



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:07 AM UTC

PDB ID : 6E9X / pdb\_00006e9x  
EMDB ID : EMD-9019  
Title : DHF91 filament  
Authors : Lynch, E.M.; Shen, H.; Fallas, J.A.; Kollman, J.M.; Baker, D.  
Deposited on : 2018-08-01  
Resolution : 7.80 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : **NOT EXECUTED**  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

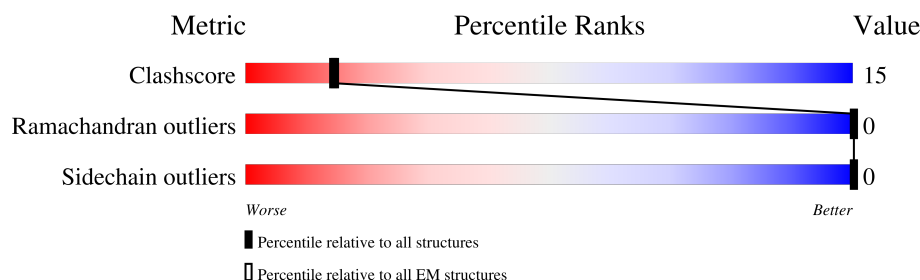
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.80 Å.

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) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 229148                      | 23984                       |
| Ramachandran outliers | 224038                      | 23583                       |
| Sidechain outliers    | 223484                      | 23102                       |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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     | 168    | 71% 24% .        |
| 1   | B     | 168    | 72% 24% .        |
| 1   | C     | 168    | 71% 24% .        |
| 1   | D     | 168    | 73% 24% .        |
| 1   | E     | 168    | 72% 24% .        |
| 1   | F     | 168    | 71% 24% .        |
| 1   | G     | 168    | 71% 24% .        |
| 1   | H     | 168    | 73% 23% .        |
| 1   | I     | 168    | 71% 26% .        |

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| Mol | Chain | Length | Quality of chain                                                                              |
|-----|-------|--------|-----------------------------------------------------------------------------------------------|
| 1   | J     | 168    |  74% 23% .  |
| 1   | K     | 168    |  72% 24% .  |
| 1   | L     | 168    |  72% 24% .  |
| 1   | M     | 168    |  71% 24% .  |
| 1   | N     | 168    |  71% 24% .  |
| 1   | O     | 168    |  73% 25% .  |
| 1   | P     | 168    |  74% 23% .  |
| 1   | Q     | 168    |  73% 23% .  |
| 1   | R     | 168    |  71% 24% .  |
| 1   | S     | 168    |  73% 23% .  |
| 1   | T     | 168    |  73% 23% .  |
| 1   | U     | 168    |  71% 26% . |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 54201 atoms, of which 27993 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DHF91 filament.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 1   | C     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | A     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | B     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | P     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | D     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | J     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | Q     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | E     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | K     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | R     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | F     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | L     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | S     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | G     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | M     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | T     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | H     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |

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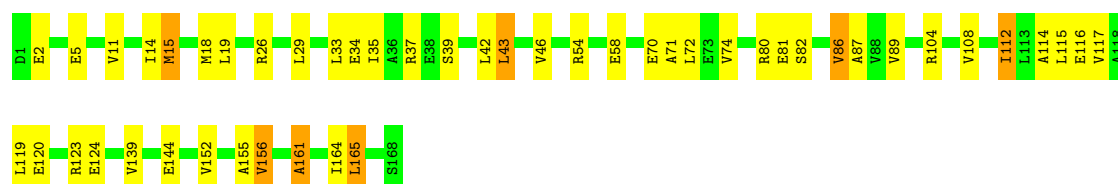
| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 1   | N     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | U     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | I     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |
| 1   | O     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2581  | 775 | 1333 | 226 | 245 | 2 |         |       |

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

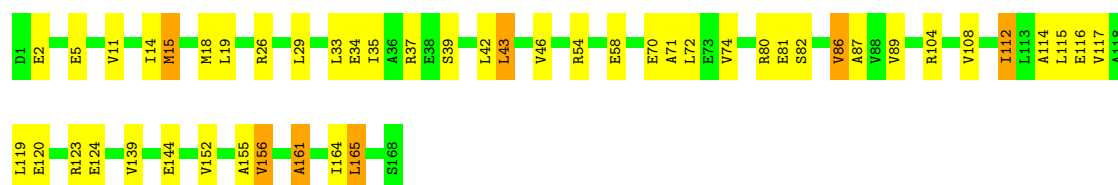
- Molecule 1: DHF91 filament

Chain C: 



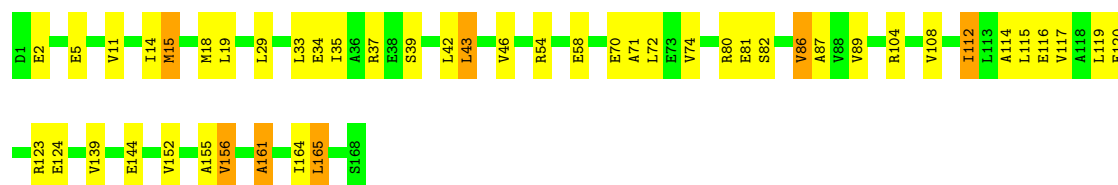
- Molecule 1: DHF91 filament

Chain A: 



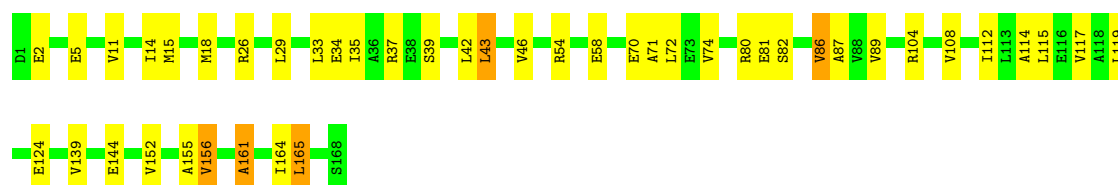
- Molecule 1: DHF91 filament

Chain B: 

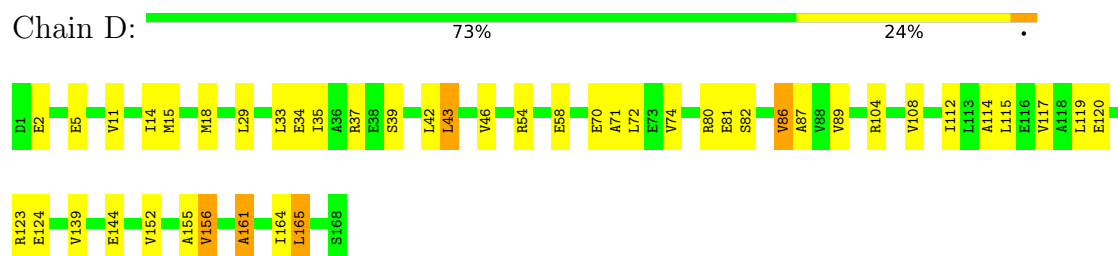


- Molecule 1: DHF91 filament

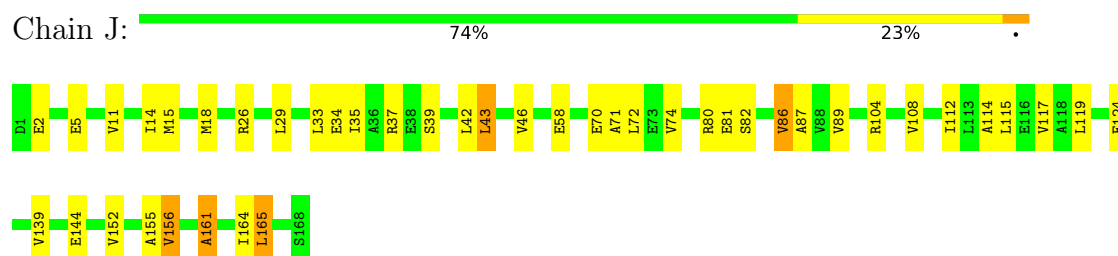
Chain P: 



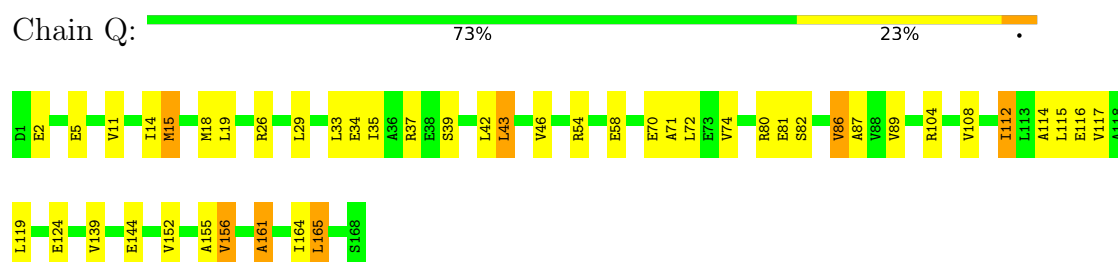
## • Molecule 1: DHF91 filament



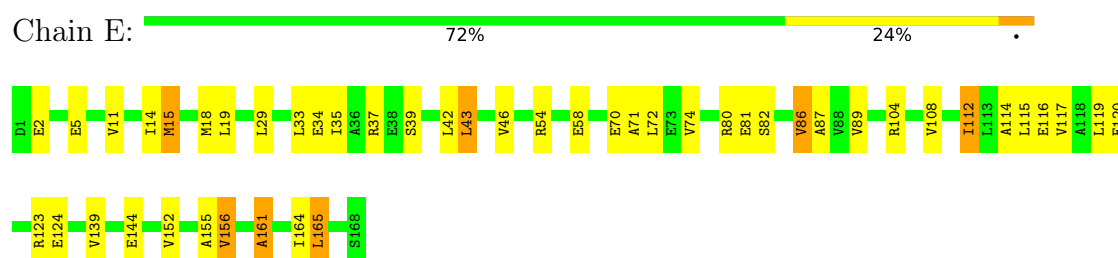
## • Molecule 1: DHF91 filament



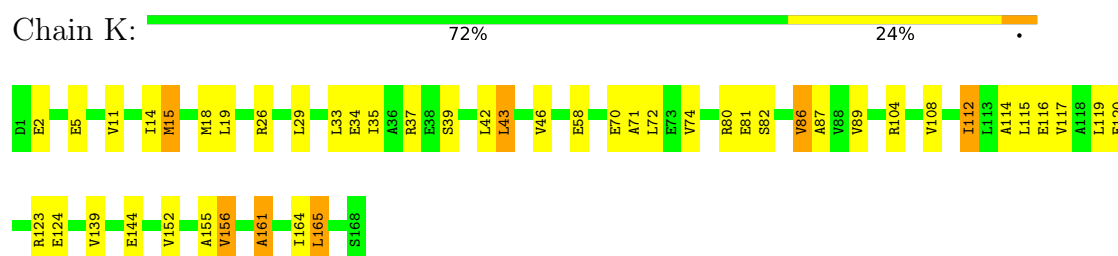
## • Molecule 1: DHF91 filament



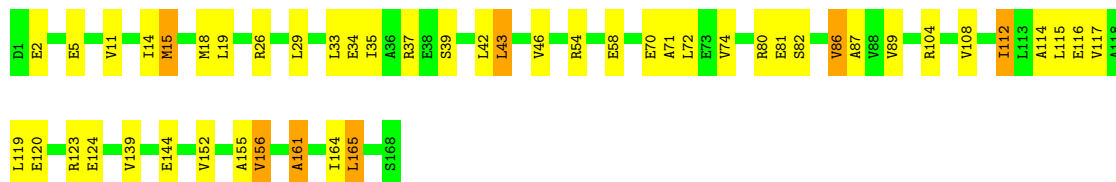
## • Molecule 1: DHF91 filament



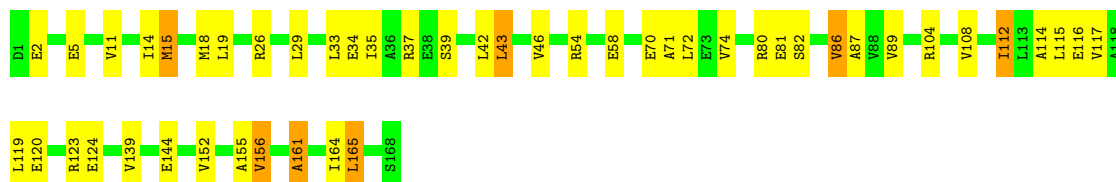
## • Molecule 1: DHF91 filament



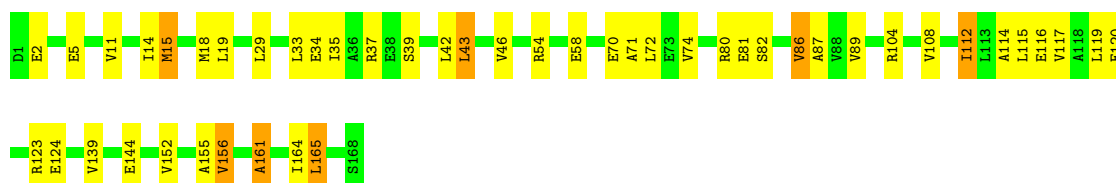
## ● Molecule 1: DHF91 filament

Chain R:  71% 24% .

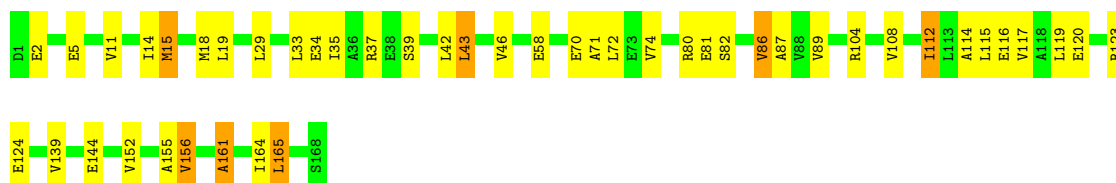
## ● Molecule 1: DHF91 filament

Chain F:  71% 24% .

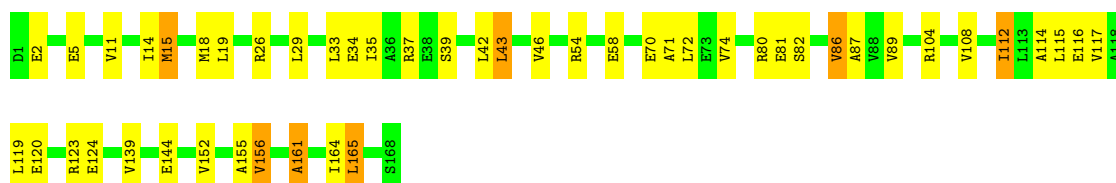
## ● Molecule 1: DHF91 filament

Chain L:  72% 24% .

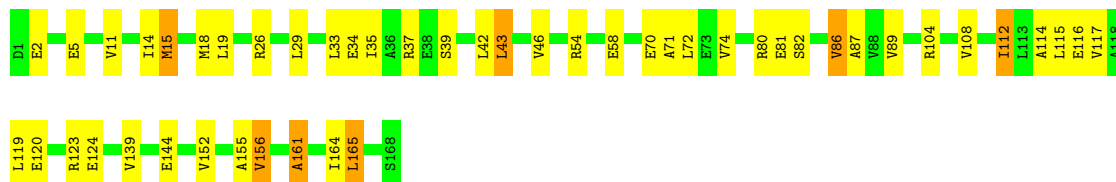
## ● Molecule 1: DHF91 filament

Chain S:  73% 23% .

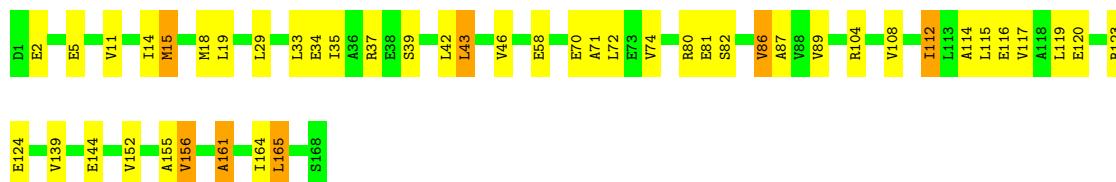
## ● Molecule 1: DHF91 filament

Chain G:  71% 24% .

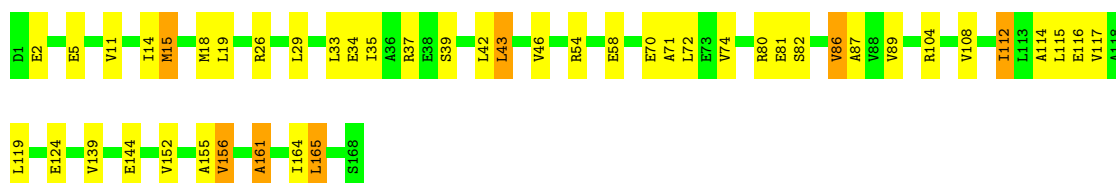
## • Molecule 1: DHF91 filament

Chain M:  71% 24% .

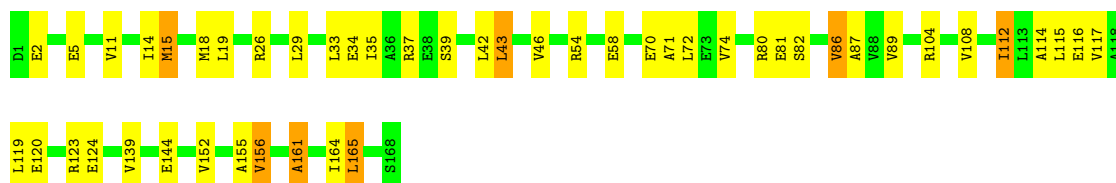
## • Molecule 1: DHF91 filament

Chain T:  73% 23% .

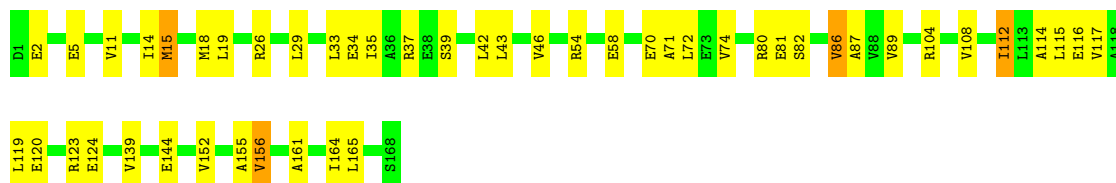
## • Molecule 1: DHF91 filament

Chain H:  73% 23% .

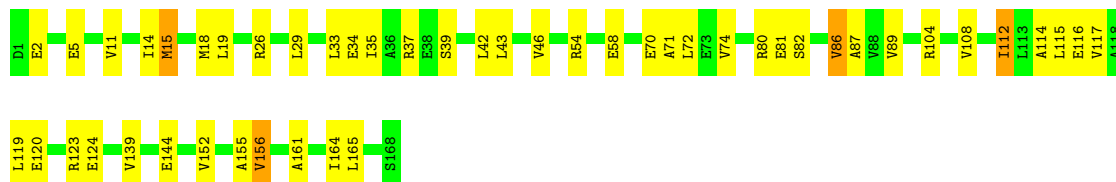
## • Molecule 1: DHF91 filament

Chain N:  71% 24% .

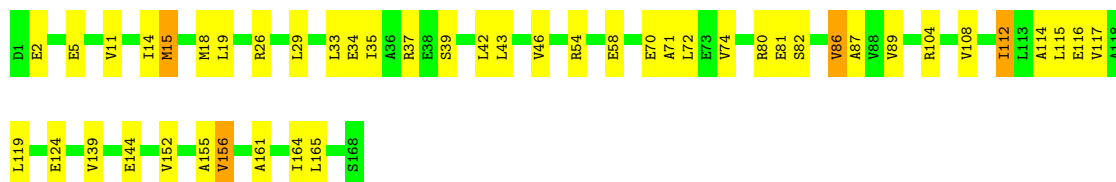
## • Molecule 1: DHF91 filament

Chain U:  71% 26% .

## • Molecule 1: DHF91 filament

Chain I:  71% 26% .

## • Molecule 1: DHF91 filament

Chain O:  73% 25% .

## 4 Experimental information

| Property                             | Value                                                 | Source    |
|--------------------------------------|-------------------------------------------------------|-----------|
| EM reconstruction method             | HELICAL                                               | Depositor |
| Imposed symmetry                     | HELICAL, twist=50.1109°, rise=24.1338 Å, axial sym=C3 | Depositor |
| Number of segments used              | 15670                                                 | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                                     | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION               | Depositor |
| Microscope                           | FEI TECNAI F20                                        | Depositor |
| Voltage (kV)                         | 200                                                   | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 45                                                    | Depositor |
| Minimum defocus (nm)                 | Not provided                                          |           |
| Maximum defocus (nm)                 | Not provided                                          |           |
| Magnification                        | Not provided                                          |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)                             | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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 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     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | B     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | C     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | D     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | E     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | F     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | G     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | H     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | I     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | J     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | K     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | L     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | M     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | N     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | O     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | P     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | Q     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | R     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | S     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | T     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| 1   | U     | 1.12         | 9/1247 (0.7%)    | 0.98        | 7/1684 (0.4%)    |
| All | All   | 1.12         | 189/26187 (0.7%) | 0.98        | 147/35364 (0.4%) |

All (189) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | I     | 89  | VAL  | CA-CB | -12.02 | 1.39        | 1.54     |
| 1   | G     | 89  | VAL  | CA-CB | -12.02 | 1.39        | 1.54     |
| 1   | F     | 89  | VAL  | CA-CB | -12.02 | 1.39        | 1.54     |
| 1   | E     | 89  | VAL  | CA-CB | -12.02 | 1.39        | 1.54     |
| 1   | A     | 89  | VAL  | CA-CB | -12.01 | 1.39        | 1.54     |
| 1   | D     | 89  | VAL  | CA-CB | -12.00 | 1.39        | 1.54     |
| 1   | H     | 89  | VAL  | CA-CB | -12.00 | 1.39        | 1.54     |

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| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | S     | 89  | VAL  | CA-CB | -12.00 | 1.39        | 1.54     |
| 1   | Q     | 89  | VAL  | CA-CB | -11.99 | 1.39        | 1.54     |
| 1   | R     | 89  | VAL  | CA-CB | -11.99 | 1.39        | 1.54     |
| 1   | U     | 89  | VAL  | CA-CB | -11.99 | 1.39        | 1.54     |
| 1   | C     | 89  | VAL  | CA-CB | -11.98 | 1.39        | 1.54     |
| 1   | P     | 89  | VAL  | CA-CB | -11.98 | 1.39        | 1.54     |
| 1   | K     | 89  | VAL  | CA-CB | -11.97 | 1.39        | 1.54     |
| 1   | T     | 89  | VAL  | CA-CB | -11.97 | 1.39        | 1.54     |
| 1   | M     | 89  | VAL  | CA-CB | -11.95 | 1.39        | 1.54     |
| 1   | B     | 89  | VAL  | CA-CB | -11.95 | 1.39        | 1.54     |
| 1   | L     | 89  | VAL  | CA-CB | -11.95 | 1.39        | 1.54     |
| 1   | O     | 89  | VAL  | CA-CB | -11.95 | 1.39        | 1.54     |
| 1   | J     | 89  | VAL  | CA-CB | -11.95 | 1.39        | 1.54     |
| 1   | N     | 89  | VAL  | CA-CB | -11.95 | 1.39        | 1.54     |
| 1   | L     | 155 | ALA  | CA-CB | 9.41   | 1.68        | 1.53     |
| 1   | B     | 155 | ALA  | CA-CB | 9.40   | 1.68        | 1.53     |
| 1   | M     | 155 | ALA  | CA-CB | 9.40   | 1.68        | 1.53     |
| 1   | K     | 155 | ALA  | CA-CB | 9.40   | 1.68        | 1.53     |
| 1   | N     | 155 | ALA  | CA-CB | 9.40   | 1.68        | 1.53     |
| 1   | O     | 155 | ALA  | CA-CB | 9.40   | 1.68        | 1.53     |
| 1   | J     | 155 | ALA  | CA-CB | 9.40   | 1.68        | 1.53     |
| 1   | U     | 155 | ALA  | CA-CB | 9.37   | 1.68        | 1.53     |
| 1   | T     | 155 | ALA  | CA-CB | 9.37   | 1.68        | 1.53     |
| 1   | C     | 155 | ALA  | CA-CB | 9.37   | 1.68        | 1.53     |
| 1   | R     | 155 | ALA  | CA-CB | 9.37   | 1.68        | 1.53     |
| 1   | S     | 155 | ALA  | CA-CB | 9.37   | 1.68        | 1.53     |
| 1   | Q     | 155 | ALA  | CA-CB | 9.36   | 1.68        | 1.53     |
| 1   | I     | 155 | ALA  | CA-CB | 9.36   | 1.68        | 1.53     |
| 1   | P     | 155 | ALA  | CA-CB | 9.36   | 1.68        | 1.53     |
| 1   | D     | 155 | ALA  | CA-CB | 9.36   | 1.68        | 1.53     |
| 1   | H     | 155 | ALA  | CA-CB | 9.35   | 1.68        | 1.53     |
| 1   | A     | 155 | ALA  | CA-CB | 9.35   | 1.68        | 1.53     |
| 1   | E     | 155 | ALA  | CA-CB | 9.35   | 1.68        | 1.53     |
| 1   | F     | 155 | ALA  | CA-CB | 9.35   | 1.68        | 1.53     |
| 1   | G     | 155 | ALA  | CA-CB | 9.35   | 1.68        | 1.53     |
| 1   | S     | 11  | VAL  | CA-CB | -8.27  | 1.45        | 1.54     |
| 1   | O     | 18  | MET  | CA-CB | -8.26  | 1.39        | 1.53     |
| 1   | R     | 11  | VAL  | CA-CB | -8.25  | 1.45        | 1.54     |
| 1   | M     | 18  | MET  | CA-CB | -8.24  | 1.39        | 1.53     |
| 1   | K     | 18  | MET  | CA-CB | -8.23  | 1.39        | 1.53     |
| 1   | H     | 11  | VAL  | CA-CB | -8.23  | 1.45        | 1.54     |
| 1   | O     | 11  | VAL  | CA-CB | -8.23  | 1.45        | 1.54     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 18  | MET  | CA-CB | -8.23 | 1.39        | 1.53     |
| 1   | J     | 18  | MET  | CA-CB | -8.23 | 1.39        | 1.53     |
| 1   | N     | 18  | MET  | CA-CB | -8.23 | 1.39        | 1.53     |
| 1   | P     | 18  | MET  | CA-CB | -8.22 | 1.39        | 1.53     |
| 1   | Q     | 11  | VAL  | CA-CB | -8.21 | 1.45        | 1.54     |
| 1   | B     | 18  | MET  | CA-CB | -8.21 | 1.39        | 1.53     |
| 1   | Q     | 18  | MET  | CA-CB | -8.21 | 1.39        | 1.53     |
| 1   | T     | 18  | MET  | CA-CB | -8.21 | 1.39        | 1.53     |
| 1   | S     | 18  | MET  | CA-CB | -8.20 | 1.39        | 1.53     |
| 1   | T     | 11  | VAL  | CA-CB | -8.20 | 1.45        | 1.54     |
| 1   | H     | 18  | MET  | CA-CB | -8.20 | 1.39        | 1.53     |
| 1   | U     | 18  | MET  | CA-CB | -8.20 | 1.39        | 1.53     |
| 1   | C     | 11  | VAL  | CA-CB | -8.19 | 1.45        | 1.54     |
| 1   | B     | 11  | VAL  | CA-CB | -8.18 | 1.45        | 1.54     |
| 1   | R     | 18  | MET  | CA-CB | -8.18 | 1.39        | 1.53     |
| 1   | D     | 18  | MET  | CA-CB | -8.18 | 1.39        | 1.53     |
| 1   | E     | 18  | MET  | CA-CB | -8.18 | 1.39        | 1.53     |
| 1   | F     | 18  | MET  | CA-CB | -8.17 | 1.39        | 1.53     |
| 1   | G     | 18  | MET  | CA-CB | -8.17 | 1.39        | 1.53     |
| 1   | A     | 18  | MET  | CA-CB | -8.17 | 1.39        | 1.53     |
| 1   | U     | 11  | VAL  | CA-CB | -8.17 | 1.45        | 1.54     |
| 1   | L     | 18  | MET  | CA-CB | -8.17 | 1.39        | 1.53     |
| 1   | I     | 18  | MET  | CA-CB | -8.17 | 1.39        | 1.53     |
| 1   | J     | 11  | VAL  | CA-CB | -8.16 | 1.45        | 1.54     |
| 1   | K     | 11  | VAL  | CA-CB | -8.16 | 1.45        | 1.54     |
| 1   | G     | 11  | VAL  | CA-CB | -8.16 | 1.45        | 1.54     |
| 1   | A     | 11  | VAL  | CA-CB | -8.15 | 1.45        | 1.54     |
| 1   | P     | 11  | VAL  | CA-CB | -8.15 | 1.45        | 1.54     |
| 1   | L     | 11  | VAL  | CA-CB | -8.15 | 1.45        | 1.54     |
| 1   | N     | 11  | VAL  | CA-CB | -8.14 | 1.45        | 1.54     |
| 1   | F     | 11  | VAL  | CA-CB | -8.14 | 1.45        | 1.54     |
| 1   | M     | 11  | VAL  | CA-CB | -8.14 | 1.45        | 1.54     |
| 1   | D     | 11  | VAL  | CA-CB | -8.13 | 1.45        | 1.54     |
| 1   | E     | 11  | VAL  | CA-CB | -8.13 | 1.45        | 1.54     |
| 1   | I     | 11  | VAL  | CA-CB | -8.12 | 1.45        | 1.54     |
| 1   | R     | 139 | VAL  | CA-CB | -7.63 | 1.45        | 1.54     |
| 1   | Q     | 139 | VAL  | CA-CB | -7.62 | 1.45        | 1.54     |
| 1   | S     | 139 | VAL  | CA-CB | -7.62 | 1.45        | 1.54     |
| 1   | T     | 139 | VAL  | CA-CB | -7.61 | 1.45        | 1.54     |
| 1   | U     | 139 | VAL  | CA-CB | -7.61 | 1.45        | 1.54     |
| 1   | C     | 139 | VAL  | CA-CB | -7.61 | 1.45        | 1.54     |
| 1   | G     | 139 | VAL  | CA-CB | -7.59 | 1.45        | 1.54     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | P     | 139 | VAL  | CA-CB | -7.59 | 1.45        | 1.54     |
| 1   | H     | 139 | VAL  | CA-CB | -7.59 | 1.45        | 1.54     |
| 1   | E     | 139 | VAL  | CA-CB | -7.58 | 1.45        | 1.54     |
| 1   | A     | 139 | VAL  | CA-CB | -7.58 | 1.45        | 1.54     |
| 1   | K     | 139 | VAL  | CA-CB | -7.58 | 1.45        | 1.54     |
| 1   | M     | 139 | VAL  | CA-CB | -7.58 | 1.45        | 1.54     |
| 1   | D     | 139 | VAL  | CA-CB | -7.58 | 1.45        | 1.54     |
| 1   | I     | 139 | VAL  | CA-CB | -7.58 | 1.45        | 1.54     |
| 1   | L     | 139 | VAL  | CA-CB | -7.58 | 1.45        | 1.54     |
| 1   | B     | 139 | VAL  | CA-CB | -7.57 | 1.45        | 1.54     |
| 1   | O     | 139 | VAL  | CA-CB | -7.57 | 1.45        | 1.54     |
| 1   | F     | 139 | VAL  | CA-CB | -7.56 | 1.45        | 1.54     |
| 1   | N     | 139 | VAL  | CA-CB | -7.56 | 1.45        | 1.54     |
| 1   | J     | 139 | VAL  | CA-CB | -7.55 | 1.45        | 1.54     |
| 1   | J     | 86  | VAL  | CA-CB | 6.55  | 1.62        | 1.54     |
| 1   | L     | 86  | VAL  | CA-CB | 6.55  | 1.62        | 1.54     |
| 1   | T     | 86  | VAL  | CA-CB | 6.55  | 1.62        | 1.54     |
| 1   | R     | 86  | VAL  | CA-CB | 6.54  | 1.62        | 1.54     |
| 1   | S     | 86  | VAL  | CA-CB | 6.53  | 1.62        | 1.54     |
| 1   | C     | 86  | VAL  | CA-CB | 6.52  | 1.62        | 1.54     |
| 1   | N     | 46  | VAL  | CA-CB | 6.52  | 1.62        | 1.54     |
| 1   | O     | 86  | VAL  | CA-CB | 6.52  | 1.62        | 1.54     |
| 1   | Q     | 86  | VAL  | CA-CB | 6.51  | 1.62        | 1.54     |
| 1   | I     | 86  | VAL  | CA-CB | 6.51  | 1.62        | 1.54     |
| 1   | P     | 86  | VAL  | CA-CB | 6.51  | 1.62        | 1.54     |
| 1   | F     | 86  | VAL  | CA-CB | 6.50  | 1.62        | 1.54     |
| 1   | M     | 46  | VAL  | CA-CB | 6.50  | 1.62        | 1.54     |
| 1   | L     | 46  | VAL  | CA-CB | 6.49  | 1.61        | 1.54     |
| 1   | B     | 46  | VAL  | CA-CB | 6.49  | 1.61        | 1.54     |
| 1   | B     | 86  | VAL  | CA-CB | 6.49  | 1.62        | 1.54     |
| 1   | S     | 46  | VAL  | CA-CB | 6.49  | 1.61        | 1.54     |
| 1   | E     | 46  | VAL  | CA-CB | 6.49  | 1.61        | 1.54     |
| 1   | U     | 46  | VAL  | CA-CB | 6.49  | 1.61        | 1.54     |
| 1   | J     | 46  | VAL  | CA-CB | 6.48  | 1.61        | 1.54     |
| 1   | O     | 46  | VAL  | CA-CB | 6.48  | 1.61        | 1.54     |
| 1   | K     | 46  | VAL  | CA-CB | 6.48  | 1.61        | 1.54     |
| 1   | U     | 86  | VAL  | CA-CB | 6.48  | 1.62        | 1.54     |
| 1   | D     | 86  | VAL  | CA-CB | 6.48  | 1.62        | 1.54     |
| 1   | D     | 46  | VAL  | CA-CB | 6.47  | 1.61        | 1.54     |
| 1   | K     | 86  | VAL  | CA-CB | 6.47  | 1.62        | 1.54     |
| 1   | T     | 46  | VAL  | CA-CB | 6.47  | 1.61        | 1.54     |
| 1   | A     | 46  | VAL  | CA-CB | 6.47  | 1.61        | 1.54     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | E     | 86  | VAL  | CA-CB | 6.46  | 1.62        | 1.54     |
| 1   | Q     | 46  | VAL  | CA-CB | 6.46  | 1.61        | 1.54     |
| 1   | A     | 86  | VAL  | CA-CB | 6.46  | 1.62        | 1.54     |
| 1   | M     | 86  | VAL  | CA-CB | 6.46  | 1.62        | 1.54     |
| 1   | I     | 46  | VAL  | CA-CB | 6.46  | 1.61        | 1.54     |
| 1   | C     | 46  | VAL  | CA-CB | 6.46  | 1.61        | 1.54     |
| 1   | G     | 46  | VAL  | CA-CB | 6.46  | 1.61        | 1.54     |
| 1   | F     | 46  | VAL  | CA-CB | 6.45  | 1.61        | 1.54     |
| 1   | H     | 86  | VAL  | CA-CB | 6.44  | 1.62        | 1.54     |
| 1   | P     | 46  | VAL  | CA-CB | 6.43  | 1.61        | 1.54     |
| 1   | H     | 46  | VAL  | CA-CB | 6.43  | 1.61        | 1.54     |
| 1   | R     | 46  | VAL  | CA-CB | 6.43  | 1.61        | 1.54     |
| 1   | G     | 86  | VAL  | CA-CB | 6.41  | 1.62        | 1.54     |
| 1   | N     | 86  | VAL  | CA-CB | 6.41  | 1.62        | 1.54     |
| 1   | K     | 165 | LEU  | CA-CB | -5.44 | 1.44        | 1.53     |
| 1   | U     | 165 | LEU  | CA-CB | -5.43 | 1.44        | 1.53     |
| 1   | S     | 165 | LEU  | CA-CB | -5.42 | 1.44        | 1.53     |
| 1   | R     | 165 | LEU  | CA-CB | -5.41 | 1.44        | 1.53     |
| 1   | B     | 165 | LEU  | CA-CB | -5.39 | 1.44        | 1.53     |
| 1   | N     | 165 | LEU  | CA-CB | -5.39 | 1.44        | 1.53     |
| 1   | M     | 165 | LEU  | CA-CB | -5.39 | 1.44        | 1.53     |
| 1   | C     | 165 | LEU  | CA-CB | -5.38 | 1.44        | 1.53     |
| 1   | F     | 165 | LEU  | CA-CB | -5.37 | 1.44        | 1.53     |
| 1   | O     | 165 | LEU  | CA-CB | -5.37 | 1.44        | 1.53     |
| 1   | J     | 165 | LEU  | CA-CB | -5.36 | 1.44        | 1.53     |
| 1   | Q     | 165 | LEU  | CA-CB | -5.35 | 1.44        | 1.53     |
| 1   | T     | 165 | LEU  | CA-CB | -5.34 | 1.44        | 1.53     |
| 1   | P     | 165 | LEU  | CA-CB | -5.31 | 1.44        | 1.53     |
| 1   | G     | 165 | LEU  | CA-CB | -5.21 | 1.44        | 1.53     |
| 1   | H     | 156 | VAL  | CA-CB | 5.20  | 1.60        | 1.54     |
| 1   | M     | 156 | VAL  | CA-CB | 5.19  | 1.60        | 1.54     |
| 1   | I     | 165 | LEU  | CA-CB | -5.18 | 1.44        | 1.53     |
| 1   | A     | 165 | LEU  | CA-CB | -5.17 | 1.44        | 1.53     |
| 1   | E     | 165 | LEU  | CA-CB | -5.17 | 1.44        | 1.53     |
| 1   | D     | 165 | LEU  | CA-CB | -5.16 | 1.44        | 1.53     |
| 1   | J     | 156 | VAL  | CA-CB | 5.16  | 1.60        | 1.54     |
| 1   | H     | 165 | LEU  | CA-CB | -5.15 | 1.44        | 1.53     |
| 1   | D     | 156 | VAL  | CA-CB | 5.15  | 1.60        | 1.54     |
| 1   | L     | 165 | LEU  | CA-CB | -5.14 | 1.44        | 1.53     |
| 1   | F     | 156 | VAL  | CA-CB | 5.14  | 1.60        | 1.54     |
| 1   | A     | 156 | VAL  | CA-CB | 5.14  | 1.60        | 1.54     |
| 1   | O     | 156 | VAL  | CA-CB | 5.13  | 1.60        | 1.54     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | G     | 156 | VAL  | CA-CB | 5.13 | 1.60        | 1.54     |
| 1   | C     | 156 | VAL  | CA-CB | 5.12 | 1.60        | 1.54     |
| 1   | Q     | 156 | VAL  | CA-CB | 5.12 | 1.60        | 1.54     |
| 1   | B     | 156 | VAL  | CA-CB | 5.12 | 1.60        | 1.54     |
| 1   | P     | 156 | VAL  | CA-CB | 5.12 | 1.60        | 1.54     |
| 1   | I     | 156 | VAL  | CA-CB | 5.11 | 1.60        | 1.54     |
| 1   | S     | 156 | VAL  | CA-CB | 5.11 | 1.60        | 1.54     |
| 1   | T     | 156 | VAL  | CA-CB | 5.11 | 1.60        | 1.54     |
| 1   | U     | 156 | VAL  | CA-CB | 5.10 | 1.60        | 1.54     |
| 1   | L     | 156 | VAL  | CA-CB | 5.10 | 1.60        | 1.54     |
| 1   | E     | 156 | VAL  | CA-CB | 5.09 | 1.60        | 1.54     |
| 1   | N     | 156 | VAL  | CA-CB | 5.08 | 1.60        | 1.54     |
| 1   | R     | 156 | VAL  | CA-CB | 5.07 | 1.60        | 1.54     |
| 1   | K     | 156 | VAL  | CA-CB | 5.06 | 1.60        | 1.54     |

All (147) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | R     | 86  | VAL  | CB-CA-C | -10.43 | 98.06       | 112.14   |
| 1   | Q     | 86  | VAL  | CB-CA-C | -10.43 | 98.06       | 112.14   |
| 1   | J     | 86  | VAL  | CB-CA-C | -10.42 | 98.07       | 112.14   |
| 1   | F     | 86  | VAL  | CB-CA-C | -10.42 | 98.07       | 112.14   |
| 1   | I     | 86  | VAL  | CB-CA-C | -10.42 | 98.07       | 112.14   |
| 1   | C     | 86  | VAL  | CB-CA-C | -10.41 | 98.08       | 112.14   |
| 1   | T     | 86  | VAL  | CB-CA-C | -10.41 | 98.08       | 112.14   |
| 1   | H     | 86  | VAL  | CB-CA-C | -10.41 | 98.08       | 112.14   |
| 1   | P     | 86  | VAL  | CB-CA-C | -10.41 | 98.09       | 112.14   |
| 1   | D     | 86  | VAL  | CB-CA-C | -10.41 | 98.09       | 112.14   |
| 1   | A     | 86  | VAL  | CB-CA-C | -10.41 | 98.09       | 112.14   |
| 1   | L     | 86  | VAL  | CB-CA-C | -10.40 | 98.09       | 112.14   |
| 1   | O     | 86  | VAL  | CB-CA-C | -10.40 | 98.09       | 112.14   |
| 1   | S     | 86  | VAL  | CB-CA-C | -10.40 | 98.10       | 112.14   |
| 1   | B     | 86  | VAL  | CB-CA-C | -10.39 | 98.11       | 112.14   |
| 1   | E     | 86  | VAL  | CB-CA-C | -10.39 | 98.11       | 112.14   |
| 1   | M     | 86  | VAL  | CB-CA-C | -10.39 | 98.11       | 112.14   |
| 1   | U     | 86  | VAL  | CB-CA-C | -10.39 | 98.11       | 112.14   |
| 1   | G     | 86  | VAL  | CB-CA-C | -10.38 | 98.12       | 112.14   |
| 1   | K     | 86  | VAL  | CB-CA-C | -10.38 | 98.13       | 112.14   |
| 1   | N     | 86  | VAL  | CB-CA-C | -10.36 | 98.15       | 112.14   |
| 1   | R     | 15  | MET  | CB-CA-C | -9.09  | 95.70       | 110.79   |
| 1   | U     | 15  | MET  | CB-CA-C | -9.09  | 95.70       | 110.79   |
| 1   | L     | 15  | MET  | CB-CA-C | -9.08  | 95.72       | 110.79   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | M     | 15  | MET  | CB-CA-C | -9.08 | 95.72       | 110.79   |
| 1   | T     | 15  | MET  | CB-CA-C | -9.07 | 95.73       | 110.79   |
| 1   | B     | 15  | MET  | CB-CA-C | -9.07 | 95.73       | 110.79   |
| 1   | S     | 15  | MET  | CB-CA-C | -9.07 | 95.73       | 110.79   |
| 1   | C     | 15  | MET  | CB-CA-C | -9.07 | 95.73       | 110.79   |
| 1   | K     | 15  | MET  | CB-CA-C | -9.07 | 95.73       | 110.79   |
| 1   | J     | 15  | MET  | CB-CA-C | -9.07 | 95.74       | 110.79   |
| 1   | O     | 15  | MET  | CB-CA-C | -9.07 | 95.74       | 110.79   |
| 1   | Q     | 15  | MET  | CB-CA-C | -9.06 | 95.74       | 110.79   |
| 1   | N     | 15  | MET  | CB-CA-C | -9.06 | 95.75       | 110.79   |
| 1   | I     | 15  | MET  | CB-CA-C | -9.06 | 95.75       | 110.79   |
| 1   | D     | 15  | MET  | CB-CA-C | -9.05 | 95.77       | 110.79   |
| 1   | A     | 15  | MET  | CB-CA-C | -9.05 | 95.77       | 110.79   |
| 1   | P     | 15  | MET  | CB-CA-C | -9.05 | 95.77       | 110.79   |
| 1   | F     | 15  | MET  | CB-CA-C | -9.04 | 95.78       | 110.79   |
| 1   | H     | 15  | MET  | CB-CA-C | -9.04 | 95.78       | 110.79   |
| 1   | E     | 15  | MET  | CB-CA-C | -9.04 | 95.79       | 110.79   |
| 1   | G     | 15  | MET  | CB-CA-C | -9.03 | 95.81       | 110.79   |
| 1   | F     | 112 | ILE  | CB-CA-C | -8.07 | 101.64      | 111.97   |
| 1   | R     | 112 | ILE  | CB-CA-C | -8.06 | 101.65      | 111.97   |
| 1   | A     | 112 | ILE  | CB-CA-C | -8.06 | 101.65      | 111.97   |
| 1   | D     | 112 | ILE  | CB-CA-C | -8.06 | 101.66      | 111.97   |
| 1   | Q     | 112 | ILE  | CB-CA-C | -8.06 | 101.66      | 111.97   |
| 1   | S     | 112 | ILE  | CB-CA-C | -8.06 | 101.66      | 111.97   |
| 1   | C     | 112 | ILE  | CB-CA-C | -8.05 | 101.66      | 111.97   |
| 1   | I     | 112 | ILE  | CB-CA-C | -8.05 | 101.66      | 111.97   |
| 1   | O     | 112 | ILE  | CB-CA-C | -8.05 | 101.67      | 111.97   |
| 1   | G     | 112 | ILE  | CB-CA-C | -8.05 | 101.67      | 111.97   |
| 1   | P     | 112 | ILE  | CB-CA-C | -8.05 | 101.67      | 111.97   |
| 1   | N     | 112 | ILE  | CB-CA-C | -8.04 | 101.67      | 111.97   |
| 1   | U     | 112 | ILE  | CB-CA-C | -8.04 | 101.68      | 111.97   |
| 1   | B     | 112 | ILE  | CB-CA-C | -8.04 | 101.68      | 111.97   |
| 1   | J     | 112 | ILE  | CB-CA-C | -8.04 | 101.68      | 111.97   |
| 1   | E     | 112 | ILE  | CB-CA-C | -8.04 | 101.68      | 111.97   |
| 1   | M     | 112 | ILE  | CB-CA-C | -8.03 | 101.69      | 111.97   |
| 1   | H     | 112 | ILE  | CB-CA-C | -8.03 | 101.69      | 111.97   |
| 1   | L     | 112 | ILE  | CB-CA-C | -8.03 | 101.70      | 111.97   |
| 1   | T     | 112 | ILE  | CB-CA-C | -8.02 | 101.70      | 111.97   |
| 1   | K     | 112 | ILE  | CB-CA-C | -8.01 | 101.72      | 111.97   |
| 1   | F     | 165 | LEU  | N-CA-CB | 7.70  | 121.56      | 110.16   |
| 1   | N     | 165 | LEU  | N-CA-CB | 7.69  | 121.54      | 110.16   |
| 1   | Q     | 165 | LEU  | N-CA-CB | 7.68  | 121.53      | 110.16   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | O     | 165 | LEU  | N-CA-CB | 7.68  | 121.53      | 110.16   |
| 1   | K     | 165 | LEU  | N-CA-CB | 7.68  | 121.53      | 110.16   |
| 1   | R     | 165 | LEU  | N-CA-CB | 7.68  | 121.52      | 110.16   |
| 1   | B     | 165 | LEU  | N-CA-CB | 7.68  | 121.52      | 110.16   |
| 1   | J     | 165 | LEU  | N-CA-CB | 7.67  | 121.51      | 110.16   |
| 1   | M     | 165 | LEU  | N-CA-CB | 7.67  | 121.51      | 110.16   |
| 1   | P     | 165 | LEU  | N-CA-CB | 7.67  | 121.51      | 110.16   |
| 1   | S     | 165 | LEU  | N-CA-CB | 7.67  | 121.51      | 110.16   |
| 1   | U     | 165 | LEU  | N-CA-CB | 7.67  | 121.51      | 110.16   |
| 1   | C     | 165 | LEU  | N-CA-CB | 7.67  | 121.50      | 110.16   |
| 1   | T     | 165 | LEU  | N-CA-CB | 7.64  | 121.47      | 110.16   |
| 1   | G     | 165 | LEU  | N-CA-CB | 7.28  | 121.57      | 110.28   |
| 1   | I     | 165 | LEU  | N-CA-CB | 7.27  | 121.56      | 110.28   |
| 1   | A     | 165 | LEU  | N-CA-CB | 7.27  | 121.55      | 110.28   |
| 1   | D     | 165 | LEU  | N-CA-CB | 7.27  | 121.55      | 110.28   |
| 1   | E     | 165 | LEU  | N-CA-CB | 7.27  | 121.55      | 110.28   |
| 1   | H     | 165 | LEU  | N-CA-CB | 7.26  | 121.53      | 110.28   |
| 1   | L     | 165 | LEU  | N-CA-CB | 7.24  | 121.51      | 110.28   |
| 1   | I     | 161 | ALA  | N-CA-CB | -6.52 | 100.56      | 110.01   |
| 1   | H     | 161 | ALA  | N-CA-CB | -6.52 | 100.56      | 110.01   |
| 1   | E     | 161 | ALA  | N-CA-CB | -6.51 | 100.56      | 110.01   |
| 1   | A     | 161 | ALA  | N-CA-CB | -6.51 | 100.57      | 110.01   |
| 1   | D     | 161 | ALA  | N-CA-CB | -6.51 | 100.57      | 110.01   |
| 1   | F     | 161 | ALA  | N-CA-CB | -6.51 | 100.57      | 110.01   |
| 1   | G     | 161 | ALA  | N-CA-CB | -6.50 | 100.58      | 110.01   |
| 1   | S     | 161 | ALA  | N-CA-CB | -6.50 | 100.59      | 110.01   |
| 1   | U     | 161 | ALA  | N-CA-CB | -6.49 | 100.60      | 110.01   |
| 1   | P     | 161 | ALA  | N-CA-CB | -6.49 | 100.60      | 110.01   |
| 1   | C     | 161 | ALA  | N-CA-CB | -6.49 | 100.61      | 110.01   |
| 1   | L     | 161 | ALA  | N-CA-CB | -6.48 | 100.61      | 110.01   |
| 1   | T     | 161 | ALA  | N-CA-CB | -6.48 | 100.61      | 110.01   |
| 1   | O     | 161 | ALA  | N-CA-CB | -6.48 | 100.61      | 110.01   |
| 1   | Q     | 161 | ALA  | N-CA-CB | -6.48 | 100.61      | 110.01   |
| 1   | M     | 161 | ALA  | N-CA-CB | -6.48 | 100.61      | 110.01   |
| 1   | N     | 161 | ALA  | N-CA-CB | -6.48 | 100.62      | 110.01   |
| 1   | B     | 161 | ALA  | N-CA-CB | -6.47 | 100.62      | 110.01   |
| 1   | K     | 161 | ALA  | N-CA-CB | -6.47 | 100.63      | 110.01   |
| 1   | R     | 161 | ALA  | N-CA-CB | -6.46 | 100.64      | 110.01   |
| 1   | J     | 161 | ALA  | N-CA-CB | -6.46 | 100.64      | 110.01   |
| 1   | I     | 43  | LEU  | CB-CA-C | 6.07  | 120.87      | 110.79   |
| 1   | T     | 43  | LEU  | CB-CA-C | 6.07  | 120.86      | 110.79   |
| 1   | L     | 43  | LEU  | CB-CA-C | 6.06  | 120.85      | 110.79   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | M     | 43  | LEU  | CB-CA-C | 6.06  | 120.85      | 110.79   |
| 1   | J     | 43  | LEU  | CB-CA-C | 6.05  | 120.84      | 110.79   |
| 1   | E     | 43  | LEU  | CB-CA-C | 6.05  | 120.84      | 110.79   |
| 1   | S     | 43  | LEU  | CB-CA-C | 6.05  | 120.84      | 110.79   |
| 1   | B     | 43  | LEU  | CB-CA-C | 6.05  | 120.83      | 110.79   |
| 1   | D     | 43  | LEU  | CB-CA-C | 6.05  | 120.83      | 110.79   |
| 1   | Q     | 43  | LEU  | CB-CA-C | 6.05  | 120.83      | 110.79   |
| 1   | H     | 43  | LEU  | CB-CA-C | 6.05  | 120.83      | 110.79   |
| 1   | C     | 43  | LEU  | CB-CA-C | 6.04  | 120.82      | 110.79   |
| 1   | K     | 43  | LEU  | CB-CA-C | 6.04  | 120.82      | 110.79   |
| 1   | A     | 43  | LEU  | CB-CA-C | 6.04  | 120.82      | 110.79   |
| 1   | R     | 43  | LEU  | CB-CA-C | 6.04  | 120.81      | 110.79   |
| 1   | P     | 43  | LEU  | CB-CA-C | 6.04  | 120.81      | 110.79   |
| 1   | G     | 43  | LEU  | CB-CA-C | 6.04  | 120.81      | 110.79   |
| 1   | O     | 43  | LEU  | CB-CA-C | 6.03  | 120.80      | 110.79   |
| 1   | F     | 43  | LEU  | CB-CA-C | 6.03  | 120.80      | 110.79   |
| 1   | N     | 43  | LEU  | CB-CA-C | 6.03  | 120.80      | 110.79   |
| 1   | U     | 43  | LEU  | CB-CA-C | 6.02  | 120.78      | 110.79   |
| 1   | M     | 155 | ALA  | N-CA-CB | -5.25 | 102.39      | 110.16   |
| 1   | N     | 155 | ALA  | N-CA-CB | -5.24 | 102.40      | 110.16   |
| 1   | R     | 155 | ALA  | N-CA-CB | -5.24 | 102.40      | 110.16   |
| 1   | Q     | 155 | ALA  | N-CA-CB | -5.24 | 102.40      | 110.16   |
| 1   | K     | 155 | ALA  | N-CA-CB | -5.24 | 102.40      | 110.16   |
| 1   | S     | 155 | ALA  | N-CA-CB | -5.24 | 102.41      | 110.16   |
| 1   | P     | 155 | ALA  | N-CA-CB | -5.24 | 102.41      | 110.16   |
| 1   | C     | 155 | ALA  | N-CA-CB | -5.24 | 102.41      | 110.16   |
| 1   | T     | 155 | ALA  | N-CA-CB | -5.24 | 102.41      | 110.16   |
| 1   | O     | 155 | ALA  | N-CA-CB | -5.24 | 102.41      | 110.16   |
| 1   | E     | 155 | ALA  | N-CA-CB | -5.23 | 102.42      | 110.16   |
| 1   | U     | 155 | ALA  | N-CA-CB | -5.23 | 102.42      | 110.16   |
| 1   | B     | 155 | ALA  | N-CA-CB | -5.23 | 102.42      | 110.16   |
| 1   | L     | 155 | ALA  | N-CA-CB | -5.23 | 102.42      | 110.16   |
| 1   | A     | 155 | ALA  | N-CA-CB | -5.22 | 102.44      | 110.16   |
| 1   | J     | 155 | ALA  | N-CA-CB | -5.22 | 102.43      | 110.16   |
| 1   | G     | 155 | ALA  | N-CA-CB | -5.22 | 102.44      | 110.16   |
| 1   | F     | 155 | ALA  | N-CA-CB | -5.22 | 102.44      | 110.16   |
| 1   | H     | 155 | ALA  | N-CA-CB | -5.21 | 102.45      | 110.16   |
| 1   | I     | 155 | ALA  | N-CA-CB | -5.20 | 102.47      | 110.16   |
| 1   | D     | 155 | ALA  | N-CA-CB | -5.20 | 102.47      | 110.16   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1248  | 1333     | 1333     | 59      | 0            |
| 1   | B     | 1248  | 1333     | 1333     | 55      | 0            |
| 1   | C     | 1248  | 1333     | 1333     | 58      | 0            |
| 1   | D     | 1248  | 1333     | 1333     | 42      | 0            |
| 1   | E     | 1248  | 1333     | 1333     | 57      | 0            |
| 1   | F     | 1248  | 1333     | 1333     | 58      | 0            |
| 1   | G     | 1248  | 1333     | 1333     | 59      | 0            |
| 1   | H     | 1248  | 1333     | 1333     | 57      | 0            |
| 1   | I     | 1248  | 1333     | 1333     | 42      | 0            |
| 1   | J     | 1248  | 1333     | 1333     | 40      | 0            |
| 1   | K     | 1248  | 1333     | 1333     | 59      | 0            |
| 1   | L     | 1248  | 1333     | 1333     | 56      | 0            |
| 1   | M     | 1248  | 1333     | 1333     | 56      | 0            |
| 1   | N     | 1248  | 1333     | 1333     | 58      | 0            |
| 1   | O     | 1248  | 1333     | 1333     | 41      | 0            |
| 1   | P     | 1248  | 1333     | 1333     | 40      | 0            |
| 1   | Q     | 1248  | 1333     | 1333     | 58      | 0            |
| 1   | R     | 1248  | 1333     | 1333     | 61      | 0            |
| 1   | S     | 1248  | 1333     | 1333     | 58      | 0            |
| 1   | T     | 1248  | 1333     | 1333     | 57      | 0            |
| 1   | U     | 1248  | 1333     | 1333     | 41      | 0            |
| All | All   | 26208 | 27993    | 27993    | 823     | 0            |

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 15.

All (823) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:165:LEU:CD1 | 1:K:19:LEU:HD12 | 1.51                     | 1.41              |
| 1:G:165:LEU:CD1 | 1:N:19:LEU:HD12 | 1.51                     | 1.41              |
| 1:T:165:LEU:CD1 | 1:I:19:LEU:HD12 | 1.50                     | 1.41              |
| 1:A:165:LEU:CD1 | 1:M:19:LEU:HD12 | 1.51                     | 1.41              |
| 1:E:165:LEU:CD1 | 1:L:19:LEU:HD12 | 1.51                     | 1.41              |
| 1:H:165:LEU:CD1 | 1:O:19:LEU:HD12 | 1.51                     | 1.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:19:LEU:HD12  | 1:F:165:LEU:CD1  | 1.51                     | 1.40              |
| 1:S:165:LEU:CD1  | 1:H:19:LEU:HD12  | 1.50                     | 1.40              |
| 1:C:165:LEU:CD1  | 1:G:19:LEU:HD12  | 1.50                     | 1.40              |
| 1:A:19:LEU:HD12  | 1:R:165:LEU:CD1  | 1.50                     | 1.39              |
| 1:J:165:LEU:CD1  | 1:Q:19:LEU:HD12  | 1.52                     | 1.39              |
| 1:Q:165:LEU:CD1  | 1:F:19:LEU:HD12  | 1.50                     | 1.39              |
| 1:K:165:LEU:CD1  | 1:R:19:LEU:HD12  | 1.52                     | 1.38              |
| 1:C:19:LEU:HD12  | 1:L:165:LEU:CD1  | 1.52                     | 1.38              |
| 1:P:165:LEU:CD1  | 1:E:19:LEU:HD12  | 1.50                     | 1.38              |
| 1:B:165:LEU:CD1  | 1:S:19:LEU:HD12  | 1.52                     | 1.38              |
| 1:M:165:LEU:CD1  | 1:T:19:LEU:HD12  | 1.52                     | 1.37              |
| 1:N:165:LEU:CD1  | 1:U:19:LEU:HD12  | 1.51                     | 1.37              |
| 1:T:165:LEU:HD11 | 1:I:19:LEU:CD1   | 1.82                     | 1.09              |
| 1:S:165:LEU:HD11 | 1:H:19:LEU:CD1   | 1.82                     | 1.09              |
| 1:K:165:LEU:HD11 | 1:R:19:LEU:CD1   | 1.83                     | 1.09              |
| 1:C:19:LEU:CD1   | 1:L:165:LEU:HD11 | 1.83                     | 1.09              |
| 1:J:165:LEU:HD11 | 1:Q:19:LEU:CD1   | 1.83                     | 1.09              |
| 1:B:165:LEU:HD11 | 1:S:19:LEU:CD1   | 1.83                     | 1.08              |
| 1:C:165:LEU:HD11 | 1:G:19:LEU:CD1   | 1.82                     | 1.08              |
| 1:P:165:LEU:CD1  | 1:E:19:LEU:CD1   | 2.31                     | 1.08              |
| 1:D:165:LEU:HD11 | 1:K:19:LEU:CD1   | 1.83                     | 1.08              |
| 1:G:165:LEU:HD11 | 1:N:19:LEU:CD1   | 1.83                     | 1.08              |
| 1:M:165:LEU:HD11 | 1:T:19:LEU:CD1   | 1.83                     | 1.08              |
| 1:N:165:LEU:HD11 | 1:U:19:LEU:CD1   | 1.83                     | 1.08              |
| 1:T:165:LEU:CD1  | 1:I:19:LEU:CD1   | 2.31                     | 1.08              |
| 1:A:165:LEU:HD11 | 1:M:19:LEU:CD1   | 1.83                     | 1.08              |
| 1:Q:165:LEU:CD1  | 1:F:19:LEU:CD1   | 2.31                     | 1.08              |
| 1:E:165:LEU:HD11 | 1:L:19:LEU:CD1   | 1.83                     | 1.08              |
| 1:H:165:LEU:HD11 | 1:O:19:LEU:CD1   | 1.83                     | 1.08              |
| 1:A:19:LEU:CD1   | 1:R:165:LEU:CD1  | 2.31                     | 1.08              |
| 1:A:19:LEU:CD1   | 1:R:165:LEU:HD11 | 1.82                     | 1.08              |
| 1:B:19:LEU:CD1   | 1:F:165:LEU:HD11 | 1.83                     | 1.08              |
| 1:D:165:LEU:CD1  | 1:K:19:LEU:CD1   | 2.32                     | 1.08              |
| 1:A:165:LEU:CD1  | 1:M:19:LEU:CD1   | 2.32                     | 1.07              |
| 1:Q:165:LEU:HD11 | 1:F:19:LEU:CD1   | 1.82                     | 1.07              |
| 1:C:165:LEU:CD1  | 1:G:19:LEU:CD1   | 2.31                     | 1.07              |
| 1:B:19:LEU:CD1   | 1:F:165:LEU:CD1  | 2.32                     | 1.07              |
| 1:S:165:LEU:CD1  | 1:H:19:LEU:CD1   | 2.31                     | 1.07              |
| 1:P:165:LEU:HD11 | 1:E:19:LEU:CD1   | 1.83                     | 1.07              |
| 1:H:165:LEU:CD1  | 1:O:19:LEU:CD1   | 2.32                     | 1.07              |
| 1:C:19:LEU:CD1   | 1:L:165:LEU:CD1  | 2.33                     | 1.07              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:165:LEU:CD1  | 1:T:19:LEU:CD1   | 2.33                     | 1.07              |
| 1:N:165:LEU:CD1  | 1:U:19:LEU:CD1   | 2.33                     | 1.07              |
| 1:J:165:LEU:CD1  | 1:Q:19:LEU:CD1   | 2.33                     | 1.07              |
| 1:G:165:LEU:CD1  | 1:N:19:LEU:CD1   | 2.32                     | 1.06              |
| 1:E:165:LEU:CD1  | 1:L:19:LEU:CD1   | 2.32                     | 1.06              |
| 1:B:165:LEU:CD1  | 1:S:19:LEU:CD1   | 2.33                     | 1.06              |
| 1:K:165:LEU:CD1  | 1:R:19:LEU:CD1   | 2.33                     | 1.05              |
| 1:T:43:LEU:HD21  | 1:U:112:ILE:HG21 | 1.45                     | 0.99              |
| 1:P:43:LEU:HD21  | 1:Q:112:ILE:HG21 | 1.45                     | 0.98              |
| 1:E:43:LEU:HD21  | 1:F:112:ILE:HG21 | 1.45                     | 0.98              |
| 1:A:112:ILE:HG21 | 1:F:43:LEU:HD21  | 1.45                     | 0.98              |
| 1:D:43:LEU:HD21  | 1:E:112:ILE:HG21 | 1.45                     | 0.97              |
| 1:S:43:LEU:HD21  | 1:T:112:ILE:HG21 | 1.45                     | 0.97              |
| 1:Q:43:LEU:HD21  | 1:R:112:ILE:HG21 | 1.45                     | 0.96              |
| 1:J:43:LEU:HD21  | 1:K:112:ILE:HG21 | 1.46                     | 0.96              |
| 1:M:43:LEU:HD21  | 1:N:112:ILE:HG21 | 1.46                     | 0.96              |
| 1:A:43:LEU:HD21  | 1:G:112:ILE:HG21 | 1.45                     | 0.96              |
| 1:B:43:LEU:HD21  | 1:M:112:ILE:HG21 | 1.46                     | 0.96              |
| 1:K:43:LEU:HD21  | 1:L:112:ILE:HG21 | 1.46                     | 0.96              |
| 1:C:112:ILE:HG21 | 1:R:43:LEU:HD21  | 1.45                     | 0.95              |
| 1:C:43:LEU:HD21  | 1:S:112:ILE:HG21 | 1.45                     | 0.95              |
| 1:N:43:LEU:HD21  | 1:O:112:ILE:HG21 | 1.46                     | 0.95              |
| 1:H:43:LEU:HD21  | 1:I:112:ILE:HG21 | 1.45                     | 0.95              |
| 1:G:43:LEU:HD21  | 1:H:112:ILE:HG21 | 1.45                     | 0.94              |
| 1:B:112:ILE:HG21 | 1:L:43:LEU:HD21  | 1.46                     | 0.94              |
| 1:B:19:LEU:HD12  | 1:F:165:LEU:HD11 | 0.91                     | 0.91              |
| 1:G:165:LEU:HD11 | 1:N:19:LEU:HD12  | 0.91                     | 0.90              |
| 1:M:165:LEU:HD11 | 1:T:19:LEU:HD12  | 0.90                     | 0.90              |
| 1:Q:165:LEU:HD11 | 1:F:19:LEU:HD12  | 0.90                     | 0.90              |
| 1:D:165:LEU:HD11 | 1:K:19:LEU:HD12  | 0.91                     | 0.90              |
| 1:N:165:LEU:HD11 | 1:U:19:LEU:HD12  | 0.90                     | 0.90              |
| 1:A:19:LEU:HD12  | 1:R:165:LEU:HD11 | 0.90                     | 0.89              |
| 1:E:165:LEU:HD11 | 1:L:19:LEU:HD12  | 0.91                     | 0.89              |
| 1:A:165:LEU:HD11 | 1:M:19:LEU:HD12  | 0.91                     | 0.89              |
| 1:P:165:LEU:HD11 | 1:E:19:LEU:HD12  | 0.90                     | 0.89              |
| 1:T:165:LEU:HD11 | 1:I:19:LEU:HD12  | 0.90                     | 0.89              |
| 1:H:165:LEU:HD11 | 1:O:19:LEU:HD12  | 0.91                     | 0.89              |
| 1:J:165:LEU:HD11 | 1:Q:19:LEU:HD12  | 0.90                     | 0.89              |
| 1:C:19:LEU:HD12  | 1:L:165:LEU:HD11 | 0.90                     | 0.89              |
| 1:S:165:LEU:HD11 | 1:H:19:LEU:HD12  | 0.90                     | 0.88              |
| 1:B:165:LEU:HD11 | 1:S:19:LEU:HD12  | 0.90                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:165:LEU:HD11 | 1:R:19:LEU:HD12  | 0.90                     | 0.88              |
| 1:C:165:LEU:HD11 | 1:G:19:LEU:HD12  | 0.90                     | 0.87              |
| 1:B:15:MET:HB3   | 1:F:165:LEU:HD21 | 1.60                     | 0.84              |
| 1:E:165:LEU:HD21 | 1:L:15:MET:HB3   | 1.60                     | 0.84              |
| 1:S:165:LEU:HD21 | 1:H:15:MET:HB3   | 1.59                     | 0.84              |
| 1:N:165:LEU:HD21 | 1:U:15:MET:HB3   | 1.60                     | 0.84              |
| 1:T:165:LEU:HD21 | 1:I:15:MET:HB3   | 1.59                     | 0.84              |
| 1:A:15:MET:HB3   | 1:R:165:LEU:HD21 | 1.59                     | 0.84              |
| 1:M:165:LEU:HD21 | 1:T:15:MET:HB3   | 1.60                     | 0.83              |
| 1:P:165:LEU:HD21 | 1:E:15:MET:HB3   | 1.59                     | 0.83              |
| 1:A:165:LEU:HD21 | 1:M:15:MET:HB3   | 1.60                     | 0.83              |
| 1:D:165:LEU:HD21 | 1:K:15:MET:HB3   | 1.59                     | 0.83              |
| 1:H:165:LEU:HD21 | 1:O:15:MET:HB3   | 1.60                     | 0.83              |
| 1:C:15:MET:HB3   | 1:L:165:LEU:HD21 | 1.60                     | 0.83              |
| 1:Q:165:LEU:HD21 | 1:F:15:MET:HB3   | 1.59                     | 0.83              |
| 1:G:165:LEU:HD21 | 1:N:15:MET:HB3   | 1.60                     | 0.83              |
| 1:K:165:LEU:HD21 | 1:R:15:MET:HB3   | 1.60                     | 0.82              |
| 1:B:165:LEU:HD21 | 1:S:15:MET:HB3   | 1.60                     | 0.82              |
| 1:C:165:LEU:HD21 | 1:G:15:MET:HB3   | 1.59                     | 0.81              |
| 1:J:165:LEU:HD21 | 1:Q:15:MET:HB3   | 1.60                     | 0.81              |
| 1:P:165:LEU:CG   | 1:E:19:LEU:HD12  | 2.12                     | 0.80              |
| 1:Q:165:LEU:CG   | 1:F:19:LEU:HD12  | 2.12                     | 0.79              |
| 1:A:19:LEU:HD12  | 1:R:165:LEU:CG   | 2.12                     | 0.79              |
| 1:C:165:LEU:CG   | 1:G:19:LEU:HD12  | 2.12                     | 0.79              |
| 1:A:165:LEU:CG   | 1:M:19:LEU:HD12  | 2.13                     | 0.79              |
| 1:S:165:LEU:CG   | 1:H:19:LEU:HD12  | 2.12                     | 0.79              |
| 1:G:165:LEU:CG   | 1:N:19:LEU:HD12  | 2.13                     | 0.79              |
| 1:H:165:LEU:CG   | 1:O:19:LEU:HD12  | 2.13                     | 0.79              |
| 1:B:19:LEU:HD12  | 1:F:165:LEU:CG   | 2.13                     | 0.79              |
| 1:D:165:LEU:CG   | 1:K:19:LEU:HD12  | 2.13                     | 0.78              |
| 1:T:165:LEU:CG   | 1:I:19:LEU:HD12  | 2.12                     | 0.78              |
| 1:E:165:LEU:CG   | 1:L:19:LEU:HD12  | 2.13                     | 0.78              |
| 1:I:80:ARG:NH2   | 1:I:124:GLU:OE2  | 2.16                     | 0.78              |
| 1:D:80:ARG:NH2   | 1:D:124:GLU:OE2  | 2.16                     | 0.78              |
| 1:L:80:ARG:NH2   | 1:L:124:GLU:OE2  | 2.16                     | 0.78              |
| 1:T:80:ARG:NH2   | 1:T:124:GLU:OE2  | 2.16                     | 0.78              |
| 1:C:80:ARG:NH2   | 1:C:124:GLU:OE2  | 2.16                     | 0.78              |
| 1:B:80:ARG:NH2   | 1:B:124:GLU:OE2  | 2.16                     | 0.78              |
| 1:Q:80:ARG:NH2   | 1:Q:124:GLU:OE2  | 2.16                     | 0.78              |
| 1:H:80:ARG:NH2   | 1:H:124:GLU:OE2  | 2.16                     | 0.78              |
| 1:F:80:ARG:NH2   | 1:F:124:GLU:OE2  | 2.16                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:80:ARG:NH2   | 1:N:124:GLU:OE2  | 2.16                     | 0.78              |
| 1:O:80:ARG:NH2   | 1:O:124:GLU:OE2  | 2.16                     | 0.78              |
| 1:U:80:ARG:NH2   | 1:U:124:GLU:OE2  | 2.16                     | 0.77              |
| 1:J:80:ARG:NH2   | 1:J:124:GLU:OE2  | 2.16                     | 0.77              |
| 1:A:80:ARG:NH2   | 1:A:124:GLU:OE2  | 2.16                     | 0.77              |
| 1:R:80:ARG:NH2   | 1:R:124:GLU:OE2  | 2.16                     | 0.77              |
| 1:S:80:ARG:NH2   | 1:S:124:GLU:OE2  | 2.16                     | 0.77              |
| 1:G:80:ARG:NH2   | 1:G:124:GLU:OE2  | 2.16                     | 0.77              |
| 1:N:165:LEU:CG   | 1:U:19:LEU:HD12  | 2.15                     | 0.77              |
| 1:C:19:LEU:HD12  | 1:L:165:LEU:CG   | 2.15                     | 0.77              |
| 1:K:80:ARG:NH2   | 1:K:124:GLU:OE2  | 2.16                     | 0.77              |
| 1:B:165:LEU:CG   | 1:S:19:LEU:HD12  | 2.15                     | 0.77              |
| 1:K:165:LEU:CG   | 1:R:19:LEU:HD12  | 2.15                     | 0.77              |
| 1:M:165:LEU:CG   | 1:T:19:LEU:HD12  | 2.15                     | 0.77              |
| 1:P:80:ARG:NH2   | 1:P:124:GLU:OE2  | 2.16                     | 0.77              |
| 1:E:80:ARG:NH2   | 1:E:124:GLU:OE2  | 2.16                     | 0.77              |
| 1:J:165:LEU:CG   | 1:Q:19:LEU:HD12  | 2.15                     | 0.76              |
| 1:M:80:ARG:NH2   | 1:M:124:GLU:OE2  | 2.16                     | 0.76              |
| 1:G:43:LEU:CD2   | 1:H:112:ILE:HD13 | 2.18                     | 0.74              |
| 1:E:43:LEU:CD2   | 1:F:112:ILE:HD13 | 2.18                     | 0.74              |
| 1:A:43:LEU:CD2   | 1:G:112:ILE:HD13 | 2.18                     | 0.74              |
| 1:A:112:ILE:HD13 | 1:F:43:LEU:CD2   | 2.18                     | 0.74              |
| 1:H:43:LEU:CD2   | 1:I:112:ILE:HD13 | 2.18                     | 0.74              |
| 1:D:43:LEU:CD2   | 1:E:112:ILE:HD13 | 2.18                     | 0.73              |
| 1:T:43:LEU:CD2   | 1:U:112:ILE:HD13 | 2.19                     | 0.73              |
| 1:P:43:LEU:CD2   | 1:Q:112:ILE:HD13 | 2.19                     | 0.73              |
| 1:S:43:LEU:CD2   | 1:T:112:ILE:HD13 | 2.19                     | 0.72              |
| 1:C:43:LEU:CD2   | 1:S:112:ILE:HD13 | 2.19                     | 0.72              |
| 1:Q:43:LEU:CD2   | 1:R:112:ILE:HD13 | 2.19                     | 0.72              |
| 1:C:112:ILE:HD13 | 1:R:43:LEU:CD2   | 2.19                     | 0.72              |
| 1:B:43:LEU:CD2   | 1:M:112:ILE:HD13 | 2.22                     | 0.70              |
| 1:J:43:LEU:CD2   | 1:K:112:ILE:HD13 | 2.22                     | 0.70              |
| 1:B:112:ILE:HD13 | 1:L:43:LEU:CD2   | 2.22                     | 0.69              |
| 1:K:43:LEU:CD2   | 1:L:112:ILE:HD13 | 2.22                     | 0.69              |
| 1:A:43:LEU:HD21  | 1:G:112:ILE:HD13 | 1.74                     | 0.69              |
| 1:G:43:LEU:HD21  | 1:H:112:ILE:HD13 | 1.74                     | 0.69              |
| 1:A:112:ILE:HD13 | 1:F:43:LEU:HD21  | 1.74                     | 0.69              |
| 1:N:43:LEU:CD2   | 1:O:112:ILE:HD13 | 2.22                     | 0.69              |
| 1:M:43:LEU:CD2   | 1:N:112:ILE:HD13 | 2.22                     | 0.69              |
| 1:D:43:LEU:HD21  | 1:E:112:ILE:HD13 | 1.74                     | 0.68              |
| 1:E:43:LEU:HD21  | 1:F:112:ILE:HD13 | 1.74                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:43:LEU:HD21  | 1:I:112:ILE:HD13 | 1.74                     | 0.68              |
| 1:C:112:ILE:HD13 | 1:R:43:LEU:HD21  | 1.75                     | 0.68              |
| 1:T:43:LEU:HD21  | 1:U:112:ILE:HD13 | 1.75                     | 0.68              |
| 1:Q:43:LEU:HD21  | 1:R:112:ILE:HD13 | 1.75                     | 0.68              |
| 1:S:43:LEU:HD21  | 1:T:112:ILE:HD13 | 1.75                     | 0.68              |
| 1:C:43:LEU:HD21  | 1:S:112:ILE:HD13 | 1.75                     | 0.67              |
| 1:P:43:LEU:HD21  | 1:Q:112:ILE:HD13 | 1.75                     | 0.67              |
| 1:N:43:LEU:HD21  | 1:O:112:ILE:HD13 | 1.79                     | 0.65              |
| 1:J:43:LEU:HD21  | 1:K:112:ILE:HD13 | 1.79                     | 0.64              |
| 1:Q:165:LEU:HD12 | 1:F:19:LEU:CD1   | 2.28                     | 0.64              |
| 1:M:43:LEU:HD21  | 1:N:112:ILE:HD13 | 1.79                     | 0.64              |
| 1:P:165:LEU:HD12 | 1:E:19:LEU:CD1   | 2.28                     | 0.64              |
| 1:B:112:ILE:HD13 | 1:L:43:LEU:HD21  | 1.79                     | 0.63              |
| 1:B:43:LEU:HD21  | 1:M:112:ILE:HD13 | 1.79                     | 0.63              |
| 1:T:165:LEU:HD12 | 1:I:19:LEU:CD1   | 2.27                     | 0.63              |
| 1:K:43:LEU:HD21  | 1:L:112:ILE:HD13 | 1.79                     | 0.63              |
| 1:B:165:LEU:HD12 | 1:S:19:LEU:CD1   | 2.28                     | 0.63              |
| 1:E:165:LEU:HD12 | 1:L:19:LEU:CD1   | 2.28                     | 0.62              |
| 1:A:19:LEU:CD1   | 1:R:165:LEU:HD12 | 2.28                     | 0.62              |
| 1:S:165:LEU:HD12 | 1:H:19:LEU:CD1   | 2.28                     | 0.62              |
| 1:J:165:LEU:HD12 | 1:Q:19:LEU:CD1   | 2.28                     | 0.61              |
| 1:G:165:LEU:HD12 | 1:N:19:LEU:CD1   | 2.28                     | 0.61              |
| 1:D:165:LEU:HD12 | 1:K:19:LEU:CD1   | 2.28                     | 0.61              |
| 1:H:165:LEU:HD12 | 1:O:19:LEU:CD1   | 2.28                     | 0.61              |
| 1:N:165:LEU:HD12 | 1:U:19:LEU:CD1   | 2.28                     | 0.61              |
| 1:R:5:GLU:HG3    | 1:R:35:ILE:HD11  | 1.83                     | 0.61              |
| 1:J:5:GLU:HG3    | 1:J:35:ILE:HD11  | 1.83                     | 0.60              |
| 1:G:5:GLU:HG3    | 1:G:35:ILE:HD11  | 1.83                     | 0.60              |
| 1:H:5:GLU:HG3    | 1:H:35:ILE:HD11  | 1.83                     | 0.60              |
| 1:I:5:GLU:HG3    | 1:I:35:ILE:HD11  | 1.83                     | 0.60              |
| 1:C:5:GLU:HG3    | 1:C:35:ILE:HD11  | 1.84                     | 0.60              |
| 1:C:165:LEU:HD12 | 1:G:19:LEU:CD1   | 2.27                     | 0.60              |
| 1:D:5:GLU:HG3    | 1:D:35:ILE:HD11  | 1.83                     | 0.60              |
| 1:Q:5:GLU:HG3    | 1:Q:35:ILE:HD11  | 1.83                     | 0.60              |
| 1:S:5:GLU:HG3    | 1:S:35:ILE:HD11  | 1.83                     | 0.60              |
| 1:K:5:GLU:HG3    | 1:K:35:ILE:HD11  | 1.83                     | 0.60              |
| 1:L:5:GLU:HG3    | 1:L:35:ILE:HD11  | 1.83                     | 0.60              |
| 1:T:5:GLU:HG3    | 1:T:35:ILE:HD11  | 1.83                     | 0.60              |
| 1:O:5:GLU:HG3    | 1:O:35:ILE:HD11  | 1.83                     | 0.60              |
| 1:P:165:LEU:CG   | 1:E:19:LEU:CD1   | 2.77                     | 0.60              |
| 1:E:5:GLU:HG3    | 1:E:35:ILE:HD11  | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:5:GLU:HG3    | 1:A:35:ILE:HD11  | 1.83                     | 0.60              |
| 1:B:5:GLU:HG3    | 1:B:35:ILE:HD11  | 1.83                     | 0.60              |
| 1:P:5:GLU:HG3    | 1:P:35:ILE:HD11  | 1.83                     | 0.60              |
| 1:K:165:LEU:HD12 | 1:R:19:LEU:CD1   | 2.28                     | 0.60              |
| 1:U:5:GLU:HG3    | 1:U:35:ILE:HD11  | 1.83                     | 0.60              |
| 1:T:165:LEU:CG   | 1:I:19:LEU:CD1   | 2.77                     | 0.60              |
| 1:A:29:LEU:HD13  | 1:A:71:ALA:HA    | 1.84                     | 0.60              |
| 1:P:29:LEU:HD13  | 1:P:71:ALA:HA    | 1.84                     | 0.60              |
| 1:F:5:GLU:HG3    | 1:F:35:ILE:HD11  | 1.83                     | 0.60              |
| 1:G:29:LEU:HD13  | 1:G:71:ALA:HA    | 1.84                     | 0.60              |
| 1:N:5:GLU:HG3    | 1:N:35:ILE:HD11  | 1.83                     | 0.60              |
| 1:U:29:LEU:HD13  | 1:U:71:ALA:HA    | 1.84                     | 0.60              |
| 1:C:19:LEU:CD1   | 1:L:165:LEU:HD12 | 2.28                     | 0.60              |
| 1:J:29:LEU:HD13  | 1:J:71:ALA:HA    | 1.84                     | 0.60              |
| 1:R:29:LEU:HD13  | 1:R:71:ALA:HA    | 1.84                     | 0.60              |
| 1:F:29:LEU:HD13  | 1:F:71:ALA:HA    | 1.84                     | 0.60              |
| 1:H:29:LEU:HD13  | 1:H:71:ALA:HA    | 1.84                     | 0.60              |
| 1:O:29:LEU:HD13  | 1:O:71:ALA:HA    | 1.84                     | 0.60              |
| 1:Q:29:LEU:HD13  | 1:Q:71:ALA:HA    | 1.84                     | 0.60              |
| 1:E:29:LEU:HD13  | 1:E:71:ALA:HA    | 1.84                     | 0.60              |
| 1:K:29:LEU:HD13  | 1:K:71:ALA:HA    | 1.84                     | 0.60              |
| 1:M:5:GLU:HG3    | 1:M:35:ILE:HD11  | 1.84                     | 0.60              |
| 1:N:29:LEU:HD13  | 1:N:71:ALA:HA    | 1.84                     | 0.59              |
| 1:C:29:LEU:HD13  | 1:C:71:ALA:HA    | 1.84                     | 0.59              |
| 1:A:19:LEU:CD1   | 1:R:165:LEU:CG   | 2.77                     | 0.59              |
| 1:M:29:LEU:HD13  | 1:M:71:ALA:HA    | 1.84                     | 0.59              |
| 1:B:19:LEU:CD1   | 1:F:165:LEU:CG   | 2.77                     | 0.59              |
| 1:D:29:LEU:HD13  | 1:D:71:ALA:HA    | 1.84                     | 0.59              |
| 1:T:29:LEU:HD13  | 1:T:71:ALA:HA    | 1.84                     | 0.59              |
| 1:I:29:LEU:HD13  | 1:I:71:ALA:HA    | 1.84                     | 0.59              |
| 1:A:19:LEU:CD1   | 1:R:165:LEU:HG   | 2.33                     | 0.59              |
| 1:A:165:LEU:CG   | 1:M:19:LEU:CD1   | 2.77                     | 0.59              |
| 1:A:165:LEU:HD12 | 1:M:19:LEU:CD1   | 2.28                     | 0.59              |
| 1:B:29:LEU:HD13  | 1:B:71:ALA:HA    | 1.84                     | 0.59              |
| 1:S:29:LEU:HD13  | 1:S:71:ALA:HA    | 1.84                     | 0.59              |
| 1:L:29:LEU:HD13  | 1:L:71:ALA:HA    | 1.84                     | 0.59              |
| 1:Q:165:LEU:HG   | 1:F:19:LEU:CD1   | 2.33                     | 0.59              |
| 1:S:165:LEU:HG   | 1:H:19:LEU:CD1   | 2.33                     | 0.59              |
| 1:N:33:LEU:HD21  | 1:N:37:ARG:NH2   | 2.18                     | 0.59              |
| 1:A:165:LEU:HG   | 1:M:19:LEU:CD1   | 2.33                     | 0.59              |
| 1:P:33:LEU:HD21  | 1:P:37:ARG:NH2   | 2.18                     | 0.59              |

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| Atom-1          | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:D:33:LEU:HD21 | 1:D:37:ARG:NH2 | 2.18                     | 0.59              |
| 1:Q:33:LEU:HD21 | 1:Q:37:ARG:NH2 | 2.18                     | 0.59              |
| 1:R:33:LEU:HD21 | 1:R:37:ARG:NH2 | 2.18                     | 0.59              |
| 1:L:33:LEU:HD21 | 1:L:37:ARG:NH2 | 2.18                     | 0.59              |
| 1:A:29:LEU:HD12 | 1:A:70:GLU:HG3 | 1.85                     | 0.59              |
| 1:A:33:LEU:HD21 | 1:A:37:ARG:NH2 | 2.18                     | 0.59              |
| 1:D:29:LEU:HD12 | 1:D:70:GLU:HG3 | 1.85                     | 0.59              |
| 1:Q:165:LEU:CG  | 1:F:19:LEU:CD1 | 2.77                     | 0.59              |
| 1:E:29:LEU:HD12 | 1:E:70:GLU:HG3 | 1.85                     | 0.59              |
| 1:K:33:LEU:HD21 | 1:K:37:ARG:NH2 | 2.18                     | 0.59              |
| 1:F:33:LEU:HD21 | 1:F:37:ARG:NH2 | 2.18                     | 0.59              |
| 1:S:33:LEU:HD21 | 1:S:37:ARG:NH2 | 2.18                     | 0.59              |
| 1:M:33:LEU:HD21 | 1:M:37:ARG:NH2 | 2.18                     | 0.59              |
| 1:I:33:LEU:HD21 | 1:I:37:ARG:NH2 | 2.18                     | 0.59              |
| 1:C:33:LEU:HD21 | 1:C:37:ARG:NH2 | 2.18                     | 0.58              |
| 1:B:29:LEU:HD12 | 1:B:70:GLU:HG3 | 1.85                     | 0.58              |
| 1:D:165:LEU:CG  | 1:K:19:LEU:CD1 | 2.77                     | 0.58              |
| 1:E:33:LEU:HD21 | 1:E:37:ARG:NH2 | 2.18                     | 0.58              |
| 1:F:29:LEU:HD12 | 1:F:70:GLU:HG3 | 1.85                     | 0.58              |
| 1:T:33:LEU:HD21 | 1:T:37:ARG:NH2 | 2.18                     | 0.58              |
| 1:H:165:LEU:HG  | 1:O:19:LEU:CD1 | 2.33                     | 0.58              |
| 1:N:29:LEU:HD12 | 1:N:70:GLU:HG3 | 1.85                     | 0.58              |
| 1:O:33:LEU:HD21 | 1:O:37:ARG:NH2 | 2.18                     | 0.58              |
| 1:B:33:LEU:HD21 | 1:B:37:ARG:NH2 | 2.18                     | 0.58              |
| 1:S:165:LEU:CG  | 1:H:19:LEU:CD1 | 2.77                     | 0.58              |
| 1:M:29:LEU:HD12 | 1:M:70:GLU:HG3 | 1.85                     | 0.58              |
| 1:U:33:LEU:HD21 | 1:U:37:ARG:NH2 | 2.18                     | 0.58              |
| 1:O:29:LEU:HD12 | 1:O:70:GLU:HG3 | 1.86                     | 0.58              |
| 1:B:165:LEU:CG  | 1:S:19:LEU:CD1 | 2.80                     | 0.58              |
| 1:P:29:LEU:HD12 | 1:P:70:GLU:HG3 | 1.85                     | 0.58              |
| 1:J:33:LEU:HD21 | 1:J:37:ARG:NH2 | 2.18                     | 0.58              |
| 1:L:29:LEU:HD12 | 1:L:70:GLU:HG3 | 1.85                     | 0.58              |
| 1:G:29:LEU:HD12 | 1:G:70:GLU:HG3 | 1.85                     | 0.58              |
| 1:H:33:LEU:HD21 | 1:H:37:ARG:NH2 | 2.18                     | 0.58              |
| 1:C:165:LEU:HG  | 1:G:19:LEU:CD1 | 2.33                     | 0.58              |
| 1:P:165:LEU:HG  | 1:E:19:LEU:CD1 | 2.33                     | 0.58              |
| 1:J:165:LEU:CG  | 1:Q:19:LEU:CD1 | 2.80                     | 0.58              |
| 1:E:165:LEU:HG  | 1:L:19:LEU:CD1 | 2.33                     | 0.58              |
| 1:U:29:LEU:HD12 | 1:U:70:GLU:HG3 | 1.86                     | 0.58              |
| 1:G:33:LEU:HD21 | 1:G:37:ARG:NH2 | 2.18                     | 0.58              |
| 1:T:29:LEU:HD12 | 1:T:70:GLU:HG3 | 1.86                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:19:LEU:CD1   | 1:F:165:LEU:HG   | 2.33                     | 0.58              |
| 1:D:165:LEU:HG   | 1:K:19:LEU:CD1   | 2.33                     | 0.58              |
| 1:Q:29:LEU:HD12  | 1:Q:70:GLU:HG3   | 1.86                     | 0.58              |
| 1:G:165:LEU:HG   | 1:N:19:LEU:CD1   | 2.33                     | 0.58              |
| 1:M:165:LEU:HD12 | 1:T:19:LEU:CD1   | 2.28                     | 0.58              |
| 1:I:29:LEU:HD12  | 1:I:70:GLU:HG3   | 1.85                     | 0.58              |
| 1:J:29:LEU:HD12  | 1:J:70:GLU:HG3   | 1.85                     | 0.58              |
| 1:H:29:LEU:HD12  | 1:H:70:GLU:HG3   | 1.85                     | 0.58              |
| 1:R:29:LEU:HD12  | 1:R:70:GLU:HG3   | 1.85                     | 0.58              |
| 1:S:29:LEU:HD12  | 1:S:70:GLU:HG3   | 1.85                     | 0.58              |
| 1:H:165:LEU:CG   | 1:O:19:LEU:CD1   | 2.78                     | 0.58              |
| 1:N:165:LEU:CG   | 1:U:19:LEU:CD1   | 2.80                     | 0.58              |
| 1:K:29:LEU:HD12  | 1:K:70:GLU:HG3   | 1.86                     | 0.58              |
| 1:T:165:LEU:HG   | 1:I:19:LEU:CD1   | 2.33                     | 0.57              |
| 1:C:29:LEU:HD12  | 1:C:70:GLU:HG3   | 1.85                     | 0.57              |
| 1:G:165:LEU:CG   | 1:N:19:LEU:CD1   | 2.77                     | 0.57              |
| 1:C:19:LEU:CD1   | 1:L:165:LEU:CG   | 2.80                     | 0.57              |
| 1:M:165:LEU:CG   | 1:T:19:LEU:CD1   | 2.80                     | 0.57              |
| 1:C:165:LEU:CG   | 1:G:19:LEU:CD1   | 2.77                     | 0.56              |
| 1:E:165:LEU:CG   | 1:L:19:LEU:CD1   | 2.77                     | 0.56              |
| 1:J:165:LEU:HG   | 1:Q:19:LEU:CD1   | 2.36                     | 0.56              |
| 1:B:165:LEU:HG   | 1:S:19:LEU:CD1   | 2.36                     | 0.56              |
| 1:M:165:LEU:HG   | 1:T:19:LEU:CD1   | 2.36                     | 0.56              |
| 1:B:19:LEU:CD1   | 1:F:165:LEU:HD12 | 2.28                     | 0.56              |
| 1:C:19:LEU:CD1   | 1:L:165:LEU:HG   | 2.36                     | 0.56              |
| 1:K:165:LEU:HG   | 1:R:19:LEU:CD1   | 2.36                     | 0.56              |
| 1:N:165:LEU:HG   | 1:U:19:LEU:CD1   | 2.36                     | 0.56              |
| 1:D:108:VAL:HG11 | 1:D:152:VAL:HG11 | 1.89                     | 0.55              |
| 1:E:108:VAL:HG11 | 1:E:152:VAL:HG11 | 1.89                     | 0.55              |
| 1:L:108:VAL:HG11 | 1:L:152:VAL:HG11 | 1.89                     | 0.55              |
| 1:B:108:VAL:HG11 | 1:B:152:VAL:HG11 | 1.89                     | 0.55              |
| 1:T:108:VAL:HG11 | 1:T:152:VAL:HG11 | 1.88                     | 0.55              |
| 1:C:29:LEU:HB3   | 1:C:74:VAL:HG21  | 1.88                     | 0.55              |
| 1:K:29:LEU:HB3   | 1:K:74:VAL:HG21  | 1.88                     | 0.55              |
| 1:U:108:VAL:HG11 | 1:U:152:VAL:HG11 | 1.89                     | 0.55              |
| 1:C:37:ARG:NH2   | 1:C:81:GLU:OE2   | 2.40                     | 0.55              |
| 1:J:29:LEU:HB3   | 1:J:74:VAL:HG21  | 1.88                     | 0.55              |
| 1:S:108:VAL:HG11 | 1:S:152:VAL:HG11 | 1.88                     | 0.55              |
| 1:M:108:VAL:HG11 | 1:M:152:VAL:HG11 | 1.89                     | 0.55              |
| 1:H:37:ARG:NH2   | 1:H:81:GLU:OE2   | 2.40                     | 0.55              |
| 1:I:108:VAL:HG11 | 1:I:152:VAL:HG11 | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:37:ARG:NH2   | 1:K:81:GLU:OE2   | 2.40                     | 0.55              |
| 1:K:108:VAL:HG11 | 1:K:152:VAL:HG11 | 1.89                     | 0.55              |
| 1:F:108:VAL:HG11 | 1:F:152:VAL:HG11 | 1.89                     | 0.55              |
| 1:S:29:LEU:HB3   | 1:S:74:VAL:HG21  | 1.88                     | 0.55              |
| 1:I:29:LEU:HB3   | 1:I:74:VAL:HG21  | 1.88                     | 0.55              |
| 1:A:115:LEU:HD12 | 1:A:156:VAL:HG12 | 1.89                     | 0.55              |
| 1:D:37:ARG:NH2   | 1:D:81:GLU:OE2   | 2.40                     | 0.55              |
| 1:F:29:LEU:HB3   | 1:F:74:VAL:HG21  | 1.88                     | 0.55              |
| 1:F:115:LEU:HD12 | 1:F:156:VAL:HG12 | 1.89                     | 0.55              |
| 1:H:29:LEU:HB3   | 1:H:74:VAL:HG21  | 1.88                     | 0.55              |
| 1:U:37:ARG:NH2   | 1:U:81:GLU:OE2   | 2.40                     | 0.55              |
| 1:P:115:LEU:HD12 | 1:P:156:VAL:HG12 | 1.89                     | 0.55              |
| 1:R:29:LEU:HB3   | 1:R:74:VAL:HG21  | 1.88                     | 0.55              |
| 1:L:29:LEU:HB3   | 1:L:74:VAL:HG21  | 1.88                     | 0.55              |
| 1:L:37:ARG:NH2   | 1:L:81:GLU:OE2   | 2.40                     | 0.55              |
| 1:K:165:LEU:CG   | 1:R:19:LEU:CD1   | 2.80                     | 0.55              |
| 1:H:108:VAL:HG11 | 1:H:152:VAL:HG11 | 1.88                     | 0.55              |
| 1:U:29:LEU:HB3   | 1:U:74:VAL:HG21  | 1.88                     | 0.55              |
| 1:C:108:VAL:HG11 | 1:C:152:VAL:HG11 | 1.89                     | 0.55              |
| 1:Q:37:ARG:NH2   | 1:Q:81:GLU:OE2   | 2.40                     | 0.55              |
| 1:S:37:ARG:NH2   | 1:S:81:GLU:OE2   | 2.40                     | 0.55              |
| 1:M:37:ARG:NH2   | 1:M:81:GLU:OE2   | 2.40                     | 0.55              |
| 1:N:108:VAL:HG11 | 1:N:152:VAL:HG11 | 1.88                     | 0.55              |
| 1:O:115:LEU:HD12 | 1:O:156:VAL:HG12 | 1.89                     | 0.55              |
| 1:A:29:LEU:HB3   | 1:A:74:VAL:HG21  | 1.88                     | 0.54              |
| 1:P:108:VAL:HG11 | 1:P:152:VAL:HG11 | 1.89                     | 0.54              |
| 1:D:29:LEU:HB3   | 1:D:74:VAL:HG21  | 1.88                     | 0.54              |
| 1:T:37:ARG:NH2   | 1:T:81:GLU:OE2   | 2.40                     | 0.54              |
| 1:N:115:LEU:HD12 | 1:N:156:VAL:HG12 | 1.89                     | 0.54              |
| 1:A:37:ARG:NH2   | 1:A:81:GLU:OE2   | 2.40                     | 0.54              |
| 1:B:37:ARG:NH2   | 1:B:81:GLU:OE2   | 2.40                     | 0.54              |
| 1:P:37:ARG:NH2   | 1:P:81:GLU:OE2   | 2.40                     | 0.54              |
| 1:F:37:ARG:NH2   | 1:F:81:GLU:OE2   | 2.40                     | 0.54              |
| 1:I:37:ARG:NH2   | 1:I:81:GLU:OE2   | 2.40                     | 0.54              |
| 1:J:108:VAL:HG11 | 1:J:152:VAL:HG11 | 1.89                     | 0.54              |
| 1:E:37:ARG:NH2   | 1:E:81:GLU:OE2   | 2.40                     | 0.54              |
| 1:A:108:VAL:HG11 | 1:A:152:VAL:HG11 | 1.89                     | 0.54              |
| 1:Q:115:LEU:HD12 | 1:Q:156:VAL:HG12 | 1.89                     | 0.54              |
| 1:G:29:LEU:HB3   | 1:G:74:VAL:HG21  | 1.88                     | 0.54              |
| 1:G:115:LEU:HD12 | 1:G:156:VAL:HG12 | 1.89                     | 0.54              |
| 1:T:29:LEU:HB3   | 1:T:74:VAL:HG21  | 1.88                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:37:ARG:NH2   | 1:N:81:GLU:OE2   | 2.40                     | 0.54              |
| 1:E:29:LEU:HB3   | 1:E:74:VAL:HG21  | 1.88                     | 0.54              |
| 1:E:115:LEU:HD12 | 1:E:156:VAL:HG12 | 1.89                     | 0.54              |
| 1:G:108:VAL:HG11 | 1:G:152:VAL:HG11 | 1.88                     | 0.54              |
| 1:O:108:VAL:HG11 | 1:O:152:VAL:HG11 | 1.89                     | 0.54              |
| 1:R:108:VAL:HG11 | 1:R:152:VAL:HG11 | 1.89                     | 0.54              |
| 1:O:29:LEU:HB3   | 1:O:74:VAL:HG21  | 1.88                     | 0.54              |
| 1:B:29:LEU:HB3   | 1:B:74:VAL:HG21  | 1.88                     | 0.54              |
| 1:P:29:LEU:HB3   | 1:P:74:VAL:HG21  | 1.88                     | 0.54              |
| 1:J:37:ARG:NH2   | 1:J:81:GLU:OE2   | 2.40                     | 0.54              |
| 1:Q:29:LEU:HB3   | 1:Q:74:VAL:HG21  | 1.88                     | 0.54              |
| 1:Q:108:VAL:HG11 | 1:Q:152:VAL:HG11 | 1.89                     | 0.54              |
| 1:K:43:LEU:HD11  | 1:L:116:GLU:OE2  | 2.08                     | 0.54              |
| 1:R:37:ARG:NH2   | 1:R:81:GLU:OE2   | 2.40                     | 0.54              |
| 1:N:29:LEU:HB3   | 1:N:74:VAL:HG21  | 1.88                     | 0.54              |
| 1:O:72:LEU:HD13  | 1:O:114:ALA:HA   | 1.90                     | 0.54              |
| 1:G:37:ARG:NH2   | 1:G:81:GLU:OE2   | 2.40                     | 0.54              |
| 1:M:29:LEU:HB3   | 1:M:74:VAL:HG21  | 1.88                     | 0.54              |
| 1:M:115:LEU:HD12 | 1:M:156:VAL:HG12 | 1.89                     | 0.54              |
| 1:I:115:LEU:HD12 | 1:I:156:VAL:HG12 | 1.89                     | 0.54              |
| 1:O:37:ARG:NH2   | 1:O:81:GLU:OE2   | 2.40                     | 0.54              |
| 1:A:72:LEU:HD13  | 1:A:114:ALA:HA   | 1.91                     | 0.53              |
| 1:N:72:LEU:HD13  | 1:N:114:ALA:HA   | 1.91                     | 0.53              |
| 1:U:115:LEU:HD12 | 1:U:156:VAL:HG12 | 1.89                     | 0.53              |
| 1:Q:72:LEU:HD13  | 1:Q:114:ALA:HA   | 1.91                     | 0.53              |
| 1:K:115:LEU:HD12 | 1:K:156:VAL:HG12 | 1.89                     | 0.53              |
| 1:G:34:GLU:OE2   | 1:G:37:ARG:NH1   | 2.42                     | 0.53              |
| 1:G:72:LEU:HD13  | 1:G:114:ALA:HA   | 1.91                     | 0.53              |
| 1:C:115:LEU:HD12 | 1:C:156:VAL:HG12 | 1.89                     | 0.53              |
| 1:P:72:LEU:HD13  | 1:P:114:ALA:HA   | 1.91                     | 0.53              |
| 1:F:72:LEU:HD13  | 1:F:114:ALA:HA   | 1.91                     | 0.53              |
| 1:L:115:LEU:HD12 | 1:L:156:VAL:HG12 | 1.89                     | 0.53              |
| 1:M:34:GLU:OE2   | 1:M:37:ARG:NH1   | 2.42                     | 0.53              |
| 1:M:72:LEU:HD13  | 1:M:114:ALA:HA   | 1.91                     | 0.53              |
| 1:N:34:GLU:OE2   | 1:N:37:ARG:NH1   | 2.42                     | 0.53              |
| 1:J:43:LEU:HD11  | 1:K:116:GLU:OE2  | 2.08                     | 0.53              |
| 1:R:72:LEU:HD13  | 1:R:114:ALA:HA   | 1.91                     | 0.53              |
| 1:F:34:GLU:OE2   | 1:F:37:ARG:NH1   | 2.42                     | 0.53              |
| 1:S:115:LEU:HD12 | 1:S:156:VAL:HG12 | 1.89                     | 0.53              |
| 1:H:115:LEU:HD12 | 1:H:156:VAL:HG12 | 1.89                     | 0.53              |
| 1:U:34:GLU:OE2   | 1:U:37:ARG:NH1   | 2.42                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:115:LEU:HD12 | 1:D:156:VAL:HG12 | 1.89                     | 0.53              |
| 1:R:115:LEU:HD12 | 1:R:156:VAL:HG12 | 1.89                     | 0.53              |
| 1:H:72:LEU:HD13  | 1:H:114:ALA:HA   | 1.90                     | 0.53              |
| 1:A:34:GLU:OE2   | 1:A:37:ARG:NH1   | 2.42                     | 0.53              |
| 1:P:34:GLU:OE2   | 1:P:37:ARG:NH1   | 2.42                     | 0.53              |
| 1:D:34:GLU:OE2   | 1:D:37:ARG:NH1   | 2.42                     | 0.53              |
| 1:J:72:LEU:HD13  | 1:J:114:ALA:HA   | 1.91                     | 0.53              |
| 1:M:43:LEU:HD11  | 1:N:116:GLU:OE2  | 2.08                     | 0.53              |
| 1:E:34:GLU:OE2   | 1:E:37:ARG:NH1   | 2.42                     | 0.53              |
| 1:S:34:GLU:OE2   | 1:S:37:ARG:NH1   | 2.42                     | 0.53              |
| 1:T:34:GLU:OE2   | 1:T:37:ARG:NH1   | 2.42                     | 0.53              |
| 1:T:115:LEU:HD12 | 1:T:156:VAL:HG12 | 1.89                     | 0.53              |
| 1:U:72:LEU:HD13  | 1:U:114:ALA:HA   | 1.91                     | 0.53              |
| 1:O:34:GLU:OE2   | 1:O:37:ARG:NH1   | 2.42                     | 0.53              |
| 1:C:34:GLU:OE2   | 1:C:37:ARG:NH1   | 2.42                     | 0.53              |
| 1:B:43:LEU:HD11  | 1:M:116:GLU:OE2  | 2.08                     | 0.53              |
| 1:B:116:GLU:OE2  | 1:L:43:LEU:HD11  | 2.08                     | 0.53              |
| 1:E:72:LEU:HD13  | 1:E:114:ALA:HA   | 1.91                     | 0.53              |
| 1:R:34:GLU:OE2   | 1:R:37:ARG:NH1   | 2.42                     | 0.53              |
| 1:N:43:LEU:HD11  | 1:O:116:GLU:OE2  | 2.08                     | 0.53              |
| 1:L:34:GLU:OE2   | 1:L:37:ARG:NH1   | 2.42                     | 0.52              |
| 1:B:72:LEU:HD13  | 1:B:114:ALA:HA   | 1.90                     | 0.52              |
| 1:K:34:GLU:OE2   | 1:K:37:ARG:NH1   | 2.42                     | 0.52              |
| 1:K:72:LEU:HD13  | 1:K:114:ALA:HA   | 1.90                     | 0.52              |
| 1:C:72:LEU:HD13  | 1:C:114:ALA:HA   | 1.91                     | 0.52              |
| 1:B:115:LEU:HD12 | 1:B:156:VAL:HG12 | 1.89                     | 0.52              |
| 1:J:115:LEU:HD12 | 1:J:156:VAL:HG12 | 1.89                     | 0.52              |
| 1:H:34:GLU:OE2   | 1:H:37:ARG:NH1   | 2.42                     | 0.52              |
| 1:I:34:GLU:OE2   | 1:I:37:ARG:NH1   | 2.42                     | 0.52              |
| 1:B:34:GLU:OE2   | 1:B:37:ARG:NH1   | 2.42                     | 0.52              |
| 1:Q:34:GLU:OE2   | 1:Q:37:ARG:NH1   | 2.42                     | 0.52              |
| 1:I:72:LEU:HD13  | 1:I:114:ALA:HA   | 1.90                     | 0.52              |
| 1:J:34:GLU:OE2   | 1:J:37:ARG:NH1   | 2.42                     | 0.52              |
| 1:D:72:LEU:HD13  | 1:D:114:ALA:HA   | 1.91                     | 0.52              |
| 1:T:72:LEU:HD13  | 1:T:114:ALA:HA   | 1.91                     | 0.52              |
| 1:L:72:LEU:HD13  | 1:L:114:ALA:HA   | 1.91                     | 0.52              |
| 1:S:72:LEU:HD13  | 1:S:114:ALA:HA   | 1.91                     | 0.52              |
| 1:A:116:GLU:OE2  | 1:F:43:LEU:HD11  | 2.10                     | 0.52              |
| 1:G:43:LEU:HD11  | 1:H:116:GLU:OE2  | 2.10                     | 0.51              |
| 1:E:43:LEU:HD11  | 1:F:116:GLU:OE2  | 2.10                     | 0.51              |
| 1:H:43:LEU:HD11  | 1:I:116:GLU:OE2  | 2.10                     | 0.51              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:43:LEU:HD11 | 1:G:116:GLU:OE2 | 2.10                     | 0.51              |
| 1:D:43:LEU:HD11 | 1:E:116:GLU:OE2 | 2.10                     | 0.51              |
| 1:L:14:ILE:HG23 | 1:L:58:GLU:HG3  | 1.94                     | 0.50              |
| 1:S:14:ILE:HG23 | 1:S:58:GLU:HG3  | 1.94                     | 0.50              |
| 1:B:14:ILE:HG23 | 1:B:58:GLU:HG3  | 1.94                     | 0.50              |
| 1:T:14:ILE:HG23 | 1:T:58:GLU:HG3  | 1.94                     | 0.50              |
| 1:C:14:ILE:HG23 | 1:C:58:GLU:HG3  | 1.94                     | 0.50              |
| 1:E:14:ILE:HG23 | 1:E:58:GLU:HG3  | 1.94                     | 0.50              |
| 1:K:14:ILE:HG23 | 1:K:58:GLU:HG3  | 1.94                     | 0.50              |
| 1:D:14:ILE:HG23 | 1:D:58:GLU:HG3  | 1.94                     | 0.50              |
| 1:M:14:ILE:HG23 | 1:M:58:GLU:HG3  | 1.94                     | 0.50              |
| 1:U:14:ILE:HG23 | 1:U:58:GLU:HG3  | 1.94                     | 0.50              |
| 1:I:14:ILE:HG23 | 1:I:58:GLU:HG3  | 1.94                     | 0.50              |
| 1:D:104:ARG:HG2 | 1:D:144:GLU:OE2 | 2.12                     | 0.50              |
| 1:J:14:ILE:HG23 | 1:J:58:GLU:HG3  | 1.94                     | 0.50              |
| 1:L:104:ARG:HG2 | 1:L:144:GLU:OE2 | 2.12                     | 0.50              |
| 1:S:104:ARG:HG2 | 1:S:144:GLU:OE2 | 2.12                     | 0.50              |
| 1:H:14:ILE:HG23 | 1:H:58:GLU:HG3  | 1.94                     | 0.50              |
| 1:U:104:ARG:HG2 | 1:U:144:GLU:OE2 | 2.12                     | 0.50              |
| 1:J:104:ARG:HG2 | 1:J:144:GLU:OE2 | 2.12                     | 0.50              |
| 1:M:104:ARG:HG2 | 1:M:144:GLU:OE2 | 2.12                     | 0.50              |
| 1:I:104:ARG:HG2 | 1:I:144:GLU:OE2 | 2.12                     | 0.50              |
| 1:C:116:GLU:OE2 | 1:R:43:LEU:HD11 | 2.12                     | 0.49              |
| 1:P:43:LEU:HD11 | 1:Q:116:GLU:OE2 | 2.12                     | 0.49              |
| 1:R:14:ILE:HG23 | 1:R:58:GLU:HG3  | 1.94                     | 0.49              |
| 1:F:14:ILE:HG23 | 1:F:58:GLU:HG3  | 1.94                     | 0.49              |
| 1:Q:104:ARG:HG2 | 1:Q:144:GLU:OE2 | 2.12                     | 0.49              |
| 1:R:104:ARG:HG2 | 1:R:144:GLU:OE2 | 2.12                     | 0.49              |
| 1:A:104:ARG:HG2 | 1:A:144:GLU:OE2 | 2.12                     | 0.49              |
| 1:T:43:LEU:HD11 | 1:U:116:GLU:OE2 | 2.12                     | 0.49              |
| 1:N:14:ILE:HG23 | 1:N:58:GLU:HG3  | 1.94                     | 0.49              |
| 1:P:104:ARG:HG2 | 1:P:144:GLU:OE2 | 2.12                     | 0.49              |
| 1:F:104:ARG:HG2 | 1:F:144:GLU:OE2 | 2.12                     | 0.49              |
| 1:C:43:LEU:HD11 | 1:S:116:GLU:OE2 | 2.12                     | 0.49              |
| 1:P:14:ILE:HG23 | 1:P:58:GLU:HG3  | 1.94                     | 0.49              |
| 1:G:104:ARG:HG2 | 1:G:144:GLU:OE2 | 2.12                     | 0.49              |
| 1:N:104:ARG:HG2 | 1:N:144:GLU:OE2 | 2.12                     | 0.49              |
| 1:O:104:ARG:HG2 | 1:O:144:GLU:OE2 | 2.12                     | 0.49              |
| 1:A:14:ILE:HG23 | 1:A:58:GLU:HG3  | 1.94                     | 0.49              |
| 1:Q:14:ILE:HG23 | 1:Q:58:GLU:HG3  | 1.94                     | 0.49              |
| 1:K:104:ARG:HG2 | 1:K:144:GLU:OE2 | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:43:LEU:HD11  | 1:T:116:GLU:OE2  | 2.12                     | 0.49              |
| 1:O:14:ILE:HG23  | 1:O:58:GLU:HG3   | 1.94                     | 0.49              |
| 1:C:104:ARG:HG2  | 1:C:144:GLU:OE2  | 2.12                     | 0.49              |
| 1:G:14:ILE:HG23  | 1:G:58:GLU:HG3   | 1.94                     | 0.49              |
| 1:H:104:ARG:HG2  | 1:H:144:GLU:OE2  | 2.12                     | 0.49              |
| 1:T:104:ARG:HG2  | 1:T:144:GLU:OE2  | 2.12                     | 0.48              |
| 1:Q:43:LEU:HD11  | 1:R:116:GLU:OE2  | 2.12                     | 0.48              |
| 1:E:104:ARG:HG2  | 1:E:144:GLU:OE2  | 2.12                     | 0.48              |
| 1:B:104:ARG:HG2  | 1:B:144:GLU:OE2  | 2.12                     | 0.48              |
| 1:E:161:ALA:HB1  | 1:L:19:LEU:HD22  | 1.96                     | 0.48              |
| 1:D:161:ALA:HB1  | 1:K:19:LEU:HD22  | 1.96                     | 0.47              |
| 1:B:19:LEU:HD22  | 1:F:161:ALA:HB1  | 1.96                     | 0.47              |
| 1:A:19:LEU:HD22  | 1:R:161:ALA:HB1  | 1.96                     | 0.47              |
| 1:H:161:ALA:HB1  | 1:O:19:LEU:HD22  | 1.96                     | 0.47              |
| 1:S:161:ALA:HB1  | 1:H:19:LEU:HD22  | 1.96                     | 0.47              |
| 1:G:161:ALA:HB1  | 1:N:19:LEU:HD22  | 1.96                     | 0.47              |
| 1:I:72:LEU:HB3   | 1:I:117:VAL:HG21 | 1.97                     | 0.47              |
| 1:C:72:LEU:HB3   | 1:C:117:VAL:HG21 | 1.97                     | 0.47              |
| 1:J:72:LEU:HB3   | 1:J:117:VAL:HG21 | 1.97                     | 0.47              |
| 1:Q:161:ALA:HB1  | 1:F:19:LEU:HD22  | 1.96                     | 0.47              |
| 1:K:72:LEU:HB3   | 1:K:117:VAL:HG21 | 1.97                     | 0.47              |
| 1:S:72:LEU:HB3   | 1:S:117:VAL:HG21 | 1.97                     | 0.47              |
| 1:H:72:LEU:HB3   | 1:H:117:VAL:HG21 | 1.97                     | 0.47              |
| 1:C:161:ALA:HB1  | 1:G:19:LEU:HD22  | 1.96                     | 0.46              |
| 1:A:161:ALA:HB1  | 1:M:19:LEU:HD22  | 1.96                     | 0.46              |
| 1:R:72:LEU:HB3   | 1:R:117:VAL:HG21 | 1.97                     | 0.46              |
| 1:T:161:ALA:HB1  | 1:I:19:LEU:HD22  | 1.96                     | 0.46              |
| 1:A:42:LEU:HD21  | 1:A:86:VAL:HG11  | 1.97                     | 0.46              |
| 1:P:161:ALA:HB1  | 1:E:19:LEU:HD22  | 1.96                     | 0.46              |
| 1:D:72:LEU:HB3   | 1:D:117:VAL:HG21 | 1.97                     | 0.46              |
| 1:R:165:LEU:HD23 | 1:R:165:LEU:HA   | 1.86                     | 0.46              |
| 1:L:72:LEU:HB3   | 1:L:117:VAL:HG21 | 1.97                     | 0.46              |
| 1:R:152:VAL:O    | 1:R:156:VAL:HG23 | 2.16                     | 0.46              |
| 1:G:72:LEU:HB3   | 1:G:117:VAL:HG21 | 1.97                     | 0.46              |
| 1:O:42:LEU:HD21  | 1:O:86:VAL:HG11  | 1.97                     | 0.46              |
| 1:L:42:LEU:HD21  | 1:L:86:VAL:HG11  | 1.97                     | 0.46              |
| 1:T:72:LEU:HB3   | 1:T:117:VAL:HG21 | 1.97                     | 0.46              |
| 1:N:42:LEU:HD21  | 1:N:86:VAL:HG11  | 1.97                     | 0.46              |
| 1:F:42:LEU:HD21  | 1:F:86:VAL:HG11  | 1.97                     | 0.46              |
| 1:G:152:VAL:O    | 1:G:156:VAL:HG23 | 2.16                     | 0.46              |
| 1:B:72:LEU:HB3   | 1:B:117:VAL:HG21 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:42:LEU:HD21  | 1:P:86:VAL:HG11  | 1.97                     | 0.46              |
| 1:D:42:LEU:HD21  | 1:D:86:VAL:HG11  | 1.97                     | 0.46              |
| 1:Q:72:LEU:HB3   | 1:Q:117:VAL:HG21 | 1.97                     | 0.46              |
| 1:T:42:LEU:HD21  | 1:T:86:VAL:HG11  | 1.97                     | 0.46              |
| 1:O:72:LEU:HB3   | 1:O:117:VAL:HG21 | 1.97                     | 0.46              |
| 1:J:152:VAL:O    | 1:J:156:VAL:HG23 | 2.16                     | 0.46              |
| 1:Q:152:VAL:O    | 1:Q:156:VAL:HG23 | 2.16                     | 0.46              |
| 1:E:72:LEU:HB3   | 1:E:117:VAL:HG21 | 1.97                     | 0.46              |
| 1:K:42:LEU:HD21  | 1:K:86:VAL:HG11  | 1.97                     | 0.46              |
| 1:I:42:LEU:HD21  | 1:I:86:VAL:HG11  | 1.97                     | 0.46              |
| 1:O:152:VAL:O    | 1:O:156:VAL:HG23 | 2.16                     | 0.46              |
| 1:B:42:LEU:HD21  | 1:B:86:VAL:HG11  | 1.97                     | 0.46              |
| 1:Q:119:LEU:HD13 | 1:Q:164:ILE:HG13 | 1.98                     | 0.46              |
| 1:S:42:LEU:HD21  | 1:S:86:VAL:HG11  | 1.97                     | 0.46              |
| 1:G:42:LEU:HD21  | 1:G:86:VAL:HG11  | 1.97                     | 0.46              |
| 1:G:119:LEU:HD13 | 1:G:164:ILE:HG13 | 1.98                     | 0.46              |
| 1:H:152:VAL:O    | 1:H:156:VAL:HG23 | 2.16                     | 0.46              |
| 1:B:152:VAL:O    | 1:B:156:VAL:HG23 | 2.16                     | 0.46              |
| 1:J:119:LEU:HD13 | 1:J:164:ILE:HG13 | 1.98                     | 0.46              |
| 1:H:119:LEU:HD13 | 1:H:164:ILE:HG13 | 1.98                     | 0.46              |
| 1:A:72:LEU:HB3   | 1:A:117:VAL:HG21 | 1.97                     | 0.45              |
| 1:A:152:VAL:O    | 1:A:156:VAL:HG23 | 2.16                     | 0.45              |
| 1:D:119:LEU:HD13 | 1:D:164:ILE:HG13 | 1.98                     | 0.45              |
| 1:Q:42:LEU:HD21  | 1:Q:86:VAL:HG11  | 1.97                     | 0.45              |
| 1:L:165:LEU:HD23 | 1:L:165:LEU:HA   | 1.86                     | 0.45              |
| 1:T:152:VAL:O    | 1:T:156:VAL:HG23 | 2.16                     | 0.45              |
| 1:T:165:LEU:HD23 | 1:T:165:LEU:HA   | 1.86                     | 0.45              |
| 1:U:72:LEU:HB3   | 1:U:117:VAL:HG21 | 1.97                     | 0.45              |
| 1:U:152:VAL:O    | 1:U:156:VAL:HG23 | 2.16                     | 0.45              |
| 1:B:119:LEU:HD13 | 1:B:164:ILE:HG13 | 1.98                     | 0.45              |
| 1:P:72:LEU:HB3   | 1:P:117:VAL:HG21 | 1.97                     | 0.45              |
| 1:J:2:GLU:HG2    | 1:J:39:SER:OG    | 2.17                     | 0.45              |
| 1:E:119:LEU:HD13 | 1:E:164:ILE:HG13 | 1.98                     | 0.45              |
| 1:E:152:VAL:O    | 1:E:156:VAL:HG23 | 2.16                     | 0.45              |
| 1:K:2:GLU:HG2    | 1:K:39:SER:OG    | 2.17                     | 0.45              |
| 1:G:2:GLU:HG2    | 1:G:39:SER:OG    | 2.17                     | 0.45              |
| 1:P:119:LEU:HD13 | 1:P:164:ILE:HG13 | 1.98                     | 0.45              |
| 1:Q:2:GLU:HG2    | 1:Q:39:SER:OG    | 2.17                     | 0.45              |
| 1:K:152:VAL:O    | 1:K:156:VAL:HG23 | 2.16                     | 0.45              |
| 1:M:2:GLU:HG2    | 1:M:39:SER:OG    | 2.17                     | 0.45              |
| 1:M:72:LEU:HB3   | 1:M:117:VAL:HG21 | 1.97                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:2:GLU:HG2    | 1:T:39:SER:OG    | 2.17                     | 0.45              |
| 1:N:72:LEU:HB3   | 1:N:117:VAL:HG21 | 1.97                     | 0.45              |
| 1:O:2:GLU:HG2    | 1:O:39:SER:OG    | 2.17                     | 0.45              |
| 1:C:42:LEU:HD21  | 1:C:86:VAL:HG11  | 1.97                     | 0.45              |
| 1:C:165:LEU:HD12 | 1:G:19:LEU:HD13  | 1.98                     | 0.45              |
| 1:D:152:VAL:O    | 1:D:156:VAL:HG23 | 2.16                     | 0.45              |
| 1:F:2:GLU:HG2    | 1:F:39:SER:OG    | 2.17                     | 0.45              |
| 1:F:72:LEU:HB3   | 1:F:117:VAL:HG21 | 1.97                     | 0.45              |
| 1:M:42:LEU:HD21  | 1:M:86:VAL:HG11  | 1.97                     | 0.45              |
| 1:T:119:LEU:HD13 | 1:T:164:ILE:HG13 | 1.98                     | 0.45              |
| 1:H:42:LEU:HD21  | 1:H:86:VAL:HG11  | 1.97                     | 0.45              |
| 1:I:152:VAL:O    | 1:I:156:VAL:HG23 | 2.16                     | 0.45              |
| 1:A:2:GLU:HG2    | 1:A:39:SER:OG    | 2.17                     | 0.45              |
| 1:A:119:LEU:HD13 | 1:A:164:ILE:HG13 | 1.98                     | 0.45              |
| 1:E:42:LEU:HD21  | 1:E:86:VAL:HG11  | 1.97                     | 0.45              |
| 1:R:119:LEU:HD13 | 1:R:164:ILE:HG13 | 1.98                     | 0.45              |
| 1:L:2:GLU:HG2    | 1:L:39:SER:OG    | 2.17                     | 0.45              |
| 1:L:119:LEU:HD13 | 1:L:164:ILE:HG13 | 1.98                     | 0.45              |
| 1:S:2:GLU:HG2    | 1:S:39:SER:OG    | 2.17                     | 0.45              |
| 1:S:165:LEU:HD12 | 1:H:19:LEU:HD13  | 1.98                     | 0.45              |
| 1:N:119:LEU:HD13 | 1:N:164:ILE:HG13 | 1.98                     | 0.45              |
| 1:U:2:GLU:HG2    | 1:U:39:SER:OG    | 2.17                     | 0.45              |
| 1:U:42:LEU:HD21  | 1:U:86:VAL:HG11  | 1.97                     | 0.45              |
| 1:C:152:VAL:O    | 1:C:156:VAL:HG23 | 2.16                     | 0.45              |
| 1:J:161:ALA:HB1  | 1:Q:19:LEU:HD22  | 1.98                     | 0.45              |
| 1:K:119:LEU:HD13 | 1:K:164:ILE:HG13 | 1.98                     | 0.45              |
| 1:H:2:GLU:HG2    | 1:H:39:SER:OG    | 2.17                     | 0.45              |
| 1:O:119:LEU:HD13 | 1:O:164:ILE:HG13 | 1.98                     | 0.45              |
| 1:C:2:GLU:HG2    | 1:C:39:SER:OG    | 2.17                     | 0.45              |
| 1:D:2:GLU:HG2    | 1:D:39:SER:OG    | 2.17                     | 0.45              |
| 1:J:42:LEU:HD21  | 1:J:86:VAL:HG11  | 1.97                     | 0.45              |
| 1:E:2:GLU:HG2    | 1:E:39:SER:OG    | 2.17                     | 0.45              |
| 1:R:2:GLU:HG2    | 1:R:39:SER:OG    | 2.17                     | 0.45              |
| 1:L:152:VAL:O    | 1:L:156:VAL:HG23 | 2.16                     | 0.45              |
| 1:S:119:LEU:HD13 | 1:S:164:ILE:HG13 | 1.98                     | 0.45              |
| 1:M:152:VAL:O    | 1:M:156:VAL:HG23 | 2.16                     | 0.45              |
| 1:M:161:ALA:HB1  | 1:T:19:LEU:HD22  | 1.98                     | 0.45              |
| 1:U:119:LEU:HD13 | 1:U:164:ILE:HG13 | 1.98                     | 0.45              |
| 1:I:2:GLU:HG2    | 1:I:39:SER:OG    | 2.17                     | 0.45              |
| 1:A:19:LEU:HD13  | 1:R:165:LEU:HD12 | 1.98                     | 0.45              |
| 1:B:2:GLU:HG2    | 1:B:39:SER:OG    | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:161:ALA:HB1  | 1:S:19:LEU:HD22  | 1.98                     | 0.45              |
| 1:R:120:GLU:OE1  | 1:R:123:ARG:NH2  | 2.47                     | 0.45              |
| 1:F:152:VAL:O    | 1:F:156:VAL:HG23 | 2.16                     | 0.45              |
| 1:M:119:LEU:HD13 | 1:M:164:ILE:HG13 | 1.98                     | 0.45              |
| 1:T:165:LEU:HD12 | 1:I:19:LEU:HD13  | 1.98                     | 0.45              |
| 1:I:119:LEU:HD13 | 1:I:164:ILE:HG13 | 1.98                     | 0.44              |
| 1:P:2:GLU:HG2    | 1:P:39:SER:OG    | 2.17                     | 0.44              |
| 1:N:152:VAL:O    | 1:N:156:VAL:HG23 | 2.16                     | 0.44              |
| 1:C:119:LEU:HD13 | 1:C:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:A:119:LEU:HD13 | 1:A:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:K:165:LEU:HD12 | 1:R:19:LEU:HD13  | 1.99                     | 0.44              |
| 1:F:119:LEU:HD13 | 1:F:164:ILE:HG13 | 1.98                     | 0.44              |
| 1:M:165:LEU:HD23 | 1:M:165:LEU:HA   | 1.86                     | 0.44              |
| 1:H:119:LEU:HD13 | 1:H:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:P:119:LEU:HD13 | 1:P:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:Q:119:LEU:HD13 | 1:Q:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:R:42:LEU:HD21  | 1:R:86:VAL:HG11  | 1.97                     | 0.44              |
| 1:R:119:LEU:HD13 | 1:R:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:F:119:LEU:HD13 | 1:F:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:G:119:LEU:HD13 | 1:G:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:N:119:LEU:HD13 | 1:N:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:I:119:LEU:HD13 | 1:I:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:B:119:LEU:HD13 | 1:B:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:S:119:LEU:HD13 | 1:S:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:N:2:GLU:HG2    | 1:N:39:SER:OG    | 2.17                     | 0.44              |
| 1:N:161:ALA:HB1  | 1:U:19:LEU:HD22  | 1.98                     | 0.44              |
| 1:O:119:LEU:HD13 | 1:O:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:P:165:LEU:HD23 | 1:P:165:LEU:HA   | 1.86                     | 0.44              |
| 1:S:120:GLU:OE1  | 1:S:123:ARG:NH2  | 2.47                     | 0.44              |
| 1:S:152:VAL:O    | 1:S:156:VAL:HG23 | 2.16                     | 0.44              |
| 1:H:165:LEU:CD2  | 1:O:15:MET:HB3   | 2.39                     | 0.44              |
| 1:D:165:LEU:HD12 | 1:K:19:LEU:HD13  | 1.99                     | 0.44              |
| 1:K:161:ALA:HB1  | 1:R:19:LEU:HD22  | 1.98                     | 0.44              |
| 1:L:119:LEU:HD13 | 1:L:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:C:19:LEU:HD13  | 1:L:165:LEU:HD12 | 1.99                     | 0.44              |
| 1:J:119:LEU:HD13 | 1:J:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:K:119:LEU:HD13 | 1:K:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:M:119:LEU:HD13 | 1:M:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:C:43:LEU:HD23  | 1:S:112:ILE:HD13 | 2.00                     | 0.44              |
| 1:C:119:LEU:HD13 | 1:C:164:ILE:HG13 | 1.98                     | 0.44              |
| 1:A:15:MET:HB3   | 1:R:165:LEU:CD2  | 2.39                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:120:GLU:OE1  | 1:A:123:ARG:NH2  | 2.47                     | 0.44              |
| 1:P:152:VAL:O    | 1:P:156:VAL:HG23 | 2.16                     | 0.44              |
| 1:E:119:LEU:HD13 | 1:E:164:ILE:CG1  | 2.48                     | 0.44              |
| 1:B:82:SER:OG    | 1:B:87:ALA:HB3   | 2.18                     | 0.43              |
| 1:J:165:LEU:HD12 | 1:Q:19:LEU:HD13  | 1.99                     | 0.43              |
| 1:L:120:GLU:OE1  | 1:L:123:ARG:NH2  | 2.47                     | 0.43              |
| 1:C:165:LEU:CD2  | 1:G:15:MET:HB3   | 2.39                     | 0.43              |
| 1:D:43:LEU:HD23  | 1:E:112:ILE:HD13 | 1.99                     | 0.43              |
| 1:E:82:SER:OG    | 1:E:87:ALA:HB3   | 2.18                     | 0.43              |
| 1:H:165:LEU:HD12 | 1:O:19:LEU:HD13  | 1.99                     | 0.43              |
| 1:C:19:LEU:HD22  | 1:L:161:ALA:HB1  | 1.98                     | 0.43              |
| 1:K:165:LEU:CD2  | 1:R:15:MET:HB3   | 2.40                     | 0.43              |
| 1:R:82:SER:OG    | 1:R:87:ALA:HB3   | 2.18                     | 0.43              |
| 1:G:82:SER:OG    | 1:G:87:ALA:HB3   | 2.18                     | 0.43              |
| 1:T:119:LEU:HD13 | 1:T:164:ILE:CG1  | 2.48                     | 0.43              |
| 1:I:120:GLU:OE1  | 1:I:123:ARG:NH2  | 2.47                     | 0.43              |
| 1:A:5:GLU:HG3    | 1:A:35:ILE:CD1   | 2.49                     | 0.43              |
| 1:D:119:LEU:HD13 | 1:D:164:ILE:CG1  | 2.48                     | 0.43              |
| 1:Q:82:SER:OG    | 1:Q:87:ALA:HB3   | 2.18                     | 0.43              |
| 1:E:82:SER:OG    | 1:E:87:ALA:CB    | 2.67                     | 0.43              |
| 1:G:165:LEU:HD12 | 1:N:19:LEU:HD13  | 1.99                     | 0.43              |
| 1:H:82:SER:OG    | 1:H:87:ALA:HB3   | 2.18                     | 0.43              |
| 1:U:82:SER:OG    | 1:U:87:ALA:HB3   | 2.18                     | 0.43              |
| 1:U:82:SER:OG    | 1:U:87:ALA:CB    | 2.67                     | 0.43              |
| 1:O:82:SER:OG    | 1:O:87:ALA:HB3   | 2.18                     | 0.43              |
| 1:C:82:SER:OG    | 1:C:87:ALA:HB3   | 2.18                     | 0.43              |
| 1:A:82:SER:OG    | 1:A:87:ALA:HB3   | 2.18                     | 0.43              |
| 1:B:82:SER:OG    | 1:B:87:ALA:CB    | 2.67                     | 0.43              |
| 1:D:82:SER:OG    | 1:D:87:ALA:HB3   | 2.18                     | 0.43              |
| 1:Q:165:LEU:HD12 | 1:F:19:LEU:HD13  | 1.98                     | 0.43              |
| 1:T:82:SER:OG    | 1:T:87:ALA:HB3   | 2.18                     | 0.43              |
| 1:D:82:SER:OG    | 1:D:87:ALA:CB    | 2.67                     | 0.43              |
| 1:J:165:LEU:CD2  | 1:Q:15:MET:HB3   | 2.40                     | 0.43              |
| 1:K:120:GLU:OE1  | 1:K:123:ARG:NH2  | 2.47                     | 0.43              |
| 1:L:82:SER:OG    | 1:L:87:ALA:CB    | 2.67                     | 0.43              |
| 1:G:43:LEU:HD23  | 1:H:112:ILE:HD13 | 1.99                     | 0.43              |
| 1:M:82:SER:OG    | 1:M:87:ALA:CB    | 2.67                     | 0.43              |
| 1:S:165:LEU:CD2  | 1:H:15:MET:HB3   | 2.39                     | 0.43              |
| 1:G:165:LEU:CD2  | 1:N:15:MET:HB3   | 2.39                     | 0.43              |
| 1:U:5:GLU:HG3    | 1:U:35:ILE:CD1   | 2.49                     | 0.43              |
| 1:J:82:SER:OG    | 1:J:87:ALA:HB3   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:5:GLU:HG3    | 1:F:35:ILE:CD1   | 2.49                     | 0.43              |
| 1:F:120:GLU:OE1  | 1:F:123:ARG:NH2  | 2.47                     | 0.43              |
| 1:G:82:SER:OG    | 1:G:87:ALA:CB    | 2.67                     | 0.43              |
| 1:B:165:LEU:HD12 | 1:S:19:LEU:HD13  | 1.99                     | 0.43              |
| 1:P:82:SER:OG    | 1:P:87:ALA:CB    | 2.67                     | 0.43              |
| 1:J:82:SER:OG    | 1:J:87:ALA:CB    | 2.67                     | 0.43              |
| 1:R:82:SER:OG    | 1:R:87:ALA:CB    | 2.67                     | 0.43              |
| 1:F:82:SER:OG    | 1:F:87:ALA:CB    | 2.67                     | 0.43              |
| 1:T:82:SER:OG    | 1:T:87:ALA:CB    | 2.67                     | 0.43              |
| 1:U:119:LEU:HD13 | 1:U:164:ILE:CG1  | 2.48                     | 0.43              |
| 1:A:112:ILE:HD13 | 1:F:43:LEU:HD23  | 1.99                     | 0.43              |
| 1:P:82:SER:OG    | 1:P:87:ALA:HB3   | 2.18                     | 0.43              |
| 1:M:82:SER:OG    | 1:M:87:ALA:HB3   | 2.18                     | 0.43              |
| 1:H:82:SER:OG    | 1:H:87:ALA:CB    | 2.67                     | 0.43              |
| 1:N:82:SER:OG    | 1:N:87:ALA:CB    | 2.67                     | 0.43              |
| 1:C:82:SER:OG    | 1:C:87:ALA:CB    | 2.67                     | 0.42              |
| 1:Q:43:LEU:HD23  | 1:R:112:ILE:HD13 | 2.00                     | 0.42              |
| 1:E:165:LEU:HD23 | 1:E:165:LEU:HA   | 1.87                     | 0.42              |
| 1:I:82:SER:OG    | 1:I:87:ALA:HB3   | 2.18                     | 0.42              |
| 1:F:82:SER:OG    | 1:F:87:ALA:HB3   | 2.18                     | 0.42              |
| 1:S:82:SER:OG    | 1:S:87:ALA:HB3   | 2.18                     | 0.42              |
| 1:G:120:GLU:OE1  | 1:G:123:ARG:NH2  | 2.47                     | 0.42              |
| 1:F:29:LEU:HD12  | 1:F:70:GLU:CG    | 2.49                     | 0.42              |
| 1:L:82:SER:OG    | 1:L:87:ALA:HB3   | 2.18                     | 0.42              |
| 1:U:29:LEU:HD12  | 1:U:70:GLU:CG    | 2.49                     | 0.42              |
| 1:E:5:GLU:HG3    | 1:E:35:ILE:CD1   | 2.49                     | 0.42              |
| 1:K:82:SER:OG    | 1:K:87:ALA:HB3   | 2.18                     | 0.42              |
| 1:S:82:SER:OG    | 1:S:87:ALA:CB    | 2.67                     | 0.42              |
| 1:N:29:LEU:HD12  | 1:N:70:GLU:CG    | 2.49                     | 0.42              |
| 1:N:82:SER:OG    | 1:N:87:ALA:HB3   | 2.18                     | 0.42              |
| 1:O:82:SER:OG    | 1:O:87:ALA:CB    | 2.67                     | 0.42              |
| 1:A:19:LEU:HD13  | 1:R:165:LEU:CD1  | 2.41                     | 0.42              |
| 1:E:120:GLU:OE1  | 1:E:123:ARG:NH2  | 2.47                     | 0.42              |
| 1:S:5:GLU:HG3    | 1:S:35:ILE:CD1   | 2.49                     | 0.42              |
| 1:O:5:GLU:HG3    | 1:O:35:ILE:CD1   | 2.49                     | 0.42              |
| 1:B:29:LEU:HD12  | 1:B:70:GLU:CG    | 2.49                     | 0.42              |
| 1:P:165:LEU:HD12 | 1:E:19:LEU:HD13  | 1.98                     | 0.42              |
| 1:K:5:GLU:HG3    | 1:K:35:ILE:CD1   | 2.49                     | 0.42              |
| 1:K:82:SER:OG    | 1:K:87:ALA:CB    | 2.67                     | 0.42              |
| 1:U:120:GLU:OE1  | 1:U:123:ARG:NH2  | 2.47                     | 0.42              |
| 1:B:19:LEU:HD13  | 1:F:165:LEU:HD12 | 1.99                     | 0.42              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:120:GLU:OE1  | 1:B:123:ARG:NH2 | 2.47                     | 0.42              |
| 1:P:29:LEU:HD12  | 1:P:70:GLU:CG   | 2.49                     | 0.42              |
| 1:N:165:LEU:HD12 | 1:U:19:LEU:HD13 | 1.99                     | 0.42              |
| 1:Q:82:SER:OG    | 1:Q:87:ALA:CB   | 2.67                     | 0.42              |
| 1:A:82:SER:OG    | 1:A:87:ALA:CB   | 2.67                     | 0.42              |
| 1:Q:165:LEU:CD2  | 1:F:15:MET:HB3  | 2.39                     | 0.42              |
| 1:E:29:LEU:HD12  | 1:E:70:GLU:CG   | 2.49                     | 0.42              |
| 1:K:165:LEU:HD23 | 1:K:165:LEU:HA  | 1.86                     | 0.42              |
| 1:I:82:SER:OG    | 1:I:87:ALA:CB   | 2.67                     | 0.42              |
| 1:S:165:LEU:HD23 | 1:S:165:LEU:HA  | 1.86                     | 0.41              |
| 1:H:5:GLU:HG3    | 1:H:35:ILE:CD1  | 2.49                     | 0.41              |
| 1:N:165:LEU:HD23 | 1:N:165:LEU:HA  | 1.86                     | 0.41              |
| 1:D:5:GLU:HG3    | 1:D:35:ILE:CD1  | 2.49                     | 0.41              |
| 1:D:29:LEU:HD12  | 1:D:70:GLU:CG   | 2.49                     | 0.41              |
| 1:Q:29:LEU:HD12  | 1:Q:70:GLU:CG   | 2.49                     | 0.41              |
| 1:R:5:GLU:HG3    | 1:R:35:ILE:CD1  | 2.49                     | 0.41              |
| 1:G:165:LEU:HD23 | 1:G:165:LEU:HA  | 1.86                     | 0.41              |
| 1:I:5:GLU:HG3    | 1:I:35:ILE:CD1  | 2.49                     | 0.41              |
| 1:M:165:LEU:HD12 | 1:T:19:LEU:HD13 | 1.99                     | 0.41              |
| 1:N:5:GLU:HG3    | 1:N:35:ILE:CD1  | 2.49                     | 0.41              |
| 1:E:165:LEU:HD12 | 1:L:19:LEU:HD13 | 1.99                     | 0.41              |
| 1:G:29:LEU:HD12  | 1:G:70:GLU:CG   | 2.49                     | 0.41              |
| 1:C:15:MET:HB3   | 1:L:165:LEU:CD2 | 2.40                     | 0.41              |
| 1:C:120:GLU:OE1  | 1:C:123:ARG:NH2 | 2.47                     | 0.41              |
| 1:A:29:LEU:HD12  | 1:A:70:GLU:CG   | 2.49                     | 0.41              |
| 1:A:165:LEU:HD12 | 1:M:19:LEU:HD13 | 1.99                     | 0.41              |
| 1:Q:5:GLU:HG3    | 1:Q:35:ILE:CD1  | 2.49                     | 0.41              |
| 1:M:14:ILE:HD11  | 1:M:54:ARG:HG2  | 2.03                     | 0.41              |
| 1:M:29:LEU:HD12  | 1:M:70:GLU:CG   | 2.49                     | 0.41              |
| 1:M:120:GLU:OE1  | 1:M:123:ARG:NH2 | 2.47                     | 0.41              |
| 1:T:165:LEU:CD1  | 1:I:19:LEU:HD13 | 2.41                     | 0.41              |
| 1:F:14:ILE:HD11  | 1:F:54:ARG:HG2  | 2.03                     | 0.41              |
| 1:H:14:ILE:HD11  | 1:H:54:ARG:HG2  | 2.03                     | 0.41              |
| 1:N:14:ILE:HD11  | 1:N:54:ARG:HG2  | 2.03                     | 0.41              |
| 1:I:14:ILE:HD11  | 1:I:54:ARG:HG2  | 2.03                     | 0.41              |
| 1:B:5:GLU:HG3    | 1:B:35:ILE:CD1  | 2.49                     | 0.41              |
| 1:E:14:ILE:HD11  | 1:E:54:ARG:HG2  | 2.03                     | 0.41              |
| 1:S:29:LEU:HD12  | 1:S:70:GLU:CG   | 2.49                     | 0.41              |
| 1:T:120:GLU:OE1  | 1:T:123:ARG:NH2 | 2.47                     | 0.41              |
| 1:N:120:GLU:OE1  | 1:N:123:ARG:NH2 | 2.47                     | 0.41              |
| 1:A:14:ILE:HD11  | 1:A:54:ARG:HG2  | 2.03                     | 0.41              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:26:ARG:HA   | 1:A:70:GLU:HG2   | 2.03                     | 0.41              |
| 1:P:26:ARG:HA   | 1:P:70:GLU:HG2   | 2.03                     | 0.41              |
| 1:D:14:ILE:HD11 | 1:D:54:ARG:HG2   | 2.03                     | 0.41              |
| 1:J:26:ARG:HA   | 1:J:70:GLU:HG2   | 2.03                     | 0.41              |
| 1:Q:26:ARG:HA   | 1:Q:70:GLU:HG2   | 2.03                     | 0.41              |
| 1:R:26:ARG:HA   | 1:R:70:GLU:HG2   | 2.03                     | 0.41              |
| 1:F:26:ARG:HA   | 1:F:70:GLU:HG2   | 2.03                     | 0.41              |
| 1:L:5:GLU:HG3   | 1:L:35:ILE:CD1   | 2.49                     | 0.41              |
| 1:G:14:ILE:HD11 | 1:G:54:ARG:HG2   | 2.03                     | 0.41              |
| 1:G:26:ARG:HA   | 1:G:70:GLU:HG2   | 2.03                     | 0.41              |
| 1:O:14:ILE:HD11 | 1:O:54:ARG:HG2   | 2.03                     | 0.41              |
| 1:C:5:GLU:HG3   | 1:C:35:ILE:CD1   | 2.49                     | 0.41              |
| 1:C:14:ILE:HD11 | 1:C:54:ARG:HG2   | 2.03                     | 0.41              |
| 1:B:14:ILE:HD11 | 1:B:54:ARG:HG2   | 2.03                     | 0.41              |
| 1:D:120:GLU:OE1 | 1:D:123:ARG:NH2  | 2.47                     | 0.41              |
| 1:J:5:GLU:HG3   | 1:J:35:ILE:CD1   | 2.49                     | 0.41              |
| 1:J:43:LEU:HD23 | 1:K:112:ILE:HD13 | 2.03                     | 0.41              |
| 1:R:29:LEU:HD12 | 1:R:70:GLU:CG    | 2.49                     | 0.41              |
| 1:S:43:LEU:HD23 | 1:T:112:ILE:HD13 | 2.00                     | 0.41              |
| 1:T:29:LEU:HD12 | 1:T:70:GLU:CG    | 2.49                     | 0.41              |
| 1:H:26:ARG:HA   | 1:H:70:GLU:HG2   | 2.03                     | 0.41              |
| 1:U:14:ILE:HD11 | 1:U:54:ARG:HG2   | 2.03                     | 0.41              |
| 1:O:26:ARG:HA   | 1:O:70:GLU:HG2   | 2.03                     | 0.41              |
| 1:C:26:ARG:HA   | 1:C:70:GLU:HG2   | 2.03                     | 0.40              |
| 1:K:29:LEU:HD12 | 1:K:70:GLU:CG    | 2.49                     | 0.40              |
| 1:N:26:ARG:HA   | 1:N:70:GLU:HG2   | 2.03                     | 0.40              |
| 1:D:165:LEU:CD2 | 1:K:15:MET:HB3   | 2.39                     | 0.40              |
| 1:R:14:ILE:HD11 | 1:R:54:ARG:HG2   | 2.03                     | 0.40              |
| 1:M:26:ARG:HA   | 1:M:70:GLU:HG2   | 2.03                     | 0.40              |
| 1:T:5:GLU:HG3   | 1:T:35:ILE:CD1   | 2.49                     | 0.40              |
| 1:P:14:ILE:HD11 | 1:P:54:ARG:HG2   | 2.03                     | 0.40              |
| 1:I:26:ARG:HA   | 1:I:70:GLU:HG2   | 2.03                     | 0.40              |
| 1:I:29:LEU:HD12 | 1:I:70:GLU:CG    | 2.49                     | 0.40              |
| 1:O:29:LEU:HD12 | 1:O:70:GLU:CG    | 2.49                     | 0.40              |
| 1:Q:14:ILE:HD11 | 1:Q:54:ARG:HG2   | 2.03                     | 0.40              |
| 1:K:26:ARG:HA   | 1:K:70:GLU:HG2   | 2.03                     | 0.40              |
| 1:L:14:ILE:HD11 | 1:L:54:ARG:HG2   | 2.03                     | 0.40              |
| 1:U:26:ARG:HA   | 1:U:70:GLU:HG2   | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 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 EM 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     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | B     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | C     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | D     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | E     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | F     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | G     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | H     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | I     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | J     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | K     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | L     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | M     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | N     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | O     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | P     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | Q     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | R     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | S     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | T     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| 1   | U     | 166/168 (99%)   | 166 (100%)  | 0       | 0        | 100         | 100 |
| All | All   | 3486/3528 (99%) | 3486 (100%) | 0       | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 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 EM 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     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | B     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | C     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | D     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | E     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | F     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | G     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | H     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | I     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | J     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | K     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | L     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | M     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | N     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | O     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | P     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | Q     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | R     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | S     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | T     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| 1   | U     | 126/126 (100%)   | 126 (100%)  | 0        | 100         | 100 |
| All | All   | 2646/2646 (100%) | 2646 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9019. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit ⓘ

This section was not generated.