 1: ubiquitin



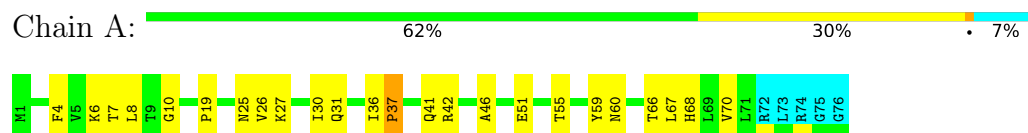
4.2.2 Score per residue for model 2

- Molecule 1: ubiquitin



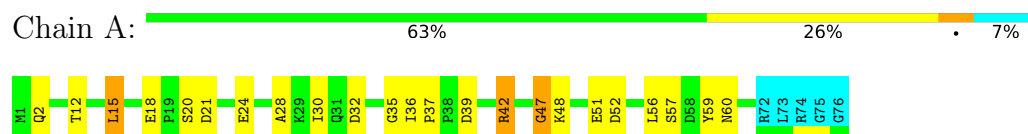
4.2.3 Score per residue for model 3

- Molecule 1: ubiquitin



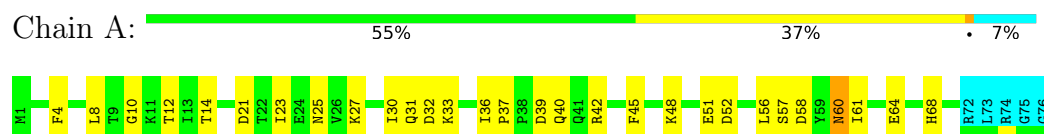
4.2.4 Score per residue for model 4

- Molecule 1: ubiquitin



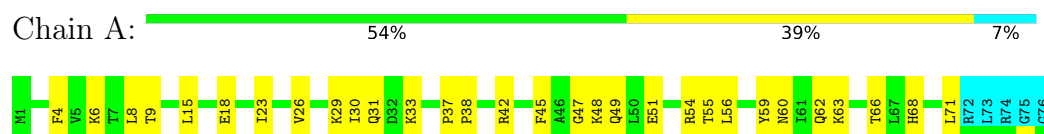
4.2.5 Score per residue for model 5

- Molecule 1: ubiquitin



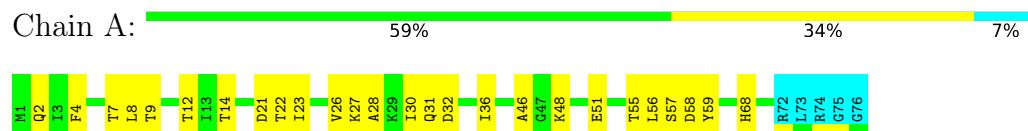
4.2.6 Score per residue for model 6

- Molecule 1: ubiquitin



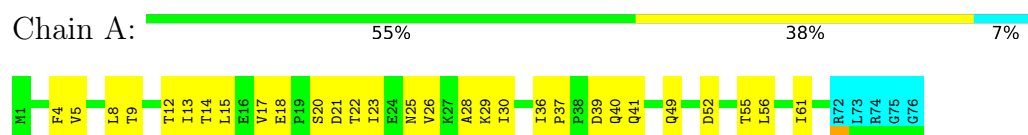
4.2.7 Score per residue for model 7

- Molecule 1: ubiquitin



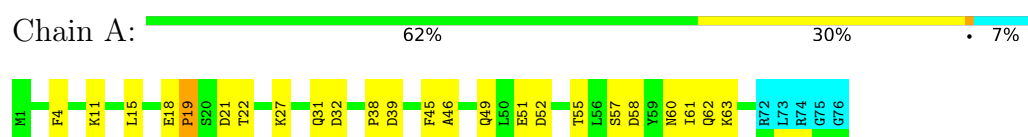
4.2.8 Score per residue for model 8

- Molecule 1: ubiquitin



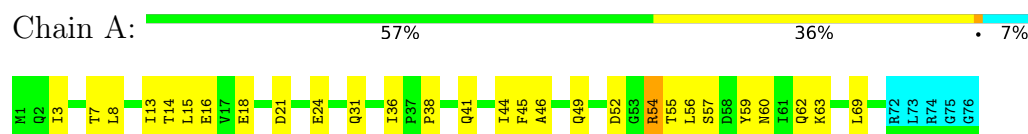
4.2.9 Score per residue for model 9

- Molecule 1: ubiquitin



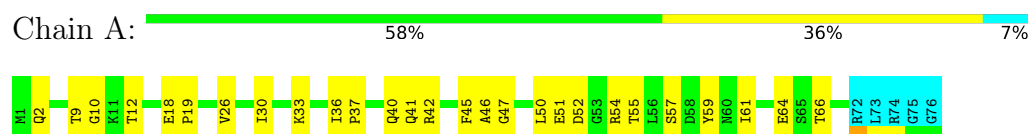
4.2.10 Score per residue for model 10

- Molecule 1: ubiquitin



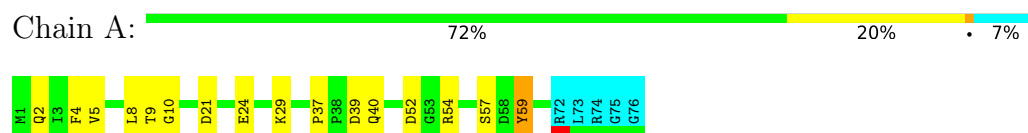
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: ubiquitin



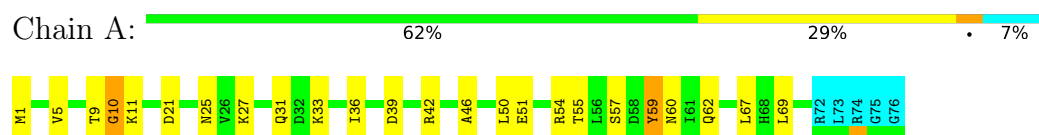
4.2.12 Score per residue for model 12

- Molecule 1: ubiquitin



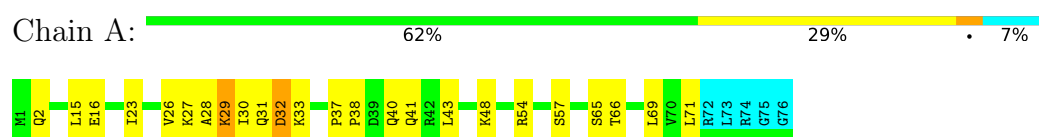
4.2.13 Score per residue for model 13

- Molecule 1: ubiquitin



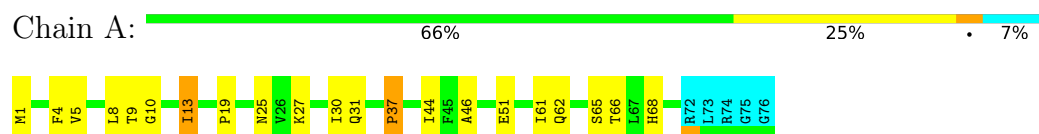
4.2.14 Score per residue for model 14

- Molecule 1: ubiquitin



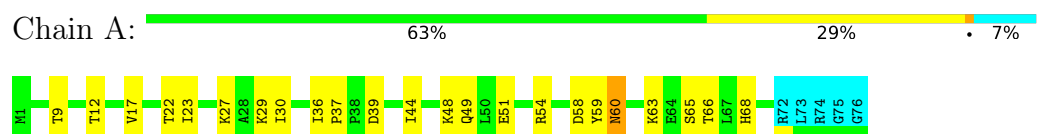
4.2.15 Score per residue for model 15

- Molecule 1: ubiquitin



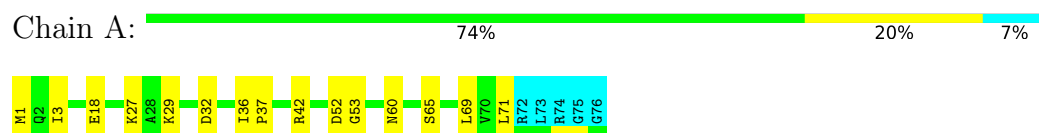
4.2.16 Score per residue for model 16

- Molecule 1: ubiquitin



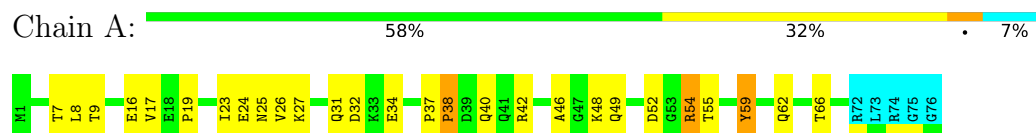
4.2.17 Score per residue for model 17

- Molecule 1: ubiquitin



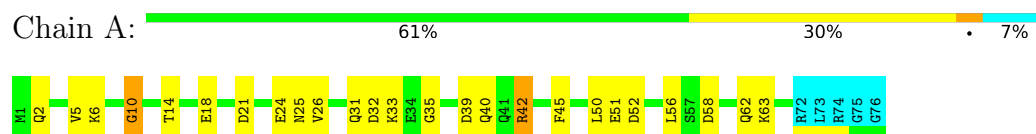
4.2.18 Score per residue for model 18

- Molecule 1: ubiquitin



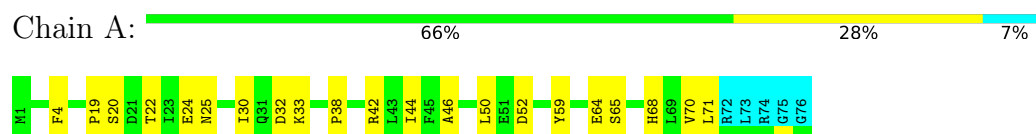
4.2.19 Score per residue for model 19

- Molecule 1: ubiquitin



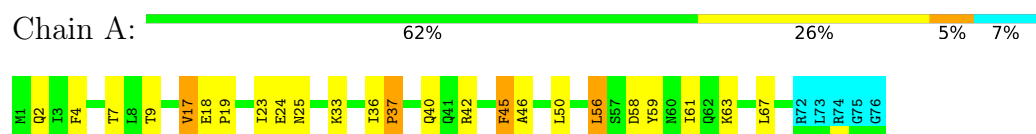
4.2.20 Score per residue for model 20

- Molecule 1: ubiquitin



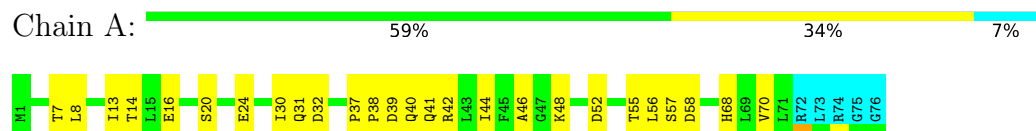
4.2.21 Score per residue for model 21

- Molecule 1: ubiquitin



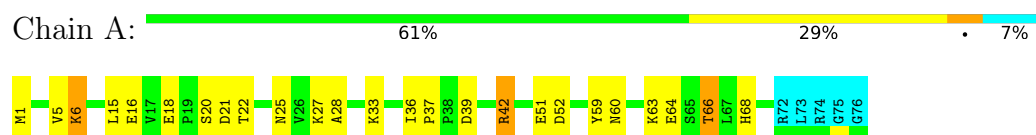
4.2.22 Score per residue for model 22

- Molecule 1: ubiquitin



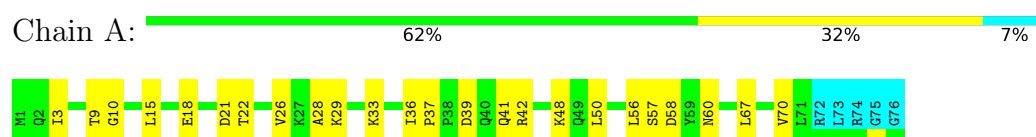
4.2.23 Score per residue for model 23

- Molecule 1: ubiquitin



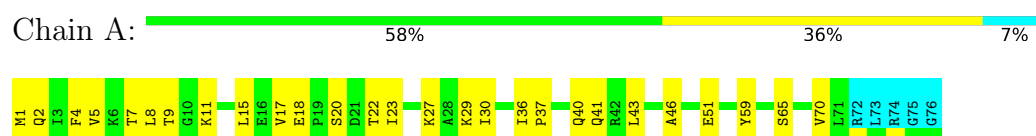
4.2.24 Score per residue for model 24

- Molecule 1: ubiquitin



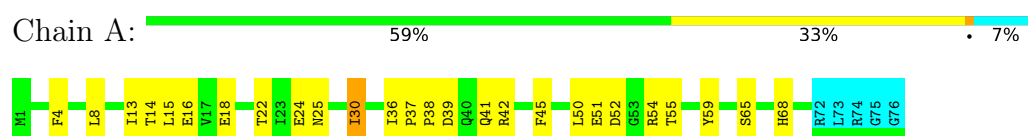
4.2.25 Score per residue for model 25

- Molecule 1: ubiquitin



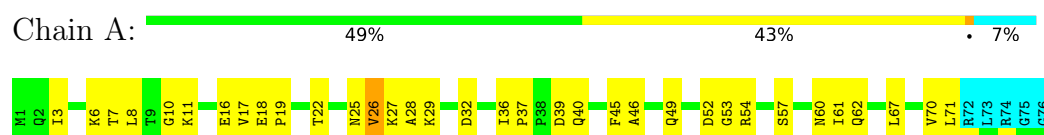
4.2.26 Score per residue for model 26

- Molecule 1: ubiquitin



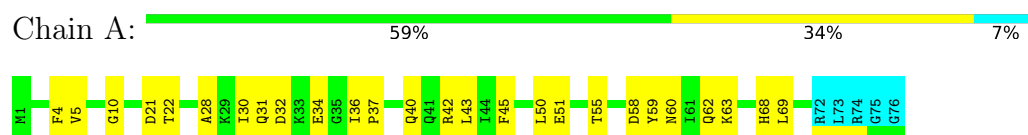
4.2.27 Score per residue for model 27

- Molecule 1: ubiquitin



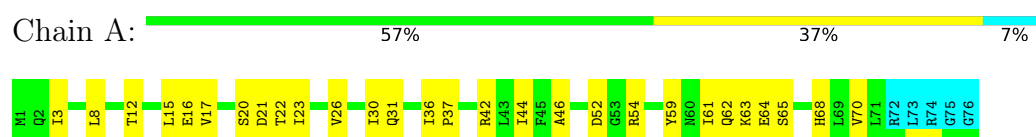
4.2.28 Score per residue for model 28

- Molecule 1: ubiquitin



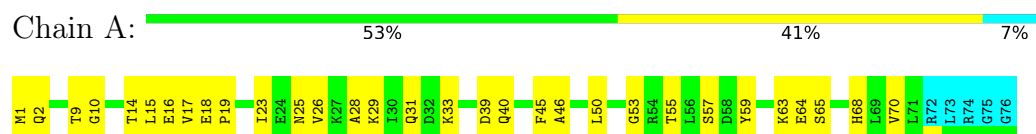
4.2.29 Score per residue for model 29

- Molecule 1: ubiquitin



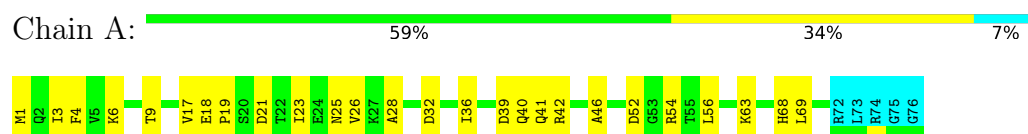
4.2.30 Score per residue for model 30

- Molecule 1: ubiquitin



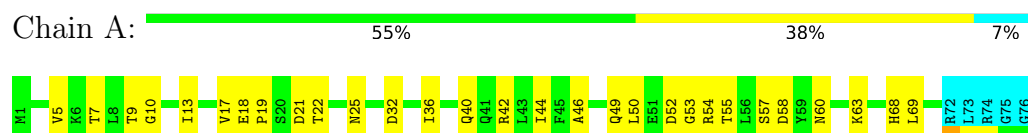
4.2.31 Score per residue for model 31

- Molecule 1: ubiquitin



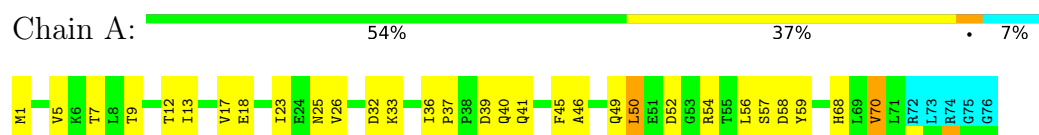
4.2.32 Score per residue for model 32

- Molecule 1: ubiquitin



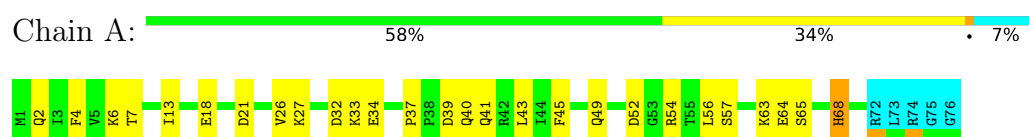
4.2.33 Score per residue for model 33

- Molecule 1: ubiquitin



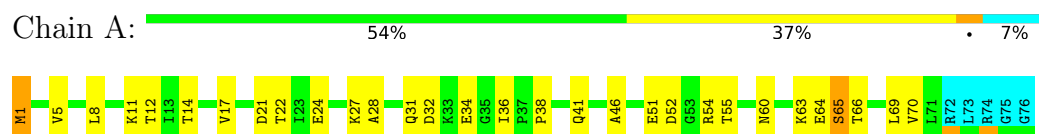
4.2.34 Score per residue for model 34

- Molecule 1: ubiquitin



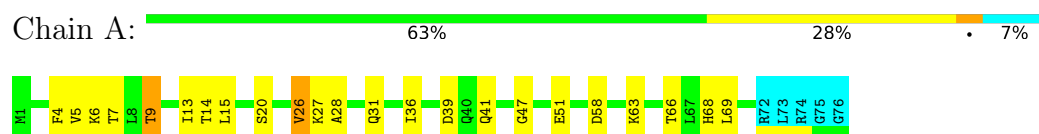
4.2.35 Score per residue for model 35

- Molecule 1: ubiquitin



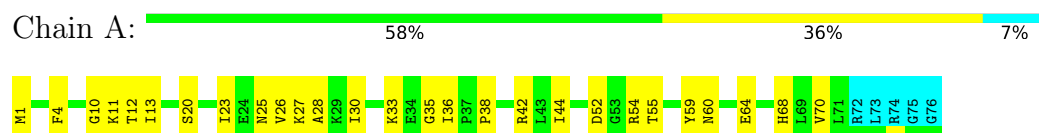
4.2.36 Score per residue for model 36

- Molecule 1: ubiquitin



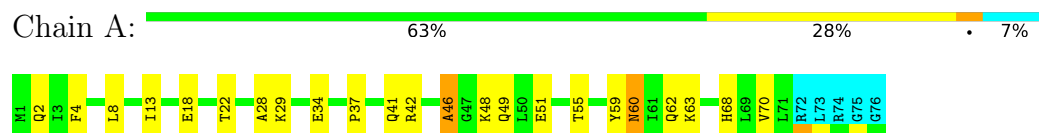
4.2.37 Score per residue for model 37

- Molecule 1: ubiquitin



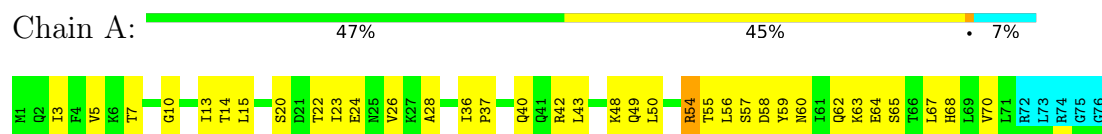
4.2.38 Score per residue for model 38

- Molecule 1: ubiquitin



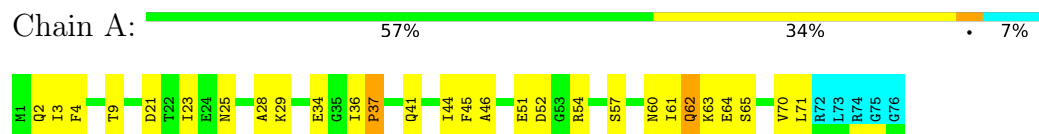
4.2.39 Score per residue for model 39

- Molecule 1: ubiquitin



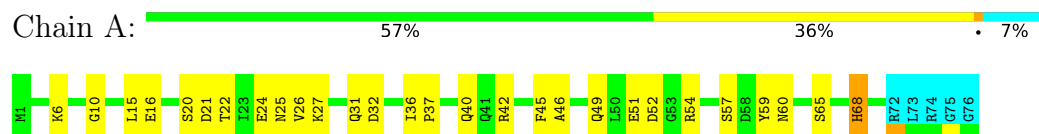
4.2.40 Score per residue for model 40

- Molecule 1: ubiquitin



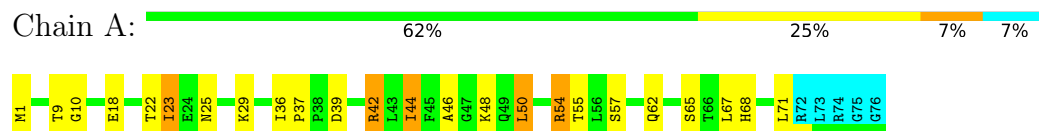
4.2.41 Score per residue for model 41

- Molecule 1: ubiquitin



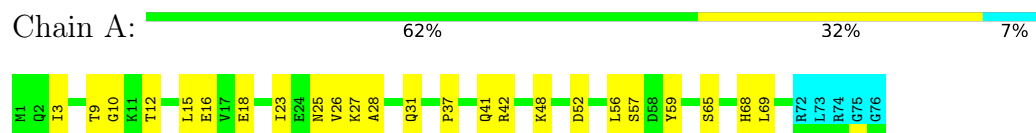
4.2.42 Score per residue for model 42

- Molecule 1: ubiquitin



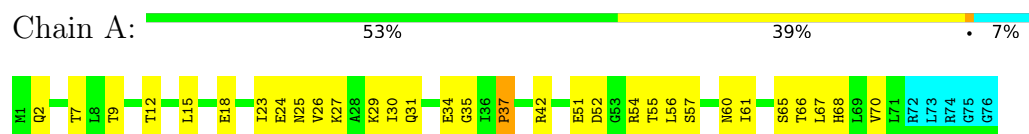
4.2.43 Score per residue for model 43

- Molecule 1: ubiquitin



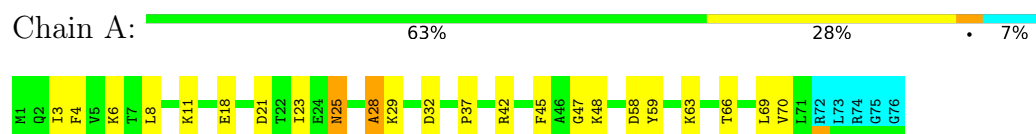
4.2.44 Score per residue for model 44

- Molecule 1: ubiquitin



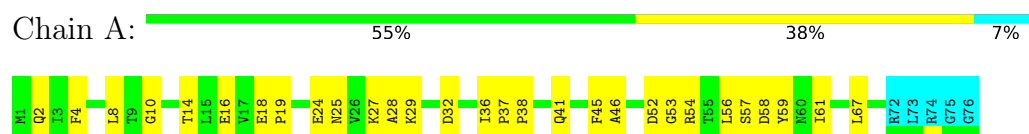
4.2.45 Score per residue for model 45

- Molecule 1: ubiquitin



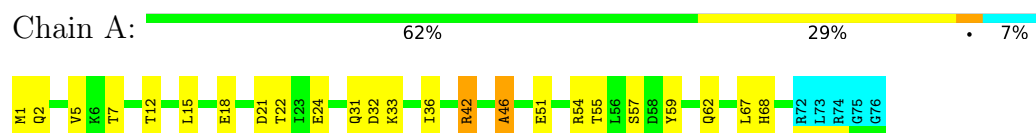
4.2.46 Score per residue for model 46

- Molecule 1: ubiquitin



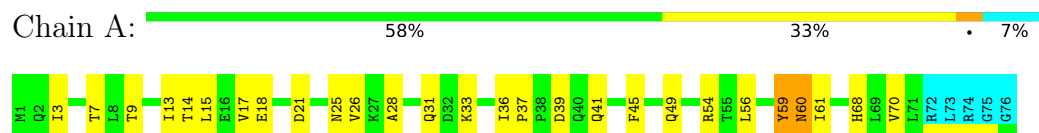
4.2.47 Score per residue for model 47

- Molecule 1: ubiquitin



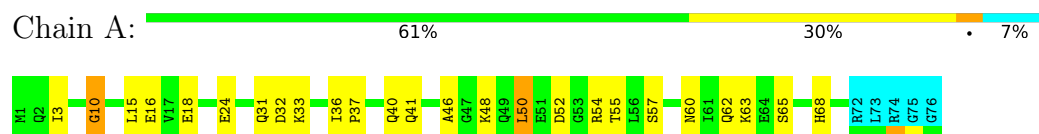
4.2.48 Score per residue for model 48

- Molecule 1: ubiquitin



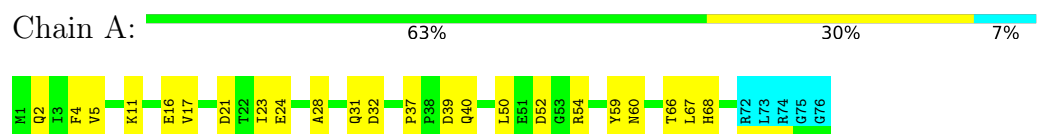
4.2.49 Score per residue for model 49

- Molecule 1: ubiquitin



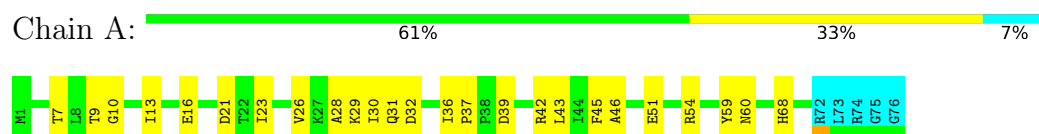
4.2.50 Score per residue for model 50

- Molecule 1: ubiquitin



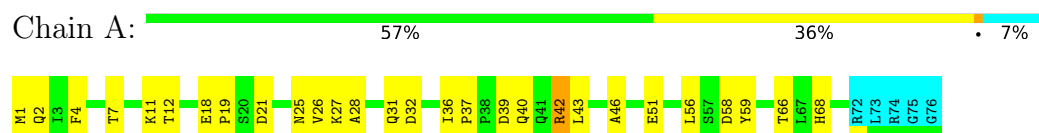
4.2.51 Score per residue for model 51

- Molecule 1: ubiquitin



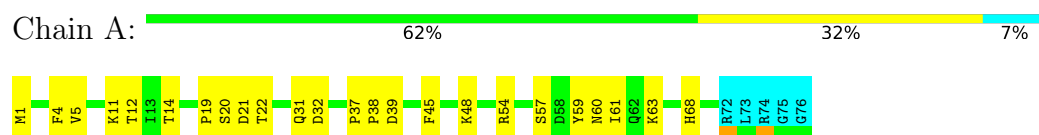
4.2.52 Score per residue for model 52

- Molecule 1: ubiquitin



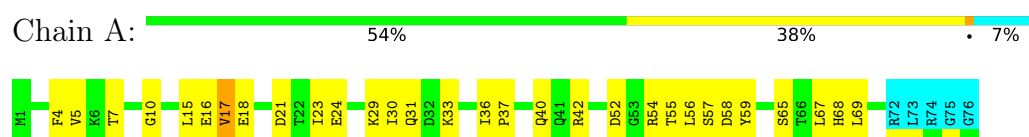
4.2.53 Score per residue for model 53

- Molecule 1: ubiquitin



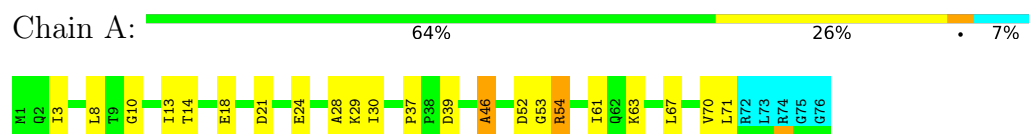
4.2.54 Score per residue for model 54

- Molecule 1: ubiquitin



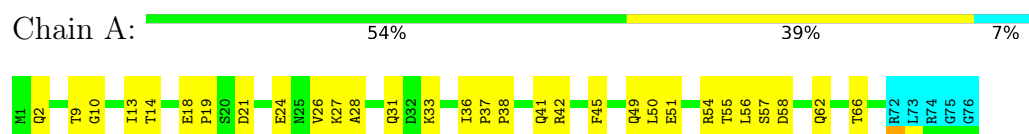
4.2.55 Score per residue for model 55

- Molecule 1: ubiquitin



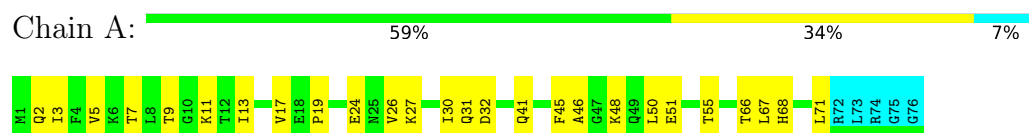
4.2.56 Score per residue for model 56

- Molecule 1: ubiquitin



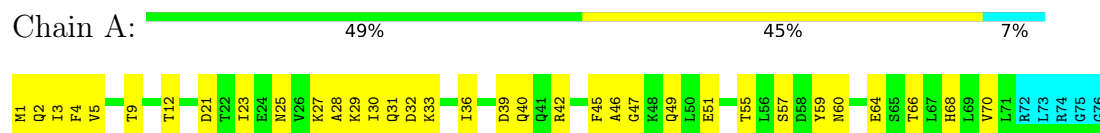
4.2.57 Score per residue for model 57

- Molecule 1: ubiquitin



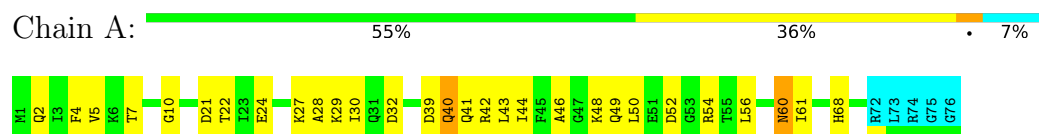
4.2.58 Score per residue for model 58

- Molecule 1: ubiquitin



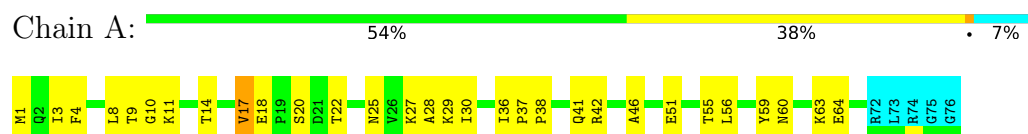
4.2.59 Score per residue for model 59

- Molecule 1: ubiquitin



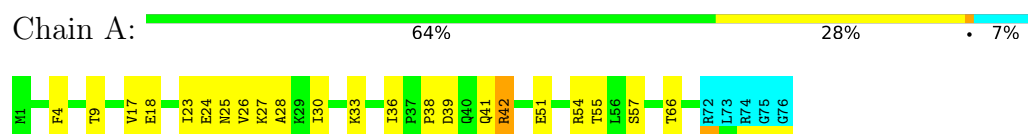
4.2.60 Score per residue for model 60

- Molecule 1: ubiquitin



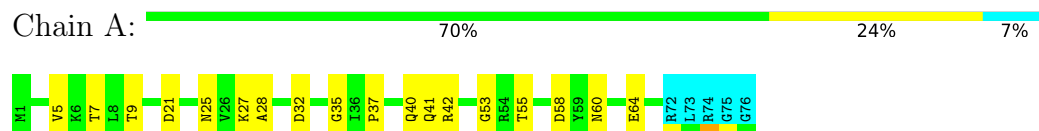
4.2.61 Score per residue for model 61

- Molecule 1: ubiquitin



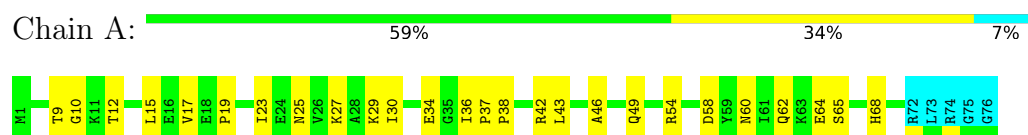
4.2.62 Score per residue for model 62

- Molecule 1: ubiquitin



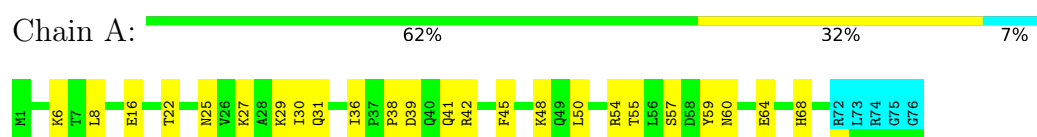
4.2.63 Score per residue for model 63

- Molecule 1: ubiquitin



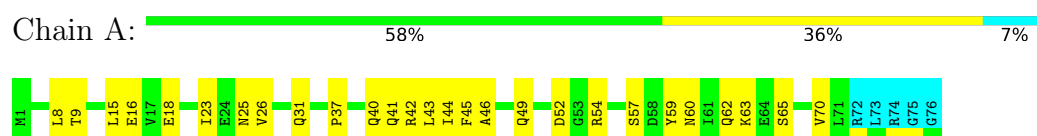
4.2.64 Score per residue for model 64

- Molecule 1: ubiquitin



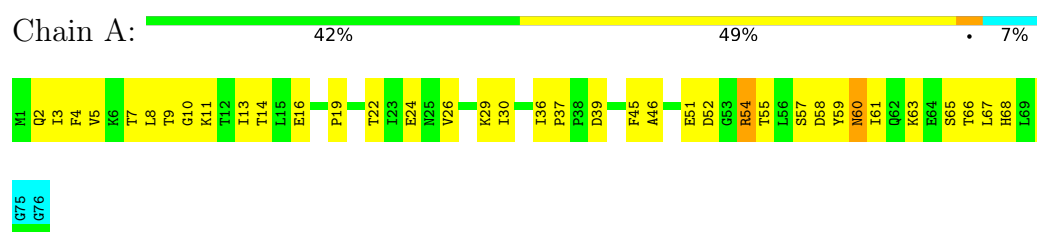
4.2.65 Score per residue for model 65

- Molecule 1: ubiquitin



4.2.66 Score per residue for model 66

- Molecule 1: ubiquitin



4.2.67 Score per residue for model 67

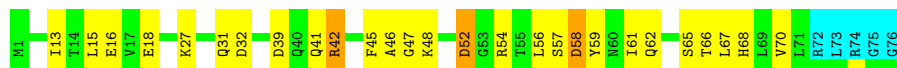
- Molecule 1: ubiquitin





4.2.68 Score per residue for model 68

- Molecule 1: ubiquitin



4.2.69 Score per residue for model 69

- Molecule 1: ubiquitin



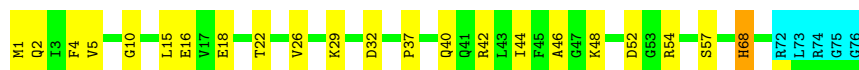
4.2.70 Score per residue for model 70

- Molecule 1: ubiquitin



4.2.71 Score per residue for model 71

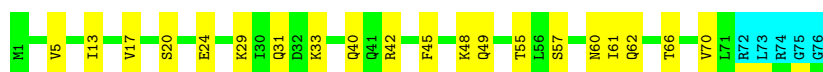
- Molecule 1: ubiquitin



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



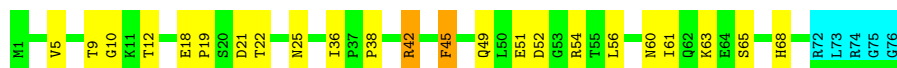
4.2.75 Score per residue for model 75

- Molecule 1: ubiquitin



4.2.76 Score per residue for model 76

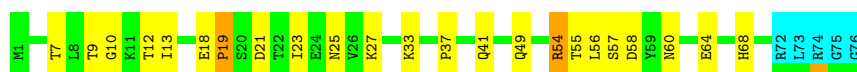
- Molecule 1: ubiquitin



4.2.77 Score per residue for model 77

- Molecule 1: ubiquitin





4.2.78 Score per residue for model 78

- Molecule 1: ubiquitin

Chain A: 66% 28% 7%



4.2.79 Score per residue for model 79

- Molecule 1: ubiquitin

Chain A: 59% 32% 7%



4.2.80 Score per residue for model 80

- Molecule 1: ubiquitin

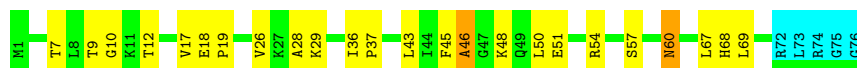
Chain A: 66% 28% 7%



4.2.81 Score per residue for model 81

- Molecule 1: ubiquitin

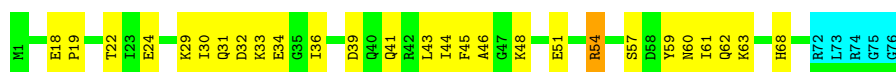
Chain A: 62% 29% 7%



4.2.82 Score per residue for model 82

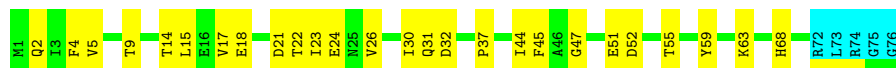
- Molecule 1: ubiquitin

Chain A: 58% 34% 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

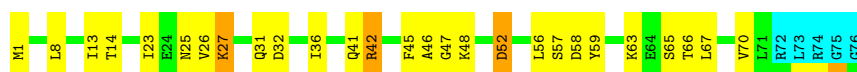
- Molecule 1: ubiquitin



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



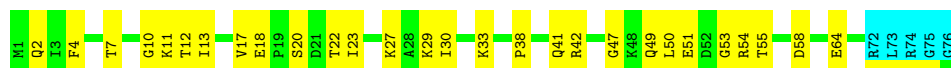
4.2.90 Score per residue for model 90

- 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

Chain A: 63% 28% 7%



4.2.94 Score per residue for model 94

- Molecule 1: ubiquitin

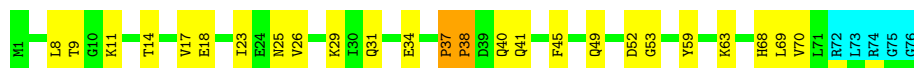
Chain A: 46% 43% 7%



4.2.95 Score per residue for model 95

- Molecule 1: ubiquitin

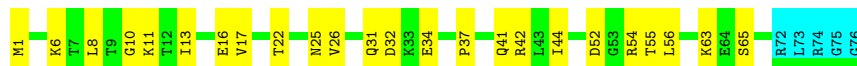
Chain A: 61% 30% 7%



4.2.96 Score per residue for model 96

- Molecule 1: ubiquitin

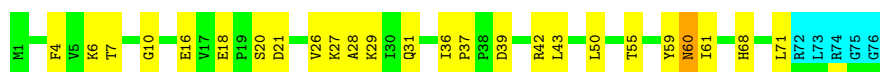
Chain A: 62% 32% 7%



4.2.97 Score per residue for model 97

- Molecule 1: ubiquitin

Chain A: 61% 32% 7%



4.2.98 Score per residue for model 98

- Molecule 1: ubiquitin

Chain A: 61% 33% 7%



4.2.99 Score per residue for model 99

- Molecule 1: ubiquitin

Chain A: 63% 29% 7%



4.2.100 Score per residue for model 100

- Molecule 1: ubiquitin

Chain A: 63% 30% 7%



4.2.101 Score per residue for model 101

- Molecule 1: ubiquitin

Chain A: 63% 28% 7%



4.2.102 Score per residue for model 102

- Molecule 1: ubiquitin

Chain A: 58% 32% 7%



4.2.103 Score per residue for model 103

- Molecule 1: ubiquitin

Chain A: 59% 32% 7%



4.2.104 Score per residue for model 104

- Molecule 1: ubiquitin

Chain A: 66% 24% 7%



4.2.105 Score per residue for model 105

- Molecule 1: ubiquitin

Chain A: 53% 39% 7%



4.2.106 Score per residue for model 106

- Molecule 1: ubiquitin

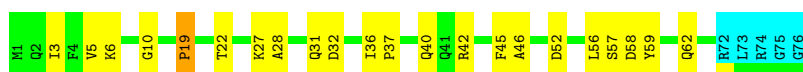
Chain A: 63% 30% 7%



4.2.107 Score per residue for model 107

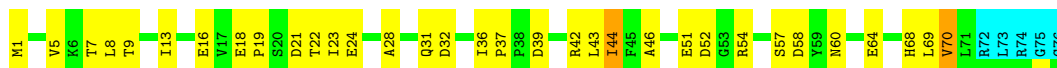
- Molecule 1: ubiquitin

Chain A: 64% 28% 7%



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

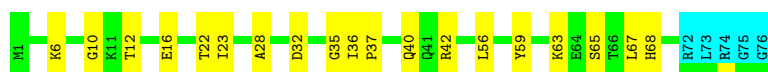
- Molecule 1: ubiquitin



4.2.112 Score per residue for model 112

- Molecule 1: ubiquitin





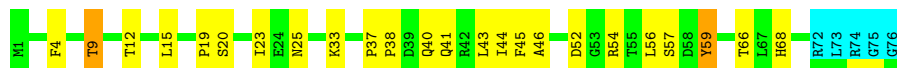
4.2.113 Score per residue for model 113

- Molecule 1: ubiquitin



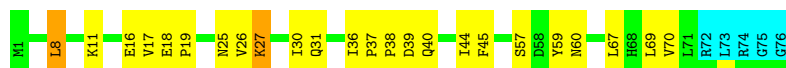
4.2.114 Score per residue for model 114

- Molecule 1: ubiquitin



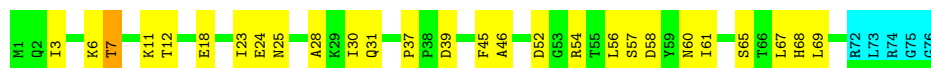
4.2.115 Score per residue for model 115

- 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



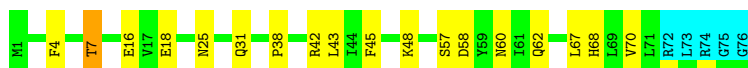
4.2.119 Score per residue for model 119

- 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

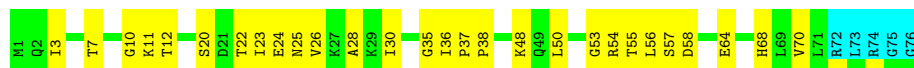
- Molecule 1: ubiquitin





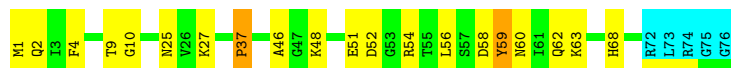
4.2.123 Score per residue for model 123

- Molecule 1: ubiquitin



4.2.124 Score per residue for model 124

- Molecule 1: ubiquitin



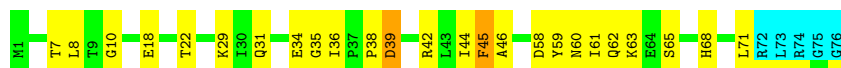
4.2.125 Score per residue for model 125

- Molecule 1: ubiquitin



4.2.126 Score per residue for model 126

- Molecule 1: ubiquitin



4.2.127 Score per residue for model 127

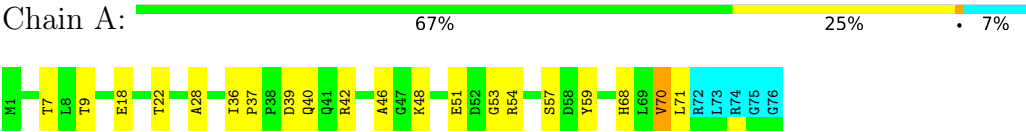
- Molecule 1: ubiquitin





4.2.128 Score per residue for model 128

- Molecule 1: ubiquitin



5 Refinement protocol and experimental data overview ⓘ

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

Of the 128 calculated structures, 128 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 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	1.46±0.01	0±0/570 (0.0± 0.0%)	2.39±0.08	34±7/770 (4.4± 1.0%)
All	All	1.46	6/72960 (0.0%)	2.39	4332/98560 (4.4%)

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	1.1±0.9
All	All	0	145

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	38	PRO	N-CA	-5.40	1.43	1.47	120	1
1	A	36	ILE	CA-CB	-5.26	1.50	1.54	92	5

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	O-C-N	-18.91	112.61	121.31	25	26
1	A	58	ASP	CA-CB-CG	14.48	127.08	112.60	116	24
1	A	36	ILE	CA-C-O	-14.03	110.87	119.15	7	28
1	A	68	HIS	CA-CB-CG	-13.67	100.13	113.80	22	20
1	A	37	PRO	CA-C-O	-13.29	110.23	120.73	24	26
1	A	56	LEU	CA-C-N	12.60	136.82	120.44	100	35
1	A	56	LEU	C-N-CA	12.60	136.82	120.44	100	35
1	A	49	GLN	N-CA-C	12.33	127.78	108.67	6	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	45	PHE	CA-CB-CG	11.96	125.76	113.80	109	35
1	A	32	ASP	CA-CB-CG	11.89	124.49	112.60	7	24
1	A	21	ASP	CA-CB-CG	-11.75	100.85	112.60	78	24
1	A	29	LYS	CA-C-N	11.54	135.10	120.56	12	12
1	A	29	LYS	C-N-CA	11.54	135.10	120.56	12	12
1	A	30	ILE	O-C-N	-11.30	110.90	121.87	4	8
1	A	4	PHE	CA-CB-CG	-11.13	102.67	113.80	20	21
1	A	6	LYS	O-C-N	-10.95	110.74	123.22	27	15
1	A	60	ASN	CA-CB-CG	-10.88	101.72	112.60	69	33
1	A	52	ASP	N-CA-C	10.83	122.65	111.07	108	33
1	A	21	ASP	N-CA-C	10.68	124.42	110.43	47	7
1	A	37	PRO	N-CA-C	10.59	120.64	110.47	23	22
1	A	63	LYS	N-CA-C	10.55	123.95	110.24	53	11
1	A	2	GLN	OE1-CD-NE2	-10.48	112.12	122.60	91	13
1	A	18	GLU	CA-C-O	-10.39	111.47	120.19	32	24
1	A	36	ILE	CA-C-N	10.37	131.06	120.38	49	21
1	A	36	ILE	C-N-CA	10.37	131.06	120.38	49	21
1	A	39	ASP	CA-CB-CG	-10.34	102.26	112.60	51	21
1	A	37	PRO	CA-C-N	10.33	130.10	119.56	24	24
1	A	37	PRO	C-N-CA	10.33	130.10	119.56	24	24
1	A	23	ILE	CA-C-N	10.23	133.99	120.28	61	27
1	A	23	ILE	C-N-CA	10.23	133.99	120.28	61	27
1	A	39	ASP	CA-C-O	10.17	131.79	119.79	118	10
1	A	8	LEU	N-CA-C	-10.07	100.74	113.43	115	7
1	A	52	ASP	CA-CB-CG	-9.98	102.62	112.60	76	21
1	A	69	LEU	CA-C-N	9.94	135.46	122.93	94	8
1	A	69	LEU	C-N-CA	9.94	135.46	122.93	94	8
1	A	26	VAL	N-CA-C	9.94	119.96	110.42	74	14
1	A	27	LYS	O-C-N	-9.94	111.59	122.12	118	6
1	A	28	ALA	CA-C-O	9.87	131.01	120.55	43	6
1	A	29	LYS	N-CA-C	9.84	122.08	111.36	88	15
1	A	13	ILE	N-CA-CB	9.82	123.38	111.60	15	5
1	A	44	ILE	O-C-N	-9.80	113.14	123.14	88	21
1	A	8	LEU	CA-C-N	9.79	133.94	120.63	108	20
1	A	8	LEU	C-N-CA	9.79	133.94	120.63	108	20
1	A	27	LYS	N-CA-C	9.77	121.92	111.28	60	24
1	A	7	THR	CA-C-N	9.58	134.11	120.79	74	21
1	A	7	THR	C-N-CA	9.58	134.11	120.79	74	21
1	A	42	ARG	NE-CZ-NH1	9.57	131.07	121.50	62	15
1	A	22	THR	N-CA-C	9.46	123.32	110.55	74	8
1	A	43	LEU	CA-C-O	9.43	131.27	120.80	125	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	18	GLU	O-C-N	-9.41	114.37	121.14	56	27
1	A	28	ALA	CA-C-N	9.37	133.60	120.29	35	18
1	A	28	ALA	C-N-CA	9.37	133.60	120.29	35	18
1	A	33	LYS	N-CA-C	9.34	121.06	111.07	56	19
1	A	36	ILE	O-C-N	-9.30	115.51	121.37	10	24
1	A	36	ILE	N-CA-C	-9.30	97.13	107.73	28	11
1	A	54	ARG	O-C-N	-9.29	112.46	122.96	109	8
1	A	25	ASN	CA-C-N	9.28	132.04	120.72	44	25
1	A	25	ASN	C-N-CA	9.28	132.04	120.72	44	25
1	A	30	ILE	CA-C-N	9.27	133.06	120.54	11	26
1	A	30	ILE	C-N-CA	9.27	133.06	120.54	11	26
1	A	68	HIS	CB-CG-CD2	-9.23	119.21	131.20	81	11
1	A	59	TYR	N-CA-C	9.18	122.27	111.71	38	13
1	A	8	LEU	O-C-N	9.16	132.59	122.15	95	6
1	A	59	TYR	CA-C-N	9.16	135.94	122.74	43	21
1	A	59	TYR	C-N-CA	9.16	135.94	122.74	43	21
1	A	57	SER	CA-C-N	9.15	132.34	120.44	93	28
1	A	57	SER	C-N-CA	9.15	132.34	120.44	93	28
1	A	41	GLN	CG-CD-NE2	9.12	130.09	116.40	64	3
1	A	6	LYS	CA-C-O	9.12	130.12	120.36	27	12
1	A	26	VAL	N-CA-CB	9.12	121.22	110.55	75	10
1	A	5	VAL	O-C-N	-9.12	113.23	122.99	79	13
1	A	26	VAL	CA-C-N	9.12	132.50	120.28	127	20
1	A	26	VAL	C-N-CA	9.12	132.50	120.28	127	20
1	A	12	THR	O-C-N	-9.10	112.22	123.05	44	6
1	A	39	ASP	CA-C-N	9.09	134.13	120.31	92	13
1	A	39	ASP	C-N-CA	9.09	134.13	120.31	92	13
1	A	32	ASP	O-C-N	-9.09	110.50	122.59	101	11
1	A	34	GLU	N-CA-C	-9.06	101.79	113.12	40	9
1	A	3	ILE	N-CA-CB	9.06	123.58	111.25	117	6
1	A	40	GLN	N-CA-C	9.05	120.91	111.14	33	11
1	A	9	THR	N-CA-CB	9.01	125.09	110.40	6	18
1	A	43	LEU	CA-C-N	8.99	134.34	123.19	39	8
1	A	43	LEU	C-N-CA	8.99	134.34	123.19	39	8
1	A	41	GLN	N-CA-C	8.94	123.51	110.28	43	20
1	A	65	SER	O-C-N	8.93	133.05	122.96	103	6
1	A	27	LYS	CA-C-N	8.90	132.21	120.28	59	26
1	A	27	LYS	C-N-CA	8.90	132.21	120.28	59	26
1	A	60	ASN	CB-CA-C	8.88	123.19	111.82	44	3
1	A	57	SER	N-CA-C	8.87	123.20	112.38	81	29
1	A	17	VAL	O-C-N	-8.84	113.23	123.04	50	22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	41	GLN	OE1-CD-NE2	-8.78	113.82	122.60	64	8
1	A	51	GLU	CA-C-N	8.78	132.04	120.28	47	43
1	A	51	GLU	C-N-CA	8.78	132.04	120.28	47	43
1	A	52	ASP	CA-C-O	-8.77	111.52	120.90	76	7
1	A	54	ARG	NE-CZ-NH2	-8.75	111.32	119.20	27	15
1	A	25	ASN	CA-CB-CG	-8.75	103.85	112.60	1	22
1	A	49	GLN	CA-C-N	8.73	133.18	120.95	34	3
1	A	49	GLN	C-N-CA	8.73	133.18	120.95	34	3
1	A	58	ASP	N-CA-C	8.73	121.59	111.11	56	16
1	A	28	ALA	N-CA-C	8.67	120.73	111.28	121	22
1	A	62	GLN	O-C-N	-8.66	112.80	122.84	121	9
1	A	17	VAL	CA-C-O	-8.59	114.89	121.68	102	4
1	A	31	GLN	OE1-CD-NE2	-8.55	114.05	122.60	83	22
1	A	18	GLU	CA-C-N	8.52	128.25	119.56	46	22
1	A	18	GLU	C-N-CA	8.52	128.25	119.56	46	22
1	A	31	GLN	N-CA-C	8.48	121.29	111.11	104	13
1	A	63	LYS	CA-C-N	8.47	134.85	122.82	84	14
1	A	63	LYS	C-N-CA	8.47	134.85	122.82	84	14
1	A	56	LEU	CA-C-O	8.37	129.67	120.63	117	7
1	A	25	ASN	OD1-CG-ND2	-8.37	114.23	122.60	124	11
1	A	37	PRO	CB-CA-C	8.34	119.01	111.17	65	12
1	A	37	PRO	N-CA-CB	8.31	111.14	103.08	102	17
1	A	70	VAL	O-C-N	-8.31	114.25	122.97	121	14
1	A	42	ARG	NE-CZ-NH2	-8.29	111.74	119.20	92	16
1	A	65	SER	N-CA-CB	8.28	123.64	110.23	39	7
1	A	62	GLN	CA-C-N	8.27	133.26	121.02	40	13
1	A	62	GLN	C-N-CA	8.27	133.26	121.02	40	13
1	A	24	GLU	O-C-N	-8.26	113.36	122.12	108	13
1	A	68	HIS	CG-CD2-NE2	8.26	115.46	107.20	23	20
1	A	31	GLN	CA-C-N	8.23	131.31	120.28	54	18
1	A	31	GLN	C-N-CA	8.23	131.31	120.28	54	18
1	A	16	GLU	O-C-N	-8.20	113.29	123.05	30	7
1	A	9	THR	CA-CB-OG1	8.19	121.88	109.60	13	8
1	A	35	GLY	CA-C-N	8.19	131.54	123.02	44	5
1	A	35	GLY	C-N-CA	8.19	131.54	123.02	44	5
1	A	13	ILE	CA-C-O	8.18	129.51	120.59	10	9
1	A	13	ILE	CA-C-N	8.18	134.00	122.72	87	3
1	A	13	ILE	C-N-CA	8.18	134.00	122.72	87	3
1	A	16	GLU	CA-C-N	8.14	130.98	122.27	10	13
1	A	16	GLU	C-N-CA	8.14	130.98	122.27	10	13
1	A	63	LYS	O-C-N	-8.14	112.19	123.01	126	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	68	HIS	CA-C-O	8.12	129.15	120.46	59	9
1	A	24	GLU	CA-C-N	8.11	130.98	120.44	57	18
1	A	24	GLU	C-N-CA	8.11	130.98	120.44	57	18
1	A	68	HIS	CB-CG-ND1	8.10	134.85	122.70	81	5
1	A	32	ASP	CA-C-N	8.08	131.43	120.44	101	13
1	A	32	ASP	C-N-CA	8.08	131.43	120.44	101	13
1	A	52	ASP	O-C-N	8.08	131.95	122.17	17	5
1	A	18	GLU	N-CA-CB	-8.04	100.55	109.72	44	12
1	A	40	GLN	O-C-N	-8.03	111.90	122.42	104	5
1	A	4	PHE	O-C-N	-8.02	113.02	123.21	124	15
1	A	2	GLN	N-CA-C	8.01	121.36	109.59	117	5
1	A	39	ASP	N-CA-CB	-8.01	98.78	110.47	24	7
1	A	61	ILE	N-CA-CB	8.01	121.21	111.60	76	8
1	A	14	THR	O-C-N	-8.00	113.19	123.02	83	8
1	A	3	ILE	O-C-N	-7.99	114.55	123.18	111	10
1	A	66	THR	CA-C-O	7.99	128.84	120.54	78	7
1	A	51	GLU	O-C-N	-7.97	113.36	122.68	82	9
1	A	55	THR	O-C-N	-7.96	113.78	122.85	30	15
1	A	48	LYS	O-C-N	-7.95	113.94	123.16	87	13
1	A	55	THR	CA-C-N	7.94	131.71	120.28	8	20
1	A	55	THR	C-N-CA	7.94	131.71	120.28	8	20
1	A	68	HIS	CE1-NE2-CD2	-7.88	101.12	109.00	30	40
1	A	61	ILE	CB-CA-C	7.87	120.49	110.96	72	6
1	A	66	THR	N-CA-CB	7.86	123.22	110.42	72	6
1	A	30	ILE	CA-C-O	-7.84	113.11	121.27	59	10
1	A	67	LEU	O-C-N	-7.84	114.08	123.10	120	16
1	A	54	ARG	NE-CZ-NH1	7.84	129.34	121.50	88	18
1	A	7	THR	O-C-N	-7.83	111.82	122.23	34	8
1	A	23	ILE	CA-C-O	7.82	128.94	120.57	30	9
1	A	30	ILE	N-CA-C	7.82	118.59	110.62	101	11
1	A	2	GLN	O-C-N	-7.81	114.14	123.13	93	11
1	A	38	PRO	CA-C-N	7.78	131.34	120.29	53	14
1	A	38	PRO	C-N-CA	7.78	131.34	120.29	53	14
1	A	40	GLN	OE1-CD-NE2	-7.76	114.84	122.60	62	16
1	A	22	THR	N-CA-CB	7.75	121.44	110.36	26	17
1	A	1	MET	CG-SD-CE	-7.74	83.88	100.90	96	14
1	A	51	GLU	N-CA-C	7.72	121.71	110.28	73	6
1	A	58	ASP	O-C-N	-7.72	112.78	122.27	52	10
1	A	58	ASP	CA-C-N	7.72	131.39	120.28	5	2
1	A	58	ASP	C-N-CA	7.72	131.39	120.28	5	2
1	A	49	GLN	CA-C-O	7.70	129.35	120.80	117	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	9	THR	O-C-N	-7.70	112.35	122.59	124	4
1	A	57	SER	O-C-N	-7.70	114.08	122.09	43	14
1	A	39	ASP	N-CA-C	7.69	120.56	111.71	128	11
1	A	41	GLN	CB-CA-C	-7.66	99.03	110.67	34	9
1	A	12	THR	CA-C-N	7.61	132.39	122.95	1	9
1	A	12	THR	C-N-CA	7.61	132.39	122.95	1	9
1	A	11	LYS	O-C-N	-7.60	114.38	123.27	66	11
1	A	13	ILE	O-C-N	-7.58	114.34	122.83	66	10
1	A	12	THR	N-CA-CB	7.57	121.21	110.46	77	11
1	A	69	LEU	O-C-N	-7.56	114.61	123.22	14	4
1	A	21	ASP	O-C-N	-7.53	114.63	123.06	35	10
1	A	19	PRO	N-CA-CB	7.51	110.99	103.48	46	10
1	A	30	ILE	N-CA-CB	7.51	118.85	110.51	59	2
1	A	20	SER	N-CA-C	7.51	122.45	111.87	91	8
1	A	12	THR	CA-C-O	7.50	128.34	120.54	44	6
1	A	61	ILE	O-C-N	-7.49	113.20	122.57	102	9
1	A	16	GLU	CA-C-O	7.49	128.60	120.58	97	9
1	A	29	LYS	O-C-N	-7.49	114.18	122.12	103	9
1	A	24	GLU	N-CA-C	7.47	119.43	111.28	83	15
1	A	40	GLN	CA-C-O	7.47	127.27	119.05	32	10
1	A	26	VAL	CA-C-O	7.46	129.17	121.41	87	4
1	A	33	LYS	O-C-N	-7.45	112.68	122.59	104	8
1	A	42	ARG	CA-C-O	7.45	128.27	120.30	64	4
1	A	68	HIS	ND1-CE1-NE2	7.44	115.84	108.40	66	20
1	A	71	LEU	CA-C-N	7.44	133.07	121.99	126	2
1	A	71	LEU	C-N-CA	7.44	133.07	121.99	126	2
1	A	53	GLY	N-CA-C	7.44	122.85	114.67	102	6
1	A	22	THR	CA-CB-OG1	7.44	120.75	109.60	93	8
1	A	54	ARG	CA-C-O	-7.43	112.92	121.68	105	3
1	A	36	ILE	CB-CA-C	-7.41	102.67	110.16	63	9
1	A	58	ASP	CA-C-O	7.40	128.47	120.10	45	8
1	A	22	THR	O-C-N	-7.38	114.67	122.94	67	12
1	A	68	HIS	CB-CA-C	-7.36	97.60	109.75	118	1
1	A	32	ASP	CA-C-O	7.35	128.22	120.42	27	10
1	A	1	MET	CA-C-N	7.33	131.80	121.24	124	8
1	A	1	MET	C-N-CA	7.33	131.80	121.24	124	8
1	A	48	LYS	CA-C-O	7.33	129.41	121.05	4	8
1	A	32	ASP	N-CA-C	7.32	119.90	111.11	111	13
1	A	71	LEU	O-C-N	-7.32	114.63	123.19	121	3
1	A	60	ASN	OD1-CG-ND2	-7.32	115.28	122.60	120	20
1	A	8	LEU	CA-C-O	7.31	128.17	120.42	2	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	56	LEU	O-C-N	-7.31	114.37	122.12	87	8
1	A	17	VAL	N-CA-CB	7.30	120.72	112.32	61	2
1	A	65	SER	CA-C-N	7.29	132.15	122.30	30	6
1	A	65	SER	C-N-CA	7.29	132.15	122.30	30	6
1	A	25	ASN	CB-CA-C	-7.29	98.47	110.85	43	2
1	A	65	SER	CB-CA-C	-7.28	97.52	109.53	29	9
1	A	46	ALA	CB-CA-C	7.28	124.90	110.42	100	3
1	A	64	GLU	O-C-N	-7.28	112.86	122.47	77	6
1	A	38	PRO	N-CD-CG	7.27	114.11	103.20	104	2
1	A	11	LYS	N-CA-CB	7.26	121.21	109.95	45	2
1	A	44	ILE	N-CA-C	-7.25	97.69	108.12	105	8
1	A	31	GLN	CA-C-O	-7.24	113.15	120.90	108	10
1	A	57	SER	CB-CA-C	-7.24	98.77	110.79	67	4
1	A	19	PRO	N-CA-C	-7.24	105.12	114.03	31	6
1	A	28	ALA	O-C-N	-7.23	112.74	122.43	79	7
1	A	62	GLN	OE1-CD-NE2	-7.20	115.40	122.60	49	15
1	A	41	GLN	O-C-N	-7.20	114.11	122.89	117	8
1	A	56	LEU	N-CA-C	7.19	120.03	111.33	6	16
1	A	60	ASN	CA-C-N	-7.19	113.33	123.11	9	7
1	A	60	ASN	C-N-CA	-7.19	113.33	123.11	9	7
1	A	67	LEU	CB-CA-C	-7.17	97.97	109.80	50	1
1	A	63	LYS	N-CA-CB	7.17	120.49	110.17	45	8
1	A	22	THR	CA-C-N	7.15	130.61	120.53	112	11
1	A	22	THR	C-N-CA	7.15	130.61	120.53	112	11
1	A	55	THR	N-CA-CB	7.13	122.03	110.41	49	13
1	A	70	VAL	N-CA-CB	-7.12	103.96	112.07	25	5
1	A	5	VAL	CA-C-N	7.11	131.88	122.42	35	3
1	A	5	VAL	C-N-CA	7.11	131.88	122.42	35	3
1	A	21	ASP	CA-C-N	7.10	133.18	121.39	50	3
1	A	21	ASP	C-N-CA	7.10	133.18	121.39	50	3
1	A	65	SER	N-CA-C	7.09	120.52	110.23	43	6
1	A	57	SER	CA-C-O	7.09	127.94	120.42	71	6
1	A	52	ASP	N-CA-CB	-7.09	99.73	110.01	33	1
1	A	9	THR	CB-CA-C	-7.07	99.78	110.88	121	5
1	A	42	ARG	NH1-CZ-NH2	-7.07	110.11	119.30	31	6
1	A	26	VAL	O-C-N	-7.05	114.68	121.94	93	8
1	A	16	GLU	N-CA-C	7.05	120.35	108.23	29	4
1	A	45	PHE	O-C-N	-7.04	114.39	122.84	114	4
1	A	42	ARG	N-CA-CB	-7.04	100.14	110.84	88	3
1	A	14	THR	CB-CA-C	-7.03	99.34	111.30	22	5
1	A	49	GLN	OE1-CD-NE2	-7.03	115.57	122.60	16	11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	3	ILE	CA-C-O	7.03	129.43	121.28	31	4
1	A	58	ASP	CB-CA-C	-7.03	98.73	110.68	19	2
1	A	60	ASN	N-CA-CB	7.00	122.32	110.49	59	13
1	A	26	VAL	CB-CA-C	-6.99	103.03	111.97	125	10
1	A	47	GLY	N-CA-C	6.98	122.61	114.16	92	1
1	A	42	ARG	O-C-N	-6.97	115.15	123.31	47	10
1	A	42	ARG	CG-CD-NE	-6.97	96.67	112.00	43	6
1	A	64	GLU	CA-C-O	6.96	128.53	120.32	62	5
1	A	61	ILE	CA-C-O	6.95	129.47	120.78	102	4
1	A	44	ILE	CA-C-O	6.95	128.00	120.57	10	3
1	A	15	LEU	N-CA-C	6.95	120.47	109.50	68	5
1	A	71	LEU	CA-C-O	6.95	128.51	120.80	27	4
1	A	58	ASP	N-CA-CB	-6.94	99.92	110.12	77	7
1	A	28	ALA	N-CA-CB	-6.94	99.61	110.30	28	7
1	A	28	ALA	CB-CA-C	-6.94	99.28	110.79	81	3
1	A	16	GLU	N-CA-CB	6.93	121.02	109.94	54	5
1	A	55	THR	N-CA-C	6.92	121.33	110.32	58	4
1	A	46	ALA	CA-C-N	6.92	134.97	121.41	7	1
1	A	46	ALA	C-N-CA	6.92	134.97	121.41	7	1
1	A	14	THR	CA-CB-CG2	6.92	122.26	110.50	69	1
1	A	35	GLY	CA-C-O	6.91	125.86	118.95	62	4
1	A	24	GLU	CA-C-O	-6.91	113.22	120.55	61	7
1	A	7	THR	N-CA-C	6.91	119.65	110.53	123	7
1	A	27	LYS	CA-C-O	-6.90	113.23	120.55	115	6
1	A	23	ILE	N-CA-C	6.89	117.65	110.62	122	8
1	A	66	THR	O-C-N	-6.87	115.30	123.27	118	7
1	A	54	ARG	CG-CD-NE	-6.87	96.88	112.00	16	2
1	A	38	PRO	N-CA-CB	6.85	110.08	103.51	9	7
1	A	15	LEU	O-C-N	-6.84	115.30	123.03	6	8
1	A	35	GLY	O-C-N	6.83	131.58	122.70	118	4
1	A	36	ILE	N-CA-CB	6.83	119.63	111.23	127	2
1	A	26	VAL	CA-CB-CG2	-6.82	98.81	110.40	67	3
1	A	41	GLN	CA-C-N	6.81	132.47	122.39	95	4
1	A	41	GLN	C-N-CA	6.81	132.47	122.39	95	4
1	A	2	GLN	N-CA-CB	6.81	120.00	109.85	110	6
1	A	16	GLU	CB-CA-C	6.80	121.67	110.78	30	2
1	A	15	LEU	CA-C-N	6.79	132.40	122.41	43	6
1	A	15	LEU	C-N-CA	6.79	132.40	122.41	43	6
1	A	23	ILE	O-C-N	-6.79	114.13	121.80	98	12
1	A	68	HIS	O-C-N	-6.78	115.49	123.22	77	9
1	A	11	LYS	N-CA-C	-6.78	97.53	109.06	52	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	14	THR	N-CA-CB	6.78	122.06	110.68	117	3
1	A	63	LYS	CA-C-O	-6.76	112.93	120.70	36	7
1	A	11	LYS	CA-C-O	6.75	129.65	121.68	96	6
1	A	5	VAL	N-CA-CB	6.73	120.97	111.82	119	9
1	A	45	PHE	CA-C-N	6.73	134.39	121.54	125	8
1	A	45	PHE	C-N-CA	6.73	134.39	121.54	125	8
1	A	50	LEU	N-CA-C	6.72	119.24	108.41	121	5
1	A	50	LEU	N-CA-CB	6.71	121.10	110.57	33	4
1	A	25	ASN	N-CA-C	6.70	118.24	111.07	31	11
1	A	34	GLU	N-CA-CB	6.67	120.07	110.40	28	1
1	A	43	LEU	N-CA-C	6.64	120.32	109.76	119	3
1	A	10	GLY	CA-C-N	6.63	132.07	122.85	74	4
1	A	10	GLY	C-N-CA	6.63	132.07	122.85	74	4
1	A	61	ILE	CA-C-N	6.63	134.56	122.02	48	4
1	A	61	ILE	C-N-CA	6.63	134.56	122.02	48	4
1	A	19	PRO	CB-CA-C	-6.63	102.44	111.85	114	7
1	A	31	GLN	CB-CG-CD	6.62	123.86	112.60	116	2
1	A	3	ILE	CB-CA-C	6.62	120.70	111.70	10	3
1	A	3	ILE	CA-CB-CG1	6.62	121.65	110.40	60	5
1	A	5	VAL	CA-C-O	6.61	126.78	120.31	25	8
1	A	69	LEU	CB-CA-C	6.61	120.64	109.80	45	6
1	A	43	LEU	O-C-N	-6.60	115.69	123.22	109	10
1	A	55	THR	CA-CB-OG1	6.59	119.49	109.60	64	14
1	A	14	THR	CA-C-O	-6.59	112.85	120.49	7	8
1	A	64	GLU	CA-C-N	6.59	130.07	120.71	91	7
1	A	64	GLU	C-N-CA	6.59	130.07	120.71	91	7
1	A	19	PRO	CA-C-O	6.57	127.67	118.99	3	2
1	A	66	THR	N-CA-C	6.57	119.40	108.96	121	3
1	A	20	SER	CA-C-N	6.56	133.44	122.87	123	6
1	A	20	SER	C-N-CA	6.56	133.44	122.87	123	6
1	A	70	VAL	CA-C-O	6.56	128.98	120.78	86	5
1	A	71	LEU	N-CA-C	6.55	119.37	108.96	40	2
1	A	9	THR	CA-C-O	-6.54	111.16	120.51	110	6
1	A	18	GLU	N-CA-C	-6.54	101.89	110.39	86	8
1	A	4	PHE	CA-C-N	6.53	131.78	123.10	91	5
1	A	4	PHE	C-N-CA	6.53	131.78	123.10	91	5
1	A	21	ASP	CB-CA-C	-6.52	98.51	109.53	85	1
1	A	70	VAL	CA-C-N	6.51	131.37	122.19	33	1
1	A	70	VAL	C-N-CA	6.51	131.37	122.19	33	1
1	A	2	GLN	CA-C-O	-6.50	113.03	120.58	117	7
1	A	45	PHE	CA-C-O	-6.47	113.38	120.30	115	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	33	LYS	N-CA-CB	-6.46	100.56	110.13	6	2
1	A	41	GLN	CA-C-O	6.46	128.06	120.69	125	9
1	A	62	GLN	CB-CG-CD	6.46	123.59	112.60	119	1
1	A	50	LEU	O-C-N	-6.46	115.67	123.16	19	6
1	A	15	LEU	N-CA-CB	6.45	121.17	110.85	9	3
1	A	68	HIS	CA-C-N	6.45	131.00	122.42	28	1
1	A	68	HIS	C-N-CA	6.45	131.00	122.42	28	1
1	A	69	LEU	CA-C-O	6.45	127.41	120.32	78	6
1	A	4	PHE	CB-CG-CD2	-6.44	109.75	120.70	79	1
1	A	32	ASP	CB-CA-C	6.43	121.61	110.68	103	3
1	A	13	ILE	CB-CG1-CD1	6.42	127.27	113.80	22	1
1	A	7	THR	N-CA-CB	6.41	119.69	110.45	57	10
1	A	55	THR	CA-C-O	-6.41	114.43	121.87	6	6
1	A	53	GLY	O-C-N	-6.41	114.37	122.70	91	7
1	A	20	SER	CA-C-O	6.40	127.02	119.28	60	4
1	A	54	ARG	CD-NE-CZ	-6.39	115.45	124.40	125	7
1	A	48	LYS	N-CA-CB	6.38	120.96	110.69	59	3
1	A	6	LYS	N-CA-CB	-6.37	99.64	110.16	3	3
1	A	10	GLY	O-C-N	-6.36	114.43	122.70	24	4
1	A	38	PRO	CB-CA-C	-6.35	102.41	111.68	95	3
1	A	53	GLY	CA-C-N	6.35	132.93	122.07	89	3
1	A	53	GLY	C-N-CA	6.35	132.93	122.07	89	3
1	A	46	ALA	CA-C-O	-6.34	111.44	120.51	40	2
1	A	23	ILE	CA-CB-CG2	6.34	121.28	110.50	87	6
1	A	21	ASP	N-CA-CB	6.34	119.30	110.17	89	8
1	A	67	LEU	CA-C-N	6.32	131.73	123.00	111	3
1	A	67	LEU	C-N-CA	6.32	131.73	123.00	111	3
1	A	65	SER	CA-C-O	-6.32	114.20	121.47	103	11
1	A	20	SER	N-CA-CB	6.32	120.11	110.44	23	1
1	A	66	THR	CA-CB-OG1	6.31	119.06	109.60	6	3
1	A	7	THR	CA-CB-OG1	6.31	119.06	109.60	121	11
1	A	48	LYS	CA-C-N	6.30	130.31	121.24	64	7
1	A	48	LYS	C-N-CA	6.30	130.31	121.24	64	7
1	A	31	GLN	O-C-N	-6.29	114.86	122.22	28	7
1	A	57	SER	N-CA-CB	6.29	119.47	110.16	22	4
1	A	12	THR	CA-CB-OG1	6.29	119.03	109.60	33	1
1	A	36	ILE	CA-CB-CG1	6.29	121.08	110.40	60	1
1	A	62	GLN	N-CA-C	6.28	118.44	110.33	119	3
1	A	54	ARG	NH1-CZ-NH2	-6.28	111.13	119.30	118	8
1	A	19	PRO	CA-C-N	6.28	133.82	121.58	27	6
1	A	19	PRO	C-N-CA	6.28	133.82	121.58	27	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	44	ILE	CA-CB-CG1	6.27	121.06	110.40	59	2
1	A	51	GLU	CA-C-O	6.27	128.13	120.92	83	6
1	A	1	MET	O-C-N	-6.26	112.98	123.00	42	2
1	A	25	ASN	CB-CG-ND2	6.25	125.78	116.40	19	2
1	A	12	THR	N-CA-C	6.25	118.15	109.15	16	3
1	A	22	THR	CA-C-O	-6.25	114.03	121.66	89	4
1	A	34	GLU	O-C-N	-6.25	114.92	122.48	121	6
1	A	34	GLU	CA-C-N	6.21	130.59	122.26	96	2
1	A	34	GLU	C-N-CA	6.21	130.59	122.26	96	2
1	A	67	LEU	N-CA-C	-6.21	100.79	110.42	122	6
1	A	30	ILE	CB-CA-C	-6.21	103.76	112.14	14	4
1	A	4	PHE	CA-C-O	6.20	127.39	120.70	125	5
1	A	30	ILE	CA-CB-CG2	6.20	121.03	110.50	3	2
1	A	6	LYS	N-CA-C	6.19	118.27	108.67	117	3
1	A	67	LEU	CA-C-O	6.17	128.09	121.11	46	3
1	A	64	GLU	CB-CA-C	6.17	122.70	110.42	5	5
1	A	47	GLY	O-C-N	-6.15	114.70	122.70	58	5
1	A	17	VAL	N-CA-C	6.13	117.19	108.42	35	4
1	A	59	TYR	CA-CB-CG	-6.13	102.87	113.90	66	2
1	A	68	HIS	N-CA-C	6.12	119.22	109.24	39	3
1	A	18	GLU	CB-CG-CD	-6.11	102.21	112.60	98	1
1	A	64	GLU	CB-CG-CD	-6.11	102.21	112.60	117	1
1	A	6	LYS	CA-C-N	6.11	131.91	121.29	36	1
1	A	6	LYS	C-N-CA	6.11	131.91	121.29	36	1
1	A	62	GLN	CG-CD-NE2	6.10	125.55	116.40	39	5
1	A	50	LEU	CA-C-N	6.10	131.74	122.65	81	4
1	A	50	LEU	C-N-CA	6.10	131.74	122.65	81	4
1	A	70	VAL	CA-CB-CG1	6.09	120.76	110.40	58	3
1	A	50	LEU	CA-C-O	6.09	126.97	120.46	123	3
1	A	14	THR	CA-CB-OG1	6.08	118.73	109.60	26	3
1	A	5	VAL	N-CA-C	6.07	117.21	107.73	101	6
1	A	54	ARG	N-CA-C	-6.07	100.11	109.52	114	3
1	A	4	PHE	N-CA-CB	6.05	120.68	110.69	12	3
1	A	49	GLN	N-CA-CB	6.05	119.03	109.71	76	2
1	A	17	VAL	CB-CA-C	-6.05	100.08	110.30	21	3
1	A	40	GLN	CA-C-N	6.04	130.71	122.19	121	8
1	A	40	GLN	C-N-CA	6.04	130.71	122.19	121	8
1	A	27	LYS	N-CA-CB	6.03	119.08	110.16	35	3
1	A	44	ILE	CA-C-N	6.03	131.23	122.85	32	2
1	A	44	ILE	C-N-CA	6.03	131.23	122.85	32	2
1	A	66	THR	CA-CB-CG2	6.02	120.74	110.50	101	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	4	PHE	CB-CA-C	-6.02	101.05	110.74	101	5
1	A	33	LYS	CA-C-O	-6.00	114.72	120.90	98	4
1	A	48	LYS	N-CA-C	5.99	118.50	108.73	82	3
1	A	26	VAL	CA-CB-CG1	5.99	120.58	110.40	79	4
1	A	12	THR	CA-CB-CG2	5.98	120.67	110.50	116	1
1	A	21	ASP	CA-C-O	-5.98	114.60	121.47	97	6
1	A	5	VAL	CG1-CB-CG2	5.97	123.94	110.80	28	1
1	A	32	ASP	N-CA-CB	-5.96	101.42	110.07	22	9
1	A	29	LYS	N-CA-CB	5.96	118.89	110.12	16	4
1	A	59	TYR	CA-C-O	5.96	126.80	119.05	33	1
1	A	42	ARG	N-CA-C	-5.96	100.00	109.23	68	2
1	A	61	ILE	CA-CB-CG1	5.96	120.52	110.40	94	1
1	A	29	LYS	CA-C-O	5.95	127.06	120.82	63	8
1	A	20	SER	O-C-N	-5.94	114.18	122.37	60	3
1	A	23	ILE	CA-CB-CG1	5.93	120.48	110.40	90	1
1	A	64	GLU	N-CA-C	5.93	119.73	111.90	23	3
1	A	43	LEU	CB-CA-C	5.92	120.11	110.22	59	4
1	A	4	PHE	CB-CG-CD1	5.91	130.74	120.70	37	3
1	A	15	LEU	CB-CA-C	-5.89	99.55	109.50	71	1
1	A	48	LYS	CA-CB-CG	-5.89	102.33	114.10	72	1
1	A	60	ASN	N-CA-C	5.88	119.75	111.52	94	3
1	A	46	ALA	O-C-N	-5.87	114.78	122.59	1	4
1	A	37	PRO	N-CD-CG	5.87	112.00	103.20	11	1
1	A	70	VAL	CA-CB-CG2	-5.87	100.43	110.40	27	5
1	A	13	ILE	CB-CA-C	-5.86	103.04	111.19	127	6
1	A	41	GLN	CB-CG-CD	-5.85	102.65	112.60	35	5
1	A	49	GLN	CB-CA-C	-5.85	100.30	109.84	92	2
1	A	3	ILE	CA-C-N	5.83	131.34	122.65	73	1
1	A	3	ILE	C-N-CA	5.83	131.34	122.65	73	1
1	A	49	GLN	O-C-N	5.82	129.46	122.94	63	8
1	A	68	HIS	N-CA-CB	5.82	119.81	110.85	66	5
1	A	25	ASN	CA-C-O	-5.82	114.39	120.55	115	3
1	A	36	ILE	CA-CB-CG2	-5.81	100.62	110.50	108	1
1	A	18	GLU	CB-CA-C	-5.81	100.02	108.91	47	3
1	A	59	TYR	CB-CG-CD1	-5.80	112.09	120.80	26	4
1	A	9	THR	OG1-CB-CG2	-5.80	97.69	109.30	83	3
1	A	59	TYR	O-C-N	-5.80	114.90	122.39	52	3
1	A	20	SER	CB-CA-C	-5.78	102.15	111.28	91	2
1	A	40	GLN	CB-CA-C	-5.77	100.96	110.72	84	1
1	A	27	LYS	CG-CD-CE	5.77	124.57	111.30	13	1
1	A	4	PHE	N-CA-C	-5.77	99.99	109.40	122	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	71	LEU	CB-CA-C	5.77	119.25	109.50	97	3
1	A	24	GLU	N-CA-CB	5.76	118.71	110.06	92	4
1	A	69	LEU	N-CA-C	5.75	118.27	108.90	84	2
1	A	63	LYS	CB-CA-C	-5.74	100.48	109.84	34	3
1	A	33	LYS	CG-CD-CE	5.74	124.51	111.30	77	1
1	A	48	LYS	CB-CA-C	5.73	119.18	109.50	68	1
1	A	67	LEU	N-CA-CB	5.73	119.91	110.69	13	2
1	A	34	GLU	CA-C-O	5.72	126.79	120.90	110	2
1	A	34	GLU	CB-CG-CD	5.72	122.32	112.60	111	2
1	A	8	LEU	N-CA-CB	5.71	118.89	110.33	26	3
1	A	14	THR	N-CA-C	5.71	117.37	109.15	55	1
1	A	51	GLU	CB-CG-CD	-5.71	102.90	112.60	86	1
1	A	66	THR	OG1-CB-CG2	-5.71	97.89	109.30	36	2
1	A	12	THR	OG1-CB-CG2	-5.70	97.91	109.30	81	2
1	A	26	VAL	CG1-CB-CG2	-5.70	98.27	110.80	41	1
1	A	59	TYR	CB-CA-C	-5.69	100.24	110.37	126	3
1	A	44	ILE	N-CA-CB	5.68	119.82	111.52	106	3
1	A	70	VAL	N-CA-C	-5.68	100.90	108.96	66	3
1	A	2	GLN	CG-CD-NE2	-5.67	107.89	116.40	19	1
1	A	9	THR	CA-C-N	5.67	132.53	121.41	44	2
1	A	9	THR	C-N-CA	5.67	132.53	121.41	44	2
1	A	31	GLN	N-CA-CB	5.66	119.01	109.78	67	2
1	A	68	HIS	ND1-CG-CD2	-5.64	100.46	106.10	23	1
1	A	43	LEU	N-CA-CB	5.64	120.64	110.83	14	4
1	A	13	ILE	N-CA-C	5.64	116.06	108.17	56	3
1	A	9	THR	CA-CB-CG2	5.64	120.08	110.50	121	2
1	A	5	VAL	CA-CB-CG1	5.63	119.98	110.40	36	1
1	A	40	GLN	N-CA-CB	-5.62	101.24	110.40	21	2
1	A	49	GLN	CG-CD-NE2	5.61	124.82	116.40	48	2
1	A	9	THR	N-CA-C	5.59	117.06	110.97	42	6
1	A	6	LYS	CB-CA-C	5.59	118.97	109.75	97	3
1	A	49	GLN	CB-CG-CD	5.58	122.08	112.60	65	2
1	A	39	ASP	O-C-N	-5.57	114.14	122.39	126	2
1	A	25	ASN	O-C-N	-5.57	115.42	122.27	90	4
1	A	42	ARG	CB-CG-CD	5.56	124.09	111.30	105	1
1	A	61	ILE	N-CA-C	5.56	115.66	107.15	68	3
1	A	5	VAL	CB-CA-C	-5.55	104.24	110.96	13	3
1	A	16	GLU	CB-CG-CD	5.55	122.04	112.60	71	3
1	A	51	GLU	N-CA-CB	5.54	119.66	110.52	25	3
1	A	18	GLU	CA-CB-CG	5.54	125.18	114.10	118	1
1	A	70	VAL	CB-CA-C	5.54	118.37	110.84	93	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	66	THR	CA-C-N	5.53	130.64	123.00	67	7
1	A	66	THR	C-N-CA	5.53	130.64	123.00	67	7
1	A	47	GLY	CA-C-N	5.53	130.95	122.93	36	4
1	A	47	GLY	C-N-CA	5.53	130.95	122.93	36	4
1	A	52	ASP	CB-CA-C	-5.52	102.46	110.96	107	2
1	A	51	GLU	CB-CA-C	5.50	119.61	109.71	44	3
1	A	69	LEU	N-CA-CB	-5.49	102.16	110.35	54	3
1	A	50	LEU	CB-CA-C	-5.49	101.28	110.29	42	1
1	A	44	ILE	CA-CB-CG2	5.48	119.82	110.50	20	2
1	A	24	GLU	CB-CG-CD	-5.47	103.30	112.60	12	1
1	A	71	LEU	CD1-CG-CD2	-5.47	98.77	110.80	55	2
1	A	42	ARG	CA-C-N	5.45	130.67	123.05	41	4
1	A	42	ARG	C-N-CA	5.45	130.67	123.05	41	4
1	A	41	GLN	N-CA-CB	5.44	118.09	109.71	8	1
1	A	48	LYS	CB-CG-CD	5.44	123.81	111.30	49	2
1	A	47	GLY	CA-C-O	-5.43	111.11	120.57	87	1
1	A	44	ILE	CB-CA-C	-5.43	102.59	110.63	119	1
1	A	56	LEU	N-CA-CB	5.43	118.66	110.30	77	1
1	A	71	LEU	N-CA-CB	5.43	118.37	109.95	20	1
1	A	31	GLN	CG-CD-NE2	-5.43	108.26	116.40	9	1
1	A	8	LEU	CB-CA-C	-5.43	101.67	110.79	55	2
1	A	15	LEU	CA-C-O	5.42	126.33	120.32	23	3
1	A	34	GLU	CB-CA-C	-5.41	100.27	109.03	18	1
1	A	33	LYS	CA-C-N	5.41	129.83	120.58	37	2
1	A	33	LYS	C-N-CA	5.41	129.83	120.58	37	2
1	A	22	THR	CA-CB-CG2	-5.40	101.31	110.50	126	2
1	A	29	LYS	CB-CA-C	-5.40	102.36	110.90	81	2
1	A	22	THR	OG1-CB-CG2	-5.40	98.50	109.30	96	1
1	A	38	PRO	N-CA-C	5.40	120.67	114.03	18	5
1	A	19	PRO	O-C-N	5.40	129.77	122.37	21	2
1	A	40	GLN	CG-CD-OE1	5.37	131.55	120.80	107	1
1	A	38	PRO	CA-C-O	-5.37	111.48	119.00	126	1
1	A	12	THR	CB-CA-C	-5.36	101.99	111.05	58	1
1	A	60	ASN	CB-CG-ND2	5.34	124.41	116.40	82	1
1	A	16	GLU	CG-CD-OE2	5.33	130.66	118.40	22	1
1	A	62	GLN	CA-C-O	5.33	128.07	121.94	88	3
1	A	27	LYS	CB-CA-C	-5.33	100.78	110.63	78	3
1	A	27	LYS	CB-CG-CD	5.32	123.54	111.30	98	1
1	A	23	ILE	CB-CG1-CD1	5.32	124.97	113.80	5	1
1	A	7	THR	CA-C-O	5.32	128.15	121.50	62	2
1	A	45	PHE	N-CA-C	5.32	117.32	108.02	48	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	2	GLN	CA-C-N	5.29	131.29	122.57	44	2
1	A	2	GLN	C-N-CA	5.29	131.29	122.57	44	2
1	A	42	ARG	CD-NE-CZ	5.29	131.80	124.40	5	3
1	A	46	ALA	N-CA-CB	5.26	119.39	110.49	80	2
1	A	60	ASN	O-C-N	5.26	129.42	122.47	101	1
1	A	46	ALA	N-CA-C	-5.26	104.54	111.96	3	2
1	A	40	GLN	CB-CG-CD	-5.26	103.66	112.60	94	2
1	A	3	ILE	N-CA-C	-5.25	102.41	108.82	1	2
1	A	31	GLN	CA-CB-CG	5.25	124.60	114.10	41	1
1	A	29	LYS	CA-CB-CG	-5.25	103.61	114.10	109	1
1	A	29	LYS	CB-CG-CD	5.25	123.36	111.30	58	1
1	A	49	GLN	CA-CB-CG	5.21	124.52	114.10	89	1
1	A	60	ASN	CA-C-O	5.21	127.96	120.51	81	1
1	A	66	THR	CB-CA-C	-5.21	101.76	110.19	67	2
1	A	37	PRO	CA-CB-CG	-5.19	94.63	104.50	124	1
1	A	1	MET	CA-CB-CG	5.18	124.47	114.10	2	1
1	A	63	LYS	CG-CD-CE	5.18	123.22	111.30	112	1
1	A	38	PRO	O-C-N	-5.17	115.27	122.30	123	1
1	A	24	GLU	CB-CA-C	5.15	119.05	110.81	67	1
1	A	2	GLN	CB-CA-C	-5.15	101.62	110.22	93	1
1	A	34	GLU	CA-CB-CG	5.15	124.39	114.10	34	1
1	A	25	ASN	CB-CG-OD1	-5.13	110.54	120.80	77	1
1	A	62	GLN	CB-CA-C	-5.12	101.36	111.60	82	1
1	A	59	TYR	CB-CG-CD2	5.12	128.47	120.80	117	3
1	A	29	LYS	CG-CD-CE	5.10	123.02	111.30	25	1
1	A	62	GLN	CG-CD-OE1	5.09	130.98	120.80	10	1
1	A	6	LYS	CA-CB-CG	-5.08	103.94	114.10	90	1
1	A	54	ARG	CA-C-N	5.08	132.24	122.03	94	1
1	A	54	ARG	C-N-CA	5.08	132.24	122.03	94	1
1	A	45	PHE	CB-CG-CD1	5.06	129.31	120.70	64	1
1	A	19	PRO	N-CD-CG	5.06	110.78	103.20	30	1
1	A	6	LYS	CG-CD-CE	5.05	122.92	111.30	106	1
1	A	42	ARG	CB-CA-C	-5.05	104.06	111.23	109	1
1	A	30	ILE	CA-CB-CG1	5.03	118.96	110.40	54	1
1	A	3	ILE	CA-CB-CG2	-5.03	101.95	110.50	40	1
1	A	15	LEU	CD1-CG-CD2	5.02	121.85	110.80	29	1
1	A	8	LEU	CD1-CG-CD2	-5.02	99.75	110.80	18	1
1	A	54	ARG	CB-CA-C	5.01	118.59	109.83	128	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	38
1	A	54	ARG	Sidechain	38
1	A	59	TYR	Sidechain	36
1	A	45	PHE	Sidechain	8
1	A	68	HIS	Sidechain	6
1	A	4	PHE	Sidechain	5
1	A	37	PRO	Peptide	4
1	A	51	GLU	Peptide	4
1	A	10	GLY	Peptide	1
1	A	41	GLN	Peptide	1
1	A	71	LEU	Peptide	1
1	A	40	GLN	Peptide	1
1	A	15	LEU	Peptide	1
1	A	2	GLN	Peptide	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	72064	75008	75008	33

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:50:LEU:H	1:A:50:LEU:HD22	0.55	1.60	49	1
1:A:7:THR:HG22	1:A:69:LEU:HD23	0.55	1.78	116	1
1:A:22:THR:O	1:A:26:VAL:HG23	0.54	2.01	27	2
1:A:23:ILE:HG23	1:A:43:LEU:HD23	0.54	1.79	114	1
1:A:23:ILE:HB	1:A:52:ASP:HA	0.54	1.79	110	2
1:A:15:LEU:HD22	1:A:29:LYS:HB3	0.53	1.80	24	1
1:A:56:LEU:HD23	1:A:61:ILE:HD12	0.46	1.86	99	1
1:A:25:ASN:O	1:A:28:ALA:HB3	0.46	2.10	45	1
1:A:19:PRO:HA	1:A:56:LEU:HB2	0.45	1.87	104	1
1:A:15:LEU:HD22	1:A:29:LYS:CB	0.44	2.42	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:LEU:CD1	1:A:26:VAL:HG13	0.44	2.42	48	2
1:A:44:ILE:HD12	1:A:49:GLN:HG2	0.44	1.88	125	1
1:A:5:VAL:HG21	1:A:15:LEU:HD12	0.43	1.88	83	1
1:A:44:ILE:HD12	1:A:70:VAL:HG21	0.43	1.89	108	1
1:A:50:LEU:HD22	1:A:59:TYR:CD2	0.43	2.48	70	3
1:A:27:LYS:HD3	1:A:38:PRO:O	0.43	2.13	115	1
1:A:16:GLU:O	1:A:29:LYS:NZ	0.43	2.51	14	1
1:A:51:GLU:CD	1:A:54:ARG:HE	0.43	2.20	104	1
1:A:54:ARG:HB2	1:A:59:TYR:CE2	0.43	2.49	18	1
1:A:23:ILE:HD12	1:A:50:LEU:HD13	0.42	1.91	42	1
1:A:43:LEU:O	1:A:50:LEU:HD12	0.42	2.14	92	1
1:A:23:ILE:HB	1:A:51:GLU:O	0.42	2.15	58	1
1:A:8:LEU:HD11	1:A:71:LEU:H	0.41	1.75	6	1
1:A:8:LEU:HD23	1:A:68:HIS:CE1	0.41	2.51	94	1
1:A:50:LEU:HD22	1:A:59:TYR:CE2	0.41	2.50	20	1
1:A:13:ILE:HD11	1:A:30:ILE:HG23	0.41	1.91	26	1
1:A:27:LYS:NZ	1:A:52:ASP:OD2	0.40	2.54	87	1
1:A:45:PHE:HB3	1:A:50:LEU:HD21	0.40	1.93	30	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%)	64±2 (92±3%)	5±2 (6±3%)	1±1 (2±1%)	9	53
All	All	8960/9728 (92%)	8231 (92%)	579 (6%)	150 (2%)	9	53

All 12 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	46	ALA	54
1	A	10	GLY	53
1	A	60	ASN	17
1	A	47	GLY	6

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Mol	Chain	Res	Type	Models (Total)
1	A	52	ASP	6
1	A	33	LYS	4
1	A	9	THR	3
1	A	64	GLU	2
1	A	35	GLY	2
1	A	11	LYS	1
1	A	7	THR	1
1	A	45	PHE	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	65/68 (96%)	64±1 (98±2%)	1±1 (2±2%)	49	91
All	All	8320/8704 (96%)	8164 (98%)	156 (2%)	49	91

All 46 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	9	THR	14
1	A	37	PRO	11
1	A	70	VAL	10
1	A	1	MET	9
1	A	15	LEU	8
1	A	17	VAL	8
1	A	50	LEU	7
1	A	38	PRO	6
1	A	19	PRO	5
1	A	65	SER	5
1	A	21	ASP	4
1	A	57	SER	4
1	A	48	LYS	4
1	A	67	LEU	4
1	A	14	THR	3
1	A	52	ASP	3
1	A	13	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	8	LEU	3
1	A	39	ASP	3
1	A	49	GLN	3
1	A	58	ASP	3
1	A	20	SER	3
1	A	44	ILE	2
1	A	60	ASN	2
1	A	31	GLN	2
1	A	7	THR	2
1	A	63	LYS	2
1	A	36	ILE	2
1	A	2	GLN	2
1	A	71	LEU	2
1	A	3	ILE	2
1	A	26	VAL	1
1	A	32	ASP	1
1	A	56	LEU	1
1	A	6	LYS	1
1	A	66	THR	1
1	A	30	ILE	1
1	A	40	GLN	1
1	A	62	GLN	1
1	A	68	HIS	1
1	A	24	GLU	1
1	A	55	THR	1
1	A	69	LEU	1
1	A	23	ILE	1
1	A	12	THR	1
1	A	43	LEU	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

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided