



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 10, 2026 – 12:11 AM UTC

PDB ID : 2EKJ / pdb\_00002ekj  
Title : Solution structures of the fn3 domain of human collagen alpha-1(XX) chain  
Authors : Sato, M.; Koshiba, S.; Inoue, M.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2007-03-23

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                                                             |

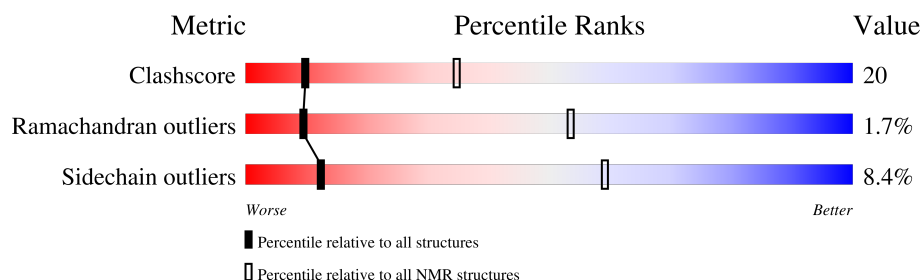
# 1 Overall quality at a glance

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     | 105    | <div> <div>50%</div> <div>28%</div> <div>•</div> <div>21%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 20 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:8-A:44, A:52-A:97 (83) | 0.32              | 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 3 clusters and 4 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1482 atoms, of which 736 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Collagen alpha-1(XX) chain.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 105      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1482  | 464 | 736 | 132 | 149 | 1 |       |

There are 13 discrepancies between the modelled and reference sequences:

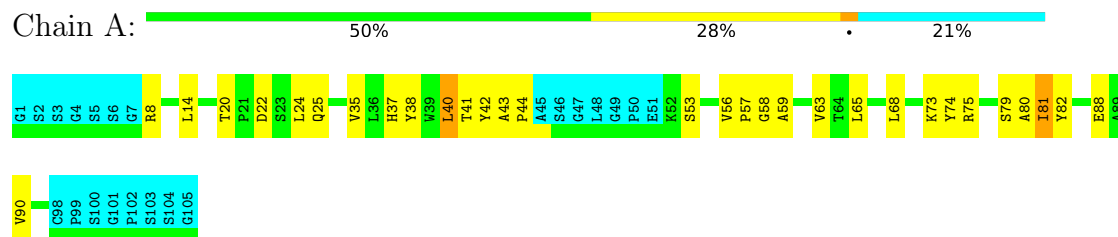
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1       | GLY      | -      | expression tag | UNP Q9P218 |
| A     | 2       | SER      | -      | expression tag | UNP Q9P218 |
| A     | 3       | SER      | -      | expression tag | UNP Q9P218 |
| A     | 4       | GLY      | -      | expression tag | UNP Q9P218 |
| A     | 5       | SER      | -      | expression tag | UNP Q9P218 |
| A     | 6       | SER      | -      | expression tag | UNP Q9P218 |
| A     | 7       | GLY      | -      | expression tag | UNP Q9P218 |
| A     | 100     | SER      | -      | expression tag | UNP Q9P218 |
| A     | 101     | GLY      | -      | expression tag | UNP Q9P218 |
| A     | 102     | PRO      | -      | expression tag | UNP Q9P218 |
| A     | 103     | SER      | -      | expression tag | UNP Q9P218 |
| A     | 104     | SER      | -      | expression tag | UNP Q9P218 |
| A     | 105     | GLY      | -      | expression tag | UNP Q9P218 |

## 4 Residue-property plots [i](#)

### 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: Collagen alpha-1(XX) chain

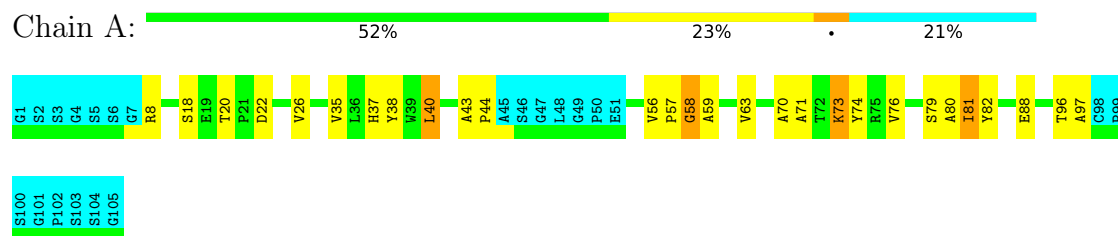


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

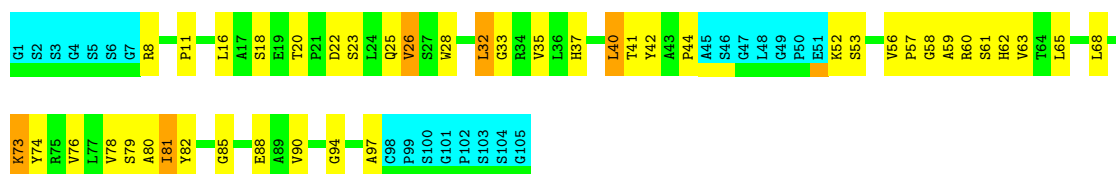
- Molecule 1: Collagen alpha-1(XX) chain



#### 4.2.2 Score per residue for model 2

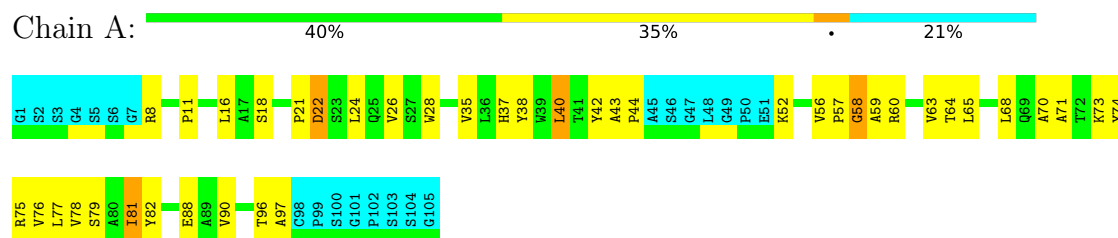
- Molecule 1: Collagen alpha-1(XX) chain





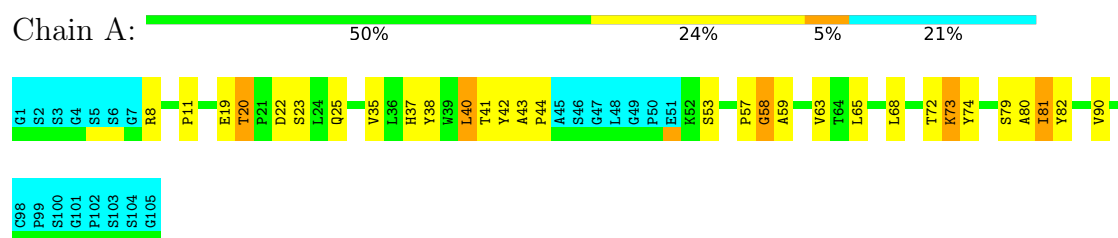
#### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Collagen alpha-1(XX) chain



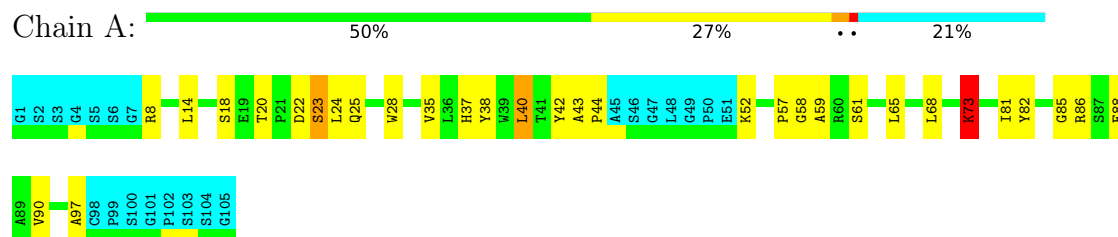
#### 4.2.4 Score per residue for model 4

- Molecule 1: Collagen alpha-1(XX) chain



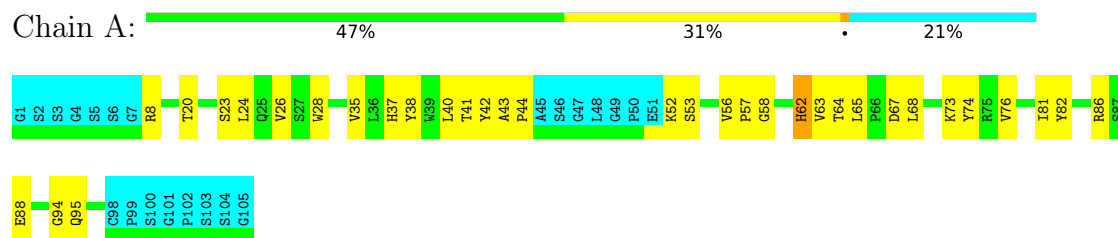
#### 4.2.5 Score per residue for model 5

- Molecule 1: Collagen alpha-1(XX) chain



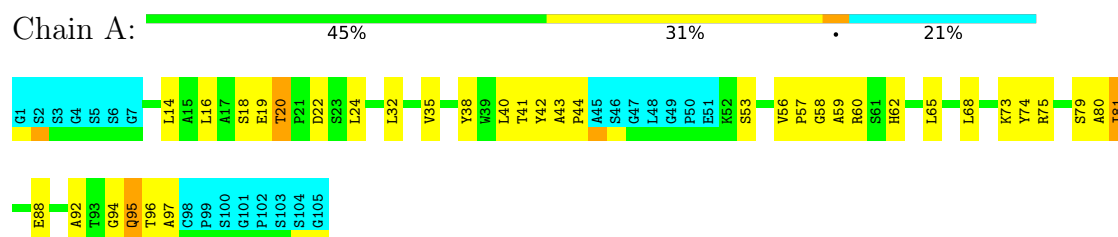
#### 4.2.6 Score per residue for model 6

- Molecule 1: Collagen alpha-1(XX) chain



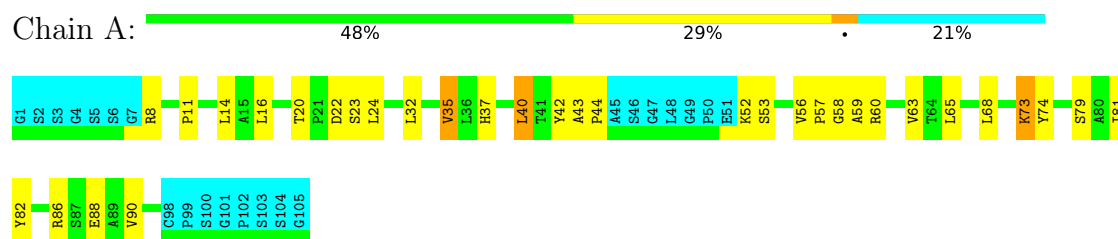
#### 4.2.7 Score per residue for model 7

- Molecule 1: Collagen alpha-1(XX) chain



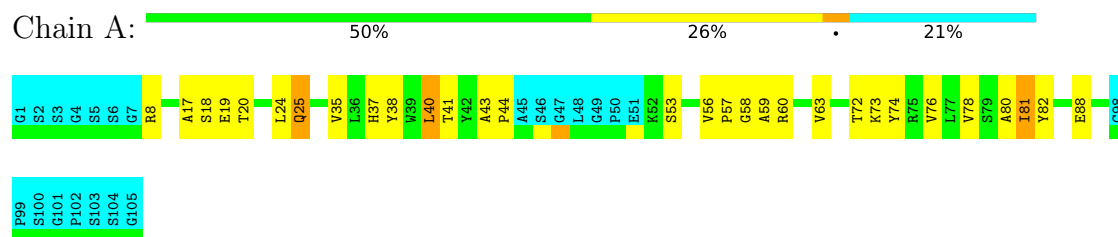
#### 4.2.8 Score per residue for model 8

- Molecule 1: Collagen alpha-1(XX) chain



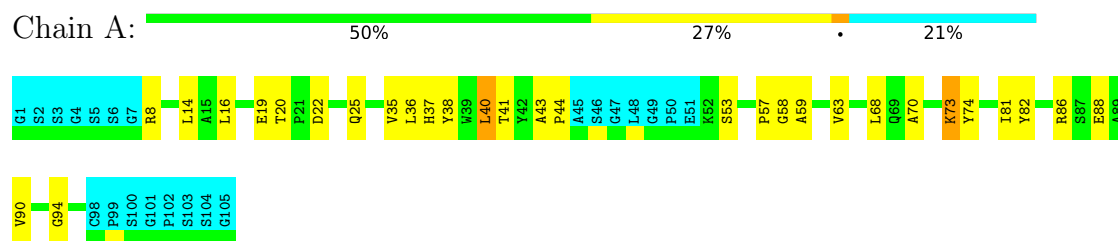
#### 4.2.9 Score per residue for model 9

- Molecule 1: Collagen alpha-1(XX) chain



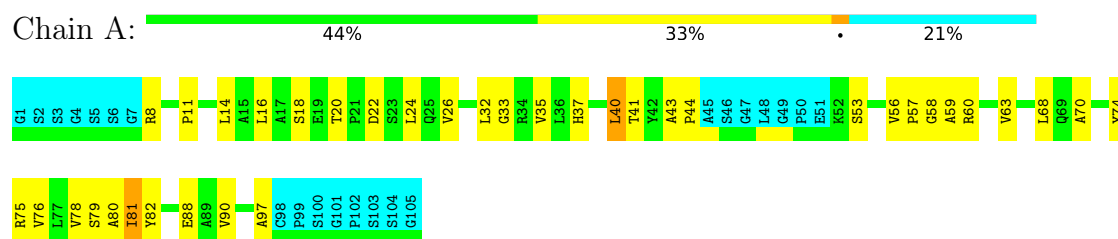
### 4.2.10 Score per residue for model 10

- Molecule 1: Collagen alpha-1(XX) chain



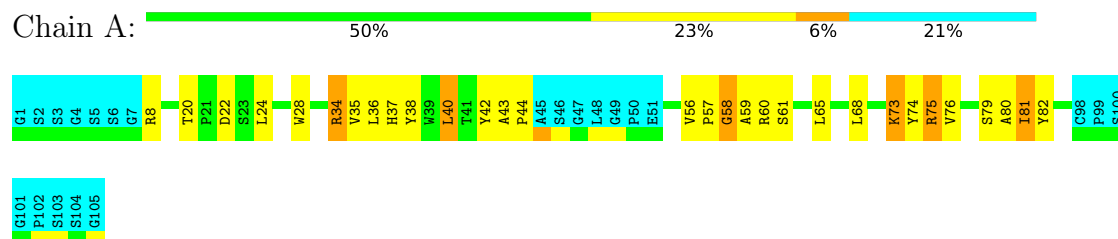
### 4.2.11 Score per residue for model 11

- Molecule 1: Collagen alpha-1(XX) chain



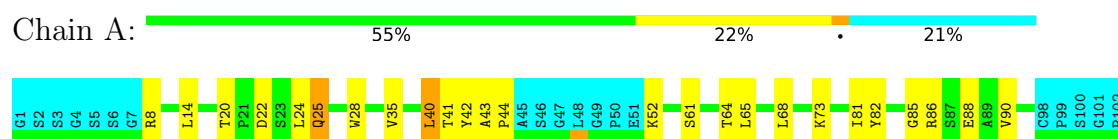
### 4.2.12 Score per residue for model 12

- Molecule 1: Collagen alpha-1(XX) chain



### 4.2.13 Score per residue for model 13

- Molecule 1: Collagen alpha-1(XX) chain



S103  
S104  
G105

#### 4.2.14 Score per residue for model 14

- Molecule 1: Collagen alpha-1(XX) chain

Chain A: 

G1 S2 S3 S4 S5 S6 S7 R8 L14 A17 S18 E19 T20 D22 S23 L24 Q25 L32 G33 H37 L40 T41 Y42 A43 A44 A45 S46 G47 G48 G49 P50 E51 E52 S53 P57 R60 V63 T64 L65 L68 K73 Y74 A80 I81 Y82 E88 A89

V90 C98 P99 S100 G101 S102 S103 S104 G105

#### 4.2.15 Score per residue for model 15

- Molecule 1: Collagen alpha-1(XX) chain

Chain A: 

G1 S2 S3 S4 S5 S6 S7 L14 A15 L16 D22 Q25 V26 L32 G33 R34 V35 L36 H37 Y38 Y39 L40 T41 Y42 A45 S46 G47 L48 G49 P50 E51 E52 S53 V63 T64 L65 L68 K73 Y74 R75 V76 L77 V78 I81 R86 S87 E88 V90

C98 P99 S100 G101 S102 S103 S104 G105

#### 4.2.16 Score per residue for model 16

- Molecule 1: Collagen alpha-1(XX) chain

Chain A: 

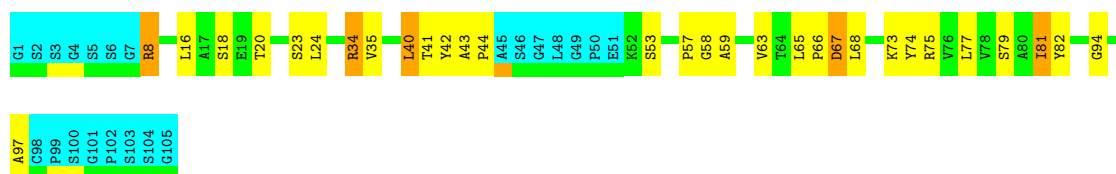
G1 S2 S3 S4 S5 S6 S7 R8 L14 T20 P21 D22 S23 V26 L32 G33 R34 V35 L36 H37 Y38 Y39 L40 T41 Y42 A43 A44 A45 S46 G47 G48 G49 P50 E51 E52 S53 V56 P57 G58 A59 R60 V63 T64 L65 L68 K73 Y74 R75 V76 A80 I81

Y82 E88 A92 C98 P99 S100 G101 P102 S103 S104 G105

#### 4.2.17 Score per residue for model 17

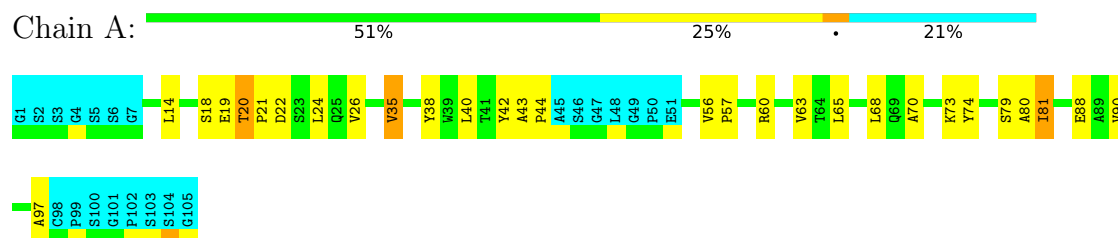
- Molecule 1: Collagen alpha-1(XX) chain

Chain A: 



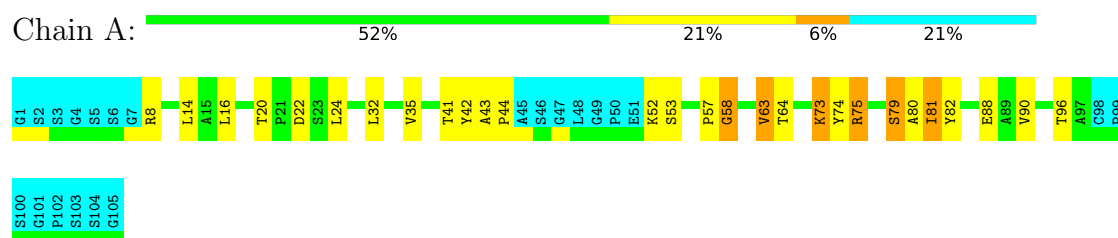
#### 4.2.18 Score per residue for model 18

- Molecule 1: Collagen alpha-1(XX) chain



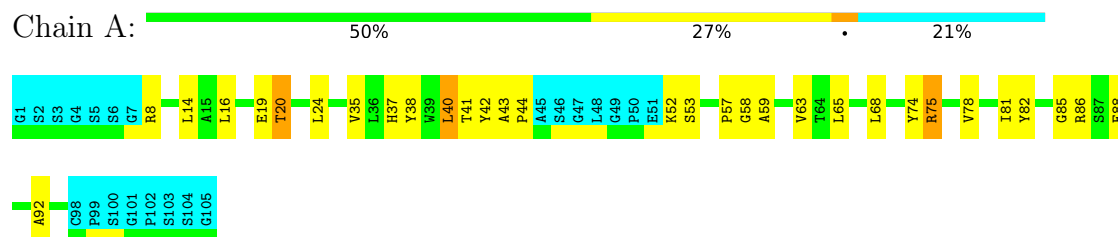
#### 4.2.19 Score per residue for model 19

- Molecule 1: Collagen alpha-1(XX) chain



#### 4.2.20 Score per residue for model 20

- Molecule 1: Collagen alpha-1(XX) chain



## 5 Refinement protocol and experimental data overview

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

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CYANA         | structure solution | 2.0.17  |
| CYANA         | refinement         | 2.0.17  |

No chemical shift data was provided.

## 6 Model quality

### 6.1 Standard geometry

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

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     | 621   | 627      | 625      | 24±5    |
| All | All   | 12420 | 12540    | 12500    | 488     |

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 20.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:68:LEU:HD22 | 1:A:74:TYR:CE2  | 0.87     | 2.05        | 15     | 8     |
| 1:A:42:TYR:CD1  | 1:A:65:LEU:HD22 | 0.84     | 2.07        | 2      | 9     |
| 1:A:40:LEU:HD13 | 1:A:63:VAL:HG11 | 0.81     | 1.50        | 15     | 10    |
| 1:A:42:TYR:CD2  | 1:A:65:LEU:HD22 | 0.80     | 2.11        | 20     | 4     |
| 1:A:26:VAL:HG21 | 1:A:76:VAL:HG11 | 0.79     | 1.54        | 16     | 5     |
| 1:A:37:HIS:NE2  | 1:A:81:ILE:HG21 | 0.75     | 1.96        | 12     | 4     |
| 1:A:40:LEU:HD13 | 1:A:63:VAL:CG1  | 0.74     | 2.12        | 15     | 8     |
| 1:A:35:VAL:HG22 | 1:A:82:TYR:CE1  | 0.71     | 2.20        | 11     | 10    |
| 1:A:35:VAL:HG11 | 1:A:38:TYR:CE1  | 0.71     | 2.21        | 5      | 7     |
| 1:A:43:ALA:HB1  | 1:A:44:PRO:HD2  | 0.70     | 1.63        | 3      | 16    |
| 1:A:28:TRP:CD1  | 1:A:61:SER:HG   | 0.69     | 2.04        | 12     | 2     |
| 1:A:68:LEU:CD2  | 1:A:74:TYR:CE2  | 0.67     | 2.78        | 11     | 4     |
| 1:A:40:LEU:O    | 1:A:41:THR:HG23 | 0.66     | 1.91        | 13     | 1     |
| 1:A:81:ILE:HD13 | 1:A:86:ARG:HB3  | 0.65     | 1.68        | 13     | 6     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:73:LYS:C    | 1:A:74:TYR:CD1  | 0.65     | 2.74        | 14     | 8     |
| 1:A:41:THR:HG22 | 1:A:53:SER:OG   | 0.65     | 1.92        | 19     | 5     |
| 1:A:32:LEU:O    | 1:A:32:LEU:HD13 | 0.64     | 1.92        | 7      | 2     |
| 1:A:41:THR:HG22 | 1:A:53:SER:HB3  | 0.63     | 1.70        | 11     | 8     |
| 1:A:24:LEU:N    | 1:A:68:LEU:HD12 | 0.63     | 2.09        | 5      | 5     |
| 1:A:18:SER:CB   | 1:A:24:LEU:HD12 | 0.63     | 2.22        | 9      | 2     |
| 1:A:40:LEU:HD21 | 1:A:76:VAL:HG13 | 0.61     | 1.72        | 2      | 7     |
| 1:A:18:SER:HB3  | 1:A:24:LEU:HD12 | 0.61     | 1.73        | 9      | 2     |
| 1:A:75:ARG:HD3  | 1:A:77:LEU:HD11 | 0.60     | 1.71        | 17     | 2     |
| 1:A:40:LEU:CD2  | 1:A:65:LEU:HD21 | 0.60     | 2.26        | 13     | 1     |
| 1:A:81:ILE:N    | 1:A:81:ILE:HD12 | 0.60     | 2.12        | 18     | 13    |
| 1:A:81:ILE:CD1  | 1:A:81:ILE:N    | 0.60     | 2.64        | 7      | 11    |
| 1:A:14:LEU:HD11 | 1:A:90:VAL:HG23 | 0.60     | 1.73        | 15     | 9     |
| 1:A:73:LYS:O    | 1:A:74:TYR:CD1  | 0.59     | 2.55        | 14     | 13    |
| 1:A:42:TYR:CZ   | 1:A:52:LYS:CB   | 0.59     | 2.85        | 15     | 8     |
| 1:A:81:ILE:N    | 1:A:81:ILE:CD1  | 0.59     | 2.65        | 18     | 2     |
| 1:A:16:LEU:HD21 | 1:A:76:VAL:CG2  | 0.59     | 2.27        | 15     | 1     |
| 1:A:81:ILE:HD13 | 1:A:86:ARG:CB   | 0.59     | 2.28        | 15     | 7     |
| 1:A:68:LEU:HD22 | 1:A:74:TYR:CZ   | 0.59     | 2.32        | 6      | 7     |
| 1:A:32:LEU:HD12 | 1:A:33:GLY:N    | 0.58     | 2.14        | 11     | 3     |
| 1:A:18:SER:HA   | 1:A:24:LEU:HD12 | 0.57     | 1.75        | 18     | 1     |
| 1:A:40:LEU:HG   | 1:A:78:VAL:HG22 | 0.57     | 1.77        | 20     | 4     |
| 1:A:11:PRO:O    | 1:A:90:VAL:HG21 | 0.57     | 1.99        | 2      | 5     |
| 1:A:66:PRO:C    | 1:A:67:ASP:CG   | 0.56     | 2.73        | 17     | 1     |
| 1:A:8:ARG:HB3   | 1:A:82:TYR:CD2  | 0.55     | 2.36        | 17     | 1     |
| 1:A:26:VAL:HG12 | 1:A:63:VAL:O    | 0.54     | 2.03        | 18     | 1     |
| 1:A:28:TRP:CE2  | 1:A:61:SER:O    | 0.54     | 2.61        | 5      | 3     |
| 1:A:16:LEU:HD21 | 1:A:76:VAL:HG23 | 0.53     | 1.78        | 15     | 1     |
| 1:A:35:VAL:HG21 | 1:A:38:TYR:CE1  | 0.53     | 2.38        | 15     | 2     |
| 1:A:63:VAL:HG22 | 1:A:64:THR:H    | 0.53     | 1.63        | 19     | 3     |
| 1:A:14:LEU:HD13 | 1:A:92:ALA:HB2  | 0.53     | 1.79        | 16     | 3     |
| 1:A:23:SER:C    | 1:A:68:LEU:HD12 | 0.53     | 2.29        | 5      | 1     |
| 1:A:16:LEU:HD23 | 1:A:94:GLY:HA3  | 0.53     | 1.80        | 10     | 3     |
| 1:A:56:VAL:HG13 | 1:A:57:PRO:HD2  | 0.52     | 1.81        | 12     | 10    |
| 1:A:8:ARG:CB    | 1:A:82:TYR:CD2  | 0.52     | 2.92        | 17     | 1     |
| 1:A:32:LEU:HD13 | 1:A:32:LEU:C    | 0.51     | 2.31        | 7      | 2     |
| 1:A:62:HIS:CD2  | 1:A:62:HIS:N    | 0.51     | 2.77        | 6      | 1     |
| 1:A:79:SER:O    | 1:A:81:ILE:CD1  | 0.51     | 2.59        | 4      | 7     |
| 1:A:16:LEU:HD23 | 1:A:24:LEU:HD21 | 0.51     | 1.83        | 19     | 5     |
| 1:A:41:THR:HG22 | 1:A:53:SER:HG   | 0.51     | 1.64        | 19     | 2     |
| 1:A:32:LEU:HD23 | 1:A:32:LEU:O    | 0.50     | 2.06        | 8      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:32:LEU:HD23 | 1:A:32:LEU:C    | 0.50     | 2.31        | 8      | 1     |
| 1:A:70:ALA:O    | 1:A:97:ALA:C    | 0.50     | 2.54        | 11     | 1     |
| 1:A:35:VAL:HG23 | 1:A:81:ILE:O    | 0.50     | 2.06        | 8      | 3     |
| 1:A:57:PRO:O    | 1:A:58:GLY:C    | 0.50     | 2.55        | 4      | 14    |
| 1:A:58:GLY:O    | 1:A:59:ALA:C    | 0.50     | 2.55        | 8      | 10    |
| 1:A:28:TRP:CD1  | 1:A:61:SER:OG   | 0.50     | 2.63        | 12     | 2     |
| 1:A:82:TYR:N    | 1:A:85:GLY:O    | 0.49     | 2.45        | 13     | 3     |
| 1:A:95:GLN:CD   | 1:A:96:THR:O    | 0.49     | 2.55        | 7      | 1     |
| 1:A:66:PRO:O    | 1:A:67:ASP:CG   | 0.49     | 2.56        | 17     | 1     |
| 1:A:80:ALA:C    | 1:A:81:ILE:HD12 | 0.49     | 2.33        | 2      | 11    |
| 1:A:18:SER:CA   | 1:A:24:LEU:HD12 | 0.49     | 2.38        | 18     | 1     |
| 1:A:43:ALA:O    | 1:A:75:ARG:N    | 0.49     | 2.46        | 7      | 4     |
| 1:A:63:VAL:HG22 | 1:A:64:THR:N    | 0.49     | 2.23        | 16     | 1     |
| 1:A:41:THR:HG22 | 1:A:53:SER:CB   | 0.49     | 2.38        | 11     | 2     |
| 1:A:17:ALA:O    | 1:A:25:GLN:N    | 0.49     | 2.45        | 9      | 2     |
| 1:A:8:ARG:HG2   | 1:A:82:TYR:CD2  | 0.48     | 2.44        | 2      | 14    |
| 1:A:22:ASP:N    | 1:A:22:ASP:OD1  | 0.48     | 2.45        | 3      | 1     |
| 1:A:40:LEU:O    | 1:A:41:THR:CG2  | 0.48     | 2.60        | 13     | 1     |
| 1:A:37:HIS:CE1  | 1:A:81:ILE:HG12 | 0.48     | 2.44        | 12     | 9     |
| 1:A:40:LEU:HD22 | 1:A:65:LEU:HD21 | 0.48     | 1.84        | 5      | 2     |
| 1:A:8:ARG:HA    | 1:A:82:TYR:CE2  | 0.48     | 2.44        | 13     | 1     |
| 1:A:38:TYR:O    | 1:A:56:VAL:HG23 | 0.47     | 2.09        | 18     | 1     |
| 1:A:24:LEU:CB   | 1:A:68:LEU:CD1  | 0.47     | 2.93        | 12     | 3     |
| 1:A:42:TYR:CZ   | 1:A:52:LYS:HB2  | 0.47     | 2.44        | 2      | 7     |
| 1:A:62:HIS:CD2  | 1:A:62:HIS:C    | 0.47     | 2.92        | 7      | 1     |
| 1:A:57:PRO:O    | 1:A:59:ALA:N    | 0.47     | 2.48        | 4      | 4     |
| 1:A:38:TYR:CE2  | 1:A:58:GLY:HA2  | 0.47     | 2.45        | 7      | 6     |
| 1:A:38:TYR:O    | 1:A:56:VAL:CG2  | 0.47     | 2.63        | 18     | 1     |
| 1:A:42:TYR:CE2  | 1:A:52:LYS:HB2  | 0.47     | 2.44        | 3      | 1     |
| 1:A:37:HIS:CE1  | 1:A:81:ILE:HG13 | 0.47     | 2.45        | 20     | 6     |
| 1:A:19:GLU:CD   | 1:A:25:GLN:NE2  | 0.47     | 2.73        | 9      | 1     |
| 1:A:72:THR:O    | 1:A:74:TYR:CD1  | 0.46     | 2.68        | 4      | 1     |
| 1:A:40:LEU:CD1  | 1:A:63:VAL:CG1  | 0.46     | 2.91        | 15     | 1     |
| 1:A:19:GLU:CG   | 1:A:20:THR:HG22 | 0.46     | 2.41        | 4      | 5     |
| 1:A:75:ARG:HD2  | 1:A:77:LEU:HD11 | 0.46     | 1.86        | 15     | 1     |
| 1:A:38:TYR:CD2  | 1:A:58:GLY:HA2  | 0.46     | 2.46        | 3      | 4     |
| 1:A:24:LEU:C    | 1:A:64:THR:HG23 | 0.46     | 2.35        | 6      | 1     |
| 1:A:11:PRO:HG3  | 1:A:78:VAL:HG12 | 0.46     | 1.87        | 3      | 2     |
| 1:A:28:TRP:CH2  | 1:A:40:LEU:HD12 | 0.46     | 2.46        | 3      | 2     |
| 1:A:72:THR:O    | 1:A:74:TYR:CE1  | 0.46     | 2.68        | 4      | 2     |
| 1:A:14:LEU:HD11 | 1:A:90:VAL:CG2  | 0.46     | 2.41        | 15     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:26:VAL:CG1  | 1:A:63:VAL:O    | 0.45     | 2.64        | 2      | 3     |
| 1:A:35:VAL:HG13 | 1:A:81:ILE:O    | 0.45     | 2.10        | 2      | 1     |
| 1:A:19:GLU:HG3  | 1:A:20:THR:HG22 | 0.45     | 1.88        | 10     | 3     |
| 1:A:18:SER:OG   | 1:A:97:ALA:N    | 0.45     | 2.50        | 7      | 8     |
| 1:A:68:LEU:HD22 | 1:A:74:TYR:CE1  | 0.45     | 2.47        | 12     | 1     |
| 1:A:70:ALA:O    | 1:A:71:ALA:HB3  | 0.45     | 2.12        | 3      | 1     |
| 1:A:32:LEU:C    | 1:A:32:LEU:CD1  | 0.45     | 2.90        | 7      | 1     |
| 1:A:21:PRO:CB   | 1:A:70:ALA:HB2  | 0.44     | 2.42        | 3      | 1     |
| 1:A:42:TYR:CZ   | 1:A:52:LYS:HB3  | 0.44     | 2.47        | 15     | 1     |
| 1:A:35:VAL:O    | 1:A:36:LEU:C    | 0.44     | 2.60        | 12     | 2     |
| 1:A:34:ARG:O    | 1:A:34:ARG:CD   | 0.44     | 2.66        | 17     | 1     |
| 1:A:61:SER:O    | 1:A:62:HIS:CD2  | 0.44     | 2.71        | 2      | 1     |
| 1:A:40:LEU:CD1  | 1:A:63:VAL:HG11 | 0.43     | 2.42        | 1      | 1     |
| 1:A:17:ALA:O    | 1:A:25:GLN:CB   | 0.43     | 2.66        | 9      | 1     |
| 1:A:73:LYS:O    | 1:A:74:TYR:CG   | 0.43     | 2.71        | 16     | 1     |
| 1:A:24:LEU:HB2  | 1:A:68:LEU:CD1  | 0.43     | 2.44        | 7      | 5     |
| 1:A:57:PRO:C    | 1:A:59:ALA:N    | 0.43     | 2.76        | 3      | 2     |
| 1:A:8:ARG:HB3   | 1:A:82:TYR:CE2  | 0.43     | 2.49        | 2      | 1     |
| 1:A:37:HIS:CE1  | 1:A:81:ILE:HG21 | 0.42     | 2.49        | 12     | 1     |
| 1:A:20:THR:CG2  | 1:A:22:ASP:OD1  | 0.42     | 2.67        | 19     | 1     |
| 1:A:21:PRO:HB3  | 1:A:70:ALA:HB2  | 0.42     | 1.90        | 3      | 1     |
| 1:A:56:VAL:CG1  | 1:A:57:PRO:HD2  | 0.42     | 2.44        | 18     | 1     |
| 1:A:20:THR:C    | 1:A:22:ASP:H    | 0.42     | 2.23        | 19     | 1     |
| 1:A:67:ASP:O    | 1:A:67:ASP:CG   | 0.42     | 2.61        | 6      | 1     |
| 1:A:42:TYR:CB   | 1:A:65:LEU:HD13 | 0.42     | 2.44        | 12     | 1     |
| 1:A:35:VAL:HG11 | 1:A:38:TYR:OH   | 0.42     | 2.14        | 20     | 2     |
| 1:A:57:PRO:HG2  | 1:A:60:ARG:NE   | 0.42     | 2.30        | 14     | 4     |
| 1:A:73:LYS:HD2  | 1:A:73:LYS:C    | 0.42     | 2.39        | 5      | 1     |
| 1:A:75:ARG:CD   | 1:A:77:LEU:HD11 | 0.42     | 2.44        | 15     | 1     |
| 1:A:18:SER:HB3  | 1:A:24:LEU:CD1  | 0.42     | 2.44        | 9      | 1     |
| 1:A:40:LEU:HD23 | 1:A:65:LEU:HD21 | 0.42     | 1.89        | 13     | 1     |
| 1:A:57:PRO:HG2  | 1:A:60:ARG:CD   | 0.42     | 2.45        | 7      | 9     |
| 1:A:8:ARG:CG    | 1:A:82:TYR:CD2  | 0.42     | 3.03        | 16     | 1     |
| 1:A:94:GLY:O    | 1:A:95:GLN:C    | 0.42     | 2.63        | 6      | 1     |
| 1:A:61:SER:C    | 1:A:62:HIS:CG   | 0.41     | 2.98        | 2      | 1     |
| 1:A:24:LEU:N    | 1:A:68:LEU:CD1  | 0.41     | 2.83        | 5      | 1     |
| 1:A:25:GLN:NE2  | 1:A:64:THR:OG1  | 0.41     | 2.53        | 13     | 1     |
| 1:A:28:TRP:CD2  | 1:A:61:SER:O    | 0.41     | 2.73        | 2      | 1     |
| 1:A:70:ALA:HB1  | 1:A:97:ALA:O    | 0.41     | 2.16        | 11     | 1     |
| 1:A:8:ARG:HB3   | 1:A:82:TYR:CE1  | 0.41     | 2.50        | 19     | 1     |
| 1:A:60:ARG:HB3  | 1:A:60:ARG:CZ   | 0.41     | 2.46        | 9      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:70:ALA:O    | 1:A:71:ALA:C    | 0.41     | 2.64        | 1      | 1     |
| 1:A:8:ARG:HG2   | 1:A:82:TYR:CG   | 0.41     | 2.51        | 16     | 1     |
| 1:A:16:LEU:HD22 | 1:A:94:GLY:N    | 0.41     | 2.31        | 7      | 1     |
| 1:A:57:PRO:CG   | 1:A:60:ARG:HD3  | 0.41     | 2.45        | 18     | 1     |
| 1:A:20:THR:O    | 1:A:23:SER:O    | 0.41     | 2.39        | 16     | 3     |
| 1:A:16:LEU:CD2  | 1:A:94:GLY:HA3  | 0.41     | 2.46        | 10     | 1     |
| 1:A:17:ALA:N    | 1:A:25:GLN:O    | 0.41     | 2.54        | 14     | 1     |
| 1:A:32:LEU:H    | 1:A:32:LEU:HD23 | 0.41     | 1.75        | 19     | 1     |
| 1:A:8:ARG:CD    | 1:A:85:GLY:O    | 0.41     | 2.69        | 2      | 1     |
| 1:A:21:PRO:O    | 1:A:68:LEU:O    | 0.40     | 2.40        | 18     | 1     |
| 1:A:37:HIS:O    | 1:A:81:ILE:CG1  | 0.40     | 2.70        | 5      | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured     | Allowed      | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|--------------|------------|-------------|----|
| 1   | A     | 83/105 (79%)    | 71±2 (86±2%) | 10±2 (12±3%) | 1±1 (2±1%) | 9           | 53 |
| All | All   | 1660/2100 (79%) | 1428 (86%)   | 203 (12%)    | 29 (2%)    | 9           | 53 |

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     | 88  | GLU  | 17             |
| 1   | A     | 58  | GLY  | 5              |
| 1   | A     | 75  | ARG  | 3              |
| 1   | A     | 33  | GLY  | 1              |
| 1   | A     | 73  | LYS  | 1              |
| 1   | A     | 34  | ARG  | 1              |
| 1   | A     | 63  | VAL  | 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     | 67/81 (83%)     | 61±2 (92±3%) | 6±2 (8±3%) | 12 59       |
| All | All   | 1340/1620 (83%) | 1228 (92%)   | 112 (8%)   | 12 59       |

All 18 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  | LEU  | 17             |
| 1   | A     | 20  | THR  | 16             |
| 1   | A     | 22  | ASP  | 15             |
| 1   | A     | 81  | ILE  | 13             |
| 1   | A     | 73  | LYS  | 12             |
| 1   | A     | 25  | GLN  | 8              |
| 1   | A     | 23  | SER  | 6              |
| 1   | A     | 35  | VAL  | 6              |
| 1   | A     | 79  | SER  | 5              |
| 1   | A     | 96  | THR  | 3              |
| 1   | A     | 34  | ARG  | 3              |
| 1   | A     | 32  | LEU  | 2              |
| 1   | A     | 26  | VAL  | 1              |
| 1   | A     | 62  | HIS  | 1              |
| 1   | A     | 95  | GLN  | 1              |
| 1   | A     | 53  | SER  | 1              |
| 1   | A     | 8   | ARG  | 1              |
| 1   | A     | 67  | ASP  | 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