



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 4, 2026 – 09:09 PM UTC

PDB ID : 2KJ5 / pdb\_00002kj5  
BMRB ID : 16312  
Title : Solution NMR structure of a domain from a putative phage integrase protein Nmul\_A0064 from Nitrosospira multiformis, Northeast Structural Genomics Consortium Target NmR46C  
Authors : Mills, J.L.; Eletsky, A.; Ghosh, A.; Wang, D.; Lee, H.; Ciccocanti, C.; Jiang, M.; Nair, R.; Rost, B.; Swapna, G.V.T.; Acton, T.B.; Xiao, R.; Everett, J.K.; Prestegard, J.H.; Montelione, G.T.; Szyperski, T.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2009-05-21

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.

The types of validation reports are described at

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

---

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

MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

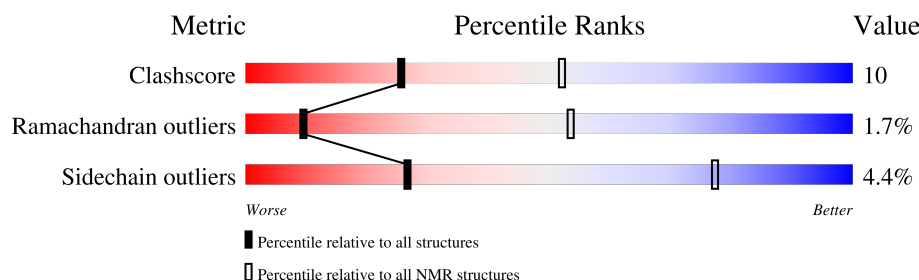
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 84%.

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<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 229148                      | 14424                     |
| Ramachandran outliers | 224038                      | 12848                     |
| Sidechain outliers    | 223484                      | 12823                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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     | 116    | <div> <div></div> <div>66%</div> <div>16%</div> <div>19%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 8 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:7-A:100 (94)        | 1.16              | 8            |

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 3 clusters and 1 single-model cluster was found.

| Cluster number        | Models                            |
|-----------------------|-----------------------------------|
| 1                     | 3, 4, 6, 7, 9, 11, 14, 17, 19, 20 |
| 2                     | 2, 8, 12, 13, 15, 16, 18          |
| 3                     | 5, 10                             |
| Single-model clusters | 1                                 |

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1897 atoms, of which 954 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Phage integrase.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 116      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1897  | 598 | 954 | 180 | 161 | 4 |       |

There are 9 discrepancies between the modelled and reference sequences:

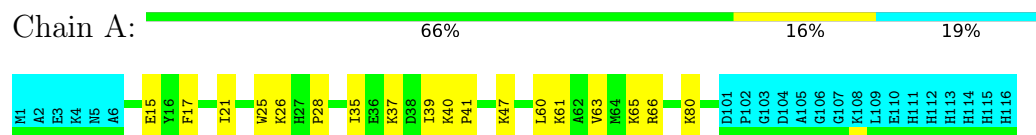
| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 1       | MET      | -      | initiating methionine | UNP Q2YCZ8 |
| A     | 109     | LEU      | -      | expression tag        | UNP Q2YCZ8 |
| A     | 110     | GLU      | -      | expression tag        | UNP Q2YCZ8 |
| A     | 111     | HIS      | -      | expression tag        | UNP Q2YCZ8 |
| A     | 112     | HIS      | -      | expression tag        | UNP Q2YCZ8 |
| A     | 113     | HIS      | -      | expression tag        | UNP Q2YCZ8 |
| A     | 114     | HIS      | -      | expression tag        | UNP Q2YCZ8 |
| A     | 115     | HIS      | -      | expression tag        | UNP Q2YCZ8 |
| A     | 116     | HIS      | -      | expression tag        | UNP Q2YCZ8 |

## 4 Residue-property plots

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

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

- Molecule 1: Phage integrase

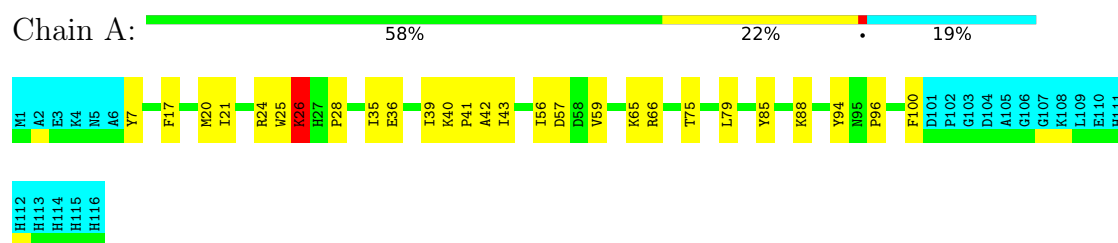


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

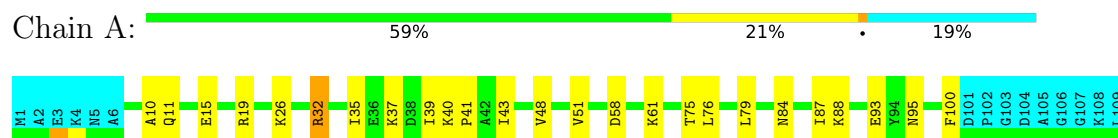
#### 4.2.1 Score per residue for model 1

- Molecule 1: Phage integrase



#### 4.2.2 Score per residue for model 2

- Molecule 1: Phage integrase



H110  
H111  
H112  
H113  
H114  
H115  
H116

### 4.2.3 Score per residue for model 3

- Molecule 1: Phage integrase

Chain A:  59% 22% 19%

M1 A2 E3 K4 N5 A6 E18 R19 M20 W25 P28 I35 I39 K40 P41 L46 K47 V48 E49 D50 D57 D58 V59 L60 K61 A62 V63 K65 R66 N73 L76 I91 F100 D101 P102 G103 D104 A105 G106 G107 K108 L109 E110 H111 H112 H113 H114 H115

H116

### 4.2.4 Score per residue for model 4

- Molecule 1: Phage integrase

Chain A:  54% 24% 19%

M1 A2 E3 K4 N5 A6 Y7 T8 Y16 R19 M20 W25 K26 H27 P28 S33 R34 K37 D38 I39 K40 P41 S45 L46 K47 D50 P53 I56 L60 K61 A62 V63 K65 R66 A72 N73 D74 T75 L76 R77 W78 L79 R89 P96 D101

P102 G103 D104 A105 G106 G107 K108 L109 H110 H111 H112 H113 H114 H115 H116

### 4.2.5 Score per residue for model 5

- Molecule 1: Phage integrase

Chain A:  62% 16% 19%

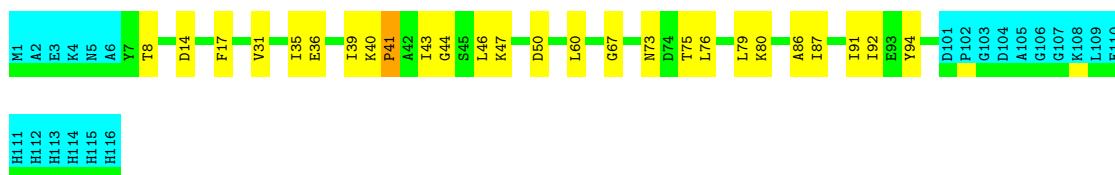
M1 A2 E3 K4 N5 A6 Y7 L12 A13 D14 F17 I21 K26 R32 S33 I35 E36 K37 D38 I39 K40 I43 L46 K47 D50 V51 K52 P53 R54 H55 K65 K80 R89 H90 I91 D101 P102 G103 D104 A105 G106 G107 K108 L109 E110 H111 H112

H113  
H114  
H115  
H116

### 4.2.6 Score per residue for model 6

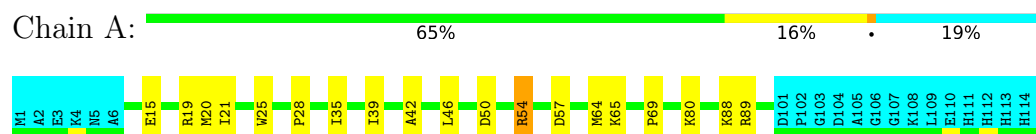
- Molecule 1: Phage integrase

Chain A:  59% 22% 19%



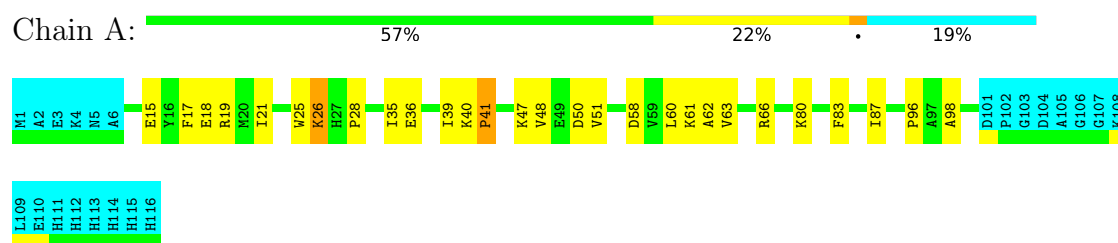
#### 4.2.7 Score per residue for model 7

- Molecule 1: Phage integrase



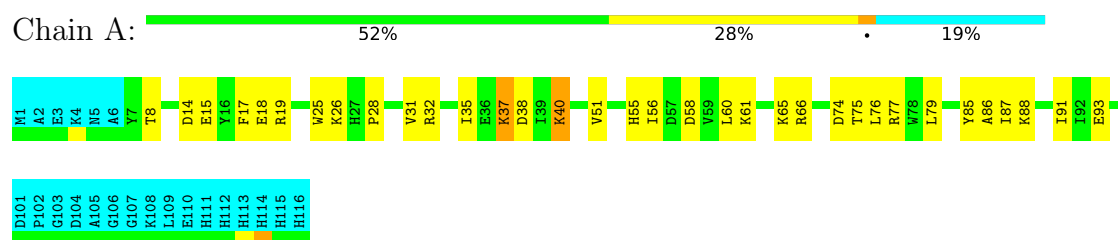
#### 4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Phage integrase



#### 4.2.9 Score per residue for model 9

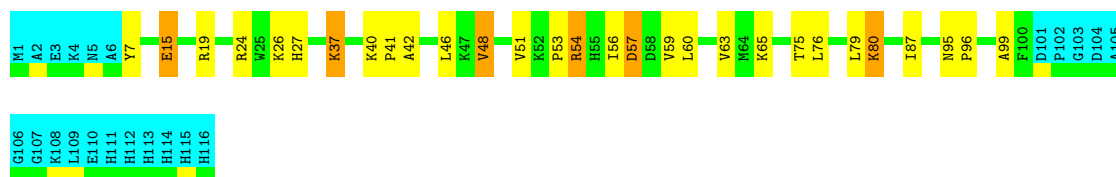
- Molecule 1: Phage integrase



#### 4.2.10 Score per residue for model 10

- Molecule 1: Phage integrase





#### 4.2.11 Score per residue for model 11

- Molecule 1: Phage integrase

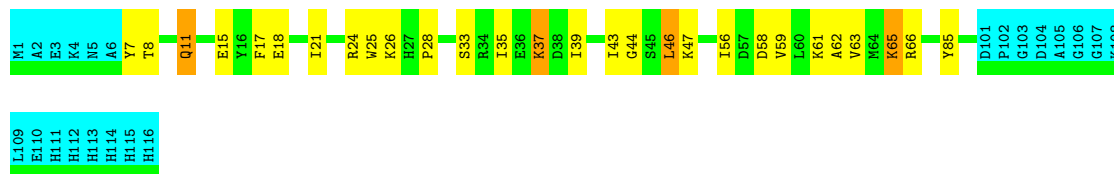
Chain A: 63% 17% 19%



#### 4.2.12 Score per residue for model 12

- Molecule 1: Phage integrase

Chain A: 57% 21% 19%



#### 4.2.13 Score per residue for model 13

- Molecule 1: Phage integrase

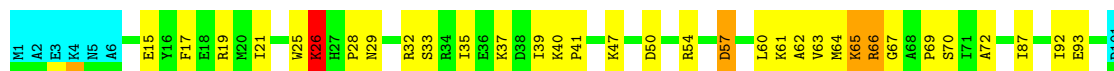
Chain A: 69% 12% 19%



#### 4.2.14 Score per residue for model 14

- Molecule 1: Phage integrase

Chain A: 53% 25% 19%



P102  
G103  
D104  
A105  
G106  
G107  
K108  
L109  
E110  
H111  
H112  
H113  
H114  
H115  
H116

#### 4.2.15 Score per residue for model 15

- Molecule 1: Phage integrase

Chain A: 49% 30% 19%

M1 A2 E3 K4 N5 A6 Y7 T8 Q11 D14 E15 Y16 F17 M20 I21 R24 W25 K26 H27 P28 V31 I35 E36 K40 K47 V51 K52 H55 D58 V59 L60 K61 A62 V63 R66 T75 L79 Y85 A86 I87 K88 R89 H90 I91 I92

A97 F100 P102 G103 D104 A105 G106 G107 K108 L109 E110 H111 H112 H113 H114 H115 H116

#### 4.2.16 Score per residue for model 16

- Molecule 1: Phage integrase

Chain A: 61% 18% 19%

M1 A2 E3 K4 N5 A6 Y7 M20 V25 K26 H27 P28 R29 I30 I32 R32 E36 K37 K40 V43 P53 D58 V59 L60 K61 A62 V63 K65 R66 T75 L79 I92 A99 F100 P102 G103 D104 A105 G106 G107 K108 L109 E110 H111 H112 H113 H114

H115 H116

#### 4.2.17 Score per residue for model 17

- Molecule 1: Phage integrase

Chain A: 60% 18% 19%

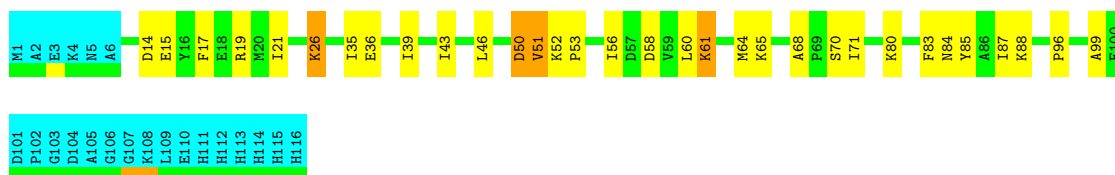
M1 A2 E3 K4 N5 A6 F17 I21 K26 S33 R34 I35 E36 K37 D38 I39 K40 P41 V43 V51 I56 V59 L60 V63 R66 W78 L79 K80 F83 I87 H90 P96 D101 P102 G103 D104 A105 G106 G107 K108 L109 E110 H111 H112

H113 H114 H115 H116

#### 4.2.18 Score per residue for model 18

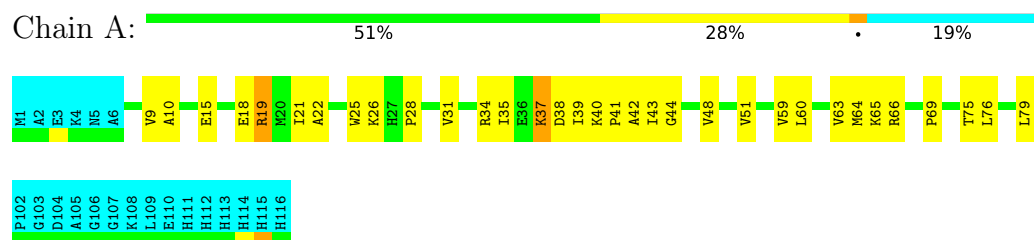
- Molecule 1: Phage integrase

Chain A: 53% 24% 19%



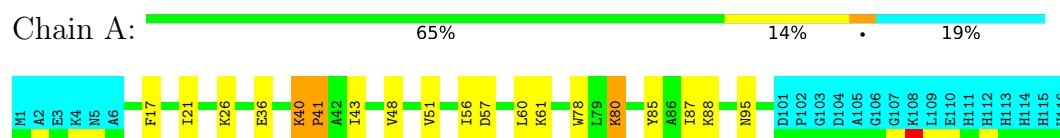
#### 4.2.19 Score per residue for model 19

- Molecule 1: Phage integrase



#### 4.2.20 Score per residue for model 20

- Molecule 1: Phage integrase



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| TALOS         | geometry optimization |         |
| CYANA         | structure solution    |         |
| CYANA         | refinement            |         |
| CNS           | structure solution    |         |
| CNS           | refinement            |         |
| MOLMOL        | refinement            |         |
| MOLMOL        | structure solution    |         |
| AutoStructure | structure solution    |         |
| AutoStructure | refinement            |         |
| PSVS          | 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)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1346           |
| Number of shifts mapped to atoms             | 1346           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 84%            |

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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     | 773   | 801      | 798      | 16±5    |
| All | All   | 15460 | 16020    | 15960    | 325     |

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 10.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:58:ASP:HA   | 1:A:61:LYS:HE2  | 0.98     | 1.30        | 8      | 4     |
| 1:A:58:ASP:HA   | 1:A:61:LYS:HD2  | 0.93     | 1.39        | 18     | 1     |
| 1:A:17:PHE:HA   | 1:A:21:ILE:HD13 | 0.93     | 1.41        | 17     | 5     |
| 1:A:47:LYS:HG2  | 1:A:49:GLU:HG2  | 0.88     | 1.45        | 3      | 1     |
| 1:A:26:LYS:HE3  | 1:A:26:LYS:HA   | 0.86     | 1.47        | 1      | 3     |
| 1:A:58:ASP:HA   | 1:A:61:LYS:HD3  | 0.85     | 1.47        | 12     | 1     |
| 1:A:47:LYS:HB2  | 1:A:50:ASP:HB2  | 0.80     | 1.50        | 11     | 2     |
| 1:A:26:LYS:HA   | 1:A:26:LYS:HE3  | 0.79     | 1.55        | 17     | 1     |
| 1:A:8:THR:HA    | 1:A:47:LYS:HA   | 0.78     | 1.51        | 15     | 4     |
| 1:A:17:PHE:HB2  | 1:A:21:ILE:HD12 | 0.77     | 1.56        | 15     | 3     |
| 1:A:87:ILE:HG13 | 1:A:93:GLU:HA   | 0.76     | 1.57        | 9      | 1     |
| 1:A:37:LYS:HE3  | 1:A:66:ARG:HD2  | 0.76     | 1.57        | 17     | 1     |
| 1:A:35:ILE:HG22 | 1:A:40:LYS:HD2  | 0.74     | 1.57        | 15     | 1     |
| 1:A:85:TYR:HA   | 1:A:88:LYS:HD3  | 0.72     | 1.61        | 15     | 3     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:36:GLU:HA   | 1:A:40:LYS:HD3  | 0.71     | 1.62        | 1      | 1     |
| 1:A:87:ILE:HD11 | 1:A:95:ASN:HB2  | 0.71     | 1.62        | 10     | 3     |
| 1:A:41:PRO:HG2  | 1:A:59:VAL:HB   | 0.70     | 1.63        | 10     | 1     |
| 1:A:20:MET:HE2  | 1:A:20:MET:HA   | 0.69     | 1.61        | 15     | 5     |
| 1:A:25:TRP:CD1  | 1:A:28:PRO:HG3  | 0.69     | 2.23        | 7      | 3     |
| 1:A:41:PRO:HB3  | 1:A:59:VAL:HB   | 0.66     | 1.67        | 19     | 1     |
| 1:A:25:TRP:HE1  | 1:A:28:PRO:HG3  | 0.66     | 1.50        | 9      | 6     |
| 1:A:64:MET:HG2  | 1:A:69:PRO:HA   | 0.65     | 1.68        | 14     | 4     |
| 1:A:35:ILE:HG23 | 1:A:39:ILE:HD12 | 0.65     | 1.69        | 18     | 2     |
| 1:A:20:MET:HA   | 1:A:20:MET:HE3  | 0.64     | 1.67        | 1      | 1     |
| 1:A:17:PHE:O    | 1:A:21:ILE:HB   | 0.63     | 1.93        | 1      | 4     |
| 1:A:41:PRO:HG3  | 1:A:59:VAL:HG23 | 0.63     | 1.68        | 17     | 1     |
| 1:A:36:GLU:HA   | 1:A:40:LYS:HG3  | 0.62     | 1.69        | 8      | 2     |
| 1:A:26:LYS:HE2  | 1:A:26:LYS:HA   | 0.62     | 1.69        | 18     | 3     |
| 1:A:35:ILE:HA   | 1:A:39:ILE:HD13 | 0.62     | 1.71        | 8      | 1     |
| 1:A:35:ILE:HG12 | 1:A:39:ILE:HD12 | 0.61     | 1.70        | 3      | 1     |
| 1:A:53:PRO:HB3  | 1:A:99:ALA:HB2  | 0.61     | 1.72        | 18     | 3     |
| 1:A:27:HIS:HB2  | 1:A:30:ILE:HB   | 0.61     | 1.71        | 11     | 1     |
| 1:A:37:LYS:HA   | 1:A:37:LYS:HE3  | 0.61     | 1.71        | 9      | 1     |
| 1:A:46:LEU:O    | 1:A:50:ASP:HB2  | 0.60     | 1.97        | 5      | 2     |
| 1:A:60:LEU:HD11 | 1:A:76:LEU:HD21 | 0.60     | 1.73        | 9      | 3     |
| 1:A:35:ILE:O    | 1:A:40:LYS:HG2  | 0.59     | 1.96        | 6      | 1     |
| 1:A:46:LEU:HB2  | 1:A:50:ASP:HB2  | 0.59     | 1.74        | 7      | 1     |
| 1:A:54:ARG:O    | 1:A:54:ARG:HD3  | 0.59     | 1.98        | 7      | 1     |
| 1:A:74:ASP:O    | 1:A:77:ARG:HG2  | 0.58     | 1.98        | 4      | 2     |
| 1:A:76:LEU:O    | 1:A:80:LYS:HD2  | 0.58     | 1.97        | 19     | 1     |
| 1:A:87:ILE:HA   | 1:A:92:ILE:O    | 0.58     | 1.97        | 14     | 3     |
| 1:A:36:GLU:HA   | 1:A:40:LYS:HE2  | 0.58     | 1.74        | 5      | 1     |
| 1:A:15:GLU:O    | 1:A:19:ARG:HD3  | 0.57     | 1.99        | 14     | 1     |
| 1:A:80:LYS:HG2  | 1:A:95:ASN:HD21 | 0.56     | 1.60        | 11     | 1     |
| 1:A:48:VAL:O    | 1:A:51:VAL:HG12 | 0.56     | 2.00        | 10     | 6     |
| 1:A:53:PRO:HG3  | 1:A:96:PRO:HA   | 0.56     | 1.77        | 4      | 1     |
| 1:A:75:THR:O    | 1:A:79:LEU:HG   | 0.56     | 2.01        | 6      | 8     |
| 1:A:89:ARG:HD3  | 1:A:91:ILE:HD11 | 0.56     | 1.78        | 5      | 1     |
| 1:A:39:ILE:HG23 | 1:A:79:LEU:HD21 | 0.55     | 1.77        | 4      | 1     |
| 1:A:65:LYS:HE2  | 1:A:65:LYS:HA   | 0.55     | 1.78        | 5      | 1     |
| 1:A:35:ILE:O    | 1:A:39:ILE:HB   | 0.54     | 2.02        | 19     | 4     |
| 1:A:97:ALA:HA   | 1:A:100:PHE:HD2 | 0.54     | 1.62        | 15     | 1     |
| 1:A:36:GLU:HA   | 1:A:40:LYS:CG   | 0.54     | 2.32        | 8      | 2     |
| 1:A:7:TYR:CE1   | 1:A:12:LEU:HA   | 0.54     | 2.38        | 5      | 1     |
| 1:A:14:ASP:HA   | 1:A:17:PHE:CD1  | 0.54     | 2.37        | 9      | 3     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:65:LYS:HD2  | 1:A:65:LYS:C    | 0.54     | 2.28        | 19     | 4     |
| 1:A:8:THR:HB    | 1:A:45:SER:HA   | 0.54     | 1.78        | 4      | 1     |
| 1:A:52:LYS:H    | 1:A:52:LYS:HD2  | 0.54     | 1.63        | 11     | 1     |
| 1:A:48:VAL:HG12 | 1:A:92:ILE:HD13 | 0.54     | 1.80        | 19     | 2     |
| 1:A:10:ALA:HA   | 1:A:40:LYS:CD   | 0.53     | 2.34        | 2      | 1     |
| 1:A:32:ARG:HE   | 1:A:36:GLU:CD   | 0.53     | 2.11        | 16     | 1     |
| 1:A:68:ALA:HB3  | 1:A:71:ILE:HD13 | 0.53     | 1.80        | 18     | 1     |
| 1:A:51:VAL:HG22 | 1:A:96:PRO:HG3  | 0.53     | 1.79        | 17     | 2     |
| 1:A:24:ARG:O    | 1:A:24:ARG:HD2  | 0.53     | 2.03        | 10     | 1     |
| 1:A:26:LYS:HA   | 1:A:26:LYS:CE   | 0.53     | 2.32        | 8      | 5     |
| 1:A:62:ALA:O    | 1:A:65:LYS:HG3  | 0.53     | 2.03        | 11     | 3     |
| 1:A:35:ILE:HA   | 1:A:39:ILE:CG1  | 0.53     | 2.33        | 19     | 2     |
| 1:A:15:GLU:O    | 1:A:19:ARG:HG2  | 0.52     | 2.04        | 10     | 6     |
| 1:A:21:ILE:HG23 | 1:A:25:TRP:HB2  | 0.52     | 1.81        | 7      | 1     |
| 1:A:54:ARG:HA   | 1:A:57:ASP:OD2  | 0.52     | 2.03        | 14     | 2     |
| 1:A:33:SER:O    | 1:A:37:LYS:HG3  | 0.52     | 2.04        | 12     | 1     |
| 1:A:61:LYS:O    | 1:A:64:MET:HG2  | 0.52     | 2.04        | 3      | 1     |
| 1:A:92:ILE:HG12 | 1:A:94:TYR:H    | 0.52     | 1.64        | 6      | 1     |
| 1:A:29:ASN:HA   | 1:A:32:ARG:HB2  | 0.52     | 1.82        | 14     | 1     |
| 1:A:39:ILE:O    | 1:A:41:PRO:HD3  | 0.51     | 2.05        | 1      | 3     |
| 1:A:25:TRP:HE1  | 1:A:28:PRO:HB3  | 0.51     | 1.65        | 12     | 3     |
| 1:A:76:LEU:HG   | 1:A:100:PHE:HD2 | 0.51     | 1.65        | 2      | 1     |
| 1:A:60:LEU:HA   | 1:A:63:VAL:HG22 | 0.51     | 1.82        | 19     | 10    |
| 1:A:60:LEU:HD22 | 1:A:72:ALA:HB1  | 0.51     | 1.82        | 4      | 1     |
| 1:A:37:LYS:HD2  | 1:A:37:LYS:C    | 0.51     | 2.31        | 19     | 3     |
| 1:A:54:ARG:HA   | 1:A:57:ASP:HB3  | 0.51     | 1.82        | 7      | 1     |
| 1:A:21:ILE:HG21 | 1:A:31:VAL:HG21 | 0.51     | 1.82        | 13     | 1     |
| 1:A:56:ILE:O    | 1:A:59:VAL:HG22 | 0.51     | 2.05        | 12     | 1     |
| 1:A:34:ARG:O    | 1:A:38:ASP:HB2  | 0.51     | 2.05        | 17     | 1     |
| 1:A:87:ILE:HA   | 1:A:93:GLU:HA   | 0.51     | 1.82        | 2      | 1     |
| 1:A:53:PRO:HB3  | 1:A:99:ALA:CB   | 0.51     | 2.36        | 18     | 1     |
| 1:A:41:PRO:HA   | 1:A:66:ARG:HH22 | 0.50     | 1.65        | 1      | 1     |
| 1:A:80:LYS:HA   | 1:A:80:LYS:HE3  | 0.50     | 1.83        | 5      | 2     |
| 1:A:10:ALA:HA   | 1:A:40:LYS:HE2  | 0.50     | 1.83        | 19     | 1     |
| 1:A:61:LYS:O    | 1:A:65:LYS:HG3  | 0.50     | 2.06        | 3      | 1     |
| 1:A:76:LEU:HG   | 1:A:100:PHE:CD2 | 0.50     | 2.41        | 2      | 1     |
| 1:A:33:SER:O    | 1:A:37:LYS:HB3  | 0.50     | 2.06        | 17     | 3     |
| 1:A:76:LEU:HD23 | 1:A:79:LEU:HD12 | 0.50     | 1.83        | 10     | 2     |
| 1:A:58:ASP:CA   | 1:A:61:LYS:HD2  | 0.50     | 2.25        | 18     | 1     |
| 1:A:17:PHE:CD2  | 1:A:21:ILE:HD12 | 0.50     | 2.41        | 5      | 1     |
| 1:A:15:GLU:O    | 1:A:19:ARG:HD2  | 0.49     | 2.07        | 19     | 1     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:89:ARG:HE   | 1:A:89:ARG:HA   | 0.49     | 1.68        | 7      | 1     |
| 1:A:80:LYS:HE2  | 1:A:80:LYS:O    | 0.49     | 2.08        | 20     | 1     |
| 1:A:60:LEU:O    | 1:A:64:MET:HG3  | 0.49     | 2.08        | 19     | 3     |
| 1:A:7:TYR:CD1   | 1:A:11:GLN:HB3  | 0.49     | 2.43        | 15     | 1     |
| 1:A:58:ASP:O    | 1:A:61:LYS:HG2  | 0.49     | 2.07        | 16     | 1     |
| 1:A:35:ILE:HA   | 1:A:39:ILE:HB   | 0.49     | 1.83        | 3      | 2     |
| 1:A:35:ILE:HG22 | 1:A:40:LYS:HE2  | 0.49     | 1.85        | 17     | 3     |
| 1:A:56:ILE:O    | 1:A:60:LEU:HG   | 0.49     | 2.08        | 20     | 5     |
| 1:A:83:PHE:O    | 1:A:87:ILE:HG13 | 0.49     | 2.08        | 8      | 3     |
| 1:A:39:ILE:HD13 | 1:A:75:THR:HG23 | 0.48     | 1.84        | 1      | 1     |
| 1:A:61:LYS:HA   | 1:A:64:MET:HE2  | 0.48     | 1.86        | 14     | 1     |
| 1:A:55:HIS:HA   | 1:A:58:ASP:OD2  | 0.48     | 2.09        | 9      | 1     |
| 1:A:89:ARG:HG3  | 1:A:91:ILE:HG13 | 0.48     | 1.85        | 15     | 1     |
| 1:A:57:ASP:O    | 1:A:61:LYS:HD3  | 0.48     | 2.08        | 20     | 1     |
| 1:A:52:LYS:HB2  | 1:A:54:ARG:HG2  | 0.48     | 1.85        | 5      | 1     |
| 1:A:21:ILE:HD11 | 1:A:78:TRP:CZ2  | 0.48     | 2.43        | 20     | 2     |
| 1:A:40:LYS:HE2  | 1:A:44:GLY:HA2  | 0.48     | 1.85        | 6      | 1     |
| 1:A:56:ILE:HA   | 1:A:59:VAL:HG22 | 0.48     | 1.86        | 1      | 1     |
| 1:A:57:ASP:HB2  | 1:A:100:PHE:HZ  | 0.48     | 1.69        | 1      | 1     |
| 1:A:41:PRO:HD2  | 1:A:43:ILE:HG12 | 0.47     | 1.86        | 2      | 3     |
| 1:A:51:VAL:HG13 | 1:A:96:PRO:HG2  | 0.47     | 1.84        | 8      | 1     |
| 1:A:46:LEU:HG   | 1:A:50:ASP:HB2  | 0.47     | 1.86        | 6      | 1     |
| 1:A:43:ILE:HG13 | 1:A:44:GLY:H    | 0.46     | 1.70        | 19     | 1     |
| 1:A:62:ALA:O    | 1:A:66:ARG:HG3  | 0.46     | 2.10        | 8      | 3     |
| 1:A:25:TRP:NE1  | 1:A:28:PRO:HG3  | 0.46     | 2.23        | 9      | 3     |
| 1:A:35:ILE:HA   | 1:A:39:ILE:HD12 | 0.46     | 1.88        | 12     | 2     |
| 1:A:14:ASP:HA   | 1:A:17:PHE:HD1  | 0.46     | 1.69        | 9      | 1     |
| 1:A:65:LYS:HD3  | 1:A:66:ARG:N    | 0.46     | 2.26        | 14     | 2     |
| 1:A:51:VAL:HA   | 1:A:55:HIS:HD2  | 0.46     | 1.71        | 9      | 2     |
| 1:A:95:ASN:ND2  | 1:A:98:ALA:HB2  | 0.45     | 2.25        | 11     | 1     |
| 1:A:31:VAL:O    | 1:A:35:ILE:HG13 | 0.45     | 2.11        | 9      | 3     |
| 1:A:39:ILE:C    | 1:A:41:PRO:HD3  | 0.45     | 2.36        | 8      | 1     |
| 1:A:63:VAL:HA   | 1:A:66:ARG:HG2  | 0.45     | 1.89        | 19     | 1     |
| 1:A:21:ILE:HD11 | 1:A:78:TRP:HZ2  | 0.45     | 1.71        | 17     | 1     |
| 1:A:14:ASP:HA   | 1:A:17:PHE:CD2  | 0.45     | 2.46        | 6      | 1     |
| 1:A:9:VAL:HG21  | 1:A:43:ILE:HD12 | 0.45     | 1.87        | 19     | 1     |
| 1:A:76:LEU:O    | 1:A:80:LYS:HG3  | 0.45     | 2.12        | 6      | 1     |
| 1:A:56:ILE:HG13 | 1:A:96:PRO:HB2  | 0.44     | 1.89        | 10     | 1     |
| 1:A:50:ASP:C    | 1:A:52:LYS:H    | 0.44     | 2.21        | 18     | 1     |
| 1:A:46:LEU:HB2  | 1:A:50:ASP:CB   | 0.44     | 2.42        | 7      | 1     |
| 1:A:32:ARG:HD3  | 1:A:32:ARG:O    | 0.44     | 2.13        | 2      | 1     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:76:LEU:HA   | 1:A:79:LEU:HD12 | 0.44     | 1.90        | 19     | 1     |
| 1:A:47:LYS:HB2  | 1:A:50:ASP:OD2  | 0.44     | 2.13        | 8      | 1     |
| 1:A:35:ILE:HA   | 1:A:39:ILE:HG12 | 0.44     | 1.90        | 19     | 1     |
| 1:A:85:TYR:HA   | 1:A:88:LYS:HE2  | 0.44     | 1.90        | 20     | 1     |
| 1:A:7:TYR:HB3   | 1:A:11:GLN:HB2  | 0.44     | 1.88        | 12     | 1     |
| 1:A:62:ALA:O    | 1:A:66:ARG:HG2  | 0.43     | 2.13        | 16     | 3     |
| 1:A:52:LYS:N    | 1:A:55:HIS:HD2  | 0.43     | 2.11        | 5      | 1     |
| 1:A:34:ARG:HD3  | 1:A:38:ASP:OD2  | 0.43     | 2.13        | 4      | 1     |
| 1:A:80:LYS:O    | 1:A:84:ASN:HB2  | 0.43     | 2.13        | 13     | 1     |
| 1:A:25:TRP:HD1  | 1:A:28:PRO:HG3  | 0.43     | 1.69        | 7      | 1     |
| 1:A:86:ALA:HA   | 1:A:91:ILE:HD12 | 0.43     | 1.90        | 9      | 2     |
| 1:A:62:ALA:O    | 1:A:65:LYS:HG2  | 0.43     | 2.13        | 16     | 1     |
| 1:A:26:LYS:O    | 1:A:27:HIS:HB2  | 0.43     | 2.14        | 15     | 1     |
| 1:A:27:HIS:HD2  | 1:A:31:VAL:HB   | 0.43     | 1.74        | 11     | 1     |
| 1:A:46:LEU:O    | 1:A:46:LEU:HG   | 0.43     | 2.13        | 11     | 2     |
| 1:A:51:VAL:HG13 | 1:A:96:PRO:HG3  | 0.43     | 1.91        | 18     | 1     |
| 1:A:15:GLU:OE2  | 1:A:19:ARG:HD3  | 0.43     | 2.14        | 19     | 1     |
| 1:A:68:ALA:HB3  | 1:A:71:ILE:CD1  | 0.42     | 2.44        | 18     | 1     |
| 1:A:85:TYR:HA   | 1:A:88:LYS:HG2  | 0.42     | 1.90        | 1      | 1     |
| 1:A:34:ARG:HA   | 1:A:38:ASP:OD1  | 0.42     | 2.14        | 19     | 1     |
| 1:A:47:LYS:HB3  | 1:A:50:ASP:HB2  | 0.42     | 1.92        | 3      | 1     |
| 1:A:47:LYS:HB3  | 1:A:50:ASP:OD2  | 0.42     | 2.14        | 14     | 1     |
| 1:A:11:GLN:NE2  | 1:A:14:ASP:HB3  | 0.42     | 2.30        | 15     | 1     |
| 1:A:57:ASP:HB2  | 1:A:100:PHE:CZ  | 0.42     | 2.49        | 1      | 2     |
| 1:A:10:ALA:HA   | 1:A:40:LYS:HD2  | 0.42     | 1.90        | 2      | 1     |
| 1:A:32:ARG:O    | 1:A:36:GLU:HG3  | 0.42     | 2.13        | 5      | 1     |
| 1:A:43:ILE:HA   | 1:A:46:LEU:HD21 | 0.42     | 1.92        | 12     | 1     |
| 1:A:60:LEU:HD22 | 1:A:72:ALA:HA   | 0.42     | 1.91        | 14     | 1     |
| 1:A:63:VAL:HA   | 1:A:66:ARG:CG   | 0.42     | 2.45        | 14     | 1     |
| 1:A:18:GLU:O    | 1:A:22:ALA:HB2  | 0.42     | 2.14        | 19     | 1     |
| 1:A:65:LYS:HE3  | 1:A:66:ARG:HB3  | 0.41     | 1.92        | 11     | 1     |
| 1:A:43:ILE:HG13 | 1:A:44:GLY:N    | 0.41     | 2.29        | 19     | 1     |
| 1:A:65:LYS:C    | 1:A:65:LYS:HD2  | 0.41     | 2.41        | 1      | 1     |
| 1:A:84:ASN:O    | 1:A:88:LYS:HD3  | 0.41     | 2.14        | 2      | 1     |
| 1:A:89:ARG:HA   | 1:A:89:ARG:NE   | 0.41     | 2.30        | 7      | 1     |
| 1:A:15:GLU:HG3  | 1:A:85:TYR:HE2  | 0.41     | 1.75        | 12     | 1     |
| 1:A:19:ARG:N    | 1:A:19:ARG:HD2  | 0.41     | 2.30        | 4      | 1     |
| 1:A:21:ILE:HG22 | 1:A:21:ILE:O    | 0.41     | 2.16        | 14     | 1     |
| 1:A:21:ILE:HD13 | 1:A:31:VAL:HG11 | 0.41     | 1.92        | 19     | 1     |
| 1:A:41:PRO:HG3  | 1:A:59:VAL:HB   | 0.41     | 1.90        | 3      | 1     |
| 1:A:94:TYR:O    | 1:A:96:PRO:HD3  | 0.41     | 2.16        | 1      | 1     |

*Continued on next page...*

Continued from previous page...

| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:51:VAL:O   | 1:A:51:VAL:HG13 | 0.41     | 2.15        | 10     | 1     |
| 1:A:43:ILE:HA  | 1:A:46:LEU:HD13 | 0.41     | 1.92        | 18     | 1     |
| 1:A:24:ARG:HG3 | 1:A:24:ARG:O    | 0.41     | 2.16        | 11     | 1     |
| 1:A:61:LYS:HE2 | 1:A:61:LYS:HB3  | 0.41     | 1.80        | 15     | 1     |
| 1:A:24:ARG:HD3 | 1:A:24:ARG:O    | 0.40     | 2.16        | 12     | 1     |
| 1:A:59:VAL:O   | 1:A:63:VAL:HG13 | 0.40     | 2.15        | 16     | 1     |
| 1:A:16:TYR:CZ  | 1:A:20:MET:HG3  | 0.40     | 2.51        | 4      | 1     |
| 1:A:34:ARG:HA  | 1:A:38:ASP:OD2  | 0.40     | 2.16        | 5      | 1     |
| 1:A:63:VAL:HA  | 1:A:66:ARG:CZ   | 0.40     | 2.46        | 12     | 1     |
| 1:A:52:LYS:H   | 1:A:55:HIS:CD2  | 0.40     | 2.35        | 15     | 1     |
| 1:A:26:LYS:HD3 | 1:A:26:LYS:HA   | 0.40     | 1.82        | 16     | 1     |
| 1:A:36:GLU:HA  | 1:A:40:LYS:HE3  | 0.40     | 1.93        | 20     | 1     |
| 1:A:84:ASN:O   | 1:A:88:LYS:HG3  | 0.40     | 2.15        | 18     | 1     |
| 1:A:47:LYS:HG3 | 1:A:48:VAL:N    | 0.40     | 2.32        | 3      | 1     |
| 1:A:65:LYS:HG3 | 1:A:66:ARG:N    | 0.40     | 2.31        | 9      | 1     |
| 1:A:24:ARG:HD3 | 1:A:24:ARG:C    | 0.40     | 2.42        | 12     | 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     | 94/116 (81%)    | 84±2 (89±2%) | 8±2 (9±2%) | 2±1 (2±1%) | 9           | 53 |
| All | All   | 1880/2320 (81%) | 1678 (89%)   | 170 (9%)   | 32 (2%)    | 9           | 53 |

All 9 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     | 26  | LYS  | 12             |
| 1   | A     | 41  | PRO  | 6              |
| 1   | A     | 42  | ALA  | 4              |
| 1   | A     | 47  | LYS  | 3              |
| 1   | A     | 43  | ILE  | 2              |
| 1   | A     | 67  | GLY  | 2              |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 44  | GLY  | 1              |
| 1   | A     | 24  | ARG  | 1              |
| 1   | A     | 51  | VAL  | 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     | 80/96 (83%)     | 76±4 (95±4%) | 4±2 (4±2%) | 27          | 77 |
| All | All   | 1588/1920 (83%) | 1518 (96%)   | 70 (4%)    | 27          | 77 |

All 32 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     | 40  | LYS  | 8              |
| 1   | A     | 80  | LYS  | 7              |
| 1   | A     | 37  | LYS  | 6              |
| 1   | A     | 26  | LYS  | 5              |
| 1   | A     | 18  | GLU  | 4              |
| 1   | A     | 65  | LYS  | 4              |
| 1   | A     | 32  | ARG  | 3              |
| 1   | A     | 54  | ARG  | 3              |
| 1   | A     | 36  | GLU  | 3              |
| 1   | A     | 27  | HIS  | 2              |
| 1   | A     | 57  | ASP  | 2              |
| 1   | A     | 52  | LYS  | 2              |
| 1   | A     | 70  | SER  | 2              |
| 1   | A     | 73  | ASN  | 1              |
| 1   | A     | 89  | ARG  | 1              |
| 1   | A     | 7   | TYR  | 1              |
| 1   | A     | 14  | ASP  | 1              |
| 1   | A     | 88  | LYS  | 1              |
| 1   | A     | 8   | THR  | 1              |
| 1   | A     | 38  | ASP  | 1              |
| 1   | A     | 15  | GLU  | 1              |
| 1   | A     | 48  | VAL  | 1              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 11  | GLN  | 1              |
| 1   | A     | 46  | LEU  | 1              |
| 1   | A     | 24  | ARG  | 1              |
| 1   | A     | 66  | ARG  | 1              |
| 1   | A     | 93  | GLU  | 1              |
| 1   | A     | 30  | ILE  | 1              |
| 1   | A     | 90  | HIS  | 1              |
| 1   | A     | 50  | ASP  | 1              |
| 1   | A     | 61  | LYS  | 1              |
| 1   | A     | 19  | ARG  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

There are no such molecules in this entry.

### 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 81% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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                  | 1346 |
| Number of shifts mapped to atoms        | 1346 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 1    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 115      | $-0.08 \pm 0.20$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 109      | $0.47 \pm 0.14$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 109      | $0.79 \pm 0.54$                 | None needed (imprecise)    |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 84%, i.e. 1157 atoms were assigned a chemical shift out of a possible 1384. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 369/463 (80%) | 186/186 (100%) | 94/188 (50%)    | 89/89 (100%)    |
| Sidechain | 715/807 (89%) | 486/524 (93%)  | 217/242 (90%)   | 12/41 (29%)     |

*Continued on next page...*

Continued from previous page...

|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 73/114 (64%)    | 43/55 (78%)          | 28/51 (55%)           | 2/8 (25%)             |
| Overall  | 1157/1384 (84%) | 715/765 (93%)        | 339/481 (70%)         | 103/138 (75%)         |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1346 atoms were assigned a chemical shift out of a possible 1660. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 454/574 (79%)   | 230/232 (99%)        | 115/232 (50%)         | 109/110 (99%)         |
| Sidechain | 819/924 (89%)   | 557/599 (93%)        | 249/281 (89%)         | 13/44 (30%)           |
| Aromatic  | 73/162 (45%)    | 43/79 (54%)          | 28/63 (44%)           | 2/20 (10%)            |
| Overall   | 1346/1660 (81%) | 830/910 (91%)        | 392/576 (68%)         | 124/174 (71%)         |

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

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 52  | LYS  | H    | 11.84      | 5.24 – 11.12        | 6.2     |

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

The image below reports *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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

