



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:59 AM UTC

PDB ID : 7LRG / pdb\_00007lrg  
EMDB ID : EMD-23497  
Title : Filamentous actin decorated with human cardiac myosin binding protein C C2 domain  
Authors : Galkin, V.E.  
Deposited on : 2021-02-16  
Resolution : 6.10 Å (reported)  
Based on initial models : 5K6P, 7JH7

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>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

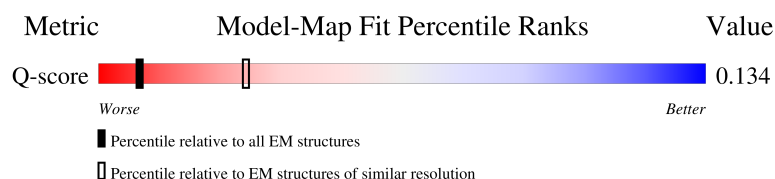
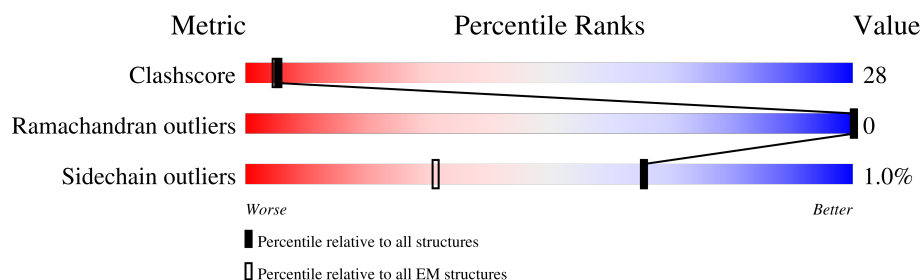
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 6.10 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) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 531 ( 5.60 - 6.60 )                                      |

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 377    |  |
| 1   | B     | 377    |  |
| 1   | C     | 377    |  |
| 1   | D     | 377    |  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain                                                              |
|-----|-------|--------|-------------------------------------------------------------------------------|
| 1   | E     | 377    | <div><div></div><div>77%</div><div>21%</div><div></div></div>                 |
| 1   | F     | 377    | <div><div></div><div>78%</div><div>21%</div><div></div></div>                 |
| 2   | G     | 94     | <div><div>20%</div><div>24%</div><div>67%</div><div>6%</div><div></div></div> |
| 2   | H     | 94     | <div><div>20%</div><div>24%</div><div>67%</div><div>6%</div><div></div></div> |
| 2   | I     | 94     | <div><div>18%</div><div>24%</div><div>67%</div><div>6%</div><div></div></div> |
| 2   | J     | 94     | <div><div>19%</div><div>23%</div><div>69%</div><div>5%</div><div></div></div> |
| 2   | K     | 94     | <div><div>19%</div><div>24%</div><div>68%</div><div>5%</div><div></div></div> |
| 2   | L     | 94     | <div><div>19%</div><div>24%</div><div>67%</div><div>6%</div><div></div></div> |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 26256 atoms, of which 4428 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 Actin, alpha cardiac muscle 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 371      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2903  | 1840 | 489 | 553 | 21 |         |       |
| 1   | B     | 371      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2903  | 1840 | 489 | 553 | 21 |         |       |
| 1   | C     | 371      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2903  | 1840 | 489 | 553 | 21 |         |       |
| 1   | D     | 371      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2903  | 1840 | 489 | 553 | 21 |         |       |
| 1   | E     | 371      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2903  | 1840 | 489 | 553 | 21 |         |       |
| 1   | F     | 371      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2903  | 1840 | 489 | 553 | 21 |         |       |

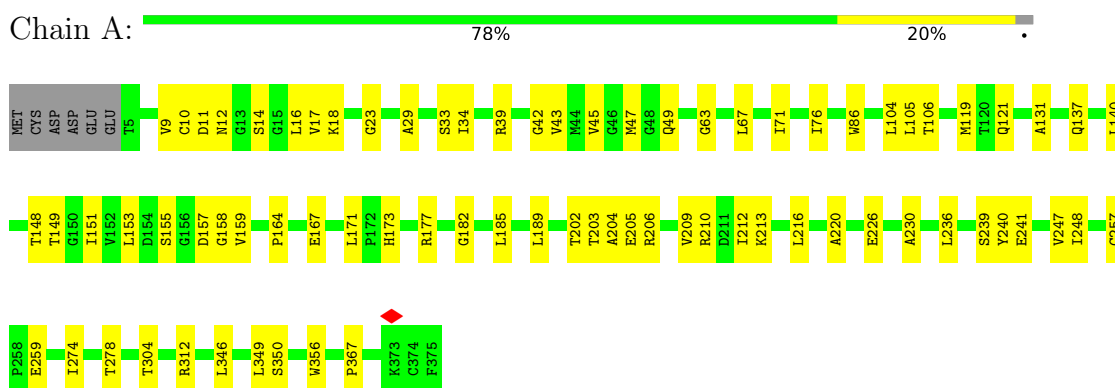
- Molecule 2 is a protein called Myosin-binding protein C, cardiac-type.

| Mol | Chain | Residues | Atoms         |          |          |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|----------|--------|---------|-------|
| 2   | G     | 94       | Total<br>1473 | C<br>461 | H<br>738 | N<br>124 | O<br>146 | S<br>4 | 0       | 0     |
| 2   | H     | 94       | Total<br>1473 | C<br>461 | H<br>738 | N<br>124 | O<br>146 | S<br>4 | 0       | 0     |
| 2   | I     | 94       | Total<br>1473 | C<br>461 | H<br>738 | N<br>124 | O<br>146 | S<br>4 | 0       | 0     |
| 2   | J     | 94       | Total<br>1473 | C<br>461 | H<br>738 | N<br>124 | O<br>146 | S<br>4 | 0       | 0     |
| 2   | K     | 94       | Total<br>1473 | C<br>461 | H<br>738 | N<br>124 | O<br>146 | S<br>4 | 0       | 0     |
| 2   | L     | 94       | Total<br>1473 | C<br>461 | H<br>738 | N<br>124 | O<br>146 | S<br>4 | 0       | 0     |

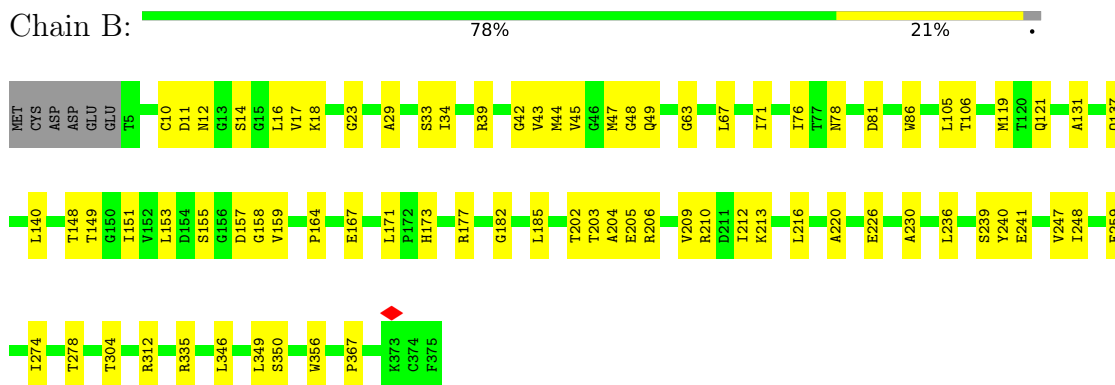
### 3 Residue-property plots

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

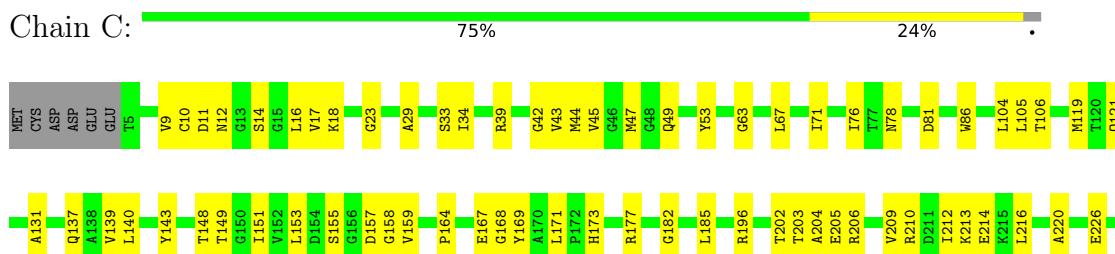
#### • Molecule 1: Actin, alpha cardiac muscle 1



#### • Molecule 1: Actin, alpha cardiac muscle 1



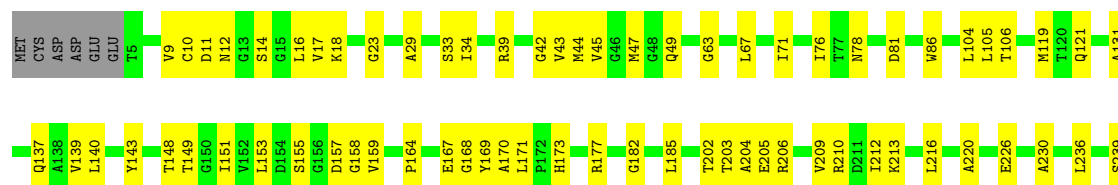
#### • Molecule 1: Actin, alpha cardiac muscle 1





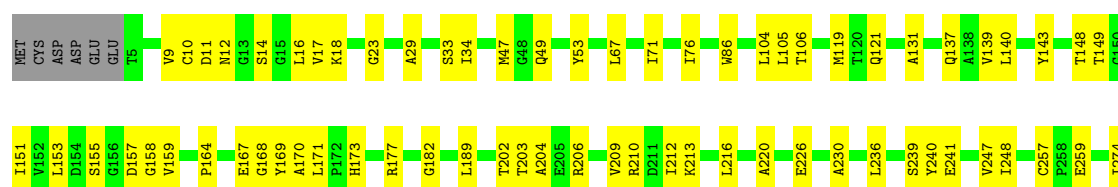
- Molecule 1: Actin, alpha cardiac muscle 1

Chain D: 75% 23%



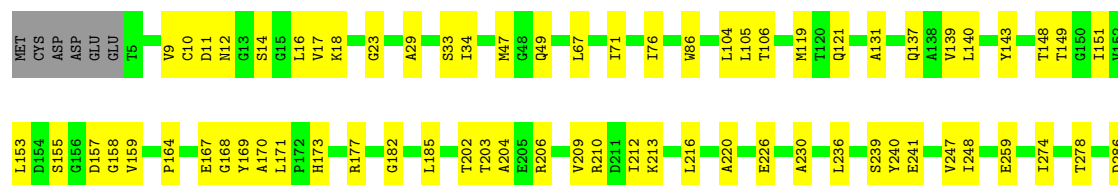
- Molecule 1: Actin, alpha cardiac muscle 1

Chain E: 77% 21%



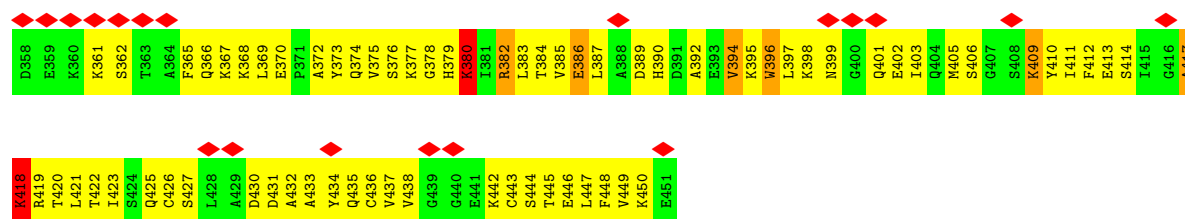
- Molecule 1: Actin, alpha cardiac muscle 1

Chain F: 78% 21%

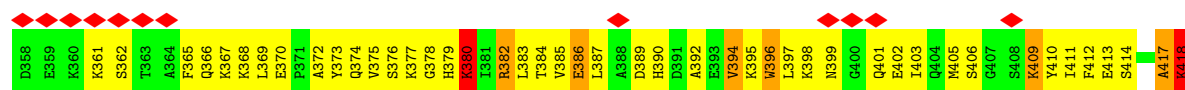


- Molecule 2: Myosin-binding protein C, cardiac-type

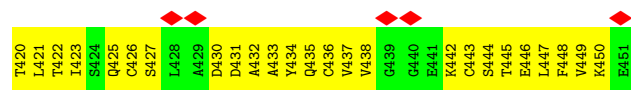
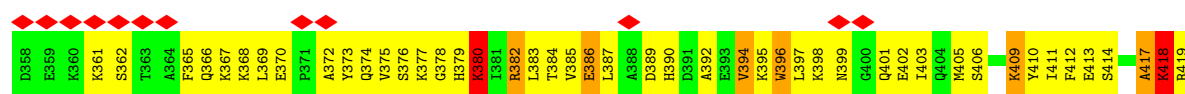
Chain G: 20% 24% 67% 6%



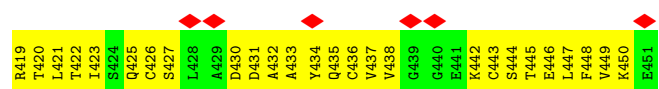
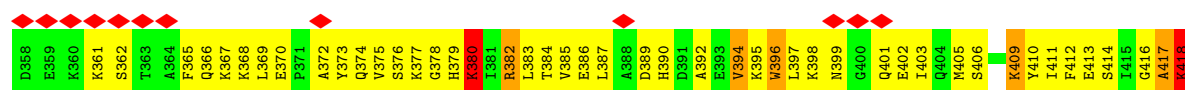
• Molecule 2: Myosin-binding protein C, cardiac-type



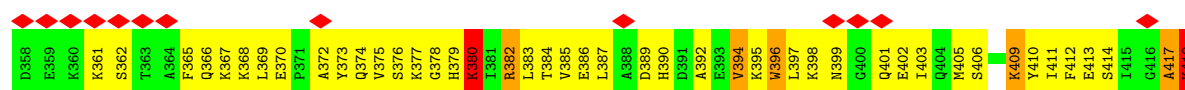
• Molecule 2: Myosin-binding protein C, cardiac-type

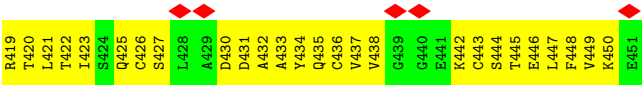


• Molecule 2: Myosin-binding protein C, cardiac-type

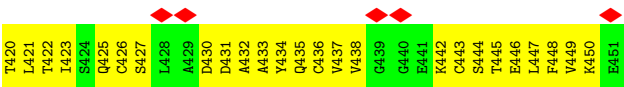
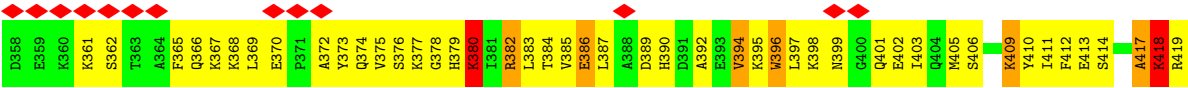


• Molecule 2: Myosin-binding protein C, cardiac-type





• Molecule 2: Myosin-binding protein C, cardiac-type



## 4 Experimental information

| Property                           | Value                                             | Source    |
|------------------------------------|---------------------------------------------------|-----------|
| EM reconstruction method           | HELICAL                                           | Depositor |
| Imposed symmetry                   | HELICAL, twist=-166.5°, rise=27.3 Å, axial sym=C1 | Depositor |
| Number of segments used            | 43047                                             | Depositor |
| Resolution determination method    | FSC 0.143 CUT-OFF                                 | Depositor |
| CTF correction method              | PHASE FLIPPING AND AMPLITUDE CORRECTION           | Depositor |
| Microscope                         | FEI TITAN KRIOS                                   | Depositor |
| Voltage (kV)                       | 300                                               | Depositor |
| Electron dose ( $e^-/\text{Å}^2$ ) | 35                                                | Depositor |
| Minimum defocus (nm)               | Not provided                                      |           |
| Maximum defocus (nm)               | Not provided                                      |           |
| Magnification                      | Not provided                                      |           |
| Image detector                     | GATAN K3 (6k x 4k)                                | Depositor |
| Maximum map value                  | 11.255                                            | Depositor |
| Minimum map value                  | -3.586                                            | Depositor |
| Average map value                  | -0.000                                            | Depositor |
| Map value standard deviation       | 1.000                                             | Depositor |
| Recommended contour level          | 0.75                                              | Depositor |
| Map size (Å)                       | 116.64001, 118.8, 276.48                          | wwPDB     |
| Map dimensions                     | 108, 110, 256                                     | wwPDB     |
| Map angles (°)                     | 90.0, 90.0, 90.0                                  | wwPDB     |
| Pixel spacing (Å)                  | 1.08, 1.08, 1.08                                  | 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     | 0.31         | 0/2969      | 0.56        | 0/4021          |
| 1   | B     | 0.31         | 0/2969      | 0.55        | 0/4021          |
| 1   | C     | 0.31         | 0/2969      | 0.56        | 0/4021          |
| 1   | D     | 0.31         | 0/2969      | 0.55        | 0/4021          |
| 1   | E     | 0.31         | 0/2969      | 0.56        | 0/4021          |
| 1   | F     | 0.31         | 0/2969      | 0.56        | 0/4021          |
| 2   | G     | 0.40         | 0/745       | 0.99        | 7/996 (0.7%)    |
| 2   | H     | 0.40         | 0/745       | 0.99        | 7/996 (0.7%)    |
| 2   | I     | 0.40         | 0/745       | 0.99        | 7/996 (0.7%)    |
| 2   | J     | 0.40         | 0/745       | 0.98        | 6/996 (0.6%)    |
| 2   | K     | 0.40         | 0/745       | 0.99        | 6/996 (0.6%)    |
| 2   | L     | 0.40         | 0/745       | 1.00        | 7/996 (0.7%)    |
| All | All   | 0.33         | 0/22284     | 0.67        | 40/30102 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | G     | 0                   | 2                   |
| 2   | H     | 0                   | 2                   |
| 2   | I     | 0                   | 2                   |
| 2   | J     | 0                   | 2                   |
| 2   | K     | 0                   | 2                   |
| 2   | L     | 0                   | 2                   |
| All | All   | 0                   | 12                  |

There are no bond length outliers.

All (40) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | K     | 396 | TRP  | N-CA-C | -7.17 | 96.83       | 108.52   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | I     | 396 | TRP  | N-CA-C   | -7.14 | 96.89       | 108.52   |
| 2   | G     | 396 | TRP  | N-CA-C   | -7.13 | 96.89       | 108.52   |
| 2   | L     | 396 | TRP  | N-CA-C   | -7.12 | 96.92       | 108.52   |
| 2   | H     | 396 | TRP  | N-CA-C   | -7.12 | 96.92       | 108.52   |
| 2   | H     | 380 | LYS  | CG-CD-CE | 6.28  | 125.73      | 111.30   |
| 2   | J     | 380 | LYS  | CG-CD-CE | 6.27  | 125.72      | 111.30   |
| 2   | G     | 380 | LYS  | CG-CD-CE | 6.26  | 125.70      | 111.30   |
| 2   | L     | 380 | LYS  | CG-CD-CE | 6.25  | 125.67      | 111.30   |
| 2   | K     | 380 | LYS  | CG-CD-CE | 6.24  | 125.65      | 111.30   |
| 2   | I     | 380 | LYS  | CG-CD-CE | 6.22  | 125.60      | 111.30   |
| 2   | J     | 382 | ARG  | CA-C-N   | 6.05  | 129.46      | 120.87   |
| 2   | J     | 382 | ARG  | C-N-CA   | 6.05  | 129.46      | 120.87   |
| 2   | H     | 382 | ARG  | CA-C-N   | 6.03  | 129.43      | 120.87   |
| 2   | H     | 382 | ARG  | C-N-CA   | 6.03  | 129.43      | 120.87   |
| 2   | L     | 382 | ARG  | CA-C-N   | 6.03  | 129.43      | 120.87   |
| 2   | L     | 382 | ARG  | C-N-CA   | 6.03  | 129.43      | 120.87   |
| 2   | I     | 382 | ARG  | CA-C-N   | 6.03  | 129.43      | 120.87   |
| 2   | I     | 382 | ARG  | C-N-CA   | 6.03  | 129.43      | 120.87   |
| 2   | K     | 382 | ARG  | CA-C-N   | 6.03  | 129.43      | 120.87   |
| 2   | K     | 382 | ARG  | C-N-CA   | 6.03  | 129.43      | 120.87   |
| 2   | J     | 396 | TRP  | N-CA-C   | -6.02 | 97.91       | 108.20   |
| 2   | G     | 382 | ARG  | CA-C-N   | 6.01  | 129.40      | 120.87   |
| 2   | G     | 382 | ARG  | C-N-CA   | 6.01  | 129.40      | 120.87   |
| 2   | J     | 418 | LYS  | CG-CD-CE | -6.00 | 97.50       | 111.30   |
| 2   | I     | 418 | LYS  | CG-CD-CE | -6.00 | 97.51       | 111.30   |
| 2   | K     | 418 | LYS  | CG-CD-CE | -5.99 | 97.52       | 111.30   |
| 2   | H     | 418 | LYS  | CG-CD-CE | -5.97 | 97.56       | 111.30   |
| 2   | L     | 418 | LYS  | CG-CD-CE | -5.97 | 97.56       | 111.30   |
| 2   | G     | 418 | LYS  | CG-CD-CE | -5.97 | 97.57       | 111.30   |
| 2   | L     | 418 | LYS  | CB-CG-CD | 5.29  | 123.46      | 111.30   |
| 2   | J     | 418 | LYS  | CB-CG-CD | 5.27  | 123.41      | 111.30   |
| 2   | H     | 418 | LYS  | CB-CG-CD | 5.27  | 123.41      | 111.30   |
| 2   | K     | 418 | LYS  | CB-CG-CD | 5.27  | 123.41      | 111.30   |
| 2   | G     | 418 | LYS  | CB-CG-CD | 5.26  | 123.41      | 111.30   |
| 2   | I     | 418 | LYS  | CB-CG-CD | 5.24  | 123.34      | 111.30   |
| 2   | G     | 386 | GLU  | N-CA-C   | -5.03 | 100.84      | 109.24   |
| 2   | L     | 386 | GLU  | N-CA-C   | -5.02 | 100.86      | 109.24   |
| 2   | H     | 386 | GLU  | N-CA-C   | -5.02 | 100.86      | 109.24   |
| 2   | I     | 386 | GLU  | N-CA-C   | -5.01 | 100.88      | 109.24   |

There are no chirality outliers.

All (12) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | G     | 394 | VAL  | Peptide |
| 2   | G     | 417 | ALA  | Peptide |
| 2   | H     | 394 | VAL  | Peptide |
| 2   | H     | 417 | ALA  | Peptide |
| 2   | I     | 394 | VAL  | Peptide |
| 2   | I     | 417 | ALA  | Peptide |
| 2   | J     | 394 | VAL  | Peptide |
| 2   | J     | 417 | ALA  | Peptide |
| 2   | K     | 394 | VAL  | Peptide |
| 2   | K     | 417 | ALA  | Peptide |
| 2   | L     | 394 | VAL  | Peptide |
| 2   | L     | 417 | ALA  | Peptide |

## 5.2 Too-close contacts [i](#)

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     | 2903  | 0        | 2880     | 78      | 0            |
| 1   | B     | 2903  | 0        | 2880     | 79      | 0            |
| 1   | C     | 2903  | 0        | 2880     | 105     | 0            |
| 1   | D     | 2903  | 0        | 2880     | 101     | 0            |
| 1   | E     | 2903  | 0        | 2880     | 80      | 0            |
| 1   | F     | 2903  | 0        | 2880     | 78      | 0            |
| 2   | G     | 735   | 738      | 737      | 143     | 0            |
| 2   | H     | 735   | 738      | 737      | 146     | 0            |
| 2   | I     | 735   | 738      | 737      | 148     | 0            |
| 2   | J     | 735   | 738      | 737      | 147     | 0            |
| 2   | K     | 735   | 738      | 737      | 146     | 0            |
| 2   | L     | 735   | 738      | 737      | 143     | 0            |
| All | All   | 21828 | 4428     | 21702    | 1222    | 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 28.

All (1222) 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:F:350:SER:HB2  | 2:L:382:ARG:NH1  | 1.25                     | 1.47              |
| 1:D:350:SER:HB2  | 2:J:382:ARG:NH1  | 1.33                     | 1.40              |
| 1:A:350:SER:HB2  | 2:G:382:ARG:NH1  | 1.38                     | 1.38              |
| 1:C:350:SER:HB2  | 2:I:382:ARG:NH1  | 1.39                     | 1.36              |
| 1:E:350:SER:HB2  | 2:K:382:ARG:NH1  | 1.40                     | 1.35              |
| 1:F:350:SER:CB   | 2:L:382:ARG:NH1  | 1.96                     | 1.26              |
| 1:B:350:SER:HB2  | 2:H:382:ARG:NH1  | 1.48                     | 1.26              |
| 1:D:350:SER:CB   | 2:J:382:ARG:NH1  | 2.03                     | 1.21              |
| 1:C:39:ARG:NH1   | 1:E:286:ASP:OD2  | 1.75                     | 1.20              |
| 1:C:350:SER:CB   | 2:I:382:ARG:NH1  | 2.05                     | 1.20              |
| 1:A:350:SER:CB   | 2:G:382:ARG:NH1  | 2.03                     | 1.19              |
| 1:B:39:ARG:NH1   | 1:D:286:ASP:OD2  | 1.75                     | 1.19              |
| 1:E:350:SER:CB   | 2:K:382:ARG:NH1  | 2.07                     | 1.17              |
| 1:F:350:SER:CB   | 2:L:382:ARG:HH11 | 1.56                     | 1.17              |
| 1:D:39:ARG:NH1   | 1:F:286:ASP:OD2  | 1.78                     | 1.16              |
| 1:B:23:GLY:HA3   | 2:H:425:GLN:HE22 | 1.05                     | 1.15              |
| 1:A:39:ARG:NH1   | 1:C:286:ASP:OD2  | 1.78                     | 1.15              |
| 1:D:23:GLY:HA3   | 2:J:425:GLN:HE22 | 1.08                     | 1.12              |
| 1:E:23:GLY:HA3   | 2:K:425:GLN:HE22 | 1.10                     | 1.11              |
| 1:D:350:SER:CB   | 2:J:382:ARG:HH11 | 1.63                     | 1.08              |
| 1:A:23:GLY:HA3   | 2:G:425:GLN:HE22 | 1.14                     | 1.08              |
| 1:B:350:SER:CB   | 2:H:382:ARG:NH1  | 2.15                     | 1.08              |
| 1:C:23:GLY:HA3   | 2:I:425:GLN:HE22 | 1.14                     | 1.05              |
| 1:E:17:VAL:HG23  | 1:E:33:SER:HB3   | 1.39                     | 1.05              |
| 1:B:17:VAL:HG23  | 1:B:33:SER:HB3   | 1.39                     | 1.04              |
| 1:A:17:VAL:HG23  | 1:A:33:SER:HB3   | 1.39                     | 1.04              |
| 1:D:17:VAL:HG23  | 1:D:33:SER:HB3   | 1.39                     | 1.04              |
| 1:C:17:VAL:HG23  | 1:C:33:SER:HB3   | 1.39                     | 1.04              |
| 1:F:17:VAL:HG23  | 1:F:33:SER:HB3   | 1.39                     | 1.03              |
| 1:F:23:GLY:HA3   | 2:L:425:GLN:HE22 | 1.18                     | 1.02              |
| 2:K:369:LEU:HD22 | 2:K:383:LEU:HD12 | 1.42                     | 1.01              |
| 1:B:43:VAL:HG11  | 1:D:139:VAL:HG21 | 1.42                     | 1.01              |
| 2:H:369:LEU:HD22 | 2:H:383:LEU:HD12 | 1.42                     | 1.01              |
| 2:I:369:LEU:HD22 | 2:I:383:LEU:HD12 | 1.42                     | 1.01              |
| 1:C:43:VAL:HG11  | 1:E:139:VAL:HG21 | 1.41                     | 1.00              |
| 1:E:350:SER:CB   | 2:K:382:ARG:HH11 | 1.70                     | 1.00              |
| 2:G:369:LEU:HD22 | 2:G:383:LEU:HD12 | 1.42                     | 1.00              |
| 1:B:349:LEU:HD22 | 2:H:413:GLU:OE2  | 1.62                     | 0.99              |
| 2:L:369:LEU:HD22 | 2:L:383:LEU:HD12 | 1.42                     | 0.99              |
| 2:J:369:LEU:HD22 | 2:J:383:LEU:HD12 | 1.42                     | 0.99              |
| 1:C:350:SER:CB   | 2:I:382:ARG:HH11 | 1.69                     | 0.98              |
| 1:D:43:VAL:HG11  | 1:F:139:VAL:HG21 | 1.44                     | 0.98              |

Continued on next page...

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:350:SER:CB   | 2:G:382:ARG:HH11 | 1.69                     | 0.97              |
| 1:D:23:GLY:HA3   | 2:J:425:GLN:NE2  | 1.81                     | 0.96              |
| 1:B:350:SER:CB   | 2:H:382:ARG:HH11 | 1.77                     | 0.95              |
| 1:B:350:SER:HB2  | 2:H:382:ARG:HH12 | 1.21                     | 0.95              |
| 1:B:42:GLY:HA2   | 1:D:169:TYR:HA   | 1.49                     | 0.95              |
| 1:A:43:VAL:HG11  | 1:C:139:VAL:HG21 | 1.46                     | 0.94              |
| 1:B:23:GLY:HA3   | 2:H:425:GLN:NE2  | 1.81                     | 0.94              |
| 1:D:42:GLY:HA2   | 1:F:169:TYR:HA   | 1.50                     | 0.93              |
| 1:D:205:GLU:HG2  | 1:F:287:ILE:HD11 | 1.52                     | 0.92              |
| 1:C:42:GLY:HA2   | 1:E:169:TYR:HA   | 1.49                     | 0.91              |
| 1:E:349:LEU:HD22 | 2:K:413:GLU:OE2  | 1.71                     | 0.90              |
| 1:B:349:LEU:HD22 | 2:H:413:GLU:CD   | 1.96                     | 0.90              |
| 1:C:205:GLU:HG2  | 1:E:287:ILE:HD11 | 1.52                     | 0.90              |
| 1:C:350:SER:HB2  | 2:I:382:ARG:HH12 | 1.07                     | 0.90              |
| 1:E:23:GLY:HA3   | 2:K:425:GLN:NE2  | 1.85                     | 0.89              |
| 1:B:205:GLU:HG2  | 1:D:287:ILE:HD11 | 1.55                     | 0.89              |
| 1:C:349:LEU:HD22 | 2:I:413:GLU:OE2  | 1.73                     | 0.89              |
| 1:A:349:LEU:HD22 | 2:G:413:GLU:OE2  | 1.73                     | 0.88              |
| 1:C:14:SER:O     | 1:C:157:ASP:HB3  | 1.74                     | 0.88              |
| 1:A:14:SER:O     | 1:A:157:ASP:HB3  | 1.74                     | 0.88              |
| 1:A:42:GLY:HA2   | 1:C:169:TYR:HA   | 1.53                     | 0.88              |
| 1:E:14:SER:O     | 1:E:157:ASP:HB3  | 1.74                     | 0.88              |
| 1:D:350:SER:HB2  | 2:J:382:ARG:HH12 | 1.09                     | 0.88              |
| 1:F:14:SER:O     | 1:F:157:ASP:HB3  | 1.74                     | 0.88              |
| 1:F:23:GLY:HA3   | 2:L:425:GLN:NE2  | 1.89                     | 0.87              |
| 1:A:205:GLU:HG2  | 1:C:287:ILE:HD11 | 1.54                     | 0.87              |
| 1:B:14:SER:O     | 1:B:157:ASP:HB3  | 1.74                     | 0.87              |
| 1:E:350:SER:HB2  | 2:K:382:ARG:HH12 | 1.11                     | 0.86              |
| 1:D:14:SER:O     | 1:D:157:ASP:HB3  | 1.74                     | 0.86              |
| 1:A:350:SER:HB2  | 2:G:382:ARG:HH12 | 1.05                     | 0.86              |
| 1:C:23:GLY:HA3   | 2:I:425:GLN:NE2  | 1.89                     | 0.86              |
| 1:A:23:GLY:HA3   | 2:G:425:GLN:NE2  | 1.90                     | 0.86              |
| 1:D:349:LEU:HD22 | 2:J:413:GLU:OE2  | 1.77                     | 0.85              |
| 1:B:23:GLY:CA    | 2:H:425:GLN:HE22 | 1.88                     | 0.84              |
| 1:E:349:LEU:HD22 | 2:K:413:GLU:CD   | 2.04                     | 0.83              |
| 2:J:386:GLU:HG3  | 2:J:418:LYS:HB2  | 1.60                     | 0.82              |
| 2:L:386:GLU:HG3  | 2:L:418:LYS:HB2  | 1.60                     | 0.82              |
| 2:K:386:GLU:HG3  | 2:K:418:LYS:HB2  | 1.60                     | 0.82              |
| 2:H:386:GLU:HG3  | 2:H:418:LYS:HB2  | 1.60                     | 0.82              |
| 1:D:349:LEU:HD22 | 2:J:413:GLU:CD   | 2.04                     | 0.81              |
| 2:I:418:LYS:NZ   | 2:I:420:THR:OG1  | 2.13                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:G:386:GLU:HG3   | 2:G:418:LYS:HB2  | 1.60                     | 0.81              |
| 2:K:418:LYS:NZ    | 2:K:420:THR:OG1  | 2.13                     | 0.81              |
| 2:L:418:LYS:NZ    | 2:L:420:THR:OG1  | 2.13                     | 0.81              |
| 2:G:418:LYS:NZ    | 2:G:420:THR:OG1  | 2.13                     | 0.81              |
| 2:I:386:GLU:HG3   | 2:I:418:LYS:HB2  | 1.60                     | 0.80              |
| 1:C:43:VAL:CG1    | 1:E:139:VAL:HG21 | 2.11                     | 0.80              |
| 2:H:418:LYS:NZ    | 2:H:420:THR:OG1  | 2.13                     | 0.80              |
| 1:F:350:SER:HB2   | 2:L:382:ARG:HH12 | 0.98                     | 0.80              |
| 2:J:418:LYS:NZ    | 2:J:420:THR:OG1  | 2.13                     | 0.80              |
| 1:C:47[B]:MET:HE3 | 1:E:168:GLY:HA3  | 1.65                     | 0.80              |
| 1:B:43:VAL:CG1    | 1:D:139:VAL:HG21 | 2.12                     | 0.79              |
| 1:C:349:LEU:HD22  | 2:I:413:GLU:CD   | 2.07                     | 0.79              |
| 1:A:349:LEU:HD22  | 2:G:413:GLU:CD   | 2.07                     | 0.79              |
| 1:C:47[B]:MET:CE  | 1:E:168:GLY:HA3  | 2.14                     | 0.78              |
| 1:D:43:VAL:CG1    | 1:F:139:VAL:HG21 | 2.13                     | 0.78              |
| 1:D:47[B]:MET:HE3 | 1:F:168:GLY:HA3  | 1.65                     | 0.78              |
| 1:D:47[B]:MET:CE  | 1:F:168:GLY:HA3  | 2.14                     | 0.78              |
| 1:E:23:GLY:CA     | 2:K:425:GLN:HE22 | 1.95                     | 0.77              |
| 1:D:23:GLY:CA     | 2:J:425:GLN:HE22 | 1.94                     | 0.77              |
| 1:B:47[B]:MET:CE  | 1:D:168:GLY:HA3  | 2.16                     | 0.76              |
| 1:B:47[B]:MET:HE3 | 1:D:168:GLY:HA3  | 1.66                     | 0.76              |
| 1:A:47[B]:MET:HE3 | 1:C:168:GLY:HA3  | 1.69                     | 0.76              |
| 1:C:205:GLU:OE2   | 1:E:287:ILE:HG12 | 1.87                     | 0.75              |
| 1:D:205:GLU:OE2   | 1:F:287:ILE:HG12 | 1.87                     | 0.75              |
| 1:A:43:VAL:CG1    | 1:C:139:VAL:HG21 | 2.16                     | 0.74              |
| 2:H:394:VAL:HA    | 2:H:438:VAL:HG22 | 1.69                     | 0.74              |
| 1:A:47[B]:MET:CE  | 1:C:168:GLY:HA3  | 2.17                     | 0.74              |
| 2:G:394:VAL:HA    | 2:G:438:VAL:HG22 | 1.69                     | 0.74              |
| 2:J:394:VAL:HA    | 2:J:438:VAL:HG22 | 1.69                     | 0.74              |
| 2:K:394:VAL:HA    | 2:K:438:VAL:HG22 | 1.69                     | 0.74              |
| 1:B:23:GLY:O      | 2:H:425:GLN:CD   | 2.31                     | 0.74              |
| 2:L:394:VAL:HA    | 2:L:438:VAL:HG22 | 1.69                     | 0.74              |
| 1:F:349:LEU:HD22  | 2:L:413:GLU:OE2  | 1.88                     | 0.73              |
| 1:A:17:VAL:CG2    | 1:A:33:SER:HB3   | 2.18                     | 0.73              |
| 1:B:205:GLU:OE2   | 1:D:287:ILE:HG12 | 1.88                     | 0.73              |
| 1:C:17:VAL:CG2    | 1:C:33:SER:HB3   | 2.18                     | 0.73              |
| 2:I:394:VAL:HA    | 2:I:438:VAL:HG22 | 1.69                     | 0.73              |
| 1:B:17:VAL:CG2    | 1:B:33:SER:HB3   | 2.18                     | 0.73              |
| 1:E:17:VAL:CG2    | 1:E:33:SER:HB3   | 2.18                     | 0.72              |
| 1:B:12:ASN:OD1    | 1:B:119:MET:HE1  | 1.89                     | 0.72              |
| 1:C:12:ASN:OD1    | 1:C:119:MET:HE1  | 1.89                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:12:ASN:OD1   | 1:A:119:MET:HE1  | 1.89                     | 0.72              |
| 1:E:12:ASN:OD1   | 1:E:119:MET:HE1  | 1.89                     | 0.72              |
| 1:A:205:GLU:OE2  | 1:C:287:ILE:HG12 | 1.89                     | 0.72              |
| 1:F:349:LEU:HD22 | 2:L:413:GLU:CD   | 2.15                     | 0.72              |
| 1:D:12:ASN:OD1   | 1:D:119:MET:HE1  | 1.89                     | 0.71              |
| 1:D:17:VAL:CG2   | 1:D:33:SER:HB3   | 2.18                     | 0.71              |
| 1:F:12:ASN:OD1   | 1:F:119:MET:HE1  | 1.89                     | 0.71              |
| 2:H:369:LEU:HD22 | 2:H:383:LEU:CD1  | 2.21                     | 0.71              |
| 1:C:63:GLY:HA3   | 1:E:289:ILE:HG23 | 1.73                     | 0.70              |
| 1:A:63:GLY:HA3   | 1:C:289:ILE:HG23 | 1.73                     | 0.70              |
| 2:K:387:LEU:HD12 | 2:K:419:ARG:HD3  | 1.74                     | 0.70              |
| 2:J:369:LEU:HD22 | 2:J:383:LEU:CD1  | 2.21                     | 0.70              |
| 2:I:387:LEU:HD12 | 2:I:419:ARG:HD3  | 1.74                     | 0.69              |
| 2:L:427:SER:C    | 2:L:449:VAL:HG11 | 2.17                     | 0.69              |
| 2:H:427:SER:C    | 2:H:449:VAL:HG11 | 2.17                     | 0.69              |
| 1:F:17:VAL:CG2   | 1:F:33:SER:HB3   | 2.18                     | 0.69              |
| 1:D:63:GLY:HA3   | 1:F:289:ILE:HG23 | 1.73                     | 0.69              |
| 2:I:398:LYS:N    | 2:I:401:GLN:O    | 2.26                     | 0.69              |
| 2:L:387:LEU:HD12 | 2:L:419:ARG:HD3  | 1.74                     | 0.69              |
| 2:I:378:GLY:N    | 2:I:426:CYS:O    | 2.26                     | 0.69              |
| 2:J:387:LEU:HD12 | 2:J:419:ARG:HD3  | 1.74                     | 0.69              |
| 2:J:427:SER:O    | 2:J:430:ASP:N    | 2.26                     | 0.69              |
| 2:K:366:GLN:HB3  | 2:K:386:GLU:HG2  | 1.75                     | 0.69              |
| 2:K:378:GLY:N    | 2:K:426:CYS:O    | 2.26                     | 0.69              |
| 2:L:369:LEU:HD22 | 2:L:383:LEU:CD1  | 2.21                     | 0.69              |
| 2:L:378:GLY:N    | 2:L:426:CYS:O    | 2.26                     | 0.69              |
| 2:G:387:LEU:HD12 | 2:G:419:ARG:HD3  | 1.74                     | 0.69              |
| 2:H:387:LEU:HD12 | 2:H:419:ARG:HD3  | 1.74                     | 0.69              |
| 2:I:427:SER:C    | 2:I:449:VAL:HG11 | 2.17                     | 0.69              |
| 2:G:378:GLY:N    | 2:G:426:CYS:O    | 2.26                     | 0.68              |
| 2:G:398:LYS:N    | 2:G:401:GLN:O    | 2.26                     | 0.68              |
| 2:H:366:GLN:HB3  | 2:H:386:GLU:HG2  | 1.75                     | 0.68              |
| 2:K:427:SER:O    | 2:K:430:ASP:N    | 2.26                     | 0.68              |
| 2:G:427:SER:C    | 2:G:449:VAL:HG11 | 2.17                     | 0.68              |
| 2:J:366:GLN:HB3  | 2:J:386:GLU:HG2  | 1.75                     | 0.68              |
| 2:I:411:ILE:HB   | 2:I:422:THR:HB   | 1.76                     | 0.68              |
| 2:J:378:GLY:N    | 2:J:426:CYS:O    | 2.26                     | 0.68              |
| 1:B:63:GLY:HA3   | 1:D:289:ILE:HG23 | 1.75                     | 0.68              |
| 2:K:398:LYS:N    | 2:K:401:GLN:O    | 2.26                     | 0.68              |
| 2:H:378:GLY:N    | 2:H:426:CYS:O    | 2.26                     | 0.67              |
| 2:G:411:ILE:HB   | 2:G:422:THR:HB   | 1.76                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:398:LYS:N    | 2:H:401:GLN:O    | 2.26                     | 0.67              |
| 2:I:366:GLN:HB3  | 2:I:386:GLU:HG2  | 1.75                     | 0.67              |
| 2:K:369:LEU:HD22 | 2:K:383:LEU:CD1  | 2.21                     | 0.67              |
| 2:K:411:ILE:HB   | 2:K:422:THR:HB   | 1.76                     | 0.67              |
| 2:G:366:GLN:HB3  | 2:G:386:GLU:HG2  | 1.75                     | 0.67              |
| 2:J:398:LYS:N    | 2:J:401:GLN:O    | 2.26                     | 0.67              |
| 2:L:398:LYS:N    | 2:L:401:GLN:O    | 2.26                     | 0.67              |
| 2:J:373:TYR:O    | 2:J:448:PHE:N    | 2.28                     | 0.67              |
| 2:L:373:TYR:O    | 2:L:448:PHE:N    | 2.28                     | 0.67              |
| 2:L:369:LEU:HD21 | 2:L:436:CYS:SG   | 2.35                     | 0.67              |
| 2:G:373:TYR:O    | 2:G:448:PHE:N    | 2.28                     | 0.67              |
| 1:D:149:THR:HG22 | 1:D:167:GLU:H    | 1.60                     | 0.67              |
| 1:F:149:THR:HG22 | 1:F:167:GLU:H    | 1.60                     | 0.67              |
| 2:H:373:TYR:O    | 2:H:448:PHE:N    | 2.28                     | 0.66              |
| 2:J:369:LEU:HD21 | 2:J:436:CYS:SG   | 2.35                     | 0.66              |
| 2:K:369:LEU:HD21 | 2:K:436:CYS:SG   | 2.35                     | 0.66              |
| 2:H:369:LEU:HD21 | 2:H:436:CYS:SG   | 2.35                     | 0.66              |
| 2:I:373:TYR:O    | 2:I:448:PHE:N    | 2.28                     | 0.66              |
| 2:K:373:TYR:O    | 2:K:448:PHE:N    | 2.28                     | 0.66              |
| 2:I:369:LEU:HD21 | 2:I:436:CYS:SG   | 2.35                     | 0.66              |
| 2:L:366:GLN:HB3  | 2:L:386:GLU:HG2  | 1.75                     | 0.66              |
| 1:B:149:THR:HG22 | 1:B:167:GLU:H    | 1.60                     | 0.66              |
| 1:E:149:THR:HG22 | 1:E:167:GLU:H    | 1.60                     | 0.66              |
| 2:H:396:TRP:O    | 2:H:403:ILE:N    | 2.29                     | 0.66              |
| 2:J:382:ARG:NE   | 2:J:422:THR:OG1  | 2.29                     | 0.66              |
| 2:J:411:ILE:HB   | 2:J:422:THR:HB   | 1.76                     | 0.66              |
| 2:L:411:ILE:HB   | 2:L:422:THR:HB   | 1.76                     | 0.66              |
| 1:A:149:THR:HG22 | 1:A:167:GLU:H    | 1.60                     | 0.66              |
| 2:G:369:LEU:HD21 | 2:G:436:CYS:SG   | 2.35                     | 0.66              |
| 1:A:23:GLY:CA    | 2:G:425:GLN:HE22 | 1.99                     | 0.66              |
| 1:C:39:ARG:HH12  | 1:E:286:ASP:CG   | 2.04                     | 0.66              |
| 2:H:382:ARG:NE   | 2:H:422:THR:OG1  | 2.29                     | 0.66              |
| 2:H:373:TYR:HE2  | 2:H:383:LEU:HA   | 1.61                     | 0.66              |
| 2:G:369:LEU:HD22 | 2:G:383:LEU:CD1  | 2.21                     | 0.66              |
| 2:I:373:TYR:HE2  | 2:I:383:LEU:HA   | 1.61                     | 0.66              |
| 2:I:382:ARG:NE   | 2:I:422:THR:OG1  | 2.29                     | 0.66              |
| 1:D:182:GLY:O    | 1:D:213:LYS:NZ   | 2.29                     | 0.65              |
| 2:G:373:TYR:HE2  | 2:G:383:LEU:HA   | 1.61                     | 0.65              |
| 2:G:383:LEU:HB2  | 2:G:421:LEU:HB3  | 1.77                     | 0.65              |
| 2:G:396:TRP:O    | 2:G:403:ILE:N    | 2.28                     | 0.65              |
| 2:H:411:ILE:HB   | 2:H:422:THR:HB   | 1.76                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:L:396:TRP:O     | 2:L:403:ILE:N    | 2.29                     | 0.65              |
| 2:K:382:ARG:NE    | 2:K:422:THR:OG1  | 2.29                     | 0.65              |
| 2:K:383:LEU:HB2   | 2:K:421:LEU:HB3  | 1.78                     | 0.65              |
| 1:C:149:THR:HG22  | 1:C:167:GLU:H    | 1.60                     | 0.65              |
| 2:J:373:TYR:HE2   | 2:J:383:LEU:HA   | 1.61                     | 0.65              |
| 1:B:182:GLY:O     | 1:B:213:LYS:NZ   | 2.29                     | 0.65              |
| 2:I:383:LEU:HB2   | 2:I:421:LEU:HB3  | 1.78                     | 0.65              |
| 2:G:382:ARG:NE    | 2:G:422:THR:OG1  | 2.29                     | 0.65              |
| 1:F:182:GLY:O     | 1:F:213:LYS:NZ   | 2.29                     | 0.65              |
| 2:L:373:TYR:HE2   | 2:L:383:LEU:HA   | 1.62                     | 0.65              |
| 2:L:383:LEU:HB2   | 2:L:421:LEU:HB3  | 1.78                     | 0.65              |
| 1:E:182:GLY:O     | 1:E:213:LYS:NZ   | 2.29                     | 0.65              |
| 2:H:383:LEU:HB2   | 2:H:421:LEU:HB3  | 1.77                     | 0.65              |
| 2:K:373:TYR:HE2   | 2:K:383:LEU:HA   | 1.61                     | 0.65              |
| 2:I:396:TRP:O     | 2:I:403:ILE:N    | 2.28                     | 0.65              |
| 2:L:382:ARG:NE    | 2:L:422:THR:OG1  | 2.29                     | 0.65              |
| 1:B:39:ARG:HH12   | 1:D:286:ASP:CG   | 2.04                     | 0.65              |
| 2:I:369:LEU:HD22  | 2:I:383:LEU:CD1  | 2.21                     | 0.64              |
| 1:A:182:GLY:O     | 1:A:213:LYS:NZ   | 2.29                     | 0.64              |
| 1:C:23:GLY:CA     | 2:I:425:GLN:HE22 | 1.99                     | 0.64              |
| 2:K:396:TRP:O     | 2:K:403:ILE:N    | 2.29                     | 0.64              |
| 1:C:182:GLY:O     | 1:C:213:LYS:NZ   | 2.29                     | 0.64              |
| 2:J:383:LEU:HB2   | 2:J:421:LEU:HB3  | 1.78                     | 0.64              |
| 1:E:23:GLY:O      | 2:K:425:GLN:CD   | 2.40                     | 0.64              |
| 1:B:47[B]:MET:HE1 | 1:D:167:GLU:O    | 1.98                     | 0.64              |
| 1:C:43:VAL:HG12   | 1:E:139:VAL:HG11 | 1.79                     | 0.64              |
| 1:B:148:THR:HG23  | 1:B:149:THR:HG23 | 1.81                     | 0.63              |
| 1:F:148:THR:HG23  | 1:F:149:THR:HG23 | 1.81                     | 0.63              |
| 1:A:148:THR:HG23  | 1:A:149:THR:HG23 | 1.80                     | 0.63              |
| 1:A:159:VAL:HG21  | 1:A:177:ARG:HE   | 1.64                     | 0.63              |
| 1:D:148:THR:HG23  | 1:D:149:THR:HG23 | 1.80                     | 0.63              |
| 1:A:39:ARG:HH12   | 1:C:286:ASP:CG   | 2.07                     | 0.63              |
| 2:H:397:LEU:HA    | 2:H:402:GLU:HA   | 1.81                     | 0.63              |
| 2:J:397:LEU:HA    | 2:J:402:GLU:HA   | 1.81                     | 0.63              |
| 1:C:148:THR:HG23  | 1:C:149:THR:HG23 | 1.80                     | 0.63              |
| 2:L:397:LEU:HA    | 2:L:402:GLU:HA   | 1.81                     | 0.63              |
| 1:C:159:VAL:HG21  | 1:C:177:ARG:HE   | 1.64                     | 0.63              |
| 1:D:39:ARG:HH12   | 1:F:286:ASP:CG   | 2.06                     | 0.63              |
| 2:L:398:LYS:HE3   | 2:L:432:ALA:HB3  | 1.81                     | 0.63              |
| 1:C:47[B]:MET:HE1 | 1:E:167:GLU:O    | 1.98                     | 0.62              |
| 1:E:148:THR:HG23  | 1:E:149:THR:HG23 | 1.80                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:410:TYR:OH   | 2:L:430:ASP:OD2  | 2.11                     | 0.62              |
| 1:B:23:GLY:O     | 2:H:425:GLN:OE1  | 2.17                     | 0.62              |
| 2:J:398:LYS:HE3  | 2:J:432:ALA:HB3  | 1.81                     | 0.62              |
| 1:E:159:VAL:HG21 | 1:E:177:ARG:HE   | 1.64                     | 0.62              |
| 1:B:43:VAL:HG12  | 1:D:139:VAL:HG11 | 1.80                     | 0.62              |
| 1:D:23:GLY:O     | 2:J:425:GLN:CD   | 2.42                     | 0.62              |
| 2:G:397:LEU:HA   | 2:G:402:GLU:HA   | 1.81                     | 0.62              |
| 2:I:373:TYR:CE2  | 2:I:383:LEU:HD13 | 2.35                     | 0.62              |
| 2:J:427:SER:C    | 2:J:449:VAL:HG11 | 2.25                     | 0.62              |
| 1:F:159:VAL:HG21 | 1:F:177:ARG:HE   | 1.64                     | 0.62              |
| 2:K:398:LYS:HE3  | 2:K:432:ALA:HB3  | 1.81                     | 0.62              |
| 2:G:373:TYR:CE2  | 2:G:383:LEU:HD13 | 2.35                     | 0.62              |
| 2:I:375:VAL:O    | 2:I:450:LYS:N    | 2.33                     | 0.62              |
| 2:K:373:TYR:CE2  | 2:K:383:LEU:HD13 | 2.35                     | 0.62              |
| 2:K:397:LEU:HA   | 2:K:402:GLU:HA   | 1.81                     | 0.62              |
| 2:H:373:TYR:CE2  | 2:H:383:LEU:HD13 | 2.35                     | 0.62              |
| 2:H:398:LYS:HE3  | 2:H:432:ALA:HB3  | 1.81                     | 0.62              |
| 2:G:375:VAL:O    | 2:G:450:LYS:N    | 2.33                     | 0.62              |
| 2:G:398:LYS:HE3  | 2:G:432:ALA:HB3  | 1.81                     | 0.62              |
| 2:J:375:VAL:O    | 2:J:450:LYS:N    | 2.33                     | 0.62              |
| 2:J:373:TYR:CE2  | 2:J:383:LEU:HD13 | 2.35                     | 0.61              |
| 2:L:375:VAL:O    | 2:L:450:LYS:N    | 2.33                     | 0.61              |
| 1:D:159:VAL:HG21 | 1:D:177:ARG:HE   | 1.64                     | 0.61              |
| 1:A:23:GLY:O     | 2:G:425:GLN:CD   | 2.42                     | 0.61              |
| 1:C:23:GLY:O     | 2:I:425:GLN:CD   | 2.42                     | 0.61              |
| 2:I:397:LEU:HA   | 2:I:402:GLU:HA   | 1.81                     | 0.61              |
| 2:I:398:LYS:HE3  | 2:I:432:ALA:HB3  | 1.81                     | 0.61              |
| 1:A:43:VAL:HG12  | 1:C:139:VAL:HG11 | 1.82                     | 0.61              |
| 1:B:159:VAL:HG21 | 1:B:177:ARG:HE   | 1.64                     | 0.61              |
| 2:L:373:TYR:CE2  | 2:L:383:LEU:HD13 | 2.35                     | 0.61              |
| 2:H:362:SER:HA   | 2:H:365:PHE:HB2  | 1.83                     | 0.61              |
| 2:I:362:SER:HA   | 2:I:365:PHE:HB2  | 1.83                     | 0.61              |
| 2:J:396:TRP:O    | 2:J:403:ILE:N    | 2.34                     | 0.61              |
| 2:K:427:SER:C    | 2:K:449:VAL:HG11 | 2.25                     | 0.61              |
| 2:H:410:TYR:OH   | 2:H:430:ASP:OD2  | 2.11                     | 0.61              |
| 2:K:375:VAL:O    | 2:K:450:LYS:N    | 2.33                     | 0.61              |
| 2:I:405:MET:HG3  | 2:I:410:TYR:O    | 2.01                     | 0.60              |
| 1:B:349:LEU:CD2  | 2:H:413:GLU:CD   | 2.70                     | 0.60              |
| 2:H:375:VAL:O    | 2:H:450:LYS:N    | 2.33                     | 0.60              |
| 1:D:43:VAL:HG12  | 1:F:139:VAL:HG11 | 1.82                     | 0.60              |
| 2:K:405:MET:HG3  | 2:K:410:TYR:O    | 2.01                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:47[B]:MET:HE1 | 1:F:167:GLU:O    | 2.00                     | 0.60              |
| 2:K:362:SER:HA    | 2:K:365:PHE:HB2  | 1.83                     | 0.60              |
| 2:J:410:TYR:OH    | 2:J:430:ASP:OD2  | 2.11                     | 0.60              |
| 2:J:362:SER:HA    | 2:J:365:PHE:HB2  | 1.83                     | 0.60              |
| 1:A:12:ASN:OD1    | 1:A:119:MET:CE   | 2.50                     | 0.60              |
| 2:G:362:SER:HA    | 2:G:365:PHE:HB2  | 1.83                     | 0.60              |
| 2:G:405:MET:HG3   | 2:G:410:TYR:O    | 2.01                     | 0.60              |
| 2:H:395:LYS:HB2   | 2:H:437:VAL:O    | 2.02                     | 0.60              |
| 2:J:395:LYS:HB2   | 2:J:437:VAL:O    | 2.02                     | 0.60              |
| 2:J:405:MET:HG3   | 2:J:410:TYR:O    | 2.01                     | 0.60              |
| 2:L:395:LYS:HB2   | 2:L:437:VAL:O    | 2.02                     | 0.60              |
| 2:K:410:TYR:OH    | 2:K:430:ASP:OD2  | 2.10                     | 0.59              |
| 2:L:362:SER:HA    | 2:L:365:PHE:HB2  | 1.83                     | 0.59              |
| 1:B:12:ASN:OD1    | 1:B:119:MET:CE   | 2.50                     | 0.59              |
| 2:L:405:MET:HG3   | 2:L:410:TYR:O    | 2.01                     | 0.59              |
| 1:D:63:GLY:HA3    | 1:F:288:ASP:OD1  | 2.03                     | 0.59              |
| 2:L:369:LEU:CD2   | 2:L:383:LEU:HD12 | 2.27                     | 0.59              |
| 1:F:12:ASN:OD1    | 1:F:119:MET:CE   | 2.50                     | 0.59              |
| 1:C:63:GLY:HA3    | 1:E:288:ASP:OD1  | 2.02                     | 0.59              |
| 1:B:42:GLY:HA2    | 1:D:168:GLY:O    | 2.03                     | 0.59              |
| 1:E:12:ASN:OD1    | 1:E:119:MET:CE   | 2.50                     | 0.59              |
| 1:D:12:ASN:OD1    | 1:D:119:MET:CE   | 2.50                     | 0.59              |
| 2:H:405:MET:HG3   | 2:H:410:TYR:O    | 2.01                     | 0.59              |
| 2:K:395:LYS:HB2   | 2:K:437:VAL:O    | 2.02                     | 0.59              |
| 2:L:373:TYR:CE2   | 2:L:383:LEU:HA   | 2.38                     | 0.59              |
| 1:C:12:ASN:OD1    | 1:C:119:MET:CE   | 2.50                     | 0.59              |
| 1:C:42:GLY:HA2    | 1:E:168:GLY:O    | 2.02                     | 0.59              |
| 2:I:373:TYR:CE2   | 2:I:383:LEU:HA   | 2.37                     | 0.59              |
| 1:B:63:GLY:HA3    | 1:D:288:ASP:OD1  | 2.02                     | 0.58              |
| 1:F:47[A]:MET:HG3 | 1:F:49:GLN:HE21  | 1.68                     | 0.58              |
| 2:G:373:TYR:CE2   | 2:G:383:LEU:HA   | 2.38                     | 0.58              |
| 2:L:365:PHE:CZ    | 2:L:438:VAL:HG23 | 2.39                     | 0.58              |
| 2:J:373:TYR:CE2   | 2:J:383:LEU:HA   | 2.38                     | 0.58              |
| 2:G:395:LYS:HB2   | 2:G:437:VAL:O    | 2.02                     | 0.58              |
| 2:G:396:TRP:CD1   | 2:G:436:CYS:HG   | 2.22                     | 0.58              |
| 2:J:365:PHE:CZ    | 2:J:438:VAL:HG23 | 2.39                     | 0.58              |
| 1:D:47[A]:MET:HG3 | 1:D:49:GLN:HE21  | 1.68                     | 0.58              |
| 2:I:365:PHE:CZ    | 2:I:438:VAL:HG23 | 2.39                     | 0.58              |
| 2:I:395:LYS:HB2   | 2:I:437:VAL:O    | 2.02                     | 0.58              |
| 1:C:45:VAL:HG12   | 1:E:143:TYR:OH   | 2.04                     | 0.58              |
| 1:C:47[A]:MET:HG3 | 1:C:49:GLN:HE21  | 1.68                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:G:365:PHE:CZ    | 2:G:438:VAL:HG23 | 2.39                     | 0.58              |
| 2:K:365:PHE:CZ    | 2:K:438:VAL:HG23 | 2.38                     | 0.58              |
| 2:K:373:TYR:CE2   | 2:K:383:LEU:HA   | 2.38                     | 0.58              |
| 2:H:365:PHE:CZ    | 2:H:438:VAL:HG23 | 2.39                     | 0.58              |
| 1:A:47[B]:MET:HE1 | 1:C:167:GLU:O    | 2.03                     | 0.58              |
| 1:E:47[A]:MET:HG3 | 1:E:49:GLN:HE21  | 1.68                     | 0.58              |
| 1:A:350:SER:HG    | 2:G:382:ARG:HH11 | 1.48                     | 0.58              |
| 1:B:47[A]:MET:HG3 | 1:B:49:GLN:HE21  | 1.68                     | 0.58              |
| 2:I:396:TRP:CD1   | 2:I:436:CYS:HG   | 2.22                     | 0.58              |
| 1:A:47[A]:MET:HG3 | 1:A:49:GLN:HE21  | 1.68                     | 0.57              |
| 2:H:373:TYR:CE2   | 2:H:383:LEU:HA   | 2.37                     | 0.57              |
| 1:F:216:LEU:HD11  | 1:F:240:TYR:HB2  | 1.86                     | 0.57              |
| 2:G:412:PHE:CE1   | 2:G:421:LEU:HD13 | 2.39                     | 0.57              |
| 2:H:430:ASP:HB2   | 2:H:449:VAL:HG21 | 1.87                     | 0.57              |
| 2:J:369:LEU:CD2   | 2:J:383:LEU:HD12 | 2.27                     | 0.57              |
| 2:J:430:ASP:HB2   | 2:J:449:VAL:HG21 | 1.87                     | 0.57              |
| 2:L:412:PHE:CE1   | 2:L:421:LEU:HD13 | 2.39                     | 0.57              |
| 1:A:42:GLY:HA2    | 1:C:168:GLY:O    | 2.04                     | 0.57              |
| 1:D:216:LEU:HD11  | 1:D:240:TYR:HB2  | 1.86                     | 0.57              |
| 2:H:433:ALA:HA    | 2:H:446:GLU:HA   | 1.87                     | 0.57              |
| 1:A:216:LEU:HD11  | 1:A:240:TYR:HB2  | 1.86                     | 0.57              |
| 1:B:212:ILE:HG23  | 1:B:216:LEU:HD12 | 1.87                     | 0.57              |
| 1:F:212:ILE:HG23  | 1:F:216:LEU:HD12 | 1.87                     | 0.57              |
| 2:G:369:LEU:CD2   | 2:G:383:LEU:HD12 | 2.27                     | 0.57              |
| 2:I:412:PHE:CE1   | 2:I:421:LEU:HD13 | 2.39                     | 0.57              |
| 2:L:430:ASP:HB2   | 2:L:449:VAL:HG21 | 1.87                     | 0.57              |
| 2:L:433:ALA:HA    | 2:L:446:GLU:HA   | 1.87                     | 0.57              |
| 1:D:212:ILE:HG23  | 1:D:216:LEU:HD12 | 1.87                     | 0.57              |
| 2:J:412:PHE:CE1   | 2:J:421:LEU:HD13 | 2.39                     | 0.57              |
| 2:H:412:PHE:CE1   | 2:H:421:LEU:HD13 | 2.39                     | 0.56              |
| 2:I:369:LEU:CD2   | 2:I:383:LEU:HD12 | 2.27                     | 0.56              |
| 2:J:433:ALA:HA    | 2:J:446:GLU:HA   | 1.87                     | 0.56              |
| 2:K:369:LEU:CD2   | 2:K:383:LEU:HD12 | 2.27                     | 0.56              |
| 2:K:412:PHE:CE1   | 2:K:421:LEU:HD13 | 2.39                     | 0.56              |
| 2:G:430:ASP:HB2   | 2:G:449:VAL:HG21 | 1.87                     | 0.56              |
| 1:C:216:LEU:HD11  | 1:C:240:TYR:HB2  | 1.86                     | 0.56              |
| 1:E:212:ILE:HG23  | 1:E:216:LEU:HD12 | 1.87                     | 0.56              |
| 1:E:216:LEU:HD11  | 1:E:240:TYR:HB2  | 1.86                     | 0.56              |
| 2:I:430:ASP:HB2   | 2:I:449:VAL:HG21 | 1.87                     | 0.56              |
| 2:K:396:TRP:CD1   | 2:K:436:CYS:HG   | 2.24                     | 0.56              |
| 1:C:350:SER:HG    | 2:I:382:ARG:HH11 | 1.50                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:216:LEU:HD11  | 1:B:240:TYR:HB2  | 1.86                     | 0.56              |
| 1:F:350:SER:CB    | 2:L:382:ARG:HH12 | 1.87                     | 0.56              |
| 2:J:366:GLN:N     | 2:J:386:GLU:O    | 2.39                     | 0.56              |
| 1:A:23:GLY:O      | 2:G:425:GLN:OE1  | 2.23                     | 0.56              |
| 1:F:71:ILE:HG12   | 1:F:76:ILE:HG13  | 1.87                     | 0.56              |
| 2:K:430:ASP:HB2   | 2:K:449:VAL:HG21 | 1.87                     | 0.56              |
| 1:A:212:ILE:HG23  | 1:A:216:LEU:HD12 | 1.87                     | 0.56              |
| 1:C:212:ILE:HG23  | 1:C:216:LEU:HD12 | 1.87                     | 0.56              |
| 2:G:436:CYS:O     | 2:G:442:LYS:HA   | 2.06                     | 0.56              |
| 2:L:436:CYS:O     | 2:L:442:LYS:HA   | 2.06                     | 0.56              |
| 1:E:71:ILE:HG12   | 1:E:76:ILE:HG13  | 1.87                     | 0.56              |
| 2:I:361:LYS:HG2   | 2:I:362:SER:H    | 1.71                     | 0.56              |
| 2:L:387:LEU:O     | 2:L:417:ALA:HB1  | 2.06                     | 0.56              |
| 2:L:396:TRP:CD1   | 2:L:436:CYS:HG   | 2.23                     | 0.56              |
| 1:A:63:GLY:HA3    | 1:C:288:ASP:OD1  | 2.06                     | 0.56              |
| 1:D:42:GLY:HA2    | 1:F:168:GLY:O    | 2.05                     | 0.56              |
| 2:G:387:LEU:O     | 2:G:417:ALA:HB1  | 2.06                     | 0.56              |
| 2:K:361:LYS:HG2   | 2:K:362:SER:H    | 1.71                     | 0.56              |
| 2:L:366:GLN:N     | 2:L:386:GLU:O    | 2.39                     | 0.56              |
| 1:B:45:VAL:HG12   | 1:D:143:TYR:OH   | 2.05                     | 0.55              |
| 2:K:433:ALA:HA    | 2:K:446:GLU:HA   | 1.87                     | 0.55              |
| 1:D:23:GLY:O      | 2:J:425:GLN:OE1  | 2.25                     | 0.55              |
| 2:G:433:ALA:HA    | 2:G:446:GLU:HA   | 1.87                     | 0.55              |
| 2:H:361:LYS:HG2   | 2:H:362:SER:H    | 1.71                     | 0.55              |
| 2:I:387:LEU:O     | 2:I:417:ALA:HB1  | 2.06                     | 0.55              |
| 2:I:433:ALA:HA    | 2:I:446:GLU:HA   | 1.87                     | 0.55              |
| 2:J:387:LEU:O     | 2:J:417:ALA:HB1  | 2.06                     | 0.55              |
| 1:C:71:ILE:HG12   | 1:C:76:ILE:HG13  | 1.87                     | 0.55              |
| 1:D:71:ILE:HG12   | 1:D:76:ILE:HG13  | 1.87                     | 0.55              |
| 2:I:436:CYS:O     | 2:I:442:LYS:HA   | 2.06                     | 0.55              |
| 2:J:361:LYS:HG2   | 2:J:362:SER:H    | 1.71                     | 0.55              |
| 1:C:202:THR:HG22  | 1:C:204:ALA:H    | 1.72                     | 0.55              |
| 1:D:47[B]:MET:HE1 | 1:F:168:GLY:HA3  | 1.89                     | 0.55              |
| 1:E:349:LEU:CD2   | 2:K:413:GLU:CD   | 2.78                     | 0.55              |
| 2:H:387:LEU:O     | 2:H:417:ALA:HB1  | 2.06                     | 0.55              |
| 1:E:202:THR:HG22  | 1:E:204:ALA:H    | 1.72                     | 0.55              |
| 2:H:366:GLN:N     | 2:H:386:GLU:O    | 2.39                     | 0.55              |
| 2:J:396:TRP:CD1   | 2:J:436:CYS:HG   | 2.24                     | 0.55              |
| 2:L:361:LYS:HG2   | 2:L:362:SER:H    | 1.71                     | 0.55              |
| 2:J:436:CYS:O     | 2:J:442:LYS:HA   | 2.06                     | 0.55              |
| 1:E:23:GLY:O      | 2:K:425:GLN:OE1  | 2.24                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:G:361:LYS:HG2   | 2:G:362:SER:H    | 1.71                     | 0.55              |
| 2:I:366:GLN:N     | 2:I:386:GLU:O    | 2.39                     | 0.55              |
| 2:K:436:CYS:O     | 2:K:442:LYS:HA   | 2.06                     | 0.55              |
| 1:A:71:ILE:HG12   | 1:A:76:ILE:HG13  | 1.87                     | 0.55              |
| 2:H:377:LYS:HG2   | 2:H:427:SER:HA   | 1.89                     | 0.55              |
| 2:H:396:TRP:CD1   | 2:H:436:CYS:HG   | 2.23                     | 0.55              |
| 2:H:436:CYS:O     | 2:H:442:LYS:HA   | 2.06                     | 0.55              |
| 2:K:387:LEU:O     | 2:K:417:ALA:HB1  | 2.06                     | 0.55              |
| 1:D:45:VAL:HG12   | 1:F:143:TYR:OH   | 2.06                     | 0.55              |
| 1:D:202:THR:HG22  | 1:D:204:ALA:H    | 1.72                     | 0.55              |
| 2:K:366:GLN:N     | 2:K:386:GLU:O    | 2.39                     | 0.55              |
| 2:H:431:ASP:HB2   | 2:H:449:VAL:HB   | 1.89                     | 0.55              |
| 2:I:380:LYS:HG2   | 2:I:423:ILE:O    | 2.07                     | 0.55              |
| 1:A:202:THR:HG22  | 1:A:204:ALA:H    | 1.72                     | 0.54              |
| 1:B:71:ILE:HG12   | 1:B:76:ILE:HG13  | 1.87                     | 0.54              |
| 1:C:23:GLY:O      | 2:I:425:GLN:OE1  | 2.24                     | 0.54              |
| 2:G:366:GLN:N     | 2:G:386:GLU:O    | 2.39                     | 0.54              |
| 2:G:380:LYS:HG2   | 2:G:423:ILE:O    | 2.07                     | 0.54              |
| 2:H:369:LEU:CD2   | 2:H:383:LEU:HD12 | 2.27                     | 0.54              |
| 1:F:202:THR:HG22  | 1:F:204:ALA:H    | 1.72                     | 0.54              |
| 2:G:431:ASP:HB2   | 2:G:449:VAL:HB   | 1.89                     | 0.54              |
| 2:J:431:ASP:HB2   | 2:J:449:VAL:HB   | 1.89                     | 0.54              |
| 2:K:380:LYS:HG2   | 2:K:423:ILE:O    | 2.07                     | 0.54              |
| 2:L:377:LYS:HG2   | 2:L:427:SER:HA   | 1.89                     | 0.54              |
| 1:C:47[B]:MET:HE1 | 1:E:168:GLY:HA3  | 1.88                     | 0.54              |
| 1:C:63:GLY:N      | 1:E:288:ASP:OD2  | 2.41                     | 0.54              |
| 2:I:431:ASP:HB2   | 2:I:449:VAL:HB   | 1.89                     | 0.54              |
| 1:B:202:THR:HG22  | 1:B:204:ALA:H    | 1.72                     | 0.54              |
| 2:G:435:GLN:O     | 2:G:437:VAL:HG23 | 2.08                     | 0.54              |
| 2:L:380:LYS:HG2   | 2:L:423:ILE:O    | 2.07                     | 0.54              |
| 1:D:203:THR:O     | 1:D:206:ARG:HB3  | 2.08                     | 0.54              |
| 2:I:435:GLN:O     | 2:I:437:VAL:HG23 | 2.08                     | 0.54              |
| 2:K:435:GLN:O     | 2:K:437:VAL:HG23 | 2.08                     | 0.54              |
| 1:A:349:LEU:CD2   | 2:G:413:GLU:CD   | 2.79                     | 0.54              |
| 2:L:431:ASP:HB2   | 2:L:449:VAL:HB   | 1.89                     | 0.54              |
| 1:B:203:THR:O     | 1:B:206:ARG:HB3  | 2.08                     | 0.53              |
| 1:B:47[B]:MET:HE1 | 1:D:168:GLY:HA3  | 1.91                     | 0.53              |
| 1:E:203:THR:O     | 1:E:206:ARG:HB3  | 2.08                     | 0.53              |
| 2:K:365:PHE:HA    | 2:K:387:LEU:HA   | 1.90                     | 0.53              |
| 1:B:63:GLY:N      | 1:D:288:ASP:OD2  | 2.41                     | 0.53              |
| 1:B:239:SER:HA    | 1:B:248:ILE:O    | 2.09                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:349:LEU:CD2  | 2:I:413:GLU:CD   | 2.79                     | 0.53              |
| 1:D:86:TRP:HH2   | 1:D:119:MET:HG3  | 1.73                     | 0.53              |
| 1:E:239:SER:HA   | 1:E:248:ILE:O    | 2.09                     | 0.53              |
| 2:I:365:PHE:HA   | 2:I:387:LEU:HA   | 1.89                     | 0.53              |
| 2:I:382:ARG:HG2  | 2:I:422:THR:HG23 | 1.90                     | 0.53              |
| 2:K:431:ASP:HB2  | 2:K:449:VAL:HB   | 1.90                     | 0.53              |
| 1:D:239:SER:HA   | 1:D:248:ILE:O    | 2.09                     | 0.53              |
| 1:F:86:TRP:HH2   | 1:F:119:MET:HG3  | 1.74                     | 0.53              |
| 2:H:365:PHE:HA   | 2:H:387:LEU:HA   | 1.90                     | 0.53              |
| 2:G:435:GLN:HA   | 2:G:443:CYS:O    | 2.09                     | 0.53              |
| 2:I:435:GLN:HA   | 2:I:443:CYS:O    | 2.09                     | 0.53              |
| 1:C:350:SER:CB   | 2:I:382:ARG:HH12 | 1.91                     | 0.53              |
| 2:G:383:LEU:HD11 | 2:G:434:TYR:HD2  | 1.73                     | 0.53              |
| 2:L:365:PHE:HA   | 2:L:387:LEU:HA   | 1.90                     | 0.53              |
| 2:L:382:ARG:HG2  | 2:L:422:THR:HG23 | 1.90                     | 0.53              |
| 2:L:383:LEU:HD11 | 2:L:434:TYR:HD2  | 1.73                     | 0.53              |
| 1:B:185:LEU:HB2  | 1:B:213:LYS:HZ1  | 1.74                     | 0.53              |
| 2:G:365:PHE:HA   | 2:G:387:LEU:HA   | 1.90                     | 0.53              |
| 2:G:409:LYS:HD3  | 2:G:409:LYS:N    | 2.24                     | 0.53              |
| 2:I:377:LYS:HG2  | 2:I:427:SER:HA   | 1.90                     | 0.53              |
| 2:I:409:LYS:HD3  | 2:I:409:LYS:N    | 2.24                     | 0.53              |
| 2:J:382:ARG:HG2  | 2:J:422:THR:HG23 | 1.90                     | 0.53              |
| 2:K:409:LYS:HD3  | 2:K:409:LYS:N    | 2.24                     | 0.53              |
| 1:C:203:THR:O    | 1:C:206:ARG:HB3  | 2.08                     | 0.53              |
| 1:D:63:GLY:N     | 1:F:288:ASP:OD2  | 2.42                     | 0.53              |
| 1:F:239:SER:HA   | 1:F:248:ILE:O    | 2.09                     | 0.53              |
| 2:G:377:LYS:HG2  | 2:G:427:SER:HA   | 1.90                     | 0.53              |
| 2:H:380:LYS:HG2  | 2:H:423:ILE:O    | 2.07                     | 0.53              |
| 2:J:365:PHE:HA   | 2:J:387:LEU:HA   | 1.90                     | 0.53              |
| 2:J:380:LYS:HG2  | 2:J:423:ILE:O    | 2.07                     | 0.53              |
| 2:L:435:GLN:O    | 2:L:437:VAL:HG23 | 2.08                     | 0.53              |
| 1:C:86:TRP:HH2   | 1:C:119:MET:HG3  | 1.73                     | 0.53              |
| 1:C:239:SER:HA   | 1:C:248:ILE:O    | 2.09                     | 0.53              |
| 1:F:203:THR:O    | 1:F:206:ARG:HB3  | 2.08                     | 0.53              |
| 2:K:387:LEU:CD1  | 2:K:419:ARG:HD3  | 2.39                     | 0.53              |
| 2:K:398:LYS:CE   | 2:K:432:ALA:HB3  | 2.39                     | 0.53              |
| 1:A:86:TRP:HH2   | 1:A:119:MET:HG3  | 1.74                     | 0.52              |
| 1:A:239:SER:HA   | 1:A:248:ILE:O    | 2.09                     | 0.52              |
| 1:C:63:GLY:CA    | 1:E:288:ASP:OD1  | 2.57                     | 0.52              |
| 2:G:382:ARG:HG2  | 2:G:422:THR:HG23 | 1.90                     | 0.52              |
| 2:G:398:LYS:CE   | 2:G:432:ALA:HB3  | 2.39                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:398:LYS:CE   | 2:H:432:ALA:HB3  | 2.39                     | 0.52              |
| 2:H:435:GLN:O    | 2:H:437:VAL:HG23 | 2.08                     | 0.52              |
| 2:I:383:LEU:HD11 | 2:I:434:TYR:HD2  | 1.73                     | 0.52              |
| 2:J:383:LEU:HD11 | 2:J:434:TYR:HD2  | 1.73                     | 0.52              |
| 2:J:435:GLN:O    | 2:J:437:VAL:HG23 | 2.08                     | 0.52              |
| 2:L:435:GLN:HA   | 2:L:443:CYS:O    | 2.09                     | 0.52              |
| 1:A:185:LEU:HB2  | 1:A:213:LYS:HZ1  | 1.74                     | 0.52              |
| 2:H:387:LEU:CD1  | 2:H:419:ARG:HD3  | 2.39                     | 0.52              |
| 2:K:435:GLN:HA   | 2:K:443:CYS:O    | 2.09                     | 0.52              |
| 1:A:203:THR:O    | 1:A:206:ARG:HB3  | 2.08                     | 0.52              |
| 1:F:185:LEU:HB2  | 1:F:213:LYS:HZ1  | 1.74                     | 0.52              |
| 2:I:387:LEU:CD1  | 2:I:419:ARG:HD3  | 2.39                     | 0.52              |
| 2:J:398:LYS:CE   | 2:J:432:ALA:HB3  | 2.39                     | 0.52              |
| 2:J:398:LYS:HB2  | 2:J:403:ILE:HG12 | 1.92                     | 0.52              |
| 2:K:383:LEU:HD11 | 2:K:434:TYR:HD2  | 1.73                     | 0.52              |
| 1:D:349:LEU:CD2  | 2:J:413:GLU:CD   | 2.80                     | 0.52              |
| 2:H:382:ARG:HG2  | 2:H:422:THR:HG23 | 1.90                     | 0.52              |
| 2:J:377:LYS:HG2  | 2:J:427:SER:HA   | 1.92                     | 0.52              |
| 2:J:435:GLN:HA   | 2:J:443:CYS:O    | 2.09                     | 0.52              |
| 2:L:409:LYS:HD3  | 2:L:409:LYS:N    | 2.24                     | 0.52              |
| 1:B:34:ILE:HD12  | 1:B:67:LEU:HD22  | 1.92                     | 0.52              |
| 1:B:63:GLY:CA    | 1:D:288:ASP:OD1  | 2.58                     | 0.52              |
| 1:C:34:ILE:HD12  | 1:C:67:LEU:HD22  | 1.92                     | 0.52              |
| 1:D:34:ILE:HD12  | 1:D:67:LEU:HD22  | 1.92                     | 0.52              |
| 2:H:383:LEU:HD11 | 2:H:434:TYR:HD2  | 1.73                     | 0.52              |
| 2:H:398:LYS:HB2  | 2:H:403:ILE:HG12 | 1.92                     | 0.52              |
| 2:I:398:LYS:HB2  | 2:I:403:ILE:HG12 | 1.92                     | 0.52              |
| 1:A:45:VAL:HG12  | 1:C:143:TYR:OH   | 2.10                     | 0.52              |
| 1:B:86:TRP:HH2   | 1:B:119:MET:HG3  | 1.74                     | 0.52              |
| 1:D:63:GLY:CA    | 1:F:288:ASP:OD1  | 2.58                     | 0.52              |
| 2:G:398:LYS:HB2  | 2:G:403:ILE:HG12 | 1.92                     | 0.52              |
| 2:I:398:LYS:CE   | 2:I:432:ALA:HB3  | 2.39                     | 0.52              |
| 2:K:398:LYS:HB2  | 2:K:403:ILE:HG12 | 1.92                     | 0.52              |
| 2:L:398:LYS:HB2  | 2:L:403:ILE:HG12 | 1.92                     | 0.52              |
| 1:A:34:ILE:HD12  | 1:A:67:LEU:HD22  | 1.92                     | 0.52              |
| 1:E:34:ILE:HD12  | 1:E:67:LEU:HD22  | 1.92                     | 0.52              |
| 2:K:382:ARG:HG2  | 2:K:422:THR:HG23 | 1.90                     | 0.52              |
| 2:L:398:LYS:CE   | 2:L:432:ALA:HB3  | 2.39                     | 0.52              |
| 1:F:34:ILE:HD12  | 1:F:67:LEU:HD22  | 1.92                     | 0.52              |
| 2:I:410:TYR:OH   | 2:I:430:ASP:OD2  | 2.11                     | 0.52              |
| 2:L:394:VAL:HG12 | 2:L:438:VAL:CG2  | 2.40                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:14:SER:O     | 1:C:157:ASP:CB   | 2.54                     | 0.52              |
| 1:E:86:TRP:HH2   | 1:E:119:MET:HG3  | 1.74                     | 0.51              |
| 2:H:394:VAL:HG12 | 2:H:438:VAL:CG2  | 2.40                     | 0.51              |
| 2:H:435:GLN:HA   | 2:H:443:CYS:O    | 2.09                     | 0.51              |
| 2:J:387:LEU:CD1  | 2:J:419:ARG:HD3  | 2.39                     | 0.51              |
| 2:J:409:LYS:HD3  | 2:J:409:LYS:N    | 2.24                     | 0.51              |
| 2:J:409:LYS:O    | 2:J:423:ILE:HG23 | 2.11                     | 0.51              |
| 1:E:230:ALA:HB2  | 1:E:236:LEU:HD12 | 1.91                     | 0.51              |
| 2:G:394:VAL:HG12 | 2:G:438:VAL:CG2  | 2.40                     | 0.51              |
| 2:G:409:LYS:O    | 2:G:423:ILE:HG23 | 2.11                     | 0.51              |
| 2:H:409:LYS:HD3  | 2:H:409:LYS:N    | 2.24                     | 0.51              |
| 2:H:409:LYS:O    | 2:H:423:ILE:HG23 | 2.11                     | 0.51              |
| 2:I:409:LYS:O    | 2:I:423:ILE:HG23 | 2.10                     | 0.51              |
| 2:I:394:VAL:HG12 | 2:I:438:VAL:CG2  | 2.40                     | 0.51              |
| 1:A:153:LEU:HD21 | 1:A:274:ILE:HD12 | 1.93                     | 0.51              |
| 1:A:230:ALA:HB2  | 1:A:236:LEU:HD12 | 1.91                     | 0.51              |
| 1:B:230:ALA:HB2  | 1:B:236:LEU:HD12 | 1.91                     | 0.51              |
| 1:D:230:ALA:HB2  | 1:D:236:LEU:HD12 | 1.91                     | 0.51              |
| 2:G:374:GLN:HA   | 2:G:448:PHE:HB2  | 1.93                     | 0.51              |
| 2:I:374:GLN:HA   | 2:I:448:PHE:HB2  | 1.93                     | 0.51              |
| 2:J:374:GLN:HA   | 2:J:448:PHE:HB2  | 1.93                     | 0.51              |
| 2:L:387:LEU:CD1  | 2:L:419:ARG:HD3  | 2.39                     | 0.51              |
| 1:E:350:SER:HG   | 2:K:382:ARG:HH11 | 1.52                     | 0.51              |
| 1:F:23:GLY:CA    | 2:L:425:GLN:HE22 | 2.06                     | 0.51              |
| 2:H:374:GLN:HA   | 2:H:448:PHE:HB2  | 1.93                     | 0.51              |
| 2:I:385:VAL:O    | 2:I:419:ARG:O    | 2.29                     | 0.51              |
| 2:J:370:GLU:O    | 2:J:445:THR:HB   | 2.11                     | 0.51              |
| 2:K:377:LYS:HG2  | 2:K:427:SER:HA   | 1.92                     | 0.51              |
| 2:K:409:LYS:O    | 2:K:423:ILE:HG23 | 2.11                     | 0.51              |
| 2:L:374:GLN:HA   | 2:L:448:PHE:HB2  | 1.93                     | 0.51              |
| 1:B:153:LEU:HD21 | 1:B:274:ILE:HD12 | 1.93                     | 0.51              |
| 1:F:230:ALA:HB2  | 1:F:236:LEU:HD12 | 1.91                     | 0.51              |
| 2:G:427:SER:O    | 2:G:430:ASP:N    | 2.44                     | 0.51              |
| 2:I:399:ASN:N    | 2:I:435:GLN:OE1  | 2.44                     | 0.51              |
| 2:J:437:VAL:HG22 | 2:J:442:LYS:HB2  | 1.93                     | 0.51              |
| 2:L:409:LYS:O    | 2:L:423:ILE:HG23 | 2.11                     | 0.51              |
| 1:C:153:LEU:HD21 | 1:C:274:ILE:HD12 | 1.93                     | 0.51              |
| 1:C:230:ALA:HB2  | 1:C:236:LEU:HD12 | 1.91                     | 0.51              |
| 2:G:385:VAL:O    | 2:G:419:ARG:O    | 2.29                     | 0.51              |
| 2:H:369:LEU:HD11 | 2:H:436:CYS:SG   | 2.51                     | 0.51              |
| 2:K:369:LEU:HD11 | 2:K:436:CYS:SG   | 2.51                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:370:GLU:O    | 2:G:445:THR:HB   | 2.11                     | 0.51              |
| 2:J:399:ASN:N    | 2:J:433:ALA:O    | 2.42                     | 0.51              |
| 2:K:370:GLU:O    | 2:K:445:THR:HB   | 2.11                     | 0.51              |
| 2:K:374:GLN:HA   | 2:K:448:PHE:HB2  | 1.93                     | 0.51              |
| 2:L:369:LEU:HD11 | 2:L:436:CYS:SG   | 2.51                     | 0.51              |
| 2:L:399:ASN:N    | 2:L:435:GLN:OE1  | 2.44                     | 0.51              |
| 2:G:387:LEU:CD1  | 2:G:419:ARG:HD3  | 2.39                     | 0.51              |
| 2:G:394:VAL:HG12 | 2:G:438:VAL:HG23 | 1.93                     | 0.51              |
| 2:I:369:LEU:HD11 | 2:I:436:CYS:SG   | 2.51                     | 0.51              |
| 2:J:385:VAL:O    | 2:J:419:ARG:O    | 2.29                     | 0.51              |
| 2:K:399:ASN:N    | 2:K:435:GLN:OE1  | 2.44                     | 0.51              |
| 2:K:414:SER:HA   | 2:K:418:LYS:O    | 2.11                     | 0.51              |
| 2:L:370:GLU:O    | 2:L:445:THR:HB   | 2.11                     | 0.51              |
| 2:L:394:VAL:HG12 | 2:L:438:VAL:HG23 | 1.93                     | 0.51              |
| 1:E:153:LEU:HD21 | 1:E:274:ILE:HD12 | 1.93                     | 0.50              |
| 2:H:370:GLU:O    | 2:H:445:THR:HB   | 2.11                     | 0.50              |
| 2:H:385:VAL:O    | 2:H:419:ARG:O    | 2.29                     | 0.50              |
| 2:I:394:VAL:HG12 | 2:I:438:VAL:HG23 | 1.94                     | 0.50              |
| 2:I:414:SER:HA   | 2:I:418:LYS:O    | 2.12                     | 0.50              |
| 2:I:437:VAL:HG22 | 2:I:442:LYS:HB2  | 1.93                     | 0.50              |
| 2:J:369:LEU:HD11 | 2:J:436:CYS:SG   | 2.51                     | 0.50              |
| 2:K:394:VAL:HG12 | 2:K:438:VAL:CG2  | 2.40                     | 0.50              |
| 2:K:394:VAL:HG12 | 2:K:438:VAL:HG23 | 1.94                     | 0.50              |
| 1:D:153:LEU:HD21 | 1:D:274:ILE:HD12 | 1.93                     | 0.50              |
| 2:J:394:VAL:HG12 | 2:J:438:VAL:CG2  | 2.40                     | 0.50              |
| 2:K:385:VAL:O    | 2:K:419:ARG:O    | 2.29                     | 0.50              |
| 2:L:385:VAL:O    | 2:L:419:ARG:O    | 2.29                     | 0.50              |
| 2:L:437:VAL:HG22 | 2:L:442:LYS:HB2  | 1.93                     | 0.50              |
| 1:B:23:GLY:CA    | 2:H:425:GLN:NE2  | 2.60                     | 0.50              |
| 2:I:406:SER:HB2  | 2:I:410:TYR:HD2  | 1.77                     | 0.50              |
| 1:F:23:GLY:O     | 2:L:425:GLN:CD   | 2.55                     | 0.50              |
| 2:G:437:VAL:HG22 | 2:G:442:LYS:HB2  | 1.93                     | 0.50              |
| 2:H:394:VAL:HG12 | 2:H:438:VAL:HG23 | 1.94                     | 0.50              |
| 2:H:406:SER:HB2  | 2:H:410:TYR:HD2  | 1.77                     | 0.50              |
| 2:J:394:VAL:HG12 | 2:J:438:VAL:HG23 | 1.93                     | 0.50              |
| 2:K:437:VAL:HG22 | 2:K:442:LYS:HB2  | 1.93                     | 0.50              |
| 1:D:23:GLY:CA    | 2:J:425:GLN:NE2  | 2.64                     | 0.50              |
| 2:G:369:LEU:HD11 | 2:G:436:CYS:SG   | 2.51                     | 0.50              |
| 2:G:414:SER:HA   | 2:G:418:LYS:O    | 2.11                     | 0.50              |
| 2:I:370:GLU:O    | 2:I:445:THR:HB   | 2.11                     | 0.50              |
| 2:I:427:SER:O    | 2:I:430:ASP:N    | 2.44                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:47[B]:MET:HE1 | 1:C:168:GLY:HA3  | 1.91                     | 0.50              |
| 2:G:399:ASN:N     | 2:G:435:GLN:OE1  | 2.44                     | 0.50              |
| 2:J:410:TYR:HB3   | 2:J:421:LEU:HD11 | 1.94                     | 0.50              |
| 2:H:410:TYR:HB3   | 2:H:421:LEU:HD11 | 1.94                     | 0.50              |
| 2:J:367:LYS:HB3   | 2:J:386:GLU:N    | 2.27                     | 0.50              |
| 2:L:410:TYR:HB3   | 2:L:421:LEU:HD11 | 1.94                     | 0.50              |
| 1:F:153:LEU:HD21  | 1:F:274:ILE:HD12 | 1.93                     | 0.50              |
| 2:H:399:ASN:N     | 2:H:433:ALA:O    | 2.42                     | 0.50              |
| 2:H:399:ASN:N     | 2:H:435:GLN:OE1  | 2.44                     | 0.50              |
| 2:J:367:LYS:HB3   | 2:J:386:GLU:CB   | 2.42                     | 0.50              |
| 2:J:403:ILE:HG21  | 2:J:421:LEU:HD21 | 1.94                     | 0.50              |
| 2:L:367:LYS:HB3   | 2:L:386:GLU:CB   | 2.42                     | 0.50              |
| 2:G:384:THR:HG23  | 2:G:418:LYS:HZ1  | 1.77                     | 0.50              |
| 2:H:367:LYS:HB3   | 2:H:386:GLU:CB   | 2.42                     | 0.50              |
| 2:H:403:ILE:HG21  | 2:H:421:LEU:HD21 | 1.94                     | 0.50              |
| 2:H:437:VAL:HG22  | 2:H:442:LYS:HB2  | 1.93                     | 0.50              |
| 2:I:399:ASN:N     | 2:I:433:ALA:O    | 2.42                     | 0.50              |
| 2:J:383:LEU:O     | 2:J:420:THR:HG23 | 2.12                     | 0.50              |
| 2:J:389:ASP:OD2   | 2:J:392:ALA:N    | 2.45                     | 0.50              |
| 2:L:389:ASP:OD2   | 2:L:392:ALA:N    | 2.45                     | 0.50              |
| 2:G:367:LYS:HB3   | 2:G:386:GLU:CB   | 2.42                     | 0.49              |
| 2:G:367:LYS:HB3   | 2:G:386:GLU:N    | 2.27                     | 0.49              |
| 2:G:389:ASP:OD2   | 2:G:392:ALA:N    | 2.45                     | 0.49              |
| 2:H:427:SER:O     | 2:H:430:ASP:N    | 2.44                     | 0.49              |
| 1:A:63:GLY:N      | 1:C:288:ASP:OD2  | 2.45                     | 0.49              |
| 1:C:42:GLY:CA     | 1:E:169:TYR:HA   | 2.32                     | 0.49              |
| 1:F:209:VAL:HA    | 1:F:212:ILE:HD12 | 1.95                     | 0.49              |
| 2:H:389:ASP:OD2   | 2:H:392:ALA:N    | 2.45                     | 0.49              |
| 2:I:389:ASP:OD2   | 2:I:392:ALA:N    | 2.45                     | 0.49              |
| 2:J:406:SER:HB2   | 2:J:410:TYR:HD2  | 1.77                     | 0.49              |
| 2:L:367:LYS:HB3   | 2:L:386:GLU:N    | 2.27                     | 0.49              |
| 1:A:63:GLY:CA     | 1:C:288:ASP:OD1  | 2.60                     | 0.49              |
| 1:C:220:ALA:HB1   | 1:C:226:GLU:HG3  | 1.94                     | 0.49              |
| 1:F:131:ALA:HB1   | 1:F:356:TRP:HB3  | 1.95                     | 0.49              |
| 2:G:406:SER:HB2   | 2:G:410:TYR:HD2  | 1.77                     | 0.49              |
| 2:H:414:SER:HA    | 2:H:418:LYS:O    | 2.11                     | 0.49              |
| 2:I:367:LYS:HB3   | 2:I:386:GLU:N    | 2.27                     | 0.49              |
| 2:I:396:TRP:CZ2   | 2:I:419:ARG:HG2  | 2.48                     | 0.49              |
| 2:J:399:ASN:N     | 2:J:435:GLN:OE1  | 2.44                     | 0.49              |
| 1:E:151:ILE:HA    | 1:E:164:PRO:HA   | 1.95                     | 0.49              |
| 1:E:220:ALA:HB1   | 1:E:226:GLU:HG3  | 1.94                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:390:HIS:HA   | 2:J:417:ALA:HB2  | 1.95                     | 0.49              |
| 2:K:396:TRP:CZ2  | 2:K:419:ARG:HG2  | 2.48                     | 0.49              |
| 2:L:403:ILE:HG21 | 2:L:421:LEU:HD21 | 1.94                     | 0.49              |
| 1:A:151:ILE:HA   | 1:A:164:PRO:HA   | 1.95                     | 0.49              |
| 1:D:209:VAL:HA   | 1:D:212:ILE:HD12 | 1.95                     | 0.49              |
| 2:I:367:LYS:HB3  | 2:I:386:GLU:CB   | 2.42                     | 0.49              |
| 2:I:383:LEU:O    | 2:I:420:THR:HG23 | 2.12                     | 0.49              |
| 2:J:396:TRP:CZ2  | 2:J:419:ARG:HG2  | 2.48                     | 0.49              |
| 2:K:383:LEU:O    | 2:K:420:THR:HG23 | 2.12                     | 0.49              |
| 2:K:406:SER:HB2  | 2:K:410:TYR:HD2  | 1.77                     | 0.49              |
| 1:A:220:ALA:HB1  | 1:A:226:GLU:HG3  | 1.94                     | 0.49              |
| 1:E:209:VAL:HA   | 1:E:212:ILE:HD12 | 1.95                     | 0.49              |
| 2:H:396:TRP:CZ2  | 2:H:419:ARG:HG2  | 2.48                     | 0.49              |
| 2:L:396:TRP:CZ2  | 2:L:419:ARG:HG2  | 2.48                     | 0.49              |
| 2:L:399:ASN:N    | 2:L:433:ALA:O    | 2.42                     | 0.49              |
| 1:A:350:SER:CB   | 2:G:382:ARG:HH12 | 1.89                     | 0.49              |
| 1:B:131:ALA:HB1  | 1:B:356:TRP:HB3  | 1.95                     | 0.49              |
| 1:B:151:ILE:HA   | 1:B:164:PRO:HA   | 1.95                     | 0.49              |
| 1:D:151:ILE:HA   | 1:D:164:PRO:HA   | 1.95                     | 0.49              |
| 2:G:410:TYR:HB3  | 2:G:421:LEU:HD11 | 1.94                     | 0.49              |
| 2:H:390:HIS:HA   | 2:H:417:ALA:HB2  | 1.95                     | 0.49              |
| 2:J:414:SER:HA   | 2:J:418:LYS:O    | 2.12                     | 0.49              |
| 1:A:131:ALA:HB1  | 1:A:356:TRP:HB3  | 1.95                     | 0.49              |
| 1:F:151:ILE:HA   | 1:F:164:PRO:HA   | 1.95                     | 0.49              |
| 2:G:383:LEU:O    | 2:G:420:THR:HG23 | 2.12                     | 0.49              |
| 2:G:396:TRP:CZ2  | 2:G:419:ARG:HG2  | 2.48                     | 0.49              |
| 2:K:410:TYR:HB3  | 2:K:421:LEU:HD11 | 1.94                     | 0.49              |
| 1:B:209:VAL:HA   | 1:B:212:ILE:HD12 | 1.95                     | 0.49              |
| 1:C:151:ILE:HA   | 1:C:164:PRO:HA   | 1.95                     | 0.49              |
| 1:C:209:VAL:HA   | 1:C:212:ILE:HD12 | 1.95                     | 0.49              |
| 1:D:14:SER:O     | 1:D:157:ASP:CB   | 2.54                     | 0.49              |
| 2:G:390:HIS:HA   | 2:G:417:ALA:CA   | 2.43                     | 0.49              |
| 2:H:367:LYS:HB3  | 2:H:386:GLU:N    | 2.27                     | 0.49              |
| 2:H:383:LEU:O    | 2:H:420:THR:HG23 | 2.12                     | 0.49              |
| 2:K:367:LYS:HB3  | 2:K:386:GLU:N    | 2.27                     | 0.49              |
| 2:J:366:GLN:H    | 2:J:387:LEU:HA   | 1.78                     | 0.49              |
| 2:K:389:ASP:OD2  | 2:K:392:ALA:N    | 2.45                     | 0.49              |
| 2:L:390:HIS:HA   | 2:L:417:ALA:HB2  | 1.95                     | 0.49              |
| 2:L:406:SER:HB2  | 2:L:410:TYR:HD2  | 1.77                     | 0.49              |
| 1:A:209:VAL:HA   | 1:A:212:ILE:HD12 | 1.95                     | 0.48              |
| 1:B:220:ALA:HB1  | 1:B:226:GLU:HG3  | 1.94                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:367:LYS:HB3  | 2:K:386:GLU:CB   | 2.42                     | 0.48              |
| 2:L:383:LEU:O    | 2:L:420:THR:HG23 | 2.12                     | 0.48              |
| 2:L:414:SER:HA   | 2:L:418:LYS:O    | 2.12                     | 0.48              |
| 2:L:427:SER:O    | 2:L:430:ASP:N    | 2.44                     | 0.48              |
| 1:B:14:SER:O     | 1:B:157:ASP:CB   | 2.54                     | 0.48              |
| 1:C:131:ALA:HB1  | 1:C:356:TRP:HB3  | 1.95                     | 0.48              |
| 2:H:366:GLN:H    | 2:H:387:LEU:HA   | 1.78                     | 0.48              |
| 2:I:390:HIS:HA   | 2:I:417:ALA:CA   | 2.43                     | 0.48              |
| 2:I:410:TYR:HB3  | 2:I:421:LEU:HD11 | 1.94                     | 0.48              |
| 2:L:390:HIS:HA   | 2:L:417:ALA:HA   | 1.95                     | 0.48              |
| 1:B:42:GLY:CA    | 1:D:169:TYR:HA   | 2.33                     | 0.48              |
| 1:D:220:ALA:HB1  | 1:D:226:GLU:HG3  | 1.94                     | 0.48              |
| 2:H:383:LEU:CD1  | 2:H:445:THR:HG21 | 2.44                     | 0.48              |
| 2:I:403:ILE:HG21 | 2:I:421:LEU:HD21 | 1.94                     | 0.48              |
| 2:K:383:LEU:CD1  | 2:K:445:THR:HG21 | 2.44                     | 0.48              |
| 2:G:403:ILE:HG21 | 2:G:421:LEU:HD21 | 1.94                     | 0.48              |
| 2:K:390:HIS:HA   | 2:K:417:ALA:HB2  | 1.95                     | 0.48              |
| 2:K:403:ILE:HG21 | 2:K:421:LEU:HD21 | 1.94                     | 0.48              |
| 2:L:367:LYS:CB   | 2:L:386:GLU:HB3  | 2.43                     | 0.48              |
| 1:D:131:ALA:HB1  | 1:D:356:TRP:HB3  | 1.95                     | 0.48              |
| 2:J:383:LEU:CD1  | 2:J:445:THR:HG21 | 2.44                     | 0.48              |
| 2:L:366:GLN:H    | 2:L:387:LEU:HA   | 1.79                     | 0.48              |
| 1:D:185:LEU:HB2  | 1:D:213:LYS:HZ1  | 1.79                     | 0.48              |
| 1:E:131:ALA:HB1  | 1:E:356:TRP:HB3  | 1.95                     | 0.48              |
| 1:C:185:LEU:HB2  | 1:C:213:LYS:HZ1  | 1.79                     | 0.48              |
| 2:I:390:HIS:HA   | 2:I:417:ALA:HB2  | 1.95                     | 0.48              |
| 1:F:220:ALA:HB1  | 1:F:226:GLU:HG3  | 1.94                     | 0.48              |
| 2:H:390:HIS:HA   | 2:H:417:ALA:CA   | 2.43                     | 0.48              |
| 2:L:390:HIS:HA   | 2:L:417:ALA:CA   | 2.43                     | 0.48              |
| 2:G:390:HIS:HA   | 2:G:417:ALA:HA   | 1.95                     | 0.48              |
| 2:I:383:LEU:CD1  | 2:I:445:THR:HG21 | 2.44                     | 0.48              |
| 2:J:367:LYS:CB   | 2:J:386:GLU:HB3  | 2.43                     | 0.48              |
| 2:L:395:LYS:HA   | 2:L:395:LYS:HE2  | 1.96                     | 0.48              |
| 1:E:14:SER:O     | 1:E:157:ASP:CB   | 2.54                     | 0.48              |
| 2:G:380:LYS:HD3  | 2:G:422:THR:HG23 | 1.96                     | 0.48              |
| 2:J:390:HIS:HA   | 2:J:417:ALA:HA   | 1.96                     | 0.47              |
| 2:K:390:HIS:HA   | 2:K:417:ALA:CA   | 2.43                     | 0.47              |
| 2:L:380:LYS:HD3  | 2:L:422:THR:HG23 | 1.96                     | 0.47              |
| 2:L:383:LEU:CD1  | 2:L:445:THR:HG21 | 2.43                     | 0.47              |
| 2:H:412:PHE:HE1  | 2:H:421:LEU:HD13 | 1.79                     | 0.47              |
| 2:H:434:TYR:O    | 2:H:445:THR:HG22 | 2.14                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:395:LYS:HE2  | 2:J:395:LYS:HA   | 1.96                     | 0.47              |
| 2:J:434:TYR:O    | 2:J:445:THR:HG22 | 2.14                     | 0.47              |
| 2:K:380:LYS:HD3  | 2:K:422:THR:HG23 | 1.96                     | 0.47              |
| 2:L:412:PHE:HE1  | 2:L:421:LEU:HD13 | 1.79                     | 0.47              |
| 1:A:14:SER:O     | 1:A:157:ASP:CB   | 2.54                     | 0.47              |
| 2:G:390:HIS:HA   | 2:G:417:ALA:HB2  | 1.95                     | 0.47              |
| 2:I:367:LYS:CB   | 2:I:386:GLU:HB3  | 2.43                     | 0.47              |
| 2:I:380:LYS:HD3  | 2:I:422:THR:HG23 | 1.96                     | 0.47              |
| 2:J:412:PHE:HE1  | 2:J:421:LEU:HD13 | 1.79                     | 0.47              |
| 2:K:366:GLN:H    | 2:K:387:LEU:HA   | 1.78                     | 0.47              |
| 2:K:367:LYS:CB   | 2:K:386:GLU:HB3  | 2.43                     | 0.47              |
| 1:F:14:SER:O     | 1:F:157:ASP:CB   | 2.54                     | 0.47              |
| 2:G:367:LYS:CB   | 2:G:386:GLU:HB3  | 2.43                     | 0.47              |
| 2:G:383:LEU:CD1  | 2:G:445:THR:HG21 | 2.44                     | 0.47              |
| 2:G:423:ILE:HG22 | 2:G:426:CYS:SG   | 2.55                     | 0.47              |
| 2:I:390:HIS:HA   | 2:I:417:ALA:HA   | 1.95                     | 0.47              |
| 2:J:380:LYS:HD3  | 2:J:422:THR:HG23 | 1.96                     | 0.47              |
| 2:K:395:LYS:HE2  | 2:K:395:LYS:HA   | 1.96                     | 0.47              |
| 2:K:423:ILE:HG22 | 2:K:426:CYS:SG   | 2.55                     | 0.47              |
| 2:G:366:GLN:H    | 2:G:387:LEU:HA   | 1.78                     | 0.47              |
| 2:H:380:LYS:HD3  | 2:H:422:THR:HG23 | 1.96                     | 0.47              |
| 2:J:390:HIS:HA   | 2:J:417:ALA:CA   | 2.43                     | 0.47              |
| 2:G:398:LYS:HD2  | 2:G:434:TYR:HE1  | 1.79                     | 0.47              |
| 2:G:412:PHE:HE1  | 2:G:421:LEU:HD13 | 1.79                     | 0.47              |
| 2:H:367:LYS:CB   | 2:H:386:GLU:HB3  | 2.43                     | 0.47              |
| 2:H:384:THR:HG23 | 2:H:418:LYS:HZ1  | 1.80                     | 0.47              |
| 2:H:390:HIS:HA   | 2:H:417:ALA:HA   | 1.96                     | 0.47              |
| 2:H:395:LYS:HE2  | 2:H:395:LYS:HA   | 1.96                     | 0.47              |
| 2:I:384:THR:HG23 | 2:I:418:LYS:HZ1  | 1.80                     | 0.47              |
| 2:I:395:LYS:HE2  | 2:I:395:LYS:HA   | 1.96                     | 0.47              |
| 2:I:412:PHE:HE1  | 2:I:421:LEU:HD13 | 1.79                     | 0.47              |
| 2:J:372:ALA:HA   | 2:J:446:GLU:H    | 1.80                     | 0.47              |
| 2:J:423:ILE:HG22 | 2:J:426:CYS:SG   | 2.55                     | 0.47              |
| 2:K:390:HIS:HA   | 2:K:417:ALA:HA   | 1.96                     | 0.47              |
| 2:K:399:ASN:N    | 2:K:433:ALA:O    | 2.42                     | 0.47              |
| 2:K:434:TYR:O    | 2:K:445:THR:HG22 | 2.14                     | 0.47              |
| 2:L:372:ALA:HA   | 2:L:446:GLU:H    | 1.80                     | 0.47              |
| 2:L:434:TYR:O    | 2:L:445:THR:HG22 | 2.14                     | 0.47              |
| 2:H:403:ILE:HD13 | 2:H:421:LEU:CD2  | 2.45                     | 0.47              |
| 2:H:423:ILE:HG22 | 2:H:426:CYS:SG   | 2.55                     | 0.47              |
| 2:I:366:GLN:H    | 2:I:387:LEU:HA   | 1.78                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:398:LYS:HD2  | 2:I:434:TYR:HE1  | 1.79                     | 0.47              |
| 2:I:423:ILE:HG22 | 2:I:426:CYS:SG   | 2.55                     | 0.47              |
| 2:J:403:ILE:HD13 | 2:J:421:LEU:CD2  | 2.45                     | 0.47              |
| 1:E:23:GLY:CA    | 2:K:425:GLN:NE2  | 2.66                     | 0.47              |
| 2:G:433:ALA:HA   | 2:G:445:THR:O    | 2.15                     | 0.47              |
| 2:H:398:LYS:HD2  | 2:H:434:TYR:HE1  | 1.79                     | 0.47              |
| 2:K:398:LYS:HD2  | 2:K:434:TYR:HE1  | 1.79                     | 0.47              |
| 2:K:412:PHE:HE1  | 2:K:421:LEU:HD13 | 1.79                     | 0.47              |
| 2:L:398:LYS:HD2  | 2:L:434:TYR:CE1  | 2.49                     | 0.47              |
| 1:D:42:GLY:CA    | 1:F:169:TYR:HA   | 2.35                     | 0.46              |
| 2:G:398:LYS:HD2  | 2:G:434:TYR:CE1  | 2.50                     | 0.46              |
| 2:G:434:TYR:O    | 2:G:445:THR:HG22 | 2.14                     | 0.46              |
| 2:K:370:GLU:HG3  | 2:K:373:TYR:HE1  | 1.80                     | 0.46              |
| 2:K:384:THR:HG23 | 2:K:418:LYS:HZ1  | 1.80                     | 0.46              |
| 2:K:403:ILE:HD13 | 2:K:421:LEU:CD2  | 2.45                     | 0.46              |
| 1:A:140:LEU:HD11 | 1:A:346:LEU:HD22 | 1.98                     | 0.46              |
| 1:C:140:LEU:HD11 | 1:C:346:LEU:HD22 | 1.98                     | 0.46              |
| 1:E:140:LEU:HD11 | 1:E:346:LEU:HD22 | 1.97                     | 0.46              |
| 2:H:372:ALA:HA   | 2:H:446:GLU:H    | 1.80                     | 0.46              |
| 2:I:398:LYS:HD2  | 2:I:434:TYR:CE1  | 2.49                     | 0.46              |
| 2:L:383:LEU:HD11 | 2:L:445:THR:HG21 | 1.97                     | 0.46              |
| 2:L:403:ILE:HD13 | 2:L:421:LEU:CD2  | 2.45                     | 0.46              |
| 2:G:399:ASN:N    | 2:G:433:ALA:O    | 2.42                     | 0.46              |
| 2:H:394:VAL:CG2  | 2:H:396:TRP:CE2  | 2.99                     | 0.46              |
| 2:H:397:LEU:C    | 2:H:403:ILE:HG13 | 2.41                     | 0.46              |
| 2:J:383:LEU:HD11 | 2:J:445:THR:HG21 | 1.97                     | 0.46              |
| 2:J:398:LYS:HD2  | 2:J:434:TYR:HE1  | 1.79                     | 0.46              |
| 2:L:423:ILE:HG22 | 2:L:426:CYS:SG   | 2.55                     | 0.46              |
| 1:B:155:SER:HB3  | 1:B:304:THR:HG23 | 1.98                     | 0.46              |
| 1:D:140:LEU:HD11 | 1:D:346:LEU:HD22 | 1.97                     | 0.46              |
| 2:I:433:ALA:HA   | 2:I:445:THR:O    | 2.15                     | 0.46              |
| 2:I:434:TYR:O    | 2:I:445:THR:HG22 | 2.14                     | 0.46              |
| 1:E:210:ARG:O    | 1:E:213:LYS:HB3  | 2.16                     | 0.46              |
| 1:F:23:GLY:O     | 2:L:425:GLN:OE1  | 2.34                     | 0.46              |
| 2:H:405:MET:HA   | 2:H:410:TYR:O    | 2.16                     | 0.46              |
| 2:J:397:LEU:C    | 2:J:403:ILE:HG13 | 2.41                     | 0.46              |
| 2:L:398:LYS:HD2  | 2:L:434:TYR:HE1  | 1.79                     | 0.46              |
| 2:L:433:ALA:HA   | 2:L:445:THR:O    | 2.15                     | 0.46              |
| 1:A:210:ARG:O    | 1:A:213:LYS:HB3  | 2.16                     | 0.46              |
| 1:B:140:LEU:HD11 | 1:B:346:LEU:HD22 | 1.97                     | 0.46              |
| 1:C:210:ARG:O    | 1:C:213:LYS:HB3  | 2.16                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:259:GLU:OE2  | 1:C:312:ARG:NH2  | 2.48                     | 0.46              |
| 1:F:140:LEU:HD11 | 1:F:346:LEU:HD22 | 1.98                     | 0.46              |
| 2:G:372:ALA:HA   | 2:G:446:GLU:H    | 1.80                     | 0.46              |
| 2:G:395:LYS:HA   | 2:G:395:LYS:HE2  | 1.96                     | 0.46              |
| 2:H:383:LEU:HD11 | 2:H:445:THR:HG21 | 1.97                     | 0.46              |
| 2:H:398:LYS:HD2  | 2:H:434:TYR:CE1  | 2.49                     | 0.46              |
| 2:I:394:VAL:CG2  | 2:I:396:TRP:CE2  | 2.99                     | 0.46              |
| 2:L:365:PHE:CG   | 2:L:368:LYS:HG2  | 2.51                     | 0.46              |
| 1:E:155:SER:HB3  | 1:E:304:THR:HG23 | 1.98                     | 0.46              |
| 2:G:383:LEU:HD11 | 2:G:445:THR:HG21 | 1.97                     | 0.46              |
| 2:I:370:GLU:HG3  | 2:I:373:TYR:HE1  | 1.80                     | 0.46              |
| 2:J:394:VAL:CG2  | 2:J:396:TRP:CE2  | 2.99                     | 0.46              |
| 2:J:398:LYS:HD2  | 2:J:434:TYR:CE1  | 2.50                     | 0.46              |
| 2:J:405:MET:HA   | 2:J:410:TYR:O    | 2.16                     | 0.46              |
| 2:K:398:LYS:HD2  | 2:K:434:TYR:CE1  | 2.50                     | 0.46              |
| 2:L:394:VAL:CG2  | 2:L:396:TRP:CE2  | 2.99                     | 0.46              |
| 1:C:49:GLN:OE1   | 1:C:53:TYR:OH    | 2.23                     | 0.46              |
| 1:D:155:SER:HB3  | 1:D:304:THR:HG23 | 1.98                     | 0.46              |
| 2:G:394:VAL:CG2  | 2:G:396:TRP:CE2  | 2.99                     | 0.46              |
| 2:K:373:TYR:CD2  | 2:K:383:LEU:HD13 | 2.51                     | 0.46              |
| 2:H:370:GLU:HG3  | 2:H:373:TYR:HE1  | 1.80                     | 0.46              |
| 2:H:373:TYR:CD2  | 2:H:383:LEU:HD13 | 2.51                     | 0.46              |
| 2:I:373:TYR:CD2  | 2:I:383:LEU:HD13 | 2.51                     | 0.46              |
| 2:I:403:ILE:HD13 | 2:I:421:LEU:CD2  | 2.45                     | 0.46              |
| 2:J:373:TYR:CD2  | 2:J:383:LEU:HD13 | 2.51                     | 0.46              |
| 2:J:433:ALA:HA   | 2:J:445:THR:O    | 2.15                     | 0.46              |
| 2:K:372:ALA:HA   | 2:K:446:GLU:H    | 1.80                     | 0.46              |
| 2:K:394:VAL:CG2  | 2:K:396:TRP:CE2  | 2.99                     | 0.46              |
| 2:K:397:LEU:C    | 2:K:403:ILE:HG13 | 2.41                     | 0.46              |
| 2:L:368:LYS:HB3  | 2:L:443:CYS:HB2  | 1.98                     | 0.46              |
| 2:L:397:LEU:C    | 2:L:403:ILE:HG13 | 2.41                     | 0.46              |
| 1:C:23:GLY:CA    | 2:I:425:GLN:NE2  | 2.70                     | 0.46              |
| 1:F:155:SER:HB3  | 1:F:304:THR:HG23 | 1.98                     | 0.46              |
| 2:G:373:TYR:CD2  | 2:G:383:LEU:HD13 | 2.51                     | 0.46              |
| 2:G:397:LEU:C    | 2:G:403:ILE:HG13 | 2.41                     | 0.46              |
| 2:G:403:ILE:HD13 | 2:G:421:LEU:CD2  | 2.45                     | 0.46              |
| 2:H:433:ALA:HA   | 2:H:445:THR:O    | 2.15                     | 0.46              |
| 2:I:383:LEU:HD11 | 2:I:445:THR:HG21 | 1.97                     | 0.46              |
| 2:I:396:TRP:HZ2  | 2:I:419:ARG:CG   | 2.29                     | 0.46              |
| 2:J:365:PHE:CG   | 2:J:368:LYS:HG2  | 2.51                     | 0.46              |
| 2:K:368:LYS:HB3  | 2:K:443:CYS:HB2  | 1.98                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:370:GLU:HG3  | 2:L:373:TYR:HE1  | 1.80                     | 0.46              |
| 2:L:373:TYR:CD2  | 2:L:383:LEU:HD13 | 2.51                     | 0.46              |
| 2:G:370:GLU:HG3  | 2:G:373:TYR:HE1  | 1.80                     | 0.45              |
| 2:J:396:TRP:HZ2  | 2:J:419:ARG:CG   | 2.30                     | 0.45              |
| 2:G:365:PHE:CG   | 2:G:368:LYS:HG2  | 2.51                     | 0.45              |
| 2:G:405:MET:HA   | 2:G:410:TYR:O    | 2.16                     | 0.45              |
| 2:G:427:SER:CA   | 2:G:449:VAL:HG11 | 2.47                     | 0.45              |
| 2:I:368:LYS:HB3  | 2:I:443:CYS:HB2  | 1.99                     | 0.45              |
| 2:J:370:GLU:HG3  | 2:J:373:TYR:HE1  | 1.80                     | 0.45              |
| 2:K:396:TRP:HZ2  | 2:K:419:ARG:CG   | 2.30                     | 0.45              |
| 2:L:405:MET:HA   | 2:L:410:TYR:O    | 2.16                     | 0.45              |
| 1:B:210:ARG:O    | 1:B:213:LYS:HB3  | 2.16                     | 0.45              |
| 2:H:365:PHE:HA   | 2:H:387:LEU:HD23 | 1.99                     | 0.45              |
| 2:H:365:PHE:CG   | 2:H:368:LYS:HG2  | 2.51                     | 0.45              |
| 2:H:396:TRP:HZ2  | 2:H:419:ARG:CG   | 2.30                     | 0.45              |
| 2:H:402:GLU:OE1  | 2:H:402:GLU:O    | 2.35                     | 0.45              |
| 2:J:368:LYS:HB3  | 2:J:443:CYS:HB2  | 1.98                     | 0.45              |
| 2:K:375:VAL:CG1  | 2:K:449:VAL:HG22 | 2.46                     | 0.45              |
| 2:K:383:LEU:HD11 | 2:K:445:THR:HG21 | 1.97                     | 0.45              |
| 2:K:433:ALA:HA   | 2:K:445:THR:O    | 2.15                     | 0.45              |
| 1:C:155:SER:HB3  | 1:C:304:THR:HG23 | 1.98                     | 0.45              |
| 1:E:49:GLN:OE1   | 1:E:53:TYR:OH    | 2.23                     | 0.45              |
| 2:H:368:LYS:HB3  | 2:H:443:CYS:HB2  | 1.98                     | 0.45              |
| 2:I:372:ALA:HA   | 2:I:446:GLU:H    | 1.80                     | 0.45              |
| 2:I:397:LEU:C    | 2:I:403:ILE:HG13 | 2.41                     | 0.45              |
| 2:J:402:GLU:OE1  | 2:J:402:GLU:O    | 2.35                     | 0.45              |
| 2:J:427:SER:CA   | 2:J:449:VAL:HG11 | 2.47                     | 0.45              |
| 1:B:259:GLU:OE2  | 1:B:312:ARG:NH2  | 2.48                     | 0.45              |
| 2:G:368:LYS:HB3  | 2:G:443:CYS:HB2  | 1.98                     | 0.45              |
| 2:I:365:PHE:CG   | 2:I:368:LYS:HG2  | 2.51                     | 0.45              |
| 2:J:365:PHE:HA   | 2:J:387:LEU:HD23 | 1.99                     | 0.45              |
| 2:L:375:VAL:CG1  | 2:L:449:VAL:HG22 | 2.46                     | 0.45              |
| 2:L:396:TRP:HZ2  | 2:L:419:ARG:CG   | 2.30                     | 0.45              |
| 2:L:402:GLU:OE1  | 2:L:402:GLU:O    | 2.35                     | 0.45              |
| 2:I:405:MET:HA   | 2:I:410:TYR:O    | 2.16                     | 0.45              |
| 2:K:405:MET:HA   | 2:K:410:TYR:O    | 2.16                     | 0.45              |
| 1:A:155:SER:HB3  | 1:A:304:THR:HG23 | 1.98                     | 0.45              |
| 2:G:396:TRP:HZ2  | 2:G:419:ARG:CG   | 2.30                     | 0.45              |
| 2:G:402:GLU:OE1  | 2:G:402:GLU:O    | 2.35                     | 0.45              |
| 2:I:375:VAL:CG1  | 2:I:449:VAL:HG22 | 2.46                     | 0.45              |
| 2:K:365:PHE:CG   | 2:K:368:LYS:HG2  | 2.51                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:427:SER:CA   | 2:K:449:VAL:HG11 | 2.47                     | 0.45              |
| 2:L:365:PHE:HA   | 2:L:387:LEU:HD23 | 1.99                     | 0.45              |
| 1:D:210:ARG:O    | 1:D:213:LYS:HB3  | 2.16                     | 0.45              |
| 2:G:365:PHE:HA   | 2:G:387:LEU:HD23 | 1.99                     | 0.45              |
| 2:H:427:SER:CA   | 2:H:449:VAL:HG11 | 2.47                     | 0.45              |
| 2:K:379:HIS:O    | 2:K:426:CYS:N    | 2.47                     | 0.45              |
| 2:L:427:SER:CA   | 2:L:449:VAL:HG11 | 2.47                     | 0.45              |
| 1:F:151:ILE:HD13 | 1:F:278:THR:HG23 | 1.99                     | 0.45              |
| 1:F:210:ARG:O    | 1:F:213:LYS:HB3  | 2.16                     | 0.45              |
| 2:I:396:TRP:CZ2  | 2:I:419:ARG:CG   | 3.00                     | 0.45              |
| 2:G:396:TRP:CZ2  | 2:G:419:ARG:CG   | 3.00                     | 0.45              |
| 2:I:402:GLU:O    | 2:I:402:GLU:OE1  | 2.35                     | 0.45              |
| 2:I:427:SER:CA   | 2:I:449:VAL:HG11 | 2.47                     | 0.45              |
| 2:H:382:ARG:CZ   | 2:H:413:GLU:OE1  | 2.65                     | 0.44              |
| 2:J:375:VAL:CG1  | 2:J:449:VAL:HG22 | 2.46                     | 0.44              |
| 2:J:383:LEU:HD11 | 2:J:434:TYR:CD2  | 2.52                     | 0.44              |
| 2:L:383:LEU:HD11 | 2:L:434:TYR:CD2  | 2.52                     | 0.44              |
| 1:D:43:VAL:HG23  | 1:F:170:ALA:HB3  | 2.00                     | 0.44              |
| 1:E:12:ASN:HD21  | 1:E:105:LEU:HD12 | 1.83                     | 0.44              |
| 2:G:375:VAL:CG1  | 2:G:449:VAL:HG22 | 2.46                     | 0.44              |
| 2:K:382:ARG:CZ   | 2:K:413:GLU:OE1  | 2.65                     | 0.44              |
| 2:G:383:LEU:HD11 | 2:G:434:TYR:CD2  | 2.52                     | 0.44              |
| 2:K:362:SER:O    | 2:K:365:PHE:O    | 2.35                     | 0.44              |
| 2:L:362:SER:O    | 2:L:365:PHE:O    | 2.35                     | 0.44              |
| 2:L:382:ARG:CZ   | 2:L:413:GLU:OE1  | 2.65                     | 0.44              |
| 1:A:151:ILE:HD13 | 1:A:278:THR:HG23 | 1.99                     | 0.44              |
| 1:B:43:VAL:HG23  | 1:D:170:ALA:HB3  | 2.00                     | 0.44              |
| 2:I:382:ARG:CZ   | 2:I:413:GLU:OE1  | 2.65                     | 0.44              |
| 2:J:382:ARG:CZ   | 2:J:413:GLU:OE1  | 2.65                     | 0.44              |
| 2:K:402:GLU:O    | 2:K:402:GLU:OE1  | 2.35                     | 0.44              |
| 1:B:151:ILE:HD13 | 1:B:278:THR:HG23 | 1.99                     | 0.44              |
| 1:D:151:ILE:HD13 | 1:D:278:THR:HG23 | 1.99                     | 0.44              |
| 2:H:375:VAL:CG1  | 2:H:449:VAL:HG22 | 2.46                     | 0.44              |
| 2:K:396:TRP:CZ2  | 2:K:419:ARG:CG   | 3.00                     | 0.44              |
| 1:C:12:ASN:HD21  | 1:C:105:LEU:HD12 | 1.83                     | 0.44              |
| 1:F:259:GLU:OE2  | 1:F:312:ARG:NH2  | 2.48                     | 0.44              |
| 2:H:396:TRP:CZ2  | 2:H:419:ARG:CG   | 3.00                     | 0.44              |
| 2:H:396:TRP:HB3  | 2:H:403:ILE:HD12 | 2.00                     | 0.44              |
| 2:I:362:SER:O    | 2:I:365:PHE:O    | 2.35                     | 0.44              |
| 2:J:362:SER:O    | 2:J:365:PHE:O    | 2.35                     | 0.44              |
| 2:L:379:HIS:O    | 2:L:426:CYS:N    | 2.47                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:396:TRP:CZ2  | 2:L:419:ARG:CG   | 3.00                     | 0.44              |
| 1:A:259:GLU:OE2  | 1:A:312:ARG:NH2  | 2.48                     | 0.44              |
| 1:C:151:ILE:HD13 | 1:C:278:THR:HG23 | 1.99                     | 0.44              |
| 1:E:151:ILE:HD13 | 1:E:278:THR:HG23 | 1.99                     | 0.44              |
| 2:G:434:TYR:CE2  | 2:G:447:LEU:HB2  | 2.53                     | 0.44              |
| 2:I:410:TYR:HE1  | 2:I:434:TYR:CE1  | 2.36                     | 0.44              |
| 2:K:365:PHE:HA   | 2:K:387:LEU:HD23 | 1.99                     | 0.44              |
| 2:G:376:SER:O    | 2:G:379:HIS:HB3  | 2.18                     | 0.44              |
| 2:G:382:ARG:CZ   | 2:G:413:GLU:OE1  | 2.65                     | 0.44              |
| 2:H:362:SER:O    | 2:H:365:PHE:O    | 2.35                     | 0.44              |
| 2:I:365:PHE:HA   | 2:I:387:LEU:HD23 | 1.99                     | 0.44              |
| 2:I:395:LYS:HB3  | 2:I:397:LEU:CD1  | 2.48                     | 0.44              |
| 2:K:392:ALA:O    | 2:K:419:ARG:NH1  | 2.51                     | 0.44              |
| 1:A:42:GLY:CA    | 1:C:169:TYR:HA   | 2.37                     | 0.43              |
| 1:A:209:VAL:O    | 1:A:212:ILE:HB   | 2.18                     | 0.43              |
| 2:G:395:LYS:HB3  | 2:G:397:LEU:CD1  | 2.48                     | 0.43              |
| 2:J:396:TRP:CZ2  | 2:J:419:ARG:CG   | 3.00                     | 0.43              |
| 2:K:395:LYS:HB3  | 2:K:397:LEU:CD1  | 2.48                     | 0.43              |
| 2:L:392:ALA:O    | 2:L:419:ARG:NH1  | 2.51                     | 0.43              |
| 2:L:396:TRP:HB3  | 2:L:403:ILE:HD12 | 2.00                     | 0.43              |
| 2:G:396:TRP:HB3  | 2:G:403:ILE:HD12 | 2.00                     | 0.43              |
| 2:I:376:SER:O    | 2:I:379:HIS:HB3  | 2.18                     | 0.43              |
| 2:I:384:THR:HG23 | 2:I:418:LYS:CE   | 2.49                     | 0.43              |
| 2:I:396:TRP:HB3  | 2:I:403:ILE:HD12 | 2.00                     | 0.43              |
| 2:G:362:SER:O    | 2:G:365:PHE:O    | 2.35                     | 0.43              |
| 2:H:395:LYS:HB3  | 2:H:397:LEU:CD1  | 2.48                     | 0.43              |
| 2:H:410:TYR:HE1  | 2:H:434:TYR:CE1  | 2.36                     | 0.43              |
| 2:J:384:THR:HG23 | 2:J:418:LYS:CE   | 2.49                     | 0.43              |
| 2:J:384:THR:HG23 | 2:J:418:LYS:HZ1  | 1.82                     | 0.43              |
| 2:J:396:TRP:HB3  | 2:J:403:ILE:HD12 | 2.00                     | 0.43              |
| 2:L:376:SER:O    | 2:L:379:HIS:HB3  | 2.18                     | 0.43              |
| 2:L:435:GLN:HG3  | 2:L:444:SER:OG   | 2.19                     | 0.43              |
| 1:C:43:VAL:HG23  | 1:E:170:ALA:HB3  | 1.99                     | 0.43              |
| 1:C:209:VAL:O    | 1:C:212:ILE:HB   | 2.18                     | 0.43              |
| 2:G:384:THR:HG23 | 2:G:418:LYS:CE   | 2.49                     | 0.43              |
| 2:I:377:LYS:HA   | 2:I:426:CYS:O    | 2.18                     | 0.43              |
| 2:I:434:TYR:CE2  | 2:I:447:LEU:HB2  | 2.53                     | 0.43              |
| 2:K:405:MET:HE2  | 2:K:412:PHE:H    | 1.84                     | 0.43              |
| 2:L:405:MET:HE2  | 2:L:412:PHE:H    | 1.84                     | 0.43              |
| 1:A:121:GLN:HE21 | 1:A:367:PRO:HG3  | 1.84                     | 0.43              |
| 2:G:392:ALA:O    | 2:G:419:ARG:NH1  | 2.52                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:376:SER:O    | 2:H:379:HIS:HB3  | 2.18                     | 0.43              |
| 2:H:392:ALA:O    | 2:H:419:ARG:NH1  | 2.52                     | 0.43              |
| 2:H:405:MET:HE2  | 2:H:412:PHE:H    | 1.83                     | 0.43              |
| 2:I:383:LEU:HD11 | 2:I:434:TYR:CD2  | 2.52                     | 0.43              |
| 2:I:405:MET:HE2  | 2:I:412:PHE:H    | 1.84                     | 0.43              |
| 2:J:435:GLN:HG3  | 2:J:444:SER:OG   | 2.19                     | 0.43              |
| 2:K:376:SER:O    | 2:K:379:HIS:HB3  | 2.18                     | 0.43              |
| 2:K:384:THR:HG23 | 2:K:418:LYS:CE   | 2.49                     | 0.43              |
| 2:K:396:TRP:HB3  | 2:K:403:ILE:HD12 | 2.00                     | 0.43              |
| 2:L:434:TYR:CE2  | 2:L:447:LEU:HB2  | 2.53                     | 0.43              |
| 1:A:12:ASN:HD21  | 1:A:105:LEU:HD12 | 1.83                     | 0.43              |
| 1:B:10:CYS:SG    | 1:B:11:ASP:N     | 2.92                     | 0.43              |
| 1:E:209:VAL:O    | 1:E:212:ILE:HB   | 2.18                     | 0.43              |
| 2:L:395:LYS:HB3  | 2:L:397:LEU:CD1  | 2.48                     | 0.43              |
| 1:D:10:CYS:SG    | 1:D:11:ASP:N     | 2.92                     | 0.43              |
| 2:H:384:THR:HG23 | 2:H:418:LYS:CE   | 2.49                     | 0.43              |
| 2:J:434:TYR:CE2  | 2:J:447:LEU:HB2  | 2.53                     | 0.43              |
| 1:C:121:GLN:HE21 | 1:C:367:PRO:HG3  | 1.84                     | 0.43              |
| 1:F:209:VAL:O    | 1:F:212:ILE:HB   | 2.18                     | 0.43              |
| 2:G:405:MET:HE2  | 2:G:412:PHE:H    | 1.83                     | 0.43              |
| 2:H:435:GLN:HG3  | 2:H:444:SER:OG   | 2.19                     | 0.43              |
| 2:I:392:ALA:O    | 2:I:419:ARG:NH1  | 2.52                     | 0.43              |
| 2:J:377:LYS:HA   | 2:J:426:CYS:O    | 2.18                     | 0.43              |
| 2:J:395:LYS:HB3  | 2:J:397:LEU:CD1  | 2.48                     | 0.43              |
| 2:K:410:TYR:HE1  | 2:K:434:TYR:CE1  | 2.36                     | 0.43              |
| 2:L:377:LYS:HA   | 2:L:426:CYS:O    | 2.18                     | 0.43              |
| 1:B:43:VAL:CG2   | 1:D:170:ALA:HB3  | 2.48                     | 0.43              |
| 1:B:44:MET:HG3   | 1:D:168:GLY:HA2  | 2.00                     | 0.43              |
| 2:H:434:TYR:CE2  | 2:H:447:LEU:HB2  | 2.53                     | 0.43              |
| 2:I:435:GLN:HG3  | 2:I:444:SER:OG   | 2.19                     | 0.43              |
| 2:J:376:SER:O    | 2:J:379:HIS:HB3  | 2.18                     | 0.43              |
| 2:K:377:LYS:HA   | 2:K:426:CYS:O    | 2.18                     | 0.43              |
| 2:J:392:ALA:O    | 2:J:419:ARG:NH1  | 2.52                     | 0.43              |
| 2:J:432:ALA:O    | 2:J:447:LEU:N    | 2.52                     | 0.43              |
| 2:K:362:SER:C    | 2:K:365:PHE:O    | 2.62                     | 0.43              |
| 1:A:10:CYS:SG    | 1:A:11:ASP:N     | 2.92                     | 0.42              |
| 1:C:43:VAL:CG2   | 1:E:170:ALA:HB3  | 2.49                     | 0.42              |
| 1:D:12:ASN:HD21  | 1:D:105:LEU:HD12 | 1.83                     | 0.42              |
| 1:D:44:MET:HG3   | 1:F:168:GLY:HA2  | 2.01                     | 0.42              |
| 1:F:10:CYS:SG    | 1:F:11:ASP:N     | 2.92                     | 0.42              |
| 1:F:12:ASN:HD21  | 1:F:105:LEU:HD12 | 1.83                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:409:LYS:O    | 2:G:410:TYR:CG   | 2.72                     | 0.42              |
| 2:G:410:TYR:HE1  | 2:G:434:TYR:CE1  | 2.36                     | 0.42              |
| 2:G:435:GLN:HG3  | 2:G:444:SER:OG   | 2.19                     | 0.42              |
| 2:H:383:LEU:HD11 | 2:H:434:TYR:CD2  | 2.52                     | 0.42              |
| 2:K:435:GLN:HG3  | 2:K:444:SER:OG   | 2.19                     | 0.42              |
| 1:A:241:GLU:HA   | 1:A:247:VAL:HG12 | 2.01                     | 0.42              |
| 1:A:349:LEU:HB3  | 2:G:413:GLU:OE2  | 2.19                     | 0.42              |
| 1:C:241:GLU:HA   | 1:C:247:VAL:HG12 | 2.01                     | 0.42              |
| 2:H:377:LYS:HA   | 2:H:426:CYS:O    | 2.18                     | 0.42              |
| 2:H:437:VAL:HG13 | 2:H:442:LYS:HB3  | 2.01                     | 0.42              |
| 2:I:372:ALA:HB1  | 2:I:446:GLU:O    | 2.20                     | 0.42              |
| 2:I:409:LYS:O    | 2:I:410:TYR:CG   | 2.73                     | 0.42              |
| 2:J:390:HIS:HA   | 2:J:417:ALA:CB   | 2.49                     | 0.42              |
| 2:J:437:VAL:HG13 | 2:J:442:LYS:HB3  | 2.02                     | 0.42              |
| 2:K:394:VAL:HG23 | 2:K:396:TRP:CD2  | 2.55                     | 0.42              |
| 2:K:434:TYR:CE2  | 2:K:447:LEU:HB2  | 2.53                     | 0.42              |
| 2:L:384:THR:HG23 | 2:L:418:LYS:CE   | 2.49                     | 0.42              |
| 2:L:410:TYR:HE1  | 2:L:434:TYR:CE1  | 2.36                     | 0.42              |
| 1:B:209:VAL:O    | 1:B:212:ILE:HB   | 2.18                     | 0.42              |
| 1:C:10:CYS:SG    | 1:C:11:ASP:N     | 2.92                     | 0.42              |
| 1:D:209:VAL:O    | 1:D:212:ILE:HB   | 2.18                     | 0.42              |
| 1:F:121:GLN:HE21 | 1:F:367:PRO:HG3  | 1.84                     | 0.42              |
| 2:H:372:ALA:HB1  | 2:H:446:GLU:O    | 2.20                     | 0.42              |
| 2:H:432:ALA:O    | 2:H:447:LEU:N    | 2.52                     | 0.42              |
| 2:K:409:LYS:O    | 2:K:410:TYR:CG   | 2.73                     | 0.42              |
| 2:L:372:ALA:HB1  | 2:L:446:GLU:O    | 2.19                     | 0.42              |
| 2:L:390:HIS:HA   | 2:L:417:ALA:CB   | 2.49                     | 0.42              |
| 1:E:121:GLN:HE21 | 1:E:367:PRO:HG3  | 1.84                     | 0.42              |
| 2:G:390:HIS:HA   | 2:G:417:ALA:CB   | 2.49                     | 0.42              |
| 2:H:390:HIS:HA   | 2:H:417:ALA:CB   | 2.49                     | 0.42              |
| 2:J:372:ALA:HB1  | 2:J:446:GLU:O    | 2.19                     | 0.42              |
| 1:B:12:ASN:HD21  | 1:B:105:LEU:HD12 | 1.83                     | 0.42              |
| 1:B:48:GLY:HA3   | 2:J:416:GLY:H    | 1.84                     | 0.42              |
| 1:D:121:GLN:HE21 | 1:D:367:PRO:HG3  | 1.84                     | 0.42              |
| 2:H:362:SER:C    | 2:H:365:PHE:O    | 2.62                     | 0.42              |
| 2:J:405:MET:HE2  | 2:J:412:PHE:H    | 1.83                     | 0.42              |
| 2:J:410:TYR:HE1  | 2:J:434:TYR:CE1  | 2.36                     | 0.42              |
| 2:L:362:SER:C    | 2:L:365:PHE:O    | 2.62                     | 0.42              |
| 1:B:164:PRO:HG2  | 1:B:171:LEU:HB2  | 2.02                     | 0.42              |
| 1:E:241:GLU:HA   | 1:E:247:VAL:HG12 | 2.01                     | 0.42              |
| 2:G:372:ALA:HB1  | 2:G:446:GLU:O    | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:362:SER:C    | 2:I:365:PHE:O    | 2.62                     | 0.42              |
| 2:J:362:SER:C    | 2:J:365:PHE:O    | 2.62                     | 0.42              |
| 2:L:437:VAL:HG13 | 2:L:442:LYS:HB3  | 2.02                     | 0.42              |
| 1:D:164:PRO:HG2  | 1:D:171:LEU:HB2  | 2.02                     | 0.42              |
| 1:E:106:THR:HB   | 1:E:137:GLN:HG2  | 2.02                     | 0.42              |
| 2:H:409:LYS:O    | 2:H:410:TYR:CG   | 2.73                     | 0.42              |
| 2:I:379:HIS:O    | 2:I:426:CYS:N    | 2.47                     | 0.42              |
| 2:K:372:ALA:HB1  | 2:K:446:GLU:O    | 2.19                     | 0.42              |
| 2:K:396:TRP:CE3  | 2:K:412:PHE:CE2  | 3.08                     | 0.42              |
| 1:B:121:GLN:HE21 | 1:B:367:PRO:HG3  | 1.84                     | 0.42              |
| 1:C:44:MET:HG3   | 1:E:168:GLY:HA2  | 2.01                     | 0.42              |
| 1:C:106:THR:HB   | 1:C:137:GLN:HG2  | 2.02                     | 0.42              |
| 2:I:369:LEU:CD2  | 2:I:383:LEU:HB3  | 2.50                     | 0.42              |
| 1:A:106:THR:HB   | 1:A:137:GLN:HG2  | 2.02                     | 0.42              |
| 2:G:377:LYS:HA   | 2:G:426:CYS:O    | 2.18                     | 0.42              |
| 2:I:390:HIS:HA   | 2:I:417:ALA:CB   | 2.49                     | 0.42              |
| 2:I:432:ALA:O    | 2:I:447:LEU:N    | 2.52                     | 0.42              |
| 1:E:18:LYS:HA    | 1:E:29:ALA:O     | 2.20                     | 0.42              |
| 1:F:164:PRO:HG2  | 1:F:171:LEU:HB2  | 2.02                     | 0.42              |
| 1:F:349:LEU:CD2  | 2:L:413:GLU:CD   | 2.90                     | 0.42              |
| 2:K:383:LEU:HD11 | 2:K:434:TYR:CD2  | 2.52                     | 0.42              |
| 1:D:14:SER:OG    | 1:D:158:GLY:HA3  | 2.20                     | 0.41              |
| 1:E:10:CYS:SG    | 1:E:11:ASP:N     | 2.92                     | 0.41              |
| 2:G:369:LEU:CD2  | 2:G:383:LEU:HB3  | 2.50                     | 0.41              |
| 2:G:369:LEU:HD23 | 2:G:385:VAL:HG13 | 2.02                     | 0.41              |
| 2:I:394:VAL:HG23 | 2:I:396:TRP:CD2  | 2.55                     | 0.41              |
| 2:J:367:LYS:HB3  | 2:J:386:GLU:HB3  | 2.02                     | 0.41              |
| 2:K:361:LYS:CG   | 2:K:362:SER:H    | 2.33                     | 0.41              |
| 2:L:409:LYS:O    | 2:L:410:TYR:CG   | 2.73                     | 0.41              |
| 1:A:18:LYS:HA    | 1:A:29:ALA:O     | 2.20                     | 0.41              |
| 1:C:14:SER:OG    | 1:C:158:GLY:HA3  | 2.20                     | 0.41              |
| 2:G:362:SER:C    | 2:G:365:PHE:O    | 2.62                     | 0.41              |
| 2:H:394:VAL:HG23 | 2:H:396:TRP:CD2  | 2.55                     | 0.41              |
| 2:I:396:TRP:CE3  | 2:I:412:PHE:CE2  | 3.08                     | 0.41              |
| 2:K:369:LEU:CD2  | 2:K:383:LEU:HB3  | 2.50                     | 0.41              |
| 2:K:390:HIS:HA   | 2:K:417:ALA:CB   | 2.49                     | 0.41              |
| 2:K:437:VAL:HG13 | 2:K:442:LYS:HB3  | 2.02                     | 0.41              |
| 2:L:394:VAL:HG23 | 2:L:396:TRP:CD2  | 2.55                     | 0.41              |
| 2:L:432:ALA:O    | 2:L:447:LEU:N    | 2.52                     | 0.41              |
| 1:B:18:LYS:HA    | 1:B:29:ALA:O     | 2.20                     | 0.41              |
| 1:C:164:PRO:HG2  | 1:C:171:LEU:HB2  | 2.02                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:18:LYS:HA    | 1:D:29:ALA:O     | 2.20                     | 0.41              |
| 1:E:164:PRO:HG2  | 1:E:171:LEU:HB2  | 2.02                     | 0.41              |
| 2:H:369:LEU:CD2  | 2:H:383:LEU:HB3  | 2.50                     | 0.41              |
| 2:J:394:VAL:HG23 | 2:J:396:TRP:CD2  | 2.55                     | 0.41              |
| 2:L:369:LEU:CD2  | 2:L:383:LEU:HB3  | 2.50                     | 0.41              |
| 1:B:241:GLU:HA   | 1:B:247:VAL:HG12 | 2.01                     | 0.41              |
| 1:F:14:SER:OG    | 1:F:158:GLY:HA3  | 2.20                     | 0.41              |
| 2:G:394:VAL:HG23 | 2:G:396:TRP:CD2  | 2.55                     | 0.41              |
| 2:G:437:VAL:HG13 | 2:G:442:LYS:HB3  | 2.02                     | 0.41              |
| 2:H:369:LEU:HD23 | 2:H:385:VAL:HG13 | 2.03                     | 0.41              |
| 2:I:369:LEU:HD23 | 2:I:385:VAL:HG13 | 2.03                     | 0.41              |
| 2:I:437:VAL:HG13 | 2:I:442:LYS:HB3  | 2.02                     | 0.41              |
| 2:J:379:HIS:O    | 2:J:426:CYS:N    | 2.47                     | 0.41              |
| 2:J:396:TRP:CE3  | 2:J:412:PHE:CE2  | 3.08                     | 0.41              |
| 2:J:418:LYS:O    | 2:J:418:LYS:HG2  | 2.17                     | 0.41              |
| 1:A:14:SER:OG    | 1:A:158:GLY:HA3  | 2.20                     | 0.41              |
| 1:A:164:PRO:HG2  | 1:A:171:LEU:HB2  | 2.02                     | 0.41              |
| 1:D:241:GLU:HA   | 1:D:247:VAL:HG12 | 2.01                     | 0.41              |
| 1:F:18:LYS:HA    | 1:F:29:ALA:O     | 2.20                     | 0.41              |
| 2:G:432:ALA:O    | 2:G:447:LEU:N    | 2.52                     | 0.41              |
| 2:H:379:HIS:O    | 2:H:426:CYS:N    | 2.47                     | 0.41              |
| 2:H:396:TRP:CB   | 2:H:403:ILE:HB   | 2.51                     | 0.41              |
| 2:J:409:LYS:O    | 2:J:410:TYR:CG   | 2.72                     | 0.41              |
| 2:K:387:LEU:HD21 | 2:K:394:VAL:CG1  | 2.51                     | 0.41              |
| 2:L:376:SER:HB2  | 2:L:379:HIS:HB2  | 2.03                     | 0.41              |
| 1:D:171:LEU:HD12 | 1:D:173:HIS:CE1  | 2.56                     | 0.41              |
| 1:F:171:LEU:HD12 | 1:F:173:HIS:CE1  | 2.56                     | 0.41              |
| 1:F:241:GLU:HA   | 1:F:247:VAL:HG12 | 2.01                     | 0.41              |
| 2:G:387:LEU:HD21 | 2:G:394:VAL:CG1  | 2.51                     | 0.41              |
| 2:L:369:LEU:HD23 | 2:L:385:VAL:HG13 | 2.03                     | 0.41              |
| 1:A:9:VAL:HA     | 1:A:104:LEU:HB3  | 2.03                     | 0.41              |
| 1:A:171:LEU:HD12 | 1:A:173:HIS:CE1  | 2.56                     | 0.41              |
| 1:D:106:THR:HB   | 1:D:137:GLN:HG2  | 2.02                     | 0.41              |
| 1:E:259:GLU:OE2  | 1:E:312:ARG:NH2  | 2.48                     | 0.41              |
| 2:G:380:LYS:HD3  | 2:G:422:THR:CG2  | 2.51                     | 0.41              |
| 2:J:369:LEU:HD23 | 2:J:385:VAL:HG13 | 2.03                     | 0.41              |
| 2:J:396:TRP:CB   | 2:J:403:ILE:HB   | 2.51                     | 0.41              |
| 1:D:43:VAL:CG2   | 1:F:170:ALA:HB3  | 2.50                     | 0.41              |
| 1:F:23:GLY:CA    | 2:L:425:GLN:NE2  | 2.73                     | 0.41              |
| 1:F:106:THR:HB   | 1:F:137:GLN:HG2  | 2.02                     | 0.41              |
| 2:H:396:TRP:CE3  | 2:H:412:PHE:CE2  | 3.08                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:409:LYS:O    | 2:H:423:ILE:HA   | 2.21                     | 0.41              |
| 2:I:367:LYS:HB3  | 2:I:386:GLU:HB3  | 2.02                     | 0.41              |
| 2:K:369:LEU:HD23 | 2:K:385:VAL:HG13 | 2.03                     | 0.41              |
| 2:K:380:LYS:HD3  | 2:K:422:THR:CG2  | 2.51                     | 0.41              |
| 2:L:367:LYS:HB3  | 2:L:386:GLU:HB3  | 2.03                     | 0.41              |
| 2:L:396:TRP:CB   | 2:L:403:ILE:HB   | 2.51                     | 0.41              |
| 1:B:106:THR:HB   | 1:B:137:GLN:HG2  | 2.02                     | 0.41              |
| 1:B:171:LEU:HD12 | 1:B:173:HIS:CE1  | 2.56                     | 0.41              |
| 1:C:9:VAL:HA     | 1:C:104:LEU:HB3  | 2.03                     | 0.41              |
| 1:C:18:LYS:HA    | 1:C:29:ALA:O     | 2.20                     | 0.41              |
| 1:C:63:GLY:CA    | 1:E:288:ASP:CG   | 2.94                     | 0.41              |
| 1:C:171:LEU:HD12 | 1:C:173:HIS:CE1  | 2.56                     | 0.41              |
| 2:I:387:LEU:HD21 | 2:I:394:VAL:CG1  | 2.51                     | 0.41              |
| 2:I:450:LYS:HD2  | 2:I:450:LYS:O    | 2.21                     | 0.41              |
| 2:J:369:LEU:CD2  | 2:J:383:LEU:HB3  | 2.50                     | 0.41              |
| 2:J:376:SER:HB2  | 2:J:379:HIS:HB2  | 2.03                     | 0.41              |
| 2:J:409:LYS:O    | 2:J:423:ILE:HA   | 2.21                     | 0.41              |
| 2:L:387:LEU:HD21 | 2:L:394:VAL:CG1  | 2.51                     | 0.41              |
| 2:L:396:TRP:CE3  | 2:L:412:PHE:CE2  | 3.08                     | 0.41              |
| 1:A:14:SER:HB3   | 1:A:158:GLY:N    | 2.36                     | 0.41              |
| 2:G:367:LYS:HB3  | 2:G:386:GLU:HB3  | 2.03                     | 0.41              |
| 2:G:376:SER:HB2  | 2:G:379:HIS:HB2  | 2.03                     | 0.41              |
| 2:H:376:SER:HB2  | 2:H:379:HIS:HB2  | 2.03                     | 0.41              |
| 2:H:380:LYS:HD3  | 2:H:422:THR:CG2  | 2.51                     | 0.41              |
| 2:H:387:LEU:HD11 | 2:H:394:VAL:HG13 | 2.03                     | 0.41              |
| 2:J:380:LYS:HD3  | 2:J:422:THR:CG2  | 2.51                     | 0.41              |
| 2:J:387:LEU:HD11 | 2:J:394:VAL:HG13 | 2.03                     | 0.41              |
| 2:K:370:GLU:O    | 2:K:445:THR:CB   | 2.69                     | 0.41              |
| 2:K:387:LEU:HD11 | 2:K:394:VAL:HG13 | 2.03                     | 0.41              |
| 2:K:396:TRP:CB   | 2:K:403:ILE:HB   | 2.51                     | 0.41              |
| 1:C:196:ARG:NH2  | 1:C:253:GLU:OE1  | 2.42                     | 0.40              |
| 1:C:349:LEU:HB3  | 2:I:413:GLU:OE2  | 2.21                     | 0.40              |
| 1:D:259:GLU:OE2  | 1:D:312:ARG:NH2  | 2.48                     | 0.40              |
| 1:F:9:VAL:HA     | 1:F:104:LEU:HB3  | 2.03                     | 0.40              |
| 2:G:365:PHE:HD1  | 2:G:367:LYS:O    | 2.05                     | 0.40              |
| 2:G:396:TRP:CE3  | 2:G:412:PHE:CE2  | 3.08                     | 0.40              |
| 2:H:384:THR:HG23 | 2:H:418:LYS:NZ   | 2.36                     | 0.40              |
| 2:I:365:PHE:HD1  | 2:I:367:LYS:O    | 2.05                     | 0.40              |
| 2:I:396:TRP:CB   | 2:I:403:ILE:HB   | 2.51                     | 0.40              |
| 2:J:387:LEU:HD21 | 2:J:394:VAL:CG1  | 2.51                     | 0.40              |
| 2:K:432:ALA:O    | 2:K:447:LEU:N    | 2.52                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:14:SER:HB3   | 1:C:158:GLY:N    | 2.37                     | 0.40              |
| 2:G:387:LEU:HD11 | 2:G:394:VAL:HG13 | 2.03                     | 0.40              |
| 2:I:370:GLU:O    | 2:I:445:THR:CB   | 2.69                     | 0.40              |
| 2:K:384:THR:HG23 | 2:K:418:LYS:NZ   | 2.36                     | 0.40              |
| 2:L:380:LYS:HD3  | 2:L:422:THR:CG2  | 2.51                     | 0.40              |
| 1:C:78:ASN:ND2   | 1:C:81:ASP:OD2   | 2.55                     | 0.40              |
| 1:D:14:SER:HB3   | 1:D:158:GLY:N    | 2.37                     | 0.40              |
| 1:E:9:VAL:HA     | 1:E:104:LEU:HB3  | 2.03                     | 0.40              |
| 2:G:450:LYS:O    | 2:G:450:LYS:HD2  | 2.21                     | 0.40              |
| 2:I:387:LEU:HD11 | 2:I:394:VAL:HG13 | 2.03                     | 0.40              |
| 2:K:409:LYS:O    | 2:K:423:ILE:HA   | 2.21                     | 0.40              |
| 2:K:450:LYS:HD2  | 2:K:450:LYS:O    | 2.21                     | 0.40              |
| 2:L:387:LEU:HD11 | 2:L:394:VAL:HG13 | 2.03                     | 0.40              |
| 2:L:450:LYS:HD2  | 2:L:450:LYS:O    | 2.21                     | 0.40              |
| 1:B:14:SER:OG    | 1:B:158:GLY:HA3  | 2.20                     | 0.40              |
| 1:D:78:ASN:ND2   | 1:D:81:ASP:OD2   | 2.55                     | 0.40              |
| 1:E:189:LEU:HD13 | 1:E:257:CYS:HB2  | 2.04                     | 0.40              |
| 2:H:361:LYS:CG   | 2:H:362:SER:H    | 2.33                     | 0.40              |
| 2:H:369:LEU:HD22 | 2:H:383:LEU:HB3  | 2.04                     | 0.40              |
| 2:H:370:GLU:O    | 2:H:445:THR:CB   | 2.69                     | 0.40              |
| 2:I:369:LEU:HD22 | 2:I:383:LEU:HB3  | 2.04                     | 0.40              |
| 2:J:384:THR:HG23 | 2:J:418:LYS:NZ   | 2.36                     | 0.40              |
| 1:A:189:LEU:HD13 | 1:A:257:CYS:HB2  | 2.04                     | 0.40              |
| 1:B:78:ASN:ND2   | 1:B:81:ASP:OD2   | 2.55                     | 0.40              |
| 1:B:304:THR:O    | 1:B:335:ARG:NH2  | 2.53                     | 0.40              |
| 1:C:210:ARG:NH1  | 1:C:214:GLU:OE2  | 2.55                     | 0.40              |
| 1:D:9:VAL:HA     | 1:D:104:LEU:HB3  | 2.03                     | 0.40              |
| 1:E:14:SER:HB3   | 1:E:158:GLY:N    | 2.36                     | 0.40              |
| 1:E:171:LEU:HD12 | 1:E:173:HIS:CE1  | 2.56                     | 0.40              |
| 2:H:387:LEU:HD21 | 2:H:394:VAL:CG1  | 2.51                     | 0.40              |
| 2:I:384:THR:HG23 | 2:I:418:LYS:NZ   | 2.36                     | 0.40              |
| 2:J:369:LEU:HD22 | 2:J:383:LEU:HB3  | 2.04                     | 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     | 370/377 (98%)   | 351 (95%)  | 19 (5%)  | 0        | 100         | 100 |
| 1   | B     | 370/377 (98%)   | 351 (95%)  | 19 (5%)  | 0        | 100         | 100 |
| 1   | C     | 370/377 (98%)   | 350 (95%)  | 20 (5%)  | 0        | 100         | 100 |
| 1   | D     | 370/377 (98%)   | 351 (95%)  | 19 (5%)  | 0        | 100         | 100 |
| 1   | E     | 370/377 (98%)   | 351 (95%)  | 19 (5%)  | 0        | 100         | 100 |
| 1   | F     | 370/377 (98%)   | 351 (95%)  | 19 (5%)  | 0        | 100         | 100 |
| 2   | G     | 92/94 (98%)     | 73 (79%)   | 19 (21%) | 0        | 100         | 100 |
| 2   | H     | 92/94 (98%)     | 73 (79%)   | 19 (21%) | 0        | 100         | 100 |
| 2   | I     | 92/94 (98%)     | 73 (79%)   | 19 (21%) | 0        | 100         | 100 |
| 2   | J     | 92/94 (98%)     | 73 (79%)   | 19 (21%) | 0        | 100         | 100 |
| 2   | K     | 92/94 (98%)     | 73 (79%)   | 19 (21%) | 0        | 100         | 100 |
| 2   | L     | 92/94 (98%)     | 73 (79%)   | 19 (21%) | 0        | 100         | 100 |
| All | All   | 2772/2826 (98%) | 2543 (92%) | 229 (8%) | 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     | 315/320 (98%) | 314 (100%) | 1 (0%)   | 86          | 85 |
| 1   | B     | 315/320 (98%) | 314 (100%) | 1 (0%)   | 86          | 85 |
| 1   | C     | 315/320 (98%) | 314 (100%) | 1 (0%)   | 86          | 85 |
| 1   | D     | 315/320 (98%) | 314 (100%) | 1 (0%)   | 86          | 85 |
| 1   | E     | 315/320 (98%) | 314 (100%) | 1 (0%)   | 86          | 85 |
| 1   | F     | 315/320 (98%) | 314 (100%) | 1 (0%)   | 86          | 85 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 2   | G     | 80/80 (100%)    | 77 (96%)   | 3 (4%)   | 29          | 50 |
| 2   | H     | 80/80 (100%)    | 77 (96%)   | 3 (4%)   | 29          | 50 |
| 2   | I     | 80/80 (100%)    | 77 (96%)   | 3 (4%)   | 29          | 50 |
| 2   | J     | 80/80 (100%)    | 77 (96%)   | 3 (4%)   | 29          | 50 |
| 2   | K     | 80/80 (100%)    | 77 (96%)   | 3 (4%)   | 29          | 50 |
| 2   | L     | 80/80 (100%)    | 77 (96%)   | 3 (4%)   | 29          | 50 |
| All | All   | 2370/2400 (99%) | 2346 (99%) | 24 (1%)  | 65          | 78 |

All (24) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 16  | LEU  |
| 1   | B     | 16  | LEU  |
| 1   | C     | 16  | LEU  |
| 1   | D     | 16  | LEU  |
| 1   | E     | 16  | LEU  |
| 1   | F     | 16  | LEU  |
| 2   | G     | 380 | LYS  |
| 2   | G     | 409 | LYS  |
| 2   | G     | 418 | LYS  |
| 2   | H     | 380 | LYS  |
| 2   | H     | 409 | LYS  |
| 2   | H     | 418 | LYS  |
| 2   | I     | 380 | LYS  |
| 2   | I     | 409 | LYS  |
| 2   | I     | 418 | LYS  |
| 2   | J     | 380 | LYS  |
| 2   | J     | 409 | LYS  |
| 2   | J     | 418 | LYS  |
| 2   | K     | 380 | LYS  |
| 2   | K     | 409 | LYS  |
| 2   | K     | 418 | LYS  |
| 2   | L     | 380 | LYS  |
| 2   | L     | 409 | LYS  |
| 2   | L     | 418 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 73  | HIS  |
| 1   | A     | 78  | ASN  |
| 1   | A     | 92  | ASN  |
| 1   | A     | 121 | GLN  |
| 1   | A     | 162 | ASN  |
| 1   | A     | 173 | HIS  |
| 1   | A     | 225 | ASN  |
| 1   | B     | 40  | HIS  |
| 1   | B     | 92  | ASN  |
| 1   | B     | 121 | GLN  |
| 1   | B     | 162 | ASN  |
| 1   | B     | 173 | HIS  |
| 1   | B     | 225 | ASN  |
| 1   | C     | 92  | ASN  |
| 1   | C     | 121 | GLN  |
| 1   | C     | 162 | ASN  |
| 1   | C     | 173 | HIS  |
| 1   | C     | 225 | ASN  |
| 1   | D     | 92  | ASN  |
| 1   | D     | 121 | GLN  |
| 1   | D     | 162 | ASN  |
| 1   | D     | 173 | HIS  |
| 1   | D     | 225 | ASN  |
| 1   | E     | 40  | HIS  |
| 1   | E     | 92  | ASN  |
| 1   | E     | 121 | GLN  |
| 1   | E     | 162 | ASN  |
| 1   | E     | 173 | HIS  |
| 1   | E     | 225 | ASN  |
| 1   | F     | 40  | HIS  |
| 1   | F     | 92  | ASN  |
| 1   | F     | 121 | GLN  |
| 1   | F     | 162 | ASN  |
| 1   | F     | 173 | HIS  |
| 1   | F     | 225 | ASN  |
| 2   | G     | 390 | HIS  |
| 2   | G     | 425 | GLN  |
| 2   | H     | 390 | HIS  |
| 2   | I     | 390 | HIS  |
| 2   | I     | 425 | GLN  |
| 2   | J     | 390 | HIS  |
| 2   | K     | 390 | HIS  |
| 2   | L     | 390 | HIS  |

### 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.

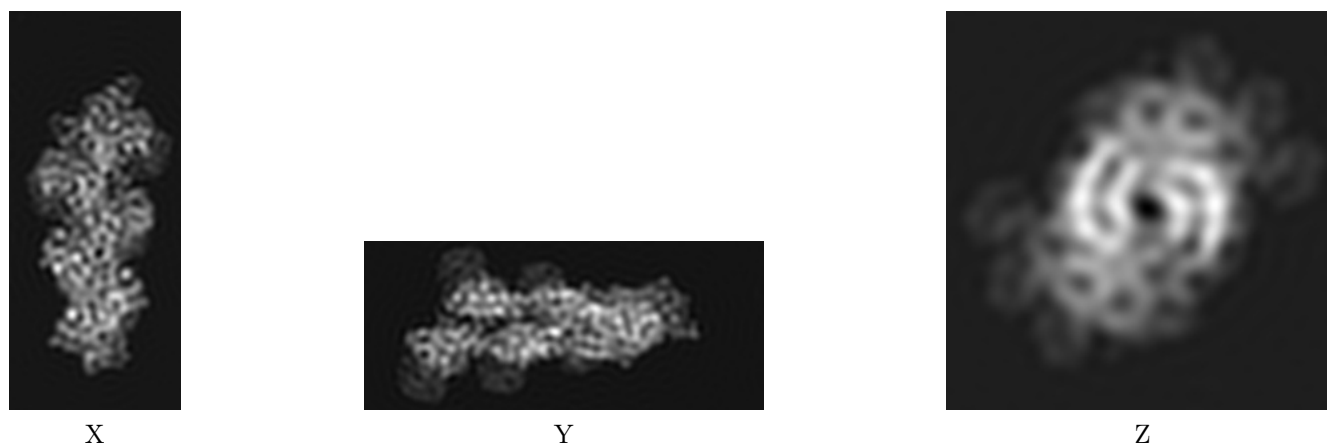
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23497. 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 [i](#)

#### 6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 48



Y Index: 57

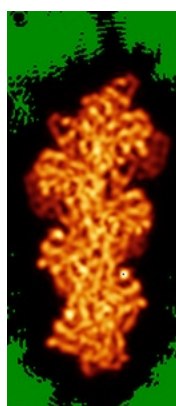


Z Index: 63

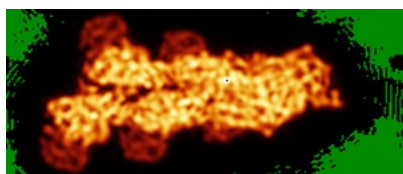
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

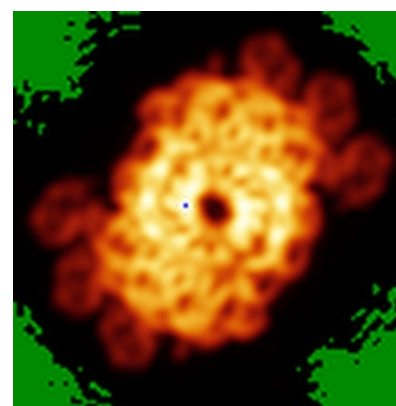
### 6.4.1 Primary map



X



Y

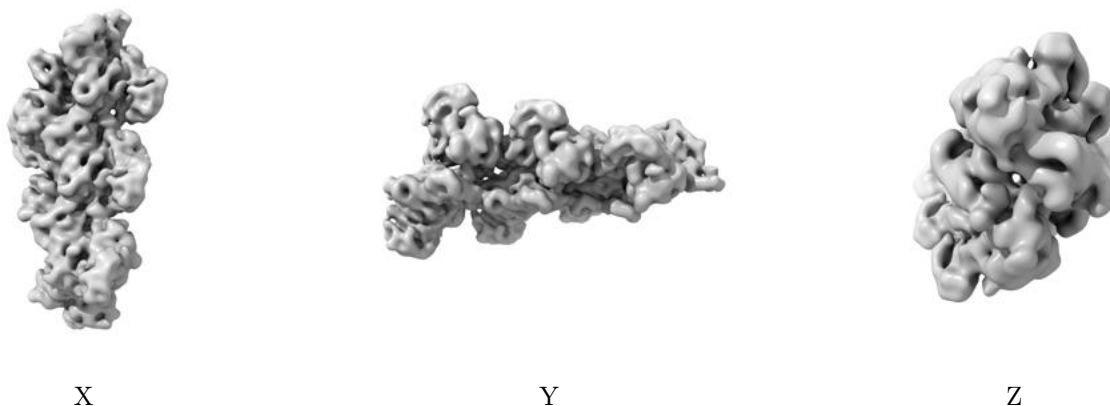


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

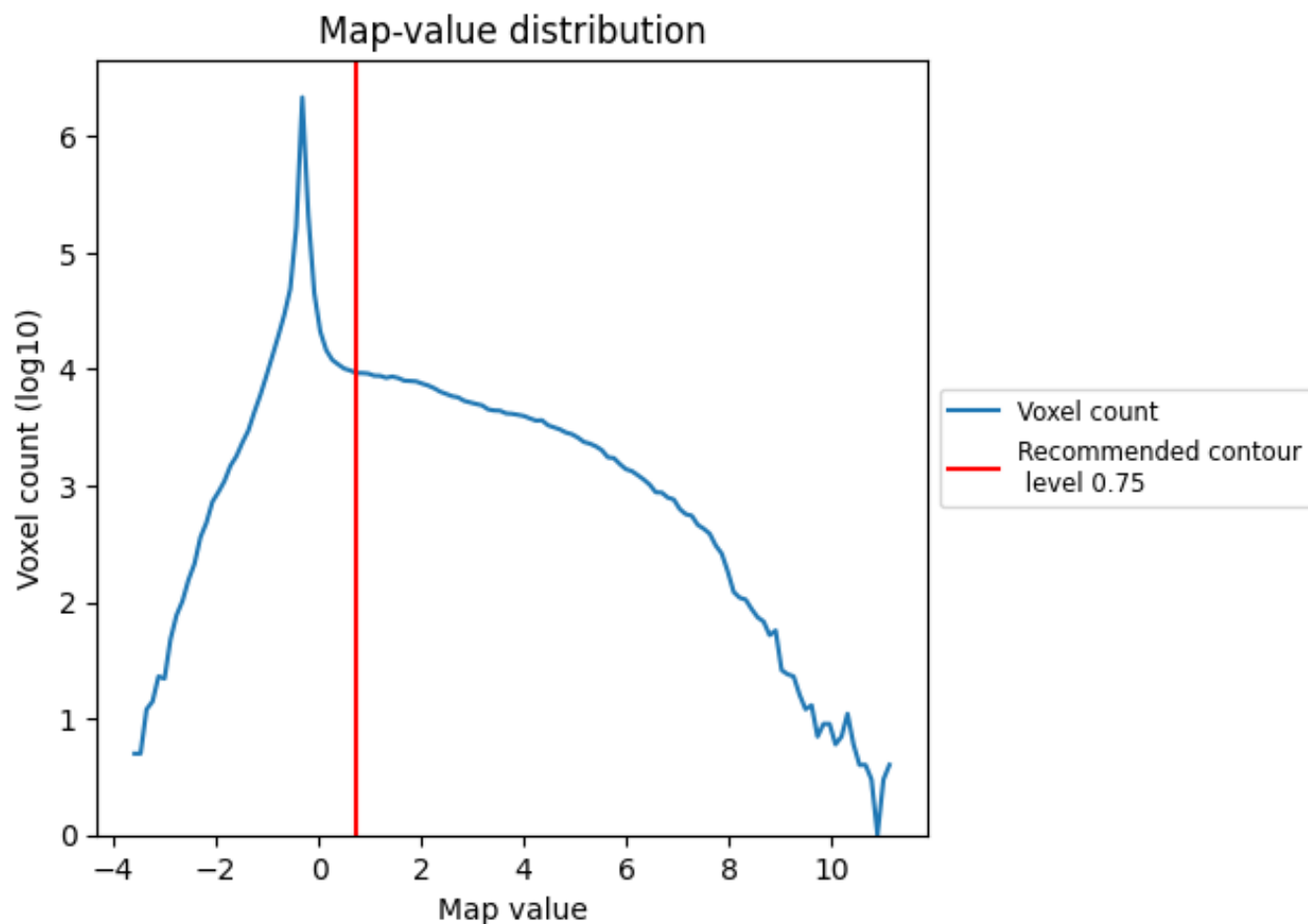
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

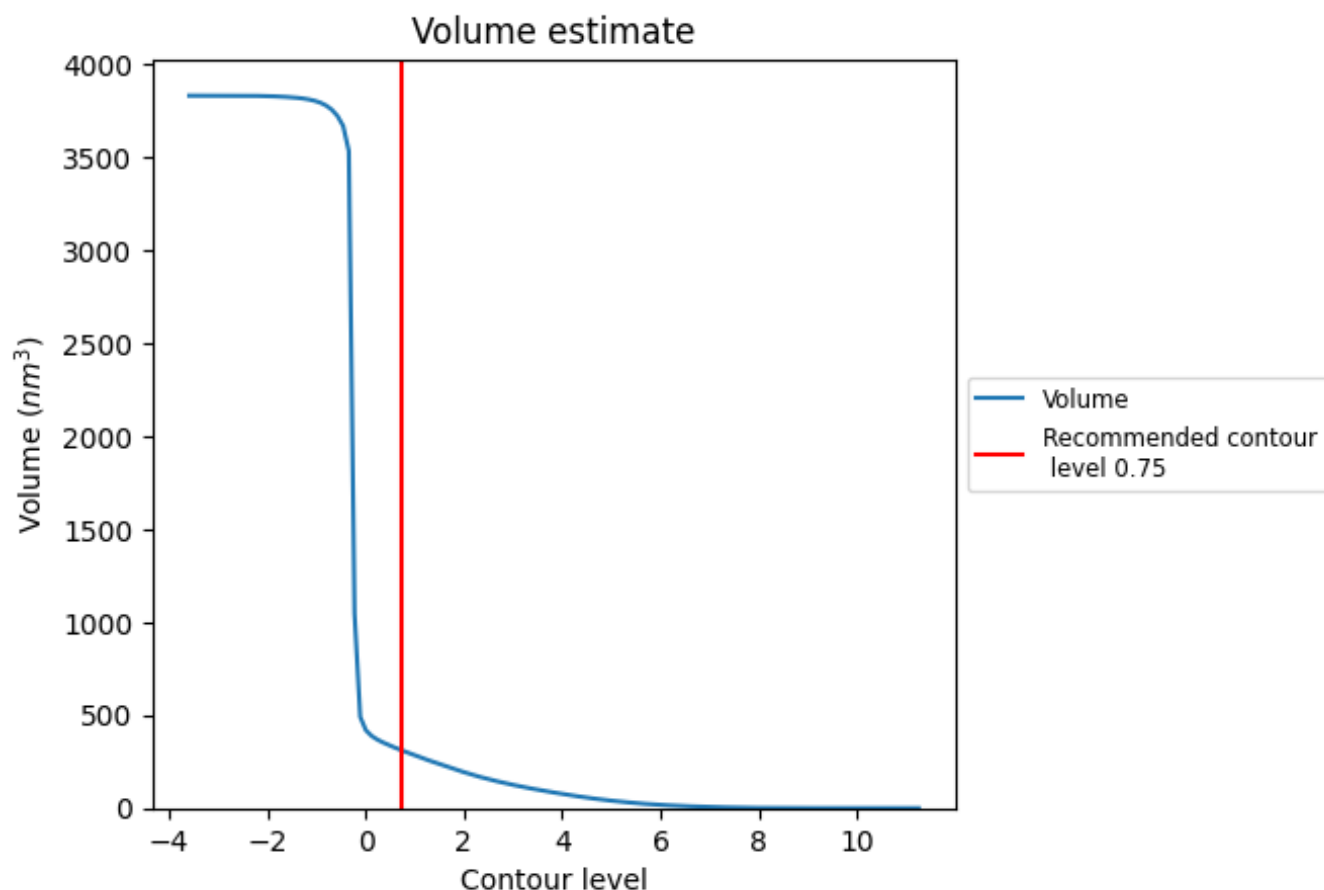
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 309 nm<sup>3</sup>; this corresponds to an approximate mass of 280 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

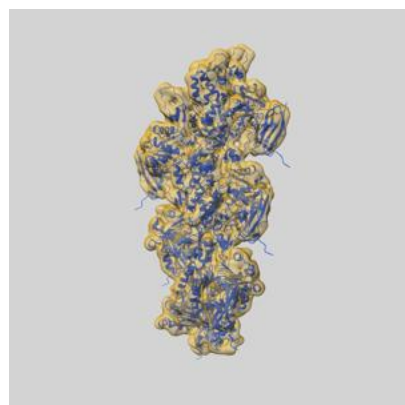
## 8 Fourier-Shell correlation

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

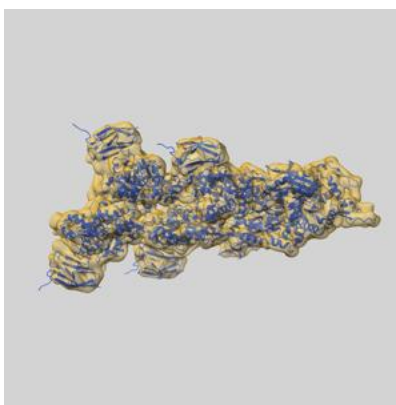
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23497 and PDB model 7LRG. Per-residue inclusion information can be found in section 3 on page 5.

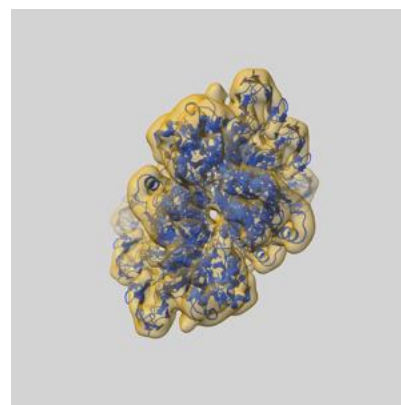
### 9.1 Map-model overlay [i](#)



X



Y



Z

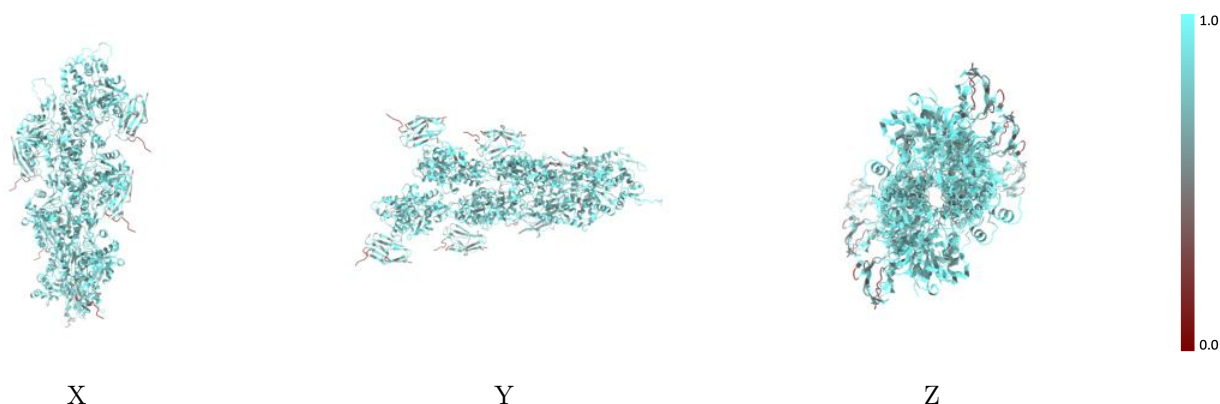
The images above show the 3D surface view of the map at the recommended contour level 0.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



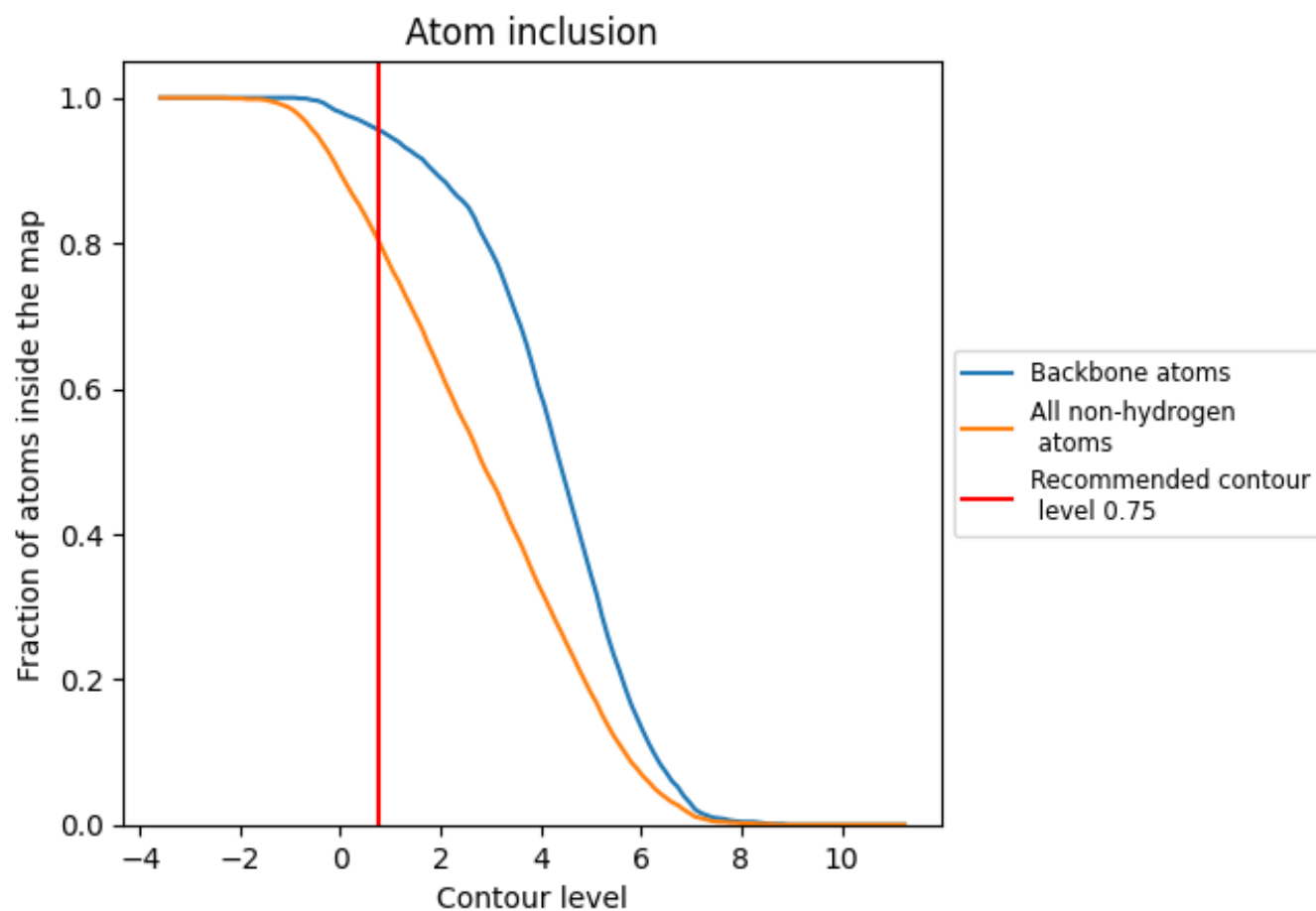
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.75).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.75) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion               | Q-score                      |
|-------|------------------------------|------------------------------|
| All   | <div><div></div>0.8050</div> | <div><div></div>0.1340</div> |
| A     | <div><div></div>0.8270</div> | <div><div></div>0.1400</div> |
| B     | <div><div></div>0.8280</div> | <div><div></div>0.1380</div> |
| C     | <div><div></div>0.8280</div> | <div><div></div>0.1400</div> |
| D     | <div><div></div>0.8260</div> | <div><div></div>0.1390</div> |
| E     | <div><div></div>0.8250</div> | <div><div></div>0.1380</div> |
| F     | <div><div></div>0.8230</div> | <div><div></div>0.1400</div> |
| G     | <div><div></div>0.6570</div> | <div><div></div>0.1090</div> |
| H     | <div><div></div>0.6630</div> | <div><div></div>0.1050</div> |
| I     | <div><div></div>0.6670</div> | <div><div></div>0.1160</div> |
| J     | <div><div></div>0.6730</div> | <div><div></div>0.1110</div> |
| K     | <div><div></div>0.6660</div> | <div><div></div>0.1140</div> |
| L     | <div><div></div>0.6590</div> | <div><div></div>0.1090</div> |

1.0

0.0

<0.0