



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 03:24 PM UTC

PDB ID : 2KDE / pdb\_00002kde  
Title : NMR structure of major S5a (196-306):K48 linked diubiquitin species  
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Deposited on : 2009-01-06

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<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                                                             |

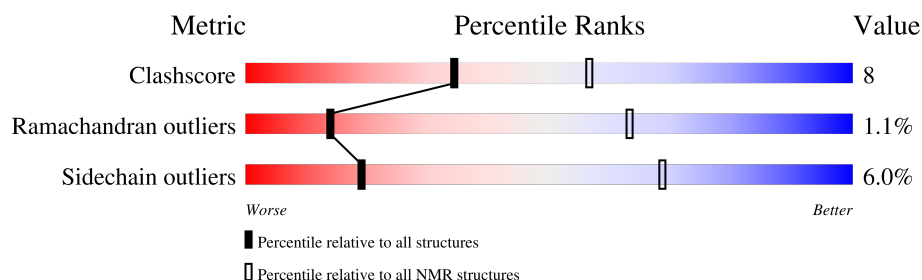
# 1 Overall quality at a glance

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     | 111    |                  |
| 2   | B     | 76     |                  |
| 2   | C     | 76     |                  |

## 2 Ensemble composition and analysis

This entry contains 7 models. Model 3 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:206-A:295, B:1-B:76,<br>C:77-C:150 (240) | 3.68              | 3            |

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 1 clusters and 2 single-model clusters were found.

| Cluster number        | Models        |
|-----------------------|---------------|
| 1                     | 1, 3, 4, 6, 7 |
| Single-model clusters | 2; 5          |

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

There are 2 unique types of molecules in this entry. The entry contains 2027 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

| Mol | Chain | Residues | Atoms |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|-------|
| 1   | A     | 111      | Total | C   | N   | O   | S | 0     |
|     |       |          | 824   | 497 | 139 | 182 | 6 |       |

- Molecule 2 is a protein called Ubiquitin.

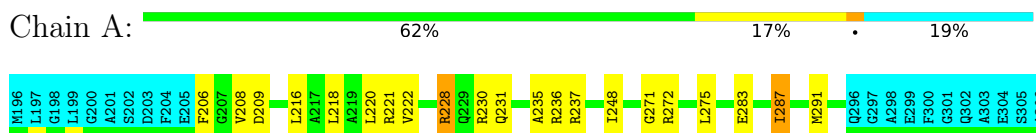
| Mol | Chain | Residues | Atoms |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|-------|
| 2   | B     | 76       | Total | C   | N   | O   | S | 0     |
|     |       |          | 601   | 378 | 105 | 117 | 1 |       |
| 2   | C     | 76       | Total | C   | N   | O   | S | 0     |
|     |       |          | 602   | 378 | 105 | 118 | 1 |       |

## 4 Residue-property plots

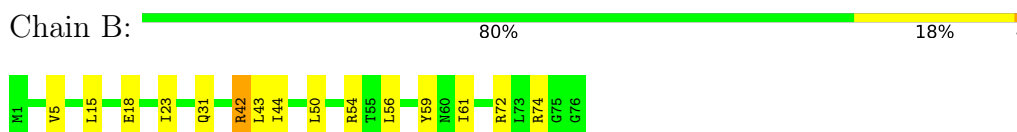
### 4.1 Average score per residue in the NMR ensemble

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.

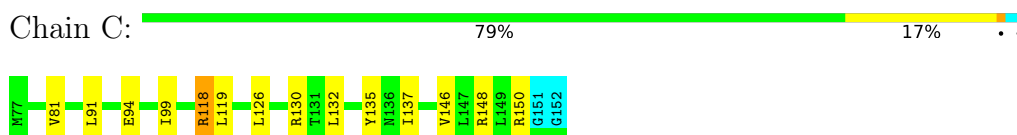
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4



- Molecule 2: Ubiquitin



- Molecule 2: Ubiquitin

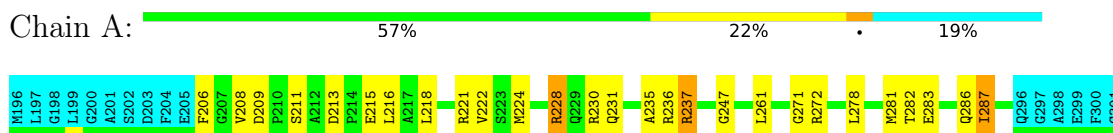


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4



Q302  
A303  
E304  
S305  
A306

- Molecule 2: Ubiquitin

Chain B:  72% 26% .

H1 F4 V5 T14 L15 I23 I30 Q31 D32 R42 L43 I44 L50 R54 T55 L56 Y59 R60 I61 S65 V70 L71 R72 L73 R74 G75 G76

- Molecule 2: Ubiquitin

Chain C:  71% 22% . .

H77 Q78 I79 F80 V81 L84 L91 F94 I99 K103 I106 R118 L119 L126 L130 T131 L132 Y135 N136 I137 D138 K139 R148 L149 R150 G151 G152

#### 4.2.2 Score per residue for model 2

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A:  61% 19% . 19%

H196 L197 G198 L199 G200 A201 S202 D203 F204 E205 L216 L217 L218 L219 L220 R221 V222 E226 Q227 R228 Q229 R230 R236 R237 T248 A249 T283 E284 G271 R272 T273 T274 L275 E283 E284 E285 I286 I287 M291 Q296 Q297 A298 E299 F300 F301 Q302 A303 E304 S305 A306

- Molecule 2: Ubiquitin

Chain B:  76% 21% .

H1 V5 R6 T12 E18 I23 R42 L43 I44 F45 L50 R54 T55 L56 Y59 R60 I61 L67 V70 L71 R72 L73 R74 G75 G76

- Molecule 2: Ubiquitin

Chain C:  71% 25% . .

H77 R82 I89 T90 L91 E92 F93 E94 I99 F100 M101 K105 R118 L119 I120 G123 K124 Q125 L126 R130 Y135 S141 V146 L147 R148 L149 R150 G151 G152

#### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A:  58% 22% . 19%

H196 L197 G198 L199 G200 A201 S202 D203 F204 E205 F206 G207 V208 D209 F210 D213 F214 E215 L216 A217 L218 A219 L220 R221 V222 R228 Q229 R230 Q231 A235 R236 R237 I248 L261 G271 R272 L275 T282 E283 I287 Q296 Q297 A298 E299 F300 F301 Q302 A303 E304 S305

A306

- Molecule 2: Ubiquitin

Chain B:  74% 20% 5%



- Molecule 2: Ubiquitin

Chain C:  79% 16% . .



#### 4.2.4 Score per residue for model 4

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A:  65% 15% 19%



- Molecule 2: Ubiquitin

Chain B:  80% 17% .



- Molecule 2: Ubiquitin

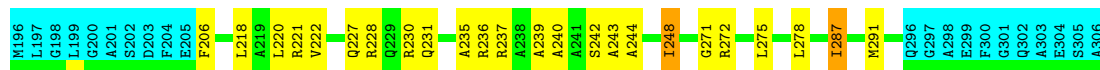
Chain C:  79% 16% . .



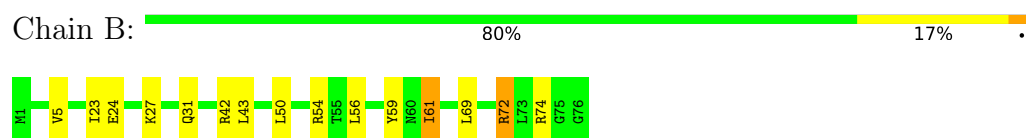
#### 4.2.5 Score per residue for model 5

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

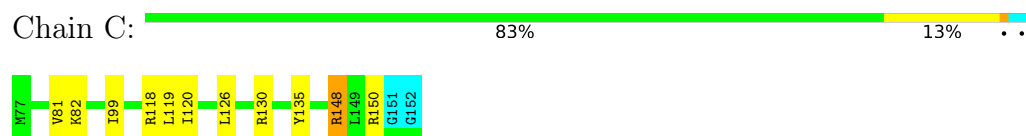
Chain A:  59% 20% 19%



- Molecule 2: Ubiquitin

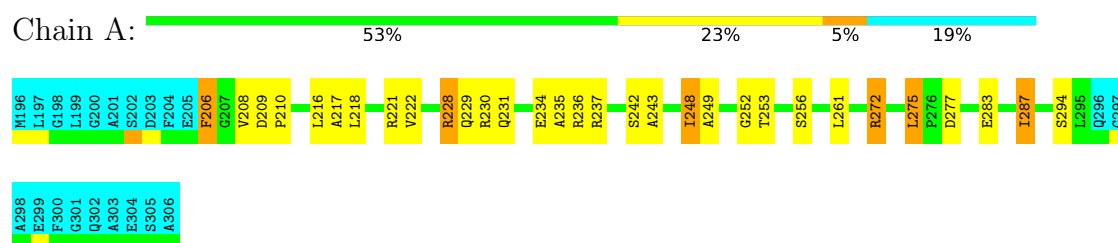


- Molecule 2: Ubiquitin

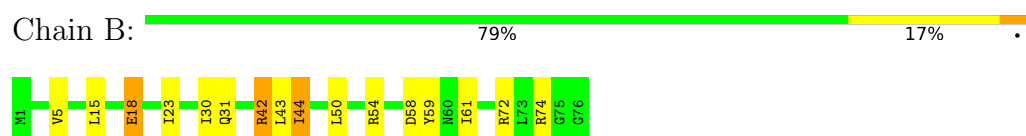


#### 4.2.6 Score per residue for model 6

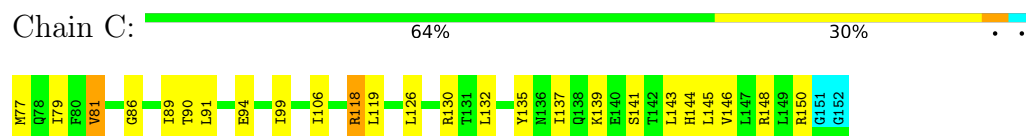
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4



- Molecule 2: Ubiquitin

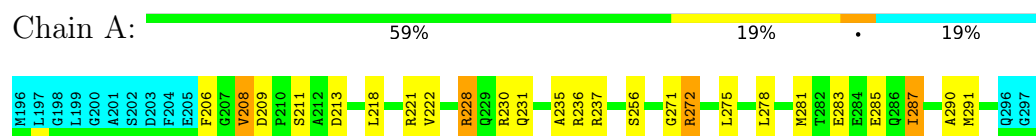


- Molecule 2: Ubiquitin



#### 4.2.7 Score per residue for model 7

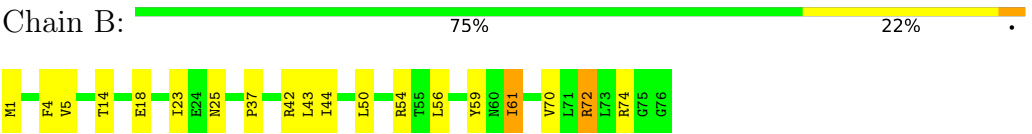
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4



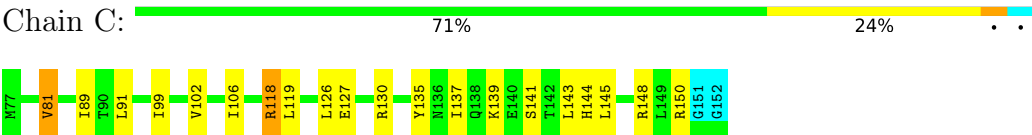




● Molecule 2: Ubiquitin



● Molecule 2: Ubiquitin



## 5 Refinement protocol and experimental data overview

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

Of the 30 calculated structures, 7 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        | structure solution |         |
| X-PLOR        | refinement         |         |

No chemical shift data was provided.

## 6 Model quality i

### 6.1 Standard geometry i

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 1.45±0.00    | 0±0/682 ( 0.0± 0.0%) | 1.48±0.01   | 0±1/920 ( 0.0± 0.1%) |
| 2   | B     | 1.43±0.01    | 0±0/607 ( 0.1± 0.1%) | 1.53±0.01   | 2±1/816 ( 0.3± 0.1%) |
| 2   | C     | 1.43±0.01    | 0±0/600 ( 0.0± 0.1%) | 1.54±0.01   | 2±1/809 ( 0.2± 0.1%) |
| All | All   | 1.44         | 4/13223 ( 0.0%)      | 1.51        | 31/17815 ( 0.2%)     |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 6.0±0.0   |
| 2   | B     | 0.0±0.0   | 4.0±0.0   |
| 2   | C     | 0.0±0.0   | 4.0±0.0   |
| All | All   | 0         | 98        |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
|     |       |     |      |       |      |             |          | Worst  | Total |
| 2   | B     | 18  | GLU  | N-CA  | 5.20 | 1.49        | 1.46     | 6      | 3     |
| 2   | C     | 94  | GLU  | N-CA  | 5.13 | 1.49        | 1.46     | 2      | 1     |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 2   | B     | 61  | ILE  | N-CA-CB | -6.29 | 105.11      | 111.90   | 2      | 6     |
| 2   | C     | 137 | ILE  | N-CA-CB | -6.06 | 105.36      | 111.90   | 4      | 4     |
| 2   | C     | 79  | ILE  | N-CA-CB | -5.74 | 105.52      | 112.07   | 1      | 1     |
| 1   | A     | 273 | THR  | N-CA-CB | -5.69 | 104.96      | 111.79   | 2      | 1     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 1   | A     | 254 | GLU  | N-CA-CB | -5.64 | 105.02      | 111.79   | 2      | 1     |
| 2   | C     | 146 | VAL  | N-CA-CB | -5.50 | 105.51      | 112.60   | 3      | 3     |
| 2   | B     | 5   | VAL  | N-CA-CB | -5.35 | 105.16      | 111.90   | 1      | 6     |
| 2   | C     | 81  | VAL  | N-CA-CB | -5.35 | 105.16      | 111.90   | 1      | 5     |
| 2   | B     | 44  | ILE  | N-CA-CB | -5.13 | 104.97      | 111.64   | 6      | 3     |
| 2   | B     | 37  | PRO  | O-C-N   | 5.08  | 123.54      | 121.15   | 7      | 1     |

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 221 | ARG  | Sidechain | 7              |
| 1   | A     | 228 | ARG  | Sidechain | 7              |
| 1   | A     | 230 | ARG  | Sidechain | 7              |
| 1   | A     | 236 | ARG  | Sidechain | 7              |
| 1   | A     | 237 | ARG  | Sidechain | 7              |
| 1   | A     | 272 | ARG  | Sidechain | 7              |
| 2   | B     | 42  | ARG  | Sidechain | 7              |
| 2   | B     | 54  | ARG  | Sidechain | 7              |
| 2   | B     | 72  | ARG  | Sidechain | 7              |
| 2   | B     | 74  | ARG  | Sidechain | 7              |
| 2   | C     | 118 | ARG  | Sidechain | 7              |
| 2   | C     | 130 | ARG  | Sidechain | 7              |
| 2   | C     | 148 | ARG  | Sidechain | 7              |
| 2   | C     | 150 | ARG  | Sidechain | 7              |

## 6.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 676   | 0        | 647      | 9±2     |
| 2   | B     | 601   | 0        | 629      | 11±2    |
| 2   | C     | 593   | 0        | 618      | 12±4    |
| All | All   | 13090 | 0        | 13258    | 213     |

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 8.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:287:ILE:HG23 | 1:A:291:MET:HE3  | 0.89     | 1.43        | 7      | 3     |
| 1:A:287:ILE:CG2  | 1:A:291:MET:HE3  | 0.76     | 2.10        | 7      | 3     |
| 2:C:119:LEU:C    | 2:C:120:ILE:HD12 | 0.73     | 2.08        | 5      | 3     |
| 1:A:218:LEU:O    | 1:A:222:VAL:HG23 | 0.72     | 1.84        | 6      | 7     |
| 2:B:50:LEU:HD22  | 2:B:59:TYR:CG    | 0.70     | 2.21        | 3      | 6     |
| 2:C:77:MET:HE2   | 2:C:94:GLU:C     | 0.70     | 2.11        | 6      | 2     |
| 2:C:81:VAL:HG21  | 2:C:91:LEU:HD22  | 0.68     | 1.63        | 1      | 3     |
| 2:B:23:ILE:HG22  | 2:B:27:LYS:CE    | 0.68     | 2.19        | 5      | 1     |
| 1:A:291:MET:HE2  | 2:C:123:GLY:C    | 0.66     | 2.15        | 2      | 1     |
| 2:B:44:ILE:HD13  | 2:B:70:VAL:CG2   | 0.66     | 2.21        | 2      | 3     |
| 2:C:106:ILE:CD1  | 2:C:145:LEU:HD13 | 0.64     | 2.22        | 6      | 2     |
| 1:A:240:ALA:O    | 1:A:244:ALA:HB3  | 0.64     | 1.93        | 5      | 1     |
| 2:B:50:LEU:HD22  | 2:B:59:TYR:CD2   | 0.63     | 2.29        | 3      | 6     |
| 2:C:126:LEU:HD22 | 2:C:135:TYR:CD2  | 0.63     | 2.28        | 1      | 5     |
| 2:C:126:LEU:HD22 | 2:C:135:TYR:CG   | 0.62     | 2.29        | 2      | 7     |
| 2:B:23:ILE:HG23  | 2:B:43:LEU:HD12  | 0.62     | 1.71        | 2      | 5     |
| 2:B:43:LEU:HB3   | 2:B:50:LEU:HD12  | 0.61     | 1.71        | 5      | 2     |
| 1:A:283:GLU:O    | 1:A:287:ILE:HD12 | 0.61     | 1.96        | 2      | 6     |
| 2:B:23:ILE:HG22  | 2:B:27:LYS:HE3   | 0.61     | 1.72        | 5      | 1     |
| 1:A:291:MET:HE2  | 2:C:124:LYS:N    | 0.61     | 2.09        | 2      | 1     |
| 2:C:90:THR:C     | 2:C:91:LEU:HD12  | 0.60     | 2.22        | 6      | 1     |
| 2:C:119:LEU:HB3  | 2:C:126:LEU:HD12 | 0.60     | 1.72        | 1      | 3     |
| 2:C:99:ILE:HG23  | 2:C:119:LEU:HD12 | 0.60     | 1.72        | 1      | 4     |
| 2:B:1:MET:HE2    | 2:B:18:GLU:C     | 0.59     | 2.23        | 7      | 1     |
| 2:B:44:ILE:HD13  | 2:B:70:VAL:HG23  | 0.58     | 1.73        | 2      | 2     |
| 2:B:44:ILE:HD12  | 2:B:44:ILE:N     | 0.58     | 2.14        | 2      | 6     |
| 2:C:120:ILE:HD12 | 2:C:120:ILE:N    | 0.57     | 2.15        | 2      | 3     |
| 1:A:290:ALA:HB1  | 2:C:144:HIS:HB3  | 0.56     | 1.75        | 7      | 1     |
| 1:A:215:GLU:OE1  | 2:B:73:LEU:HD11  | 0.55     | 2.01        | 3      | 1     |
| 2:C:106:ILE:HD13 | 2:C:145:LEU:HD13 | 0.55     | 1.78        | 6      | 1     |
| 2:C:132:LEU:HA   | 2:C:137:ILE:HD12 | 0.55     | 1.78        | 6      | 4     |
| 1:A:210:PRO:CB   | 1:A:217:ALA:HB2  | 0.54     | 2.32        | 6      | 2     |
| 1:A:278:LEU:HD12 | 1:A:281:MET:HE3  | 0.54     | 1.80        | 7      | 1     |
| 2:B:73:LEU:HD12  | 2:B:73:LEU:N     | 0.54     | 2.18        | 3      | 2     |
| 2:B:15:LEU:HD11  | 2:B:30:ILE:HG12  | 0.53     | 1.79        | 6      | 3     |
| 2:B:43:LEU:CD1   | 2:B:69:LEU:HD12  | 0.53     | 2.34        | 5      | 1     |
| 1:A:206:PHE:O    | 1:A:216:LEU:HD13 | 0.53     | 2.03        | 6      | 1     |
| 2:B:4:PHE:CZ     | 2:B:14:THR:HG23  | 0.52     | 2.40        | 1      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:239:ALA:O    | 1:A:243:ALA:HB3  | 0.52     | 2.04        | 5      | 1     |
| 1:A:253:THR:O    | 1:A:253:THR:HG23 | 0.51     | 2.06        | 2      | 2     |
| 1:A:248:ILE:HG23 | 1:A:248:ILE:O    | 0.51     | 2.05        | 3      | 3     |
| 2:B:42:ARG:HB3   | 2:B:44:ILE:HD11  | 0.51     | 1.83        | 1      | 4     |
| 1:A:278:LEU:HD22 | 2:C:84:LEU:HD13  | 0.50     | 1.82        | 1      | 1     |
| 2:B:56:LEU:HA    | 2:B:61:ILE:HD12  | 0.50     | 1.83        | 3      | 4     |
| 2:C:89:ILE:HG22  | 2:C:91:LEU:CD1   | 0.50     | 2.36        | 6      | 1     |
| 1:A:210:PRO:HB2  | 1:A:217:ALA:HB2  | 0.49     | 1.82        | 6      | 1     |
| 2:B:43:LEU:C     | 2:B:44:ILE:HD12  | 0.49     | 2.33        | 4      | 4     |
| 1:A:281:MET:HE2  | 1:A:286:GLN:HA   | 0.49     | 1.85        | 1      | 1     |
| 2:C:91:LEU:HD12  | 2:C:91:LEU:N     | 0.49     | 2.23        | 1      | 2     |
| 2:C:89:ILE:HG22  | 2:C:91:LEU:CD2   | 0.49     | 2.37        | 2      | 1     |
| 2:B:4:PHE:CE1    | 2:B:14:THR:HG23  | 0.48     | 2.42        | 7      | 1     |
| 1:A:287:ILE:HG23 | 1:A:291:MET:CE   | 0.48     | 2.37        | 5      | 2     |
| 2:C:81:VAL:HG11  | 2:C:106:ILE:HD11 | 0.48     | 1.84        | 6      | 1     |
| 2:C:99:ILE:CG2   | 2:C:119:LEU:HD12 | 0.48     | 2.38        | 1      | 4     |
| 1:A:261:LEU:C    | 1:A:261:LEU:HD23 | 0.47     | 2.34        | 3      | 2     |
| 1:A:231:GLN:O    | 1:A:235:ALA:HB2  | 0.47     | 2.08        | 3      | 6     |
| 2:C:93:VAL:HG12  | 2:C:105:LYS:CD   | 0.47     | 2.40        | 2      | 1     |
| 1:A:275:LEU:HD11 | 1:A:277:ASP:CG   | 0.46     | 2.35        | 6      | 1     |
| 2:B:23:ILE:HG22  | 2:B:27:LYS:HE2   | 0.46     | 1.86        | 5      | 1     |
| 2:C:99:ILE:HG23  | 2:C:119:LEU:CD1  | 0.46     | 2.40        | 1      | 2     |
| 2:B:23:ILE:CG2   | 2:B:43:LEU:HD12  | 0.45     | 2.41        | 2      | 2     |
| 2:C:126:LEU:CD2  | 2:C:135:TYR:CD1  | 0.45     | 3.00        | 3      | 5     |
| 2:C:89:ILE:HG22  | 2:C:91:LEU:HD12  | 0.45     | 1.86        | 7      | 1     |
| 2:C:126:LEU:CD2  | 2:C:135:TYR:CG   | 0.45     | 2.99        | 1      | 5     |
| 1:A:243:ALA:HB1  | 1:A:249:ALA:HB2  | 0.45     | 1.89        | 6      | 1     |
| 2:C:94:GLU:O     | 2:C:132:LEU:HD12 | 0.44     | 2.12        | 1      | 1     |
| 2:B:6:LYS:HG2    | 2:B:12:THR:HG23  | 0.44     | 1.89        | 2      | 1     |
| 2:C:91:LEU:HD21  | 2:C:106:ILE:CG1  | 0.44     | 2.41        | 1      | 2     |
| 1:A:294:SER:CB   | 2:C:144:HIS:CE1  | 0.44     | 3.00        | 6      | 1     |
| 2:B:4:PHE:CE1    | 2:B:14:THR:CG2   | 0.44     | 3.00        | 7      | 1     |
| 2:B:50:LEU:CD2   | 2:B:59:TYR:CD1   | 0.44     | 3.00        | 7      | 2     |
| 2:B:43:LEU:HD12  | 2:B:69:LEU:HD12  | 0.44     | 1.90        | 5      | 1     |
| 2:B:50:LEU:CD2   | 2:B:59:TYR:CG    | 0.44     | 3.00        | 5      | 2     |
| 2:C:81:VAL:CG2   | 2:C:91:LEU:HD12  | 0.44     | 2.43        | 4      | 1     |
| 2:C:79:ILE:HD12  | 2:C:143:LEU:HD12 | 0.44     | 1.90        | 6      | 1     |
| 1:A:275:LEU:HD11 | 1:A:277:ASP:OD2  | 0.44     | 2.13        | 6      | 1     |
| 2:B:18:GLU:O     | 2:B:56:LEU:HD12  | 0.43     | 2.14        | 2      | 1     |
| 2:C:81:VAL:HG11  | 2:C:106:ILE:CD1  | 0.43     | 2.44        | 6      | 1     |
| 2:B:36:ILE:HG21  | 2:B:71:LEU:HD21  | 0.43     | 1.89        | 3      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:C:126:LEU:HD22 | 2:C:135:TYR:CD1  | 0.43     | 2.49        | 4      | 1     |
| 2:C:89:ILE:CG2   | 2:C:91:LEU:HD11  | 0.43     | 2.44        | 6      | 1     |
| 1:A:213:ASP:OD2  | 1:A:216:LEU:HD13 | 0.42     | 2.14        | 1      | 1     |
| 1:A:291:MET:HE2  | 2:C:120:ILE:HG23 | 0.42     | 1.92        | 4      | 2     |
| 2:B:15:LEU:HD11  | 2:B:30:ILE:CG1   | 0.42     | 2.44        | 6      | 1     |
| 1:A:208:VAL:HG23 | 1:A:209:ASP:N    | 0.42     | 2.30        | 4      | 2     |
| 2:C:126:LEU:CD2  | 2:C:135:TYR:CD2  | 0.42     | 3.02        | 4      | 1     |
| 1:A:208:VAL:HG13 | 1:A:209:ASP:N    | 0.42     | 2.30        | 7      | 3     |
| 2:B:44:ILE:N     | 2:B:44:ILE:CD1   | 0.42     | 2.83        | 1      | 4     |
| 2:C:120:ILE:N    | 2:C:120:ILE:CD1  | 0.41     | 2.83        | 4      | 2     |
| 2:B:50:LEU:CD2   | 2:B:59:TYR:CD2   | 0.41     | 3.03        | 4      | 1     |
| 2:B:43:LEU:HD12  | 2:B:43:LEU:N     | 0.41     | 2.30        | 5      | 1     |
| 2:C:99:ILE:HG22  | 2:C:103:LYS:HE3  | 0.41     | 1.92        | 1      | 1     |
| 2:C:146:VAL:HG12 | 2:C:147:LEU:N    | 0.41     | 2.30        | 4      | 1     |
| 2:C:91:LEU:CD1   | 2:C:91:LEU:N     | 0.40     | 2.84        | 6      | 1     |
| 1:A:215:GLU:CD   | 2:B:73:LEU:HD11  | 0.40     | 2.40        | 3      | 1     |
| 2:C:118:ARG:HB3  | 2:C:120:ILE:HD11 | 0.40     | 1.92        | 4      | 1     |
| 2:B:13:ILE:HG22  | 2:B:15:LEU:CD2   | 0.40     | 2.46        | 4      | 1     |
| 2:C:91:LEU:HD23  | 2:C:102:VAL:HG13 | 0.40     | 1.92        | 7      | 1     |
| 2:C:91:LEU:N     | 2:C:91:LEU:CD1   | 0.40     | 2.85        | 1      | 1     |
| 1:A:248:ILE:HG23 | 1:A:249:ALA:N    | 0.40     | 2.31        | 2      | 1     |
| 2:B:45:PHE:HB2   | 2:B:67:LEU:HD23  | 0.40     | 1.93        | 2      | 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     | 90/111 (81%)    | 78±2 (87±2%) | 9±2 (10±3%) | 2±1 (3±1%) | 6           | 43 |
| 2   | B     | 74/76 (97%)     | 69±2 (93±3%) | 5±2 (7±3%)  | 0±0 (0±0%) | 44          | 80 |
| 2   | C     | 73/76 (96%)     | 68±1 (94±1%) | 4±1 (6±1%)  | 0±0 (0±0%) | 44          | 80 |
| All | All   | 1659/1841 (90%) | 1510 (91%)   | 131 (8%)    | 18 (1%)    | 14          | 63 |

All 8 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     | 206 | PHE  | 6              |
| 1   | A     | 271 | GLY  | 5              |
| 1   | A     | 282 | THR  | 2              |
| 1   | A     | 247 | GLY  | 1              |
| 2   | B     | 75  | GLY  | 1              |
| 1   | A     | 252 | GLY  | 1              |
| 2   | C     | 86  | GLY  | 1              |
| 1   | A     | 208 | 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     | 70/83 (84%)     | 63±2 (91±3%) | 7±2 (9±3%) | 10          | 56 |
| 2   | B     | 68/68 (100%)    | 65±1 (96±2%) | 3±1 (4±2%) | 28          | 78 |
| 2   | C     | 68/68 (100%)    | 65±2 (96±2%) | 3±2 (4±2%) | 28          | 78 |
| All | All   | 1442/1533 (94%) | 1356 (94%)   | 86 (6%)    | 19          | 68 |

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

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 287 | ILE  | 7              |
| 1   | A     | 275 | LEU  | 6              |
| 1   | A     | 228 | ARG  | 4              |
| 2   | B     | 31  | GLN  | 4              |
| 1   | A     | 220 | LEU  | 4              |
| 2   | C     | 139 | LYS  | 3              |
| 2   | C     | 118 | ARG  | 3              |
| 2   | C     | 141 | SER  | 3              |
| 2   | B     | 72  | ARG  | 3              |
| 1   | A     | 211 | SER  | 2              |
| 2   | B     | 65  | SER  | 2              |
| 1   | A     | 216 | LEU  | 2              |
| 1   | A     | 285 | GLU  | 2              |
| 2   | C     | 82  | LYS  | 2              |
| 2   | C     | 101 | ASN  | 2              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 213 | ASP  | 2              |
| 2   | B     | 42  | ARG  | 2              |
| 2   | C     | 148 | ARG  | 2              |
| 1   | A     | 242 | SER  | 2              |
| 1   | A     | 248 | ILE  | 2              |
| 1   | A     | 256 | SER  | 2              |
| 1   | A     | 272 | ARG  | 2              |
| 1   | A     | 215 | GLU  | 1              |
| 1   | A     | 224 | MET  | 1              |
| 1   | A     | 237 | ARG  | 1              |
| 1   | A     | 261 | LEU  | 1              |
| 2   | B     | 32  | ASP  | 1              |
| 2   | C     | 78  | GLN  | 1              |
| 2   | C     | 130 | ARG  | 1              |
| 2   | C     | 149 | LEU  | 1              |
| 1   | A     | 226 | GLU  | 1              |
| 2   | B     | 6   | LYS  | 1              |
| 2   | B     | 74  | ARG  | 1              |
| 2   | B     | 51  | GLU  | 1              |
| 2   | B     | 63  | LYS  | 1              |
| 1   | A     | 227 | GLN  | 1              |
| 1   | A     | 278 | LEU  | 1              |
| 2   | B     | 24  | GLU  | 1              |
| 1   | A     | 229 | GLN  | 1              |
| 1   | A     | 234 | GLU  | 1              |
| 2   | B     | 18  | GLU  | 1              |
| 2   | B     | 58  | ASP  | 1              |
| 2   | B     | 25  | ASN  | 1              |
| 2   | C     | 127 | GLU  | 1              |
| 2   | C     | 143 | LEU  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [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