



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 19, 2020 – 09:39 pm BST

PDB ID : 2N2K  
Title : Ensemble structure of the closed state of Lys63-linked diubiquitin in the absence of a ligand  
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Deposited on : 2015-05-10

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

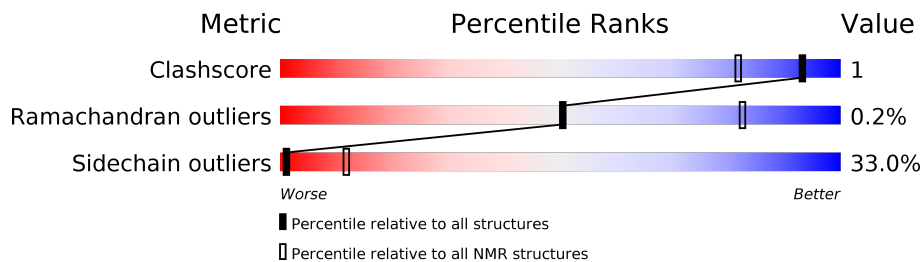
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 15%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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  $\geq 3$ , 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	B	71	

## 2 Ensemble composition and analysis i

This entry contains 70 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:72 (72)	0.09	2
2	B:1-B:71 (71)	1.12	26

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 7 clusters and 7 single-model clusters were found.

Cluster number	Models
1	2, 3, 4, 5, 8, 10, 11, 13, 14, 20, 21, 22, 30, 33, 35, 39, 43, 44, 48, 49, 50, 52, 55
2	1, 7, 9, 17, 18, 25, 28, 29, 31, 34, 36, 53, 59, 60, 63, 64
3	6, 19, 23, 24, 26, 27, 37, 47, 51, 62, 67, 70
4	16, 32, 42, 54, 56
5	40, 45, 66
6	12, 58
7	41, 57
Single-model clusters	15; 38; 46; 61; 65; 68; 69

### 3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2045 atoms, of which 445 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ubiquitin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	76	459	184	87	91	91	6	0

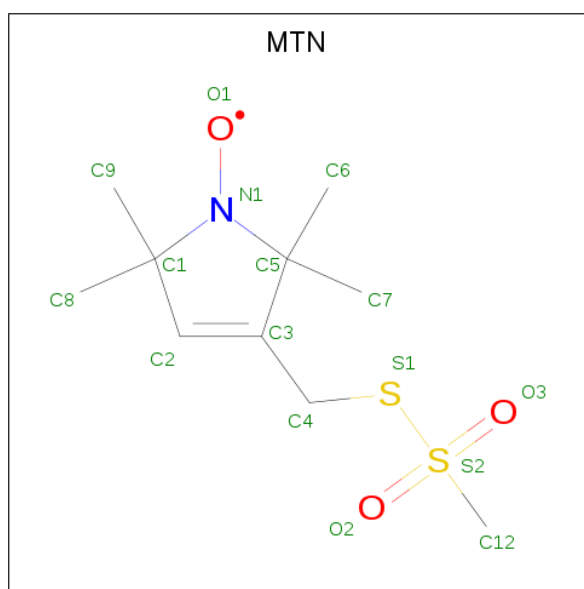
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	CYS	ASN	ENGINEERED MUTATION	UNP P0CG48
A	48	CYS	LYS	ENGINEERED MUTATION	UNP P0CG48

- Molecule 2 is a protein called ubiquitin.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	71	1424	584	268	288	284	0

- Molecule 3 is S-[(1-oxyl-2,2,5,5-tetramethyl-2,5-dihydro-1H-pyrrol-3-yl)methyl] methanesulfonothioate (three-letter code: MTN) (formula: C<sub>10</sub>H<sub>18</sub>NO<sub>3</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	S
3	A	1	81	27	45	3	3	3

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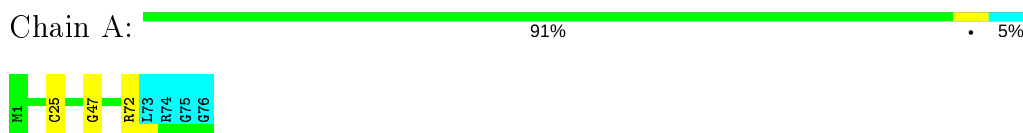
Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	S
3	A	1	81	27	45	3	3	3

## 4 Residue-property plots

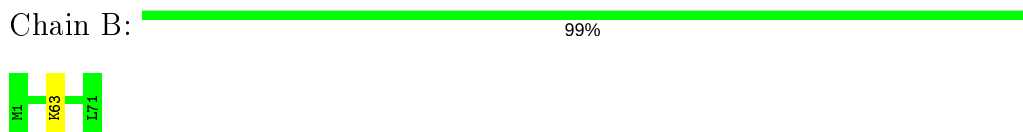
### 4.1 Average score per residue in the NMR ensemble

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



- Molecule 2: ubiquitin

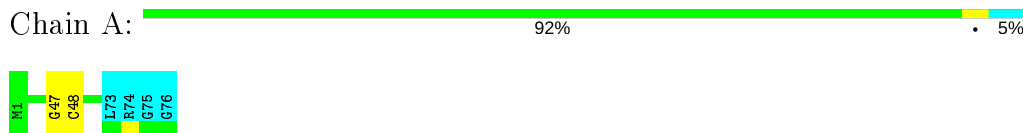


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: ubiquitin



- Molecule 2: ubiquitin



There are no outlier residues in this chain.

#### 4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: ubiquitin

Chain A:  91% • 5%



- Molecule 2: ubiquitin

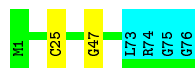
Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.3 Score per residue for model 3

- Molecule 1: ubiquitin

Chain A:  92% • 5%




- Molecule 2: ubiquitin

Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.4 Score per residue for model 4

- Molecule 1: ubiquitin

Chain A:  89% 5% 5%



- Molecule 2: ubiquitin

Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.5 Score per residue for model 5

- Molecule 1: ubiquitin

Chain A:  93% • 5%



- Molecule 2: ubiquitin

Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.6 Score per residue for model 6

- Molecule 1: ubiquitin

Chain A:  92% • 5%




- Molecule 2: ubiquitin

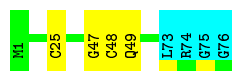
Chain B:  99%



#### 4.2.7 Score per residue for model 7

- Molecule 1: ubiquitin

Chain A:  89% 5% 5%



- Molecule 2: ubiquitin

Chain B:  100%

There are no outlier residues in this chain.



### 4.2.8 Score per residue for model 8

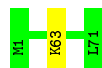
- Molecule 1: ubiquitin

Chain A:  93% • 5%



- Molecule 2: ubiquitin

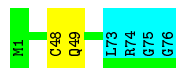
Chain B:  99% •



### 4.2.9 Score per residue for model 9

- Molecule 1: ubiquitin

Chain A:  92% • 5%




- Molecule 2: ubiquitin

Chain B:  100%

There are no outlier residues in this chain.

### 4.2.10 Score per residue for model 10

- Molecule 1: ubiquitin

Chain A:  89% • • 5%



- Molecule 2: ubiquitin

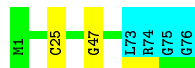
Chain B:  97% •



#### 4.2.11 Score per residue for model 11

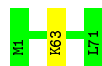
- Molecule 1: ubiquitin

Chain A:  92% 5%



- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.12 Score per residue for model 12

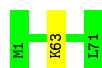
- Molecule 1: ubiquitin

Chain A:  92% 5%



- Molecule 2: ubiquitin

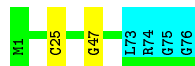
Chain B:  99%



#### 4.2.13 Score per residue for model 13

- Molecule 1: ubiquitin

Chain A:  92% 5%



- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.14 Score per residue for model 14

- Molecule 1: ubiquitin

Chain A:  93% • 5%



- Molecule 2: ubiquitin

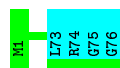
Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.15 Score per residue for model 15

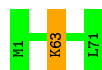
- Molecule 1: ubiquitin

Chain A:  95% 5%



- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.16 Score per residue for model 16

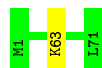
- Molecule 1: ubiquitin

Chain A:  91% • 5%



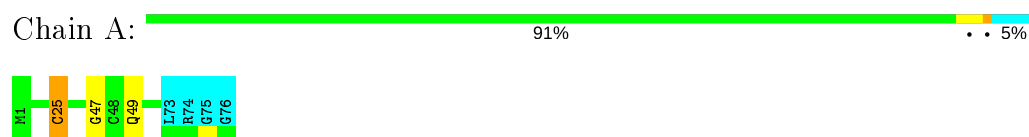
- Molecule 2: ubiquitin

Chain B:  99%

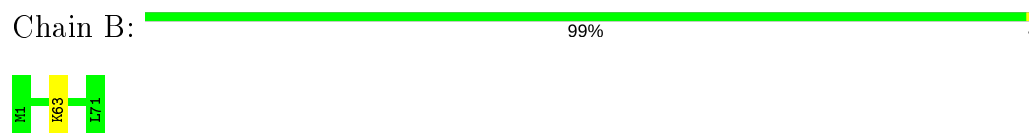


### 4.2.17 Score per residue for model 17

- Molecule 1: ubiquitin

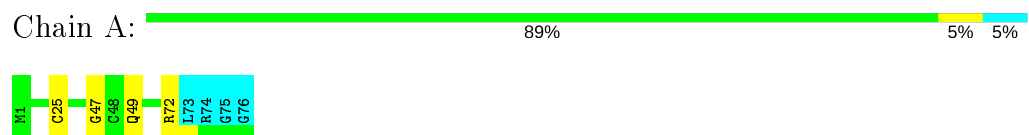


- Molecule 2: ubiquitin



### 4.2.18 Score per residue for model 18

- Molecule 1: ubiquitin



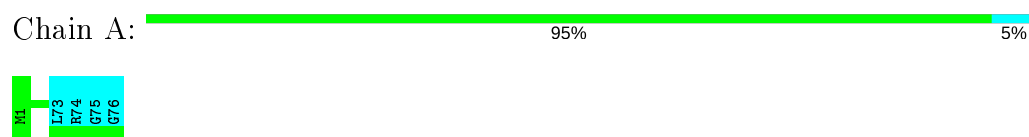
- Molecule 2: ubiquitin



There are no outlier residues in this chain.

### 4.2.19 Score per residue for model 19

- Molecule 1: ubiquitin




- Molecule 2: ubiquitin



There are no outlier residues in this chain.

#### 4.2.20 Score per residue for model 20

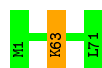
- Molecule 1: ubiquitin

Chain A:  91% • 5%



- Molecule 2: ubiquitin

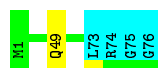
Chain B:  99% •



#### 4.2.21 Score per residue for model 21

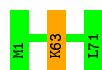
- Molecule 1: ubiquitin

Chain A:  93% • 5%



- Molecule 2: ubiquitin

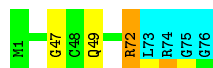
Chain B:  99% •



#### 4.2.22 Score per residue for model 22

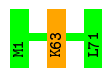
- Molecule 1: ubiquitin

Chain A:  91% • 5%



- Molecule 2: ubiquitin

Chain B:  99% •



### 4.2.23 Score per residue for model 23

- Molecule 1: ubiquitin

Chain A:  92% • 5%



- Molecule 2: ubiquitin

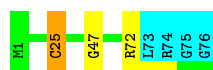
Chain B:  100%

There are no outlier residues in this chain.

### 4.2.24 Score per residue for model 24

- Molecule 1: ubiquitin

Chain A:  91% • • 5%



- Molecule 2: ubiquitin

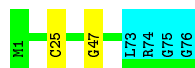
Chain B:  100%

There are no outlier residues in this chain.

### 4.2.25 Score per residue for model 25

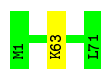
- Molecule 1: ubiquitin

Chain A:  92% • 5%



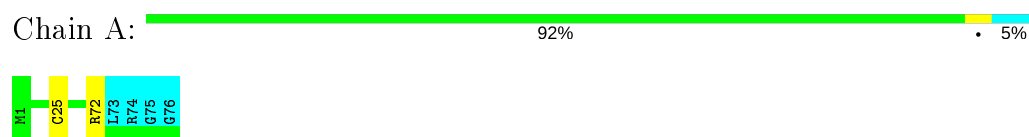
- Molecule 2: ubiquitin

Chain B:  99% •

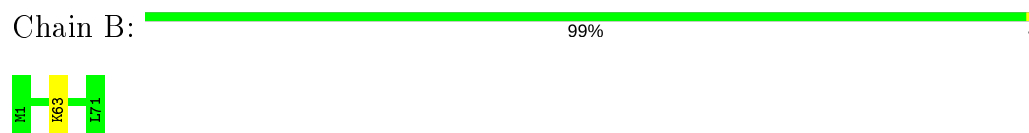


#### 4.2.26 Score per residue for model 26

- Molecule 1: ubiquitin

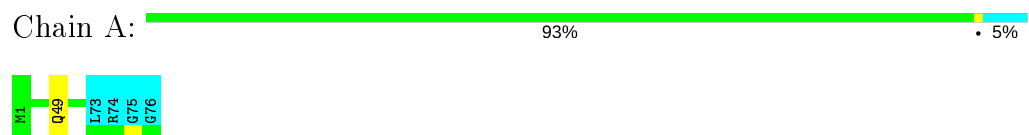


- Molecule 2: ubiquitin

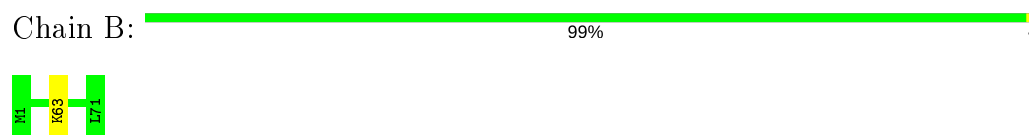


#### 4.2.27 Score per residue for model 27

- Molecule 1: ubiquitin

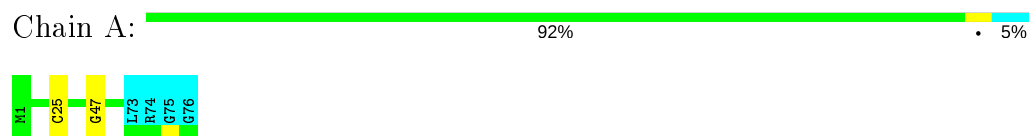


- Molecule 2: ubiquitin

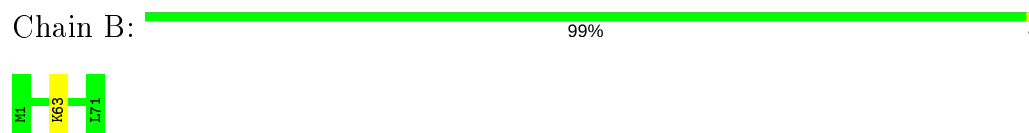


#### 4.2.28 Score per residue for model 28

- Molecule 1: ubiquitin




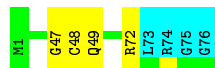
- Molecule 2: ubiquitin



#### 4.2.29 Score per residue for model 29

- Molecule 1: ubiquitin

Chain A:  89% 5% 5%



- Molecule 2: ubiquitin

Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.30 Score per residue for model 30

- Molecule 1: ubiquitin

Chain A:  92% 5%



- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.31 Score per residue for model 31

- Molecule 1: ubiquitin

Chain A:  93% 5%



- Molecule 2: ubiquitin


Chain B:  97%





#### 4.2.32 Score per residue for model 32

- Molecule 1: ubiquitin

Chain A:  89% 5% 5%



- Molecule 2: ubiquitin

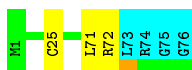
Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.33 Score per residue for model 33

- Molecule 1: ubiquitin

Chain A:  91% 5%




- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.34 Score per residue for model 34

- Molecule 1: ubiquitin

Chain A:  89% 5% 5%



- Molecule 2: ubiquitin

Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.35 Score per residue for model 35

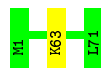
- Molecule 1: ubiquitin

Chain A:  91% 5%



- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.36 Score per residue for model 36

- Molecule 1: ubiquitin

Chain A:  89% 5% 5%



- Molecule 2: ubiquitin

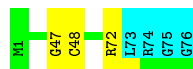
Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.37 Score per residue for model 37

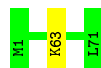
- Molecule 1: ubiquitin

Chain A:  91% 5%




- Molecule 2: ubiquitin

Chain B:  99%



### 4.2.38 Score per residue for model 38

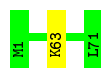
- Molecule 1: ubiquitin

Chain A:  89% 5% 5%



- Molecule 2: ubiquitin

Chain B:  99%



### 4.2.39 Score per residue for model 39

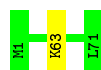
- Molecule 1: ubiquitin

Chain A:  91% 5%



- Molecule 2: ubiquitin

Chain B:  99%



### 4.2.40 Score per residue for model 40

- Molecule 1: ubiquitin

Chain A:  92% 5%



- Molecule 2: ubiquitin

Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.41 Score per residue for model 41

- Molecule 1: ubiquitin

Chain A:  91% 5%



- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.42 Score per residue for model 42

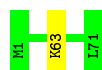
- Molecule 1: ubiquitin

Chain A:  91% 5%



- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.43 Score per residue for model 43

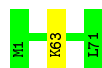
- Molecule 1: ubiquitin

Chain A:  91% 5%



- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.44 Score per residue for model 44

- Molecule 1: ubiquitin

Chain A:  92% • 5%



- Molecule 2: ubiquitin

Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.45 Score per residue for model 45

- Molecule 1: ubiquitin

Chain A:  93% • 5%



- Molecule 2: ubiquitin

Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.46 Score per residue for model 46

- Molecule 1: ubiquitin

Chain A:  95% • 5%



- Molecule 2: ubiquitin

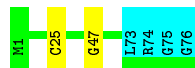
Chain B:  99% •



#### 4.2.47 Score per residue for model 47

- Molecule 1: ubiquitin

Chain A:  92% 5%




- Molecule 2: ubiquitin

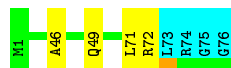
Chain B:  99%



#### 4.2.48 Score per residue for model 48

- Molecule 1: ubiquitin

Chain A:  89% 5% 5%



- Molecule 2: ubiquitin

Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.49 Score per residue for model 49

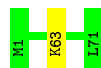
- Molecule 1: ubiquitin

Chain A:  91% 5%



- Molecule 2: ubiquitin

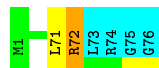
Chain B:  99%



#### 4.2.50 Score per residue for model 50

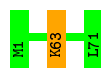
- Molecule 1: ubiquitin

Chain A:  92% .. 5%




- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.51 Score per residue for model 51

- Molecule 1: ubiquitin

Chain A:  88% 7% 5%



- Molecule 2: ubiquitin

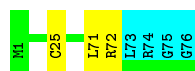
Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.52 Score per residue for model 52

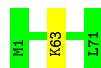
- Molecule 1: ubiquitin

Chain A:  91% • 5%



- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.53 Score per residue for model 53

- Molecule 1: ubiquitin

Chain A:  92% • 5%



- Molecule 2: ubiquitin

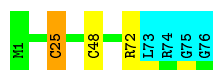
Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.54 Score per residue for model 54

- Molecule 1: ubiquitin

Chain A:  91% • • 5%



- Molecule 2: ubiquitin

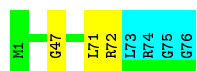
Chain B:  99% •



#### 4.2.55 Score per residue for model 55

- Molecule 1: ubiquitin

Chain A:  91% • 5%



- Molecule 2: ubiquitin


Chain B:  100%

There are no outlier residues in this chain.



#### 4.2.56 Score per residue for model 56

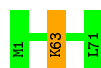
- Molecule 1: ubiquitin

Chain A:  91% 5%



- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.57 Score per residue for model 57

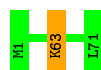
- Molecule 1: ubiquitin

Chain A:  92% 5%




- Molecule 2: ubiquitin

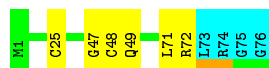
Chain B:  99%



#### 4.2.58 Score per residue for model 58

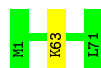
- Molecule 1: ubiquitin

Chain A:  87% 8% 5%



- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.59 Score per residue for model 59

- Molecule 1: ubiquitin

Chain A:  91% • 5%



- Molecule 2: ubiquitin

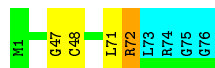
Chain B:  97% •



#### 4.2.60 Score per residue for model 60

- Molecule 1: ubiquitin

Chain A:  89% • • 5%



- Molecule 2: ubiquitin

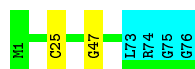
Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.61 Score per residue for model 61

- Molecule 1: ubiquitin

Chain A:  92% • 5%




- Molecule 2: ubiquitin

Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.62 Score per residue for model 62

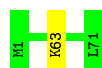
- Molecule 1: ubiquitin

Chain A:  91% 5%



- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.63 Score per residue for model 63

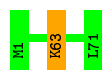
- Molecule 1: ubiquitin

Chain A:  92% 5%




- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.64 Score per residue for model 64

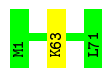
- Molecule 1: ubiquitin

Chain A:  88% 7% 5%



- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.65 Score per residue for model 65

- Molecule 1: ubiquitin

Chain A:  93% • 5%



- Molecule 2: ubiquitin

Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.66 Score per residue for model 66

- Molecule 1: ubiquitin

Chain A:  91% • • 5%




- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.67 Score per residue for model 67

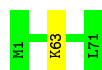
- Molecule 1: ubiquitin

Chain A:  89% • • 5%



- Molecule 2: ubiquitin

Chain B:  99%



#### 4.2.68 Score per residue for model 68

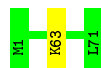
- Molecule 1: ubiquitin

Chain A:  91% • 5%



- Molecule 2: ubiquitin

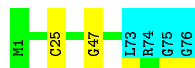
Chain B:  99% •



#### 4.2.69 Score per residue for model 69

- Molecule 1: ubiquitin

Chain A:  92% • 5%



- Molecule 2: ubiquitin

Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.70 Score per residue for model 70

- Molecule 1: ubiquitin

Chain A:  93% • 5%



- Molecule 2: ubiquitin

Chain B:  99% •



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, torsion angle dynamics*.

Of the 80 calculated structures, 70 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	270
Number of shifts mapped to atoms	270
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	15%

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

Bond lengths and bond angles in the following residue types are not validated in this section: MTN

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts i

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	116	23	92	2±1
2	B	1156	268	349	1±1
3	A	72	90	90	2±1
All	All	94080	26670	37226	166

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 1.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:GLY:O	3:A:102[X]:MTN:H73	0.65	1.91	37	3
1:A:47:GLY:O	3:A:102[Y]:MTN:H62	0.65	1.92	11	1
1:A:71:LEU:O	1:A:72[A]:ARG:O	0.64	2.16	66	3
1:A:47:GLY:O	3:A:102[Z]:MTN:H62	0.63	1.93	7	3
1:A:47:GLY:O	3:A:102[Y]:MTN:H93	0.60	1.96	10	1
1:A:71:LEU:O	1:A:72[A]:ARG:C	0.59	2.39	43	3
1:A:71:LEU:O	1:A:72[C]:ARG:C	0.59	2.39	33	8
2:B:63[D]:LYS:O	2:B:63[D]:LYS:NZ	0.57	2.37	50	1
1:A:47:GLY:O	3:A:102[Y]:MTN:H61	0.56	2.01	34	1
1:A:49:GLN:N	3:A:102[Y]:MTN:S1	0.56	2.78	35	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:63[D]:LYS:NZ	2:B:63[D]:LYS:O	0.55	2.40	66	1
1:A:25[Y]:CYS:SG	3:A:101[Y]:MTN:H2	0.54	2.42	17	6
1:A:48[Z]:CYS:SG	3:A:102[Z]:MTN:H2	0.53	2.43	67	1
3:A:101[X]:MTN:H71	3:A:101[X]:MTN:S1	0.51	2.46	61	1
1:A:47:GLY:O	3:A:102[X]:MTN:H62	0.51	2.06	59	3
1:A:71:LEU:O	1:A:72[C]:ARG:O	0.51	2.29	33	5
1:A:47:GLY:O	3:A:102[Z]:MTN:H73	0.50	2.06	13	5
1:A:47:GLY:O	3:A:102[Z]:MTN:H61	0.50	2.06	47	1
3:A:101[X]:MTN:H61	3:A:101[X]:MTN:S1	0.50	2.47	61	1
1:A:46:ALA:O	3:A:102[Z]:MTN:S1	0.50	2.70	48	1
3:A:102[X]:MTN:H71	3:A:102[X]:MTN:S1	0.50	2.47	25	1
2:B:63[D]:LYS:CE	2:B:63[D]:LYS:O	0.49	2.60	66	1
3:A:102[X]:MTN:S1	3:A:102[X]:MTN:H61	0.49	2.47	25	1
1:A:58:ASP:O	3:A:102[Y]:MTN:H81	0.49	2.07	65	1
1:A:47:GLY:O	3:A:102[X]:MTN:H61	0.49	2.07	32	1
1:A:47:GLY:O	3:A:102[Y]:MTN:S1	0.49	2.70	69	10
1:A:49:GLN:O	3:A:102[Y]:MTN:S1	0.48	2.72	35	1
1:A:71:LEU:C	1:A:72[C]:ARG:O	0.48	2.52	44	3
1:A:47:GLY:O	3:A:102[Z]:MTN:H71	0.48	2.08	47	1
1:A:47:GLY:O	3:A:102[X]:MTN:H71	0.48	2.08	32	1
1:A:47:GLY:O	3:A:102[Z]:MTN:H82	0.47	2.09	36	1
1:A:47:GLY:C	3:A:102[Y]:MTN:S1	0.47	2.93	24	13
2:B:63[B]:LYS:N	2:B:63[B]:LYS:CD	0.47	2.78	46	2
1:A:49:GLN:N	3:A:102[X]:MTN:S1	0.46	2.89	58	6
1:A:49:GLN:N	3:A:102[Z]:MTN:S1	0.46	2.89	22	5
1:A:47:GLY:C	3:A:102[X]:MTN:S1	0.46	2.95	64	4
1:A:47:GLY:C	3:A:102[Z]:MTN:S1	0.45	2.95	38	8
1:A:47:GLY:O	3:A:102[Y]:MTN:H73	0.45	2.11	22	1
2:B:63[B]:LYS:CD	2:B:63[B]:LYS:N	0.45	2.79	39	5
2:B:63[C]:LYS:CD	2:B:63[C]:LYS:N	0.45	2.80	58	2
1:A:47:GLY:O	3:A:102[X]:MTN:S1	0.45	2.74	5	2
2:B:63[D]:LYS:CD	2:B:63[D]:LYS:N	0.45	2.80	22	11
1:A:47:GLY:O	3:A:102[Z]:MTN:S1	0.45	2.74	61	5
2:B:63[A]:LYS:N	2:B:63[A]:LYS:CD	0.44	2.80	57	2
2:B:63[D]:LYS:N	2:B:63[D]:LYS:CD	0.44	2.80	41	4
2:B:63[B]:LYS:CD	2:B:63[B]:LYS:H	0.43	2.26	46	2
1:A:71:LEU:O	1:A:72[D]:ARG:C	0.43	2.56	20	1
1:A:47:GLY:O	3:A:102[X]:MTN:H82	0.43	2.14	51	1
1:A:71:LEU:C	1:A:72[A]:ARG:O	0.43	2.57	36	1
2:B:63[C]:LYS:HG2	2:B:64[C]:GLU:N	0.42	2.29	59	2
2:B:63[D]:LYS:O	2:B:63[D]:LYS:CE	0.42	2.68	50	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:63[A]:LYS:H	2:B:63[A]:LYS:HD3	0.42	1.75	20	1
2:B:63[C]:LYS:HD3	2:B:63[C]:LYS:H	0.41	1.76	67	1
2:B:63[A]:LYS:HG2	2:B:64[A]:GLU:N	0.40	2.32	31	1
1:A:47:GLY:O	3:A:102[Y]:MTN:H81	0.40	2.16	57	1
1:A:47:GLY:O	3:A:102[Z]:MTN:H93	0.40	2.16	28	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	78/76 (103%)	76±2 (98±3%)	1±2 (1±2%)	1±2 (1±2%)	20	68
2	B	276/71 (389%)	276±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	24780/10290 (241%)	24660 (100%)	64 (0%)	56 (0%)	50	82

All 4 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	72[A]	ARG	14
1	A	72[B]	ARG	14
1	A	72[C]	ARG	14
1	A	72[D]	ARG	14

### 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	6/68 (9%)	4±2 (62±32%)	2±2 (38±32%)	1	6
2	B	4/65 (6%)	3±2 (74±44%)	1±2 (26±44%)	2	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	700/9310 (8%)	469 (67%)	231 (33%)	<b>1</b> <b>12</b>

All 10 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	25[Y]	CYS	37
1	A	25[Z]	CYS	37
1	A	25[X]	CYS	37
2	B	63[C]	LYS	18
2	B	63[D]	LYS	18
2	B	63[A]	LYS	18
2	B	63[B]	LYS	18
1	A	48[Y]	CYS	16
1	A	48[X]	CYS	16
1	A	48[Z]	CYS	16

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	MTN	A	102[Z]	1	9,12,16	1.49±0.01	0±0 (0±0%)
3	MTN	A	102[X]	1	9,12,16	1.50±0.01	0±0 (0±0%)
3	MTN	A	101[Z]	1	9,12,16	1.46±0.01	0±0 (0±0%)
3	MTN	A	101[X]	1	9,12,16	1.52±0.01	0±0 (0±0%)
3	MTN	A	102[Y]	1	9,12,16	1.46±0.01	0±0 (0±0%)
3	MTN	A	101[Y]	1	9,12,16	1.49±0.01	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	MTN	A	102[Z]	1	9,20,27	1.64±0.01	0±0 (0±0%)
3	MTN	A	102[X]	1	9,20,27	1.65±0.01	0±0 (0±0%)
3	MTN	A	101[Z]	1	9,20,27	1.62±0.01	0±0 (0±0%)
3	MTN	A	101[X]	1	9,20,27	1.69±0.01	0±0 (0±0%)
3	MTN	A	102[Y]	1	9,20,27	1.64±0.01	0±0 (0±0%)
3	MTN	A	101[Y]	1	9,20,27	1.67±0.01	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MTN	A	101[Y]	1	-	0±0,0,25,29	0±0,1,1,1
3	MTN	A	102[X]	1	-	0±0,0,25,29	0±0,1,1,1
3	MTN	A	102[Y]	1	-	0±0,0,25,29	0±0,1,1,1
3	MTN	A	101[Z]	1	-	0±0,0,25,29	0±0,1,1,1
3	MTN	A	102[Z]	1	-	0±0,0,25,29	0±0,1,1,1
3	MTN	A	101[X]	1	-	0±0,0,25,29	0±0,1,1,1

There are no bond-length outliers.

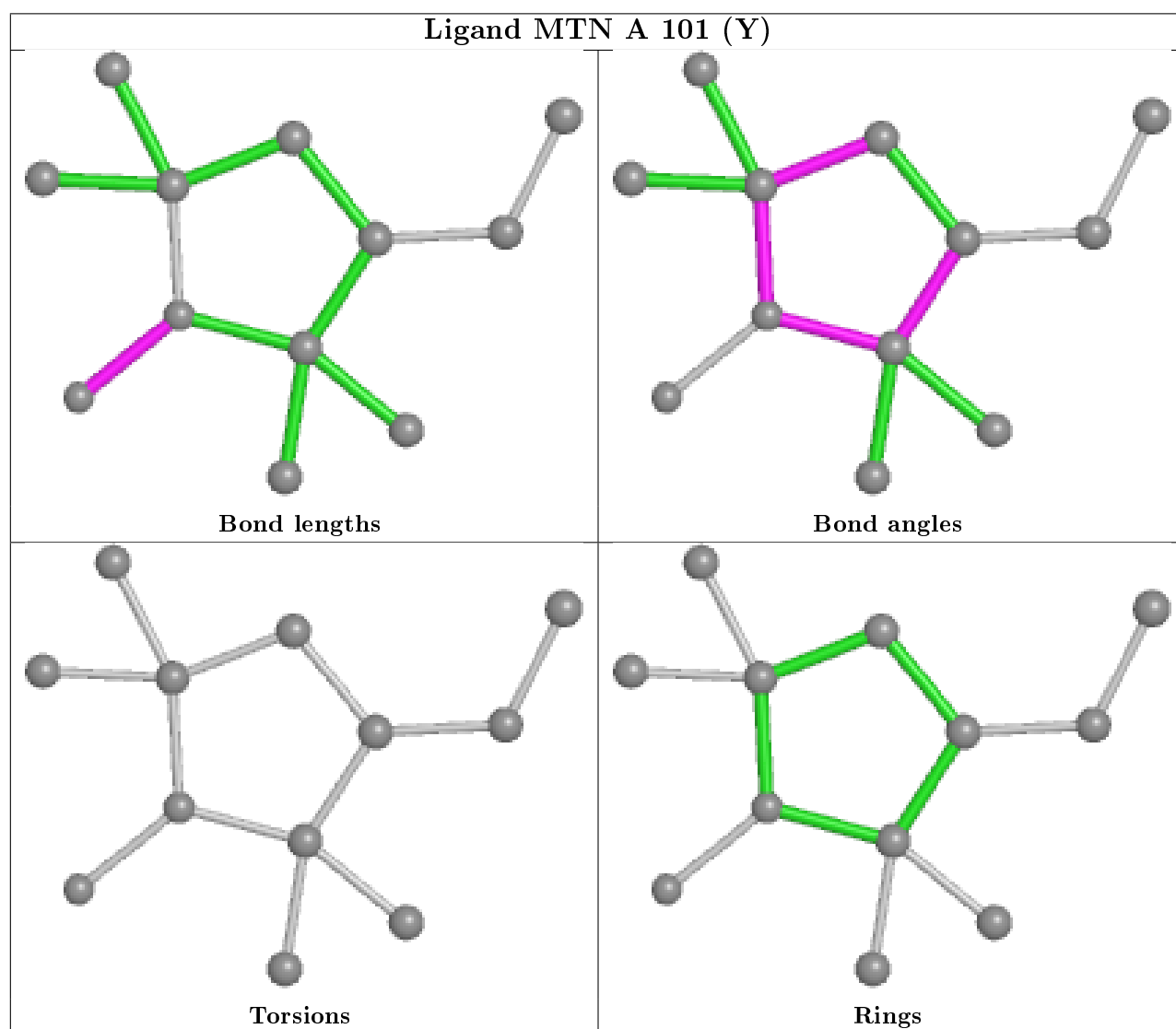
There are no bond-angle outliers.

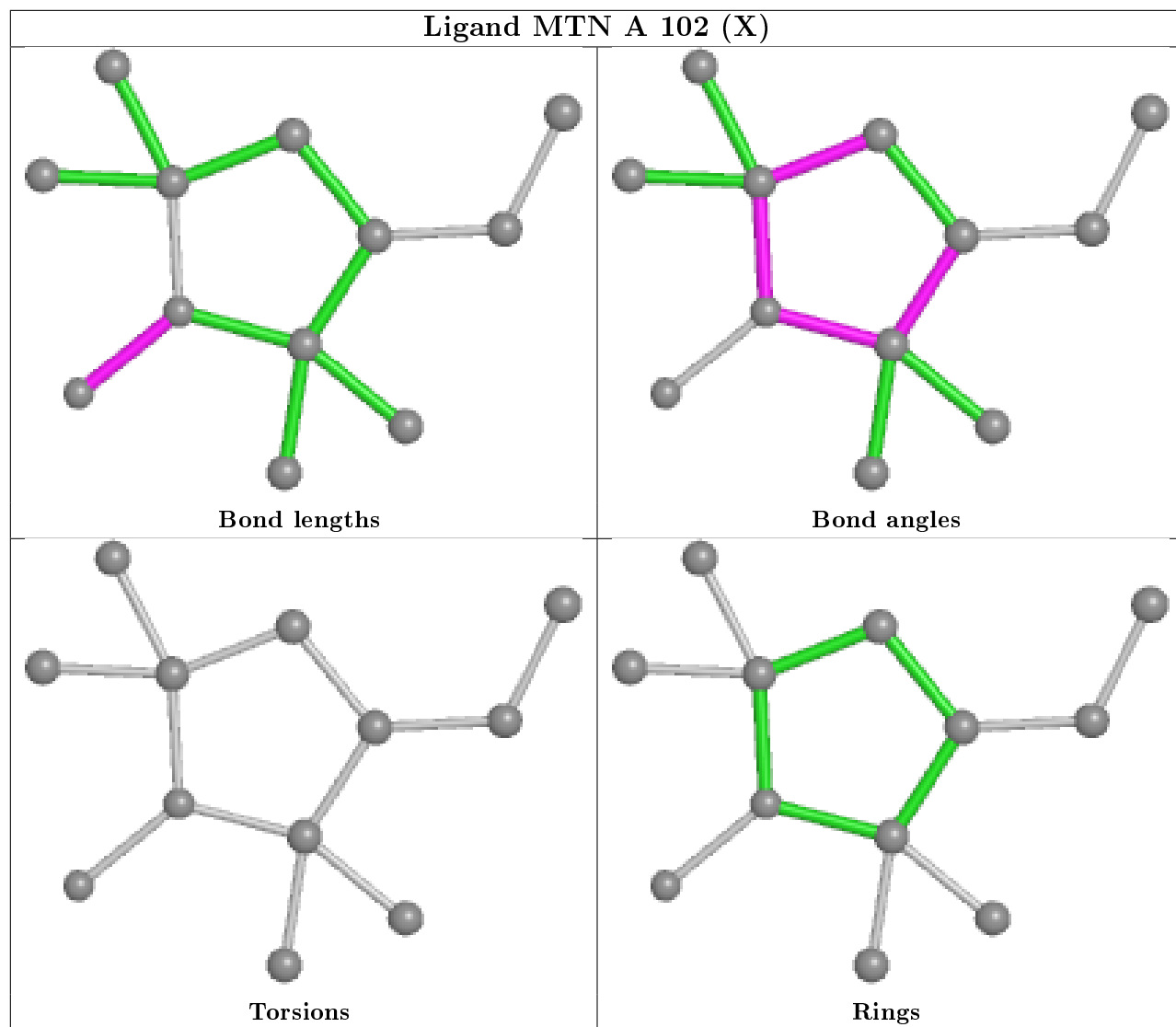
There are no chirality outliers.

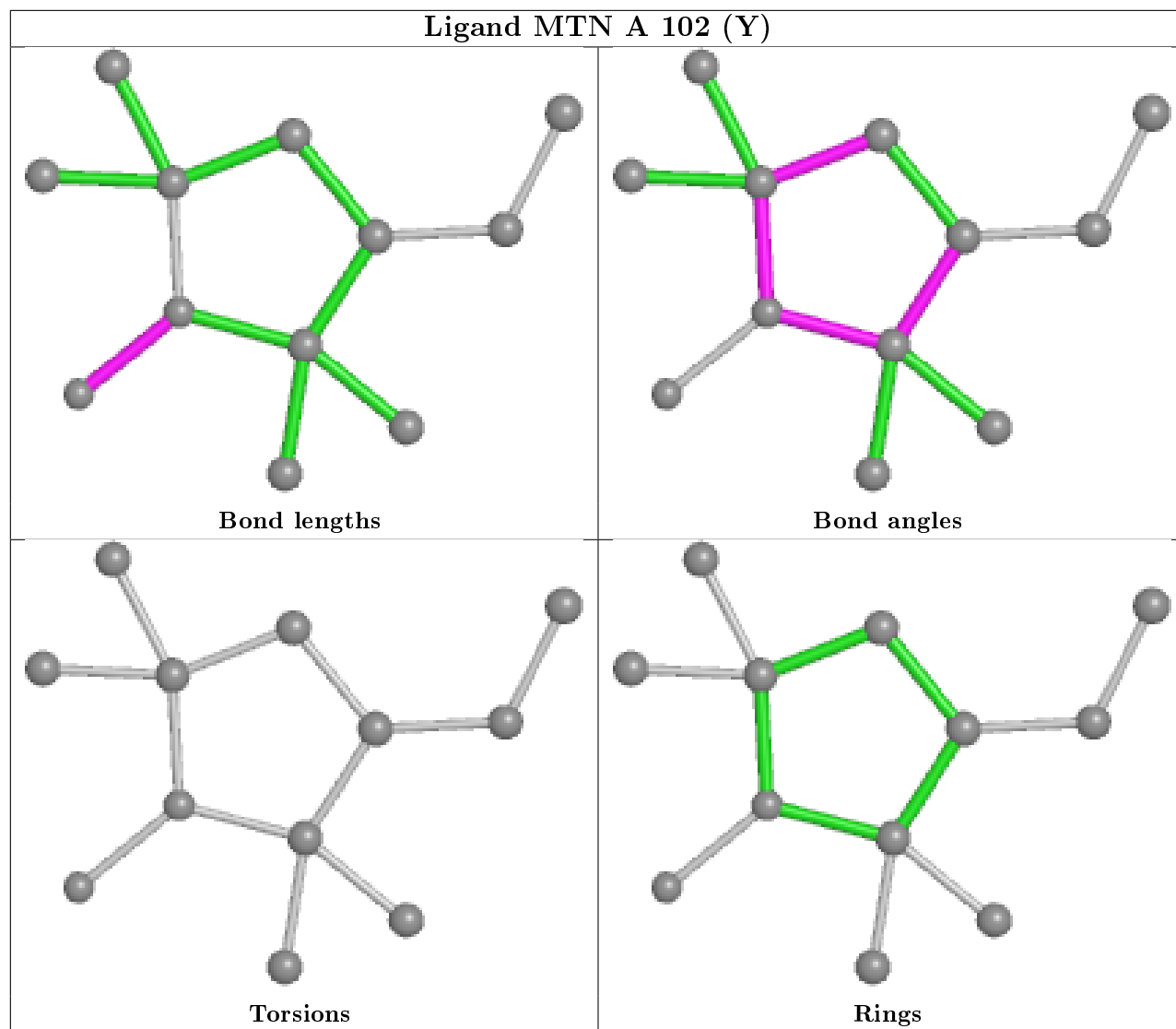
There are no torsion outliers.

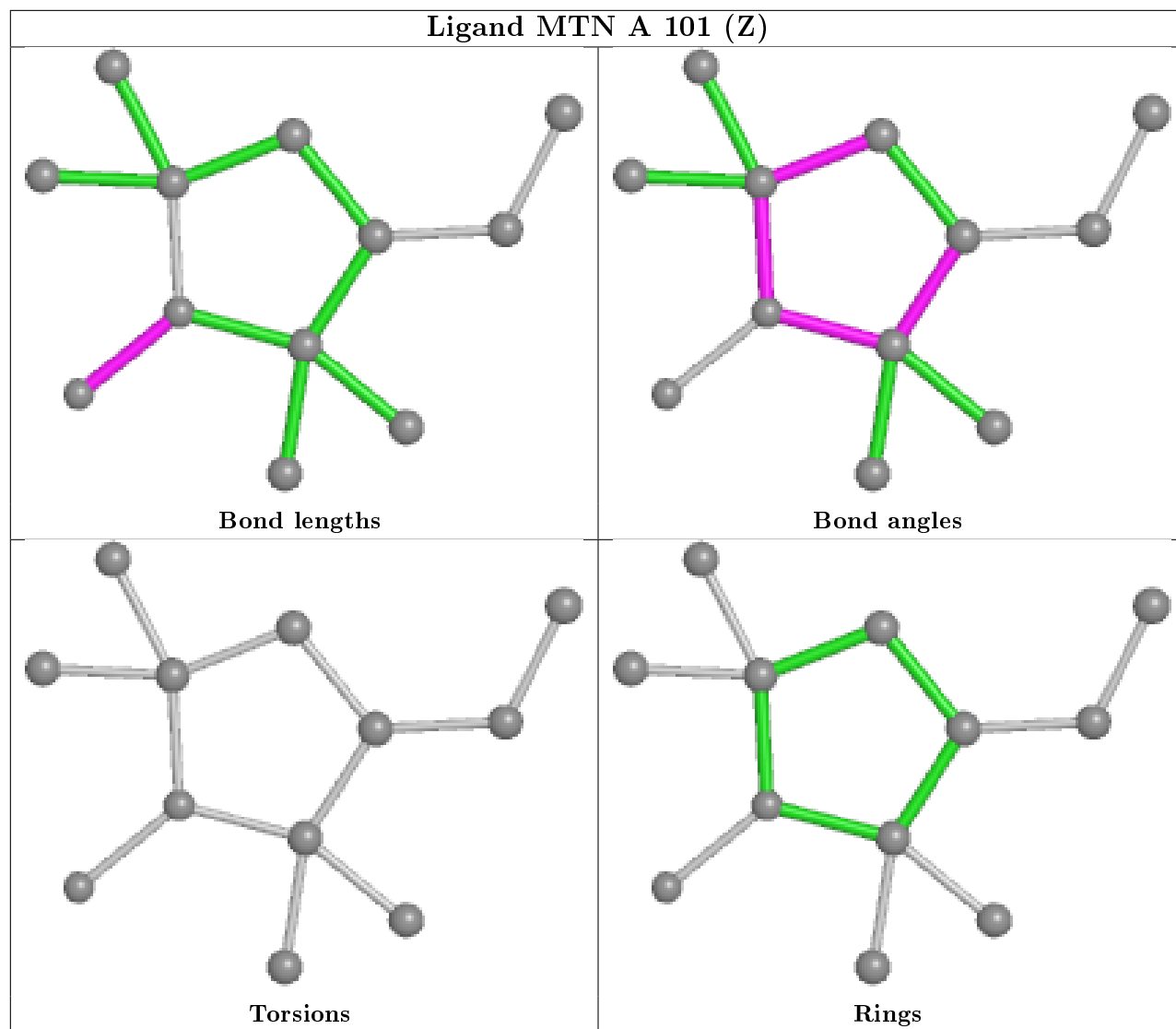
There are no ring outliers.

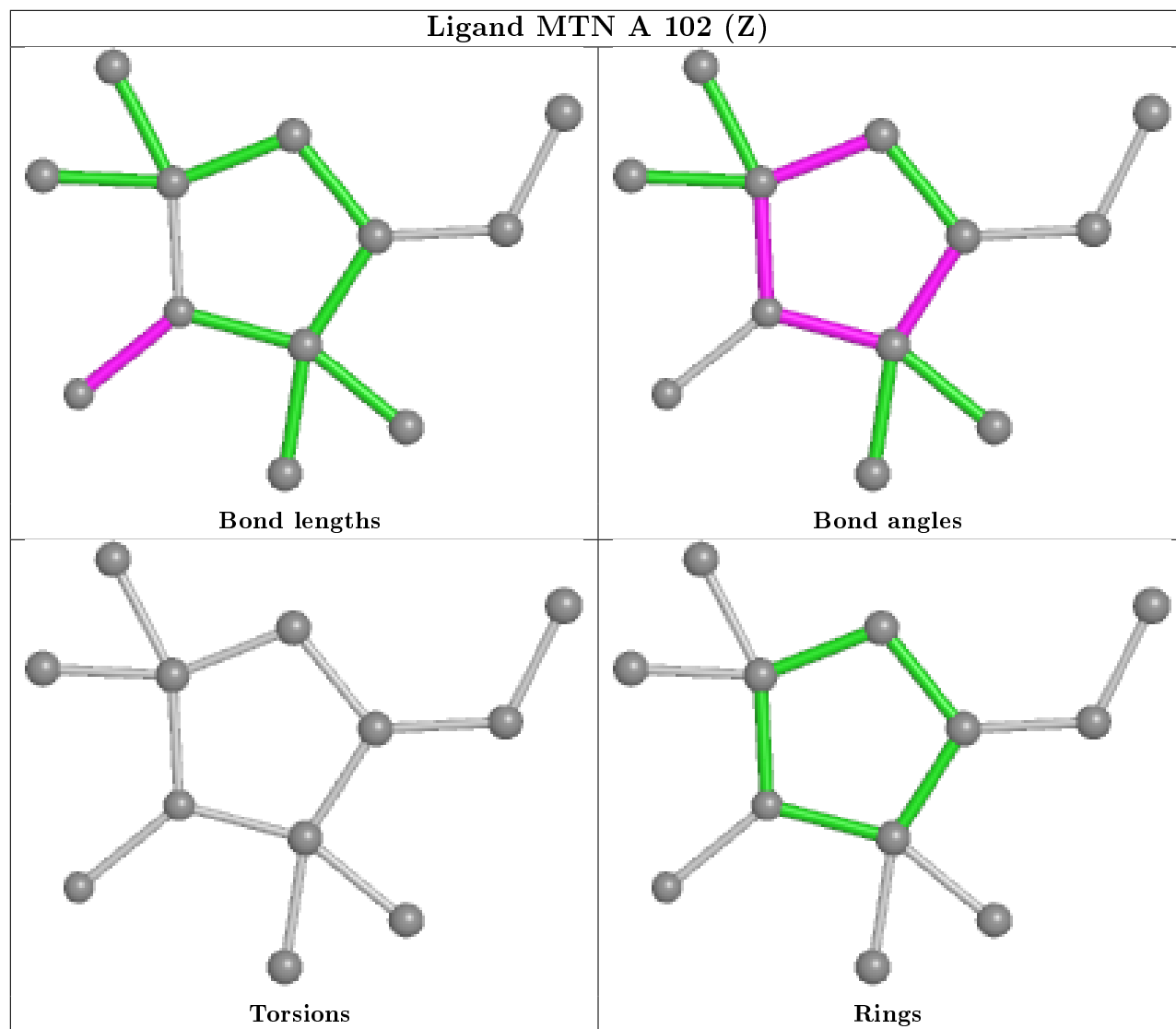
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



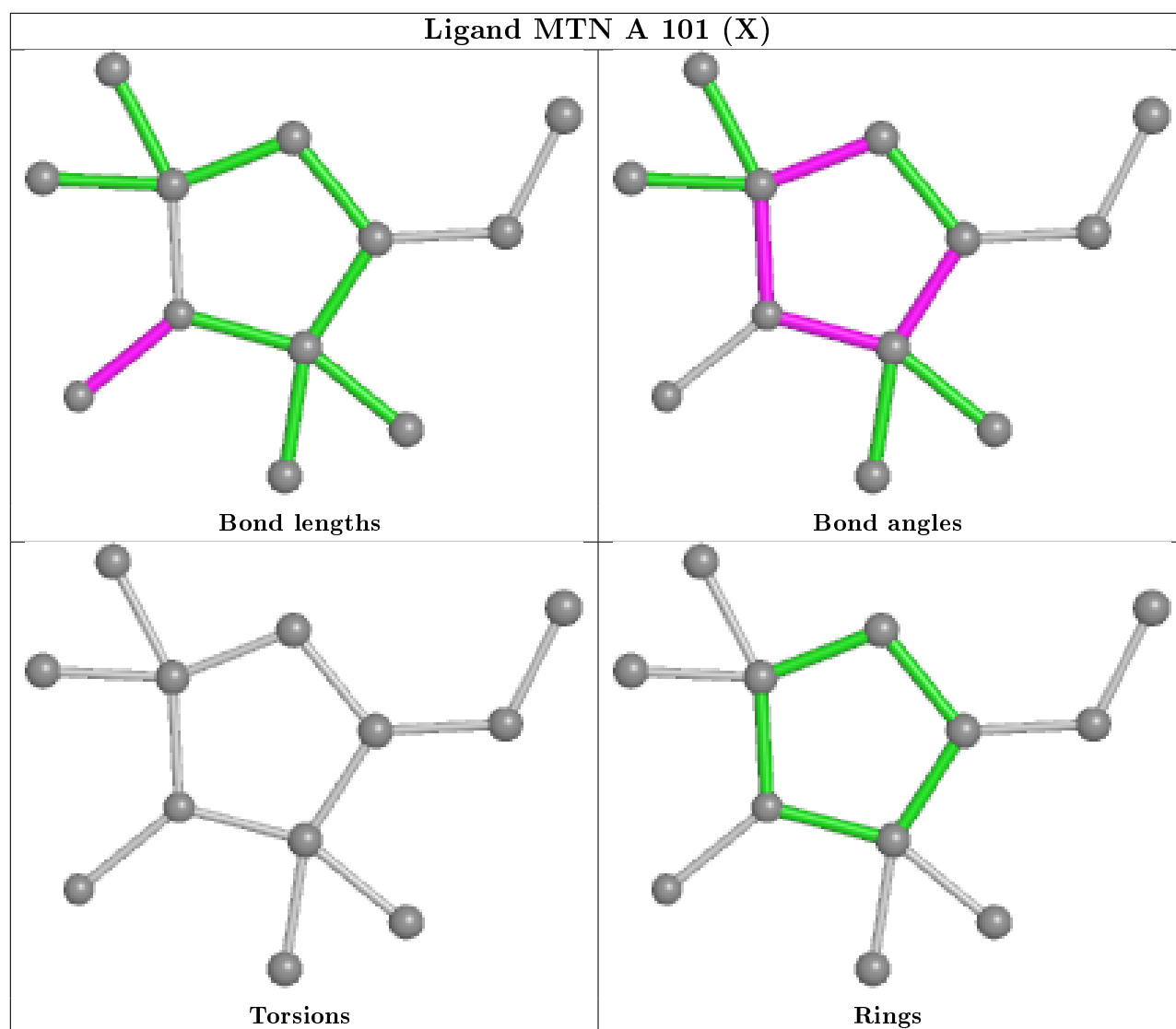












## 6.7 Other polymers [\(i\)](#)

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 i

The completeness of assignment taking into account all chemical shift lists is 15% for the well-defined parts and 15% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping i

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	270
Number of shifts mapped to atoms	270
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing i

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
<sup>13</sup> C <sub><math>\alpha</math></sub>	0	—	None (insufficient data)
<sup>13</sup> C <sub><math>\beta</math></sub>	0	—	None (insufficient data)
<sup>13</sup> C'	0	—	None (insufficient data)
<sup>15</sup> N	135	0.46 $\pm$ 0.67	None needed (< 0.5 ppm)

#### 7.1.3 Completeness of resonance assignments i

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 15%, i.e. 262 atoms were assigned a chemical shift out of a possible 1791. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	262/703 (37%)	131/280 (47%)	0/286 (0%)	131/137 (96%)
Sidechain	0/1024 (0%)	0/595 (0%)	0/386 (0%)	0/43 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/64 (0%)	0/36 (0%)	0/28 (0%)	0/0 (—%)
Overall	262/1791 (15%)	131/911 (14%)	0/700 (0%)	131/180 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 15%, i.e. 270 atoms were assigned a chemical shift out of a possible 1838. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	270/723 (37%)	135/288 (47%)	0/294 (0%)	135/141 (96%)
Sidechain	0/1051 (0%)	0/611 (0%)	0/394 (0%)	0/46 (0%)
Aromatic	0/64 (0%)	0/36 (0%)	0/28 (0%)	0/0 (—%)
Overall	270/1838 (15%)	135/935 (14%)	0/716 (0%)	135/187 (72%)

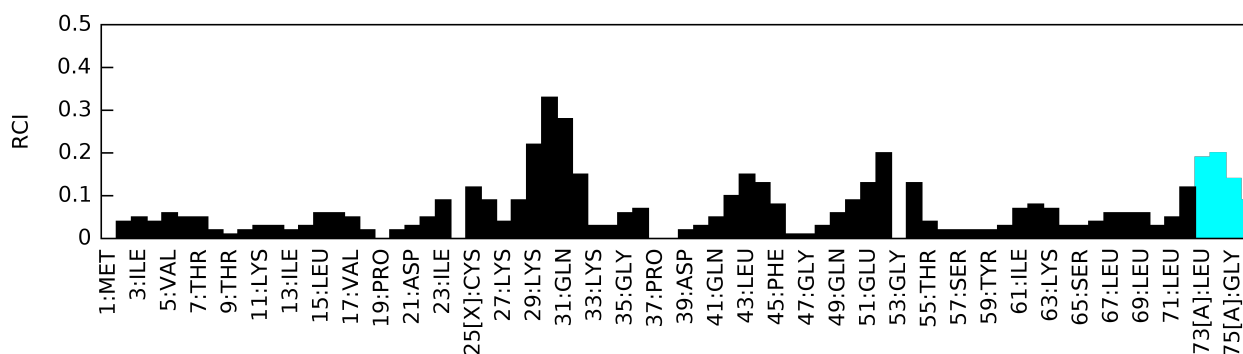
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

The images below report *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

