



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 08:44 pm GMT

PDB ID : 1XQQ
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

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

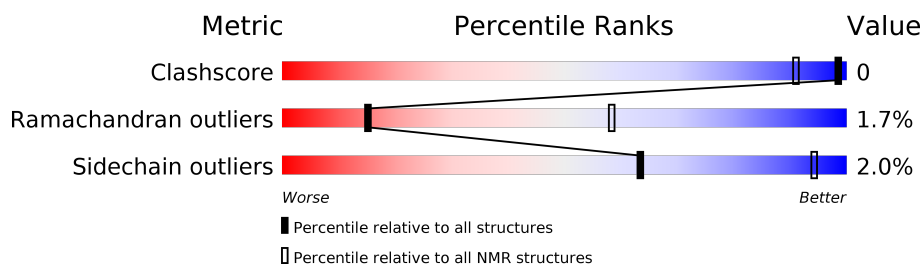
1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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

Mol	Chain	Length	Quality of chain
1	A	76	

2 Ensemble composition and analysis ⓘ

This entry contains 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)	0.41	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.

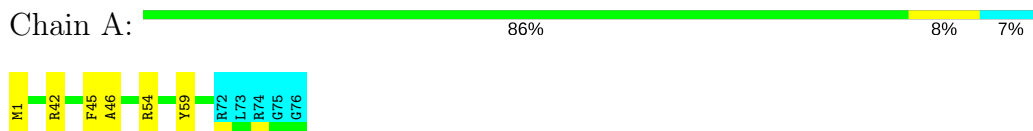
Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1231	378	629	105	118	1	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: ubiquitin

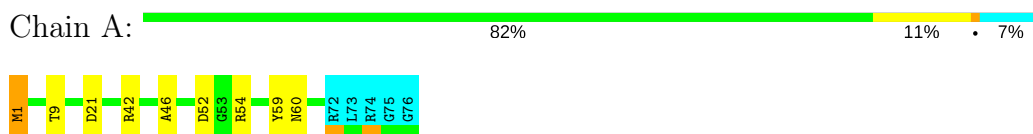


4.2 Scores per residue for each member of the ensemble

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

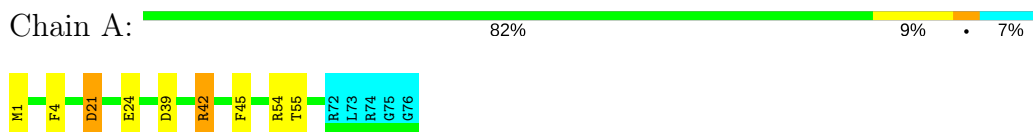
4.2.1 Score per residue for model 1

- Molecule 1: ubiquitin



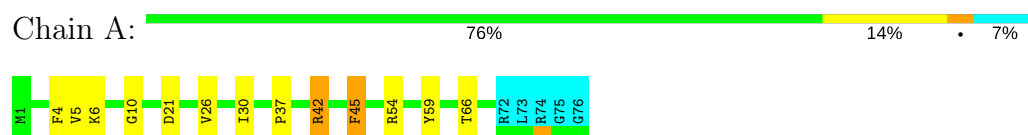
4.2.2 Score per residue for model 2

- Molecule 1: ubiquitin



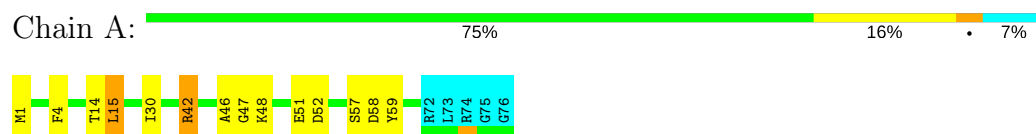
4.2.3 Score per residue for model 3

- Molecule 1: ubiquitin



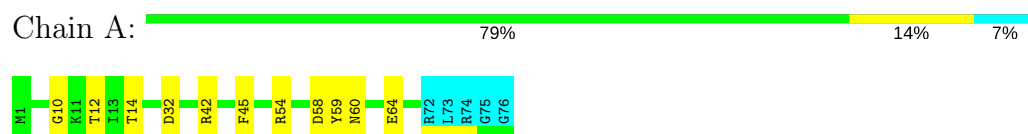
4.2.4 Score per residue for model 4

- Molecule 1: ubiquitin



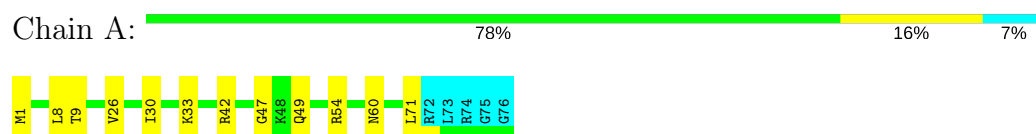
4.2.5 Score per residue for model 5

- Molecule 1: ubiquitin



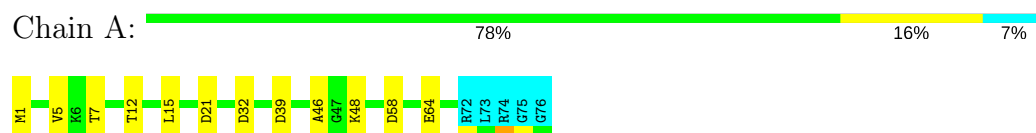
4.2.6 Score per residue for model 6

- Molecule 1: ubiquitin



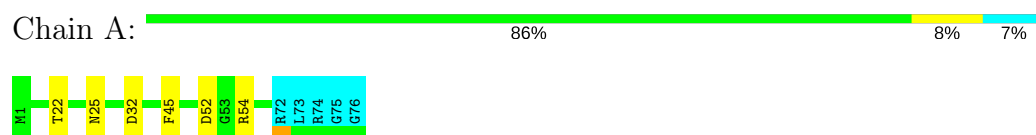
4.2.7 Score per residue for model 7

- Molecule 1: ubiquitin



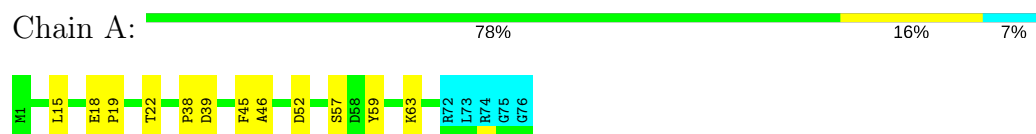
4.2.8 Score per residue for model 8

- Molecule 1: ubiquitin



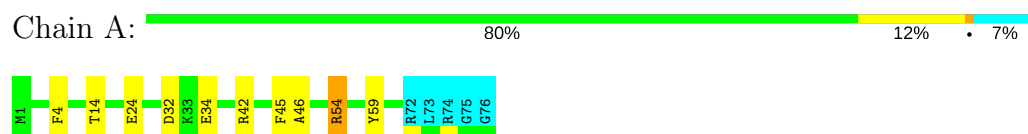
4.2.9 Score per residue for model 9

- Molecule 1: ubiquitin



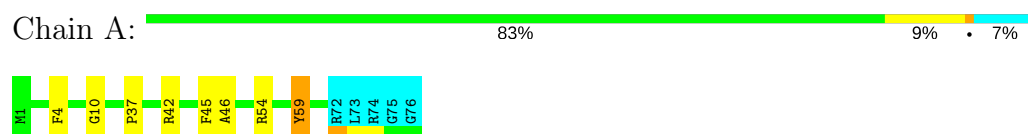
4.2.10 Score per residue for model 10

- Molecule 1: ubiquitin



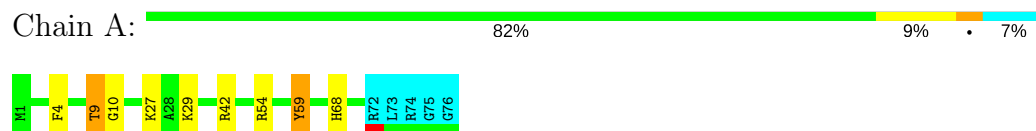
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: ubiquitin



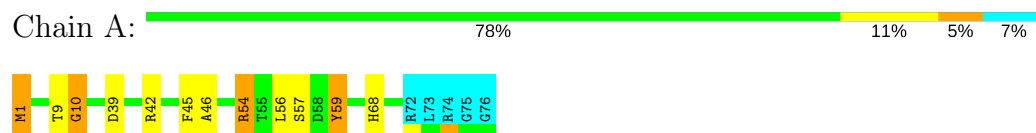
4.2.12 Score per residue for model 12

- Molecule 1: ubiquitin



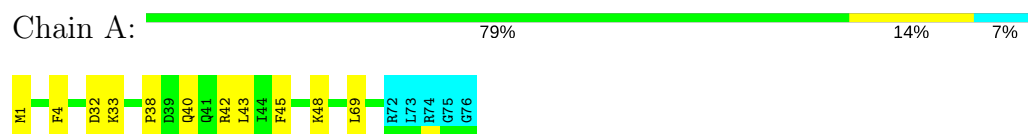
4.2.13 Score per residue for model 13

- Molecule 1: ubiquitin



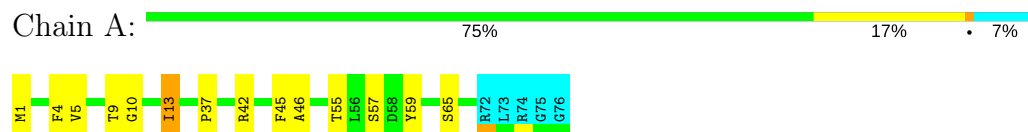
4.2.14 Score per residue for model 14

- Molecule 1: ubiquitin



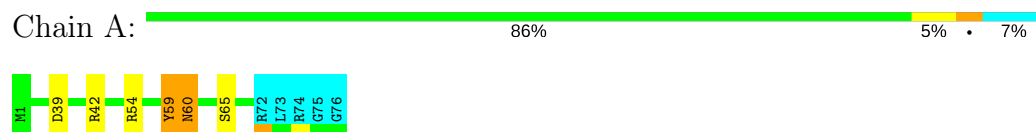
4.2.15 Score per residue for model 15

- Molecule 1: ubiquitin



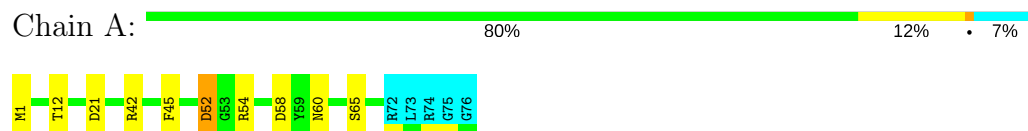
4.2.16 Score per residue for model 16

- Molecule 1: ubiquitin



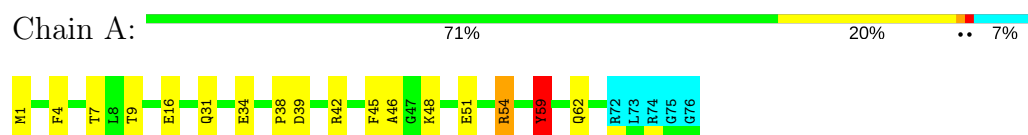
4.2.17 Score per residue for model 17

- Molecule 1: ubiquitin



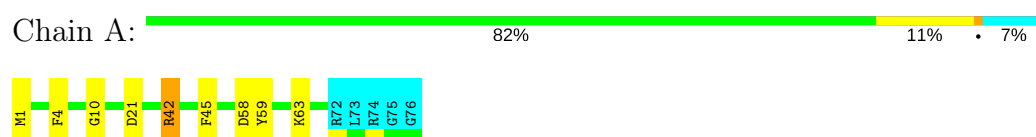
4.2.18 Score per residue for model 18

- Molecule 1: ubiquitin



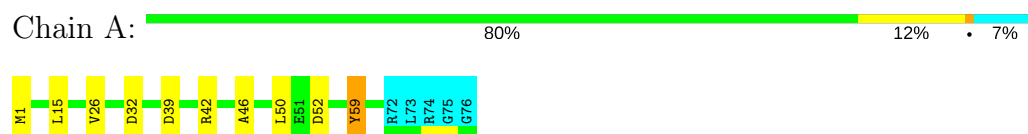
4.2.19 Score per residue for model 19

- Molecule 1: ubiquitin



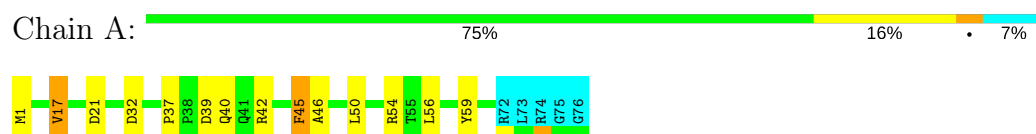
4.2.20 Score per residue for model 20

- Molecule 1: ubiquitin



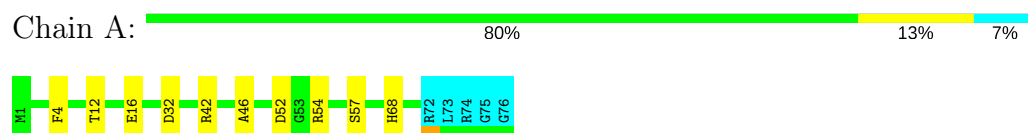
4.2.21 Score per residue for model 21

- Molecule 1: ubiquitin



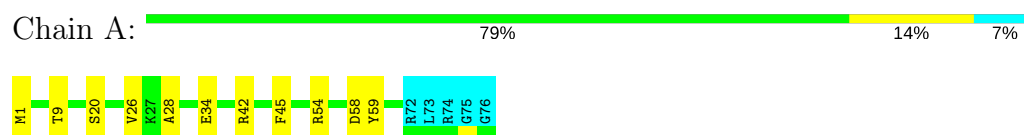
4.2.22 Score per residue for model 22

- Molecule 1: ubiquitin



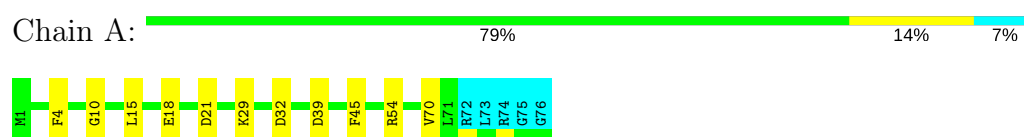
4.2.23 Score per residue for model 23

- Molecule 1: ubiquitin



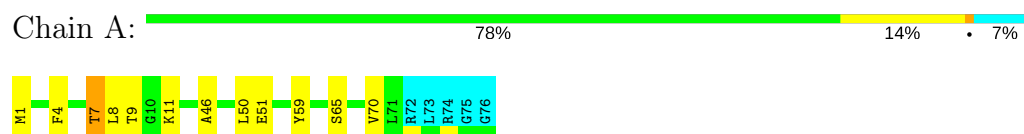
4.2.24 Score per residue for model 24

- Molecule 1: ubiquitin



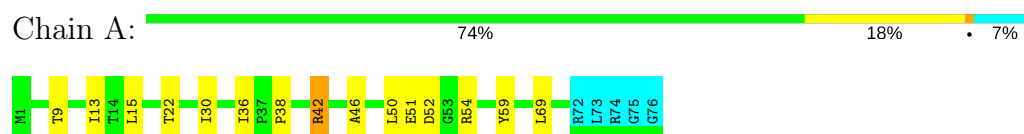
4.2.25 Score per residue for model 25

- Molecule 1: ubiquitin



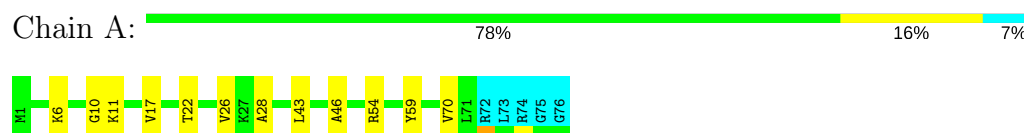
4.2.26 Score per residue for model 26

- Molecule 1: ubiquitin



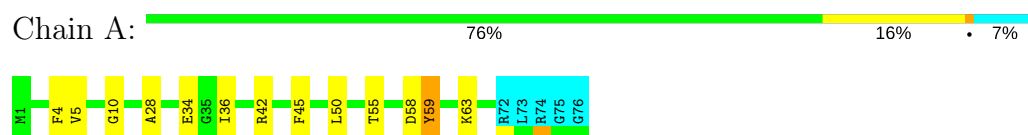
4.2.27 Score per residue for model 27

- Molecule 1: ubiquitin



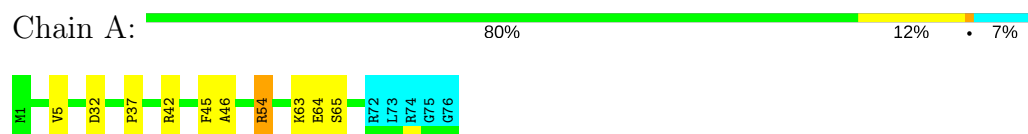
4.2.28 Score per residue for model 28

- Molecule 1: ubiquitin



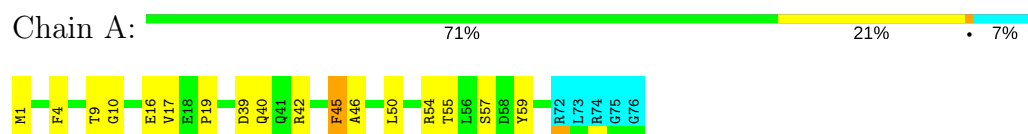
4.2.29 Score per residue for model 29

- Molecule 1: ubiquitin



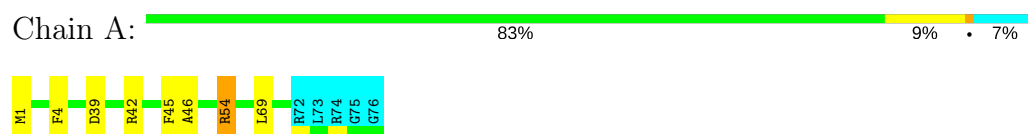
4.2.30 Score per residue for model 30

- Molecule 1: ubiquitin



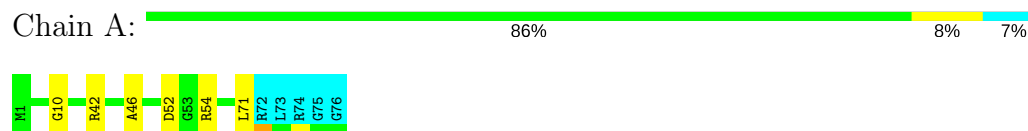
4.2.31 Score per residue for model 31

- Molecule 1: ubiquitin



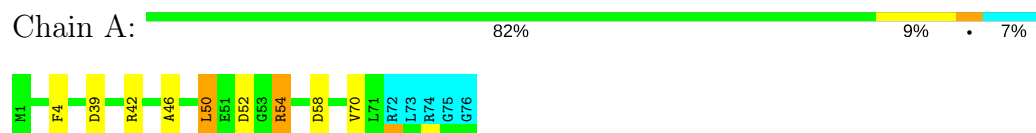
4.2.32 Score per residue for model 32

- Molecule 1: ubiquitin



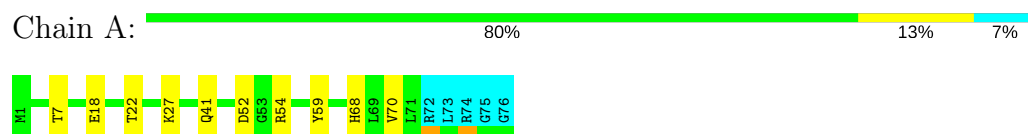
4.2.33 Score per residue for model 33

- Molecule 1: ubiquitin



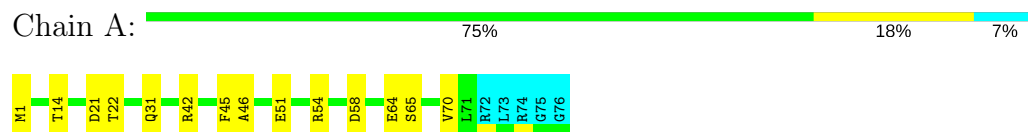
4.2.34 Score per residue for model 34

- Molecule 1: ubiquitin



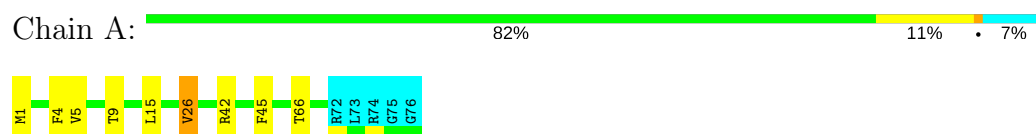
4.2.35 Score per residue for model 35

- Molecule 1: ubiquitin



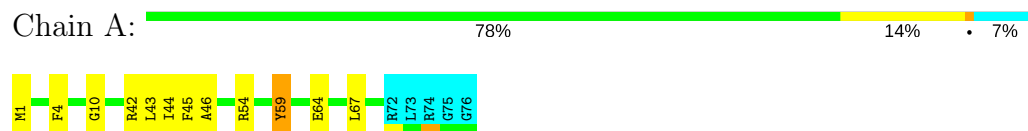
4.2.36 Score per residue for model 36

- Molecule 1: ubiquitin



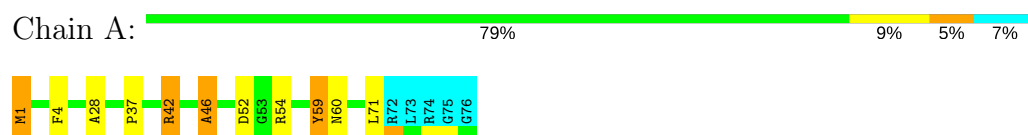
4.2.37 Score per residue for model 37

- Molecule 1: ubiquitin



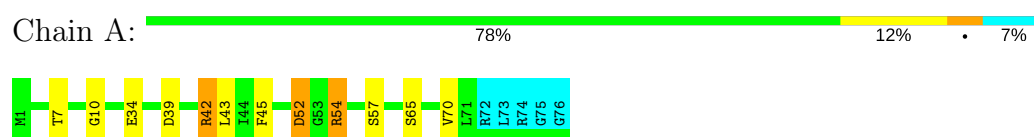
4.2.38 Score per residue for model 38

- Molecule 1: ubiquitin



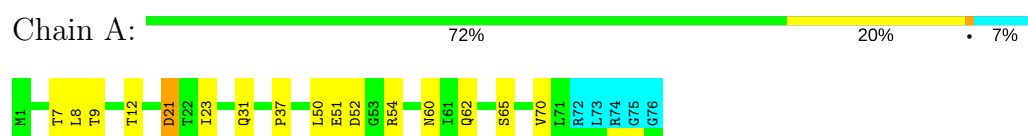
4.2.39 Score per residue for model 39

- Molecule 1: ubiquitin



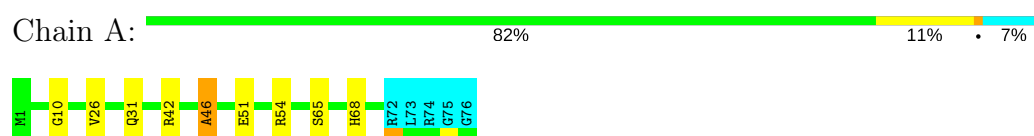
4.2.40 Score per residue for model 40

- Molecule 1: ubiquitin



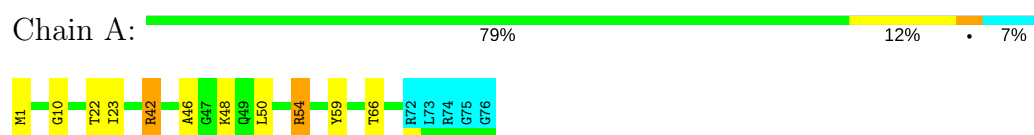
4.2.41 Score per residue for model 41

- Molecule 1: ubiquitin



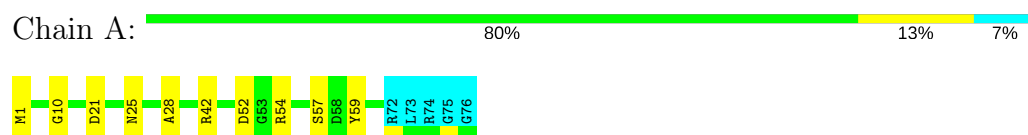
4.2.42 Score per residue for model 42

- Molecule 1: ubiquitin



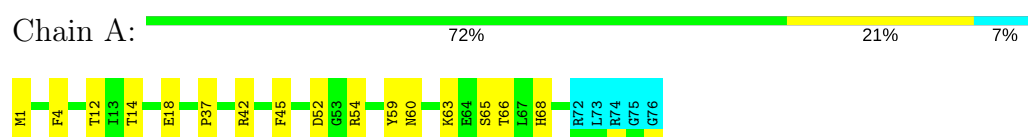
4.2.43 Score per residue for model 43

- Molecule 1: ubiquitin



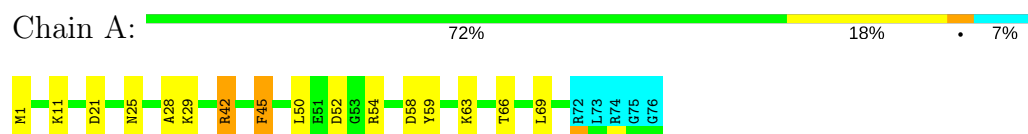
4.2.44 Score per residue for model 44

- Molecule 1: ubiquitin



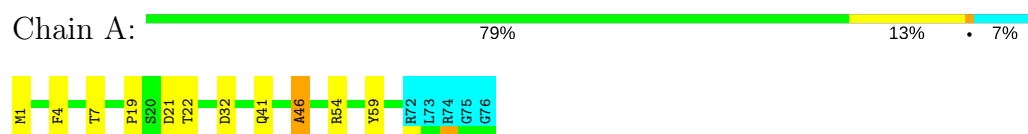
4.2.45 Score per residue for model 45

- Molecule 1: ubiquitin



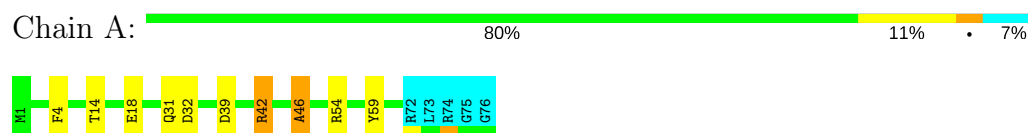
4.2.46 Score per residue for model 46

- Molecule 1: ubiquitin



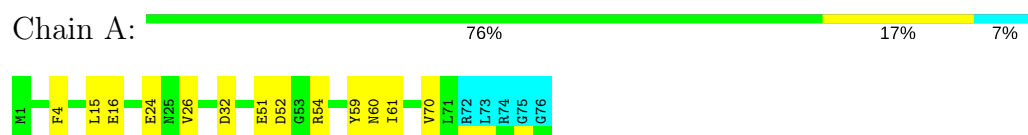
4.2.47 Score per residue for model 47

- Molecule 1: ubiquitin



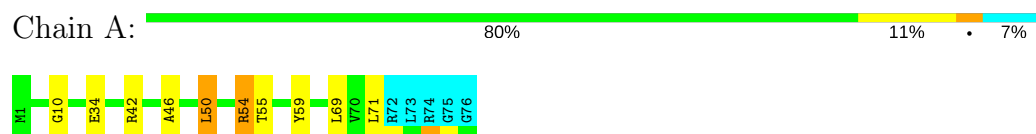
4.2.48 Score per residue for model 48

- Molecule 1: ubiquitin



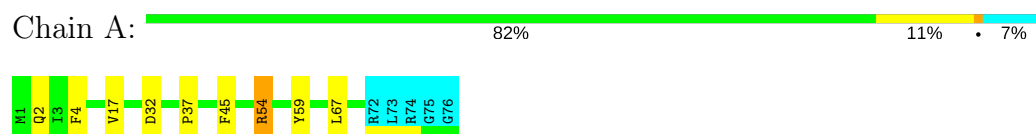
4.2.49 Score per residue for model 49

- Molecule 1: ubiquitin



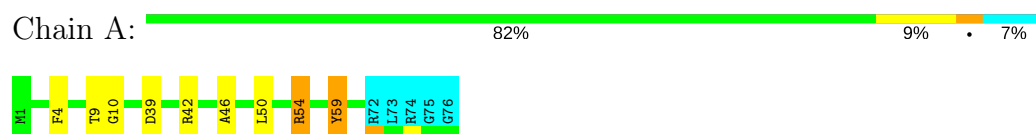
4.2.50 Score per residue for model 50

- Molecule 1: ubiquitin



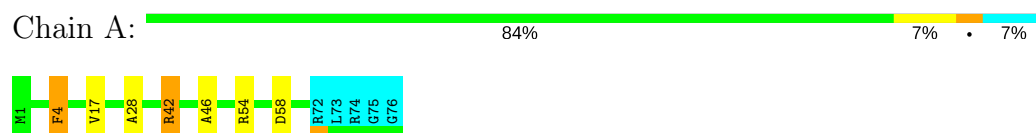
4.2.51 Score per residue for model 51

- Molecule 1: ubiquitin



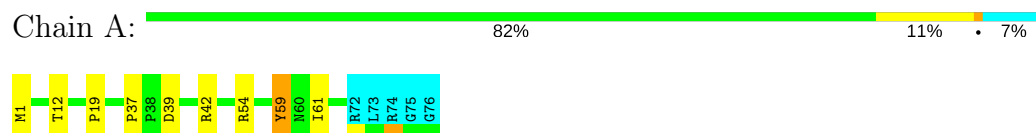
4.2.52 Score per residue for model 52

- Molecule 1: ubiquitin



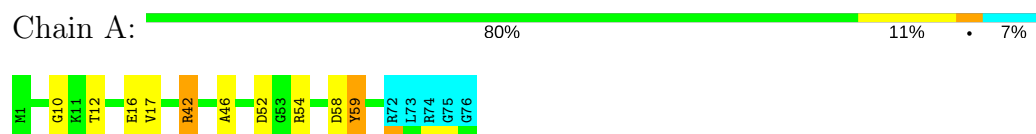
4.2.53 Score per residue for model 53

- Molecule 1: ubiquitin



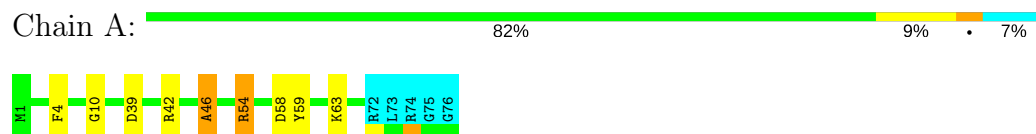
4.2.54 Score per residue for model 54

- Molecule 1: ubiquitin



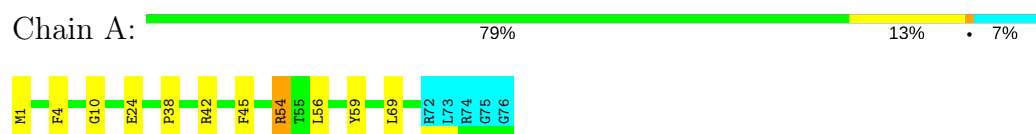
4.2.55 Score per residue for model 55

- Molecule 1: ubiquitin



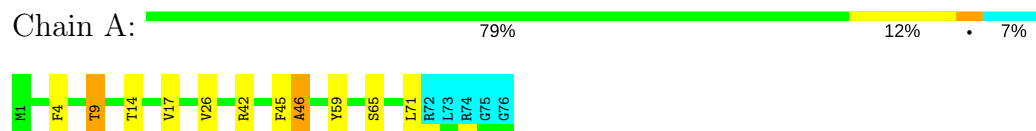
4.2.56 Score per residue for model 56

- Molecule 1: ubiquitin



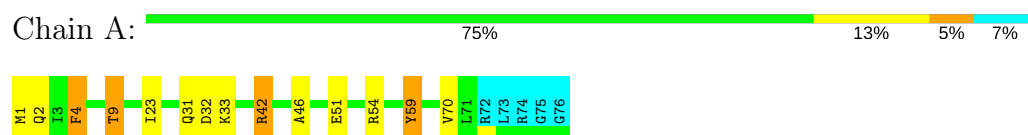
4.2.57 Score per residue for model 57

- Molecule 1: ubiquitin



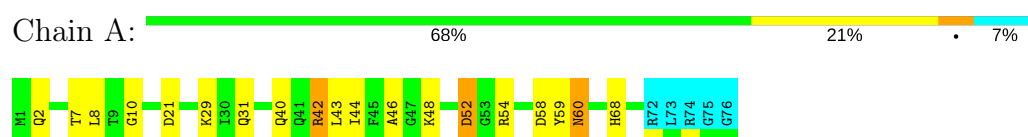
4.2.58 Score per residue for model 58

- Molecule 1: ubiquitin



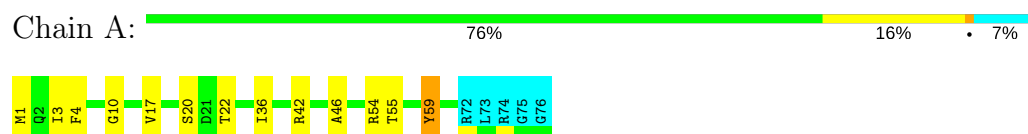
4.2.59 Score per residue for model 59

- Molecule 1: ubiquitin



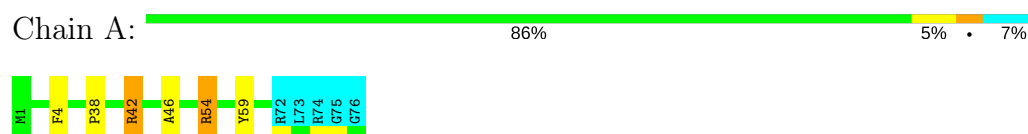
4.2.60 Score per residue for model 60

- Molecule 1: ubiquitin



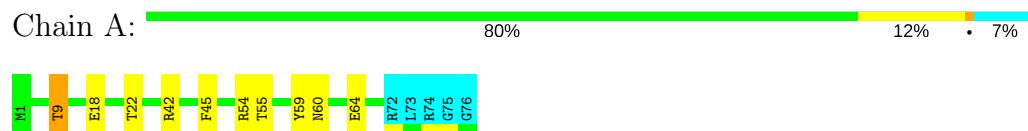
4.2.61 Score per residue for model 61

- Molecule 1: ubiquitin



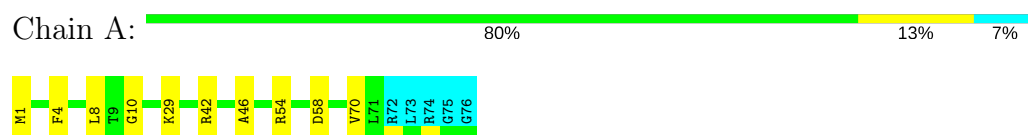
4.2.62 Score per residue for model 62

- Molecule 1: ubiquitin



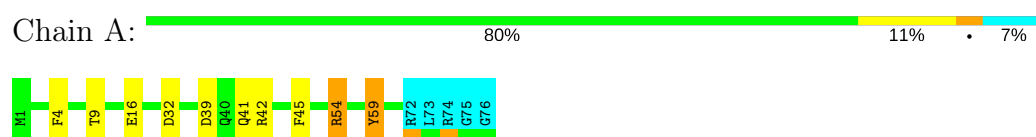
4.2.63 Score per residue for model 63

- Molecule 1: ubiquitin



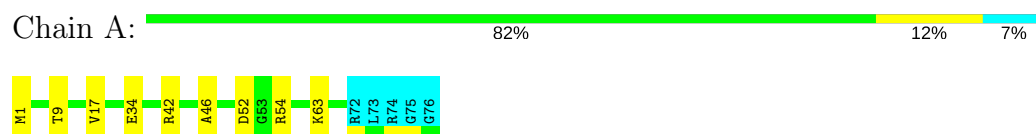
4.2.64 Score per residue for model 64

- Molecule 1: ubiquitin



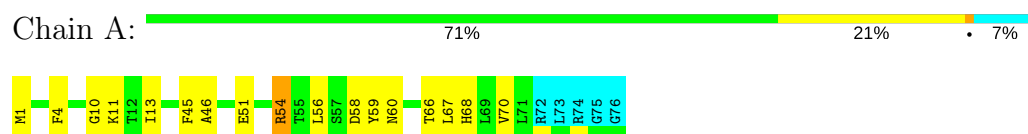
4.2.65 Score per residue for model 65

- Molecule 1: ubiquitin



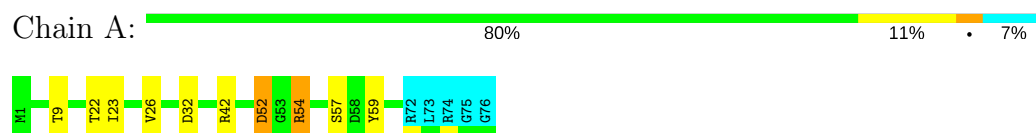
4.2.66 Score per residue for model 66

- Molecule 1: ubiquitin



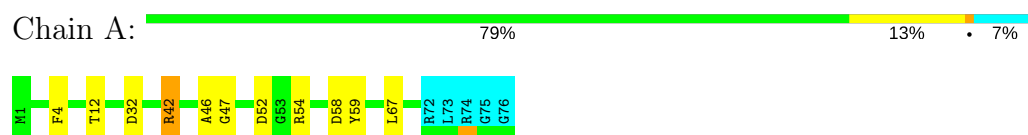
4.2.67 Score per residue for model 67

- Molecule 1: ubiquitin



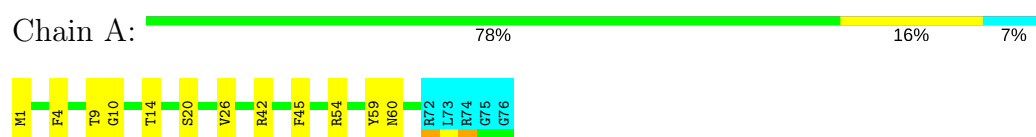
4.2.68 Score per residue for model 68

- Molecule 1: ubiquitin



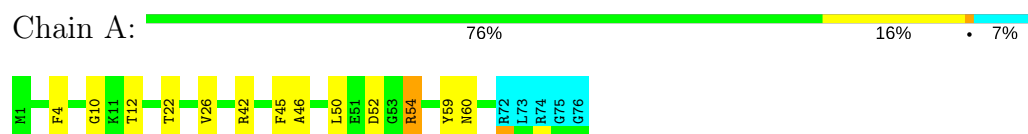
4.2.69 Score per residue for model 69

- Molecule 1: ubiquitin



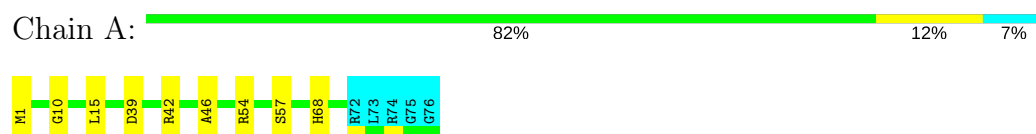
4.2.70 Score per residue for model 70

- Molecule 1: ubiquitin



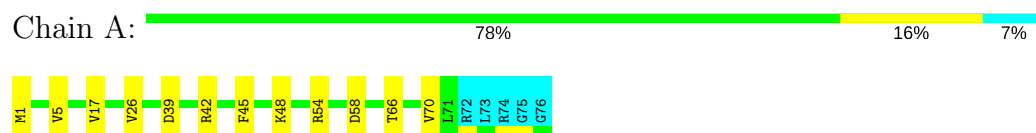
4.2.71 Score per residue for model 71

- Molecule 1: ubiquitin



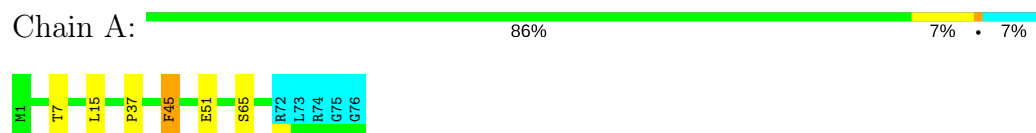
4.2.72 Score per residue for model 72

- Molecule 1: ubiquitin



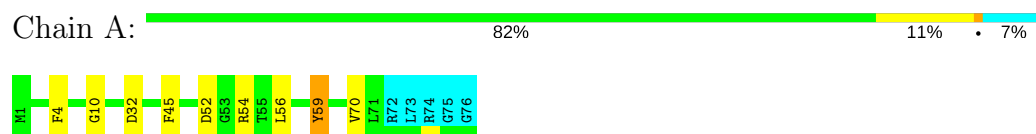
4.2.73 Score per residue for model 73

- Molecule 1: ubiquitin



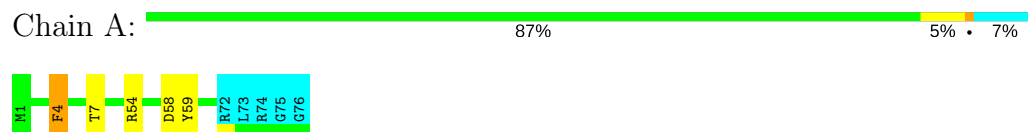
4.2.74 Score per residue for model 74

- Molecule 1: ubiquitin



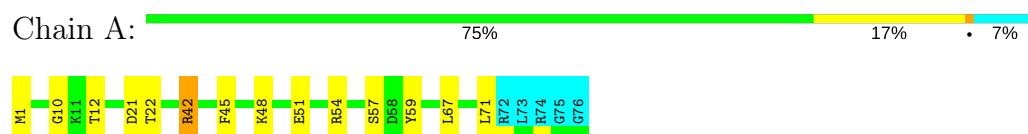
4.2.75 Score per residue for model 75

- Molecule 1: ubiquitin



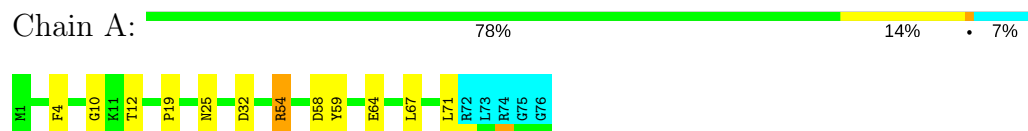
4.2.76 Score per residue for model 76

- Molecule 1: ubiquitin



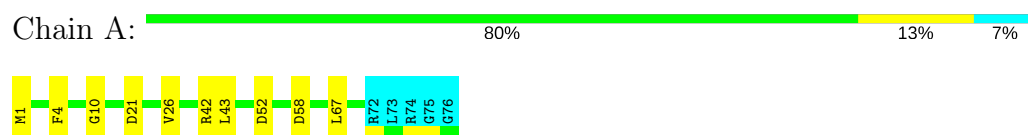
4.2.77 Score per residue for model 77

- Molecule 1: ubiquitin



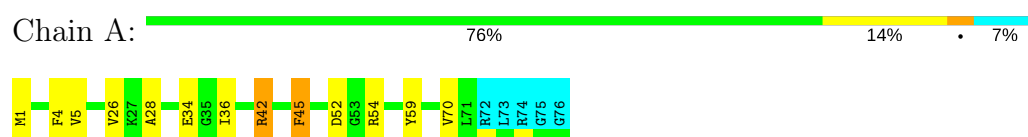
4.2.78 Score per residue for model 78

- Molecule 1: ubiquitin



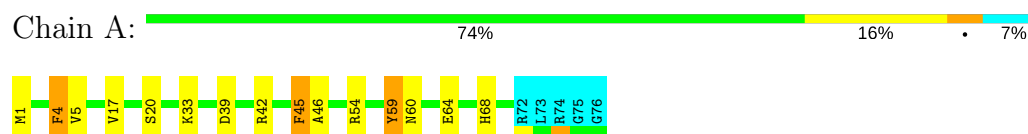
4.2.79 Score per residue for model 79

- Molecule 1: ubiquitin



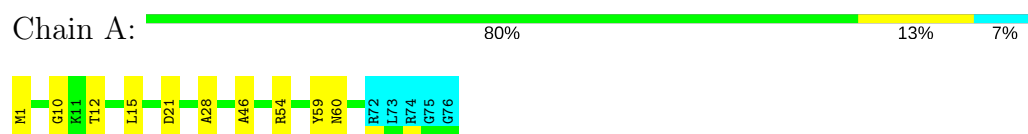
4.2.80 Score per residue for model 80

- Molecule 1: ubiquitin



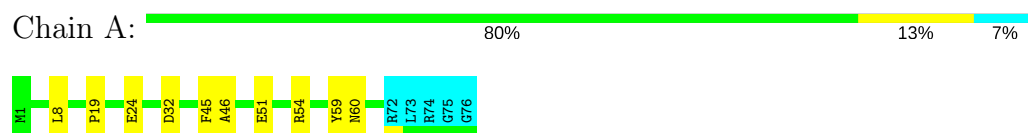
4.2.81 Score per residue for model 81

- Molecule 1: ubiquitin



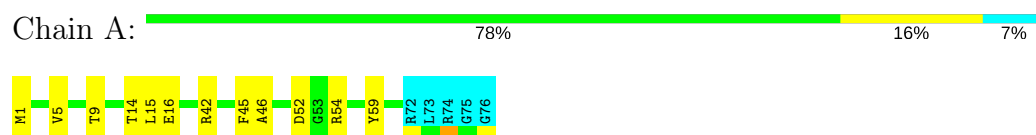
4.2.82 Score per residue for model 82

- Molecule 1: ubiquitin



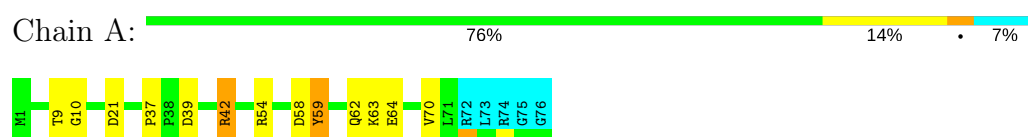
4.2.83 Score per residue for model 83

- Molecule 1: ubiquitin



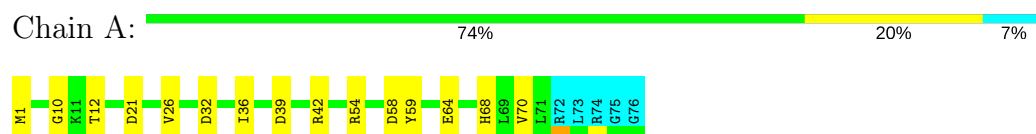
4.2.84 Score per residue for model 84

- Molecule 1: ubiquitin



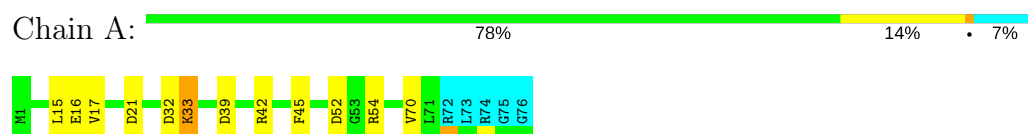
4.2.85 Score per residue for model 85

- Molecule 1: ubiquitin



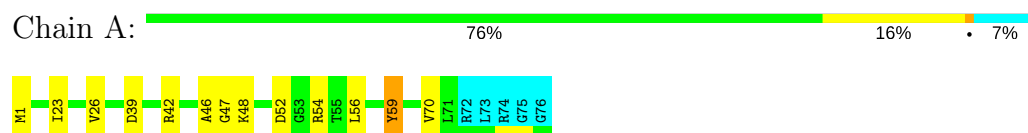
4.2.86 Score per residue for model 86

- Molecule 1: ubiquitin



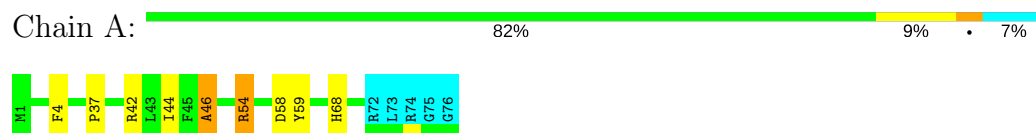
4.2.87 Score per residue for model 87

- Molecule 1: ubiquitin



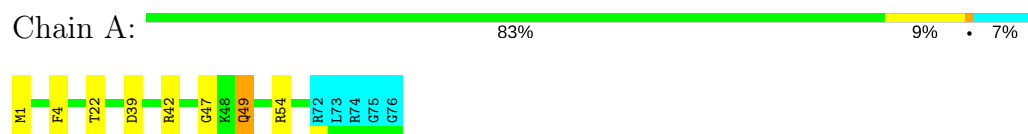
4.2.88 Score per residue for model 88

- Molecule 1: ubiquitin



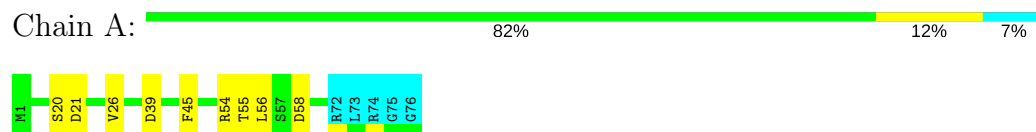
4.2.89 Score per residue for model 89

- Molecule 1: ubiquitin



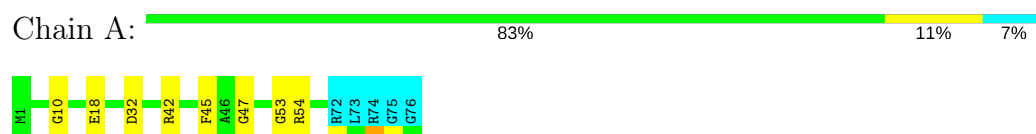
4.2.90 Score per residue for model 90

- Molecule 1: ubiquitin



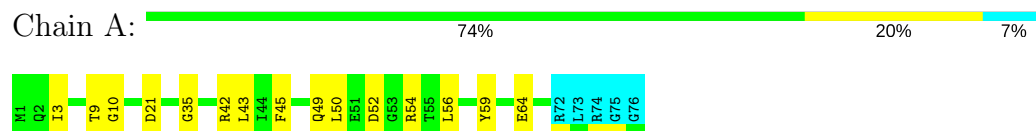
4.2.91 Score per residue for model 91

- Molecule 1: ubiquitin



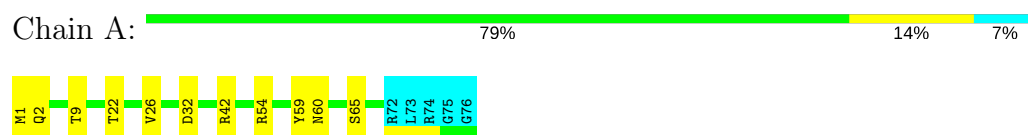
4.2.92 Score per residue for model 92

- Molecule 1: ubiquitin



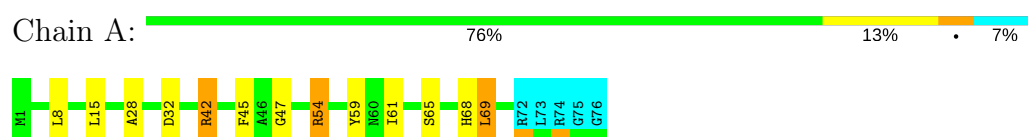
4.2.93 Score per residue for model 93

- Molecule 1: ubiquitin



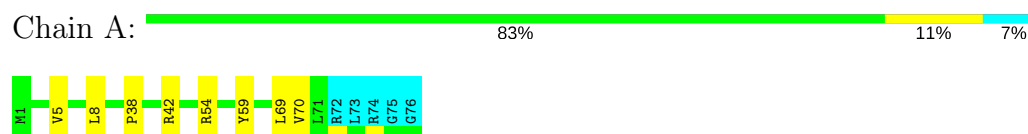
4.2.94 Score per residue for model 94

- Molecule 1: ubiquitin



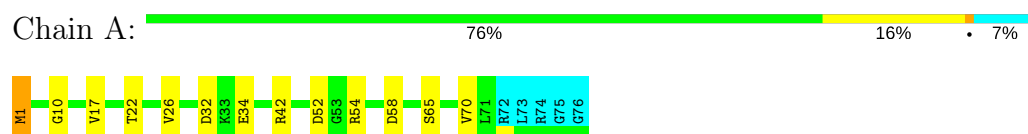
4.2.95 Score per residue for model 95

- Molecule 1: ubiquitin



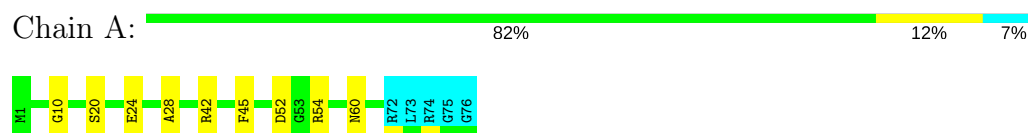
4.2.96 Score per residue for model 96

- Molecule 1: ubiquitin



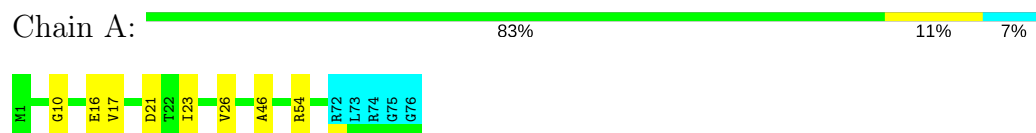
4.2.97 Score per residue for model 97

- Molecule 1: ubiquitin



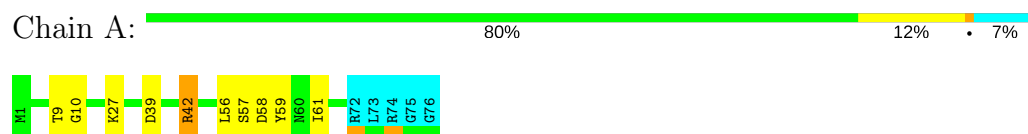
4.2.98 Score per residue for model 98

- Molecule 1: ubiquitin



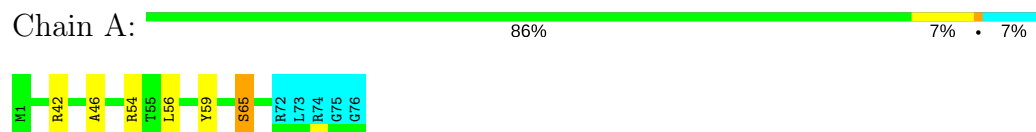
4.2.99 Score per residue for model 99

- Molecule 1: ubiquitin



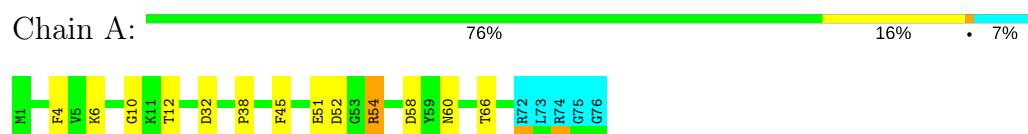
4.2.100 Score per residue for model 100

- Molecule 1: ubiquitin



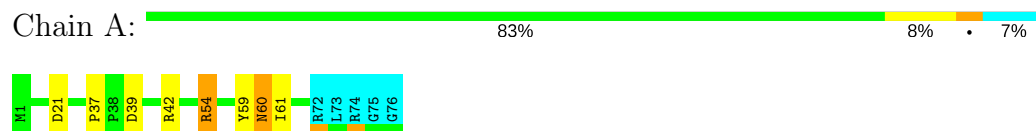
4.2.101 Score per residue for model 101

- Molecule 1: ubiquitin



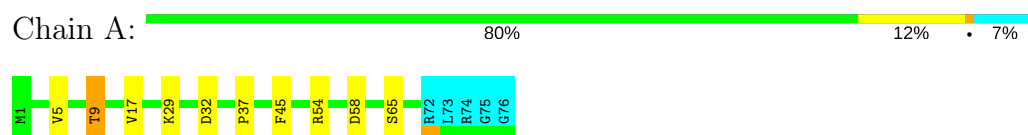
4.2.102 Score per residue for model 102

- Molecule 1: ubiquitin



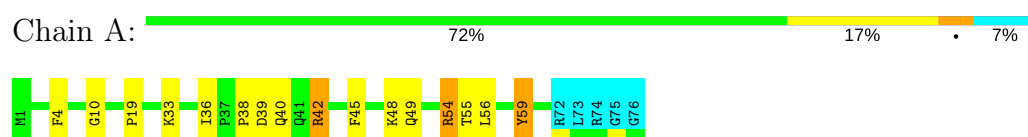
4.2.103 Score per residue for model 103

- Molecule 1: ubiquitin



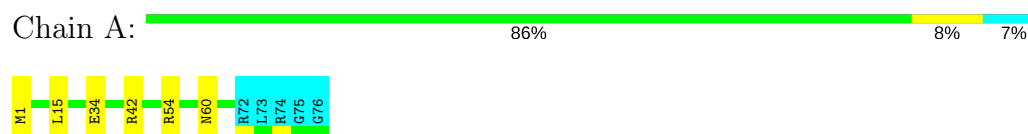
4.2.104 Score per residue for model 104

- Molecule 1: ubiquitin



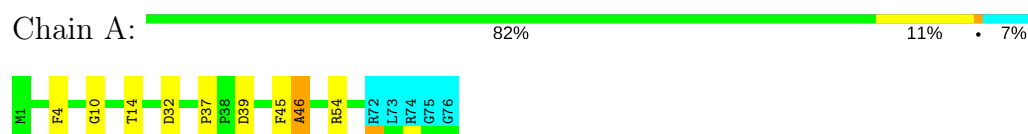
4.2.105 Score per residue for model 105

- Molecule 1: ubiquitin



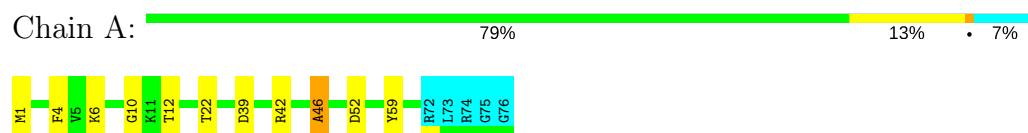
4.2.106 Score per residue for model 106

- Molecule 1: ubiquitin



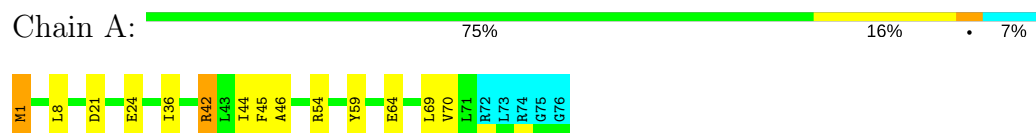
4.2.107 Score per residue for model 107

- Molecule 1: ubiquitin



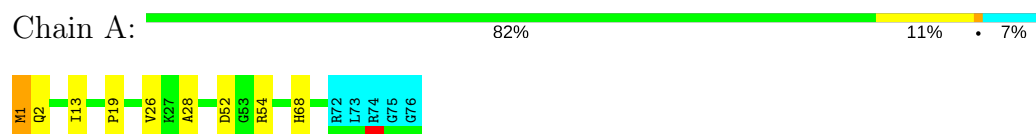
4.2.108 Score per residue for model 108

- Molecule 1: ubiquitin



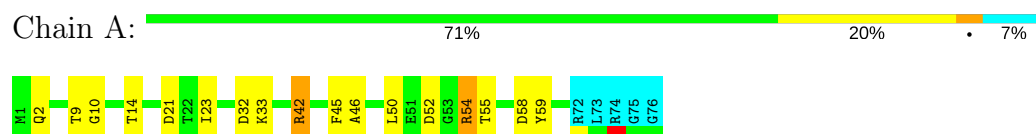
4.2.109 Score per residue for model 109

- Molecule 1: ubiquitin



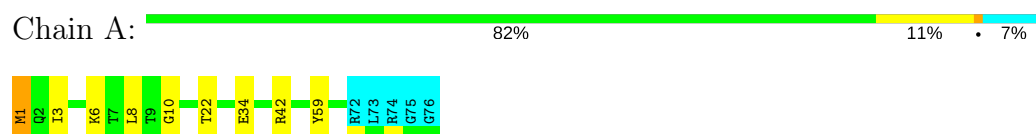
4.2.110 Score per residue for model 110

- Molecule 1: ubiquitin



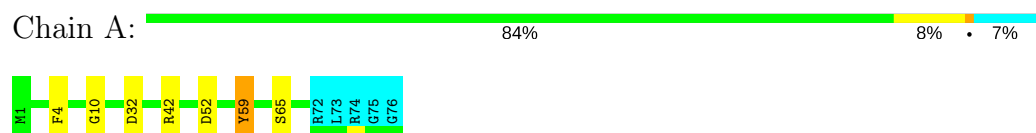
4.2.111 Score per residue for model 111

- Molecule 1: ubiquitin



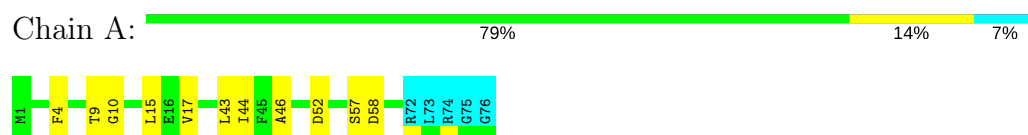
4.2.112 Score per residue for model 112

- Molecule 1: ubiquitin



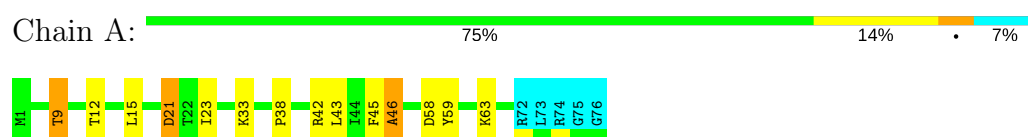
4.2.113 Score per residue for model 113

- Molecule 1: ubiquitin



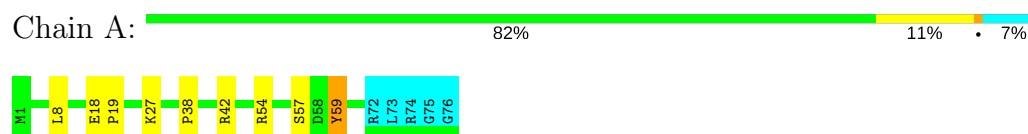
4.2.114 Score per residue for model 114

- Molecule 1: ubiquitin



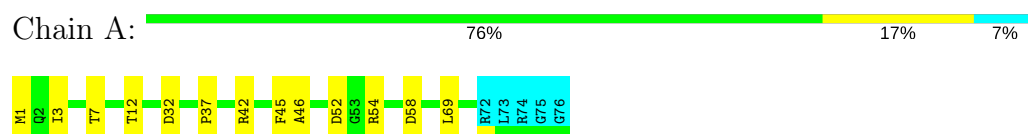
4.2.115 Score per residue for model 115

- Molecule 1: ubiquitin



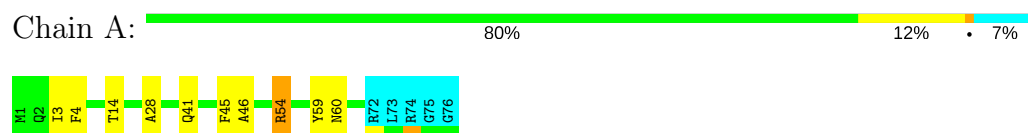
4.2.116 Score per residue for model 116

- Molecule 1: ubiquitin



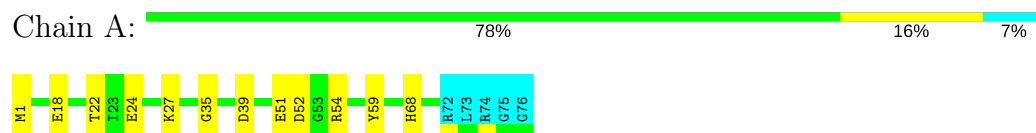
4.2.117 Score per residue for model 117

- Molecule 1: ubiquitin



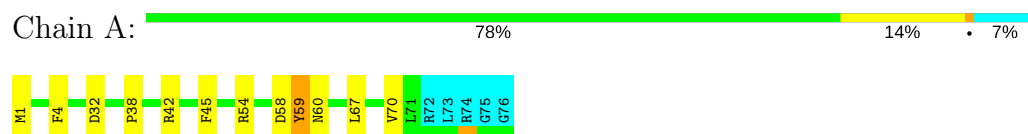
4.2.118 Score per residue for model 118

- Molecule 1: ubiquitin



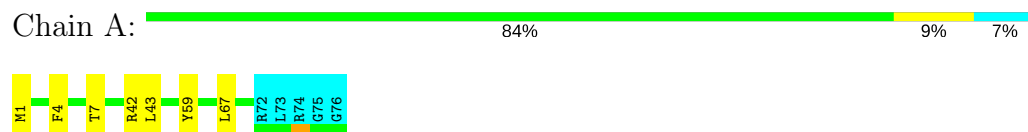
4.2.119 Score per residue for model 119

- Molecule 1: ubiquitin



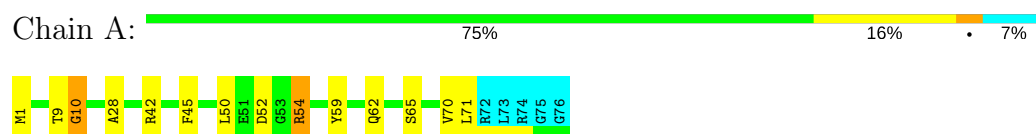
4.2.120 Score per residue for model 120

- Molecule 1: ubiquitin



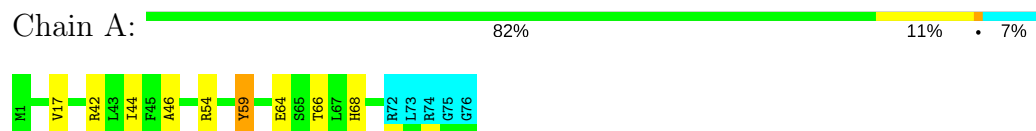
4.2.121 Score per residue for model 121

- Molecule 1: ubiquitin



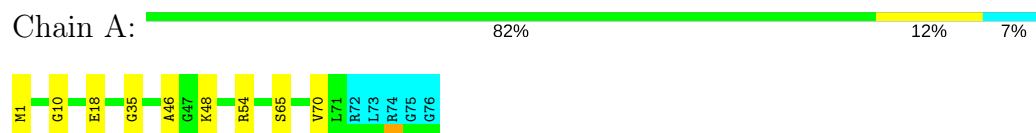
4.2.122 Score per residue for model 122

- Molecule 1: ubiquitin



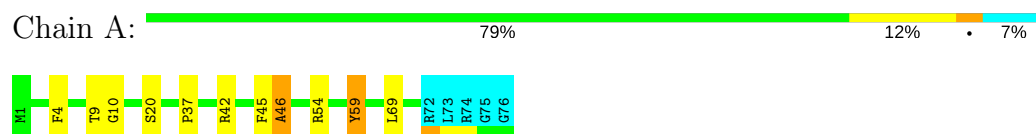
4.2.123 Score per residue for model 123

- Molecule 1: ubiquitin



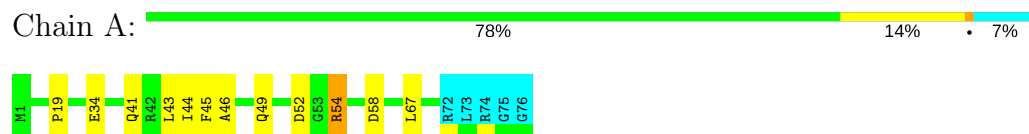
4.2.124 Score per residue for model 124

- Molecule 1: ubiquitin



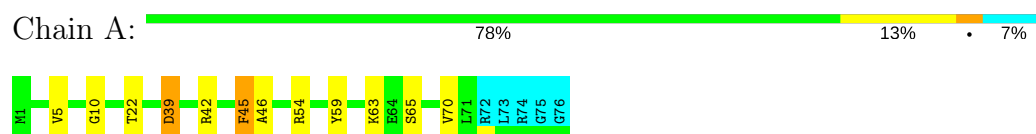
4.2.125 Score per residue for model 125

- Molecule 1: ubiquitin



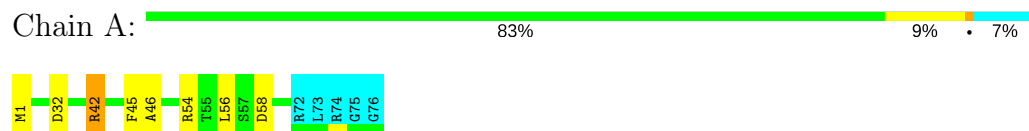
4.2.126 Score per residue for model 126

- Molecule 1: ubiquitin




4.2.127 Score per residue for model 127

- Molecule 1: ubiquitin



4.2.128 Score per residue for model 128

- Molecule 1: ubiquitin

Chain A:  83% 11% 7%



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. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.96±0.00	0±0/570 (0.0±0.0%)	1.86±0.08	10±3/770 (1.3±0.4%)
All	All	0.96	0/72960 (0.0%)	1.86	1270/98560 (1.3%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.1±0.9
All	All	0	145

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	42	ARG	NE-CZ-NH1	21.55	131.07	120.30	62	64
1	A	54	ARG	NE-CZ-NH1	18.08	129.34	120.30	88	77
1	A	54	ARG	NE-CZ-NH2	-17.95	111.32	120.30	27	53
1	A	42	ARG	NE-CZ-NH2	-17.12	111.74	120.30	92	54
1	A	4	PHE	CB-CG-CD2	-15.79	109.75	120.80	79	39
1	A	59	TYR	CB-CG-CD1	-14.84	112.09	121.00	26	39
1	A	4	PHE	CB-CG-CD1	14.21	130.74	120.80	37	30
1	A	59	TYR	CB-CG-CD2	-12.89	113.26	121.00	4	38
1	A	58	ASP	CB-CG-OD2	12.51	129.56	118.30	55	16
1	A	45	PHE	CB-CG-CD1	12.15	129.31	120.80	64	30
1	A	45	PHE	CB-CG-CD2	-11.86	112.50	120.80	127	39
1	A	21	ASP	CB-CG-OD1	11.24	128.41	118.30	90	13
1	A	1	MET	CG-SD-CE	-10.20	83.88	100.20	96	33
1	A	58	ASP	CB-CG-OD1	9.92	127.22	118.30	119	17
1	A	46	ALA	CB-CA-C	9.87	124.90	110.10	100	16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	39	ASP	CB-CG-OD1	9.46	126.81	118.30	7	21
1	A	65	SER	N-CA-CB	8.76	123.64	110.50	39	10
1	A	39	ASP	CB-CG-OD2	8.70	126.13	118.30	85	16
1	A	52	ASP	CB-CG-OD2	8.62	126.06	118.30	34	15
1	A	42	ARG	NH1-CZ-NH2	-8.44	110.11	119.40	31	13
1	A	5	VAL	CG1-CB-CG2	8.15	123.94	110.90	28	5
1	A	26	VAL	CA-CB-CG2	-8.06	98.81	110.90	67	6
1	A	32	ASP	CB-CG-OD1	8.01	125.51	118.30	48	18
1	A	59	TYR	CG-CD1-CE1	-7.99	114.91	121.30	16	8
1	A	32	ASP	CB-CG-OD2	-7.94	111.15	118.30	21	16
1	A	68	HIS	CA-CB-CG	-7.92	100.13	113.60	22	2
1	A	22	THR	CA-CB-CG2	-7.92	101.31	112.40	126	12
1	A	26	VAL	CG1-CB-CG2	-7.89	98.27	110.90	41	10
1	A	59	TYR	CG-CD2-CE2	7.86	127.59	121.30	44	7
1	A	9	THR	CA-CB-CG2	-7.82	101.45	112.40	51	14
1	A	9	THR	N-CA-CB	7.78	125.09	110.30	6	4
1	A	32	ASP	O-C-N	-7.62	110.50	122.70	101	2
1	A	56	LEU	CB-CG-CD1	7.60	123.92	111.00	74	4
1	A	28	ALA	CB-CA-C	7.59	121.48	110.10	27	4
1	A	54	ARG	NH1-CZ-NH2	-7.51	111.13	119.40	118	12
1	A	21	ASP	CB-CG-OD2	-7.50	111.55	118.30	92	14
1	A	28	ALA	N-CA-CB	-7.49	99.61	110.10	28	7
1	A	6	LYS	O-C-N	-7.48	110.74	122.70	27	3
1	A	71	LEU	CB-CG-CD1	7.45	123.67	111.00	77	2
1	A	50	LEU	CB-CG-CD1	-7.42	98.39	111.00	45	4
1	A	52	ASP	CB-CG-OD1	7.40	124.96	118.30	107	16
1	A	30	ILE	O-C-N	-7.37	110.90	122.70	4	3
1	A	38	PRO	N-CD-CG	7.27	114.11	103.20	104	2
1	A	42	ARG	CG-CD-NE	-7.20	96.67	111.80	43	7
1	A	7	THR	CA-CB-CG2	-7.13	102.42	112.40	39	6
1	A	59	TYR	CZ-CE2-CD2	-7.12	113.39	119.80	120	7
1	A	54	ARG	CG-CD-NE	-7.11	96.88	111.80	16	2
1	A	14	THR	CA-CB-CG2	7.04	122.26	112.40	69	7
1	A	55	THR	CA-CB-CG2	-6.98	102.62	112.40	15	3
1	A	70	VAL	CA-CB-CG2	-6.98	100.43	110.90	27	6
1	A	27	LYS	O-C-N	-6.95	111.59	122.70	118	1
1	A	67	LEU	CB-CG-CD1	6.90	122.73	111.00	125	4
1	A	69	LEU	CB-CG-CD2	-6.89	99.28	111.00	49	2
1	A	24	GLU	O-C-N	-6.85	111.73	122.70	118	3
1	A	69	LEU	CB-CG-CD1	6.85	122.64	111.00	26	3
1	A	56	LEU	CB-CG-CD2	6.84	122.62	111.00	21	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	66	THR	N-CA-CB	6.80	123.22	110.30	72	3
1	A	7	THR	O-C-N	-6.80	111.82	122.70	34	2
1	A	12	THR	CA-CB-CG2	-6.75	102.95	112.40	17	9
1	A	40	GLN	O-C-N	-6.75	111.90	122.70	104	2
1	A	43	LEU	CB-CG-CD1	6.74	122.45	111.00	37	2
1	A	64	GLU	OE1-CD-OE2	-6.70	115.26	123.30	85	9
1	A	46	ALA	N-CA-CB	6.63	119.39	110.10	80	7
1	A	15	LEU	CB-CG-CD1	-6.63	99.73	111.00	94	2
1	A	65	SER	CB-CA-C	-6.62	97.52	110.10	29	6
1	A	17	VAL	CG1-CB-CG2	-6.59	100.36	110.90	96	3
1	A	70	VAL	CA-CB-CG1	6.58	120.76	110.90	58	5
1	A	1	MET	CA-CB-CG	6.57	124.47	113.30	2	8
1	A	63	LYS	O-C-N	-6.57	112.19	122.70	126	2
1	A	39	ASP	N-CA-CB	-6.57	98.78	110.60	24	3
1	A	12	THR	O-C-N	-6.55	112.22	122.70	44	2
1	A	37	PRO	N-CA-CB	6.54	111.14	103.30	102	5
1	A	60	ASN	N-CA-CB	6.51	122.32	110.60	59	7
1	A	34	GLU	OE1-CD-OE2	-6.49	115.51	123.30	23	8
1	A	65	SER	O-C-N	6.47	133.05	122.70	103	1
1	A	61	ILE	O-C-N	-6.46	112.36	122.70	53	2
1	A	70	VAL	CG1-CB-CG2	-6.46	100.57	110.90	25	7
1	A	26	VAL	CA-CB-CG1	6.45	120.58	110.90	79	4
1	A	67	LEU	CB-CA-C	-6.44	97.97	110.20	50	2
1	A	8	LEU	CB-CG-CD1	6.42	121.92	111.00	82	3
1	A	19	PRO	N-CA-CB	6.41	110.99	103.30	46	4
1	A	20	SER	N-CA-CB	6.40	120.11	110.50	23	3
1	A	54	ARG	O-C-N	-6.40	112.46	122.70	109	2
1	A	71	LEU	CB-CG-CD2	-6.40	100.12	111.00	38	2
1	A	68	HIS	CB-CA-C	-6.40	97.60	110.40	118	1
1	A	60	ASN	CB-CA-C	6.39	123.19	110.40	44	1
1	A	9	THR	O-C-N	-6.38	112.35	123.20	124	2
1	A	55	THR	O-C-N	-6.33	112.57	122.70	60	3
1	A	33	LYS	O-C-N	-6.26	112.68	122.70	104	3
1	A	54	ARG	CD-NE-CZ	6.25	132.35	123.60	37	6
1	A	28	ALA	O-C-N	-6.22	112.74	122.70	79	2
1	A	58	ASP	CA-CB-CG	6.22	127.08	113.40	116	2
1	A	49	GLN	N-CA-C	6.22	127.78	111.00	6	1
1	A	58	ASP	O-C-N	-6.20	112.78	122.70	52	2
1	A	62	GLN	O-C-N	-6.19	112.80	122.70	121	3
1	A	14	THR	N-CA-CB	6.19	122.06	110.30	117	2
1	A	8	LEU	O-C-N	6.18	132.59	122.70	95	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	16	GLU	CG-CD-OE2	6.18	130.66	118.30	22	1
1	A	55	THR	N-CA-CB	6.17	122.03	110.30	49	5
1	A	64	GLU	CB-CA-C	6.15	122.70	110.40	5	2
1	A	64	GLU	O-C-N	-6.15	112.86	122.70	77	2
1	A	67	LEU	CB-CG-CD2	6.14	121.43	111.00	66	2
1	A	9	THR	CA-CB-OG1	6.13	121.88	109.00	13	1
1	A	66	THR	CA-CB-CG2	-6.12	103.84	112.40	44	5
1	A	41	GLN	CB-CA-C	-6.11	98.17	110.40	125	2
1	A	4	PHE	CG-CD2-CE2	-6.10	114.09	120.80	58	2
1	A	6	LYS	N-CA-CB	-6.09	99.64	110.60	3	2
1	A	51	GLU	OE1-CD-OE2	-6.08	116.01	123.30	18	5
1	A	1	MET	O-C-N	-6.07	112.98	122.70	42	2
1	A	5	VAL	CA-CB-CG1	6.05	119.98	110.90	36	2
1	A	56	LEU	C-N-CA	6.05	136.82	121.70	100	2
1	A	4	PHE	O-C-N	-6.05	113.02	122.70	124	3
1	A	52	ASP	N-CA-CB	-6.04	99.73	110.60	33	1
1	A	46	ALA	C-N-CA	6.03	134.97	122.30	7	1
1	A	50	LEU	CB-CG-CD2	5.99	121.19	111.00	40	1
1	A	57	SER	N-CA-CB	5.98	119.47	110.50	22	2
1	A	5	VAL	O-C-N	-5.98	113.13	122.70	103	2
1	A	44	ILE	O-C-N	-5.97	113.14	122.70	88	4
1	A	5	VAL	CA-CB-CG2	-5.97	101.94	110.90	80	4
1	A	11	LYS	N-CA-CB	-5.97	99.85	110.60	27	2
1	A	25	ASN	CB-CA-C	-5.97	98.47	110.40	43	2
1	A	57	SER	CB-CA-C	-5.97	98.77	110.10	67	3
1	A	17	VAL	CB-CA-C	-5.96	100.08	111.40	21	3
1	A	21	ASP	CB-CA-C	-5.95	98.51	110.40	85	1
1	A	14	THR	O-C-N	-5.95	113.19	122.70	83	1
1	A	58	ASP	N-CA-CB	-5.93	99.92	110.60	77	3
1	A	17	VAL	O-C-N	-5.92	113.23	122.70	50	2
1	A	16	GLU	O-C-N	-5.88	113.29	122.70	30	2
1	A	37	PRO	N-CD-CG	5.87	112.00	103.20	11	1
1	A	22	THR	N-CA-CB	5.86	121.44	110.30	26	3
1	A	42	ARG	CD-NE-CZ	5.86	131.80	123.60	5	3
1	A	51	GLU	O-C-N	-5.84	113.36	122.70	82	1
1	A	58	ASP	CB-CA-C	-5.83	98.73	110.40	19	1
1	A	16	GLU	OE1-CD-OE2	-5.83	116.31	123.30	18	6
1	A	42	ARG	N-CA-CB	-5.81	100.14	110.60	88	1
1	A	22	THR	O-C-N	-5.79	113.43	122.70	35	2
1	A	16	GLU	N-CA-CB	5.79	121.02	110.60	54	2
1	A	70	VAL	O-C-N	-5.77	113.47	122.70	123	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	51	GLU	C-N-CA	5.77	136.12	121.70	26	4
1	A	12	THR	N-CA-CB	5.76	121.25	110.30	76	5
1	A	48	LYS	N-CA-CB	5.75	120.96	110.60	59	2
1	A	15	LEU	CB-CG-CD2	-5.73	101.25	111.00	113	2
1	A	21	ASP	CA-CB-CG	-5.71	100.85	113.40	78	1
1	A	59	TYR	C-N-CA	5.69	135.94	121.70	43	2
1	A	38	PRO	N-CA-CB	5.65	110.08	103.30	9	4
1	A	18	GLU	N-CA-CB	5.65	120.77	110.60	91	5
1	A	16	GLU	CB-CA-C	5.63	121.67	110.40	30	1
1	A	3	ILE	CA-CB-CG1	5.61	121.65	111.00	60	1
1	A	32	ASP	CB-CA-C	5.61	121.61	110.40	103	1
1	A	15	LEU	CB-CA-C	-5.60	99.55	110.20	71	2
1	A	4	PHE	N-CA-CB	5.60	120.68	110.60	12	1
1	A	22	THR	CA-CB-OG1	5.60	120.75	109.00	93	1
1	A	59	TYR	CD1-CE1-CZ	5.59	124.83	119.80	51	4
1	A	4	PHE	CG-CD1-CE1	-5.58	114.66	120.80	120	2
1	A	41	GLN	CG-CD-NE2	5.58	130.09	116.70	64	1
1	A	33	LYS	N-CA-CB	-5.58	100.56	110.60	6	1
1	A	39	ASP	CA-C-O	5.57	131.79	120.10	118	1
1	A	3	ILE	N-CA-CB	5.55	123.58	110.80	117	2
1	A	35	GLY	O-C-N	5.55	131.58	122.70	118	1
1	A	59	TYR	CA-CB-CG	-5.54	102.87	113.40	66	1
1	A	45	PHE	CD1-CE1-CZ	5.54	126.74	120.10	72	4
1	A	25	ASN	CB-CG-OD1	-5.53	110.54	121.60	77	1
1	A	18	GLU	CA-C-N	5.52	132.55	117.10	34	1
1	A	8	LEU	CB-CG-CD2	-5.52	101.62	111.00	59	3
1	A	69	LEU	C-N-CA	5.50	135.46	121.70	94	1
1	A	29	LYS	O-C-N	-5.49	113.91	122.70	45	2
1	A	63	LYS	N-CA-CB	5.49	120.49	110.60	45	1
1	A	69	LEU	CB-CA-C	5.49	120.64	110.20	45	3
1	A	48	LYS	O-C-N	-5.48	113.94	122.70	87	2
1	A	15	LEU	N-CA-CB	5.47	121.34	110.40	4	2
1	A	13	ILE	N-CA-CB	5.47	123.38	110.80	15	1
1	A	56	LEU	O-C-N	-5.47	113.95	122.70	92	2
1	A	59	TYR	CB-CA-C	-5.46	99.48	110.40	4	2
1	A	45	PHE	CG-CD1-CE1	5.45	126.79	120.80	104	2
1	A	24	GLU	OE1-CD-OE2	-5.44	116.77	123.30	10	3
1	A	23	ILE	O-C-N	-5.41	114.05	122.70	40	2
1	A	67	LEU	O-C-N	-5.39	114.08	122.70	120	1
1	A	57	SER	O-C-N	-5.38	114.08	122.70	43	2
1	A	52	ASP	CB-CA-C	5.38	121.15	110.40	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	41	GLN	O-C-N	-5.37	114.11	122.70	117	1
1	A	7	THR	C-N-CA	5.37	135.11	121.70	18	1
1	A	63	LYS	CB-CA-C	-5.37	99.67	110.40	55	1
1	A	29	LYS	C-N-CA	5.36	135.10	121.70	12	1
1	A	9	THR	OG1-CB-CG2	-5.35	97.69	110.00	83	2
1	A	18	GLU	CA-CB-CG	5.35	125.18	113.40	118	1
1	A	50	LEU	N-CA-CB	5.35	121.10	110.40	33	1
1	A	39	ASP	O-C-N	-5.35	114.14	122.70	126	1
1	A	2	GLN	O-C-N	-5.35	114.14	122.70	93	2
1	A	44	ILE	CA-C-N	5.34	128.94	117.20	88	1
1	A	18	GLU	OE1-CD-OE2	-5.33	116.90	123.30	24	2
1	A	20	SER	O-C-N	-5.33	114.18	122.70	60	1
1	A	34	GLU	O-C-N	-5.32	114.15	123.20	96	2
1	A	43	LEU	CA-C-O	5.32	131.27	120.10	125	1
1	A	60	ASN	CA-CB-CG	-5.31	101.72	113.40	69	2
1	A	36	ILE	CA-CB-CG1	5.31	121.08	111.00	60	1
1	A	44	ILE	CA-CB-CG1	5.29	121.06	111.00	59	1
1	A	36	ILE	CA-C-N	5.27	131.86	117.10	26	2
1	A	47	GLY	CA-C-O	-5.27	111.11	120.60	87	1
1	A	66	THR	OG1-CB-CG2	-5.26	97.89	110.00	36	1
1	A	43	LEU	CB-CG-CD2	5.26	119.94	111.00	78	2
1	A	34	GLU	N-CA-CB	5.26	120.07	110.60	28	1
1	A	12	THR	OG1-CB-CG2	-5.26	97.91	110.00	81	1
1	A	63	LYS	C-N-CA	5.26	134.85	121.70	84	1
1	A	17	VAL	CA-CB-CG1	-5.25	103.02	110.90	86	1
1	A	45	PHE	CG-CD2-CE2	-5.25	115.03	120.80	119	1
1	A	13	ILE	O-C-N	-5.22	114.34	122.70	66	1
1	A	2	GLN	N-CA-CB	5.22	120.00	110.60	110	1
1	A	43	LEU	CB-CA-C	5.21	120.11	110.20	59	1
1	A	45	PHE	CZ-CE2-CD2	5.21	126.36	120.10	119	1
1	A	53	GLY	O-C-N	-5.21	114.37	122.70	91	1
1	A	40	GLN	N-CA-CB	-5.20	101.24	110.60	21	1
1	A	11	LYS	O-C-N	-5.20	114.38	122.70	66	1
1	A	28	ALA	CA-C-O	5.20	131.01	120.10	43	1
1	A	45	PHE	O-C-N	-5.19	114.39	122.70	114	1
1	A	7	THR	N-CA-CB	5.19	120.16	110.30	7	1
1	A	23	ILE	CA-CB-CG2	5.19	121.28	110.90	87	1
1	A	18	GLU	CB-CA-C	-5.19	100.02	110.40	47	1
1	A	10	GLY	O-C-N	-5.17	114.43	122.70	24	2
1	A	24	GLU	N-CA-CB	-5.17	101.30	110.60	97	1
1	A	27	LYS	N-CA-CB	-5.15	101.33	110.60	34	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	52	ASP	O-C-N	5.14	131.95	123.20	17	2
1	A	61	ILE	C-N-CA	5.14	134.56	121.70	48	1
1	A	27	LYS	CD-CE-NZ	-5.14	99.87	111.70	99	2
1	A	36	ILE	CA-CB-CG2	-5.14	100.62	110.90	108	1
1	A	36	ILE	N-CA-C	-5.14	97.13	111.00	28	1
1	A	43	LEU	N-CA-CB	5.12	120.64	110.40	14	1
1	A	68	HIS	N-CA-CB	5.11	119.81	110.60	66	3
1	A	66	THR	O-C-N	-5.11	114.53	122.70	45	1
1	A	32	ASP	N-CA-CB	-5.10	101.42	110.60	22	3
1	A	18	GLU	CG-CD-OE2	-5.09	108.11	118.30	62	1
1	A	3	ILE	O-C-N	-5.09	114.55	122.70	111	1
1	A	31	GLN	CA-CB-CG	5.09	124.60	113.40	41	1
1	A	17	VAL	CA-CB-CG2	-5.09	103.27	110.90	52	1
1	A	45	PHE	C-N-CA	5.08	134.39	121.70	125	1
1	A	30	ILE	CA-CB-CG2	5.07	121.03	110.90	3	1
1	A	34	GLU	CB-CA-C	-5.07	100.27	110.40	18	1
1	A	39	ASP	CA-CB-CG	-5.06	102.26	113.40	51	1
1	A	69	LEU	O-C-N	-5.06	114.61	122.70	14	2
1	A	19	PRO	N-CD-CG	5.06	110.78	103.20	30	1
1	A	49	GLN	CA-CB-CG	5.06	124.52	113.40	89	1
1	A	43	LEU	C-N-CA	5.05	134.34	121.70	39	1
1	A	36	ILE	CA-C-O	-5.05	109.49	120.10	85	1
1	A	49	GLN	CB-CA-C	-5.05	100.30	110.40	92	1
1	A	21	ASP	O-C-N	-5.04	114.63	122.70	35	1
1	A	71	LEU	O-C-N	-5.04	114.63	122.70	121	1
1	A	32	ASP	CA-CB-CG	5.04	124.49	113.40	7	1
1	A	51	GLU	N-CA-CB	5.04	119.66	110.60	25	1
1	A	48	LYS	CA-CB-CG	-5.03	102.33	113.40	72	1
1	A	34	GLU	CG-CD-OE2	-5.01	108.27	118.30	39	1
1	A	26	VAL	O-C-N	-5.01	114.68	122.70	93	1
1	A	61	ILE	CA-CB-CG1	5.01	120.52	111.00	94	1
1	A	22	THR	OG1-CB-CG2	-5.00	98.50	110.00	96	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

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Mol	Chain	Res	Type	Group	Models (Total)
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	41	GLN	Peptide	1
1	A	40	GLN	Peptide	1
1	A	15	LEU	Peptide	1
1	A	71	LEU	Peptide	1
1	A	10	GLY	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	30

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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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: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%)	15	58
All	All	8960/9728 (92%)	8231 (92%)	579 (6%)	150 (2%)	15	58

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
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

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Mol	Chain	Res	Type	Models (Total)
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%)	63	94
All	All	8320/8704 (96%)	8150 (98%)	170 (2%)	63	94

All 45 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	1	MET	25
1	A	9	THR	12
1	A	52	ASP	9
1	A	17	VAL	8
1	A	37	PRO	8
1	A	57	SER	7
1	A	31	GLN	7
1	A	63	LYS	6
1	A	21	ASP	6
1	A	48	LYS	6
1	A	70	VAL	6
1	A	38	PRO	5
1	A	65	SER	5
1	A	15	LEU	5
1	A	19	PRO	4
1	A	50	LEU	4
1	A	20	SER	3
1	A	39	ASP	3
1	A	68	HIS	3
1	A	58	ASP	3
1	A	45	PHE	3
1	A	2	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	29	LYS	2
1	A	13	ILE	2
1	A	14	THR	2
1	A	7	THR	2
1	A	60	ASN	2
1	A	49	GLN	2
1	A	8	LEU	2
1	A	56	LEU	1
1	A	32	ASP	1
1	A	69	LEU	1
1	A	62	GLN	1
1	A	42	ARG	1
1	A	24	GLU	1
1	A	4	PHE	1
1	A	71	LEU	1
1	A	3	ILE	1
1	A	36	ILE	1
1	A	67	LEU	1
1	A	12	THR	1
1	A	59	TYR	1
1	A	40	GLN	1
1	A	43	LEU	1
1	A	33	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers [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