



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 09:08 PM UTC

PDB ID : 2KF2 / pdb\_00002kf2  
Title : Solution NMR structure of of Streptomyces coelicolor polyketide cyclase SCO5315. Northeast Structural Genomics Consortium target RR365  
Authors : Cort, J.R.; Ramelot, T.A.; Ding, K.; Wang, H.; Jiang, M.; Maglaqui, M.; Xiao, R.; Nair, R.; Baran, M.C.; Everett, J.K.; Swapna, G.V.T.; Acton, T.B.; Rost, B.; Montelione, G.T.; Kennedy, M.A.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2009-02-11

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>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| wwPDB-RCI                      | : | v_1n_11_5_13_A (Berjanski et al., 2005)                          |
| PANAV                          | : | Wang et al. (2010)                                               |
| wwPDB-ShiftChecker             | : | v1.2                                                             |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

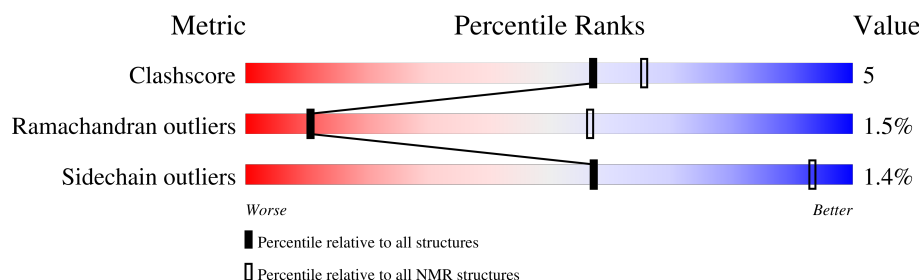
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<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     | 167    |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 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:2-A:150 (149)       | 1.04              | 1            |

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 2 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2638 atoms, of which 1285 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative polyketide cyclase.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 167      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2638  | 841 | 1285 | 244 | 259 | 9 |       |

There are 9 discrepancies between the modelled and reference sequences:

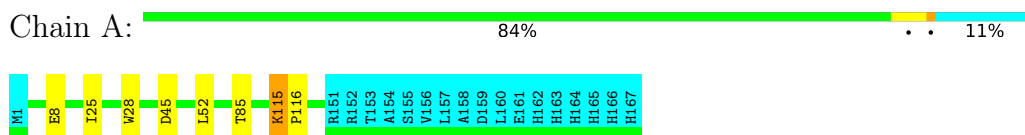
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 20      | THR      | ASN    | SEE REMARK 999 | UNP P23154 |
| A     | 160     | LEU      | -      | expression tag | UNP P23154 |
| A     | 161     | GLU      | -      | expression tag | UNP P23154 |
| A     | 162     | HIS      | -      | expression tag | UNP P23154 |
| A     | 163     | HIS      | -      | expression tag | UNP P23154 |
| A     | 164     | HIS      | -      | expression tag | UNP P23154 |
| A     | 165     | HIS      | -      | expression tag | UNP P23154 |
| A     | 166     | HIS      | -      | expression tag | UNP P23154 |
| A     | 167     | HIS      | -      | expression tag | UNP P23154 |

## 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: Putative polyketide cyclase

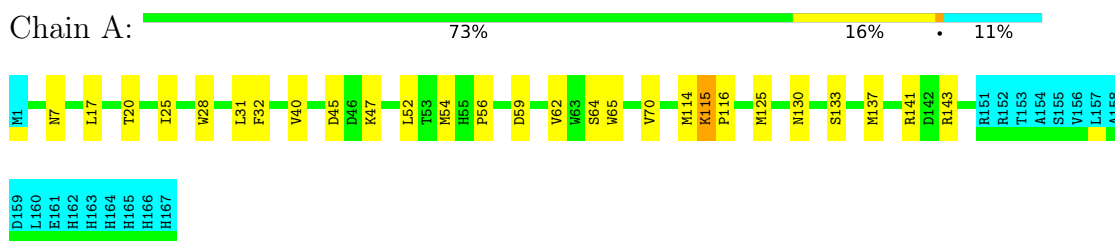


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

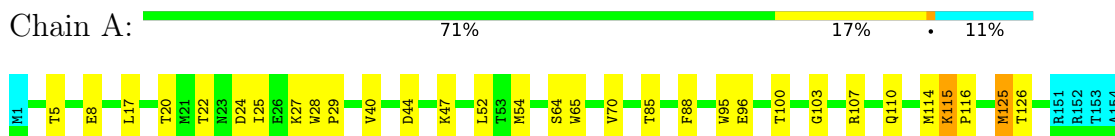
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Putative polyketide cyclase



#### 4.2.2 Score per residue for model 2

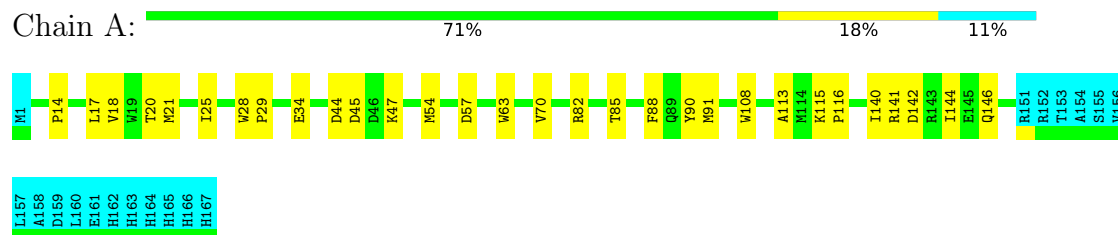
- Molecule 1: Putative polyketide cyclase





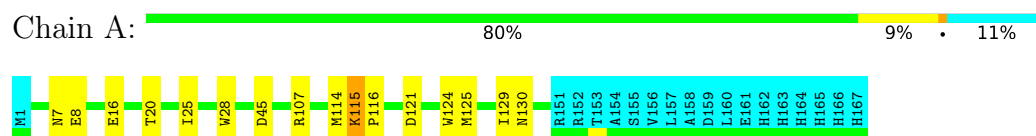
### 4.2.3 Score per residue for model 3

- Molecule 1: Putative polyketide cyclase



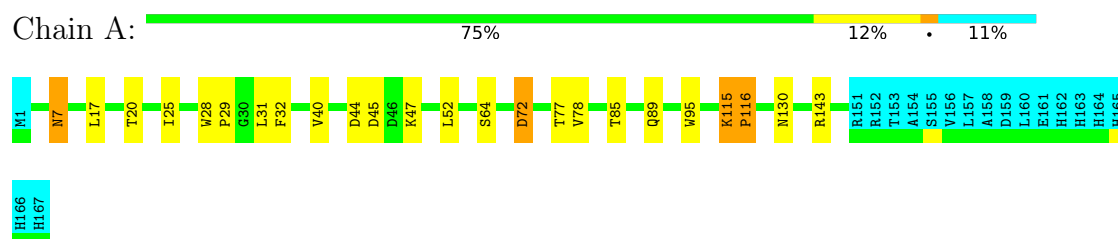
### 4.2.4 Score per residue for model 4

- Molecule 1: Putative polyketide cyclase



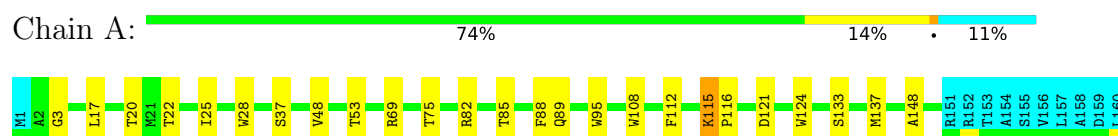
### 4.2.5 Score per residue for model 5

- Molecule 1: Putative polyketide cyclase



### 4.2.6 Score per residue for model 6

- Molecule 1: Putative polyketide cyclase



E161  
H162  
H163  
H164  
H165  
H166  
H167

#### 4.2.7 Score per residue for model 7

- Molecule 1: Putative polyketide cyclase

Chain A:  81% 6% 11%

M1 L17 T20 T25 W28 E34 D45 M54 K115 P116 D122 S133 M137 G149 E150 R151 R152 T153 A154 S155 V156 L157 A158 D159 L160 E161 H162 H163 H164 H165 H166 H167

#### 4.2.8 Score per residue for model 8

- Molecule 1: Putative polyketide cyclase

Chain A:  78% 11% 11%

M1 N7 D24 K27 L31 D45 V48 L52 S64 R69 R82 M91 K115 D122 M125 T126 D127 N128 I129 S133 M137 R143 R151 R152 T153 A154 S155 V156 L157 A158 D159 L160 E161 H162 H163 H164 H165 H166 H167

#### 4.2.9 Score per residue for model 9

- Molecule 1: Putative polyketide cyclase

Chain A:  79% 8% 11%

M1 H4 E8 E16 R43 D44 D45 V48 R107 Q110 D111 F112 K115 P116 D122 M125 I129 S133 M137 R151 R152 T153 A154 S155 V156 L157 A158 D159 L160 E161 H162 H163 H164 H165 H166 H167

#### 4.2.10 Score per residue for model 10

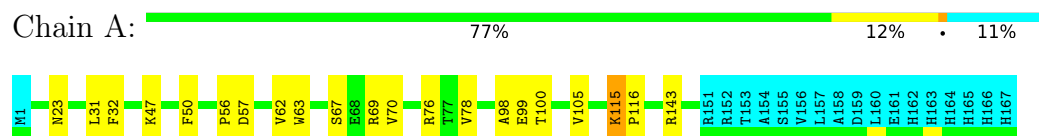
- Molecule 1: Putative polyketide cyclase

Chain A:  77% 11% 11%

M1 L17 T20 N23 D24 L25 W28 E39 D45 D46 K47 R51 R69 V70 V76 R79 T85 F88 Q89 Y90 F112 A113 M114 K115 R151 R152 T153 A154 S155 V156 L157 A158 D159 L160 E161 H162 H163 H164 H165 H166 H167

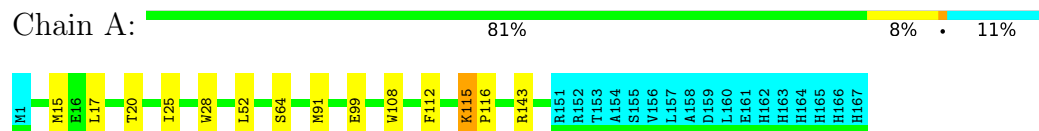
#### 4.2.11 Score per residue for model 11

- Molecule 1: Putative polyketide cyclase



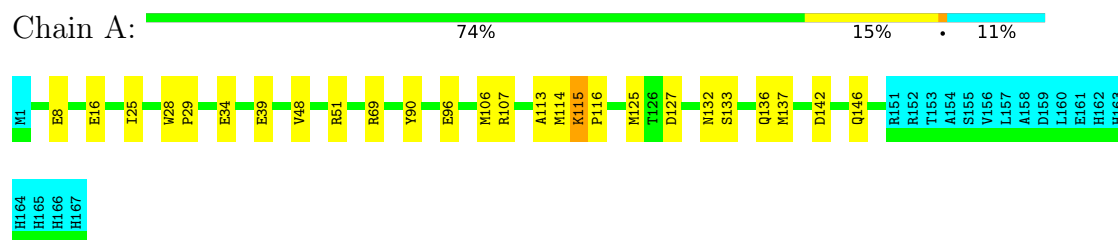
#### 4.2.12 Score per residue for model 12

- Molecule 1: Putative polyketide cyclase



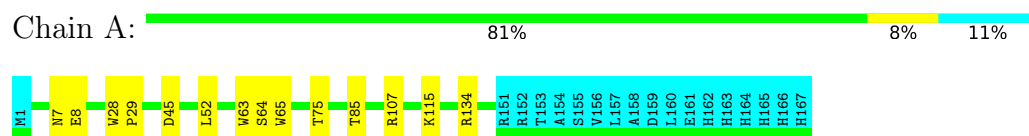
#### 4.2.13 Score per residue for model 13

- Molecule 1: Putative polyketide cyclase



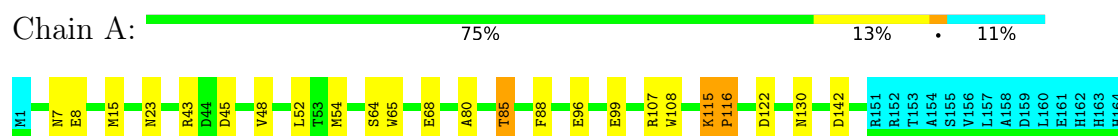
#### 4.2.14 Score per residue for model 14

- Molecule 1: Putative polyketide cyclase



#### 4.2.15 Score per residue for model 15

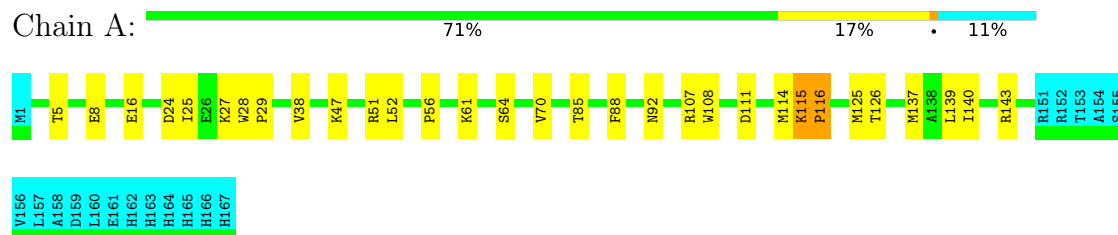
- Molecule 1: Putative polyketide cyclase



H165  
H166  
H167

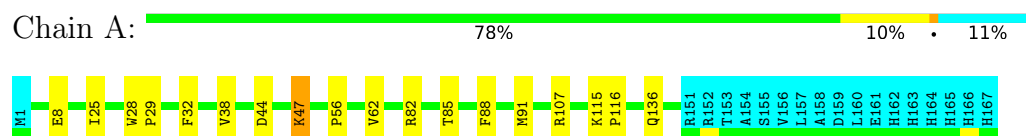
#### 4.2.16 Score per residue for model 16

- Molecule 1: Putative polyketide cyclase



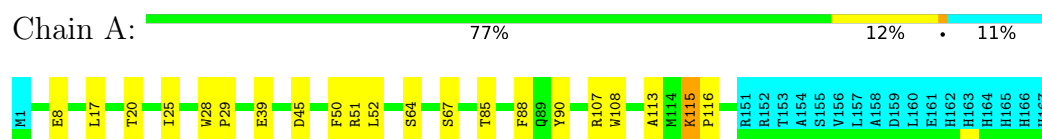
#### 4.2.17 Score per residue for model 17

- Molecule 1: Putative polyketide cyclase



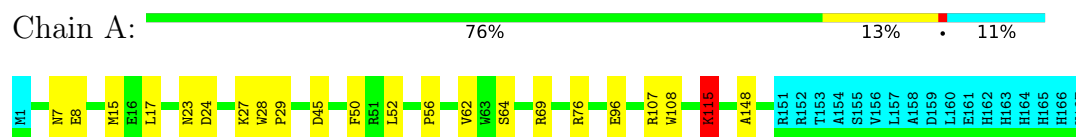
#### 4.2.18 Score per residue for model 18

- Molecule 1: Putative polyketide cyclase



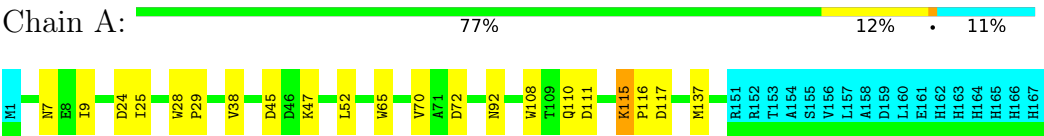
#### 4.2.19 Score per residue for model 19

- Molecule 1: Putative polyketide cyclase



4.2.20 Score per residue for model 20

- Molecule 1: Putative polyketide cyclase



## 5 Refinement protocol and experimental data overview

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

Of the 40 calculated structures, 20 were deposited, based on the following criterion: *lowest energy, fewest restraint violations, favorable backbone geometry*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| AutoStructure | structure solution | .       |
| CNS           | refinement         | .       |
| X-PLOR NIH    | refinement         | .       |
| PSVS          | structure solution | .       |

No chemical shift data was provided.

## 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     | 1199  | 1137     | 1135     | 11±4    |
| All | All   | 23980 | 22740    | 22700    | 226     |

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 5.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:31:LEU:HG   | 1:A:143:ARG:HG2 | 0.83     | 1.48        | 5      | 3     |
| 1:A:8:GLU:HG2   | 1:A:107:ARG:HG2 | 0.76     | 1.56        | 19     | 8     |
| 1:A:24:ASP:HB2  | 1:A:27:LYS:HE2  | 0.74     | 1.58        | 8      | 1     |
| 1:A:115:LYS:HA  | 1:A:115:LYS:HE3 | 0.71     | 1.61        | 19     | 1     |
| 1:A:114:MET:SD  | 1:A:125:MET:HG3 | 0.70     | 2.26        | 4      | 4     |
| 1:A:47:LYS:HG2  | 1:A:70:VAL:HG22 | 0.66     | 1.64        | 2      | 7     |
| 1:A:9:ILE:HG13  | 1:A:137:MET:HB3 | 0.66     | 1.65        | 20     | 1     |
| 1:A:52:LEU:O    | 1:A:64:SER:HA   | 0.64     | 1.92        | 16     | 10    |
| 1:A:7:ASN:HB2   | 1:A:108:TRP:HB2 | 0.63     | 1.71        | 20     | 2     |
| 1:A:48:VAL:HG13 | 1:A:69:ARG:HB3  | 0.62     | 1.70        | 13     | 3     |
| 1:A:44:ASP:HB3  | 1:A:47:LYS:HB2  | 0.62     | 1.72        | 2      | 2     |
| 1:A:15:MET:SD   | 1:A:99:GLU:HB2  | 0.62     | 2.34        | 15     | 1     |
| 1:A:96:GLU:HB2  | 1:A:107:ARG:HB2 | 0.62     | 1.72        | 2      | 1     |
| 1:A:89:GLN:HB2  | 1:A:115:LYS:HB2 | 0.61     | 1.69        | 5      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:115:LYS:HB3 | 1:A:116:PRO:HD3  | 0.61     | 1.72        | 5      | 4     |
| 1:A:44:ASP:HB2  | 1:A:47:LYS:HB2   | 0.61     | 1.70        | 17     | 2     |
| 1:A:89:GLN:HG3  | 1:A:115:LYS:HD2  | 0.60     | 1.73        | 6      | 1     |
| 1:A:17:LEU:HA   | 1:A:20:THR:HG22  | 0.60     | 1.73        | 12     | 4     |
| 1:A:54:MET:HE3  | 1:A:65:TRP:HH2   | 0.60     | 1.56        | 1      | 3     |
| 1:A:56:PRO:HB3  | 1:A:62:VAL:HG22  | 0.59     | 1.72        | 17     | 2     |
| 1:A:17:LEU:HD23 | 1:A:148:ALA:HB1  | 0.59     | 1.75        | 19     | 1     |
| 1:A:56:PRO:HG3  | 1:A:62:VAL:HG22  | 0.58     | 1.74        | 19     | 2     |
| 1:A:115:LYS:N   | 1:A:116:PRO:HD2  | 0.58     | 2.14        | 9      | 4     |
| 1:A:85:THR:HG22 | 1:A:88:PHE:HB2   | 0.58     | 1.74        | 18     | 2     |
| 1:A:7:ASN:HD21  | 1:A:129:ILE:HG22 | 0.58     | 1.59        | 4      | 1     |
| 1:A:133:SER:O   | 1:A:137:MET:HG2  | 0.57     | 1.99        | 9      | 4     |
| 1:A:108:TRP:HB3 | 1:A:110:GLN:HE21 | 0.57     | 1.59        | 20     | 1     |
| 1:A:85:THR:HB   | 1:A:88:PHE:O     | 0.57     | 1.99        | 2      | 4     |
| 1:A:7:ASN:OD1   | 1:A:130:ASN:HA   | 0.55     | 2.00        | 5      | 4     |
| 1:A:90:TYR:HB3  | 1:A:113:ALA:HB3  | 0.55     | 1.78        | 10     | 4     |
| 1:A:5:THR:HG23  | 1:A:126:THR:HG23 | 0.55     | 1.79        | 16     | 1     |
| 1:A:92:ASN:HB3  | 1:A:111:ASP:HB2  | 0.55     | 1.79        | 20     | 1     |
| 1:A:125:MET:HE2 | 1:A:125:MET:HA   | 0.53     | 1.78        | 2      | 1     |
| 1:A:34:GLU:HG2  | 1:A:54:MET:HE1   | 0.53     | 1.79        | 7      | 1     |
| 1:A:92:ASN:HB3  | 1:A:111:ASP:HB3  | 0.53     | 1.81        | 16     | 1     |
| 1:A:133:SER:O   | 1:A:137:MET:HB2  | 0.52     | 2.05        | 1      | 1     |
| 1:A:85:THR:HG21 | 1:A:88:PHE:HB2   | 0.52     | 1.80        | 17     | 2     |
| 1:A:3:GLY:HA3   | 1:A:112:PHE:CE1  | 0.52     | 2.40        | 6      | 1     |
| 1:A:125:MET:O   | 1:A:129:ILE:HG12 | 0.52     | 2.05        | 8      | 1     |
| 1:A:39:GLU:HB3  | 1:A:51:ARG:HB3   | 0.52     | 1.82        | 10     | 1     |
| 1:A:25:ILE:HG22 | 1:A:28:TRP:CZ2   | 0.51     | 2.40        | 10     | 11    |
| 1:A:69:ARG:HA   | 1:A:79:ARG:O     | 0.51     | 2.04        | 10     | 1     |
| 1:A:15:MET:SD   | 1:A:99:GLU:HG2   | 0.51     | 2.46        | 12     | 1     |
| 1:A:4:HIS:HB3   | 1:A:111:ASP:HA   | 0.50     | 1.81        | 9      | 1     |
| 1:A:85:THR:CG2  | 1:A:88:PHE:HB2   | 0.50     | 2.36        | 18     | 3     |
| 1:A:28:TRP:N    | 1:A:29:PRO:HD2   | 0.50     | 2.22        | 18     | 10    |
| 1:A:57:ASP:HB2  | 1:A:63:TRP:CZ2   | 0.50     | 2.41        | 3      | 1     |
| 1:A:115:LYS:N   | 1:A:116:PRO:CD   | 0.50     | 2.74        | 18     | 2     |
| 1:A:24:ASP:HB2  | 1:A:27:LYS:HD2   | 0.50     | 1.83        | 19     | 1     |
| 1:A:7:ASN:HD21  | 1:A:134:ARG:HB2  | 0.50     | 1.66        | 14     | 1     |
| 1:A:115:LYS:NZ  | 1:A:115:LYS:HB3  | 0.50     | 2.22        | 18     | 1     |
| 1:A:114:MET:C   | 1:A:116:PRO:HD2  | 0.49     | 2.32        | 2      | 1     |
| 1:A:8:GLU:HG2   | 1:A:107:ARG:HG3  | 0.49     | 1.85        | 4      | 1     |
| 1:A:7:ASN:ND2   | 1:A:133:SER:HB2  | 0.49     | 2.21        | 8      | 1     |
| 1:A:8:GLU:HG2   | 1:A:107:ARG:HD2  | 0.49     | 1.83        | 17     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:115:LYS:HB2 | 1:A:116:PRO:HD3  | 0.48     | 1.84        | 6      | 1     |
| 1:A:142:ASP:O   | 1:A:146:GLN:HG3  | 0.48     | 2.09        | 3      | 2     |
| 1:A:17:LEU:HA   | 1:A:20:THR:HB    | 0.48     | 1.86        | 3      | 5     |
| 1:A:137:MET:SD  | 1:A:140:ILE:HD12 | 0.48     | 2.49        | 16     | 1     |
| 1:A:22:THR:HB   | 1:A:95:TRP:HZ3   | 0.47     | 1.69        | 6      | 2     |
| 1:A:4:HIS:HA    | 1:A:110:GLN:O    | 0.47     | 2.09        | 9      | 1     |
| 1:A:82:ARG:HH21 | 1:A:85:THR:HG23  | 0.47     | 1.69        | 6      | 1     |
| 1:A:23:ASN:HA   | 1:A:69:ARG:NH2   | 0.47     | 2.24        | 11     | 1     |
| 1:A:132:ASN:O   | 1:A:136:GLN:HG2  | 0.47     | 2.09        | 13     | 1     |
| 1:A:25:ILE:HB   | 1:A:38:VAL:HG11  | 0.47     | 1.87        | 17     | 1     |
| 1:A:7:ASN:ND2   | 1:A:108:TRP:HB2  | 0.46     | 2.26        | 19     | 1     |
| 1:A:114:MET:O   | 1:A:115:LYS:HB2  | 0.46     | 2.10        | 4      | 2     |
| 1:A:96:GLU:HB3  | 1:A:107:ARG:HB2  | 0.46     | 1.87        | 15     | 3     |
| 1:A:52:LEU:HD13 | 1:A:65:TRP:CZ2   | 0.46     | 2.45        | 20     | 1     |
| 1:A:43:ARG:HB3  | 1:A:48:VAL:HG23  | 0.46     | 1.87        | 9      | 2     |
| 1:A:63:TRP:HB3  | 1:A:65:TRP:CZ3   | 0.46     | 2.46        | 14     | 1     |
| 1:A:50:PHE:CZ   | 1:A:67:SER:HB2   | 0.45     | 2.47        | 11     | 1     |
| 1:A:15:MET:HE1  | 1:A:76:ARG:HB3   | 0.45     | 1.88        | 19     | 1     |
| 1:A:57:ASP:HB2  | 1:A:63:TRP:CH2   | 0.45     | 2.47        | 11     | 1     |
| 1:A:16:GLU:H    | 1:A:16:GLU:CD    | 0.45     | 2.20        | 9      | 1     |
| 1:A:38:VAL:HG22 | 1:A:52:LEU:HG    | 0.45     | 1.89        | 20     | 1     |
| 1:A:82:ARG:HD2  | 1:A:91:MET:SD    | 0.44     | 2.52        | 8      | 1     |
| 1:A:121:ASP:H   | 1:A:124:TRP:HD1  | 0.44     | 1.56        | 6      | 2     |
| 1:A:50:PHE:CE1  | 1:A:69:ARG:HB2   | 0.44     | 2.47        | 19     | 1     |
| 1:A:34:GLU:HG2  | 1:A:54:MET:HE3   | 0.44     | 1.89        | 3      | 1     |
| 1:A:17:LEU:HD23 | 1:A:148:ALA:HB2  | 0.44     | 1.89        | 6      | 1     |
| 1:A:72:ASP:HB3  | 1:A:77:THR:O     | 0.44     | 2.13        | 5      | 1     |
| 1:A:25:ILE:HD11 | 1:A:40:VAL:HG22  | 0.43     | 1.90        | 1      | 3     |
| 1:A:137:MET:HE2 | 1:A:137:MET:HA   | 0.43     | 1.91        | 13     | 3     |
| 1:A:56:PRO:HA   | 1:A:61:LYS:O     | 0.43     | 2.12        | 16     | 1     |
| 1:A:54:MET:HE3  | 1:A:65:TRP:CH2   | 0.43     | 2.48        | 15     | 2     |
| 1:A:7:ASN:HD22  | 1:A:133:SER:HB2  | 0.43     | 1.73        | 8      | 1     |
| 1:A:70:VAL:O    | 1:A:78:VAL:HA    | 0.43     | 2.13        | 10     | 1     |
| 1:A:14:PRO:O    | 1:A:18:VAL:HG23  | 0.43     | 2.14        | 3      | 1     |
| 1:A:125:MET:HA  | 1:A:125:MET:CE   | 0.43     | 2.43        | 2      | 1     |
| 1:A:139:LEU:O   | 1:A:143:ARG:HG2  | 0.43     | 2.14        | 16     | 1     |
| 1:A:50:PHE:CE1  | 1:A:67:SER:HB2   | 0.43     | 2.49        | 18     | 1     |
| 1:A:23:ASN:HA   | 1:A:69:ARG:HH12  | 0.42     | 1.74        | 19     | 1     |
| 1:A:5:THR:OG1   | 1:A:110:GLN:HB2  | 0.42     | 2.14        | 2      | 1     |
| 1:A:24:ASP:OD2  | 1:A:27:LYS:HG2   | 0.42     | 2.14        | 2      | 1     |
| 1:A:98:ALA:HB3  | 1:A:105:VAL:HB   | 0.42     | 1.90        | 11     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:91:MET:SD   | 1:A:112:PHE:HB3  | 0.42     | 2.54        | 12     | 1     |
| 1:A:100:THR:HB  | 1:A:103:GLY:O    | 0.42     | 2.15        | 2      | 1     |
| 1:A:137:MET:O   | 1:A:141:ARG:HB2  | 0.42     | 2.14        | 1      | 1     |
| 1:A:78:VAL:HB   | 1:A:95:TRP:HB2   | 0.42     | 1.91        | 5      | 1     |
| 1:A:89:GLN:CG   | 1:A:115:LYS:HD2  | 0.42     | 2.44        | 6      | 1     |
| 1:A:39:GLU:HB2  | 1:A:51:ARG:HB3   | 0.42     | 1.90        | 13     | 2     |
| 1:A:32:PHE:HE1  | 1:A:136:GLN:HB3  | 0.42     | 1.75        | 17     | 1     |
| 1:A:25:ILE:HA   | 1:A:28:TRP:CD1   | 0.42     | 2.50        | 17     | 2     |
| 1:A:82:ARG:HB3  | 1:A:91:MET:HB2   | 0.42     | 1.91        | 17     | 1     |
| 1:A:82:ARG:HH21 | 1:A:91:MET:HG3   | 0.42     | 1.75        | 3      | 1     |
| 1:A:37:SER:HB2  | 1:A:53:THR:HB    | 0.42     | 1.92        | 6      | 1     |
| 1:A:48:VAL:CG1  | 1:A:69:ARG:HB3   | 0.41     | 2.44        | 13     | 1     |
| 1:A:133:SER:O   | 1:A:137:MET:HG3  | 0.41     | 2.15        | 8      | 1     |
| 1:A:51:ARG:HG2  | 1:A:64:SER:HB2   | 0.41     | 1.90        | 16     | 1     |
| 1:A:24:ASP:OD2  | 1:A:27:LYS:HG3   | 0.41     | 2.16        | 16     | 1     |
| 1:A:17:LEU:O    | 1:A:21:MET:HG2   | 0.41     | 2.16        | 3      | 1     |
| 1:A:125:MET:O   | 1:A:129:ILE:HG13 | 0.41     | 2.14        | 9      | 1     |
| 1:A:28:TRP:HB2  | 1:A:38:VAL:HG21  | 0.41     | 1.93        | 16     | 1     |
| 1:A:129:ILE:O   | 1:A:133:SER:HB2  | 0.41     | 2.16        | 9      | 1     |
| 1:A:115:LYS:H   | 1:A:116:PRO:CD   | 0.41     | 2.29        | 7      | 1     |
| 1:A:112:PHE:HE2 | 1:A:122:ASP:HA   | 0.41     | 1.76        | 9      | 1     |
| 1:A:90:TYR:O    | 1:A:112:PHE:HA   | 0.41     | 2.15        | 10     | 1     |
| 1:A:76:ARG:NH1  | 1:A:99:GLU:HB2   | 0.41     | 2.31        | 11     | 1     |
| 1:A:68:GLU:O    | 1:A:80:ALA:HA    | 0.41     | 2.16        | 15     | 1     |
| 1:A:115:LYS:H   | 1:A:116:PRO:HD2  | 0.41     | 1.76        | 15     | 1     |
| 1:A:5:THR:CG2   | 1:A:126:THR:HA   | 0.40     | 2.46        | 2      | 1     |
| 1:A:31:LEU:HG   | 1:A:143:ARG:HG3  | 0.40     | 1.93        | 8      | 1     |
| 1:A:140:ILE:O   | 1:A:144:ILE:HG12 | 0.40     | 2.16        | 3      | 1     |
| 1:A:89:GLN:HE21 | 1:A:115:LYS:HB2  | 0.40     | 1.76        | 10     | 1     |
| 1:A:96:GLU:O    | 1:A:106:MET:HA   | 0.40     | 2.16        | 13     | 1     |
| 1:A:69:ARG:CZ   | 1:A:78:VAL:HG11  | 0.40     | 2.47        | 11     | 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     | 149/167 (89%)   | 140±2 (94±1%) | 6±2 (4±1%) | 2±1 (2±1%) | 11          | 57 |
| All | All   | 2980/3340 (89%) | 2807 (94%)    | 127 (4%)   | 46 (2%)    | 11          | 57 |

All 7 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     | 115 | LYS  | 19             |
| 1   | A     | 45  | ASP  | 13             |
| 1   | A     | 116 | PRO  | 7              |
| 1   | A     | 122 | ASP  | 3              |
| 1   | A     | 34  | GLU  | 2              |
| 1   | A     | 16  | GLU  | 1              |
| 1   | A     | 85  | THR  | 1              |

### 6.3.2 Protein sidechains ⓘ

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     | 127/143 (89%)   | 125±1 (99±1%) | 2±1 (1±1%) | 57          | 93 |
| All | All   | 2540/2860 (89%) | 2504 (99%)    | 36 (1%)    | 57          | 93 |

All 22 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     | 108 | TRP  | 5              |
| 1   | A     | 32  | PHE  | 3              |
| 1   | A     | 115 | LYS  | 3              |
| 1   | A     | 72  | ASP  | 2              |
| 1   | A     | 85  | THR  | 2              |
| 1   | A     | 75  | THR  | 2              |
| 1   | A     | 127 | ASP  | 2              |
| 1   | A     | 16  | GLU  | 2              |
| 1   | A     | 23  | ASN  | 2              |
| 1   | A     | 59  | ASP  | 1              |
| 1   | A     | 125 | MET  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 141 | ARG  | 1              |
| 1   | A     | 20  | THR  | 1              |
| 1   | A     | 7   | ASN  | 1              |
| 1   | A     | 54  | MET  | 1              |
| 1   | A     | 8   | GLU  | 1              |
| 1   | A     | 100 | THR  | 1              |
| 1   | A     | 143 | ARG  | 1              |
| 1   | A     | 142 | ASP  | 1              |
| 1   | A     | 47  | LYS  | 1              |
| 1   | A     | 24  | ASP  | 1              |
| 1   | A     | 117 | ASP  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided