



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:11 PM BST

PDB ID : 4BKK  
EMDB ID: : EMD-2369  
Title : The Respiratory Syncytial Virus nucleoprotein-RNA complex forms a left-handed helical nucleocapsid.  
Authors : Bakker, S.E.; Duquerroy, S.; Galloux, M.; Loney, C.; Conner, E.; Eleouet, J.F.; Rey, F.A.; Bhella, D.  
Deposited on : 2013-04-26  
Resolution : unknown (reported)  
Based on PDB ID : 2WJ8

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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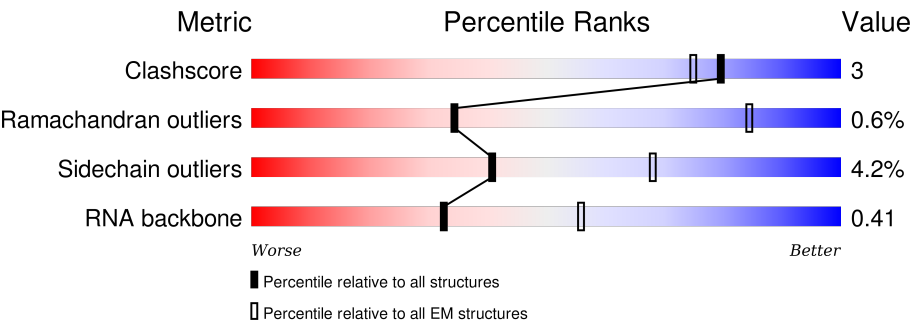
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is unknown.

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 (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore            | 114402                   | 924                      |
| Ramachandran outliers | 111179                   | 726                      |
| Sidechain outliers    | 111093                   | 686                      |
| RNA backbone          | 3027                     | 244                      |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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     | 161    | <div><div>86%14%</div></div>  |
| 2   | B     | 391    | <div><div>86%8%5%</div></div> |
| 2   | C     | 391    | <div><div>85%9%5%</div></div> |
| 2   | D     | 391    | <div><div>85%9%5%</div></div> |
| 2   | E     | 391    | <div><div>85%9%5%</div></div> |
| 2   | F     | 391    | <div><div>85%9%5%</div></div> |
| 2   | G     | 391    | <div><div>85%9%5%</div></div> |
| 2   | H     | 391    | <div><div>85%9%5%</div></div> |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 2   | I     | 391    |  85% 9% • 5%   |
| 2   | J     | 391    |  85% 9% • 5%   |
| 2   | K     | 391    |  85% 9% • 5%   |
| 2   | L     | 391    |  83% 10% • 5%  |
| 2   | M     | 391    |  83% 10% • 5%  |
| 2   | N     | 391    |  83% 10% • 5%  |
| 2   | O     | 391    |  84% 9% • 5%   |
| 2   | P     | 391    |  84% 9% • 5%   |
| 2   | Q     | 391    |  84% 9% • 5%   |
| 2   | R     | 391    |  84% 9% • 5%   |
| 2   | S     | 391    |  85% 9% • 5%   |
| 2   | T     | 391    |  84% 9% • 5%   |
| 2   | U     | 391    |  84% 9% • 5% |
| 2   | V     | 391    |  85% 8% • 5% |
| 2   | W     | 391    |  85% 9% • 5% |
| 2   | X     | 391    |  85% 9% • 5% |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 69483 atoms, of which 0 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 RNA chain called RNA (161-MER).

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 1   | A     | 161      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3220  | 1449 | 483 | 1127 | 161 |         |       |

- Molecule 2 is a protein called NUCLEOPROTEIN.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2881  | 1824 | 501 | 540 | 16 |         |       |
| 2   | C     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2881  | 1824 | 501 | 540 | 16 |         |       |
| 2   | D     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2881  | 1824 | 501 | 540 | 16 |         |       |
| 2   | E     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2881  | 1824 | 501 | 540 | 16 |         |       |
| 2   | F     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2881  | 1824 | 501 | 540 | 16 |         |       |
| 2   | G     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2881  | 1824 | 501 | 540 | 16 |         |       |
| 2   | H     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2881  | 1824 | 501 | 540 | 16 |         |       |
| 2   | I     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2881  | 1824 | 501 | 540 | 16 |         |       |
| 2   | J     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2881  | 1824 | 501 | 540 | 16 |         |       |
| 2   | K     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2881  | 1824 | 501 | 540 | 16 |         |       |
| 2   | L     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2881  | 1824 | 501 | 540 | 16 |         |       |
| 2   | M     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2881  | 1824 | 501 | 540 | 16 |         |       |
| 2   | N     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2881  | 1824 | 501 | 540 | 16 |         |       |
| 2   | O     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2881  | 1824 | 501 | 540 | 16 |         |       |

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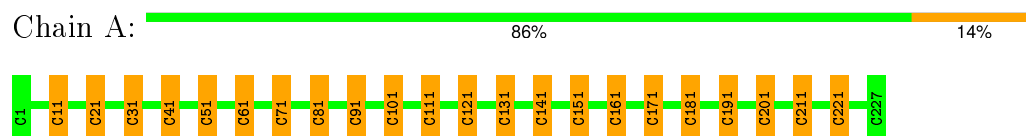
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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 2   | P     | 370      | Total<br>2881 | C<br>1824 | N<br>501 | O<br>540 | S<br>16 | 0       | 0     |
| 2   | Q     | 370      | Total<br>2881 | C<br>1824 | N<br>501 | O<br>540 | S<br>16 | 0       | 0     |
| 2   | R     | 370      | Total<br>2881 | C<br>1824 | N<br>501 | O<br>540 | S<br>16 | 0       | 0     |
| 2   | S     | 370      | Total<br>2881 | C<br>1824 | N<br>501 | O<br>540 | S<br>16 | 0       | 0     |
| 2   | T     | 370      | Total<br>2881 | C<br>1824 | N<br>501 | O<br>540 | S<br>16 | 0       | 0     |
| 2   | U     | 370      | Total<br>2881 | C<br>1824 | N<br>501 | O<br>540 | S<br>16 | 0       | 0     |
| 2   | V     | 370      | Total<br>2881 | C<br>1824 | N<br>501 | O<br>540 | S<br>16 | 0       | 0     |
| 2   | W     | 370      | Total<br>2881 | C<br>1824 | N<br>501 | O<br>540 | S<br>16 | 0       | 0     |
| 2   | X     | 370      | Total<br>2881 | C<br>1824 | N<br>501 | O<br>540 | S<br>16 | 0       | 0     |

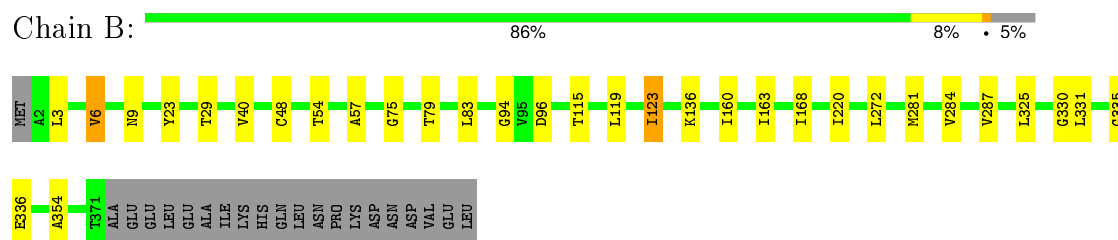
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

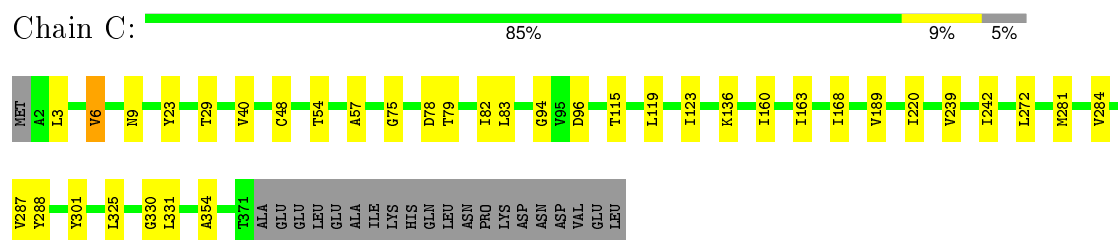
- Molecule 1: RNA (161-MER)



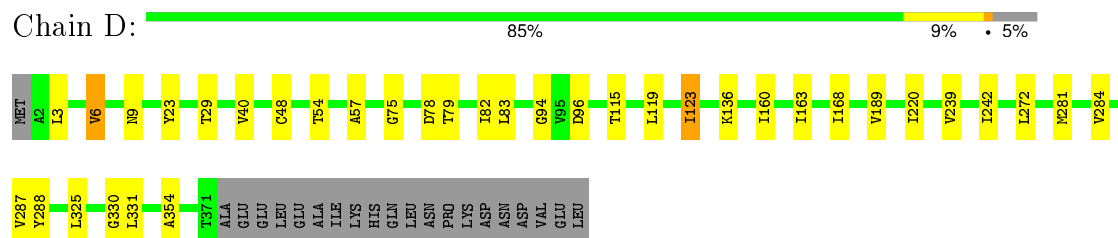
- Molecule 2: NUCLEOPROTEIN



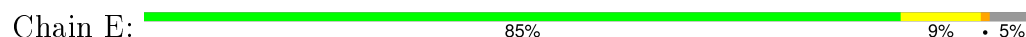
- Molecule 2: NUCLEOPROTEIN

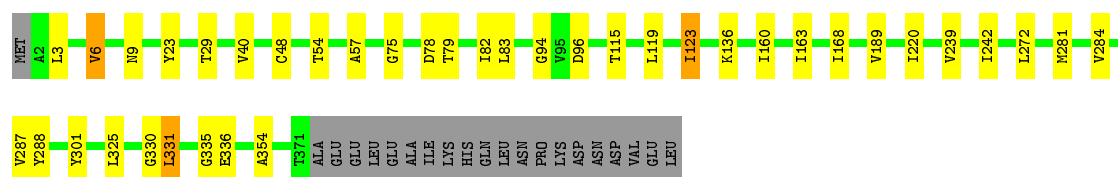


- Molecule 2: NUCLEOPROTEIN



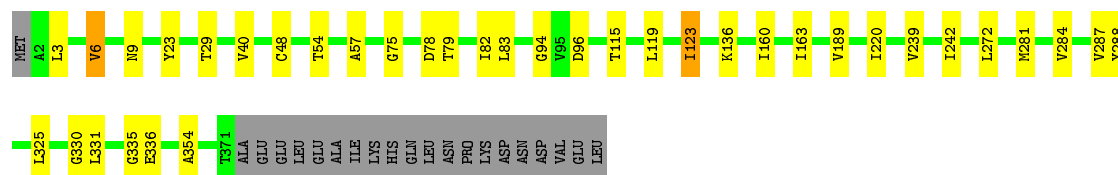
- Molecule 2: NUCLEOPROTEIN





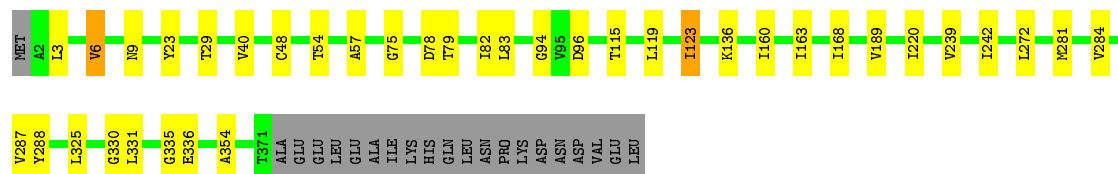
• Molecule 2: NUCLEOPROTEIN

Chain F: 85% 9% • 5%



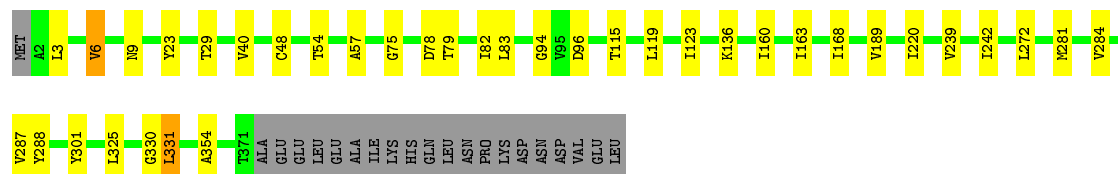
• Molecule 2: NUCLEOPROTEIN

Chain G: 85% 9% • 5%



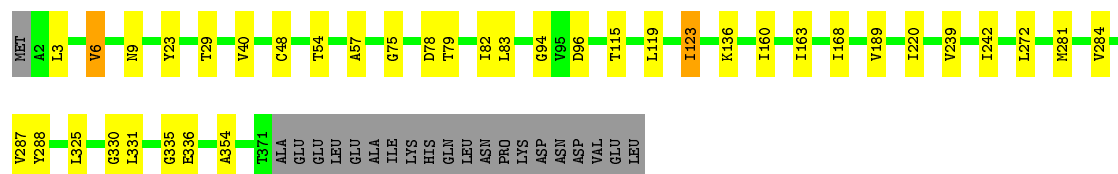
• Molecule 2: NUCLEOPROTEIN

Chain H: 85% 9% • 5%



• Molecule 2: NUCLEOPROTEIN

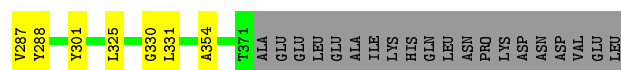
Chain I: 85% 9% • 5%



• Molecule 2: NUCLEOPROTEIN

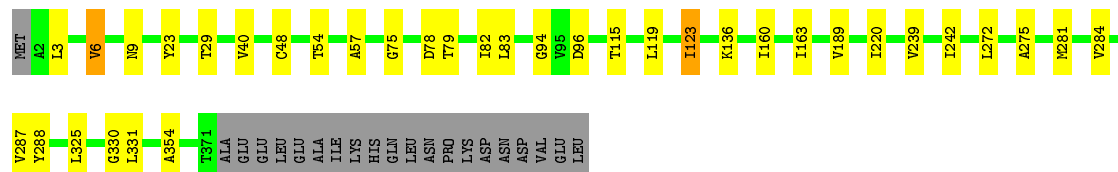
Chain J: 85% 9% • 5%





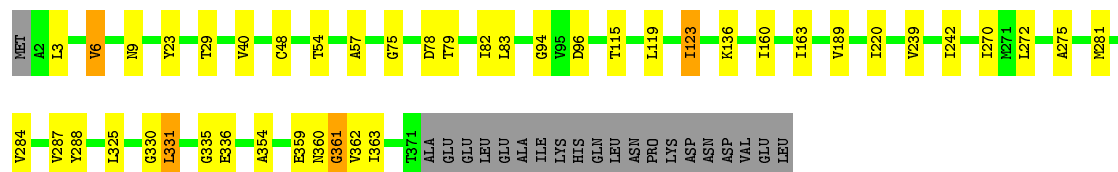
• Molecule 2: NUCLEOPROTEIN

Chain K: 85% 9% • 5%



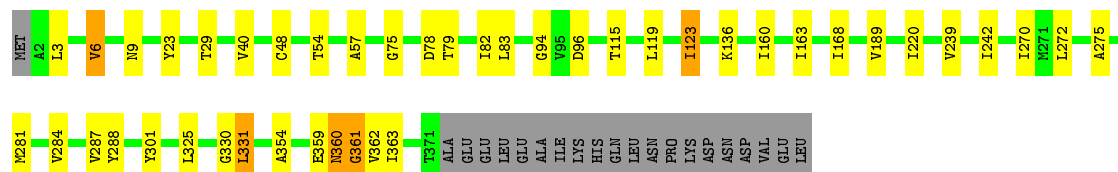
• Molecule 2: NUCLEOPROTEIN

Chain L: 83% 10% • 5%



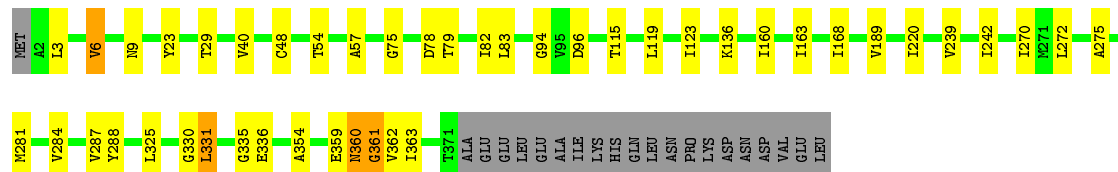
• Molecule 2: NUCLEOPROTEIN

Chain M: 83% 10% • 5%



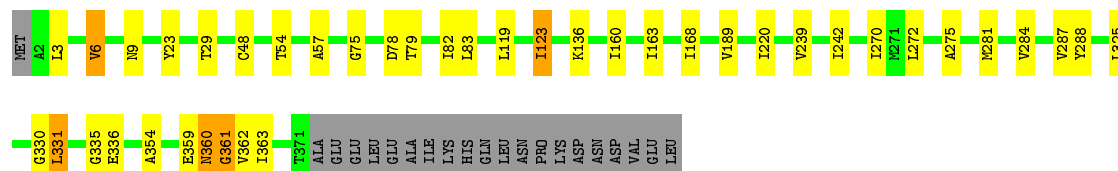
• Molecule 2: NUCLEOPROTEIN

Chain N: 83% 10% • 5%




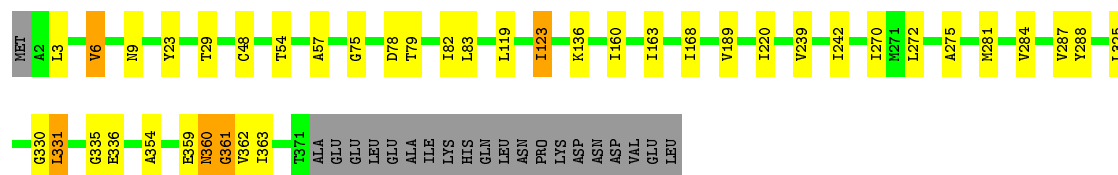
• Molecule 2: NUCLEOPROTEIN

Chain O: 84% 9% • 5%




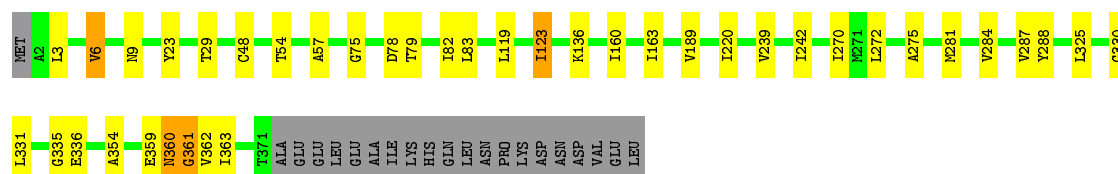
- Molecule 2: NUCLEOPROTEIN

Chain P: 




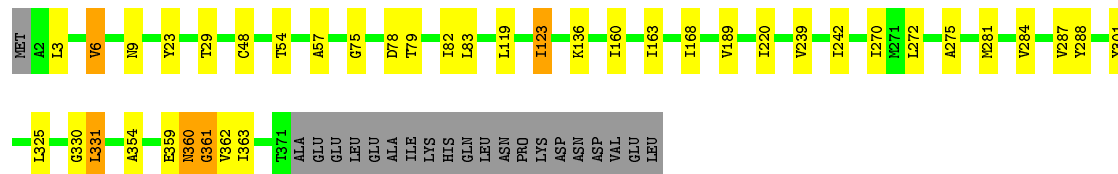
- Molecule 2: NUCLEOPROTEIN

Chain Q: 




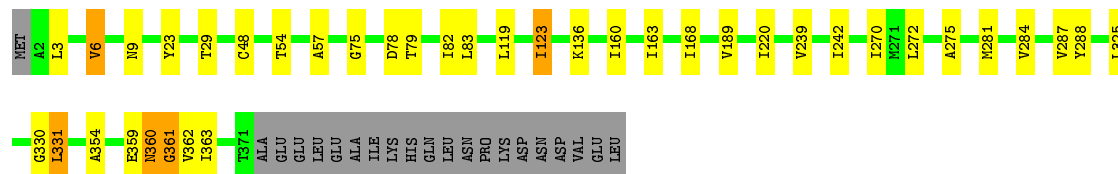
- Molecule 2: NUCLEOPROTEIN

Chain R: 




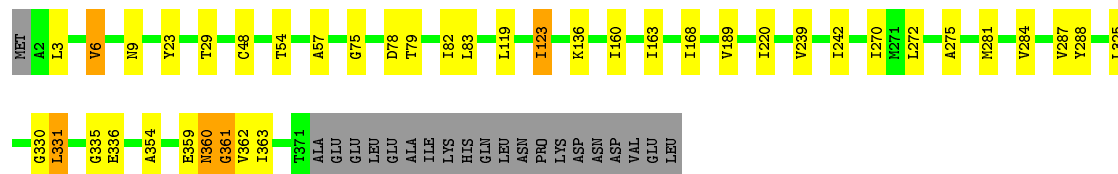
- Molecule 2: NUCLEOPROTEIN

Chain S: 

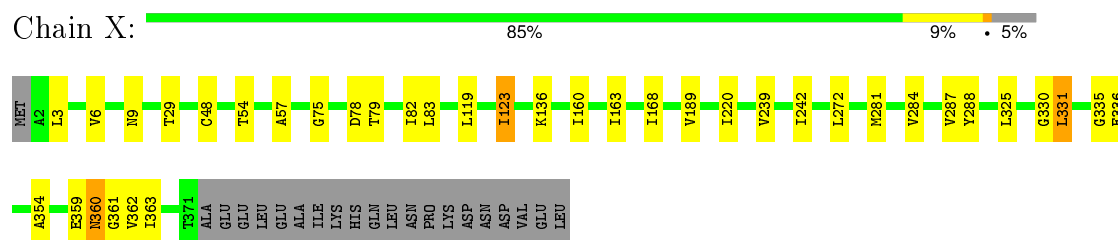


- Molecule 2: NUCLEOPROTEIN

Chain T: 



- Molecule 2: NUCLEOPROTEIN



## 4 Experimental information

| Property                             | Value                | Source    |
|--------------------------------------|----------------------|-----------|
| Reconstruction method                | TOMOGRAPHY           | Depositor |
| Imposed symmetry                     | POINT, Not provided  | Depositor |
| Number of images                     | Not provided         | Depositor |
| Resolution determination method      | Not provided         | Depositor |
| CTF correction method                | Not provided         | Depositor |
| Microscope                           | OTHER                | Depositor |
| Voltage (kV)                         | 200                  | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 131                  | Depositor |
| Minimum defocus (nm)                 | 2000                 | Depositor |
| Maximum defocus (nm)                 | 4000                 | Depositor |
| Magnification                        | 40000                | Depositor |
| Image detector                       | GATAN ULTRASCAN 4000 | 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  >2 | RMSZ        | # Z  >2 |
| 1   | A     | 0.22         | 0/3541  | 0.73        | 0/5470  |
| 2   | B     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | C     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | D     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | E     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | F     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | G     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | H     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | I     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | J     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | K     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | L     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | M     | 0.27         | 0/2929  | 0.43        | 0/3946  |
| 2   | N     | 0.27         | 0/2929  | 0.43        | 0/3946  |
| 2   | O     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | P     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | Q     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | R     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | S     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | T     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | U     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | V     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | W     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| 2   | X     | 0.27         | 0/2929  | 0.42        | 0/3946  |
| All | All   | 0.27         | 0/70908 | 0.45        | 0/96228 |

There are no bond length outliers.

There are no bond angle outliers.

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     | 3220  | 0        | 1772     | 76      | 0            |
| 2   | B     | 2881  | 0        | 2915     | 17      | 0            |
| 2   | C     | 2881  | 0        | 2915     | 24      | 0            |
| 2   | D     | 2881  | 0        | 2915     | 22      | 0            |
| 2   | E     | 2881  | 0        | 2915     | 24      | 0            |
| 2   | F     | 2881  | 0        | 2915     | 26      | 0            |
| 2   | G     | 2881  | 0        | 2915     | 23      | 0            |
| 2   | H     | 2881  | 0        | 2915     | 25      | 0            |
| 2   | I     | 2881  | 0        | 2915     | 23      | 0            |
| 2   | J     | 2881  | 0        | 2915     | 23      | 0            |
| 2   | K     | 2881  | 0        | 2915     | 25      | 0            |
| 2   | L     | 2881  | 0        | 2915     | 36      | 0            |
| 2   | M     | 2881  | 0        | 2915     | 36      | 0            |
| 2   | N     | 2881  | 0        | 2915     | 37      | 0            |
| 2   | O     | 2881  | 0        | 2915     | 28      | 0            |
| 2   | P     | 2881  | 0        | 2915     | 30      | 0            |
| 2   | Q     | 2881  | 0        | 2915     | 28      | 0            |
| 2   | R     | 2881  | 0        | 2915     | 28      | 0            |
| 2   | S     | 2881  | 0        | 2915     | 29      | 0            |
| 2   | T     | 2881  | 0        | 2915     | 27      | 0            |
| 2   | U     | 2881  | 0        | 2915     | 30      | 0            |
| 2   | V     | 2881  | 0        | 2915     | 28      | 0            |
| 2   | W     | 2881  | 0        | 2915     | 26      | 0            |
| 2   | X     | 2881  | 0        | 2915     | 25      | 0            |
| All | All   | 69483 | 0        | 68817    | 472     | 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 3.

All (472) 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:A:221:C:H5" | 2:C:189:VAL:HG22 | 1.77                     | 0.66              |
| 1:A:211:C:H5" | 2:D:189:VAL:HG22 | 1.77                     | 0.66              |
| 1:A:101:C:H5" | 2:O:189:VAL:HG22 | 1.78                     | 0.66              |

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| Atom-1         | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 1:A:11:C:H5''  | 2:X:189:VAL:HG22 | 1.78                     | 0.66              |
| 1:A:91:C:H5''  | 2:P:189:VAL:HG22 | 1.78                     | 0.66              |
| 1:A:121:C:H5'' | 2:M:189:VAL:HG22 | 1.78                     | 0.65              |
| 1:A:81:C:H5''  | 2:Q:189:VAL:HG22 | 1.78                     | 0.65              |
| 1:A:161:C:H5'' | 2:I:189:VAL:HG22 | 1.77                     | 0.65              |
| 1:A:131:C:H5'' | 2:L:189:VAL:HG22 | 1.78                     | 0.65              |
| 1:A:181:C:H5'' | 2:G:189:VAL:HG22 | 1.78                     | 0.65              |
| 1:A:191:C:H5'' | 2:F:189:VAL:HG22 | 1.78                     | 0.65              |
| 1:A:141:C:H5'' | 2:K:189:VAL:HG22 | 1.78                     | 0.65              |
| 1:A:21:C:H5''  | 2:W:189:VAL:HG22 | 1.78                     | 0.65              |
| 1:A:61:C:H5''  | 2:S:189:VAL:HG22 | 1.78                     | 0.65              |
| 1:A:151:C:H5'' | 2:J:189:VAL:HG22 | 1.78                     | 0.64              |
| 1:A:111:C:H5'' | 2:N:189:VAL:HG22 | 1.78                     | 0.64              |
| 1:A:71:C:H5''  | 2:R:189:VAL:HG22 | 1.78                     | 0.64              |
| 1:A:171:C:H5'' | 2:H:189:VAL:HG22 | 1.77                     | 0.64              |
| 1:A:201:C:H5'' | 2:E:189:VAL:HG22 | 1.78                     | 0.64              |
| 1:A:51:C:H5''  | 2:T:189:VAL:HG22 | 1.78                     | 0.64              |
| 1:A:31:C:H5''  | 2:V:189:VAL:HG22 | 1.78                     | 0.64              |
| 1:A:41:C:H5''  | 2:U:189:VAL:HG22 | 1.78                     | 0.63              |
| 1:A:161:C:C5'  | 2:I:189:VAL:HG22 | 2.30                     | 0.61              |
| 1:A:151:C:C5'  | 2:J:189:VAL:HG22 | 2.31                     | 0.61              |
| 1:A:31:C:C5'   | 2:V:189:VAL:HG22 | 2.31                     | 0.61              |
| 1:A:101:C:C5'  | 2:O:189:VAL:HG22 | 2.31                     | 0.61              |
| 1:A:81:C:C5'   | 2:Q:189:VAL:HG22 | 2.31                     | 0.61              |
| 1:A:131:C:C5'  | 2:L:189:VAL:HG22 | 2.31                     | 0.61              |
| 1:A:201:C:C5'  | 2:E:189:VAL:HG22 | 2.31                     | 0.61              |
| 1:A:211:C:C5'  | 2:D:189:VAL:HG22 | 2.30                     | 0.61              |
| 1:A:181:C:C5'  | 2:G:189:VAL:HG22 | 2.31                     | 0.61              |
| 1:A:91:C:C5'   | 2:P:189:VAL:HG22 | 2.31                     | 0.60              |
| 1:A:191:C:C5'  | 2:F:189:VAL:HG22 | 2.31                     | 0.60              |
| 1:A:171:C:C5'  | 2:H:189:VAL:HG22 | 2.31                     | 0.60              |
| 1:A:51:C:C5'   | 2:T:189:VAL:HG22 | 2.31                     | 0.60              |
| 1:A:141:C:C5'  | 2:K:189:VAL:HG22 | 2.31                     | 0.60              |
| 1:A:21:C:C5'   | 2:W:189:VAL:HG22 | 2.31                     | 0.60              |
| 1:A:221:C:C5'  | 2:C:189:VAL:HG22 | 2.31                     | 0.60              |
| 1:A:61:C:C5'   | 2:S:189:VAL:HG22 | 2.31                     | 0.60              |
| 1:A:11:C:C5'   | 2:X:189:VAL:HG22 | 2.31                     | 0.60              |
| 1:A:41:C:C5'   | 2:U:189:VAL:HG22 | 2.31                     | 0.60              |
| 1:A:71:C:C5'   | 2:R:189:VAL:HG22 | 2.31                     | 0.59              |
| 1:A:121:C:C5'  | 2:M:189:VAL:HG22 | 2.31                     | 0.59              |
| 1:A:111:C:C5'  | 2:N:189:VAL:HG22 | 2.31                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:X:119:LEU:HD11 | 2:X:123:ILE:HD11 | 1.86                     | 0.57              |
| 2:D:40:VAL:CG2   | 2:D:96:ASP:HA    | 2.34                     | 0.57              |
| 2:L:40:VAL:CG2   | 2:L:96:ASP:HA    | 2.34                     | 0.57              |
| 2:S:119:LEU:HD11 | 2:S:123:ILE:HD11 | 1.87                     | 0.57              |
| 2:G:40:VAL:CG2   | 2:G:96:ASP:HA    | 2.34                     | 0.57              |
| 2:C:119:LEU:HD11 | 2:C:123:ILE:HD11 | 1.87                     | 0.57              |
| 2:N:40:VAL:CG2   | 2:N:96:ASP:HA    | 2.35                     | 0.57              |
| 2:I:40:VAL:CG2   | 2:I:96:ASP:HA    | 2.35                     | 0.56              |
| 2:B:40:VAL:CG2   | 2:B:96:ASP:HA    | 2.35                     | 0.56              |
| 2:J:40:VAL:CG2   | 2:J:96:ASP:HA    | 2.36                     | 0.56              |
| 2:H:119:LEU:HD11 | 2:H:123:ILE:HD11 | 1.87                     | 0.56              |
| 2:H:40:VAL:CG2   | 2:H:96:ASP:HA    | 2.36                     | 0.56              |
| 2:P:119:LEU:HD11 | 2:P:123:ILE:HD11 | 1.88                     | 0.56              |
| 2:C:40:VAL:CG2   | 2:C:96:ASP:HA    | 2.36                     | 0.56              |
| 2:F:40:VAL:CG2   | 2:F:96:ASP:HA    | 2.35                     | 0.56              |
| 2:K:40:VAL:CG2   | 2:K:96:ASP:HA    | 2.35                     | 0.55              |
| 2:L:239:VAL:HA   | 2:L:242:ILE:HD12 | 1.88                     | 0.55              |
| 2:V:239:VAL:HA   | 2:V:242:ILE:HD12 | 1.88                     | 0.55              |
| 2:K:119:LEU:HD11 | 2:K:123:ILE:HD11 | 1.88                     | 0.55              |
| 2:M:40:VAL:CG2   | 2:M:96:ASP:HA    | 2.36                     | 0.55              |
| 2:E:40:VAL:CG2   | 2:E:96:ASP:HA    | 2.36                     | 0.55              |
| 2:G:239:VAL:HA   | 2:G:242:ILE:HD12 | 1.88                     | 0.55              |
| 2:Q:239:VAL:HA   | 2:Q:242:ILE:HD12 | 1.88                     | 0.55              |
| 2:F:119:LEU:HD11 | 2:F:123:ILE:HD11 | 1.89                     | 0.55              |
| 2:N:119:LEU:HD11 | 2:N:123:ILE:HD11 | 1.89                     | 0.55              |
| 2:I:239:VAL:HA   | 2:I:242:ILE:HD12 | 1.89                     | 0.55              |
| 2:C:115:THR:OG1  | 2:M:360:ASN:OD1  | 2.25                     | 0.55              |
| 2:H:115:THR:OG1  | 2:R:360:ASN:OD1  | 2.25                     | 0.55              |
| 2:W:239:VAL:HA   | 2:W:242:ILE:HD12 | 1.89                     | 0.54              |
| 2:T:239:VAL:HA   | 2:T:242:ILE:HD12 | 1.88                     | 0.54              |
| 2:M:119:LEU:HD11 | 2:M:123:ILE:HD11 | 1.89                     | 0.54              |
| 2:U:119:LEU:HD11 | 2:U:123:ILE:HD11 | 1.89                     | 0.54              |
| 2:J:239:VAL:HA   | 2:J:242:ILE:HD12 | 1.89                     | 0.54              |
| 2:H:239:VAL:HA   | 2:H:242:ILE:HD12 | 1.89                     | 0.54              |
| 2:M:239:VAL:HA   | 2:M:242:ILE:HD12 | 1.89                     | 0.54              |
| 2:R:239:VAL:HA   | 2:R:242:ILE:HD12 | 1.89                     | 0.54              |
| 2:O:239:VAL:HA   | 2:O:242:ILE:HD12 | 1.88                     | 0.54              |
| 2:K:115:THR:OG1  | 2:U:360:ASN:OD1  | 2.26                     | 0.54              |
| 2:I:119:LEU:HD11 | 2:I:123:ILE:HD11 | 1.90                     | 0.54              |
| 2:K:96:ASP:OD2   | 2:U:360:ASN:HB3  | 2.09                     | 0.53              |
| 2:Q:119:LEU:HD11 | 2:Q:123:ILE:HD11 | 1.91                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:119:LEU:HD11 | 2:R:123:ILE:HD11 | 1.91                     | 0.53              |
| 2:D:239:VAL:HA   | 2:D:242:ILE:HD12 | 1.88                     | 0.53              |
| 2:N:239:VAL:HA   | 2:N:242:ILE:HD12 | 1.89                     | 0.53              |
| 2:V:119:LEU:HD11 | 2:V:123:ILE:HD11 | 1.90                     | 0.53              |
| 2:S:239:VAL:HA   | 2:S:242:ILE:HD12 | 1.90                     | 0.53              |
| 2:E:239:VAL:HA   | 2:E:242:ILE:HD12 | 1.89                     | 0.53              |
| 2:X:239:VAL:HA   | 2:X:242:ILE:HD12 | 1.90                     | 0.53              |
| 2:K:239:VAL:HA   | 2:K:242:ILE:HD12 | 1.90                     | 0.53              |
| 2:F:239:VAL:HA   | 2:F:242:ILE:HD12 | 1.89                     | 0.53              |
| 2:D:119:LEU:HD11 | 2:D:123:ILE:HD11 | 1.91                     | 0.53              |
| 2:U:239:VAL:HA   | 2:U:242:ILE:HD12 | 1.91                     | 0.52              |
| 2:P:239:VAL:HA   | 2:P:242:ILE:HD12 | 1.90                     | 0.52              |
| 2:C:96:ASP:OD2   | 2:M:360:ASN:HB3  | 2.09                     | 0.52              |
| 2:H:96:ASP:OD2   | 2:R:360:ASN:HB3  | 2.10                     | 0.52              |
| 2:C:239:VAL:HA   | 2:C:242:ILE:HD12 | 1.90                     | 0.52              |
| 2:X:48:CYS:HB3   | 2:X:160:ILE:HD12 | 1.92                     | 0.52              |
| 2:F:96:ASP:OD2   | 2:P:360:ASN:HB3  | 2.10                     | 0.52              |
| 2:M:96:ASP:OD2   | 2:W:360:ASN:HB3  | 2.10                     | 0.51              |
| 2:D:48:CYS:HB3   | 2:D:160:ILE:HD12 | 1.92                     | 0.51              |
| 2:W:119:LEU:HD11 | 2:W:123:ILE:HD11 | 1.92                     | 0.51              |
| 2:P:48:CYS:HB3   | 2:P:160:ILE:HD12 | 1.92                     | 0.51              |
| 2:N:48:CYS:HB3   | 2:N:160:ILE:HD12 | 1.92                     | 0.51              |
| 2:I:48:CYS:HB3   | 2:I:160:ILE:HD12 | 1.92                     | 0.51              |
| 2:F:48:CYS:HB3   | 2:F:160:ILE:HD12 | 1.92                     | 0.51              |
| 2:O:48:CYS:HB3   | 2:O:160:ILE:HD12 | 1.93                     | 0.51              |
| 2:E:48:CYS:HB3   | 2:E:160:ILE:HD12 | 1.93                     | 0.51              |
| 2:B:48:CYS:HB3   | 2:B:160:ILE:HD12 | 1.92                     | 0.51              |
| 2:M:48:CYS:HB3   | 2:M:160:ILE:HD12 | 1.93                     | 0.51              |
| 2:N:96:ASP:OD2   | 2:X:360:ASN:HB3  | 2.11                     | 0.51              |
| 2:C:48:CYS:HB3   | 2:C:160:ILE:HD12 | 1.93                     | 0.51              |
| 2:L:48:CYS:HB3   | 2:L:160:ILE:HD12 | 1.92                     | 0.51              |
| 2:Q:78:ASP:O     | 2:Q:82:ILE:HG23  | 2.11                     | 0.51              |
| 2:W:48:CYS:HB3   | 2:W:160:ILE:HD12 | 1.92                     | 0.51              |
| 2:S:48:CYS:HB3   | 2:S:160:ILE:HD12 | 1.92                     | 0.51              |
| 2:L:96:ASP:OD2   | 2:V:360:ASN:HB3  | 2.11                     | 0.50              |
| 2:N:96:ASP:HB2   | 2:X:360:ASN:HB3  | 1.93                     | 0.50              |
| 2:J:78:ASP:O     | 2:J:82:ILE:HG23  | 2.11                     | 0.50              |
| 2:J:48:CYS:HB3   | 2:J:160:ILE:HD12 | 1.93                     | 0.50              |
| 2:D:78:ASP:O     | 2:D:82:ILE:HG23  | 2.11                     | 0.50              |
| 2:V:78:ASP:O     | 2:V:82:ILE:HG23  | 2.12                     | 0.50              |
| 2:Q:48:CYS:HB3   | 2:Q:160:ILE:HD12 | 1.92                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:V:48:CYS:HB3   | 2:V:160:ILE:HD12 | 1.92                     | 0.50              |
| 2:I:78:ASP:O     | 2:I:82:ILE:HG23  | 2.12                     | 0.50              |
| 2:K:48:CYS:HB3   | 2:K:160:ILE:HD12 | 1.92                     | 0.50              |
| 2:E:78:ASP:O     | 2:E:82:ILE:HG23  | 2.12                     | 0.50              |
| 2:J:96:ASP:OD2   | 2:T:360:ASN:HB3  | 2.12                     | 0.50              |
| 2:G:78:ASP:O     | 2:G:82:ILE:HG23  | 2.11                     | 0.50              |
| 2:F:78:ASP:O     | 2:F:82:ILE:HG23  | 2.12                     | 0.50              |
| 2:G:48:CYS:HB3   | 2:G:160:ILE:HD12 | 1.92                     | 0.50              |
| 2:U:78:ASP:O     | 2:U:82:ILE:HG23  | 2.12                     | 0.50              |
| 2:T:48:CYS:HB3   | 2:T:160:ILE:HD12 | 1.92                     | 0.50              |
| 2:C:78:ASP:O     | 2:C:82:ILE:HG23  | 2.12                     | 0.50              |
| 2:T:78:ASP:O     | 2:T:82:ILE:HG23  | 2.12                     | 0.50              |
| 2:D:96:ASP:HB2   | 2:N:360:ASN:HB3  | 1.94                     | 0.50              |
| 2:G:96:ASP:OD2   | 2:Q:360:ASN:HB3  | 2.12                     | 0.50              |
| 2:O:78:ASP:O     | 2:O:82:ILE:HG23  | 2.12                     | 0.50              |
| 2:G:119:LEU:HD11 | 2:G:123:ILE:HD11 | 1.94                     | 0.50              |
| 2:R:78:ASP:O     | 2:R:82:ILE:HG23  | 2.12                     | 0.50              |
| 2:R:48:CYS:HB3   | 2:R:160:ILE:HD12 | 1.93                     | 0.50              |
| 2:D:96:ASP:OD2   | 2:N:360:ASN:HB3  | 2.12                     | 0.49              |
| 2:W:78:ASP:O     | 2:W:82:ILE:HG23  | 2.12                     | 0.49              |
| 2:I:96:ASP:OD2   | 2:S:360:ASN:HB3  | 2.12                     | 0.49              |
| 2:H:48:CYS:HB3   | 2:H:160:ILE:HD12 | 1.93                     | 0.49              |
| 2:P:78:ASP:O     | 2:P:82:ILE:HG23  | 2.12                     | 0.49              |
| 2:N:78:ASP:O     | 2:N:82:ILE:HG23  | 2.12                     | 0.49              |
| 2:K:78:ASP:O     | 2:K:82:ILE:HG23  | 2.12                     | 0.49              |
| 2:P:281:MET:HA   | 2:P:284:VAL:HG22 | 1.93                     | 0.49              |
| 2:M:330:GLY:HA3  | 2:M:354:ALA:HB3  | 1.94                     | 0.49              |
| 2:E:96:ASP:OD2   | 2:O:360:ASN:HB3  | 2.12                     | 0.49              |
| 2:U:48:CYS:HB3   | 2:U:160:ILE:HD12 | 1.92                     | 0.49              |
| 2:L:78:ASP:O     | 2:L:82:ILE:HG23  | 2.11                     | 0.49              |
| 2:L:119:LEU:HD11 | 2:L:123:ILE:HD11 | 1.93                     | 0.49              |
| 2:U:281:MET:HA   | 2:U:284:VAL:HG22 | 1.93                     | 0.49              |
| 2:R:75:GLY:O     | 2:R:79:THR:HG22  | 2.13                     | 0.49              |
| 2:L:96:ASP:HB2   | 2:V:360:ASN:HB3  | 1.95                     | 0.49              |
| 2:W:75:GLY:O     | 2:W:79:THR:HG22  | 2.13                     | 0.49              |
| 2:E:75:GLY:O     | 2:E:79:THR:HG22  | 2.13                     | 0.49              |
| 2:M:78:ASP:O     | 2:M:82:ILE:HG23  | 2.12                     | 0.49              |
| 2:E:281:MET:HA   | 2:E:284:VAL:HG22 | 1.93                     | 0.49              |
| 2:W:330:GLY:HA3  | 2:W:354:ALA:HB3  | 1.94                     | 0.49              |
| 2:E:115:THR:OG1  | 2:O:360:ASN:OD1  | 2.28                     | 0.49              |
| 2:J:75:GLY:O     | 2:J:79:THR:HG22  | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:96:ASP:OD2   | 2:L:360:ASN:HB3  | 2.12                     | 0.49              |
| 2:H:78:ASP:O     | 2:H:82:ILE:HG23  | 2.12                     | 0.49              |
| 2:O:330:GLY:HA3  | 2:O:354:ALA:HB3  | 1.95                     | 0.49              |
| 2:E:119:LEU:HD11 | 2:E:123:ILE:HD11 | 1.95                     | 0.49              |
| 2:T:281:MET:HA   | 2:T:284:VAL:HG22 | 1.94                     | 0.49              |
| 2:J:281:MET:HA   | 2:J:284:VAL:HG22 | 1.94                     | 0.49              |
| 2:I:96:ASP:HB2   | 2:S:360:ASN:HB3  | 1.94                     | 0.49              |
| 2:F:281:MET:HA   | 2:F:284:VAL:HG22 | 1.94                     | 0.49              |
| 2:O:281:MET:HA   | 2:O:284:VAL:HG22 | 1.94                     | 0.49              |
| 2:R:330:GLY:HA3  | 2:R:354:ALA:HB3  | 1.94                     | 0.49              |
| 2:X:78:ASP:O     | 2:X:82:ILE:HG23  | 2.12                     | 0.48              |
| 2:S:78:ASP:O     | 2:S:82:ILE:HG23  | 2.12                     | 0.48              |
| 2:B:119:LEU:HD11 | 2:B:123:ILE:HD11 | 1.94                     | 0.48              |
| 2:C:96:ASP:HB2   | 2:M:360:ASN:HB3  | 1.95                     | 0.48              |
| 2:M:115:THR:OG1  | 2:W:360:ASN:OD1  | 2.25                     | 0.48              |
| 2:M:75:GLY:O     | 2:M:79:THR:HG22  | 2.13                     | 0.48              |
| 2:J:115:THR:OG1  | 2:T:360:ASN:OD1  | 2.29                     | 0.48              |
| 2:T:119:LEU:HD11 | 2:T:123:ILE:HD11 | 1.95                     | 0.48              |
| 2:O:75:GLY:O     | 2:O:79:THR:HG22  | 2.14                     | 0.48              |
| 2:O:119:LEU:HD11 | 2:O:123:ILE:HD11 | 1.95                     | 0.48              |
| 2:K:96:ASP:HB2   | 2:U:360:ASN:HB3  | 1.95                     | 0.48              |
| 2:H:75:GLY:O     | 2:H:79:THR:HG22  | 2.14                     | 0.48              |
| 2:K:281:MET:HA   | 2:K:284:VAL:HG22 | 1.93                     | 0.48              |
| 2:F:96:ASP:HB2   | 2:P:360:ASN:HB3  | 1.95                     | 0.48              |
| 2:P:330:GLY:HA3  | 2:P:354:ALA:HB3  | 1.96                     | 0.48              |
| 2:M:115:THR:OG1  | 2:W:359:GLU:HG3  | 2.14                     | 0.48              |
| 2:V:281:MET:HA   | 2:V:284:VAL:HG22 | 1.96                     | 0.48              |
| 2:E:96:ASP:HB2   | 2:O:360:ASN:HB3  | 1.96                     | 0.48              |
| 2:M:96:ASP:HB2   | 2:W:360:ASN:HB3  | 1.96                     | 0.48              |
| 2:K:115:THR:OG1  | 2:U:359:GLU:HG3  | 2.14                     | 0.47              |
| 2:X:281:MET:HA   | 2:X:284:VAL:HG22 | 1.96                     | 0.47              |
| 2:D:281:MET:HA   | 2:D:284:VAL:HG22 | 1.95                     | 0.47              |
| 2:G:96:ASP:HB2   | 2:Q:360:ASN:HB3  | 1.95                     | 0.47              |
| 2:J:96:ASP:HB2   | 2:T:360:ASN:HB3  | 1.96                     | 0.47              |
| 2:T:75:GLY:O     | 2:T:79:THR:HG22  | 2.14                     | 0.47              |
| 2:H:115:THR:OG1  | 2:R:359:GLU:HG3  | 2.14                     | 0.47              |
| 2:E:115:THR:OG1  | 2:O:359:GLU:HG3  | 2.14                     | 0.47              |
| 2:T:330:GLY:HA3  | 2:T:354:ALA:HB3  | 1.96                     | 0.47              |
| 2:L:115:THR:OG1  | 2:V:360:ASN:OD1  | 2.31                     | 0.47              |
| 2:J:119:LEU:HD11 | 2:J:123:ILE:HD11 | 1.96                     | 0.47              |
| 2:U:75:GLY:O     | 2:U:79:THR:HG22  | 2.15                     | 0.47              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:F:115:THR:OG1 | 2:P:360:ASN:OD1  | 2.27                     | 0.47              |
| 2:B:96:ASP:HB2  | 2:L:360:ASN:HB3  | 1.97                     | 0.47              |
| 2:J:115:THR:OG1 | 2:T:359:GLU:HG3  | 2.14                     | 0.47              |
| 2:C:115:THR:OG1 | 2:M:359:GLU:HG3  | 2.15                     | 0.47              |
| 2:C:75:GLY:O    | 2:C:79:THR:HG22  | 2.15                     | 0.47              |
| 2:L:75:GLY:O    | 2:L:79:THR:HG22  | 2.15                     | 0.47              |
| 2:B:115:THR:OG1 | 2:L:360:ASN:OD1  | 2.31                     | 0.47              |
| 2:N:281:MET:HA  | 2:N:284:VAL:HG22 | 1.96                     | 0.47              |
| 2:G:75:GLY:O    | 2:G:79:THR:HG22  | 2.14                     | 0.47              |
| 2:I:281:MET:HA  | 2:I:284:VAL:HG22 | 1.96                     | 0.47              |
| 2:B:96:ASP:CG   | 2:L:361:GLY:H    | 2.19                     | 0.46              |
| 2:B:281:MET:HA  | 2:B:284:VAL:HG22 | 1.97                     | 0.46              |
| 2:N:115:THR:OG1 | 2:X:360:ASN:OD1  | 2.30                     | 0.46              |
| 2:U:330:GLY:HA3 | 2:U:354:ALA:HB3  | 1.95                     | 0.46              |
| 2:Q:281:MET:HA  | 2:Q:284:VAL:HG22 | 1.96                     | 0.46              |
| 2:W:281:MET:HA  | 2:W:284:VAL:HG22 | 1.98                     | 0.46              |
| 2:H:96:ASP:HB2  | 2:R:360:ASN:HB3  | 1.96                     | 0.46              |
| 2:C:281:MET:HA  | 2:C:284:VAL:HG22 | 1.97                     | 0.46              |
| 2:B:75:GLY:O    | 2:B:79:THR:HG22  | 2.16                     | 0.46              |
| 2:P:75:GLY:O    | 2:P:79:THR:HG22  | 2.16                     | 0.46              |
| 2:D:23:TYR:CD1  | 2:E:82:ILE:HG22  | 2.51                     | 0.46              |
| 2:E:23:TYR:CD1  | 2:F:82:ILE:HG22  | 2.51                     | 0.46              |
| 2:M:23:TYR:CD1  | 2:N:82:ILE:HG22  | 2.51                     | 0.46              |
| 2:D:75:GLY:O    | 2:D:79:THR:HG22  | 2.16                     | 0.46              |
| 2:B:23:TYR:CD1  | 2:C:82:ILE:HG22  | 2.51                     | 0.46              |
| 2:J:23:TYR:CD1  | 2:K:82:ILE:HG22  | 2.51                     | 0.46              |
| 2:L:23:TYR:CD1  | 2:M:82:ILE:HG22  | 2.51                     | 0.46              |
| 2:G:23:TYR:CD1  | 2:H:82:ILE:HG22  | 2.51                     | 0.46              |
| 2:S:330:GLY:HA3 | 2:S:354:ALA:HB3  | 1.98                     | 0.46              |
| 2:L:330:GLY:HA3 | 2:L:354:ALA:HB3  | 1.97                     | 0.46              |
| 2:G:94:GLY:O    | 2:Q:360:ASN:ND2  | 2.49                     | 0.46              |
| 2:I:23:TYR:CD1  | 2:J:82:ILE:HG22  | 2.51                     | 0.46              |
| 2:C:23:TYR:CD1  | 2:D:82:ILE:HG22  | 2.51                     | 0.46              |
| 2:H:23:TYR:CD1  | 2:I:82:ILE:HG22  | 2.51                     | 0.46              |
| 2:S:281:MET:HA  | 2:S:284:VAL:HG22 | 1.97                     | 0.46              |
| 2:X:75:GLY:O    | 2:X:79:THR:HG22  | 2.16                     | 0.46              |
| 2:Q:330:GLY:HA3 | 2:Q:354:ALA:HB3  | 1.98                     | 0.46              |
| 2:D:94:GLY:O    | 2:N:360:ASN:ND2  | 2.49                     | 0.45              |
| 2:E:330:GLY:HA3 | 2:E:354:ALA:HB3  | 1.98                     | 0.45              |
| 2:D:115:THR:OG1 | 2:N:360:ASN:OD1  | 2.32                     | 0.45              |
| 2:G:115:THR:OG1 | 2:Q:359:GLU:HG3  | 2.16                     | 0.45              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:K:23:TYR:CD1  | 2:L:82:ILE:HG22  | 2.51                     | 0.45              |
| 2:L:281:MET:HA  | 2:L:284:VAL:HG22 | 1.97                     | 0.45              |
| 2:Q:75:GLY:O    | 2:Q:79:THR:HG22  | 2.16                     | 0.45              |
| 2:X:330:GLY:HA3 | 2:X:354:ALA:HB3  | 1.97                     | 0.45              |
| 2:F:23:TYR:CD1  | 2:G:82:ILE:HG22  | 2.52                     | 0.45              |
| 2:K:75:GLY:O    | 2:K:79:THR:HG22  | 2.16                     | 0.45              |
| 2:N:23:TYR:CD1  | 2:O:82:ILE:HG22  | 2.52                     | 0.45              |
| 2:O:23:TYR:CD1  | 2:P:82:ILE:HG22  | 2.51                     | 0.45              |
| 2:J:330:GLY:HA3 | 2:J:354:ALA:HB3  | 1.99                     | 0.45              |
| 2:N:75:GLY:O    | 2:N:79:THR:HG22  | 2.17                     | 0.45              |
| 2:Q:23:TYR:CD1  | 2:R:82:ILE:HG22  | 2.52                     | 0.45              |
| 2:R:23:TYR:CD1  | 2:S:82:ILE:HG22  | 2.51                     | 0.45              |
| 2:R:281:MET:HA  | 2:R:284:VAL:HG22 | 1.98                     | 0.45              |
| 2:M:281:MET:HA  | 2:M:284:VAL:HG22 | 1.98                     | 0.45              |
| 2:F:335:GLY:HA2 | 2:F:336:GLU:HA   | 1.82                     | 0.45              |
| 2:P:23:TYR:CD1  | 2:Q:82:ILE:HG22  | 2.52                     | 0.45              |
| 2:V:75:GLY:O    | 2:V:79:THR:HG22  | 2.17                     | 0.45              |
| 2:G:281:MET:HA  | 2:G:284:VAL:HG22 | 1.97                     | 0.45              |
| 2:H:281:MET:HA  | 2:H:284:VAL:HG22 | 1.98                     | 0.45              |
| 2:S:75:GLY:O    | 2:S:79:THR:HG22  | 2.17                     | 0.45              |
| 2:L:94:GLY:O    | 2:V:360:ASN:ND2  | 2.49                     | 0.45              |
| 2:N:115:THR:OG1 | 2:X:359:GLU:HG3  | 2.17                     | 0.45              |
| 2:B:115:THR:OG1 | 2:L:359:GLU:HG3  | 2.16                     | 0.45              |
| 2:M:94:GLY:O    | 2:W:360:ASN:ND2  | 2.50                     | 0.45              |
| 2:F:75:GLY:O    | 2:F:79:THR:HG22  | 2.17                     | 0.45              |
| 2:G:115:THR:OG1 | 2:Q:360:ASN:OD1  | 2.30                     | 0.45              |
| 2:B:94:GLY:O    | 2:L:360:ASN:ND2  | 2.50                     | 0.45              |
| 2:F:115:THR:OG1 | 2:P:359:GLU:HG3  | 2.16                     | 0.45              |
| 2:S:23:TYR:CD1  | 2:T:82:ILE:HG22  | 2.52                     | 0.45              |
| 2:I:75:GLY:O    | 2:I:79:THR:HG22  | 2.17                     | 0.45              |
| 2:I:94:GLY:O    | 2:S:360:ASN:ND2  | 2.50                     | 0.45              |
| 2:E:94:GLY:O    | 2:O:360:ASN:ND2  | 2.50                     | 0.45              |
| 2:H:330:GLY:HA3 | 2:H:354:ALA:HB3  | 1.98                     | 0.45              |
| 2:C:330:GLY:HA3 | 2:C:354:ALA:HB3  | 1.99                     | 0.45              |
| 2:N:94:GLY:O    | 2:X:360:ASN:ND2  | 2.50                     | 0.45              |
| 2:D:115:THR:OG1 | 2:N:359:GLU:HG3  | 2.17                     | 0.44              |
| 2:T:23:TYR:CD1  | 2:U:82:ILE:HG22  | 2.51                     | 0.44              |
| 2:N:335:GLY:HA2 | 2:N:336:GLU:HA   | 1.82                     | 0.44              |
| 2:B:330:GLY:HA3 | 2:B:354:ALA:HB3  | 2.00                     | 0.44              |
| 2:H:94:GLY:O    | 2:R:360:ASN:ND2  | 2.50                     | 0.44              |
| 2:W:23:TYR:CD1  | 2:X:82:ILE:HG22  | 2.51                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:94:GLY:O     | 2:T:360:ASN:ND2  | 2.50                     | 0.44              |
| 2:N:362:VAL:HG12 | 2:N:363:ILE:N    | 2.33                     | 0.44              |
| 2:H:96:ASP:N     | 2:R:360:ASN:OD1  | 2.49                     | 0.44              |
| 2:V:23:TYR:CD1   | 2:W:82:ILE:HG22  | 2.52                     | 0.44              |
| 2:V:330:GLY:HA3  | 2:V:354:ALA:HB3  | 1.98                     | 0.44              |
| 2:X:335:GLY:HA2  | 2:X:336:GLU:HA   | 1.82                     | 0.44              |
| 1:A:21:C:C4      | 2:W:242:ILE:HG12 | 2.53                     | 0.44              |
| 2:I:115:THR:OG1  | 2:S:359:GLU:HG3  | 2.17                     | 0.44              |
| 2:F:94:GLY:O     | 2:P:360:ASN:ND2  | 2.51                     | 0.44              |
| 2:N:330:GLY:HA3  | 2:N:354:ALA:HB3  | 1.98                     | 0.44              |
| 1:A:181:C:C4     | 2:G:242:ILE:HG12 | 2.53                     | 0.44              |
| 2:X:119:LEU:CD1  | 2:X:123:ILE:HD11 | 2.48                     | 0.44              |
| 2:U:23:TYR:CD1   | 2:V:82:ILE:HG22  | 2.52                     | 0.44              |
| 2:L:115:THR:OG1  | 2:V:359:GLU:HG3  | 2.17                     | 0.44              |
| 1:A:91:C:C4      | 2:P:242:ILE:HG12 | 2.53                     | 0.43              |
| 1:A:131:C:C4     | 2:L:242:ILE:HG12 | 2.53                     | 0.43              |
| 1:A:71:C:C4      | 2:R:242:ILE:HG12 | 2.53                     | 0.43              |
| 2:C:94:GLY:O     | 2:M:360:ASN:ND2  | 2.51                     | 0.43              |
| 2:K:94:GLY:O     | 2:U:360:ASN:ND2  | 2.51                     | 0.43              |
| 2:M:331:LEU:HD13 | 2:M:354:ALA:HB1  | 2.00                     | 0.43              |
| 2:C:119:LEU:CD1  | 2:C:123:ILE:HD11 | 2.48                     | 0.43              |
| 1:A:41:C:C4      | 2:U:242:ILE:HG12 | 2.53                     | 0.43              |
| 2:Q:275:ALA:HB3  | 2:R:361:GLY:HA2  | 1.99                     | 0.43              |
| 2:V:362:VAL:HG12 | 2:V:363:ILE:N    | 2.34                     | 0.43              |
| 1:A:221:C:C4     | 2:C:242:ILE:HG12 | 2.54                     | 0.43              |
| 2:W:331:LEU:HD13 | 2:W:354:ALA:HB1  | 2.00                     | 0.43              |
| 2:L:335:GLY:HA2  | 2:L:336:GLU:HA   | 1.82                     | 0.43              |
| 1:A:121:C:C4     | 2:M:242:ILE:HG12 | 2.53                     | 0.43              |
| 1:A:101:C:C4     | 2:O:242:ILE:HG12 | 2.54                     | 0.43              |
| 1:A:201:C:C4     | 2:E:242:ILE:HG12 | 2.54                     | 0.43              |
| 2:G:335:GLY:HA2  | 2:G:336:GLU:HA   | 1.82                     | 0.43              |
| 2:S:119:LEU:CD1  | 2:S:123:ILE:HD11 | 2.49                     | 0.43              |
| 2:X:362:VAL:HG12 | 2:X:363:ILE:N    | 2.34                     | 0.43              |
| 1:A:191:C:C4     | 2:F:242:ILE:HG12 | 2.53                     | 0.43              |
| 2:T:362:VAL:HG12 | 2:T:363:ILE:N    | 2.34                     | 0.43              |
| 2:L:275:ALA:HB3  | 2:M:361:GLY:HA2  | 2.00                     | 0.43              |
| 2:V:275:ALA:HB3  | 2:W:361:GLY:HA2  | 2.00                     | 0.43              |
| 1:A:11:C:C4      | 2:X:242:ILE:HG12 | 2.54                     | 0.42              |
| 1:A:151:C:C4     | 2:J:242:ILE:HG12 | 2.54                     | 0.42              |
| 1:A:31:C:C4      | 2:V:242:ILE:HG12 | 2.53                     | 0.42              |
| 2:U:335:GLY:HA2  | 2:U:336:GLU:HA   | 1.82                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:275:ALA:HB3  | 2:U:361:GLY:HA2  | 2.01                     | 0.42              |
| 1:A:211:C:C4     | 2:D:242:ILE:HG12 | 2.55                     | 0.42              |
| 1:A:141:C:C4     | 2:K:242:ILE:HG12 | 2.53                     | 0.42              |
| 1:A:61:C:C4      | 2:S:242:ILE:HG12 | 2.54                     | 0.42              |
| 1:A:171:C:C4     | 2:H:242:ILE:HG12 | 2.54                     | 0.42              |
| 1:A:51:C:C4      | 2:T:242:ILE:HG12 | 2.54                     | 0.42              |
| 1:A:161:C:C4     | 2:I:242:ILE:HG12 | 2.55                     | 0.42              |
| 2:M:96:ASP:N     | 2:W:360:ASN:OD1  | 2.49                     | 0.42              |
| 2:R:331:LEU:HD13 | 2:R:354:ALA:HB1  | 2.01                     | 0.42              |
| 2:I:335:GLY:HA2  | 2:I:336:GLU:HA   | 1.82                     | 0.42              |
| 2:S:275:ALA:HB3  | 2:T:361:GLY:HA2  | 2.01                     | 0.42              |
| 2:S:6:VAL:HG23   | 2:T:288:TYR:CE2  | 2.55                     | 0.42              |
| 2:L:270:ILE:HG23 | 2:M:363:ILE:HG21 | 2.02                     | 0.42              |
| 2:S:362:VAL:HG12 | 2:S:363:ILE:N    | 2.34                     | 0.42              |
| 2:O:335:GLY:HA2  | 2:O:336:GLU:HA   | 1.82                     | 0.42              |
| 1:A:81:C:C4      | 2:Q:242:ILE:HG12 | 2.53                     | 0.42              |
| 1:A:111:C:C4     | 2:N:242:ILE:HG12 | 2.55                     | 0.42              |
| 2:O:331:LEU:HD13 | 2:O:354:ALA:HB1  | 2.02                     | 0.42              |
| 2:O:362:VAL:HG12 | 2:O:363:ILE:N    | 2.34                     | 0.42              |
| 2:N:275:ALA:HB3  | 2:O:361:GLY:HA2  | 2.01                     | 0.42              |
| 2:Q:335:GLY:HA2  | 2:Q:336:GLU:HA   | 1.82                     | 0.42              |
| 2:K:330:GLY:HA3  | 2:K:354:ALA:HB3  | 2.01                     | 0.42              |
| 2:N:6:VAL:HG23   | 2:O:288:TYR:CE2  | 2.55                     | 0.42              |
| 2:O:275:ALA:HB3  | 2:P:361:GLY:HA2  | 2.02                     | 0.42              |
| 2:C:6:VAL:HG23   | 2:D:288:TYR:CE2  | 2.55                     | 0.42              |
| 2:K:275:ALA:HB3  | 2:L:361:GLY:HA2  | 2.02                     | 0.42              |
| 2:H:119:LEU:CD1  | 2:H:123:ILE:HD11 | 2.49                     | 0.42              |
| 2:S:270:ILE:HG23 | 2:T:363:ILE:HG21 | 2.02                     | 0.42              |
| 2:L:362:VAL:HG12 | 2:L:363:ILE:N    | 2.35                     | 0.42              |
| 2:I:6:VAL:HG23   | 2:J:288:TYR:CE2  | 2.55                     | 0.42              |
| 2:O:270:ILE:HG23 | 2:P:363:ILE:HG21 | 2.02                     | 0.42              |
| 2:H:54:THR:HB    | 2:H:57:ALA:HB2   | 2.02                     | 0.42              |
| 2:Q:270:ILE:HG23 | 2:R:363:ILE:HG21 | 2.02                     | 0.42              |
| 2:K:119:LEU:CD1  | 2:K:123:ILE:HD11 | 2.50                     | 0.42              |
| 2:X:331:LEU:HD13 | 2:X:354:ALA:HB1  | 2.02                     | 0.42              |
| 2:I:330:GLY:HA3  | 2:I:354:ALA:HB3  | 2.02                     | 0.42              |
| 2:H:6:VAL:HG23   | 2:I:288:TYR:CE2  | 2.55                     | 0.42              |
| 2:F:330:GLY:HA3  | 2:F:354:ALA:HB3  | 2.02                     | 0.42              |
| 2:G:330:GLY:HA3  | 2:G:354:ALA:HB3  | 2.01                     | 0.42              |
| 2:D:96:ASP:CB    | 2:N:360:ASN:HB3  | 2.50                     | 0.41              |
| 2:N:96:ASP:CB    | 2:X:360:ASN:HB3  | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:54:THR:HB    | 2:R:57:ALA:HB2   | 2.02                     | 0.41              |
| 2:F:6:VAL:HG23   | 2:G:288:TYR:CE2  | 2.55                     | 0.41              |
| 2:I:96:ASP:CB    | 2:S:360:ASN:HB3  | 2.50                     | 0.41              |
| 2:U:270:ILE:HD13 | 2:U:270:ILE:HA   | 1.97                     | 0.41              |
| 2:V:270:ILE:HG23 | 2:W:363:ILE:HG21 | 2.02                     | 0.41              |
| 2:P:6:VAL:HG23   | 2:Q:288:TYR:CE2  | 2.55                     | 0.41              |
| 2:U:331:LEU:HD13 | 2:U:354:ALA:HB1  | 2.01                     | 0.41              |
| 2:S:54:THR:HB    | 2:S:57:ALA:HB2   | 2.03                     | 0.41              |
| 2:M:54:THR:HB    | 2:M:57:ALA:HB2   | 2.02                     | 0.41              |
| 2:P:54:THR:HB    | 2:P:57:ALA:HB2   | 2.03                     | 0.41              |
| 2:I:115:THR:OG1  | 2:S:360:ASN:OD1  | 2.31                     | 0.41              |
| 2:P:331:LEU:HD13 | 2:P:354:ALA:HB1  | 2.02                     | 0.41              |
| 2:W:362:VAL:HG12 | 2:W:363:ILE:N    | 2.35                     | 0.41              |
| 2:T:335:GLY:HA2  | 2:T:336:GLU:HA   | 1.82                     | 0.41              |
| 2:X:54:THR:HB    | 2:X:57:ALA:HB2   | 2.02                     | 0.41              |
| 2:M:119:LEU:CD1  | 2:M:123:ILE:HD11 | 2.51                     | 0.41              |
| 2:M:362:VAL:HG12 | 2:M:363:ILE:N    | 2.36                     | 0.41              |
| 2:U:275:ALA:HB3  | 2:V:361:GLY:HA2  | 2.02                     | 0.41              |
| 2:Q:6:VAL:HG23   | 2:R:288:TYR:CE2  | 2.56                     | 0.41              |
| 2:K:54:THR:HB    | 2:K:57:ALA:HB2   | 2.03                     | 0.41              |
| 2:F:54:THR:HB    | 2:F:57:ALA:HB2   | 2.03                     | 0.41              |
| 2:P:335:GLY:HA2  | 2:P:336:GLU:HA   | 1.82                     | 0.41              |
| 2:U:54:THR:HB    | 2:U:57:ALA:HB2   | 2.03                     | 0.41              |
| 2:C:54:THR:HB    | 2:C:57:ALA:HB2   | 2.02                     | 0.41              |
| 2:C:96:ASP:N     | 2:M:360:ASN:OD1  | 2.49                     | 0.41              |
| 2:N:119:LEU:CD1  | 2:N:123:ILE:HD11 | 2.50                     | 0.41              |
| 2:L:331:LEU:HD13 | 2:L:354:ALA:HB1  | 2.02                     | 0.41              |
| 2:N:331:LEU:HD13 | 2:N:354:ALA:HB1  | 2.03                     | 0.41              |
| 2:S:270:ILE:HA   | 2:S:270:ILE:HD13 | 1.97                     | 0.41              |
| 2:B:335:GLY:HA2  | 2:B:336:GLU:HA   | 1.82                     | 0.41              |
| 2:T:270:ILE:HG23 | 2:U:363:ILE:HG21 | 2.03                     | 0.41              |
| 2:U:362:VAL:HG12 | 2:U:363:ILE:N    | 2.35                     | 0.41              |
| 2:B:96:ASP:OD2   | 2:L:361:GLY:N    | 2.41                     | 0.41              |
| 2:E:23:TYR:CG    | 2:F:82:ILE:HG22  | 2.56                     | 0.41              |
| 2:J:23:TYR:CG    | 2:K:82:ILE:HG22  | 2.56                     | 0.41              |
| 2:N:270:ILE:HG23 | 2:O:363:ILE:HG21 | 2.03                     | 0.41              |
| 2:R:362:VAL:HG12 | 2:R:363:ILE:N    | 2.36                     | 0.41              |
| 2:T:6:VAL:HG23   | 2:U:288:TYR:CE2  | 2.56                     | 0.41              |
| 2:V:6:VAL:HG23   | 2:W:288:TYR:CE2  | 2.55                     | 0.41              |
| 2:P:362:VAL:HG12 | 2:P:363:ILE:N    | 2.35                     | 0.41              |
| 2:Q:270:ILE:HD13 | 2:Q:270:ILE:HA   | 1.96                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:54:THR:HB    | 2:Q:57:ALA:HB2   | 2.03                     | 0.41              |
| 2:R:6:VAL:HG23   | 2:S:288:TYR:CE2  | 2.56                     | 0.41              |
| 2:M:275:ALA:HB3  | 2:N:361:GLY:HA2  | 2.02                     | 0.41              |
| 2:D:6:VAL:HG23   | 2:E:288:TYR:CE2  | 2.55                     | 0.41              |
| 2:L:96:ASP:CB    | 2:V:360:ASN:HB3  | 2.51                     | 0.41              |
| 2:P:119:LEU:CD1  | 2:P:123:ILE:HD11 | 2.50                     | 0.41              |
| 2:T:331:LEU:HD13 | 2:T:354:ALA:HB1  | 2.02                     | 0.41              |
| 2:W:54:THR:HB    | 2:W:57:ALA:HB2   | 2.03                     | 0.41              |
| 2:K:6:VAL:HG23   | 2:L:288:TYR:CE2  | 2.55                     | 0.41              |
| 2:M:6:VAL:HG23   | 2:N:288:TYR:CE2  | 2.55                     | 0.41              |
| 2:E:54:THR:HB    | 2:E:57:ALA:HB2   | 2.03                     | 0.41              |
| 2:G:6:VAL:HG23   | 2:H:288:TYR:CE2  | 2.56                     | 0.41              |
| 2:E:335:GLY:HA2  | 2:E:336:GLU:HA   | 1.82                     | 0.41              |
| 2:J:6:VAL:HG23   | 2:K:288:TYR:CE2  | 2.56                     | 0.41              |
| 2:U:119:LEU:CD1  | 2:U:123:ILE:HD11 | 2.51                     | 0.41              |
| 2:S:331:LEU:HD13 | 2:S:354:ALA:HB1  | 2.02                     | 0.41              |
| 2:H:331:LEU:HD13 | 2:H:354:ALA:HB1  | 2.03                     | 0.41              |
| 2:W:6:VAL:HG23   | 2:X:288:TYR:CE2  | 2.56                     | 0.41              |
| 2:E:6:VAL:HG23   | 2:F:288:TYR:CE2  | 2.56                     | 0.41              |
| 2:G:54:THR:HB    | 2:G:57:ALA:HB2   | 2.03                     | 0.41              |
| 2:T:54:THR:HB    | 2:T:57:ALA:HB2   | 2.03                     | 0.41              |
| 2:I:54:THR:HB    | 2:I:57:ALA:HB2   | 2.03                     | 0.41              |
| 2:U:6:VAL:HG23   | 2:V:288:TYR:CE2  | 2.56                     | 0.41              |
| 2:D:330:GLY:HA3  | 2:D:354:ALA:HB3  | 2.02                     | 0.41              |
| 1:A:221:C:C2     | 2:C:242:ILE:HA   | 2.56                     | 0.40              |
| 2:U:270:ILE:HG23 | 2:V:363:ILE:HG21 | 2.03                     | 0.40              |
| 2:J:54:THR:HB    | 2:J:57:ALA:HB2   | 2.03                     | 0.40              |
| 1:A:11:C:C2      | 2:X:242:ILE:HA   | 2.57                     | 0.40              |
| 1:A:191:C:C2     | 2:F:242:ILE:HA   | 2.57                     | 0.40              |
| 2:G:96:ASP:CB    | 2:Q:360:ASN:HB3  | 2.52                     | 0.40              |
| 2:F:96:ASP:CB    | 2:P:360:ASN:HB3  | 2.50                     | 0.40              |
| 2:F:119:LEU:CD1  | 2:F:123:ILE:HD11 | 2.50                     | 0.40              |
| 2:M:23:TYR:CG    | 2:N:82:ILE:HG22  | 2.56                     | 0.40              |
| 2:V:331:LEU:HD13 | 2:V:354:ALA:HB1  | 2.03                     | 0.40              |
| 2:W:270:ILE:HG23 | 2:X:363:ILE:HG21 | 2.03                     | 0.40              |
| 2:R:275:ALA:HB3  | 2:S:361:GLY:HA2  | 2.02                     | 0.40              |
| 2:L:54:THR:HB    | 2:L:57:ALA:HB2   | 2.03                     | 0.40              |
| 2:P:270:ILE:HG23 | 2:Q:363:ILE:HG21 | 2.03                     | 0.40              |
| 2:N:54:THR:HB    | 2:N:57:ALA:HB2   | 2.03                     | 0.40              |
| 2:B:54:THR:HB    | 2:B:57:ALA:HB2   | 2.03                     | 0.40              |
| 2:P:275:ALA:HB3  | 2:Q:361:GLY:HA2  | 2.02                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:91:C:C2      | 2:P:242:ILE:HA   | 2.57                     | 0.40              |
| 1:A:171:C:C2     | 2:H:242:ILE:HA   | 2.57                     | 0.40              |
| 2:B:6:VAL:HG23   | 2:C:288:TYR:CE2  | 2.56                     | 0.40              |
| 2:O:6:VAL:HG23   | 2:P:288:TYR:CE2  | 2.56                     | 0.40              |
| 2:V:54:THR:HB    | 2:V:57:ALA:HB2   | 2.03                     | 0.40              |
| 1:A:101:C:C2     | 2:O:242:ILE:HA   | 2.57                     | 0.40              |
| 1:A:131:C:C2     | 2:L:242:ILE:HA   | 2.57                     | 0.40              |
| 1:A:71:C:C2      | 2:R:242:ILE:HA   | 2.57                     | 0.40              |
| 2:K:96:ASP:CB    | 2:U:360:ASN:HB3  | 2.51                     | 0.40              |
| 2:E:331:LEU:HD13 | 2:E:354:ALA:HB1  | 2.03                     | 0.40              |
| 2:M:270:ILE:HG23 | 2:N:363:ILE:HG21 | 2.03                     | 0.40              |
| 2:R:270:ILE:HG23 | 2:S:363:ILE:HG21 | 2.03                     | 0.40              |
| 2:O:54:THR:HB    | 2:O:57:ALA:HB2   | 2.03                     | 0.40              |
| 2:D:54:THR:HB    | 2:D:57:ALA:HB2   | 2.03                     | 0.40              |
| 1:A:151:C:C2     | 2:J:242:ILE:HA   | 2.57                     | 0.40              |
| 1:A:31:C:C2      | 2:V:242:ILE:HA   | 2.57                     | 0.40              |
| 2:Q:362:VAL:HG12 | 2:Q:363:ILE:N    | 2.35                     | 0.40              |
| 2:L:6:VAL:HG23   | 2:M:288:TYR:CE2  | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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 |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 2   | B     | 368/391 (94%) | 354 (96%) | 13 (4%) | 1 (0%)   | 46          | 46 |
| 2   | C     | 368/391 (94%) | 352 (96%) | 15 (4%) | 1 (0%)   | 46          | 46 |
| 2   | D     | 368/391 (94%) | 352 (96%) | 15 (4%) | 1 (0%)   | 46          | 46 |
| 2   | E     | 368/391 (94%) | 353 (96%) | 14 (4%) | 1 (0%)   | 46          | 46 |
| 2   | F     | 368/391 (94%) | 352 (96%) | 15 (4%) | 1 (0%)   | 46          | 46 |
| 2   | G     | 368/391 (94%) | 353 (96%) | 14 (4%) | 1 (0%)   | 46          | 46 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 2   | H     | 368/391 (94%)   | 353 (96%)  | 14 (4%)  | 1 (0%)   | 46          | 46 |
| 2   | I     | 368/391 (94%)   | 352 (96%)  | 15 (4%)  | 1 (0%)   | 46          | 46 |
| 2   | J     | 368/391 (94%)   | 353 (96%)  | 14 (4%)  | 1 (0%)   | 46          | 46 |
| 2   | K     | 368/391 (94%)   | 352 (96%)  | 15 (4%)  | 1 (0%)   | 46          | 46 |
| 2   | L     | 368/391 (94%)   | 353 (96%)  | 13 (4%)  | 2 (0%)   | 34          | 34 |
| 2   | M     | 368/391 (94%)   | 353 (96%)  | 12 (3%)  | 3 (1%)   | 24          | 24 |
| 2   | N     | 368/391 (94%)   | 352 (96%)  | 13 (4%)  | 3 (1%)   | 24          | 24 |
| 2   | O     | 368/391 (94%)   | 353 (96%)  | 12 (3%)  | 3 (1%)   | 24          | 24 |
| 2   | P     | 368/391 (94%)   | 352 (96%)  | 13 (4%)  | 3 (1%)   | 24          | 24 |
| 2   | Q     | 368/391 (94%)   | 352 (96%)  | 13 (4%)  | 3 (1%)   | 24          | 24 |
| 2   | R     | 368/391 (94%)   | 353 (96%)  | 12 (3%)  | 3 (1%)   | 24          | 24 |
| 2   | S     | 368/391 (94%)   | 352 (96%)  | 13 (4%)  | 3 (1%)   | 24          | 24 |
| 2   | T     | 368/391 (94%)   | 353 (96%)  | 12 (3%)  | 3 (1%)   | 24          | 24 |
| 2   | U     | 368/391 (94%)   | 353 (96%)  | 12 (3%)  | 3 (1%)   | 24          | 24 |
| 2   | V     | 368/391 (94%)   | 352 (96%)  | 13 (4%)  | 3 (1%)   | 24          | 24 |
| 2   | W     | 368/391 (94%)   | 353 (96%)  | 12 (3%)  | 3 (1%)   | 24          | 24 |
| 2   | X     | 368/391 (94%)   | 352 (96%)  | 13 (4%)  | 3 (1%)   | 24          | 24 |
| All | All   | 8464/8993 (94%) | 8109 (96%) | 307 (4%) | 48 (1%)  | 34          | 30 |

All (48) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 360 | ASN  |
| 2   | O     | 360 | ASN  |
| 2   | P     | 360 | ASN  |
| 2   | R     | 360 | ASN  |
| 2   | U     | 360 | ASN  |
| 2   | W     | 360 | ASN  |
| 2   | X     | 360 | ASN  |
| 2   | M     | 361 | GLY  |
| 2   | O     | 361 | GLY  |
| 2   | P     | 361 | GLY  |
| 2   | R     | 361 | GLY  |
| 2   | S     | 360 | ASN  |
| 2   | S     | 361 | GLY  |
| 2   | T     | 360 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | W     | 361 | GLY  |
| 2   | X     | 361 | GLY  |
| 2   | N     | 360 | ASN  |
| 2   | N     | 361 | GLY  |
| 2   | Q     | 360 | ASN  |
| 2   | Q     | 361 | GLY  |
| 2   | T     | 361 | GLY  |
| 2   | U     | 361 | GLY  |
| 2   | V     | 360 | ASN  |
| 2   | V     | 361 | GLY  |
| 2   | L     | 361 | GLY  |
| 2   | C     | 6   | VAL  |
| 2   | D     | 6   | VAL  |
| 2   | E     | 6   | VAL  |
| 2   | H     | 6   | VAL  |
| 2   | I     | 6   | VAL  |
| 2   | J     | 6   | VAL  |
| 2   | M     | 6   | VAL  |
| 2   | N     | 6   | VAL  |
| 2   | O     | 6   | VAL  |
| 2   | S     | 6   | VAL  |
| 2   | T     | 6   | VAL  |
| 2   | W     | 6   | VAL  |
| 2   | X     | 6   | VAL  |
| 2   | B     | 6   | VAL  |
| 2   | F     | 6   | VAL  |
| 2   | G     | 6   | VAL  |
| 2   | K     | 6   | VAL  |
| 2   | L     | 6   | VAL  |
| 2   | P     | 6   | VAL  |
| 2   | Q     | 6   | VAL  |
| 2   | R     | 6   | VAL  |
| 2   | U     | 6   | VAL  |
| 2   | V     | 6   | VAL  |

### 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 |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 2   | B     | 309/328 (94%)   | 296 (96%)  | 13 (4%)  | 36          | 36 |
| 2   | C     | 309/328 (94%)   | 296 (96%)  | 13 (4%)  | 36          | 36 |
| 2   | D     | 309/328 (94%)   | 296 (96%)  | 13 (4%)  | 36          | 36 |
| 2   | E     | 309/328 (94%)   | 295 (96%)  | 14 (4%)  | 34          | 34 |
| 2   | F     | 309/328 (94%)   | 297 (96%)  | 12 (4%)  | 39          | 39 |
| 2   | G     | 309/328 (94%)   | 296 (96%)  | 13 (4%)  | 36          | 36 |
| 2   | H     | 309/328 (94%)   | 296 (96%)  | 13 (4%)  | 36          | 36 |
| 2   | I     | 309/328 (94%)   | 296 (96%)  | 13 (4%)  | 36          | 36 |
| 2   | J     | 309/328 (94%)   | 295 (96%)  | 14 (4%)  | 34          | 34 |
| 2   | K     | 309/328 (94%)   | 297 (96%)  | 12 (4%)  | 39          | 39 |
| 2   | L     | 309/328 (94%)   | 297 (96%)  | 12 (4%)  | 39          | 39 |
| 2   | M     | 309/328 (94%)   | 295 (96%)  | 14 (4%)  | 34          | 34 |
| 2   | N     | 309/328 (94%)   | 297 (96%)  | 12 (4%)  | 39          | 39 |
| 2   | O     | 309/328 (94%)   | 296 (96%)  | 13 (4%)  | 36          | 36 |
| 2   | P     | 309/328 (94%)   | 296 (96%)  | 13 (4%)  | 36          | 36 |
| 2   | Q     | 309/328 (94%)   | 297 (96%)  | 12 (4%)  | 39          | 39 |
| 2   | R     | 309/328 (94%)   | 295 (96%)  | 14 (4%)  | 34          | 34 |
| 2   | S     | 309/328 (94%)   | 296 (96%)  | 13 (4%)  | 36          | 36 |
| 2   | T     | 309/328 (94%)   | 296 (96%)  | 13 (4%)  | 36          | 36 |
| 2   | U     | 309/328 (94%)   | 295 (96%)  | 14 (4%)  | 34          | 34 |
| 2   | V     | 309/328 (94%)   | 297 (96%)  | 12 (4%)  | 39          | 39 |
| 2   | W     | 309/328 (94%)   | 295 (96%)  | 14 (4%)  | 34          | 34 |
| 2   | X     | 309/328 (94%)   | 296 (96%)  | 13 (4%)  | 36          | 36 |
| All | All   | 7107/7544 (94%) | 6808 (96%) | 299 (4%) | 41          | 36 |

All (299) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 3   | LEU  |
| 2   | B     | 9   | ASN  |
| 2   | B     | 29  | THR  |
| 2   | B     | 83  | LEU  |
| 2   | B     | 123 | ILE  |
| 2   | B     | 136 | LYS  |
| 2   | B     | 163 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 168 | ILE  |
| 2   | B     | 220 | ILE  |
| 2   | B     | 272 | LEU  |
| 2   | B     | 287 | VAL  |
| 2   | B     | 325 | LEU  |
| 2   | B     | 331 | LEU  |
| 2   | C     | 3   | LEU  |
| 2   | C     | 9   | ASN  |
| 2   | C     | 29  | THR  |
| 2   | C     | 83  | LEU  |
| 2   | C     | 136 | LYS  |
| 2   | C     | 163 | ILE  |
| 2   | C     | 168 | ILE  |
| 2   | C     | 220 | ILE  |
| 2   | C     | 272 | LEU  |
| 2   | C     | 287 | VAL  |
| 2   | C     | 301 | TYR  |
| 2   | C     | 325 | LEU  |
| 2   | C     | 331 | LEU  |
| 2   | D     | 3   | LEU  |
| 2   | D     | 9   | ASN  |
| 2   | D     | 29  | THR  |
| 2   | D     | 83  | LEU  |
| 2   | D     | 123 | ILE  |
| 2   | D     | 136 | LYS  |
| 2   | D     | 163 | ILE  |
| 2   | D     | 168 | ILE  |
| 2   | D     | 220 | ILE  |
| 2   | D     | 272 | LEU  |
| 2   | D     | 287 | VAL  |
| 2   | D     | 325 | LEU  |
| 2   | D     | 331 | LEU  |
| 2   | E     | 3   | LEU  |
| 2   | E     | 9   | ASN  |
| 2   | E     | 29  | THR  |
| 2   | E     | 83  | LEU  |
| 2   | E     | 123 | ILE  |
| 2   | E     | 136 | LYS  |
| 2   | E     | 163 | ILE  |
| 2   | E     | 168 | ILE  |
| 2   | E     | 220 | ILE  |
| 2   | E     | 272 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 287 | VAL  |
| 2   | E     | 301 | TYR  |
| 2   | E     | 325 | LEU  |
| 2   | E     | 331 | LEU  |
| 2   | F     | 3   | LEU  |
| 2   | F     | 9   | ASN  |
| 2   | F     | 29  | THR  |
| 2   | F     | 83  | LEU  |
| 2   | F     | 123 | ILE  |
| 2   | F     | 136 | LYS  |
| 2   | F     | 163 | ILE  |
| 2   | F     | 220 | ILE  |
| 2   | F     | 272 | LEU  |
| 2   | F     | 287 | VAL  |
| 2   | F     | 325 | LEU  |
| 2   | F     | 331 | LEU  |
| 2   | G     | 3   | LEU  |
| 2   | G     | 9   | ASN  |
| 2   | G     | 29  | THR  |
| 2   | G     | 83  | LEU  |
| 2   | G     | 123 | ILE  |
| 2   | G     | 136 | LYS  |
| 2   | G     | 163 | ILE  |
| 2   | G     | 168 | ILE  |
| 2   | G     | 220 | ILE  |
| 2   | G     | 272 | LEU  |
| 2   | G     | 287 | VAL  |
| 2   | G     | 325 | LEU  |
| 2   | G     | 331 | LEU  |
| 2   | H     | 3   | LEU  |
| 2   | H     | 9   | ASN  |
| 2   | H     | 29  | THR  |
| 2   | H     | 83  | LEU  |
| 2   | H     | 136 | LYS  |
| 2   | H     | 163 | ILE  |
| 2   | H     | 168 | ILE  |
| 2   | H     | 220 | ILE  |
| 2   | H     | 272 | LEU  |
| 2   | H     | 287 | VAL  |
| 2   | H     | 301 | TYR  |
| 2   | H     | 325 | LEU  |
| 2   | H     | 331 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | I     | 3   | LEU  |
| 2   | I     | 9   | ASN  |
| 2   | I     | 29  | THR  |
| 2   | I     | 83  | LEU  |
| 2   | I     | 123 | ILE  |
| 2   | I     | 136 | LYS  |
| 2   | I     | 163 | ILE  |
| 2   | I     | 168 | ILE  |
| 2   | I     | 220 | ILE  |
| 2   | I     | 272 | LEU  |
| 2   | I     | 287 | VAL  |
| 2   | I     | 325 | LEU  |
| 2   | I     | 331 | LEU  |
| 2   | J     | 3   | LEU  |
| 2   | J     | 9   | ASN  |
| 2   | J     | 29  | THR  |
| 2   | J     | 83  | LEU  |
| 2   | J     | 123 | ILE  |
| 2   | J     | 136 | LYS  |
| 2   | J     | 163 | ILE  |
| 2   | J     | 168 | ILE  |
| 2   | J     | 220 | ILE  |
| 2   | J     | 272 | LEU  |
| 2   | J     | 287 | VAL  |
| 2   | J     | 301 | TYR  |
| 2   | J     | 325 | LEU  |
| 2   | J     | 331 | LEU  |
| 2   | K     | 3   | LEU  |
| 2   | K     | 9   | ASN  |
| 2   | K     | 29  | THR  |
| 2   | K     | 83  | LEU  |
| 2   | K     | 123 | ILE  |
| 2   | K     | 136 | LYS  |
| 2   | K     | 163 | ILE  |
| 2   | K     | 220 | ILE  |
| 2   | K     | 272 | LEU  |
| 2   | K     | 287 | VAL  |
| 2   | K     | 325 | LEU  |
| 2   | K     | 331 | LEU  |
| 2   | L     | 3   | LEU  |
| 2   | L     | 9   | ASN  |
| 2   | L     | 29  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 83  | LEU  |
| 2   | L     | 123 | ILE  |
| 2   | L     | 136 | LYS  |
| 2   | L     | 163 | ILE  |
| 2   | L     | 220 | ILE  |
| 2   | L     | 272 | LEU  |
| 2   | L     | 287 | VAL  |
| 2   | L     | 325 | LEU  |
| 2   | L     | 331 | LEU  |
| 2   | M     | 3   | LEU  |
| 2   | M     | 9   | ASN  |
| 2   | M     | 29  | THR  |
| 2   | M     | 83  | LEU  |
| 2   | M     | 123 | ILE  |
| 2   | M     | 136 | LYS  |
| 2   | M     | 163 | ILE  |
| 2   | M     | 168 | ILE  |
| 2   | M     | 220 | ILE  |
| 2   | M     | 272 | LEU  |
| 2   | M     | 287 | VAL  |
| 2   | M     | 301 | TYR  |
| 2   | M     | 325 | LEU  |
| 2   | M     | 331 | LEU  |
| 2   | N     | 3   | LEU  |
| 2   | N     | 9   | ASN  |
| 2   | N     | 29  | THR  |
| 2   | N     | 83  | LEU  |
| 2   | N     | 136 | LYS  |
| 2   | N     | 163 | ILE  |
| 2   | N     | 168 | ILE  |
| 2   | N     | 220 | ILE  |
| 2   | N     | 272 | LEU  |
| 2   | N     | 287 | VAL  |
| 2   | N     | 325 | LEU  |
| 2   | N     | 331 | LEU  |
| 2   | O     | 3   | LEU  |
| 2   | O     | 9   | ASN  |
| 2   | O     | 29  | THR  |
| 2   | O     | 83  | LEU  |
| 2   | O     | 123 | ILE  |
| 2   | O     | 136 | LYS  |
| 2   | O     | 163 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 168 | ILE  |
| 2   | O     | 220 | ILE  |
| 2   | O     | 272 | LEU  |
| 2   | O     | 287 | VAL  |
| 2   | O     | 325 | LEU  |
| 2   | O     | 331 | LEU  |
| 2   | P     | 3   | LEU  |
| 2   | P     | 9   | ASN  |
| 2   | P     | 29  | THR  |
| 2   | P     | 83  | LEU  |
| 2   | P     | 123 | ILE  |
| 2   | P     | 136 | LYS  |
| 2   | P     | 163 | ILE  |
| 2   | P     | 168 | ILE  |
| 2   | P     | 220 | ILE  |
| 2   | P     | 272 | LEU  |
| 2   | P     | 287 | VAL  |
| 2   | P     | 325 | LEU  |
| 2   | P     | 331 | LEU  |
| 2   | Q     | 3   | LEU  |
| 2   | Q     | 9   | ASN  |
| 2   | Q     | 29  | THR  |
| 2   | Q     | 83  | LEU  |
| 2   | Q     | 123 | ILE  |
| 2   | Q     | 136 | LYS  |
| 2   | Q     | 163 | ILE  |
| 2   | Q     | 220 | ILE  |
| 2   | Q     | 272 | LEU  |
| 2   | Q     | 287 | VAL  |
| 2   | Q     | 325 | LEU  |
| 2   | Q     | 331 | LEU  |
| 2   | R     | 3   | LEU  |
| 2   | R     | 9   | ASN  |
| 2   | R     | 29  | THR  |
| 2   | R     | 83  | LEU  |
| 2   | R     | 123 | ILE  |
| 2   | R     | 136 | LYS  |
| 2   | R     | 163 | ILE  |
| 2   | R     | 168 | ILE  |
| 2   | R     | 220 | ILE  |
| 2   | R     | 272 | LEU  |
| 2   | R     | 287 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | R     | 301 | TYR  |
| 2   | R     | 325 | LEU  |
| 2   | R     | 331 | LEU  |
| 2   | S     | 3   | LEU  |
| 2   | S     | 9   | ASN  |
| 2   | S     | 29  | THR  |
| 2   | S     | 83  | LEU  |
| 2   | S     | 123 | ILE  |
| 2   | S     | 136 | LYS  |
| 2   | S     | 163 | ILE  |
| 2   | S     | 168 | ILE  |
| 2   | S     | 220 | ILE  |
| 2   | S     | 272 | LEU  |
| 2   | S     | 287 | VAL  |
| 2   | S     | 325 | LEU  |
| 2   | S     | 331 | LEU  |
| 2   | T     | 3   | LEU  |
| 2   | T     | 9   | ASN  |
| 2   | T     | 29  | THR  |
| 2   | T     | 83  | LEU  |
| 2   | T     | 123 | ILE  |
| 2   | T     | 136 | LYS  |
| 2   | T     | 163 | ILE  |
| 2   | T     | 168 | ILE  |
| 2   | T     | 220 | ILE  |
| 2   | T     | 272 | LEU  |
| 2   | T     | 287 | VAL  |
| 2   | T     | 325 | LEU  |
| 2   | T     | 331 | LEU  |
| 2   | U     | 3   | LEU  |
| 2   | U     | 9   | ASN  |
| 2   | U     | 29  | THR  |
| 2   | U     | 83  | LEU  |
| 2   | U     | 123 | ILE  |
| 2   | U     | 136 | LYS  |
| 2   | U     | 163 | ILE  |
| 2   | U     | 168 | ILE  |
| 2   | U     | 220 | ILE  |
| 2   | U     | 272 | LEU  |
| 2   | U     | 287 | VAL  |
| 2   | U     | 301 | TYR  |
| 2   | U     | 325 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | U     | 331 | LEU  |
| 2   | V     | 3   | LEU  |
| 2   | V     | 9   | ASN  |
| 2   | V     | 29  | THR  |
| 2   | V     | 83  | LEU  |
| 2   | V     | 123 | ILE  |
| 2   | V     | 136 | LYS  |
| 2   | V     | 163 | ILE  |
| 2   | V     | 220 | ILE  |
| 2   | V     | 272 | LEU  |
| 2   | V     | 287 | VAL  |
| 2   | V     | 325 | LEU  |
| 2   | V     | 331 | LEU  |
| 2   | W     | 3   | LEU  |
| 2   | W     | 9   | ASN  |
| 2   | W     | 29  | THR  |
| 2   | W     | 83  | LEU  |
| 2   | W     | 123 | ILE  |
| 2   | W     | 136 | LYS  |
| 2   | W     | 163 | ILE  |
| 2   | W     | 168 | ILE  |
| 2   | W     | 220 | ILE  |
| 2   | W     | 272 | LEU  |
| 2   | W     | 287 | VAL  |
| 2   | W     | 301 | TYR  |
| 2   | W     | 325 | LEU  |
| 2   | W     | 331 | LEU  |
| 2   | X     | 3   | LEU  |
| 2   | X     | 9   | ASN  |
| 2   | X     | 29  | THR  |
| 2   | X     | 83  | LEU  |
| 2   | X     | 123 | ILE  |
| 2   | X     | 136 | LYS  |
| 2   | X     | 163 | ILE  |
| 2   | X     | 168 | ILE  |
| 2   | X     | 220 | ILE  |
| 2   | X     | 272 | LEU  |
| 2   | X     | 287 | VAL  |
| 2   | X     | 325 | LEU  |
| 2   | X     | 331 | LEU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 26  | GLN  |
| 2   | B     | 59  | HIS  |
| 2   | B     | 187 | ASN  |
| 2   | B     | 274 | HIS  |
| 2   | B     | 327 | ASN  |
| 2   | C     | 26  | GLN  |
| 2   | C     | 59  | HIS  |
| 2   | C     | 274 | HIS  |
| 2   | C     | 327 | ASN  |
| 2   | D     | 26  | GLN  |
| 2   | D     | 59  | HIS  |
| 2   | D     | 274 | HIS  |
| 2   | D     | 327 | ASN  |
| 2   | E     | 26  | GLN  |
| 2   | E     | 59  | HIS  |
| 2   | E     | 274 | HIS  |
| 2   | E     | 327 | ASN  |
| 2   | F     | 26  | GLN  |
| 2   | F     | 59  | HIS  |
| 2   | F     | 274 | HIS  |
| 2   | F     | 327 | ASN  |
| 2   | G     | 26  | GLN  |
| 2   | G     | 59  | HIS  |
| 2   | G     | 274 | HIS  |
| 2   | G     | 327 | ASN  |
| 2   | H     | 26  | GLN  |
| 2   | H     | 59  | HIS  |
| 2   | H     | 274 | HIS  |
| 2   | H     | 327 | ASN  |
| 2   | I     | 26  | GLN  |
| 2   | I     | 59  | HIS  |
| 2   | I     | 274 | HIS  |
| 2   | I     | 327 | ASN  |
| 2   | J     | 26  | GLN  |
| 2   | J     | 59  | HIS  |
| 2   | J     | 274 | HIS  |
| 2   | J     | 327 | ASN  |
| 2   | K     | 26  | GLN  |
| 2   | K     | 59  | HIS  |
| 2   | K     | 274 | HIS  |
| 2   | K     | 327 | ASN  |
| 2   | L     | 26  | GLN  |
| 2   | L     | 59  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 274 | HIS  |
| 2   | L     | 327 | ASN  |
| 2   | M     | 26  | GLN  |
| 2   | M     | 59  | HIS  |
| 2   | M     | 274 | HIS  |
| 2   | M     | 327 | ASN  |
| 2   | N     | 26  | GLN  |
| 2   | N     | 59  | HIS  |
| 2   | N     | 274 | HIS  |
| 2   | N     | 327 | ASN  |
| 2   | O     | 26  | GLN  |
| 2   | O     | 59  | HIS  |
| 2   | O     | 274 | HIS  |
| 2   | O     | 327 | ASN  |
| 2   | P     | 26  | GLN  |
| 2   | P     | 59  | HIS  |
| 2   | P     | 274 | HIS  |
| 2   | P     | 327 | ASN  |
| 2   | Q     | 26  | GLN  |
| 2   | Q     | 59  | HIS  |
| 2   | Q     | 274 | HIS  |
| 2   | Q     | 327 | ASN  |
| 2   | R     | 26  | GLN  |
| 2   | R     | 59  | HIS  |
| 2   | R     | 274 | HIS  |
| 2   | R     | 327 | ASN  |
| 2   | S     | 26  | GLN  |
| 2   | S     | 59  | HIS  |
| 2   | S     | 274 | HIS  |
| 2   | S     | 327 | ASN  |
| 2   | T     | 26  | GLN  |
| 2   | T     | 59  | HIS  |
| 2   | T     | 274 | HIS  |
| 2   | T     | 327 | ASN  |
| 2   | U     | 26  | GLN  |
| 2   | U     | 59  | HIS  |
| 2   | U     | 274 | HIS  |
| 2   | U     | 327 | ASN  |
| 2   | V     | 26  | GLN  |
| 2   | V     | 59  | HIS  |
| 2   | V     | 274 | HIS  |
| 2   | V     | 327 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | W     | 26  | GLN  |
| 2   | W     | 59  | HIS  |
| 2   | W     | 274 | HIS  |
| 2   | W     | 327 | ASN  |
| 2   | X     | 59  | HIS  |
| 2   | X     | 274 | HIS  |
| 2   | X     | 327 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed      | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 1   | A     | 160/161 (99%) | 22 (13%)          | 0               |

All (22) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | C    |
| 1   | A     | 21  | C    |
| 1   | A     | 31  | C    |
| 1   | A     | 41  | C    |
| 1   | A     | 51  | C    |
| 1   | A     | 61  | C    |
| 1   | A     | 71  | C    |
| 1   | A     | 81  | C    |
| 1   | A     | 91  | C    |
| 1   | A     | 101 | C    |
| 1   | A     | 111 | C    |
| 1   | A     | 121 | C    |
| 1   | A     | 131 | C    |
| 1   | A     | 141 | C    |
| 1   | A     | 151 | C    |
| 1   | A     | 161 | C    |
| 1   | A     | 171 | C    |
| 1   | A     | 181 | C    |
| 1   | A     | 191 | C    |
| 1   | A     | 201 | C    |
| 1   | A     | 211 | C    |
| 1   | A     | 221 | C    |

There are no RNA pucker outliers to report.

## 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 carbohydrates 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.