



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 2, 2026 – 03:18 AM UTC

PDB ID : 2JP0 / pdb\_00002jp0  
Title : Solution structure of the N-terminal extraceullular domain of the lymphocyte receptor CD5 calculated using inferential structure determination (ISD)  
Authors : Garza-Garcia, A.; Harris, R.; Esposito, D.; Driscoll, P.C.; Rieping, W.  
Deposited on : 2007-04-16

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:

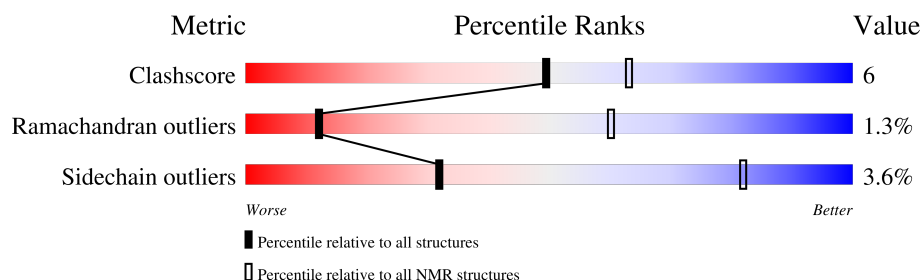
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| 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     | 131    |                  |

## 2 Ensemble composition and analysis

This entry contains 50 models. Model 41 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:26-A:134 (109)      | 0.98              | 41           |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 7 clusters and 12 single-model clusters were found.

| Cluster number        | Models                                          |
|-----------------------|-------------------------------------------------|
| 1                     | 3, 8, 9, 14, 17, 19, 20, 22, 23, 25, 28, 32, 41 |
| 2                     | 1, 10, 11, 12, 13, 15, 27, 36, 37, 38, 48       |
| 3                     | 5, 18, 33, 42                                   |
| 4                     | 4, 6, 21                                        |
| 5                     | 2, 29, 34                                       |
| 6                     | 39, 40                                          |
| 7                     | 44, 47                                          |
| Single-model clusters | 7; 16; 24; 26; 30; 31; 35; 43; 45; 46; 49; 50   |

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1677 atoms, of which 806 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called T-cell surface glycoprotein CD5.

| Mol | Chain | Residues | Atoms |     |     |     |     |    | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|-------|
| 1   | A     | 110      | Total | C   | H   | N   | O   | S  | 0     |
|     |       |          | 1677  | 538 | 806 | 156 | 167 | 10 |       |

There are 23 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 4       | MET      | -      | cloning artifact    | UNP P06127 |
| A     | 5       | GLY      | -      | cloning artifact    | UNP P06127 |
| A     | 6       | GLY      | -      | cloning artifact    | UNP P06127 |
| A     | 7       | SER      | -      | cloning artifact    | UNP P06127 |
| A     | 8       | HIS      | -      | expression tag      | UNP P06127 |
| A     | 9       | HIS      | -      | expression tag      | UNP P06127 |
| A     | 10      | HIS      | -      | expression tag      | UNP P06127 |
| A     | 11      | HIS      | -      | expression tag      | UNP P06127 |
| A     | 12      | HIS      | -      | expression tag      | UNP P06127 |
| A     | 13      | HIS      | -      | expression tag      | UNP P06127 |
| A     | 14      | SER      | -      | cloning artifact    | UNP P06127 |
| A     | 15      | SER      | -      | cloning artifact    | UNP P06127 |
| A     | 16      | GLY      | -      | cloning artifact    | UNP P06127 |
| A     | 17      | LEU      | -      | cloning artifact    | UNP P06127 |
| A     | 18      | VAL      | -      | cloning artifact    | UNP P06127 |
| A     | 19      | PRO      | -      | cloning artifact    | UNP P06127 |
| A     | 20      | ARG      | -      | cloning artifact    | UNP P06127 |
| A     | 21      | GLY      | -      | cloning artifact    | UNP P06127 |
| A     | 22      | SER      | -      | cloning artifact    | UNP P06127 |
| A     | 23      | HIS      | -      | cloning artifact    | UNP P06127 |
| A     | 24      | MET      | -      | cloning artifact    | UNP P06127 |
| A     | 88      | ASP      | VAL    | engineered mutation | UNP P06127 |
| A     | 97      | LYS      | VAL    | engineered mutation | UNP P06127 |

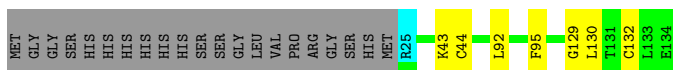
## 4 Residue-property plots [i](#)

### 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: T-cell surface glycoprotein CD5

Chain A: 



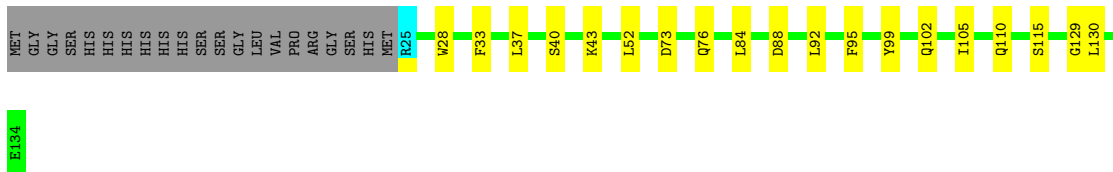
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: T-cell surface glycoprotein CD5

Chain A: 



E134

#### 4.2.2 Score per residue for model 2

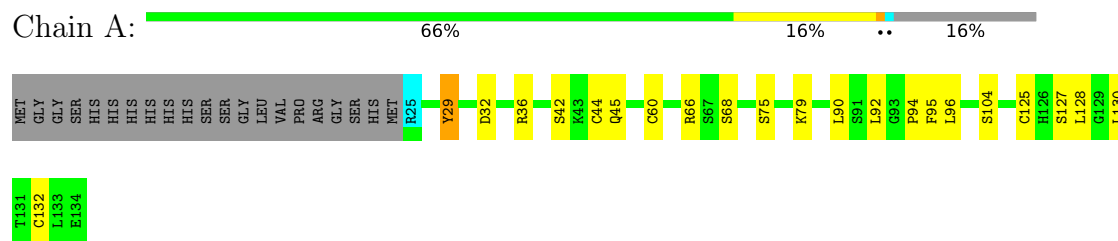
- Molecule 1: T-cell surface glycoprotein CD5

Chain A: 



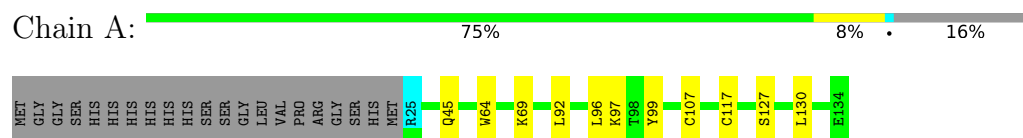
### 4.2.3 Score per residue for model 3

- Molecule 1: T-cell surface glycoprotein CD5



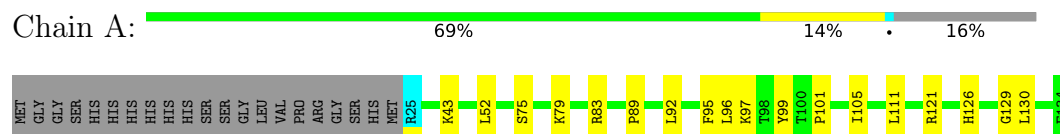
### 4.2.4 Score per residue for model 4

- Molecule 1: T-cell surface glycoprotein CD5



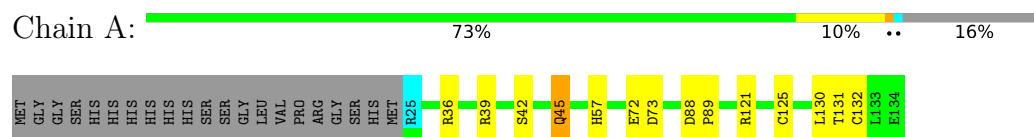
### 4.2.5 Score per residue for model 5

- Molecule 1: T-cell surface glycoprotein CD5



### 4.2.6 Score per residue for model 6

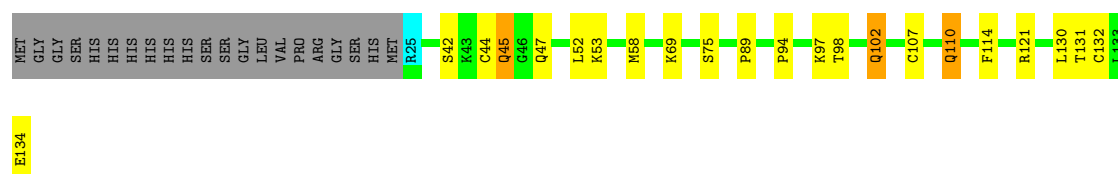
- Molecule 1: T-cell surface glycoprotein CD5



### 4.2.7 Score per residue for model 7

- Molecule 1: T-cell surface glycoprotein CD5

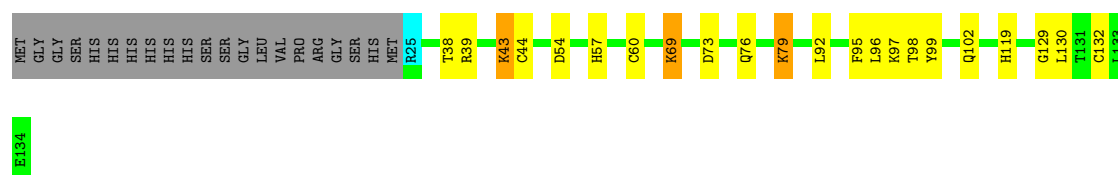




#### 4.2.8 Score per residue for model 8

- Molecule 1: T-cell surface glycoprotein CD5

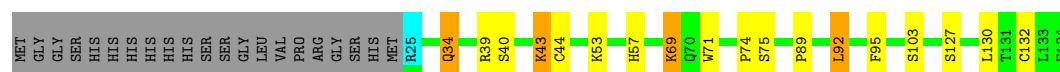
Chain A: 66% 15% .. 16%



#### 4.2.9 Score per residue for model 9

- Molecule 1: T-cell surface glycoprotein CD5

Chain A: 69% 11% .. 16%



#### 4.2.10 Score per residue for model 10

- Molecule 1: T-cell surface glycoprotein CD5

Chain A: 71% 11% .. 16%



#### 4.2.11 Score per residue for model 11

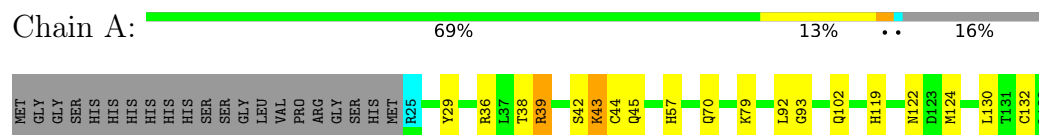
- Molecule 1: T-cell surface glycoprotein CD5

Chain A: 69% 14% . 16%



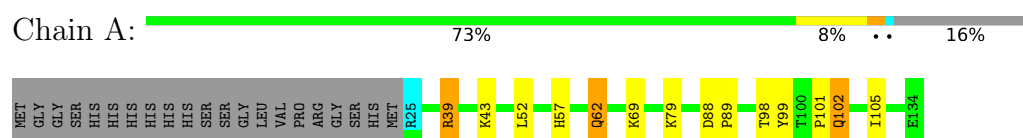
### 4.2.12 Score per residue for model 12

- Molecule 1: T-cell surface glycoprotein CD5



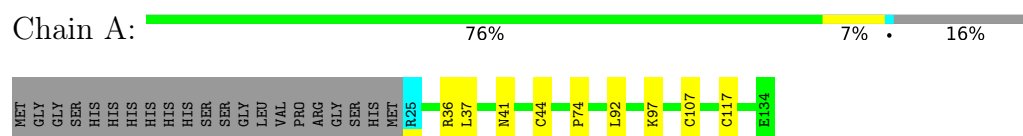
### 4.2.13 Score per residue for model 13

- Molecule 1: T-cell surface glycoprotein CD5



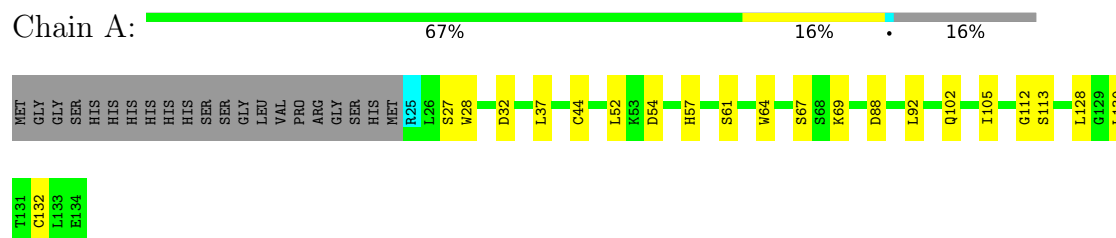
### 4.2.14 Score per residue for model 14

- Molecule 1: T-cell surface glycoprotein CD5



### 4.2.15 Score per residue for model 15

- Molecule 1: T-cell surface glycoprotein CD5



### 4.2.16 Score per residue for model 16

- Molecule 1: T-cell surface glycoprotein CD5





#### 4.2.17 Score per residue for model 17

- Molecule 1: T-cell surface glycoprotein CD5

Chain A: 63% 18% .. 16%



#### 4.2.18 Score per residue for model 18

- Molecule 1: T-cell surface glycoprotein CD5

Chain A: 70% 11% .. 16%



#### 4.2.19 Score per residue for model 19

- Molecule 1: T-cell surface glycoprotein CD5

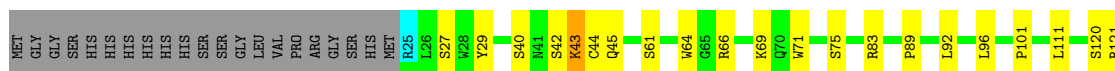
Chain A: 67% 14% .. 16%



#### 4.2.20 Score per residue for model 20

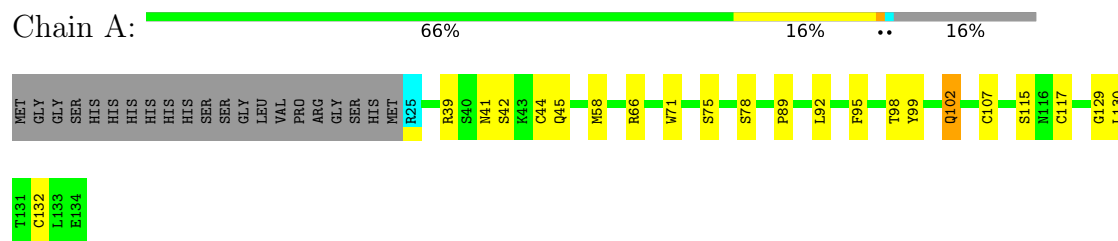
- Molecule 1: T-cell surface glycoprotein CD5

Chain A: 63% 19% .. 16%



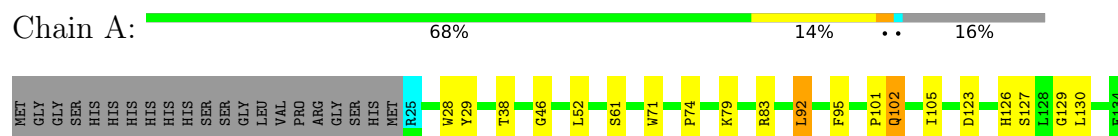
#### 4.2.21 Score per residue for model 21

- Molecule 1: T-cell surface glycoprotein CD5



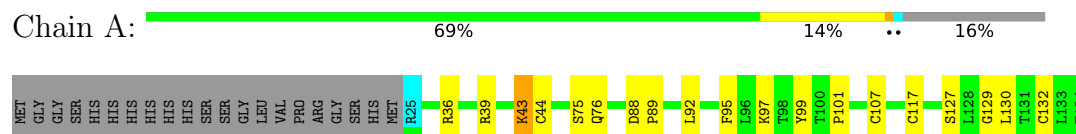
#### 4.2.22 Score per residue for model 22

- Molecule 1: T-cell surface glycoprotein CD5



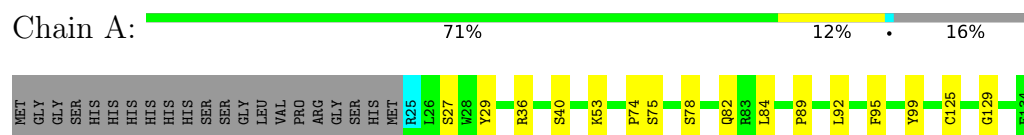
#### 4.2.23 Score per residue for model 23

- Molecule 1: T-cell surface glycoprotein CD5



#### 4.2.24 Score per residue for model 24

- Molecule 1: T-cell surface glycoprotein CD5



#### 4.2.25 Score per residue for model 25

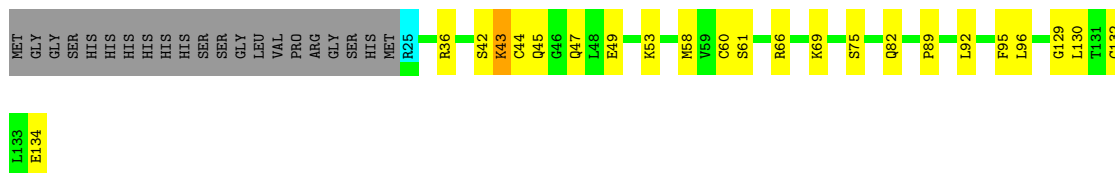
- Molecule 1: T-cell surface glycoprotein CD5





#### 4.2.26 Score per residue for model 26

- Molecule 1: T-cell surface glycoprotein CD5



#### 4.2.27 Score per residue for model 27

- Molecule 1: T-cell surface glycoprotein CD5



#### 4.2.28 Score per residue for model 28

- Molecule 1: T-cell surface glycoprotein CD5



#### 4.2.29 Score per residue for model 29

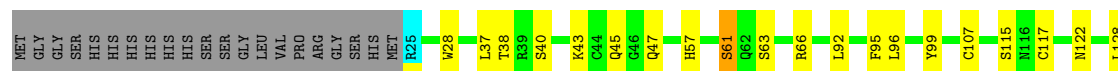
- Molecule 1: T-cell surface glycoprotein CD5



### 4.2.30 Score per residue for model 30

- Molecule 1: T-cell surface glycoprotein CD5

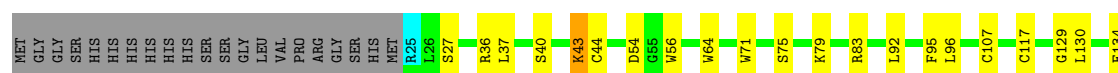
Chain A: 



### 4.2.31 Score per residue for model 31

- Molecule 1: T-cell surface glycoprotein CD5

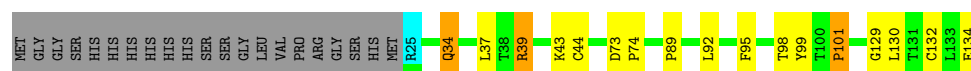
Chain A: 



### 4.2.32 Score per residue for model 32

- Molecule 1: T-cell surface glycoprotein CD5

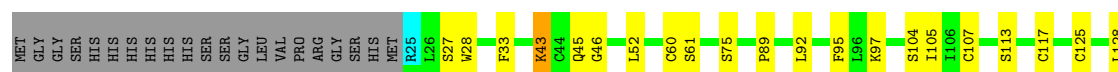
Chain A: 



### 4.2.33 Score per residue for model 33

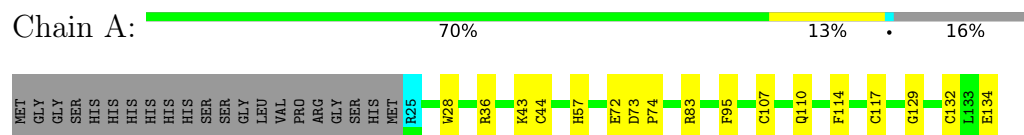
- Molecule 1: T-cell surface glycoprotein CD5

Chain A: 



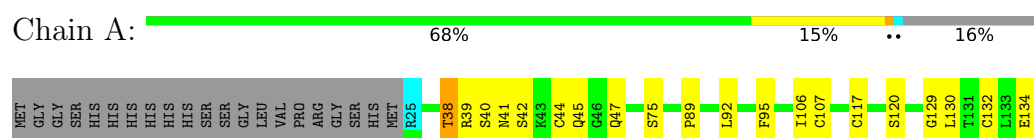
#### 4.2.34 Score per residue for model 34

- Molecule 1: T-cell surface glycoprotein CD5



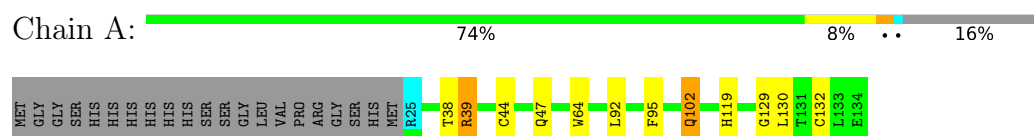
#### 4.2.35 Score per residue for model 35

- Molecule 1: T-cell surface glycoprotein CD5



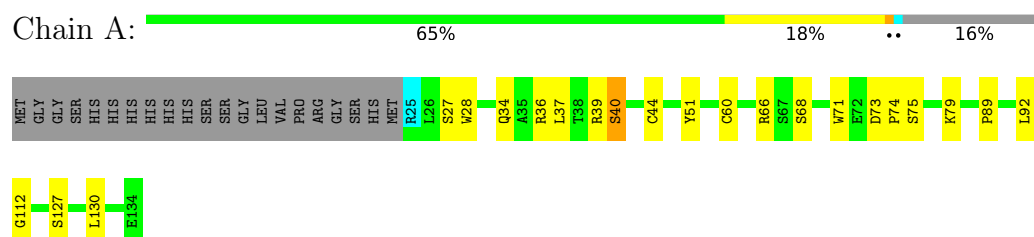
#### 4.2.36 Score per residue for model 36

- Molecule 1: T-cell surface glycoprotein CD5



#### 4.2.37 Score per residue for model 37

- Molecule 1: T-cell surface glycoprotein CD5



#### 4.2.38 Score per residue for model 38

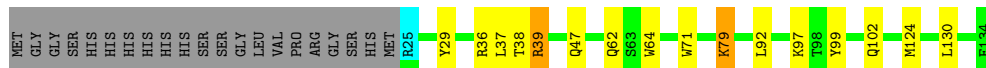
- Molecule 1: T-cell surface glycoprotein CD5





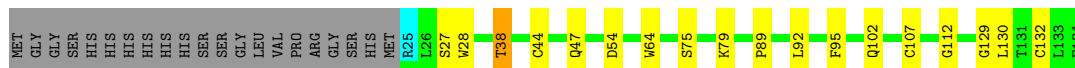
#### 4.2.39 Score per residue for model 39

- Molecule 1: T-cell surface glycoprotein CD5



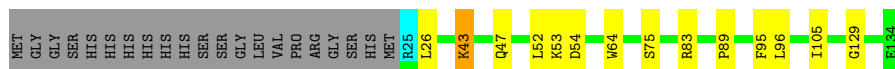
#### 4.2.40 Score per residue for model 40

- Molecule 1: T-cell surface glycoprotein CD5



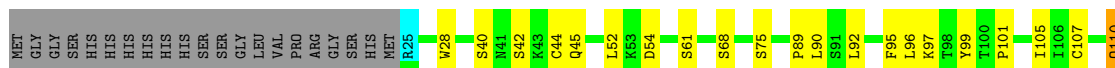
#### 4.2.41 Score per residue for model 41 (medoid)

- Molecule 1: T-cell surface glycoprotein CD5



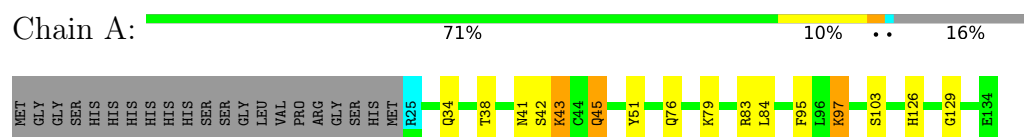
#### 4.2.42 Score per residue for model 42

- Molecule 1: T-cell surface glycoprotein CD5



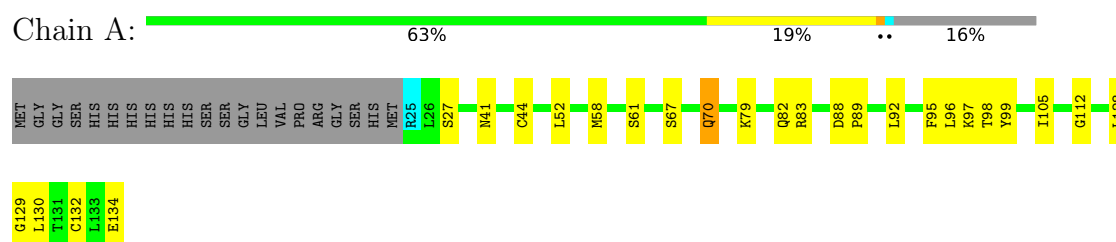
#### 4.2.43 Score per residue for model 43

- Molecule 1: T-cell surface glycoprotein CD5



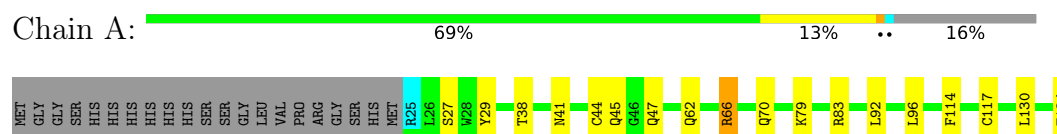
#### 4.2.44 Score per residue for model 44

- Molecule 1: T-cell surface glycoprotein CD5



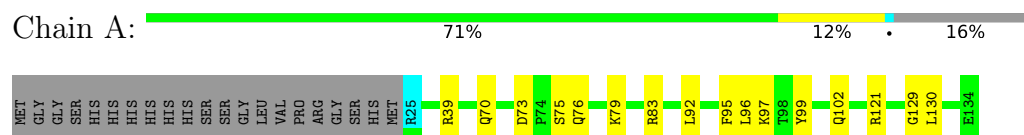
#### 4.2.45 Score per residue for model 45

- Molecule 1: T-cell surface glycoprotein CD5



#### 4.2.46 Score per residue for model 46

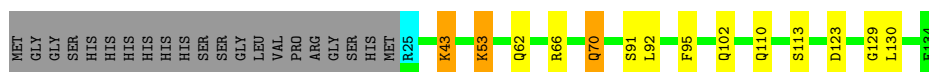
- Molecule 1: T-cell surface glycoprotein CD5



#### 4.2.47 Score per residue for model 47

- Molecule 1: T-cell surface glycoprotein CD5





#### 4.2.48 Score per residue for model 48

- Molecule 1: T-cell surface glycoprotein CD5

Chain A: 69% 12% • 16%



#### 4.2.49 Score per residue for model 49

- Molecule 1: T-cell surface glycoprotein CD5

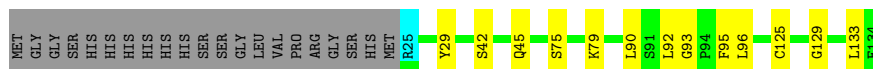
Chain A: 72% 11% • 16%



#### 4.2.50 Score per residue for model 50

- Molecule 1: T-cell surface glycoprotein CD5

Chain A: 73% 10% • 16%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *Inferential structure determination*.

Of the 500 calculated structures, 50 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 |
|-------------------------------------|--------------------|---------|
| CNS                                 | structure solution | 1.1     |
| X-PLOR NIH                          | structure solution |         |
| Inferential Structure Determination | refinement         |         |

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     | 860   | 795      | 805      | 10±3    |
| All | All   | 43000 | 39750    | 40250    | 478     |

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 6.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:95:PHE:HB2   | 1:A:129:GLY:HA3  | 0.87     | 1.41        | 41     | 26    |
| 1:A:44:CYS:HB3   | 1:A:134:GLU:HG2  | 0.83     | 1.47        | 32     | 2     |
| 1:A:75:SER:HA    | 1:A:89:PRO:HG2   | 0.81     | 1.52        | 24     | 17    |
| 1:A:42:SER:HB3   | 1:A:45:GLN:HB3   | 0.80     | 1.52        | 3      | 5     |
| 1:A:52:LEU:HD11  | 1:A:105:ILE:HD13 | 0.75     | 1.56        | 5      | 13    |
| 1:A:110:GLN:HE21 | 1:A:110:GLN:HA   | 0.74     | 1.40        | 42     | 2     |
| 1:A:74:PRO:HB3   | 1:A:92:LEU:HB2   | 0.73     | 1.60        | 17     | 4     |
| 1:A:92:LEU:HG    | 1:A:130:LEU:HD13 | 0.73     | 1.60        | 9      | 10    |
| 1:A:92:LEU:HD12  | 1:A:130:LEU:HD13 | 0.73     | 1.61        | 37     | 9     |
| 1:A:42:SER:HB2   | 1:A:45:GLN:HB3   | 0.72     | 1.59        | 7      | 2     |
| 1:A:43:LYS:HA    | 1:A:43:LYS:HE3   | 0.72     | 1.61        | 43     | 2     |
| 1:A:92:LEU:HD13  | 1:A:130:LEU:HD13 | 0.71     | 1.62        | 15     | 16    |
| 1:A:79:LYS:HA    | 1:A:79:LYS:HE3   | 0.69     | 1.62        | 38     | 2     |
| 1:A:39:ARG:H     | 1:A:39:ARG:HD3   | 0.69     | 1.48        | 21     | 6     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:36:ARG:HH11  | 1:A:39:ARG:HH21  | 0.69     | 1.30        | 18     | 1     |
| 1:A:34:GLN:HE21  | 1:A:34:GLN:HA    | 0.69     | 1.48        | 38     | 2     |
| 1:A:60:CYS:SG    | 1:A:104:SER:HB2  | 0.69     | 2.28        | 33     | 2     |
| 1:A:95:PHE:HB3   | 1:A:129:GLY:HA3  | 0.68     | 1.64        | 21     | 4     |
| 1:A:69:LYS:HA    | 1:A:69:LYS:HE2   | 0.68     | 1.65        | 20     | 1     |
| 1:A:101:PRO:HB3  | 1:A:123:ASP:HA   | 0.68     | 1.66        | 22     | 1     |
| 1:A:83:ARG:HA    | 1:A:83:ARG:NE    | 0.67     | 2.05        | 11     | 5     |
| 1:A:58:MET:HE1   | 1:A:98:THR:HG21  | 0.66     | 1.67        | 7      | 1     |
| 1:A:62:GLN:HE21  | 1:A:62:GLN:HA    | 0.66     | 1.51        | 16     | 2     |
| 1:A:44:CYS:SG    | 1:A:132:CYS:HB2  | 0.65     | 2.31        | 18     | 14    |
| 1:A:44:CYS:HB2   | 1:A:134:GLU:HB3  | 0.64     | 1.69        | 16     | 3     |
| 1:A:39:ARG:H     | 1:A:39:ARG:HD2   | 0.64     | 1.51        | 36     | 2     |
| 1:A:53:LYS:H     | 1:A:53:LYS:HD3   | 0.62     | 1.54        | 2      | 2     |
| 1:A:76:GLN:HE21  | 1:A:76:GLN:HA    | 0.62     | 1.54        | 17     | 1     |
| 1:A:44:CYS:HB3   | 1:A:132:CYS:HB2  | 0.62     | 1.72        | 44     | 11    |
| 1:A:61:SER:HB2   | 1:A:126:HIS:HD2  | 0.61     | 1.55        | 22     | 1     |
| 1:A:74:PRO:HA    | 1:A:92:LEU:HD12  | 0.61     | 1.73        | 24     | 1     |
| 1:A:89:PRO:HB3   | 1:A:130:LEU:HD21 | 0.60     | 1.73        | 6      | 2     |
| 1:A:79:LYS:HE2   | 1:A:79:LYS:HA    | 0.60     | 1.74        | 13     | 2     |
| 1:A:53:LYS:H     | 1:A:53:LYS:HD2   | 0.59     | 1.56        | 26     | 2     |
| 1:A:43:LYS:HD3   | 1:A:43:LYS:H     | 0.59     | 1.57        | 47     | 7     |
| 1:A:62:GLN:HA    | 1:A:66:ARG:HA    | 0.58     | 1.74        | 45     | 1     |
| 1:A:52:LEU:HG    | 1:A:53:LYS:H     | 0.58     | 1.58        | 29     | 2     |
| 1:A:47:GLN:HE22  | 1:A:98:THR:HB    | 0.58     | 1.59        | 16     | 1     |
| 1:A:29:TYR:HA    | 1:A:79:LYS:HD2   | 0.58     | 1.76        | 50     | 1     |
| 1:A:49:GLU:HG2   | 1:A:58:MET:HG2   | 0.58     | 1.76        | 27     | 2     |
| 1:A:42:SER:HB3   | 1:A:45:GLN:HG2   | 0.58     | 1.75        | 42     | 2     |
| 1:A:61:SER:HB2   | 1:A:126:HIS:CD2  | 0.58     | 2.34        | 22     | 1     |
| 1:A:42:SER:HB2   | 1:A:45:GLN:HB2   | 0.57     | 1.75        | 35     | 2     |
| 1:A:70:GLN:HE21  | 1:A:70:GLN:HA    | 0.57     | 1.59        | 47     | 1     |
| 1:A:37:LEU:HD12  | 1:A:44:CYS:HA    | 0.57     | 1.77        | 17     | 6     |
| 1:A:58:MET:HE1   | 1:A:98:THR:HB    | 0.57     | 1.74        | 44     | 2     |
| 1:A:97:LYS:HD3   | 1:A:97:LYS:H     | 0.57     | 1.58        | 43     | 1     |
| 1:A:102:GLN:HE21 | 1:A:102:GLN:HA   | 0.56     | 1.59        | 13     | 3     |
| 1:A:95:PHE:CB    | 1:A:129:GLY:HA3  | 0.56     | 2.31        | 27     | 17    |
| 1:A:27:SER:HA    | 1:A:113:SER:HA   | 0.56     | 1.78        | 15     | 2     |
| 1:A:102:GLN:HA   | 1:A:119:HIS:CE1  | 0.56     | 2.36        | 12     | 3     |
| 1:A:102:GLN:HA   | 1:A:119:HIS:NE2  | 0.56     | 2.15        | 36     | 3     |
| 1:A:71:TRP:CZ2   | 1:A:92:LEU:HD22  | 0.55     | 2.36        | 22     | 4     |
| 1:A:43:LYS:NZ    | 1:A:43:LYS:HB2   | 0.55     | 2.16        | 19     | 1     |
| 1:A:28:TRP:CE2   | 1:A:112:GLY:HA2  | 0.55     | 2.37        | 42     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:54:ASP:HB2   | 1:A:57:HIS:HE1   | 0.55     | 1.61        | 15     | 1     |
| 1:A:44:CYS:SG    | 1:A:134:GLU:HB2  | 0.55     | 2.42        | 26     | 2     |
| 1:A:61:SER:HA    | 1:A:128:LEU:HD12 | 0.55     | 1.79        | 15     | 5     |
| 1:A:97:LYS:HA    | 1:A:126:HIS:HD2  | 0.55     | 1.61        | 43     | 1     |
| 1:A:39:ARG:HD2   | 1:A:40:SER:N     | 0.55     | 2.17        | 37     | 1     |
| 1:A:96:LEU:HG    | 1:A:97:LYS:H     | 0.54     | 1.62        | 44     | 1     |
| 1:A:122:ASN:OD1  | 1:A:124:MET:HG2  | 0.54     | 2.02        | 12     | 2     |
| 1:A:66:ARG:HH12  | 1:A:111:LEU:HD11 | 0.54     | 1.63        | 38     | 1     |
| 1:A:44:CYS:HB2   | 1:A:134:GLU:HB2  | 0.54     | 1.79        | 19     | 3     |
| 1:A:43:LYS:H     | 1:A:43:LYS:HD2   | 0.53     | 1.63        | 23     | 3     |
| 1:A:99:TYR:C     | 1:A:101:PRO:HD3  | 0.53     | 2.28        | 23     | 3     |
| 1:A:58:MET:HE1   | 1:A:99:TYR:HA    | 0.53     | 1.79        | 16     | 1     |
| 1:A:39:ARG:HH11  | 1:A:39:ARG:HG2   | 0.53     | 1.62        | 6      | 1     |
| 1:A:69:LYS:HA    | 1:A:94:PRO:HD2   | 0.53     | 1.80        | 7      | 1     |
| 1:A:73:ASP:OD1   | 1:A:76:GLN:HG2   | 0.53     | 2.04        | 1      | 4     |
| 1:A:95:PHE:HB2   | 1:A:129:GLY:CA   | 0.53     | 2.33        | 24     | 2     |
| 1:A:72:GLU:HG3   | 1:A:73:ASP:H     | 0.53     | 1.64        | 6      | 1     |
| 1:A:27:SER:HA    | 1:A:112:GLY:O    | 0.52     | 2.04        | 44     | 3     |
| 1:A:66:ARG:HD3   | 1:A:71:TRP:HD1   | 0.52     | 1.64        | 21     | 1     |
| 1:A:66:ARG:N     | 1:A:66:ARG:HD2   | 0.52     | 2.19        | 48     | 1     |
| 1:A:95:PHE:CD2   | 1:A:96:LEU:HG    | 0.52     | 2.39        | 26     | 8     |
| 1:A:38:THR:HB    | 1:A:39:ARG:NH1   | 0.51     | 2.19        | 12     | 1     |
| 1:A:28:TRP:HA    | 1:A:33:PHE:CD2   | 0.51     | 2.40        | 1      | 2     |
| 1:A:37:LEU:H     | 1:A:84:LEU:HD21  | 0.51     | 1.65        | 1      | 1     |
| 1:A:121:ARG:O    | 1:A:121:ARG:HD2  | 0.51     | 2.06        | 27     | 1     |
| 1:A:61:SER:HB3   | 1:A:128:LEU:HA   | 0.51     | 1.83        | 30     | 1     |
| 1:A:47:GLN:NE2   | 1:A:58:MET:HE3   | 0.51     | 2.21        | 7      | 1     |
| 1:A:107:CYS:SG   | 1:A:114:PHE:HA   | 0.51     | 2.46        | 34     | 4     |
| 1:A:70:GLN:HB3   | 1:A:92:LEU:O     | 0.51     | 2.06        | 19     | 1     |
| 1:A:79:LYS:O     | 1:A:83:ARG:HG2   | 0.51     | 2.05        | 31     | 9     |
| 1:A:78:SER:HA    | 1:A:89:PRO:HG3   | 0.51     | 1.83        | 29     | 1     |
| 1:A:78:SER:HA    | 1:A:89:PRO:HD3   | 0.50     | 1.83        | 21     | 1     |
| 1:A:71:TRP:HZ2   | 1:A:92:LEU:HD22  | 0.50     | 1.64        | 20     | 1     |
| 1:A:45:GLN:HA    | 1:A:130:LEU:O    | 0.50     | 2.06        | 30     | 2     |
| 1:A:63:SER:O     | 1:A:66:ARG:HG2   | 0.50     | 2.05        | 30     | 1     |
| 1:A:130:LEU:HD23 | 1:A:131:THR:N    | 0.50     | 2.21        | 7      | 3     |
| 1:A:66:ARG:HG3   | 1:A:111:LEU:HD12 | 0.50     | 1.83        | 49     | 1     |
| 1:A:107:CYS:HA   | 1:A:117:CYS:HA   | 0.50     | 1.82        | 14     | 15    |
| 1:A:97:LYS:HB3   | 1:A:99:TYR:CE2   | 0.50     | 2.42        | 42     | 6     |
| 1:A:99:TYR:O     | 1:A:101:PRO:HD3  | 0.50     | 2.07        | 32     | 3     |
| 1:A:68:SER:C     | 1:A:94:PRO:HG2   | 0.50     | 2.32        | 37     | 1     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:36:ARG:HH11  | 1:A:39:ARG:NH2  | 0.49     | 2.02        | 18     | 1     |
| 1:A:66:ARG:NH1   | 1:A:71:TRP:H    | 0.49     | 2.05        | 37     | 2     |
| 1:A:29:TYR:HA    | 1:A:79:LYS:HG2  | 0.49     | 1.83        | 39     | 1     |
| 1:A:62:GLN:HG2   | 1:A:124:MET:HE3 | 0.49     | 1.84        | 39     | 1     |
| 1:A:43:LYS:O     | 1:A:84:LEU:HD13 | 0.49     | 2.08        | 43     | 1     |
| 1:A:69:LYS:HA    | 1:A:69:LYS:HE3  | 0.48     | 1.85        | 10     | 3     |
| 1:A:61:SER:O     | 1:A:66:ARG:HB2  | 0.48     | 2.08        | 26     | 1     |
| 1:A:68:SER:HA    | 1:A:94:PRO:HG2  | 0.48     | 1.84        | 3      | 1     |
| 1:A:43:LYS:N     | 1:A:43:LYS:HE3  | 0.48     | 2.22        | 26     | 1     |
| 1:A:130:LEU:HD22 | 1:A:132:CYS:SG  | 0.48     | 2.49        | 6      | 2     |
| 1:A:30:ASP:HB2   | 1:A:33:PHE:HB2  | 0.48     | 1.84        | 49     | 1     |
| 1:A:39:ARG:H     | 1:A:39:ARG:CD   | 0.48     | 2.21        | 32     | 1     |
| 1:A:36:ARG:NH1   | 1:A:39:ARG:HH21 | 0.47     | 2.02        | 18     | 1     |
| 1:A:27:SER:C     | 1:A:29:TYR:H    | 0.47     | 2.17        | 20     | 3     |
| 1:A:67:SER:HB2   | 1:A:69:LYS:HG2  | 0.47     | 1.85        | 15     | 1     |
| 1:A:42:SER:HB3   | 1:A:45:GLN:OE1  | 0.47     | 2.08        | 26     | 2     |
| 1:A:29:TYR:HA    | 1:A:79:LYS:HD3  | 0.47     | 1.86        | 12     | 2     |
| 1:A:72:GLU:C     | 1:A:74:PRO:HD3  | 0.47     | 2.34        | 34     | 1     |
| 1:A:62:GLN:HB3   | 1:A:66:ARG:HG3  | 0.47     | 1.85        | 47     | 1     |
| 1:A:83:ARG:HA    | 1:A:83:ARG:CZ   | 0.47     | 2.40        | 20     | 1     |
| 1:A:38:THR:HG21  | 1:A:47:GLN:HB2  | 0.47     | 1.86        | 40     | 1     |
| 1:A:43:LYS:HG2   | 1:A:134:GLU:OE2 | 0.47     | 2.09        | 29     | 1     |
| 1:A:42:SER:HB3   | 1:A:45:GLN:HG3  | 0.46     | 1.87        | 27     | 2     |
| 1:A:122:ASN:ND2  | 1:A:124:MET:HG2 | 0.46     | 2.25        | 49     | 1     |
| 1:A:79:LYS:HE3   | 1:A:79:LYS:CA   | 0.46     | 2.38        | 38     | 1     |
| 1:A:97:LYS:HD3   | 1:A:126:HIS:HD2 | 0.46     | 1.71        | 5      | 1     |
| 1:A:37:LEU:HD21  | 1:A:130:LEU:HB3 | 0.46     | 1.87        | 32     | 3     |
| 1:A:121:ARG:CZ   | 1:A:121:ARG:HA  | 0.46     | 2.41        | 20     | 1     |
| 1:A:102:GLN:HG3  | 1:A:119:HIS:HE1 | 0.46     | 1.70        | 25     | 1     |
| 1:A:36:ARG:NH1   | 1:A:39:ARG:HH22 | 0.45     | 2.09        | 6      | 1     |
| 1:A:99:TYR:HA    | 1:A:123:ASP:O   | 0.45     | 2.12        | 19     | 1     |
| 1:A:96:LEU:HG    | 1:A:97:LYS:N    | 0.45     | 2.26        | 44     | 1     |
| 1:A:97:LYS:NZ    | 1:A:97:LYS:HB2  | 0.45     | 2.26        | 46     | 1     |
| 1:A:61:SER:OG    | 1:A:126:HIS:HB2 | 0.45     | 2.12        | 48     | 1     |
| 1:A:61:SER:O     | 1:A:68:SER:HA   | 0.45     | 2.11        | 42     | 1     |
| 1:A:73:ASP:N     | 1:A:74:PRO:HD3  | 0.45     | 2.27        | 11     | 4     |
| 1:A:43:LYS:HD2   | 1:A:43:LYS:N    | 0.45     | 2.27        | 33     | 1     |
| 1:A:38:THR:OG1   | 1:A:47:GLN:HB2  | 0.45     | 2.12        | 36     | 4     |
| 1:A:69:LYS:HA    | 1:A:94:PRO:CD   | 0.45     | 2.42        | 7      | 1     |
| 1:A:47:GLN:HG3   | 1:A:96:LEU:HD12 | 0.45     | 1.89        | 41     | 2     |
| 1:A:122:ASN:HD22 | 1:A:124:MET:HG2 | 0.45     | 1.70        | 49     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:88:ASP:CG    | 1:A:89:PRO:HD2   | 0.44     | 2.37        | 44     | 1     |
| 1:A:42:SER:HB2   | 1:A:45:GLN:O     | 0.44     | 2.12        | 50     | 1     |
| 1:A:95:PHE:O     | 1:A:127:SER:HB2  | 0.44     | 2.12        | 3      | 1     |
| 1:A:37:LEU:HB2   | 1:A:43:LYS:O     | 0.44     | 2.12        | 30     | 1     |
| 1:A:42:SER:HB3   | 1:A:45:GLN:CG    | 0.44     | 2.43        | 42     | 1     |
| 1:A:26:LEU:HD11  | 1:A:53:LYS:HE3   | 0.44     | 1.88        | 41     | 1     |
| 1:A:44:CYS:CB    | 1:A:134:GLU:HB3  | 0.44     | 2.42        | 7      | 2     |
| 1:A:39:ARG:HD3   | 1:A:39:ARG:N     | 0.44     | 2.28        | 13     | 2     |
| 1:A:101:PRO:HB2  | 1:A:120:SER:O    | 0.44     | 2.13        | 20     | 1     |
| 1:A:62:GLN:O     | 1:A:66:ARG:HD3   | 0.44     | 2.13        | 45     | 1     |
| 1:A:92:LEU:HG    | 1:A:93:GLY:N     | 0.44     | 2.27        | 19     | 2     |
| 1:A:74:PRO:HB2   | 1:A:89:PRO:HB2   | 0.44     | 1.90        | 32     | 1     |
| 1:A:38:THR:HG21  | 1:A:47:GLN:HE21  | 0.44     | 1.73        | 40     | 1     |
| 1:A:114:PHE:HA   | 1:A:117:CYS:SG   | 0.44     | 2.53        | 45     | 1     |
| 1:A:28:TRP:HD1   | 1:A:29:TYR:HD1   | 0.43     | 1.56        | 22     | 1     |
| 1:A:88:ASP:OD1   | 1:A:89:PRO:HD2   | 0.43     | 2.13        | 13     | 1     |
| 1:A:34:GLN:HB2   | 1:A:51:TYR:HB3   | 0.43     | 1.89        | 43     | 3     |
| 1:A:42:SER:HB3   | 1:A:134:GLU:OE1  | 0.43     | 2.14        | 20     | 1     |
| 1:A:101:PRO:HB2  | 1:A:121:ARG:HD2  | 0.43     | 1.89        | 5      | 1     |
| 1:A:75:SER:HA    | 1:A:89:PRO:HB2   | 0.43     | 1.90        | 35     | 2     |
| 1:A:28:TRP:O     | 1:A:79:LYS:HB2   | 0.43     | 2.14        | 37     | 1     |
| 1:A:38:THR:CG2   | 1:A:47:GLN:HB2   | 0.43     | 2.43        | 40     | 1     |
| 1:A:70:GLN:OE1   | 1:A:91:SER:HB3   | 0.43     | 2.13        | 47     | 1     |
| 1:A:95:PHE:HB3   | 1:A:96:LEU:HD12  | 0.43     | 1.91        | 30     | 1     |
| 1:A:79:LYS:HE2   | 1:A:83:ARG:HG2   | 0.43     | 1.91        | 38     | 1     |
| 1:A:37:LEU:HA    | 1:A:47:GLN:O     | 0.43     | 2.13        | 39     | 1     |
| 1:A:70:GLN:CD    | 1:A:70:GLN:H     | 0.43     | 2.21        | 45     | 2     |
| 1:A:92:LEU:HD11  | 1:A:128:LEU:HD21 | 0.43     | 1.91        | 3      | 2     |
| 1:A:66:ARG:HD3   | 1:A:71:TRP:CD1   | 0.43     | 2.48        | 21     | 1     |
| 1:A:66:ARG:HB3   | 1:A:71:TRP:CH2   | 0.43     | 2.48        | 16     | 1     |
| 1:A:69:LYS:HG2   | 1:A:70:GLN:H     | 0.42     | 1.73        | 2      | 1     |
| 1:A:70:GLN:HG2   | 1:A:93:GLY:HA3   | 0.42     | 1.89        | 12     | 1     |
| 1:A:70:GLN:HG3   | 1:A:92:LEU:O     | 0.42     | 2.14        | 16     | 1     |
| 1:A:96:LEU:HB2   | 1:A:127:SER:HB2  | 0.42     | 1.92        | 37     | 2     |
| 1:A:42:SER:HB3   | 1:A:45:GLN:CB    | 0.42     | 2.41        | 12     | 1     |
| 1:A:43:LYS:HA    | 1:A:43:LYS:CE    | 0.42     | 2.40        | 43     | 1     |
| 1:A:110:GLN:HE21 | 1:A:110:GLN:CA   | 0.42     | 2.25        | 7      | 1     |
| 1:A:39:ARG:HG3   | 1:A:40:SER:N     | 0.42     | 2.30        | 48     | 1     |
| 1:A:121:ARG:O    | 1:A:121:ARG:HG3  | 0.42     | 2.15        | 11     | 1     |
| 1:A:36:ARG:HA    | 1:A:84:LEU:HD11  | 0.42     | 1.91        | 24     | 1     |
| 1:A:43:LYS:HG3   | 1:A:44:CYS:SG    | 0.42     | 2.55        | 29     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:61:SER:HB2   | 1:A:67:SER:HB2   | 0.42     | 1.91        | 44     | 1     |
| 1:A:38:THR:HA    | 1:A:39:ARG:HH11  | 0.42     | 1.75        | 8      | 1     |
| 1:A:26:LEU:CD1   | 1:A:52:LEU:HA    | 0.41     | 2.46        | 18     | 1     |
| 1:A:36:ARG:HG3   | 1:A:49:GLU:HB2   | 0.41     | 1.91        | 26     | 1     |
| 1:A:28:TRP:O     | 1:A:79:LYS:HB3   | 0.41     | 2.15        | 40     | 1     |
| 1:A:110:GLN:HB2  | 1:A:113:SER:OG   | 0.41     | 2.14        | 47     | 1     |
| 1:A:99:TYR:HA    | 1:A:124:MET:HA   | 0.41     | 1.92        | 49     | 1     |
| 1:A:66:ARG:HA    | 1:A:66:ARG:NE    | 0.41     | 2.30        | 3      | 1     |
| 1:A:66:ARG:HH22  | 1:A:111:LEU:HD22 | 0.41     | 1.74        | 20     | 1     |
| 1:A:78:SER:O     | 1:A:82:GLN:HG2   | 0.41     | 2.15        | 24     | 1     |
| 1:A:93:GLY:O     | 1:A:128:LEU:HA   | 0.41     | 2.16        | 19     | 1     |
| 1:A:44:CYS:HB2   | 1:A:134:GLU:HG2  | 0.41     | 1.91        | 45     | 1     |
| 1:A:53:LYS:HD3   | 1:A:53:LYS:O     | 0.41     | 2.15        | 38     | 1     |
| 1:A:43:LYS:HE3   | 1:A:43:LYS:H     | 0.41     | 1.75        | 26     | 1     |
| 1:A:42:SER:HB2   | 1:A:45:GLN:CB    | 0.41     | 2.40        | 7      | 1     |
| 1:A:79:LYS:HE2   | 1:A:79:LYS:CA    | 0.41     | 2.45        | 13     | 1     |
| 1:A:36:ARG:HG2   | 1:A:56:TRP:CZ3   | 0.41     | 2.50        | 31     | 1     |
| 1:A:44:CYS:HB2   | 1:A:134:GLU:HG3  | 0.41     | 1.93        | 35     | 1     |
| 1:A:106:ILE:HD12 | 1:A:120:SER:HA   | 0.41     | 1.93        | 35     | 1     |
| 1:A:53:LYS:H     | 1:A:53:LYS:CD    | 0.40     | 2.24        | 47     | 1     |
| 1:A:34:GLN:HE21  | 1:A:34:GLN:N     | 0.40     | 2.14        | 9      | 1     |
| 1:A:92:LEU:HD21  | 1:A:128:LEU:HD21 | 0.40     | 1.92        | 20     | 1     |
| 1:A:76:GLN:OE1   | 1:A:76:GLN:HA    | 0.40     | 2.17        | 46     | 1     |
| 1:A:101:PRO:O    | 1:A:120:SER:HB3  | 0.40     | 2.16        | 17     | 1     |
| 1:A:38:THR:O     | 1:A:46:GLY:HA3   | 0.40     | 2.15        | 22     | 1     |
| 1:A:47:GLN:OE1   | 1:A:58:MET:HE3   | 0.40     | 2.16        | 26     | 1     |
| 1:A:46:GLY:HA2   | 1:A:95:PHE:CE2   | 0.40     | 2.52        | 33     | 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     | 108/131 (82%)   | 93±3 (87±3%) | 13±3 (12±3%) | 1±1 (1±1%) | 12          | 60 |
| All | All   | 5400/6550 (82%) | 4674 (87%)   | 658 (12%)    | 68 (1%)    | 12          | 60 |

All 18 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     | 40  | SER  | 14             |
| 1   | A     | 64  | TRP  | 11             |
| 1   | A     | 102 | GLN  | 9              |
| 1   | A     | 41  | ASN  | 6              |
| 1   | A     | 96  | LEU  | 5              |
| 1   | A     | 38  | THR  | 5              |
| 1   | A     | 111 | LEU  | 3              |
| 1   | A     | 54  | ASP  | 3              |
| 1   | A     | 99  | TYR  | 2              |
| 1   | A     | 103 | SER  | 2              |
| 1   | A     | 53  | LYS  | 1              |
| 1   | A     | 120 | SER  | 1              |
| 1   | A     | 85  | ASN  | 1              |
| 1   | A     | 101 | PRO  | 1              |
| 1   | A     | 39  | ARG  | 1              |
| 1   | A     | 66  | ARG  | 1              |
| 1   | A     | 123 | ASP  | 1              |
| 1   | A     | 133 | LEU  | 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     | 99/117 (85%)    | 95±2 (96±2%) | 4±2 (4±2%) | 32          | 82 |
| All | All   | 4950/5850 (85%) | 4774 (96%)   | 176 (4%)   | 32          | 82 |

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     | 43  | LYS  | 24             |
| 1   | A     | 57  | HIS  | 13             |
| 1   | A     | 36  | ARG  | 9              |
| 1   | A     | 39  | ARG  | 9              |
| 1   | A     | 53  | LYS  | 6              |
| 1   | A     | 125 | CYS  | 6              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 45  | GLN  | 6              |
| 1   | A     | 69  | LYS  | 6              |
| 1   | A     | 70  | GLN  | 6              |
| 1   | A     | 75  | SER  | 5              |
| 1   | A     | 97  | LYS  | 5              |
| 1   | A     | 102 | GLN  | 5              |
| 1   | A     | 92  | LEU  | 5              |
| 1   | A     | 88  | ASP  | 4              |
| 1   | A     | 110 | GLN  | 4              |
| 1   | A     | 121 | ARG  | 4              |
| 1   | A     | 127 | SER  | 4              |
| 1   | A     | 107 | CYS  | 3              |
| 1   | A     | 90  | LEU  | 3              |
| 1   | A     | 60  | CYS  | 3              |
| 1   | A     | 79  | LYS  | 3              |
| 1   | A     | 98  | THR  | 3              |
| 1   | A     | 34  | GLN  | 3              |
| 1   | A     | 62  | GLN  | 3              |
| 1   | A     | 76  | GLN  | 3              |
| 1   | A     | 82  | GLN  | 3              |
| 1   | A     | 54  | ASP  | 3              |
| 1   | A     | 29  | TYR  | 2              |
| 1   | A     | 32  | ASP  | 2              |
| 1   | A     | 83  | ARG  | 2              |
| 1   | A     | 99  | TYR  | 2              |
| 1   | A     | 28  | TRP  | 2              |
| 1   | A     | 122 | ASN  | 2              |
| 1   | A     | 71  | TRP  | 2              |
| 1   | A     | 95  | PHE  | 1              |
| 1   | A     | 103 | SER  | 1              |
| 1   | A     | 44  | CYS  | 1              |
| 1   | A     | 42  | SER  | 1              |
| 1   | A     | 72  | GLU  | 1              |
| 1   | A     | 106 | ILE  | 1              |
| 1   | A     | 126 | HIS  | 1              |
| 1   | A     | 47  | GLN  | 1              |
| 1   | A     | 61  | SER  | 1              |
| 1   | A     | 27  | SER  | 1              |
| 1   | A     | 134 | GLU  | 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